Entering Gaussian System, Link 0=g09

Input=ZnTSPsim3.com

Output=ZnTSPsim3.log

Initial command:

/home/kira/g09/l1.exe "/home/kira/g09/scratch/Gau-5972.inp" -scrdir="/home/kira/g09/scratch/"

Entering Link 1 = /home/kira/g09/l1.exe PID= 5979.

Copyright (c) 1988,1990,1992,1993,1995,1998,2003,2009,2015,

Gaussian, Inc. All Rights Reserved.

This is part of the Gaussian(R) 09 program. It is based on

the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),

the Gaussian(R) 98 system (copyright 1998, Gaussian, Inc.),

the Gaussian(R) 94 system (copyright 1995, Gaussian, Inc.),

the Gaussian 92(TM) system (copyright 1992, Gaussian, Inc.),

the Gaussian 90(TM) system (copyright 1990, Gaussian, Inc.),

the Gaussian 88(TM) system (copyright 1988, Gaussian, Inc.),

the Gaussian 86(TM) system (copyright 1986, Carnegie Mellon

University), and the Gaussian 82(TM) system (copyright 1983,

Carnegie Mellon University). Gaussian is a federally registered

trademark of Gaussian, Inc.

This software contains proprietary and confidential information,

including trade secrets, belonging to Gaussian, Inc.

This software is provided under written license and may be

used, copied, transmitted, or stored only in accord with that

written license.

The following legend is applicable only to US Government

contracts under FAR:

RESTRICTED RIGHTS LEGEND

Use, reproduction and disclosure by the US Government is

subject to restrictions as set forth in subparagraphs (a)

and (c) of the Commercial Computer Software - Restricted

Rights clause in FAR 52.227-19.

Gaussian, Inc.

340 Quinnipiac St., Bldg. 40, Wallingford CT 06492

---------------------------------------------------------------

Warning -- This program may not be used in any manner that

competes with the business of Gaussian, Inc. or will provide

assistance to any competitor of Gaussian, Inc. The licensee

of this program is prohibited from giving any competitor of

Gaussian, Inc. access to this program. By using this program,

the user acknowledges that Gaussian, Inc. is engaged in the

business of creating and licensing software in the field of

computational chemistry and represents and warrants to the

licensee that it is not a competitor of Gaussian, Inc. and that

it will not use this program in any manner prohibited above.

---------------------------------------------------------------

Cite this work as:

Gaussian 09, Revision E.01,

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,

M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,

G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,

A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,

M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,

Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,

J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,

K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,

K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,

M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,

V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,

O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,

R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,

P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,

O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,

and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Gaussian 09: ES64L-G09RevE.01 30-Nov-2015

29-Jul-2019

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

%nprocshared=16

Will use up to 16 processors via shared memory.

%mem=32GB

%chk=ZnTSPsim3.chk

----------------------------------------------------------------------

#p opt=calcall b3lyp/genecp scrf=(solvent=dmso,smd) empiricaldispersio

n=gd3bj

----------------------------------------------------------------------

1/10=4,14=-1,18=20,19=15,26=3,38=1/1,3;

2/9=110,12=2,17=6,18=5,40=1/2;

3/5=7,11=2,16=1,17=8,25=1,30=1,70=32201,71=2,72=21,74=-5,124=41,140=1/1,2,3;

4//1;

5/5=2,38=5,53=21/2;

8/6=4,10=90,11=11/1;

11/6=1,8=1,9=11,15=111,16=1/1,2,10;

10/6=1/2;

6/7=2,8=2,9=2,10=2,18=1,28=1/1;

7/10=1,25=1/1,2,3,16;

1/10=4,14=-1,18=20,19=15,26=3/3(3);

2/9=110/2;

7/8=1,9=1,25=1,44=-1/16;

99//99;

2/9=110/2;

3/5=7,6=1,11=2,16=1,17=8,25=1,30=1,70=32205,71=2,72=21,74=-5,82=7,124=41,140=1/1,2,3;

4/5=5,16=3,69=1/1;

5/5=2,38=5,53=21/2;

8/6=4,10=90,11=11/1;

11/6=1,8=1,9=11,15=111,16=1/1,2,10;

10/6=1/2;

7/10=1,25=1/1,2,3,16;

1/10=4,14=-1,18=20,19=15,26=3/3(-8);

2/9=110/2;

6/7=2,8=2,9=2,10=2,18=1,19=2,28=1/1;

7/8=1,9=1,25=1,44=-1/16;

99//99;

Leave Link 1 at Mon Jul 29 21:22:50 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l101.exe)

---------

ZnTSPsim3

---------

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C -0.68116 -4.2733 -0.04119

C -1.102 -2.88919 -0.00631

N 0. -2.08169 0.01622

C 1.102 -2.88919 -0.00631

C 0.68116 -4.2733 -0.04119

C 2.44614 -2.44614 -0.01155

C 2.88919 -1.102 -0.00631

N 2.08169 0. 0.01622

C 2.88919 1.102 -0.00631

C 4.2733 0.68116 -0.04119

C 4.2733 -0.68116 -0.04119

C -2.44614 -2.44614 -0.01155

C -2.88919 -1.102 -0.00631

C -4.2733 -0.68116 -0.04119

C -4.2733 0.68116 -0.04119

C -2.88919 1.102 -0.00631

N -2.08169 0. 0.01622

C -2.44614 2.44614 -0.01155

C -1.102 2.88919 -0.00631

C -0.68116 4.2733 -0.04119

C 0.68116 4.2733 -0.04119

C 1.102 2.88919 -0.00631

N 0. 2.08169 0.01622

H -1.33968 -5.12856 -0.06729

H 1.33968 -5.12856 -0.06729

H 5.12856 1.33968 -0.06729

H 5.12856 -1.33968 -0.06729

H -5.12856 -1.33968 -0.06729

H -5.12856 1.33968 -0.06729

H -1.33968 5.12856 -0.06729

H 1.33968 5.12856 -0.06729

Zn 0. 0. 0.18878

C 2.44614 2.44614 -0.01155

C 3.45499 3.45499 -0.04062

C -3.45499 -3.45499 -0.04062

C 4.30737 4.30737 -0.06978

C -4.30737 -4.30737 -0.06978

C 3.45499 -3.45499 -0.04062

C 4.30737 -4.30737 -0.06978

C -3.45499 3.45499 -0.04062

C -4.30737 4.30737 -0.06978

H -5.06191 5.06191 -0.09298

H 5.06191 5.06191 -0.09298

H 5.06191 -5.06191 -0.09298

H -5.06191 -5.06191 -0.09298

NAtoms= 45 NQM= 45 NQMF= 0 NMMI= 0 NMMIF= 0

NMic= 0 NMicF= 0.

Isotopes and Nuclear Properties:

(Nuclear quadrupole moments (NQMom) in fm\*\*2, nuclear magnetic moments (NMagM)

in nuclear magnetons)

Atom 1 2 3 4 5 6 7 8 9 10

IAtWgt= 12 12 14 12 12 12 12 14 12 12

AtmWgt= 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000

NucSpn= 0 0 2 0 0 0 0 2 0 0

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000

Atom 11 12 13 14 15 16 17 18 19 20

IAtWgt= 12 12 12 12 12 12 14 12 12 12

AtmWgt= 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 14.0030740 12.0000000 12.0000000 12.0000000

NucSpn= 0 0 0 0 0 0 2 0 0 0

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.4037610 0.0000000 0.0000000 0.0000000

AtZNuc= 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 7.0000000 6.0000000 6.0000000 6.0000000

Atom 21 22 23 24 25 26 27 28 29 30

IAtWgt= 12 12 14 1 1 1 1 1 1 1

AtmWgt= 12.0000000 12.0000000 14.0030740 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 0 0 2 1 1 1 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 2.0440000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000 0.4037610 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 6.0000000 6.0000000 7.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Atom 31 32 33 34 35 36 37 38 39 40

IAtWgt= 1 64 12 12 12 12 12 12 12 12

AtmWgt= 1.0078250 63.9291454 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000 12.0000000

NucSpn= 1 0 0 0 0 0 0 0 0 0

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 2.7928460 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

AtZNuc= 1.0000000 30.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000 6.0000000

Atom 41 42 43 44 45

IAtWgt= 12 1 1 1 1

AtmWgt= 12.0000000 1.0078250 1.0078250 1.0078250 1.0078250

NucSpn= 0 1 1 1 1

AtZEff= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

NMagM= 0.0000000 2.7928460 2.7928460 2.7928460 2.7928460

AtZNuc= 6.0000000 1.0000000 1.0000000 1.0000000 1.0000000

Leave Link 101 at Mon Jul 29 21:22:51 2019, MaxMem= 4294967296 cpu: 7.0

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

----------------------------

! Initial Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.4471 calculate D2E/DX2 analytically !

! R2 R(1,5) 1.3623 calculate D2E/DX2 analytically !

! R3 R(1,24) 1.0797 calculate D2E/DX2 analytically !

! R4 R(2,3) 1.3664 calculate D2E/DX2 analytically !

! R5 R(2,12) 1.4153 calculate D2E/DX2 analytically !

! R6 R(3,4) 1.3664 calculate D2E/DX2 analytically !

! R7 R(3,32) 2.0888 calculate D2E/DX2 analytically !

! R8 R(4,5) 1.4471 calculate D2E/DX2 analytically !

! R9 R(4,6) 1.4153 calculate D2E/DX2 analytically !

! R10 R(5,25) 1.0797 calculate D2E/DX2 analytically !

! R11 R(6,7) 1.4153 calculate D2E/DX2 analytically !

! R12 R(6,38) 1.427 calculate D2E/DX2 analytically !

! R13 R(7,8) 1.3664 calculate D2E/DX2 analytically !

! R14 R(7,11) 1.4471 calculate D2E/DX2 analytically !

! R15 R(8,9) 1.3664 calculate D2E/DX2 analytically !

! R16 R(8,32) 2.0888 calculate D2E/DX2 analytically !

! R17 R(9,10) 1.4471 calculate D2E/DX2 analytically !

! R18 R(9,33) 1.4153 calculate D2E/DX2 analytically !

! R19 R(10,11) 1.3623 calculate D2E/DX2 analytically !

! R20 R(10,26) 1.0797 calculate D2E/DX2 analytically !

! R21 R(11,27) 1.0797 calculate D2E/DX2 analytically !

! R22 R(12,13) 1.4153 calculate D2E/DX2 analytically !

! R23 R(12,35) 1.427 calculate D2E/DX2 analytically !

! R24 R(13,14) 1.4471 calculate D2E/DX2 analytically !

! R25 R(13,17) 1.3664 calculate D2E/DX2 analytically !

! R26 R(14,15) 1.3623 calculate D2E/DX2 analytically !

! R27 R(14,28) 1.0797 calculate D2E/DX2 analytically !

! R28 R(15,16) 1.4471 calculate D2E/DX2 analytically !

! R29 R(15,29) 1.0797 calculate D2E/DX2 analytically !

! R30 R(16,17) 1.3664 calculate D2E/DX2 analytically !

! R31 R(16,18) 1.4153 calculate D2E/DX2 analytically !

! R32 R(17,32) 2.0888 calculate D2E/DX2 analytically !

! R33 R(18,19) 1.4153 calculate D2E/DX2 analytically !

! R34 R(18,40) 1.427 calculate D2E/DX2 analytically !

! R35 R(19,20) 1.4471 calculate D2E/DX2 analytically !

! R36 R(19,23) 1.3664 calculate D2E/DX2 analytically !

! R37 R(20,21) 1.3623 calculate D2E/DX2 analytically !

! R38 R(20,30) 1.0797 calculate D2E/DX2 analytically !

! R39 R(21,22) 1.4471 calculate D2E/DX2 analytically !

! R40 R(21,31) 1.0797 calculate D2E/DX2 analytically !

! R41 R(22,23) 1.3664 calculate D2E/DX2 analytically !

! R42 R(22,33) 1.4153 calculate D2E/DX2 analytically !

! R43 R(23,32) 2.0888 calculate D2E/DX2 analytically !

! R44 R(33,34) 1.427 calculate D2E/DX2 analytically !

! R45 R(34,36) 1.2058 calculate D2E/DX2 analytically !

! R46 R(35,37) 1.2058 calculate D2E/DX2 analytically !

! R47 R(36,43) 1.0673 calculate D2E/DX2 analytically !

! R48 R(37,45) 1.0673 calculate D2E/DX2 analytically !

! R49 R(38,39) 1.2058 calculate D2E/DX2 analytically !

! R50 R(39,44) 1.0673 calculate D2E/DX2 analytically !

! R51 R(40,41) 1.2058 calculate D2E/DX2 analytically !

! R52 R(41,42) 1.0673 calculate D2E/DX2 analytically !

! A1 A(2,1,5) 106.9066 calculate D2E/DX2 analytically !

! A2 A(2,1,24) 125.5108 calculate D2E/DX2 analytically !

! A3 A(5,1,24) 127.5819 calculate D2E/DX2 analytically !

! A4 A(1,2,3) 109.3363 calculate D2E/DX2 analytically !

! A5 A(1,2,12) 125.1365 calculate D2E/DX2 analytically !

! A6 A(3,2,12) 125.523 calculate D2E/DX2 analytically !

! A7 A(2,3,4) 107.5139 calculate D2E/DX2 analytically !

! A8 A(2,3,32) 126.18 calculate D2E/DX2 analytically !

! A9 A(4,3,32) 126.18 calculate D2E/DX2 analytically !

! A10 A(3,4,5) 109.3363 calculate D2E/DX2 analytically !

! A11 A(3,4,6) 125.523 calculate D2E/DX2 analytically !

! A12 A(5,4,6) 125.1365 calculate D2E/DX2 analytically !

! A13 A(1,5,4) 106.9066 calculate D2E/DX2 analytically !

! A14 A(1,5,25) 127.5819 calculate D2E/DX2 analytically !

! A15 A(4,5,25) 125.5108 calculate D2E/DX2 analytically !

! A16 A(4,6,7) 126.4846 calculate D2E/DX2 analytically !

! A17 A(4,6,38) 116.7556 calculate D2E/DX2 analytically !

! A18 A(7,6,38) 116.7556 calculate D2E/DX2 analytically !

! A19 A(6,7,8) 125.523 calculate D2E/DX2 analytically !

! A20 A(6,7,11) 125.1365 calculate D2E/DX2 analytically !

! A21 A(8,7,11) 109.3363 calculate D2E/DX2 analytically !

! A22 A(7,8,9) 107.5139 calculate D2E/DX2 analytically !

! A23 A(7,8,32) 126.18 calculate D2E/DX2 analytically !

! A24 A(9,8,32) 126.18 calculate D2E/DX2 analytically !

! A25 A(8,9,10) 109.3363 calculate D2E/DX2 analytically !

! A26 A(8,9,33) 125.523 calculate D2E/DX2 analytically !

! A27 A(10,9,33) 125.1365 calculate D2E/DX2 analytically !

! A28 A(9,10,11) 106.9066 calculate D2E/DX2 analytically !

! A29 A(9,10,26) 125.5108 calculate D2E/DX2 analytically !

! A30 A(11,10,26) 127.5819 calculate D2E/DX2 analytically !

! A31 A(7,11,10) 106.9066 calculate D2E/DX2 analytically !

! A32 A(7,11,27) 125.5108 calculate D2E/DX2 analytically !

! A33 A(10,11,27) 127.5819 calculate D2E/DX2 analytically !

! A34 A(2,12,13) 126.4846 calculate D2E/DX2 analytically !

! A35 A(2,12,35) 116.7556 calculate D2E/DX2 analytically !

! A36 A(13,12,35) 116.7556 calculate D2E/DX2 analytically !

! A37 A(12,13,14) 125.1365 calculate D2E/DX2 analytically !

! A38 A(12,13,17) 125.523 calculate D2E/DX2 analytically !

! A39 A(14,13,17) 109.3363 calculate D2E/DX2 analytically !

! A40 A(13,14,15) 106.9066 calculate D2E/DX2 analytically !

! A41 A(13,14,28) 125.5108 calculate D2E/DX2 analytically !

! A42 A(15,14,28) 127.5819 calculate D2E/DX2 analytically !

! A43 A(14,15,16) 106.9066 calculate D2E/DX2 analytically !

! A44 A(14,15,29) 127.5819 calculate D2E/DX2 analytically !

! A45 A(16,15,29) 125.5108 calculate D2E/DX2 analytically !

! A46 A(15,16,17) 109.3363 calculate D2E/DX2 analytically !

! A47 A(15,16,18) 125.1365 calculate D2E/DX2 analytically !

! A48 A(17,16,18) 125.523 calculate D2E/DX2 analytically !

! A49 A(13,17,16) 107.5139 calculate D2E/DX2 analytically !

! A50 A(13,17,32) 126.18 calculate D2E/DX2 analytically !

! A51 A(16,17,32) 126.18 calculate D2E/DX2 analytically !

! A52 A(16,18,19) 126.4846 calculate D2E/DX2 analytically !

! A53 A(16,18,40) 116.7556 calculate D2E/DX2 analytically !

! A54 A(19,18,40) 116.7556 calculate D2E/DX2 analytically !

! A55 A(18,19,20) 125.1365 calculate D2E/DX2 analytically !

! A56 A(18,19,23) 125.523 calculate D2E/DX2 analytically !

! A57 A(20,19,23) 109.3363 calculate D2E/DX2 analytically !

! A58 A(19,20,21) 106.9066 calculate D2E/DX2 analytically !

! A59 A(19,20,30) 125.5108 calculate D2E/DX2 analytically !

! A60 A(21,20,30) 127.5819 calculate D2E/DX2 analytically !

! A61 A(20,21,22) 106.9066 calculate D2E/DX2 analytically !

! A62 A(20,21,31) 127.5819 calculate D2E/DX2 analytically !

! A63 A(22,21,31) 125.5108 calculate D2E/DX2 analytically !

! A64 A(21,22,23) 109.3363 calculate D2E/DX2 analytically !

! A65 A(21,22,33) 125.1365 calculate D2E/DX2 analytically !

! A66 A(23,22,33) 125.523 calculate D2E/DX2 analytically !

! A67 A(19,23,22) 107.5139 calculate D2E/DX2 analytically !

! A68 A(19,23,32) 126.18 calculate D2E/DX2 analytically !

! A69 A(22,23,32) 126.18 calculate D2E/DX2 analytically !

! A70 A(3,32,8) 89.609 calculate D2E/DX2 analytically !

! A71 A(3,32,17) 89.609 calculate D2E/DX2 analytically !

! A72 A(8,32,23) 89.609 calculate D2E/DX2 analytically !

! A73 A(17,32,23) 89.609 calculate D2E/DX2 analytically !

! A74 A(9,33,22) 126.4846 calculate D2E/DX2 analytically !

! A75 A(9,33,34) 116.7556 calculate D2E/DX2 analytically !

! A76 A(22,33,34) 116.7556 calculate D2E/DX2 analytically !

! A77 L(3,32,23,17,-1) 179.218 calculate D2E/DX2 analytically !

! A78 L(8,32,17,23,-1) 179.218 calculate D2E/DX2 analytically !

! A79 L(33,34,36,26,-1) 179.9973 calculate D2E/DX2 analytically !

! A80 L(12,35,37,24,-1) 179.9973 calculate D2E/DX2 analytically !

! A81 L(34,36,43,26,-1) 180.0017 calculate D2E/DX2 analytically !

! A82 L(35,37,45,24,-1) 180.0017 calculate D2E/DX2 analytically !

! A83 L(6,38,39,25,-1) 179.9973 calculate D2E/DX2 analytically !

! A84 L(38,39,44,25,-1) 180.0017 calculate D2E/DX2 analytically !

! A85 L(18,40,41,29,-1) 179.9973 calculate D2E/DX2 analytically !

! A86 L(40,41,42,29,-1) 180.0017 calculate D2E/DX2 analytically !

! A87 L(3,32,23,17,-2) 189.4447 calculate D2E/DX2 analytically !

! A88 L(8,32,17,23,-2) 170.5553 calculate D2E/DX2 analytically !

! A89 L(33,34,36,26,-2) 179.7801 calculate D2E/DX2 analytically !

! A90 L(12,35,37,24,-2) 180.2199 calculate D2E/DX2 analytically !

! A91 L(34,36,43,26,-2) 180.1608 calculate D2E/DX2 analytically !

! A92 L(35,37,45,24,-2) 179.8392 calculate D2E/DX2 analytically !

! A93 L(6,38,39,25,-2) 179.7801 calculate D2E/DX2 analytically !

! A94 L(38,39,44,25,-2) 180.1608 calculate D2E/DX2 analytically !

! A95 L(18,40,41,29,-2) 180.2199 calculate D2E/DX2 analytically !

! A96 L(40,41,42,29,-2) 179.8392 calculate D2E/DX2 analytically !

! D1 D(5,1,2,3) -0.0972 calculate D2E/DX2 analytically !

! D2 D(5,1,2,12) 179.1882 calculate D2E/DX2 analytically !

! D3 D(24,1,2,3) -179.8007 calculate D2E/DX2 analytically !

! D4 D(24,1,2,12) -0.5153 calculate D2E/DX2 analytically !

! D5 D(2,1,5,4) 0.0 calculate D2E/DX2 analytically !

! D6 D(2,1,5,25) -179.6955 calculate D2E/DX2 analytically !

! D7 D(24,1,5,4) 179.6955 calculate D2E/DX2 analytically !

! D8 D(24,1,5,25) 0.0 calculate D2E/DX2 analytically !

! D9 D(1,2,3,4) 0.1573 calculate D2E/DX2 analytically !

! D10 D(1,2,3,32) -175.9517 calculate D2E/DX2 analytically !

! D11 D(12,2,3,4) -179.1247 calculate D2E/DX2 analytically !

! D12 D(12,2,3,32) 4.7663 calculate D2E/DX2 analytically !

! D13 D(1,2,12,13) -178.5823 calculate D2E/DX2 analytically !

! D14 D(1,2,12,35) 0.638 calculate D2E/DX2 analytically !

! D15 D(3,2,12,13) 0.5892 calculate D2E/DX2 analytically !

! D16 D(3,2,12,35) 179.8095 calculate D2E/DX2 analytically !

! D17 D(2,3,4,5) -0.1573 calculate D2E/DX2 analytically !

! D18 D(2,3,4,6) 179.1247 calculate D2E/DX2 analytically !

! D19 D(32,3,4,5) 175.9517 calculate D2E/DX2 analytically !

! D20 D(32,3,4,6) -4.7663 calculate D2E/DX2 analytically !

! D21 D(2,3,32,8) -177.5769 calculate D2E/DX2 analytically !

! D22 D(2,3,32,17) -7.0216 calculate D2E/DX2 analytically !

! D23 D(4,3,32,8) 7.0216 calculate D2E/DX2 analytically !

! D24 D(4,3,32,17) 177.5769 calculate D2E/DX2 analytically !

! D25 D(3,4,5,1) 0.0972 calculate D2E/DX2 analytically !

! D26 D(3,4,5,25) 179.8007 calculate D2E/DX2 analytically !

! D27 D(6,4,5,1) -179.1882 calculate D2E/DX2 analytically !

! D28 D(6,4,5,25) 0.5153 calculate D2E/DX2 analytically !

! D29 D(3,4,6,7) -0.5892 calculate D2E/DX2 analytically !

! D30 D(3,4,6,38) -179.8095 calculate D2E/DX2 analytically !

! D31 D(5,4,6,7) 178.5823 calculate D2E/DX2 analytically !

! D32 D(5,4,6,38) -0.638 calculate D2E/DX2 analytically !

! D33 D(4,6,7,8) 0.5892 calculate D2E/DX2 analytically !

! D34 D(4,6,7,11) -178.5823 calculate D2E/DX2 analytically !

! D35 D(38,6,7,8) 179.8095 calculate D2E/DX2 analytically !

! D36 D(38,6,7,11) 0.638 calculate D2E/DX2 analytically !

! D37 D(6,7,8,9) -179.1247 calculate D2E/DX2 analytically !

! D38 D(6,7,8,32) 4.7663 calculate D2E/DX2 analytically !

! D39 D(11,7,8,9) 0.1573 calculate D2E/DX2 analytically !

! D40 D(11,7,8,32) -175.9517 calculate D2E/DX2 analytically !

! D41 D(6,7,11,10) 179.1882 calculate D2E/DX2 analytically !

! D42 D(6,7,11,27) -0.5153 calculate D2E/DX2 analytically !

! D43 D(8,7,11,10) -0.0972 calculate D2E/DX2 analytically !

! D44 D(8,7,11,27) -179.8007 calculate D2E/DX2 analytically !

! D45 D(7,8,9,10) -0.1573 calculate D2E/DX2 analytically !

! D46 D(7,8,9,33) 179.1247 calculate D2E/DX2 analytically !

! D47 D(32,8,9,10) 175.9517 calculate D2E/DX2 analytically !

! D48 D(32,8,9,33) -4.7663 calculate D2E/DX2 analytically !

! D49 D(7,8,32,3) -7.0216 calculate D2E/DX2 analytically !

! D50 D(7,8,32,23) -177.5769 calculate D2E/DX2 analytically !

! D51 D(9,8,32,3) 177.5769 calculate D2E/DX2 analytically !

! D52 D(9,8,32,23) 7.0216 calculate D2E/DX2 analytically !

! D53 D(8,9,10,11) 0.0972 calculate D2E/DX2 analytically !

! D54 D(8,9,10,26) 179.8007 calculate D2E/DX2 analytically !

! D55 D(33,9,10,11) -179.1882 calculate D2E/DX2 analytically !

! D56 D(33,9,10,26) 0.5153 calculate D2E/DX2 analytically !

! D57 D(8,9,33,22) -0.5892 calculate D2E/DX2 analytically !

! D58 D(8,9,33,34) -179.8095 calculate D2E/DX2 analytically !

! D59 D(10,9,33,22) 178.5823 calculate D2E/DX2 analytically !

! D60 D(10,9,33,34) -0.638 calculate D2E/DX2 analytically !

! D61 D(9,10,11,7) 0.0 calculate D2E/DX2 analytically !

! D62 D(9,10,11,27) 179.6955 calculate D2E/DX2 analytically !

! D63 D(26,10,11,7) -179.6955 calculate D2E/DX2 analytically !

! D64 D(26,10,11,27) 0.0 calculate D2E/DX2 analytically !

! D65 D(2,12,13,14) 178.5823 calculate D2E/DX2 analytically !

! D66 D(2,12,13,17) -0.5892 calculate D2E/DX2 analytically !

! D67 D(35,12,13,14) -0.638 calculate D2E/DX2 analytically !

! D68 D(35,12,13,17) -179.8095 calculate D2E/DX2 analytically !

! D69 D(12,13,14,15) -179.1882 calculate D2E/DX2 analytically !

! D70 D(12,13,14,28) 0.5153 calculate D2E/DX2 analytically !

! D71 D(17,13,14,15) 0.0972 calculate D2E/DX2 analytically !

! D72 D(17,13,14,28) 179.8007 calculate D2E/DX2 analytically !

! D73 D(12,13,17,16) 179.1247 calculate D2E/DX2 analytically !

! D74 D(12,13,17,32) -4.7663 calculate D2E/DX2 analytically !

! D75 D(14,13,17,16) -0.1573 calculate D2E/DX2 analytically !

! D76 D(14,13,17,32) 175.9517 calculate D2E/DX2 analytically !

! D77 D(13,14,15,16) 0.0 calculate D2E/DX2 analytically !

! D78 D(13,14,15,29) 179.6955 calculate D2E/DX2 analytically !

! D79 D(28,14,15,16) -179.6955 calculate D2E/DX2 analytically !

! D80 D(28,14,15,29) 0.0 calculate D2E/DX2 analytically !

! D81 D(14,15,16,17) -0.0972 calculate D2E/DX2 analytically !

! D82 D(14,15,16,18) 179.1882 calculate D2E/DX2 analytically !

! D83 D(29,15,16,17) -179.8007 calculate D2E/DX2 analytically !

! D84 D(29,15,16,18) -0.5153 calculate D2E/DX2 analytically !

! D85 D(15,16,17,13) 0.1573 calculate D2E/DX2 analytically !

! D86 D(15,16,17,32) -175.9517 calculate D2E/DX2 analytically !

! D87 D(18,16,17,13) -179.1247 calculate D2E/DX2 analytically !

! D88 D(18,16,17,32) 4.7663 calculate D2E/DX2 analytically !

! D89 D(15,16,18,19) -178.5823 calculate D2E/DX2 analytically !

! D90 D(15,16,18,40) 0.638 calculate D2E/DX2 analytically !

! D91 D(17,16,18,19) 0.5892 calculate D2E/DX2 analytically !

! D92 D(17,16,18,40) 179.8095 calculate D2E/DX2 analytically !

! D93 D(13,17,32,3) 7.0216 calculate D2E/DX2 analytically !

! D94 D(13,17,32,23) 177.5769 calculate D2E/DX2 analytically !

! D95 D(16,17,32,3) -177.5769 calculate D2E/DX2 analytically !

! D96 D(16,17,32,23) -7.0216 calculate D2E/DX2 analytically !

! D97 D(16,18,19,20) 178.5823 calculate D2E/DX2 analytically !

! D98 D(16,18,19,23) -0.5892 calculate D2E/DX2 analytically !

! D99 D(40,18,19,20) -0.638 calculate D2E/DX2 analytically !

! D100 D(40,18,19,23) -179.8095 calculate D2E/DX2 analytically !

! D101 D(18,19,20,21) -179.1882 calculate D2E/DX2 analytically !

! D102 D(18,19,20,30) 0.5153 calculate D2E/DX2 analytically !

! D103 D(23,19,20,21) 0.0972 calculate D2E/DX2 analytically !

! D104 D(23,19,20,30) 179.8007 calculate D2E/DX2 analytically !

! D105 D(18,19,23,22) 179.1247 calculate D2E/DX2 analytically !

! D106 D(18,19,23,32) -4.7663 calculate D2E/DX2 analytically !

! D107 D(20,19,23,22) -0.1573 calculate D2E/DX2 analytically !

! D108 D(20,19,23,32) 175.9517 calculate D2E/DX2 analytically !

! D109 D(19,20,21,22) 0.0 calculate D2E/DX2 analytically !

! D110 D(19,20,21,31) 179.6955 calculate D2E/DX2 analytically !

! D111 D(30,20,21,22) -179.6955 calculate D2E/DX2 analytically !

! D112 D(30,20,21,31) 0.0 calculate D2E/DX2 analytically !

! D113 D(20,21,22,23) -0.0972 calculate D2E/DX2 analytically !

! D114 D(20,21,22,33) 179.1882 calculate D2E/DX2 analytically !

! D115 D(31,21,22,23) -179.8007 calculate D2E/DX2 analytically !

! D116 D(31,21,22,33) -0.5153 calculate D2E/DX2 analytically !

! D117 D(21,22,23,19) 0.1573 calculate D2E/DX2 analytically !

! D118 D(21,22,23,32) -175.9517 calculate D2E/DX2 analytically !

! D119 D(33,22,23,19) -179.1247 calculate D2E/DX2 analytically !

! D120 D(33,22,23,32) 4.7663 calculate D2E/DX2 analytically !

! D121 D(21,22,33,9) -178.5823 calculate D2E/DX2 analytically !

! D122 D(21,22,33,34) 0.638 calculate D2E/DX2 analytically !

! D123 D(23,22,33,9) 0.5892 calculate D2E/DX2 analytically !

! D124 D(23,22,33,34) 179.8095 calculate D2E/DX2 analytically !

! D125 D(19,23,32,8) 177.5769 calculate D2E/DX2 analytically !

! D126 D(19,23,32,17) 7.0216 calculate D2E/DX2 analytically !

! D127 D(22,23,32,8) -7.0216 calculate D2E/DX2 analytically !

! D128 D(22,23,32,17) -177.5769 calculate D2E/DX2 analytically !

--------------------------------------------------------------------------------

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06

Number of steps in this run= 270 maximum allowed number of steps= 270.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Mon Jul 29 21:22:51 2019, MaxMem= 4294967296 cpu: 0.2

(Enter /home/kira/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -0.681163 -4.273295 -0.041193

2 6 0 -1.101995 -2.889186 -0.006314

3 7 0 0.000000 -2.081690 0.016222

4 6 0 1.101995 -2.889186 -0.006314

5 6 0 0.681163 -4.273295 -0.041193

6 6 0 2.446135 -2.446135 -0.011552

7 6 0 2.889186 -1.101995 -0.006314

8 7 0 2.081690 0.000000 0.016222

9 6 0 2.889186 1.101995 -0.006314

10 6 0 4.273295 0.681163 -0.041193

11 6 0 4.273295 -0.681163 -0.041193

12 6 0 -2.446135 -2.446135 -0.011552

13 6 0 -2.889186 -1.101995 -0.006314

14 6 0 -4.273295 -0.681163 -0.041193

15 6 0 -4.273295 0.681163 -0.041193

16 6 0 -2.889186 1.101995 -0.006314

17 7 0 -2.081690 0.000000 0.016222

18 6 0 -2.446135 2.446135 -0.011552

19 6 0 -1.101995 2.889186 -0.006314

20 6 0 -0.681163 4.273295 -0.041193

21 6 0 0.681163 4.273295 -0.041193

22 6 0 1.101995 2.889186 -0.006314

23 7 0 0.000000 2.081690 0.016222

24 1 0 -1.339682 -5.128561 -0.067294

25 1 0 1.339682 -5.128561 -0.067294

26 1 0 5.128561 1.339682 -0.067294

27 1 0 5.128561 -1.339682 -0.067294

28 1 0 -5.128561 -1.339682 -0.067294

29 1 0 -5.128561 1.339682 -0.067294

30 1 0 -1.339682 5.128561 -0.067294

31 1 0 1.339682 5.128561 -0.067294

32 30 0 0.000000 0.000000 0.188776

33 6 0 2.446135 2.446135 -0.011552

34 6 0 3.454989 3.454989 -0.040621

35 6 0 -3.454989 -3.454989 -0.040621

36 6 0 4.307371 4.307371 -0.069779

37 6 0 -4.307371 -4.307371 -0.069779

38 6 0 3.454989 -3.454989 -0.040621

39 6 0 4.307371 -4.307371 -0.069779

40 6 0 -3.454989 3.454989 -0.040621

41 6 0 -4.307371 4.307371 -0.069779

42 1 0 -5.061915 5.061915 -0.092982

43 1 0 5.061915 5.061915 -0.092982

44 1 0 5.061915 -5.061915 -0.092982

45 1 0 -5.061915 -5.061915 -0.092982

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.447092 0.000000

3 N 2.295738 1.366364 0.000000

4 C 2.257571 2.203990 1.366364 0.000000

5 C 1.362326 2.257571 2.295738 1.447092 0.000000

6 C 3.622069 3.575688 2.473291 1.415286 2.540574

7 C 4.775537 4.373051 3.050853 2.527470 3.864418

8 N 5.088979 4.299274 2.943954 3.050853 4.497313

9 C 6.453088 5.644382 4.299274 4.373051 5.811224

10 C 7.006662 6.453088 5.088979 4.775537 6.119646

11 C 6.119646 5.811224 4.497313 3.864418 5.080042

12 C 2.540574 1.415286 2.473291 3.575688 3.622069

13 C 3.864418 2.527470 3.050853 4.373051 4.775537

14 C 5.080042 3.864418 4.497313 5.811224 6.119646

15 C 6.119646 4.775537 5.088979 6.453088 7.006662

16 C 5.811224 4.373051 4.299274 5.644382 6.453088

17 N 4.497313 3.050853 2.943954 4.299274 5.088979

18 C 6.947427 5.502035 5.146411 6.407410 7.411586

19 C 7.174918 5.778372 5.091612 6.184428 7.381193

20 C 8.546590 7.174918 6.391644 7.381193 8.654486

21 C 8.654486 7.381193 6.391644 7.174918 8.546590

22 C 7.381193 6.184428 5.091612 5.778372 7.174918

23 N 6.391644 5.091612 4.163380 5.091612 6.391644

24 H 1.079726 2.252779 3.329436 3.313654 2.194533

25 H 2.194533 3.313654 3.329436 2.252779 1.079726

26 H 8.078310 7.530396 6.165622 5.839544 7.161392

27 H 6.508430 6.420632 5.182633 4.314848 5.327862

28 H 5.327862 4.314848 5.182633 6.420632 6.508430

29 H 7.161392 5.839544 6.165622 7.530396 8.078310

30 H 9.424926 8.021501 7.334129 8.381514 9.616621

31 H 9.616621 8.381514 7.334129 8.021501 9.424926

32 Zn 4.333350 3.098362 2.088829 3.098362 4.333350

33 C 7.411586 6.407410 5.146411 5.502035 6.947427

34 C 8.765508 7.811263 6.526484 6.766559 8.210998

35 C 2.892012 2.420308 3.718350 4.592103 4.216323

36 C 9.925428 9.003094 7.705903 7.878382 9.315473

37 C 3.626481 3.505669 4.849175 5.592541 4.988732

38 C 4.216323 4.592103 3.718350 2.420308 2.892012

39 C 4.988732 5.592541 4.849175 3.505669 3.626481

40 C 8.210998 6.766559 6.526484 7.811263 8.765508

41 C 9.315473 7.878382 7.705903 9.003094 9.925428

42 H 10.312120 8.883045 8.755912 10.060880 10.960464

43 H 10.960464 10.060880 8.755912 8.883045 10.312120

44 H 5.797202 6.536211 5.875087 4.517657 4.451471

45 H 4.451471 4.517657 5.875087 6.536211 5.797202

6 7 8 9 10

6 C 0.000000

7 C 1.415286 0.000000

8 N 2.473291 1.366364 0.000000

9 C 3.575688 2.203990 1.366364 0.000000

10 C 3.622069 2.257571 2.295738 1.447092 0.000000

11 C 2.540574 1.447092 2.295738 2.257571 1.362326

12 C 4.892270 5.502035 5.146411 6.407410 7.411586

13 C 5.502035 5.778372 5.091612 6.184428 7.381193

14 C 6.947427 7.174918 6.391644 7.381193 8.654486

15 C 7.411586 7.381193 6.391644 7.174918 8.546590

16 C 6.407410 6.184428 5.091612 5.778372 7.174918

17 N 5.146411 5.091612 4.163380 5.091612 6.391644

18 C 6.918715 6.407410 5.146411 5.502035 6.947427

19 C 6.407410 5.644382 4.299274 4.373051 5.811224

20 C 7.411586 6.453088 5.088979 4.775537 6.119646

21 C 6.947427 5.811224 4.497313 3.864418 5.080042

22 C 5.502035 4.373051 3.050853 2.527470 3.864418

23 N 5.146411 4.299274 2.943954 3.050853 4.497313

24 H 4.640143 5.839544 6.165622 7.530396 8.078310

25 H 2.902198 4.314848 5.182633 6.420632 6.508430

26 H 4.640143 3.313654 3.329436 2.252779 1.079726

27 H 2.902198 2.252779 3.329436 3.313654 2.194533

28 H 7.655283 8.021501 7.334129 8.381514 9.616621

29 H 8.468266 8.381514 7.334129 8.021501 9.424926

30 H 8.468266 7.530396 6.165622 5.839544 7.161392

31 H 7.655283 6.420632 5.182633 4.314848 5.327862

32 Zn 3.465153 3.098362 2.088829 3.098362 4.333350

33 C 4.892270 3.575688 2.473291 1.415286 2.540574

34 C 5.986810 4.592103 3.718350 2.420308 2.892012

35 C 5.986810 6.766559 6.526484 7.811263 8.765508

36 C 7.005529 5.592541 4.849175 3.505669 3.626481

37 C 7.005529 7.878382 7.705903 9.003094 9.925428

38 C 1.427031 2.420308 3.718350 4.592103 4.216323

39 C 2.632829 3.505669 4.849175 5.592541 4.988732

40 C 8.345500 7.811263 6.526484 6.766559 8.210998

41 C 9.551077 9.003094 7.705903 7.878382 9.315473

42 H 10.618298 10.060880 8.755912 8.883045 10.312120

43 H 7.951085 6.536211 5.875087 4.517657 4.451471

44 H 3.700168 4.517657 5.875087 6.536211 5.797202

45 H 7.951085 8.883045 8.755912 10.060880 10.960464

11 12 13 14 15

11 C 0.000000

12 C 6.947427 0.000000

13 C 7.174918 1.415286 0.000000

14 C 8.546590 2.540574 1.447092 0.000000

15 C 8.654486 3.622069 2.257571 1.362326 0.000000

16 C 7.381193 3.575688 2.203990 2.257571 1.447092

17 N 6.391644 2.473291 1.366364 2.295738 2.295738

18 C 7.411586 4.892270 3.575688 3.622069 2.540574

19 C 6.453088 5.502035 4.373051 4.775537 3.864418

20 C 7.006662 6.947427 5.811224 6.119646 5.080042

21 C 6.119646 7.411586 6.453088 7.006662 6.119646

22 C 4.775537 6.407410 5.644382 6.453088 5.811224

23 N 5.088979 5.146411 4.299274 5.088979 4.497313

24 H 7.161392 2.902198 4.314848 5.327862 6.508430

25 H 5.327862 4.640143 5.839544 7.161392 8.078310

26 H 2.194533 8.468266 8.381514 9.616621 9.424926

27 H 1.079726 7.655283 8.021501 9.424926 9.616621

28 H 9.424926 2.902198 2.252779 1.079726 2.194533

29 H 9.616621 4.640143 3.313654 2.194533 1.079726

30 H 8.078310 7.655283 6.420632 6.508430 5.327862

31 H 6.508430 8.468266 7.530396 8.078310 7.161392

32 Zn 4.333350 3.465153 3.098362 4.333350 4.333350

33 C 3.622069 6.918715 6.407410 7.411586 6.947427

34 C 4.216323 8.345500 7.811263 8.765508 8.210998

35 C 8.210998 1.427031 2.420308 2.892012 4.216323

36 C 4.988732 9.551077 9.003094 9.925428 9.315473

37 C 9.315473 2.632829 3.505669 3.626481 4.988732

38 C 2.892012 5.986810 6.766559 8.210998 8.765508

39 C 3.626481 7.005529 7.878382 9.315473 9.925428

40 C 8.765508 5.986810 4.592103 4.216323 2.892012

41 C 9.925428 7.005529 5.592541 4.988732 3.626481

42 H 10.960464 7.951085 6.536211 5.797202 4.451471

43 H 5.797202 10.618298 10.060880 10.960464 10.312120

44 H 4.451471 7.951085 8.883045 10.312120 10.960464

45 H 10.312120 3.700168 4.517657 4.451471 5.797202

16 17 18 19 20

16 C 0.000000

17 N 1.366364 0.000000

18 C 1.415286 2.473291 0.000000

19 C 2.527470 3.050853 1.415286 0.000000

20 C 3.864418 4.497313 2.540574 1.447092 0.000000

21 C 4.775537 5.088979 3.622069 2.257571 1.362326

22 C 4.373051 4.299274 3.575688 2.203990 2.257571

23 N 3.050853 2.943954 2.473291 1.366364 2.295738

24 H 6.420632 5.182633 7.655283 8.021501 9.424926

25 H 7.530396 6.165622 8.468266 8.381514 9.616621

26 H 8.021501 7.334129 7.655283 6.420632 6.508430

27 H 8.381514 7.334129 8.468266 7.530396 8.078310

28 H 3.313654 3.329436 4.640143 5.839544 7.161392

29 H 2.252779 3.329436 2.902198 4.314848 5.327862

30 H 4.314848 5.182633 2.902198 2.252779 1.079726

31 H 5.839544 6.165622 4.640143 3.313654 2.194533

32 Zn 3.098362 2.088829 3.465153 3.098362 4.333350

33 C 5.502035 5.146411 4.892270 3.575688 3.622069

34 C 6.766559 6.526484 5.986810 4.592103 4.216323

35 C 4.592103 3.718350 5.986810 6.766559 8.210998

36 C 7.878382 7.705903 7.005529 5.592541 4.988732

37 C 5.592541 4.849175 7.005529 7.878382 9.315473

38 C 7.811263 6.526484 8.345500 7.811263 8.765508

39 C 9.003094 7.705903 9.551077 9.003094 9.925428

40 C 2.420308 3.718350 1.427031 2.420308 2.892012

41 C 3.505669 4.849175 2.632829 3.505669 3.626481

42 H 4.517657 5.875087 3.700168 4.517657 4.451471

43 H 8.883045 8.755912 7.951085 6.536211 5.797202

44 H 10.060880 8.755912 10.618298 10.060880 10.960464

45 H 6.536211 5.875087 7.951085 8.883045 10.312120

21 22 23 24 25

21 C 0.000000

22 C 1.447092 0.000000

23 N 2.295738 1.366364 0.000000

24 H 9.616621 8.381514 7.334129 0.000000

25 H 9.424926 8.021501 7.334129 2.679364 0.000000

26 H 5.327862 4.314848 5.182633 9.147477 7.496251

27 H 7.161392 5.839544 6.165622 7.496251 5.358284

28 H 8.078310 7.530396 6.165622 5.358284 7.496251

29 H 6.508430 6.420632 5.182633 7.496251 9.147477

30 H 2.194533 3.313654 3.329436 10.257122 10.601299

31 H 1.079726 2.252779 3.329436 10.601299 10.257122

32 Zn 4.333350 3.098362 2.088829 5.306831 5.306831

33 C 2.540574 1.415286 2.473291 8.468266 7.655283

34 C 2.892012 2.420308 3.718350 9.831933 8.840394

35 C 8.765508 7.811263 6.526484 2.697421 5.078427

36 C 3.626481 3.505669 4.849175 10.996637 9.891612

37 C 9.925428 9.003094 7.705903 3.079210 5.706450

38 C 8.210998 6.766559 6.526484 5.078427 2.697421

39 C 9.315473 7.878382 7.705903 5.706450 3.079210

40 C 4.216323 4.592103 3.718350 8.840394 9.831933

41 C 4.988732 5.592541 4.849175 9.891612 10.996637

42 H 5.797202 6.536211 5.875087 10.849031 12.034405

43 H 4.451471 4.517657 5.875087 12.034405 10.849031

44 H 10.312120 8.883045 8.755912 6.401995 3.722918

45 H 10.960464 10.060880 8.755912 3.722918 6.401995

26 27 28 29 30

26 H 0.000000

27 H 2.679364 0.000000

28 H 10.601299 10.257122 0.000000

29 H 10.257122 10.601299 2.679364 0.000000

30 H 7.496251 9.147477 7.496251 5.358284 0.000000

31 H 5.358284 7.496251 9.147477 7.496251 2.679364

32 Zn 5.306831 5.306831 5.306831 5.306831 5.306831

33 C 2.902198 4.640143 8.468266 7.655283 4.640143

34 C 2.697421 5.078427 9.831933 8.840394 5.078427

35 C 9.831933 8.840394 2.697421 5.078427 8.840394

36 C 3.079210 5.706450 10.996637 9.891612 5.706450

37 C 10.996637 9.891612 3.079210 5.706450 9.891612

38 C 5.078427 2.697421 8.840394 9.831933 9.831933

39 C 5.706450 3.079210 9.891612 10.996637 10.996637

40 C 8.840394 9.831933 5.078427 2.697421 2.697421

41 C 9.891612 10.996637 5.706450 3.079210 3.079210

42 H 10.849031 12.034405 6.401995 3.722918 3.722918

43 H 3.722918 6.401995 12.034405 10.849031 6.401995

44 H 6.401995 3.722918 10.849031 12.034405 12.034405

45 H 12.034405 10.849031 3.722918 6.401995 10.849031

31 32 33 34 35

31 H 0.000000

32 Zn 5.306831 0.000000

33 C 2.902198 3.465153 0.000000

34 C 2.697421 4.891474 1.427031 0.000000

35 C 9.831933 4.891474 8.345500 9.772185 0.000000

36 C 3.079210 6.097027 2.632829 1.205803 10.977674

37 C 10.996637 6.097027 9.551077 10.977674 1.205803

38 C 8.840394 4.891474 5.986810 6.909978 6.909978

39 C 9.891612 6.097027 7.005529 7.809074 7.809074

40 C 5.078427 4.891474 5.986810 6.909978 6.909978

41 C 5.706450 6.097027 7.005529 7.809074 7.809074

42 H 6.401995 7.164172 7.951085 8.667330 8.667330

43 H 3.722918 7.164172 3.700168 2.273140 12.044835

44 H 10.849031 7.164172 7.951085 8.667330 8.667330

45 H 12.034405 7.164172 10.618298 12.044835 2.273140

36 37 38 39 40

36 C 0.000000

37 C 12.183085 0.000000

38 C 7.809074 7.809074 0.000000

39 C 8.614742 8.614742 1.205803 0.000000

40 C 7.809074 7.809074 9.772185 10.977674 0.000000

41 C 8.614742 8.614742 10.977674 12.183085 1.205803

42 H 9.399649 9.399649 12.044835 13.250192 2.273140

43 H 1.067339 13.250192 8.667330 9.399649 8.667330

44 H 9.399649 9.399649 2.273140 1.067339 12.044835

45 H 13.250192 1.067339 8.667330 9.399649 8.667330

41 42 43 44 45

41 C 0.000000

42 H 1.067339 0.000000

43 H 9.399649 10.123830 0.000000

44 H 13.250192 14.317258 10.123830 0.000000

45 H 9.399649 10.123830 14.317258 10.123830 0.000000

Stoichiometry C28H12N4Zn(3)

Framework group C4V[C4(Zn),2SGV(N2),2SGD(C6H2),X(C16H8)]

Deg. of freedom 19

Full point group C4V NOp 8

Largest Abelian subgroup C2V NOp 4

Largest concise Abelian subgroup C2V NOp 4

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.681163 4.273295 -0.041193

2 6 0 1.101995 2.889186 -0.006314

3 7 0 0.000000 2.081690 0.016222

4 6 0 -1.101995 2.889186 -0.006314

5 6 0 -0.681163 4.273295 -0.041193

6 6 0 -2.446135 2.446135 -0.011552

7 6 0 -2.889186 1.101995 -0.006314

8 7 0 -2.081690 0.000000 0.016222

9 6 0 -2.889186 -1.101995 -0.006314

10 6 0 -4.273295 -0.681163 -0.041193

11 6 0 -4.273295 0.681163 -0.041193

12 6 0 2.446135 2.446135 -0.011552

13 6 0 2.889186 1.101995 -0.006314

14 6 0 4.273295 0.681163 -0.041193

15 6 0 4.273295 -0.681163 -0.041193

16 6 0 2.889186 -1.101995 -0.006314

17 7 0 2.081690 -0.000000 0.016222

18 6 0 2.446135 -2.446135 -0.011552

19 6 0 1.101995 -2.889186 -0.006314

20 6 0 0.681163 -4.273295 -0.041193

21 6 0 -0.681163 -4.273295 -0.041193

22 6 0 -1.101995 -2.889186 -0.006314

23 7 0 -0.000000 -2.081690 0.016222

24 1 0 1.339682 5.128561 -0.067294

25 1 0 -1.339682 5.128561 -0.067294

26 1 0 -5.128561 -1.339682 -0.067294

27 1 0 -5.128561 1.339682 -0.067294

28 1 0 5.128561 1.339682 -0.067294

29 1 0 5.128561 -1.339682 -0.067294

30 1 0 1.339682 -5.128561 -0.067294

31 1 0 -1.339682 -5.128561 -0.067294

32 30 0 0.000000 0.000000 0.188776

33 6 0 -2.446135 -2.446135 -0.011552

34 6 0 -3.454989 -3.454989 -0.040621

35 6 0 3.454989 3.454989 -0.040621

36 6 0 -4.307371 -4.307371 -0.069779

37 6 0 4.307371 4.307371 -0.069779

38 6 0 -3.454989 3.454989 -0.040621

39 6 0 -4.307371 4.307371 -0.069779

40 6 0 3.454989 -3.454989 -0.040621

41 6 0 4.307371 -4.307371 -0.069779

42 1 0 5.061915 -5.061915 -0.092982

43 1 0 -5.061915 -5.061915 -0.092982

44 1 0 -5.061915 5.061915 -0.092982

45 1 0 5.061915 5.061915 -0.092982

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1465170 0.1465170 0.0733190

Leave Link 202 at Mon Jul 29 21:22:51 2019, MaxMem= 4294967296 cpu: 0.2

(Enter /home/kira/g09/l301.exe)

General basis read from cards: (5D, 7F)

Centers: 32

S 1 1.00

Exponent= 7.9970000000D-01 Coefficients= 1.0000000000D+00

S 1 1.00

Exponent= 1.7520000000D-01 Coefficients= 1.0000000000D+00

S 1 1.00

Exponent= 5.5600000000D-02 Coefficients= 1.0000000000D+00

P 1 1.00

Exponent= 1.2020000000D-01 Coefficients= 1.0000000000D+00

P 1 1.00

Exponent= 3.5100000000D-02 Coefficients= 1.0000000000D+00

D 3 1.00

Exponent= 6.8850000000D+01 Coefficients= 2.5853200000D-02

Exponent= 1.8320000000D+01 Coefficients= 1.6511950000D-01

Exponent= 5.9220000000D+00 Coefficients= 4.4682120000D-01

D 1 1.00

Exponent= 1.9270000000D+00 Coefficients= 1.0000000000D+00

D 1 1.00

Exponent= 5.5280000000D-01 Coefficients= 1.0000000000D+00

\*\*\*\*

Centers: 24 25 26 27 28 29 30 31 42 43

Centers: 44 45 1 2 4 5 6 7 9 10

Centers: 11 12 13 14 15 16 18 19 20 21

Centers: 22 33 34 35 36 37 38 39 40 41

Centers: 3 8 17 23

6-311G\*

\*\*\*\*

======================================================================================================

Pseudopotential Parameters

======================================================================================================

Center Atomic Valence Angular Power

Number Number Electrons Momentum of R Exponent Coefficient SO-Coeffient

======================================================================================================

1 6

No pseudopotential on this center.

2 6

No pseudopotential on this center.

3 7

No pseudopotential on this center.

4 6

No pseudopotential on this center.

5 6

No pseudopotential on this center.

6 6

No pseudopotential on this center.

7 6

No pseudopotential on this center.

8 7

No pseudopotential on this center.

9 6

No pseudopotential on this center.

10 6

No pseudopotential on this center.

11 6

No pseudopotential on this center.

12 6

No pseudopotential on this center.

13 6

No pseudopotential on this center.

14 6

No pseudopotential on this center.

15 6

No pseudopotential on this center.

16 6

No pseudopotential on this center.

17 7

No pseudopotential on this center.

18 6

No pseudopotential on this center.

19 6

No pseudopotential on this center.

20 6

No pseudopotential on this center.

21 6

No pseudopotential on this center.

22 6

No pseudopotential on this center.

23 7

No pseudopotential on this center.

24 1

No pseudopotential on this center.

25 1

No pseudopotential on this center.

26 1

No pseudopotential on this center.

27 1

No pseudopotential on this center.

28 1

No pseudopotential on this center.

29 1

No pseudopotential on this center.

30 1

No pseudopotential on this center.

31 1

No pseudopotential on this center.

32 30 12

F and up

1 386.7379660 -18.00000000 0.00000000

2 72.8587359 -124.35274030 0.00000000

2 15.9066170 -30.66018220 0.00000000

2 4.3502340 -10.63589890 0.00000000

2 1.2842199 -0.76836230 0.00000000

S - F

0 19.0867858 3.00000000 0.00000000

1 5.0231080 22.52342250 0.00000000

2 1.2701744 48.44659420 0.00000000

2 1.0671287 -44.55601190 0.00000000

2 0.9264190 12.99839580 0.00000000

P - F

0 43.4927750 5.00000000 0.00000000

1 20.8692669 20.74355890 0.00000000

2 21.7118378 90.30271580 0.00000000

2 6.3616915 74.66103160 0.00000000

2 1.2291195 9.88944240 0.00000000

D - F

2 13.5851800 -4.84903590 0.00000000

2 9.8373050 3.69133790 0.00000000

2 0.8373113 -0.50373190 0.00000000

33 6

No pseudopotential on this center.

34 6

No pseudopotential on this center.

35 6

No pseudopotential on this center.

36 6

No pseudopotential on this center.

37 6

No pseudopotential on this center.

38 6

No pseudopotential on this center.

39 6

No pseudopotential on this center.

40 6

No pseudopotential on this center.

41 6

No pseudopotential on this center.

42 1

No pseudopotential on this center.

43 1

No pseudopotential on this center.

44 1

No pseudopotential on this center.

45 1

No pseudopotential on this center.

======================================================================================================

Ernie: Thresh= 0.10000D-02 Tol= 0.10000D-05 Strict=F.

There are 184 symmetry adapted cartesian basis functions of A1 symmetry.

There are 155 symmetry adapted cartesian basis functions of A2 symmetry.

There are 166 symmetry adapted cartesian basis functions of B1 symmetry.

There are 166 symmetry adapted cartesian basis functions of B2 symmetry.

There are 172 symmetry adapted basis functions of A1 symmetry.

There are 148 symmetry adapted basis functions of A2 symmetry.

There are 158 symmetry adapted basis functions of B1 symmetry.

There are 158 symmetry adapted basis functions of B2 symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

111 alpha electrons 109 beta electrons

nuclear repulsion energy 3060.6075869192 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 45 NActive= 45 NUniq= 9 SFac= 4.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1305299058 Hartrees.

Nuclear repulsion after empirical dispersion term = 3060.4770570133 Hartrees.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: York/Karplus (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3898

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.63D-06

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 148

GePol: Fraction of low-weight points (<1% of avg) = 3.80%

GePol: Cavity surface area = 415.581 Ang\*\*2

GePol: Cavity volume = 419.954 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = 0.0082950066 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3060.4853520199 Hartrees.

Leave Link 301 at Mon Jul 29 21:22:51 2019, MaxMem= 4294967296 cpu: 2.0

(Enter /home/kira/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

One-electron integral symmetry used in STVInt

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 3.40D-05 NBF= 172 148 158 158

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 172 148 158 158

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Mon Jul 29 21:22:52 2019, MaxMem= 4294967296 cpu: 12.0

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Mon Jul 29 21:22:52 2019, MaxMem= 4294967296 cpu: 1.3

(Enter /home/kira/g09/l401.exe)

ExpMin= 3.51D-02 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1359.39225070913

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Alpha Orbitals:

Occupied (E) (E) (A1) (B2) (B1) (E) (E) (A1) (B1) (E) (E)

(A1) (B2) (E) (E) (A1) (A2) (E) (E) (B1) (B1)

(E) (E) (A1) (B2) (E) (E) (A2) (A1) (E) (E) (B1)

(A1) (E) (E) (B2) (B1) (E) (E) (A1) (B1) (E) (E)

(A1) (B2) (E) (E) (A1) (A2) (E) (E) (B2) (B1)

(A1) (E) (E) (B1) (B2) (B1) (E) (E) (A2) (E) (E)

(A1) (A1) (E) (E) (B1) (B2) (E) (E) (A1) (A2)

(E) (E) (A1) (B1) (E) (E) (A1) (B2) (B1) (E) (E)

(E) (E) (A2) (B2) (A1) (B1) (E) (E) (A1) (E) (E)

(B2) (E) (E) (A2) (B2) (B1) (E) (E) (A1) (B2)

(E) (E) (A2) (A1) (E)

Virtual (E) (B1) (B2) (E) (E) (B2) (A2) (B1) (A1) (E)

(E) (E) (E) (A2) (A1) (A1) (A1) (E) (E) (B1) (E)

(E) (A1) (B2) (B1) (E) (E) (E) (E) (A1) (A1) (B1)

(E) (E) (E) (E) (A2) (B1) (B1) (E) (E) (A1) (B2)

(A1) (A2) (A1) (E) (E) (B2) (E) (E) (B1) (A1)

(E) (E) (E) (E) (A1) (B1) (B2) (E) (E) (A1) (A2)

(E) (E) (B1) (E) (E) (A1) (A2) (B2) (B1) (B1)

(A1) (E) (E) (A1) (E) (E) (B2) (B2) (B1) (E) (E)

(A2) (E) (E) (A1) (E) (E) (E) (E) (A2) (B1) (B1)

(E) (E) (A2) (E) (E) (B2) (E) (E) (A1) (A1) (B1)

(B2) (A2) (E) (E) (A1) (E) (E) (A1) (B2) (E) (E)

(A1) (E) (E) (B1) (A2) (E) (E) (B1) (E) (E) (B2)

(B1) (E) (E) (A1) (A1) (A2) (B1) (A2) (E) (E)

(B2) (A1) (E) (E) (B1) (E) (E) (B2) (E) (E) (A1)

(E) (E) (E) (E) (B1) (A2) (B2) (E) (E) (B1) (B1)

(A1) (E) (E) (B2) (A1) (E) (E) (A1) (A2) (E) (E)

(B1) (A2) (B1) (A1) (B2) (E) (E) (A1) (E) (E)

(E) (E) (B1) (E) (E) (A2) (B2) (B2) (A1) (E) (E)

(B1) (A2) (B1) (E) (E) (E) (E) (B2) (A1) (A1)

(B2) (E) (E) (B1) (E) (E) (A2) (B2) (A1) (A2)

(E) (E) (E) (E) (A1) (B1) (A1) (B1) (E) (E) (A2)

(B2) (E) (E) (E) (E) (B1) (B2) (E) (E) (A1) (A2)

(B1) (E) (E) (A1) (A2) (E) (E) (B2) (A1) (E) (E)

(A1) (B1) (B2) (E) (E) (E) (E) (B2) (E) (E) (A2)

(A1) (B2) (E) (E) (B2) (E) (E) (A1) (A2) (E) (E)

(E) (E) (B1) (A1) (B1) (A1) (E) (E) (A2) (E) (E)

(B1) (B2) (A1) (B2) (E) (E) (B1) (E) (E) (A1)

(E) (E) (A2) (B1) (A2) (E) (E) (B2) (A2) (E) (E)

(B2) (A1) (E) (E) (B1) (A1) (A1) (B1) (A2) (E)

(E) (B2) (E) (E) (B1) (E) (E) (A2) (A1) (B1) (E)

(E) (E) (E) (B1) (E) (E) (B2) (A2) (B2) (B1) (A2)

(E) (E) (A1) (B1) (A1) (E) (E) (A2) (E) (E) (A1)

(B2) (B1) (E) (E) (E) (E) (A1) (E) (E) (B1) (A2)

(B1) (E) (E) (A1) (B1) (E) (E) (A1) (B1) (B2)

(E) (E) (B2) (A2) (E) (E) (B2) (A2) (E) (E) (B2)

(A1) (E) (E) (B1) (A1) (E) (E) (A1) (A2) (E) (E)

(A1) (B1) (E) (E) (A2) (B2) (E) (E) (A1) (B1)

(E) (E) (B2) (B1) (E) (E) (E) (E) (B2) (E) (E)

(A1) (A2) (A1) (A2) (A2) (B1) (B2) (E) (E) (E)

(E) (A1) (E) (E) (B1) (B1) (B2) (B1) (A1) (E)

(E) (E) (E) (B1) (A2) (E) (E) (A1) (B2) (E) (E)

(B1) (A1) (E) (E) (B2) (A2) (E) (E) (A2) (A1)

(E) (E) (B1) (A1) (E) (E) (A2) (B1) (B1) (E) (E)

(E) (E) (B2) (B2) (E) (E) (A1) (A1) (E) (E) (B1)

(A2) (A1) (E) (E) (B2) (B1) (A1) (E) (E) (B2)

(E) (E) (A2) (B1) (E) (E) (A2) (E) (E) (A1) (B1)

(B2) (A1) (A1) (E) (E) (B1) (A1) (E) (E) (B2)

(B1) (E) (E) (A1) (A2) (E) (E) (B2) (B1) (E) (E)

(A1) (B1) (E) (E) (A2) (B1) (A1) (E) (E) (B2)

(A1) (E) (E)

Beta Orbitals:

Occupied (E) (E) (A1) (B2) (B1) (E) (E) (A1) (B1) (E) (E)

(A1) (B2) (E) (E) (A1) (A2) (E) (E) (B1) (B1)

(E) (E) (A1) (B2) (E) (E) (A2) (A1) (E) (E) (B1)

(A1) (E) (E) (B2) (B1) (E) (E) (A1) (B1) (E) (E)

(A1) (B2) (E) (E) (A1) (A2) (E) (E) (B2) (B1)

(A1) (E) (E) (B1) (B2) (B1) (E) (E) (A2) (E) (E)

(A1) (A1) (E) (E) (B1) (B2) (E) (E) (A1) (A2)

(E) (E) (A1) (B1) (E) (E) (A1) (B2) (B1) (E) (E)

(E) (E) (A2) (B2) (A1) (B1) (E) (E) (A1) (E) (E)

(B2) (E) (E) (A2) (B2) (B1) (E) (E) (A1) (B2)

(E) (E) (A2)

Virtual (A1) (E) (E) (B1) (B2) (E) (E) (B2) (A2) (B1)

(A1) (E) (E) (E) (E) (A2) (A1) (A1) (A1) (E) (E)

(B1) (E) (E) (A1) (B2) (B1) (E) (E) (E) (E) (A1)

(A1) (B1) (E) (E) (E) (E) (A2) (B1) (B1) (E) (E)

(A1) (B2) (A1) (A2) (A1) (E) (E) (B2) (E) (E)

(B1) (A1) (E) (E) (E) (E) (A1) (B1) (B2) (E) (E)

(A1) (A2) (E) (E) (B1) (E) (E) (A1) (A2) (B2)

(B1) (B1) (A1) (E) (E) (A1) (E) (E) (B2) (B2)

(B1) (E) (E) (A2) (E) (E) (A1) (E) (E) (E) (E)

(A2) (B1) (B1) (E) (E) (A2) (E) (E) (B2) (E) (E)

(A1) (A1) (B1) (B2) (A2) (E) (E) (A1) (E) (E)

(A1) (B2) (E) (E) (A1) (E) (E) (B1) (A2) (E) (E)

(B1) (E) (E) (B2) (B1) (E) (E) (A1) (A1) (A2)

(B1) (A2) (E) (E) (B2) (A1) (E) (E) (B1) (E) (E)

(B2) (E) (E) (A1) (E) (E) (E) (E) (B1) (A2) (B2)

(E) (E) (B1) (B1) (A1) (E) (E) (B2) (A1) (E) (E)

(A1) (A2) (E) (E) (B1) (A2) (B1) (A1) (B2) (E)

(E) (A1) (E) (E) (E) (E) (B1) (E) (E) (A2) (B2)

(B2) (A1) (E) (E) (B1) (A2) (B1) (E) (E) (E) (E)

(B2) (A1) (A1) (B2) (E) (E) (B1) (E) (E) (A2)

(B2) (A1) (A2) (E) (E) (E) (E) (A1) (B1) (A1)

(B1) (E) (E) (A2) (B2) (E) (E) (E) (E) (B1) (B2)

(E) (E) (A1) (A2) (B1) (E) (E) (A1) (A2) (E) (E)

(B2) (A1) (E) (E) (A1) (B1) (B2) (E) (E) (E) (E)

(B2) (E) (E) (A2) (A1) (B2) (E) (E) (B2) (E) (E)

(A1) (A2) (E) (E) (E) (E) (B1) (A1) (B1) (A1)

(E) (E) (A2) (E) (E) (B1) (B2) (A1) (B2) (E) (E)

(B1) (E) (E) (A1) (E) (E) (A2) (B1) (A2) (E) (E)

(B2) (A2) (E) (E) (B2) (A1) (E) (E) (B1) (A1)

(A1) (B1) (A2) (E) (E) (B2) (E) (E) (B1) (E) (E)

(A2) (A1) (B1) (E) (E) (E) (E) (B1) (E) (E) (B2)

(A2) (B2) (B1) (A2) (E) (E) (A1) (B1) (A1) (E)

(E) (A2) (E) (E) (A1) (B2) (B1) (E) (E) (E) (E)

(A1) (E) (E) (B1) (A2) (B1) (E) (E) (A1) (B1)

(E) (E) (A1) (B1) (B2) (E) (E) (B2) (A2) (E) (E)

(B2) (A2) (E) (E) (B2) (A1) (E) (E) (B1) (A1)

(E) (E) (A1) (A2) (E) (E) (A1) (B1) (E) (E) (A2)

(B2) (E) (E) (A1) (B1) (E) (E) (B2) (B1) (E) (E)

(E) (E) (B2) (E) (E) (A1) (A2) (A1) (A2) (A2)

(B1) (B2) (E) (E) (E) (E) (A1) (E) (E) (B1) (B1)

(B2) (B1) (A1) (E) (E) (E) (E) (B1) (A2) (E) (E)

(A1) (B2) (E) (E) (B1) (A1) (E) (E) (B2) (A2)

(E) (E) (A2) (A1) (E) (E) (B1) (A1) (E) (E) (A2)

(B1) (B1) (E) (E) (E) (E) (B2) (B2) (E) (E) (A1)

(A1) (E) (E) (B1) (A2) (A1) (E) (E) (B2) (B1)

(A1) (E) (E) (B2) (E) (E) (A2) (B1) (E) (E) (A2)

(E) (E) (A1) (B1) (B2) (A1) (A1) (E) (E) (B1)

(A1) (E) (E) (B2) (B1) (E) (E) (A1) (A2) (E) (E)

(B2) (B1) (E) (E) (A1) (B1) (E) (E) (A2) (B1)

(A1) (E) (E) (B2) (A1) (E) (E)

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0000 S= 1.0000

Leave Link 401 at Mon Jul 29 21:22:53 2019, MaxMem= 4294967296 cpu: 23.2

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1388313 IEndB= 1388313 NGot= 4294967296 MDV= 4294046536

LenX= 4294046536 LenY= 4293595624

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 660000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Inv3: Mode=1 IEnd= 45583212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.33D-15 for 3879.

Iteration 1 A\*A^-1 deviation from orthogonality is 4.06D-15 for 2188 2002.

Iteration 1 A^-1\*A deviation from unit magnitude is 6.11D-15 for 3879.

Iteration 1 A^-1\*A deviation from orthogonality is 1.87D-14 for 2173 2129.

E= -1358.28180751023

DIIS: error= 8.32D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1358.28180751023 IErMin= 1 ErrMin= 8.32D-02

ErrMax= 8.32D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.80D+00 BMatP= 3.80D+00

IDIUse=3 WtCom= 1.68D-01 WtEn= 8.32D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.019 Goal= None Shift= 0.000

Gap= 0.037 Goal= None Shift= 0.000

GapD= 0.019 DampG=0.250 DampE=0.250 DampFc=0.1250 IDamp=-1.

Damping current iteration by 1.25D-01

RMSDP=2.71D-03 MaxDP=1.14D-01 OVMax= 2.05D-01

Cycle 2 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.37D-04 CP: 9.96D-01

E= -1358.43026087832 Delta-E= -0.148453368090 Rises=F Damp=T

DIIS: error= 5.97D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1358.43026087832 IErMin= 2 ErrMin= 5.97D-02

ErrMax= 5.97D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.21D+00 BMatP= 3.80D+00

IDIUse=3 WtCom= 4.03D-01 WtEn= 5.97D-01

Coeff-Com: -0.297D+01 0.397D+01

Coeff-En: 0.000D+00 0.100D+01

Coeff: -0.120D+01 0.220D+01

Gap= 0.025 Goal= None Shift= 0.000

Gap= 0.039 Goal= None Shift= 0.000

RMSDP=1.56D-03 MaxDP=6.40D-02 DE=-1.48D-01 OVMax= 8.56D-02

Cycle 3 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 9.33D-04 CP: 9.63D-01 3.00D+00

E= -1358.89578995565 Delta-E= -0.465529077328 Rises=F Damp=F

DIIS: error= 3.59D-02 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1358.89578995565 IErMin= 3 ErrMin= 3.59D-02

ErrMax= 3.59D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.64D-01 BMatP= 2.21D+00

IDIUse=3 WtCom= 6.41D-01 WtEn= 3.59D-01

Coeff-Com: 0.141D+01-0.139D+01 0.973D+00

Coeff-En: 0.643D-02 0.000D+00 0.994D+00

Coeff: 0.907D+00-0.888D+00 0.980D+00

Gap= 0.028 Goal= None Shift= 0.000

Gap= 0.040 Goal= None Shift= 0.000

RMSDP=7.67D-04 MaxDP=3.45D-02 DE=-4.66D-01 OVMax= 5.26D-02

Cycle 4 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 5.37D-04 CP: 9.71D-01 3.00D+00 4.16D-01

E= -1358.98929019292 Delta-E= -0.093500237279 Rises=F Damp=F

DIIS: error= 1.50D-02 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1358.98929019292 IErMin= 4 ErrMin= 1.50D-02

ErrMax= 1.50D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.19D-02 BMatP= 5.64D-01

IDIUse=3 WtCom= 8.50D-01 WtEn= 1.50D-01

Coeff-Com: -0.648D-01 0.118D+00 0.308D+00 0.639D+00

Coeff-En: 0.000D+00 0.000D+00 0.530D-01 0.947D+00

Coeff: -0.551D-01 0.100D+00 0.270D+00 0.685D+00

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.042 Goal= None Shift= 0.000

RMSDP=2.36D-04 MaxDP=9.96D-03 DE=-9.35D-02 OVMax= 2.11D-02

Cycle 5 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 8.77D-05 CP: 9.69D-01 3.00D+00 5.67D-01 6.89D-01

E= -1359.00486064467 Delta-E= -0.015570451746 Rises=F Damp=F

DIIS: error= 2.64D-03 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.00486064467 IErMin= 5 ErrMin= 2.64D-03

ErrMax= 2.64D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.11D-03 BMatP= 9.19D-02

IDIUse=3 WtCom= 9.74D-01 WtEn= 2.64D-02

Coeff-Com: -0.165D+00 0.193D+00 0.102D+00 0.450D+00 0.420D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.160D+00 0.188D+00 0.991D-01 0.438D+00 0.435D+00

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.043 Goal= None Shift= 0.000

RMSDP=5.52D-05 MaxDP=3.14D-03 DE=-1.56D-02 OVMax= 8.37D-03

Cycle 6 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.93D-05 CP: 9.69D-01 3.00D+00 5.63D-01 7.46D-01 5.98D-01

E= -1359.00670184438 Delta-E= -0.001841199705 Rises=F Damp=F

DIIS: error= 4.50D-04 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.00670184438 IErMin= 6 ErrMin= 4.50D-04

ErrMax= 4.50D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.81D-04 BMatP= 8.11D-03

IDIUse=3 WtCom= 9.95D-01 WtEn= 4.50D-03

Coeff-Com: -0.516D-01 0.572D-01 0.900D-02 0.931D-01 0.167D+00 0.725D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.513D-01 0.570D-01 0.896D-02 0.927D-01 0.166D+00 0.726D+00

Gap= 0.029 Goal= None Shift= 0.000

Gap= 0.044 Goal= None Shift= 0.000

RMSDP=1.35D-05 MaxDP=6.20D-04 DE=-1.84D-03 OVMax= 3.65D-03

Cycle 7 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.24D-05 CP: 9.69D-01 3.00D+00 5.65D-01 7.46D-01 6.54D-01

CP: 9.88D-01

E= -1359.00678145664 Delta-E= -0.000079612262 Rises=F Damp=F

DIIS: error= 1.77D-04 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.00678145664 IErMin= 7 ErrMin= 1.77D-04

ErrMax= 1.77D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.09D-05 BMatP= 1.81D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.77D-03

Coeff-Com: 0.136D-01-0.170D-01-0.184D-01-0.603D-01-0.326D-01 0.200D+00

Coeff-Com: 0.914D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00

Coeff-En: 0.100D+01

Coeff: 0.135D-01-0.169D-01-0.184D-01-0.602D-01-0.326D-01 0.200D+00

Coeff: 0.914D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=1.01D-05 MaxDP=5.41D-04 DE=-7.96D-05 OVMax= 3.19D-03

Cycle 8 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 5.91D-06 CP: 9.69D-01 3.00D+00 5.66D-01 7.48D-01 6.94D-01

CP: 1.18D+00 1.38D+00

E= -1359.00681299170 Delta-E= -0.000031535066 Rises=F Damp=F

DIIS: error= 1.31D-04 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.00681299170 IErMin= 8 ErrMin= 1.31D-04

ErrMax= 1.31D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.71D-05 BMatP= 3.09D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.31D-03

Coeff-Com: 0.433D-01-0.497D-01-0.139D-01-0.849D-01-0.988D-01-0.214D+00

Coeff-Com: 0.543D+00 0.875D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00 0.000D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.433D-01-0.496D-01-0.138D-01-0.848D-01-0.987D-01-0.214D+00

Coeff: 0.542D+00 0.876D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=8.74D-06 MaxDP=4.25D-04 DE=-3.15D-05 OVMax= 2.88D-03

Cycle 9 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 3.60D-06 CP: 9.69D-01 3.00D+00 5.66D-01 7.49D-01 7.31D-01

CP: 1.34D+00 1.81D+00 1.12D+00

E= -1359.00682649959 Delta-E= -0.000013507890 Rises=F Damp=F

DIIS: error= 4.96D-05 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.00682649959 IErMin= 9 ErrMin= 4.96D-05

ErrMax= 4.96D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.59D-06 BMatP= 1.71D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.176D-01-0.201D-01-0.377D-02-0.289D-01-0.372D-01-0.108D+00

Coeff-Com: 0.996D-01 0.424D+00 0.657D+00

Coeff: 0.176D-01-0.201D-01-0.377D-02-0.289D-01-0.372D-01-0.108D+00

Coeff: 0.996D-01 0.424D+00 0.657D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=2.06D-06 MaxDP=1.09D-04 DE=-1.35D-05 OVMax= 5.35D-04

Cycle 10 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.43D-06 CP: 9.69D-01 3.00D+00 5.66D-01 7.50D-01 7.31D-01

CP: 1.37D+00 1.89D+00 1.27D+00 1.01D+00

E= -1359.00682746303 Delta-E= -0.000000963434 Rises=F Damp=F

DIIS: error= 2.16D-05 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.00682746303 IErMin=10 ErrMin= 2.16D-05

ErrMax= 2.16D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.54D-07 BMatP= 2.59D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.173D-02 0.210D-02 0.143D-02 0.618D-02 0.503D-02-0.434D-02

Coeff-Com: -0.104D+00 0.348D-01 0.434D+00 0.627D+00

Coeff: -0.173D-02 0.210D-02 0.143D-02 0.618D-02 0.503D-02-0.434D-02

Coeff: -0.104D+00 0.348D-01 0.434D+00 0.627D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=1.06D-06 MaxDP=5.36D-05 DE=-9.63D-07 OVMax= 2.22D-04

Cycle 11 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 7.42D-07 CP: 9.69D-01 3.00D+00 5.66D-01 7.50D-01 7.33D-01

CP: 1.37D+00 1.91D+00 1.33D+00 1.15D+00 9.11D-01

E= -1359.00682785075 Delta-E= -0.000000387717 Rises=F Damp=F

DIIS: error= 1.16D-05 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1359.00682785075 IErMin=11 ErrMin= 1.16D-05

ErrMax= 1.16D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.05D-07 BMatP= 9.54D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.418D-02 0.482D-02 0.109D-02 0.735D-02 0.838D-02 0.176D-01

Coeff-Com: -0.542D-01-0.653D-01 0.282D-01 0.216D+00 0.841D+00

Coeff: -0.418D-02 0.482D-02 0.109D-02 0.735D-02 0.838D-02 0.176D-01

Coeff: -0.542D-01-0.653D-01 0.282D-01 0.216D+00 0.841D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=5.89D-07 MaxDP=2.58D-05 DE=-3.88D-07 OVMax= 1.17D-04

Cycle 12 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 4.00D-07 CP: 9.69D-01 3.00D+00 5.66D-01 7.50D-01 7.33D-01

CP: 1.37D+00 1.92D+00 1.35D+00 1.21D+00 1.10D+00

CP: 1.23D+00

E= -1359.00682793235 Delta-E= -0.000000081600 Rises=F Damp=F

DIIS: error= 6.98D-06 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1359.00682793235 IErMin=12 ErrMin= 6.98D-06

ErrMax= 6.98D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.99D-08 BMatP= 1.05D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.209D-02 0.237D-02 0.159D-03 0.240D-02 0.346D-02 0.123D-01

Coeff-Com: 0.627D-02-0.578D-01-0.137D+00-0.830D-01 0.538D+00 0.715D+00

Coeff: -0.209D-02 0.237D-02 0.159D-03 0.240D-02 0.346D-02 0.123D-01

Coeff: 0.627D-02-0.578D-01-0.137D+00-0.830D-01 0.538D+00 0.715D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=3.77D-07 MaxDP=1.70D-05 DE=-8.16D-08 OVMax= 7.79D-05

Cycle 13 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 2.21D-07 CP: 9.69D-01 3.00D+00 5.66D-01 7.50D-01 7.33D-01

CP: 1.37D+00 1.92D+00 1.37D+00 1.24D+00 1.18D+00

CP: 1.54D+00 1.07D+00

E= -1359.00682796825 Delta-E= -0.000000035906 Rises=F Damp=F

DIIS: error= 2.67D-06 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1359.00682796825 IErMin=13 ErrMin= 2.67D-06

ErrMax= 2.67D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.41D-09 BMatP= 5.99D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.188D-03-0.236D-03-0.735D-04-0.424D-03-0.144D-03 0.109D-02

Coeff-Com: 0.133D-01-0.130D-01-0.571D-01-0.667D-01 0.893D-02 0.273D+00

Coeff-Com: 0.841D+00

Coeff: 0.188D-03-0.236D-03-0.735D-04-0.424D-03-0.144D-03 0.109D-02

Coeff: 0.133D-01-0.130D-01-0.571D-01-0.667D-01 0.893D-02 0.273D+00

Coeff: 0.841D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=1.79D-07 MaxDP=7.31D-06 DE=-3.59D-08 OVMax= 3.66D-05

Cycle 14 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.06D-07 CP: 9.69D-01 3.00D+00 5.66D-01 7.50D-01 7.33D-01

CP: 1.37D+00 1.92D+00 1.37D+00 1.26D+00 1.23D+00

CP: 1.64D+00 1.24D+00 1.01D+00

E= -1359.00682797389 Delta-E= -0.000000005642 Rises=F Damp=F

DIIS: error= 1.59D-06 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1359.00682797389 IErMin=14 ErrMin= 1.59D-06

ErrMax= 1.59D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.57D-09 BMatP= 8.41D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.615D-03-0.713D-03-0.728D-04-0.790D-03-0.824D-03-0.181D-02

Coeff-Com: 0.681D-02 0.472D-02-0.475D-02-0.229D-01-0.115D+00 0.656D-02

Coeff-Com: 0.521D+00 0.607D+00

Coeff: 0.615D-03-0.713D-03-0.728D-04-0.790D-03-0.824D-03-0.181D-02

Coeff: 0.681D-02 0.472D-02-0.475D-02-0.229D-01-0.115D+00 0.656D-02

Coeff: 0.521D+00 0.607D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=7.81D-08 MaxDP=3.72D-06 DE=-5.64D-09 OVMax= 1.44D-05

Cycle 15 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 4.57D-08 CP: 9.69D-01 3.00D+00 5.66D-01 7.50D-01 7.33D-01

CP: 1.37D+00 1.92D+00 1.37D+00 1.26D+00 1.24D+00

CP: 1.67D+00 1.29D+00 1.18D+00 8.58D-01

E= -1359.00682797527 Delta-E= -0.000000001376 Rises=F Damp=F

DIIS: error= 5.52D-07 at cycle 15 NSaved= 15.

NSaved=15 IEnMin=15 EnMin= -1359.00682797527 IErMin=15 ErrMin= 5.52D-07

ErrMax= 5.52D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.01D-10 BMatP= 3.57D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.149D-03-0.170D-03-0.331D-04-0.236D-03-0.310D-03-0.661D-03

Coeff-Com: 0.592D-03 0.351D-02 0.428D-02-0.316D-02-0.359D-01-0.297D-01

Coeff-Com: 0.699D-01 0.243D+00 0.749D+00

Coeff: 0.149D-03-0.170D-03-0.331D-04-0.236D-03-0.310D-03-0.661D-03

Coeff: 0.592D-03 0.351D-02 0.428D-02-0.316D-02-0.359D-01-0.297D-01

Coeff: 0.699D-01 0.243D+00 0.749D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=2.85D-08 MaxDP=1.98D-06 DE=-1.38D-09 OVMax= 8.01D-06

Cycle 16 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 1.95D-08 CP: 9.69D-01 3.00D+00 5.66D-01 7.50D-01 7.33D-01

CP: 1.37D+00 1.92D+00 1.37D+00 1.26D+00 1.24D+00

CP: 1.68D+00 1.30D+00 1.21D+00 9.61D-01 9.92D-01

E= -1359.00682797545 Delta-E= -0.000000000181 Rises=F Damp=F

DIIS: error= 4.20D-07 at cycle 16 NSaved= 16.

NSaved=16 IEnMin=16 EnMin= -1359.00682797545 IErMin=16 ErrMin= 4.20D-07

ErrMax= 4.20D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.12D-10 BMatP= 4.01D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.825D-04 0.976D-04-0.489D-05 0.640D-04 0.768D-05 0.124D-04

Coeff-Com: -0.170D-02 0.152D-02 0.539D-02 0.465D-02 0.612D-02-0.240D-01

Coeff-Com: -0.105D+00-0.666D-02 0.527D+00 0.593D+00

Coeff: -0.825D-04 0.976D-04-0.489D-05 0.640D-04 0.768D-05 0.124D-04

Coeff: -0.170D-02 0.152D-02 0.539D-02 0.465D-02 0.612D-02-0.240D-01

Coeff: -0.105D+00-0.666D-02 0.527D+00 0.593D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=1.31D-08 MaxDP=1.02D-06 DE=-1.81D-10 OVMax= 2.53D-06

Cycle 17 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

RMSU= 8.66D-09 CP: 9.69D-01 3.00D+00 5.66D-01 7.50D-01 7.33D-01

CP: 1.37D+00 1.92D+00 1.37D+00 1.26D+00 1.24D+00

CP: 1.69D+00 1.30D+00 1.22D+00 1.02D+00 1.11D+00

CP: 8.74D-01

E= -1359.00682797550 Delta-E= -0.000000000049 Rises=F Damp=F

DIIS: error= 1.51D-07 at cycle 17 NSaved= 17.

NSaved=17 IEnMin=17 EnMin= -1359.00682797550 IErMin=17 ErrMin= 1.51D-07

ErrMax= 1.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.76D-12 BMatP= 2.12D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.194D-04 0.229D-04 0.987D-06 0.177D-04 0.823D-05-0.129D-04

Coeff-Com: -0.334D-03 0.130D-03 0.122D-02 0.204D-02 0.312D-02-0.268D-02

Coeff-Com: -0.305D-01-0.349D-01 0.359D-01 0.136D+00 0.890D+00

Coeff: -0.194D-04 0.229D-04 0.987D-06 0.177D-04 0.823D-05-0.129D-04

Coeff: -0.334D-03 0.130D-03 0.122D-02 0.204D-02 0.312D-02-0.268D-02

Coeff: -0.305D-01-0.349D-01 0.359D-01 0.136D+00 0.890D+00

Gap= 0.030 Goal= None Shift= 0.000

Gap= 0.045 Goal= None Shift= 0.000

RMSDP=5.61D-09 MaxDP=3.02D-07 DE=-4.91D-11 OVMax= 1.63D-06

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

Error on total polarization charges = 0.06194

SCF Done: E(UB3LYP) = -1359.00682798 A.U. after 17 cycles

NFock= 17 Conv=0.56D-08 -V/T= 1.9681

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0541 S= 1.0179

<L.S>= 0.000000000000E+00

KE= 1.403834754201D+03 PE=-9.363387609646D+03 EE= 3.540060675450D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.21

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0541, after 2.0016

Leave Link 502 at Mon Jul 29 21:24:33 2019, MaxMem= 4294967296 cpu: 1559.6

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 109 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 109 NVA= 525 NVB= 527

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13822739D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.29905579D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13809866D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.45348544D-01

Leave Link 801 at Mon Jul 29 21:24:33 2019, MaxMem= 4294967296 cpu: 0.6

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

8 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Mon Jul 29 21:24:37 2019, MaxMem= 4294967296 cpu: 59.0

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Mon Jul 29 21:24:37 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

Density matrix has lower than full symmetry, NOpUse= 4 NOpAll= 8.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 260

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Mon Jul 29 21:26:47 2019, MaxMem= 4294967296 cpu: 2076.6

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Density matrix has lower than full symmetry, NOpUse= 4 NOpAll= 8.

Using symmetry in CPHF.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 660000000 NMat= 42 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 2.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 42 NMatS0= 42 NMatT0= 0 NMatD0= 42 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 42 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 42.

42 vectors produced by pass 0 Test12= 2.76D-13 2.38D-09 XBig12= 7.50D+03 6.12D+01.

AX will form 42 AO Fock derivatives at one time.

42 vectors produced by pass 1 Test12= 2.76D-13 2.38D-09 XBig12= 8.46D+02 4.95D+00.

42 vectors produced by pass 2 Test12= 2.76D-13 2.38D-09 XBig12= 1.82D+02 3.92D+00.

42 vectors produced by pass 3 Test12= 2.76D-13 2.38D-09 XBig12= 3.81D+01 1.24D+00.

42 vectors produced by pass 4 Test12= 2.76D-13 2.38D-09 XBig12= 3.10D+00 3.06D-01.

42 vectors produced by pass 5 Test12= 2.76D-13 2.38D-09 XBig12= 1.33D-01 5.28D-02.

42 vectors produced by pass 6 Test12= 2.76D-13 2.38D-09 XBig12= 4.68D-03 8.73D-03.

42 vectors produced by pass 7 Test12= 2.76D-13 2.38D-09 XBig12= 1.22D-04 1.01D-03.

40 vectors produced by pass 8 Test12= 2.76D-13 2.38D-09 XBig12= 2.33D-06 1.35D-04.

25 vectors produced by pass 9 Test12= 2.76D-13 2.38D-09 XBig12= 3.35D-08 1.26D-05.

8 vectors produced by pass 10 Test12= 2.76D-13 2.38D-09 XBig12= 4.00D-10 1.75D-06.

2 vectors produced by pass 11 Test12= 2.76D-13 2.38D-09 XBig12= 4.95D-12 1.74D-07.

2 vectors produced by pass 12 Test12= 2.76D-13 2.38D-09 XBig12= 8.26D-14 1.92D-08.

InvSVY: IOpt=1 It= 1 EMax= 4.26D-14

Solved reduced A of dimension 413 with 42 vectors.

FullF1: Do perturbations 1 to 42.

Isotropic polarizability for W= 0.000000 1036.61 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Mon Jul 29 22:43:18 2019, MaxMem= 4294967296 cpu: 73445.6

(Enter /home/kira/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Alpha Orbitals:

Occupied (E) (E) (E) (E) (B2) (?A) (?A) (?B) (?A) (?B)

(B2) (?A) (?A) (B2) (?B) (?A) (B1) (E) (E) (A1)

(B1) (E) (E) (A1) (E) (E) (E) (E) (E) (E) (E)

(E) (?C) (?D) (?D) (?C) (?E) (?D) (?D) (?C) (?D)

(?C) (?D) (?C) (?E) (?D) (?D) (?C) (?E) (?D) (?D)

(?E) (?C) (?E) (?D) (?D) (?C) (?C) (?D) (?D) (?E)

(?C) (?E) (?D) (?D) (?C) (?E) (?D) (?D) (?D) (?D)

(?C) (?C) (?E) (?D) (?D) (?F) (?E) (?G) (?G) (?C)

(?D) (?D) (?F) (?E) (?C) (?E) (?D) (?C) (?D) (?E)

(?G) (?G) (?F) (?D) (?D) (?C) (?D) (?D) (?E) (?H)

(?G) (?G) (?C) (?F) (?G) (?F) (?G) (?F) (?H) (?G)

Virtual (?G) (?H) (?F) (B2) (?F) (E) (E) (E) (A2) (?G)

(?G) (?F) (?G) (?G) (?F) (E) (E) (E) (?F) (E)

(E) (?I) (?F) (E) (?F) (E) (?I) (E) (E) (?I) (A1)

(?J) (E) (?H) (E) (?K) (?K) (?J) (?K) (A1) (?K)

(?K) (?J) (?J) (?K) (?K) (?K) (?K) (?K) (?J) (?J)

(?K) (?K) (?K) (?K) (?J) (?K) (?K) (?K) (?J) (?K)

(?K) (?K) (?J) (?K) (?K) (?K) (B1) (?K) (?J) (?J)

(?J) (?K) (?K) (?J) (?K) (?K) (?K) (?K) (?J) (?K)

(?K) (?K) (?K) (?K) (?K) (?J) (?J) (?K) (B1) (?K)

(?K) (?K) (?K) (?K) (?J) (?K) (?K) (?K) (?K) (?K)

(?K) (?J) (?J) (?J) (?K) (?K) (?K) (A1) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?J) (?K) (?K) (?K) (?K)

(?J) (?J) (?K) (?J) (?K) (?J) (?K) (?K) (?K) (?J)

(?K) (?K) (?K) (?K) (?K) (?K) (?J) (?K) (?J) (?K)

(?K) (?K) (?K) (?K) (?K) (?J) (?K) (?K) (?K) (?K)

(?J) (?K) (?K) (?K) (?K) (?J) (B1) (?K) (?K) (?J)

(?K) (?J) (?K) (?K) (?J) (?K) (?K) (?K) (?J) (?K)

(?K) (?J) (?K) (?K) (?K) (?K) (?K) (?J) (?K) (?K)

(?K) (?K) (?K) (?K) (?J) (?J) (?K) (?K) (?J) (?J)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?J) (?K) (?J)

(B1) (?K) (?K) (?K) (?J) (?J) (?J) (?K) (?K) (?K)

(?K) (?J) (?K) (A2) (?K) (?K) (?K) (?J) (?J) (?K)

(?K) (?K) (?K) (?J) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?J) (?J) (?K) (E) (E) (?J) (?K) (?J)

(?K) (?K) (?J) (?J) (?K) (?K) (E) (?K) (?K) (?J)

(?K) (?J) (?K) (E) (?K) (?K) (?J) (?J) (?K) (?K)

(?J) (?K) (?K) (?J) (?K) (?K) (?K) (?K) (?K) (?K)

(?J) (?K) (?K) (?J) (?K) (?K) (?K) (?K) (?K) (?J)

(?J) (?J) (?K) (?K) (?K) (?K) (?K) (?J) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?J) (?K) (?K) (?K) (?K)

(?J) (?K) (?K) (?J) (?J) (?J) (?K) (?K) (?K) (?J)

(?K) (?K) (?K) (?K) (?K) (?K) (?J) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?J) (?J) (?K)

(?K) (A1) (A1) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (A2)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (A1) (?K) (?K) (?K) (?K) (E) (E) (?K) (?K)

(E) (E) (?K) (E) (?K) (E) (?K) (?K) (E) (E) (E)

(?K) (?K) (E) (E) (E) (?K) (?K) (E) (?K) (?K)

(E) (E) (E) (E) (E) (E) (E) (A1) (B1) (B2) (A1)

(?K) (?K) (?K) (B1) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(E) (E) (E) (E) (B1) (A1) (E) (E) (E) (E) (E)

(E)

Beta Orbitals:

Occupied (E) (E) (E) (E) (B2) (?A) (?A) (?B) (?A) (?B)

(B2) (?A) (?A) (?B) (B2) (?A) (B1) (E) (E) (A1)

(B1) (E) (E) (A1) (E) (E) (E) (E) (E) (E) (E)

(E) (?C) (?D) (?D) (?C) (?E) (?D) (?D) (?C) (?D)

(?C) (?D) (?C) (?E) (?D) (?D) (A1) (?E) (?D) (?D)

(?E) (?E) (?F) (?D) (?D) (?F) (?F) (?D) (?D) (?E)

(?F) (?E) (?D) (?D) (?F) (?E) (?D) (?D) (?D) (?D)

(?F) (?F) (?E) (?D) (?D) (?F) (?E) (?D) (?F) (?D)

(?D) (?D) (?E) (?F) (?F) (?D) (?F) (?D) (?E) (?G)

(?D) (?D) (?D) (?D) (?F) (?F) (?D) (?D) (?E) (?G)

(?F) (?D) (?F) (?D) (?F) (?D) (?D) (?G)

Virtual (?F) (?D) (?D) (?G) (?F) (?F) (E) (E) (A2) (?G)

(?F) (?D) (?D) (?F) (?D) (?F) (?D) (?D) (?D) (?G)

(?F) (?D) (?D) (?G) (?F) (?D) (?F) (?D) (?G) (?D)

(?D) (?G) (?F) (?F) (?G) (?D) (?D) (?D) (?D) (?F)

(?G) (?F) (?D) (?D) (?F) (?F) (?G) (?D) (?D) (?D)

(?D) (?F) (?F) (?G) (?G) (?D) (?D) (?F) (?G) (?D)

(?D) (?F) (?G) (?D) (?D) (?F) (?D) (?D) (?D) (?D)

(?F) (?G) (?F) (?F) (?G) (?G) (?F) (?D) (?G) (?D)

(?D) (?F) (?D) (?D) (?D) (?G) (?D) (?D) (?F) (?G)

(?F) (?G) (?D) (?D) (?D) (?D) (?G) (?F) (?D) (?D)

(?D) (?D) (?G) (?G) (?F) (?F) (?F) (?D) (?D) (?G)

(?F) (?D) (?D) (?D) (?D) (?D) (?G) (?F) (?D) (?G)

(?D) (?D) (?G) (?F) (?F) (?D) (?F) (?D) (?D) (?F)

(?D) (?G) (?F) (?G) (?D) (?G) (?D) (?D) (?D) (?F)

(?G) (?F) (?G) (?D) (?D) (?D) (?D) (?F) (?D) (?D)

(?G) (?D) (?D) (?F) (?G) (?D) (?D) (?G) (?F) (?G)

(?D) (?D) (?F) (?G) (?F) (?D) (?D) (?D) (?D) (?F)

(?G) (A1) (?G) (?G) (?F) (?D) (?D) (?G) (?D) (?D)

(?F) (?D) (?D) (?G) (?D) (?G) (?D) (?F) (?F) (?D)

(?D) (?F) (?F) (?D) (?D) (?G) (?G) (?G) (?D) (?D)

(?F) (?D) (?F) (?G) (?D) (?D) (?D) (?F) (?F) (?F)

(?D) (?D) (?D) (?D) (?G) (?F) (?G) (?D) (?D) (?G)

(?F) (A1) (?D) (?D) (?G) (?G) (?F) (?D) (?D) (?G)

(?D) (?D) (?D) (?D) (?G) (?F) (?F) (?G) (?D) (?D)

(?F) (?G) (?F) (?H) (?H) (?F) (?F) (?H) (?H) (?I)

(?H) (?H) (?F) (?H) (?H) (?F) (?H) (?I) (?H) (?F)

(?F) (?F) (?H) (?H) (?H) (?H) (?F) (?I) (?H) (?H)

(?H) (?H) (?I) (?F) (?I) (?I) (?H) (?F) (?H) (?H)

(?H) (?I) (?F) (?F) (?F) (?I) (?H) (?H) (?H) (?F)

(?H) (?H) (?H) (?I) (?I) (?I) (?H) (?H) (?F) (?I)

(?H) (?H) (?F) (?I) (?H) (?H) (?F) (?F) (?F) (?I)

(?I) (?H) (?F) (?I) (?H) (?H) (?H) (?H) (?H) (?F)

(?I) (?I) (?H) (?H) (?H) (?I) (?H) (?H) (?H) (?F)

(?I) (?F) (?I) (?I) (?F) (A1) (?H) (?I) (?H) (?H)

(?H) (?H) (?H) (?I) (?J) (?I) (?H) (?H) (?K) (?H)

(?H) (?H) (?H) (?K) (?I) (?I) (?I) (?H) (?H) (?K)

(?I) (?J) (?I) (?H) (?H) (?H) (?H) (?J) (?I) (?H)

(?H) (?J) (?I) (?J) (?J) (?H) (?H) (?I) (?H) (?H)

(?J) (?J) (?H) (?H) (?J) (?I) (?H) (?H) (?J) (?I)

(?H) (A2) (?H) (?J) (?H) (?H) (?H) (?H) (?J) (?I)

(?J) (?I) (?H) (?H) (?H) (?H) (?J) (?J) (?H) (?H)

(?I) (?I) (?J) (?I) (?H) (?J) (?I) (?H) (?H) (?H)

(?J) (?I) (?H) (?H) (?I) (?J) (?I) (?J) (?H) (?H)

(?I) (?H) (?H) (?I) (?H) (?H) (?J) (?J) (?I) (?J)

(?H) (?H) (?H) (?H) (?I) (?J) (?H) (?H) (?I) (?J)

(?H) (?H) (?I) (?H) (A1) (?I) (?H) (?I) (?I) (E)

(E) (?K) (E) (?K) (E) (?K) (?K) (E) (E) (?K) (?K)

(?I) (?I) (E) (?K) (?K) (E) (E) (E) (?K) (?K)

(E) (?K) (?K) (E) (E) (E) (E) (E) (E) (E) (A1)

(B1) (B2) (A1) (?K) (?K) (?K) (B1) (?K) (?K) (?K)

(?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K) (?K)

(?K) (?K) (?K) (E) (E) (E) (E) (B1) (A1) (E) (E)

(E) (E) (E) (E)

Unable to determine electronic state: an orbital has unidentified symmetry.

Alpha occ. eigenvalues -- -14.31825 -14.31824 -14.31734 -14.31733 -10.22735

Alpha occ. eigenvalues -- -10.22735 -10.22735 -10.22735 -10.22092 -10.22092

Alpha occ. eigenvalues -- -10.22091 -10.22091 -10.20915 -10.20915 -10.20915

Alpha occ. eigenvalues -- -10.20915 -10.18836 -10.18836 -10.18836 -10.18836

Alpha occ. eigenvalues -- -10.18107 -10.18107 -10.18107 -10.18107 -10.17585

Alpha occ. eigenvalues -- -10.17585 -10.17518 -10.17518 -10.16310 -10.16310

Alpha occ. eigenvalues -- -10.16244 -10.16244 -0.97672 -0.97069 -0.96378

Alpha occ. eigenvalues -- -0.95712 -0.85581 -0.83611 -0.83539 -0.81674

Alpha occ. eigenvalues -- -0.77697 -0.77522 -0.76994 -0.76538 -0.76022

Alpha occ. eigenvalues -- -0.75290 -0.75233 -0.73749 -0.72829 -0.67886

Alpha occ. eigenvalues -- -0.67785 -0.63100 -0.60016 -0.60001 -0.59389

Alpha occ. eigenvalues -- -0.59057 -0.58365 -0.57441 -0.56406 -0.56373

Alpha occ. eigenvalues -- -0.56111 -0.55663 -0.55507 -0.55084 -0.55073

Alpha occ. eigenvalues -- -0.53151 -0.52699 -0.52555 -0.52199 -0.51760

Alpha occ. eigenvalues -- -0.51564 -0.50291 -0.49788 -0.46169 -0.45304

Alpha occ. eigenvalues -- -0.45158 -0.44739 -0.43447 -0.43352 -0.43049

Alpha occ. eigenvalues -- -0.42620 -0.41327 -0.41113 -0.40349 -0.39831

Alpha occ. eigenvalues -- -0.38779 -0.38438 -0.38257 -0.37998 -0.37921

Alpha occ. eigenvalues -- -0.37725 -0.34893 -0.34860 -0.33276 -0.32890

Alpha occ. eigenvalues -- -0.32435 -0.30089 -0.29779 -0.29765 -0.29434

Alpha occ. eigenvalues -- -0.28413 -0.27516 -0.27376 -0.27126 -0.26942

Alpha occ. eigenvalues -- -0.25954 -0.25626 -0.25364 -0.21813 -0.21290

Alpha occ. eigenvalues -- -0.14196

Alpha virt. eigenvalues -- -0.11206 -0.06836 0.02238 0.02543 0.02794

Alpha virt. eigenvalues -- 0.02869 0.02870 0.03299 0.03433 0.03595

Alpha virt. eigenvalues -- 0.03714 0.04428 0.04996 0.05021 0.05213

Alpha virt. eigenvalues -- 0.05648 0.05704 0.06643 0.07793 0.08394

Alpha virt. eigenvalues -- 0.08431 0.08432 0.09710 0.09793 0.09830

Alpha virt. eigenvalues -- 0.09913 0.11465 0.12457 0.12577 0.13663

Alpha virt. eigenvalues -- 0.13669 0.15250 0.15736 0.15742 0.15797

Alpha virt. eigenvalues -- 0.17171 0.17435 0.19154 0.19815 0.21986

Alpha virt. eigenvalues -- 0.23046 0.23276 0.23750 0.24029 0.24149

Alpha virt. eigenvalues -- 0.24812 0.24915 0.25558 0.25622 0.26381

Alpha virt. eigenvalues -- 0.26493 0.26716 0.28123 0.29712 0.29831

Alpha virt. eigenvalues -- 0.30895 0.30996 0.32420 0.32463 0.32562

Alpha virt. eigenvalues -- 0.35049 0.35100 0.35128 0.35222 0.35506

Alpha virt. eigenvalues -- 0.35618 0.36188 0.36220 0.36311 0.36563

Alpha virt. eigenvalues -- 0.36704 0.38068 0.38400 0.39732 0.40184

Alpha virt. eigenvalues -- 0.40186 0.40498 0.40767 0.41223 0.41262

Alpha virt. eigenvalues -- 0.41324 0.42076 0.42171 0.43381 0.43469

Alpha virt. eigenvalues -- 0.43588 0.43709 0.44275 0.44485 0.44861

Alpha virt. eigenvalues -- 0.45523 0.45525 0.47142 0.47229 0.47875

Alpha virt. eigenvalues -- 0.48137 0.48836 0.48861 0.49314 0.49367

Alpha virt. eigenvalues -- 0.50795 0.51127 0.51207 0.51417 0.51617

Alpha virt. eigenvalues -- 0.51918 0.52005 0.52099 0.54757 0.56082

Alpha virt. eigenvalues -- 0.56143 0.57005 0.57005 0.57473 0.57497

Alpha virt. eigenvalues -- 0.57576 0.57576 0.57934 0.58601 0.58693

Alpha virt. eigenvalues -- 0.61320 0.61695 0.62116 0.62236 0.62367

Alpha virt. eigenvalues -- 0.62519 0.63254 0.63341 0.63701 0.63974

Alpha virt. eigenvalues -- 0.64464 0.65062 0.65217 0.65468 0.65489

Alpha virt. eigenvalues -- 0.68312 0.68429 0.68896 0.69222 0.69833

Alpha virt. eigenvalues -- 0.70049 0.70238 0.70260 0.71611 0.71638

Alpha virt. eigenvalues -- 0.73456 0.73553 0.73602 0.74548 0.74601

Alpha virt. eigenvalues -- 0.74651 0.74809 0.74951 0.75272 0.75360

Alpha virt. eigenvalues -- 0.76959 0.77350 0.78681 0.81300 0.81358

Alpha virt. eigenvalues -- 0.81970 0.82456 0.83302 0.84288 0.84395

Alpha virt. eigenvalues -- 0.85564 0.85691 0.85957 0.88321 0.89733

Alpha virt. eigenvalues -- 0.90874 0.91092 0.91261 0.92662 0.92688

Alpha virt. eigenvalues -- 0.94627 0.95445 0.95531 0.95929 0.97510

Alpha virt. eigenvalues -- 0.97629 0.99808 0.99939 1.00143 1.00414

Alpha virt. eigenvalues -- 1.00885 1.01600 1.01815 1.01827 1.04443

Alpha virt. eigenvalues -- 1.04768 1.05303 1.05422 1.05816 1.06641

Alpha virt. eigenvalues -- 1.06779 1.08612 1.08623 1.11520 1.12214

Alpha virt. eigenvalues -- 1.12301 1.12332 1.12639 1.13178 1.13264

Alpha virt. eigenvalues -- 1.13773 1.14013 1.14595 1.15141 1.15399

Alpha virt. eigenvalues -- 1.16206 1.16248 1.16946 1.17051 1.17741

Alpha virt. eigenvalues -- 1.18407 1.18560 1.18987 1.19213 1.20727

Alpha virt. eigenvalues -- 1.20907 1.21102 1.21109 1.22311 1.23752

Alpha virt. eigenvalues -- 1.24506 1.24509 1.25142 1.25662 1.25696

Alpha virt. eigenvalues -- 1.27936 1.28230 1.28381 1.29019 1.31446

Alpha virt. eigenvalues -- 1.31678 1.33707 1.33778 1.34058 1.37478

Alpha virt. eigenvalues -- 1.42188 1.42511 1.42735 1.47323 1.47602

Alpha virt. eigenvalues -- 1.48354 1.48443 1.49306 1.51492 1.51767

Alpha virt. eigenvalues -- 1.52627 1.54796 1.54799 1.54815 1.54890

Alpha virt. eigenvalues -- 1.54964 1.55129 1.56373 1.57708 1.58195

Alpha virt. eigenvalues -- 1.58371 1.58371 1.58678 1.58867 1.59198

Alpha virt. eigenvalues -- 1.60934 1.61335 1.61518 1.62749 1.62765

Alpha virt. eigenvalues -- 1.62767 1.64478 1.64884 1.65509 1.66498

Alpha virt. eigenvalues -- 1.66541 1.66873 1.70066 1.70163 1.72260

Alpha virt. eigenvalues -- 1.72402 1.73896 1.75257 1.76652 1.77029

Alpha virt. eigenvalues -- 1.77238 1.78907 1.79026 1.79341 1.79945

Alpha virt. eigenvalues -- 1.80078 1.80194 1.81013 1.81176 1.83897

Alpha virt. eigenvalues -- 1.84027 1.85153 1.86474 1.87459 1.87703

Alpha virt. eigenvalues -- 1.88247 1.88375 1.89101 1.89130 1.89264

Alpha virt. eigenvalues -- 1.89848 1.90452 1.93554 1.94019 1.94606

Alpha virt. eigenvalues -- 1.94884 1.94928 1.95200 1.95493 1.95626

Alpha virt. eigenvalues -- 1.97360 1.97456 1.99045 1.99843 2.00554

Alpha virt. eigenvalues -- 2.03123 2.03146 2.03976 2.04183 2.04221

Alpha virt. eigenvalues -- 2.09198 2.09222 2.11615 2.11633 2.13674

Alpha virt. eigenvalues -- 2.18228 2.20085 2.25313 2.26460 2.27815

Alpha virt. eigenvalues -- 2.27969 2.28418 2.30746 2.30818 2.33344

Alpha virt. eigenvalues -- 2.33659 2.35042 2.35408 2.36245 2.36267

Alpha virt. eigenvalues -- 2.36432 2.37808 2.40461 2.40648 2.40989

Alpha virt. eigenvalues -- 2.41326 2.41349 2.41505 2.43320 2.45287

Alpha virt. eigenvalues -- 2.48336 2.48431 2.49170 2.49975 2.51963

Alpha virt. eigenvalues -- 2.53114 2.53640 2.53722 2.55816 2.56096

Alpha virt. eigenvalues -- 2.56752 2.56768 2.57668 2.57745 2.58175

Alpha virt. eigenvalues -- 2.59901 2.60159 2.61583 2.62338 2.62645

Alpha virt. eigenvalues -- 2.64149 2.64457 2.64566 2.66538 2.67249

Alpha virt. eigenvalues -- 2.70960 2.70966 2.73457 2.76887 2.77900

Alpha virt. eigenvalues -- 2.77915 2.79991 2.80718 2.82837 2.82969

Alpha virt. eigenvalues -- 2.83094 2.84242 2.87034 2.87340 2.87936

Alpha virt. eigenvalues -- 2.87979 2.87980 2.87990 2.91835 2.95277

Alpha virt. eigenvalues -- 2.95482 2.95708 2.95949 2.95979 2.96010

Alpha virt. eigenvalues -- 2.97573 2.98627 2.98667 2.99876 3.00650

Alpha virt. eigenvalues -- 3.01265 3.02742 3.03205 3.03487 3.04091

Alpha virt. eigenvalues -- 3.04131 3.05163 3.05182 3.06790 3.07089

Alpha virt. eigenvalues -- 3.08447 3.08463 3.09134 3.16928 3.17853

Alpha virt. eigenvalues -- 3.18261 3.18423 3.18582 3.21124 3.21666

Alpha virt. eigenvalues -- 3.21980 3.24617 3.25657 3.25756 3.28542

Alpha virt. eigenvalues -- 3.29877 3.30793 3.31857 3.32294 3.32294

Alpha virt. eigenvalues -- 3.33198 3.33890 3.35251 3.36223 3.37531

Alpha virt. eigenvalues -- 3.37861 3.44704 3.48109 3.51813 3.51903

Alpha virt. eigenvalues -- 3.52801 3.56883 3.56888 3.57635 3.57786

Alpha virt. eigenvalues -- 3.58950 3.62973 3.65305 3.65455 3.81721

Alpha virt. eigenvalues -- 3.82346 3.82390 3.84698 3.85133 3.85268

Alpha virt. eigenvalues -- 3.85701 3.89048 3.92887 3.93251 3.96427

Alpha virt. eigenvalues -- 3.99819 4.11135 4.19885 4.20082 4.32338

Alpha virt. eigenvalues -- 4.33197 4.46795 4.51295 4.51545 4.61267

Alpha virt. eigenvalues -- 4.65157 4.65234 4.65846 5.14238 5.19136

Alpha virt. eigenvalues -- 5.19518 5.31865 7.78487 7.78503 7.86600

Alpha virt. eigenvalues -- 7.92450 8.12814 11.11492 23.26672 23.31762

Alpha virt. eigenvalues -- 23.31828 23.34596 23.51803 23.54767 23.55783

Alpha virt. eigenvalues -- 23.57606 23.74612 23.76370 23.76418 23.78265

Alpha virt. eigenvalues -- 23.91331 23.93725 23.93868 23.96551 24.00032

Alpha virt. eigenvalues -- 24.01547 24.01898 24.02758 24.13004 24.13116

Alpha virt. eigenvalues -- 24.14359 24.14690 24.93582 24.93641 24.93955

Alpha virt. eigenvalues -- 24.93955 35.62183 35.63658 35.64774 35.64894

Beta occ. eigenvalues -- -14.31608 -14.31608 -14.31493 -14.31493 -10.22316

Beta occ. eigenvalues -- -10.22316 -10.22316 -10.22316 -10.22205 -10.22205

Beta occ. eigenvalues -- -10.22205 -10.22205 -10.20840 -10.20840 -10.20840

Beta occ. eigenvalues -- -10.20839 -10.18943 -10.18943 -10.18943 -10.18942

Beta occ. eigenvalues -- -10.17873 -10.17873 -10.17873 -10.17873 -10.17597

Beta occ. eigenvalues -- -10.17597 -10.17531 -10.17531 -10.16223 -10.16223

Beta occ. eigenvalues -- -10.16157 -10.16157 -0.97335 -0.96767 -0.96010

Beta occ. eigenvalues -- -0.95389 -0.84955 -0.83043 -0.82879 -0.81079

Beta occ. eigenvalues -- -0.77538 -0.77370 -0.76726 -0.76244 -0.75676

Beta occ. eigenvalues -- -0.74876 -0.74850 -0.73053 -0.72696 -0.67678

Beta occ. eigenvalues -- -0.67221 -0.62704 -0.59837 -0.59830 -0.59284

Beta occ. eigenvalues -- -0.58813 -0.58291 -0.57406 -0.56354 -0.56352

Beta occ. eigenvalues -- -0.56092 -0.55412 -0.55396 -0.54884 -0.54876

Beta occ. eigenvalues -- -0.53057 -0.52478 -0.52430 -0.51986 -0.51553

Beta occ. eigenvalues -- -0.51399 -0.50197 -0.49568 -0.45931 -0.45067

Beta occ. eigenvalues -- -0.44913 -0.43778 -0.43213 -0.42603 -0.42544

Beta occ. eigenvalues -- -0.41877 -0.41247 -0.41052 -0.39801 -0.39660

Beta occ. eigenvalues -- -0.38681 -0.38229 -0.37817 -0.37769 -0.37624

Beta occ. eigenvalues -- -0.36841 -0.33678 -0.33656 -0.32614 -0.32254

Beta occ. eigenvalues -- -0.32128 -0.29986 -0.29657 -0.29647 -0.29304

Beta occ. eigenvalues -- -0.27117 -0.26848 -0.26437 -0.26271 -0.26265

Beta occ. eigenvalues -- -0.24783 -0.24450 -0.24354 -0.20831

Beta virt. eigenvalues -- -0.16296 -0.09969 -0.09202 -0.04774 0.02449

Beta virt. eigenvalues -- 0.02614 0.02931 0.02941 0.03490 0.03776

Beta virt. eigenvalues -- 0.03813 0.04286 0.04375 0.04799 0.05395

Beta virt. eigenvalues -- 0.05602 0.05676 0.05764 0.05850 0.07006

Beta virt. eigenvalues -- 0.07867 0.08473 0.08522 0.08533 0.09755

Beta virt. eigenvalues -- 0.09841 0.09906 0.09984 0.11504 0.12473

Beta virt. eigenvalues -- 0.12655 0.13711 0.14676 0.15343 0.17033

Beta virt. eigenvalues -- 0.17036 0.17111 0.17316 0.17557 0.19326

Beta virt. eigenvalues -- 0.20024 0.22569 0.23283 0.23603 0.23807

Beta virt. eigenvalues -- 0.24278 0.24320 0.24930 0.25111 0.25808

Beta virt. eigenvalues -- 0.25821 0.26560 0.26857 0.26995 0.28170

Beta virt. eigenvalues -- 0.29889 0.30162 0.31081 0.31123 0.32541

Beta virt. eigenvalues -- 0.32576 0.32633 0.35351 0.35450 0.35503

Beta virt. eigenvalues -- 0.35506 0.35814 0.36002 0.36292 0.36407

Beta virt. eigenvalues -- 0.36608 0.36823 0.37144 0.38199 0.38555

Beta virt. eigenvalues -- 0.39840 0.40299 0.40513 0.40863 0.41022

Beta virt. eigenvalues -- 0.41463 0.41628 0.41725 0.42224 0.42297

Beta virt. eigenvalues -- 0.43485 0.43763 0.43825 0.43918 0.44629

Beta virt. eigenvalues -- 0.44718 0.45491 0.45857 0.45867 0.47485

Beta virt. eigenvalues -- 0.47613 0.48063 0.48433 0.49179 0.49260

Beta virt. eigenvalues -- 0.49589 0.49599 0.50952 0.51274 0.51347

Beta virt. eigenvalues -- 0.51509 0.51995 0.52114 0.52221 0.52269

Beta virt. eigenvalues -- 0.55121 0.56265 0.56280 0.57250 0.57252

Beta virt. eigenvalues -- 0.57740 0.57743 0.57788 0.57968 0.58179

Beta virt. eigenvalues -- 0.58770 0.58936 0.61344 0.62119 0.62357

Beta virt. eigenvalues -- 0.62377 0.62643 0.62644 0.63369 0.63410

Beta virt. eigenvalues -- 0.63793 0.64104 0.64596 0.65096 0.65252

Beta virt. eigenvalues -- 0.65539 0.65593 0.68335 0.68579 0.69017

Beta virt. eigenvalues -- 0.69230 0.70057 0.70381 0.70718 0.70814

Beta virt. eigenvalues -- 0.71814 0.71839 0.73665 0.73872 0.74033

Beta virt. eigenvalues -- 0.74678 0.74722 0.74757 0.74939 0.75011

Beta virt. eigenvalues -- 0.75382 0.75475 0.77058 0.78076 0.79533

Beta virt. eigenvalues -- 0.81336 0.81508 0.82038 0.82562 0.83393

Beta virt. eigenvalues -- 0.84340 0.84552 0.85783 0.86102 0.86106

Beta virt. eigenvalues -- 0.88439 0.89967 0.90923 0.91307 0.91468

Beta virt. eigenvalues -- 0.92729 0.92817 0.94759 0.95772 0.95785

Beta virt. eigenvalues -- 0.96454 0.97575 0.97904 0.99909 1.00552

Beta virt. eigenvalues -- 1.00775 1.00878 1.01245 1.01676 1.02081

Beta virt. eigenvalues -- 1.02148 1.04634 1.05568 1.05685 1.05852

Beta virt. eigenvalues -- 1.06236 1.07322 1.07460 1.08920 1.09041

Beta virt. eigenvalues -- 1.11660 1.12357 1.12469 1.12482 1.13008

Beta virt. eigenvalues -- 1.13395 1.13493 1.13828 1.14286 1.14998

Beta virt. eigenvalues -- 1.15327 1.15640 1.16340 1.16550 1.17179

Beta virt. eigenvalues -- 1.17287 1.18199 1.18702 1.19001 1.19221

Beta virt. eigenvalues -- 1.19355 1.21090 1.21131 1.21294 1.21455

Beta virt. eigenvalues -- 1.22386 1.23828 1.24819 1.24874 1.25283

Beta virt. eigenvalues -- 1.25911 1.26005 1.28156 1.28582 1.28603

Beta virt. eigenvalues -- 1.29404 1.31778 1.32251 1.34076 1.34146

Beta virt. eigenvalues -- 1.34442 1.37520 1.42424 1.42762 1.42954

Beta virt. eigenvalues -- 1.47688 1.47906 1.48831 1.48861 1.49810

Beta virt. eigenvalues -- 1.51794 1.52014 1.52751 1.54985 1.55170

Beta virt. eigenvalues -- 1.55201 1.55258 1.55278 1.55320 1.57174

Beta virt. eigenvalues -- 1.57817 1.58461 1.58544 1.58790 1.59056

Beta virt. eigenvalues -- 1.59267 1.59507 1.61064 1.61568 1.61783

Beta virt. eigenvalues -- 1.62952 1.62958 1.63580 1.64623 1.65058

Beta virt. eigenvalues -- 1.65576 1.66577 1.66659 1.67072 1.70247

Beta virt. eigenvalues -- 1.70270 1.72372 1.72884 1.74044 1.75556

Beta virt. eigenvalues -- 1.76907 1.77130 1.77450 1.79324 1.79360

Beta virt. eigenvalues -- 1.79488 1.79994 1.80313 1.80583 1.81105

Beta virt. eigenvalues -- 1.81154 1.83939 1.84321 1.85694 1.86549

Beta virt. eigenvalues -- 1.87847 1.88290 1.88694 1.88895 1.89595

Beta virt. eigenvalues -- 1.89656 1.89803 1.90374 1.90654 1.93782

Beta virt. eigenvalues -- 1.94488 1.94706 1.95065 1.95339 1.95716

Beta virt. eigenvalues -- 1.96018 1.96178 1.97434 1.97713 1.99180

Beta virt. eigenvalues -- 1.99905 2.00992 2.03458 2.03537 2.04332

Beta virt. eigenvalues -- 2.04587 2.04964 2.09292 2.09339 2.11721

Beta virt. eigenvalues -- 2.12178 2.13710 2.18267 2.20164 2.26091

Beta virt. eigenvalues -- 2.27274 2.27980 2.28477 2.28515 2.31440

Beta virt. eigenvalues -- 2.31510 2.33585 2.34073 2.35070 2.36108

Beta virt. eigenvalues -- 2.36561 2.36864 2.36969 2.37848 2.40468

Beta virt. eigenvalues -- 2.40670 2.41127 2.41370 2.41397 2.41597

Beta virt. eigenvalues -- 2.43398 2.45846 2.48493 2.48757 2.49366

Beta virt. eigenvalues -- 2.50226 2.52681 2.53733 2.54273 2.54329

Beta virt. eigenvalues -- 2.56182 2.56704 2.57100 2.57464 2.57851

Beta virt. eigenvalues -- 2.58025 2.58471 2.60070 2.60790 2.61773

Beta virt. eigenvalues -- 2.62675 2.63157 2.64560 2.64782 2.64934

Beta virt. eigenvalues -- 2.66957 2.67748 2.71095 2.71107 2.73664

Beta virt. eigenvalues -- 2.77058 2.78197 2.78221 2.80257 2.81147

Beta virt. eigenvalues -- 2.82966 2.83238 2.83322 2.84469 2.87125

Beta virt. eigenvalues -- 2.87453 2.88368 2.88372 2.88381 2.88389

Beta virt. eigenvalues -- 2.92004 2.95709 2.95737 2.96140 2.96165

Beta virt. eigenvalues -- 2.96576 2.97534 2.97548 2.98560 2.98605

Beta virt. eigenvalues -- 2.99868 3.00854 3.01426 3.02775 3.04075

Beta virt. eigenvalues -- 3.04221 3.04296 3.04666 3.05342 3.05367

Beta virt. eigenvalues -- 3.06966 3.08433 3.08548 3.08559 3.09224

Beta virt. eigenvalues -- 3.16969 3.17933 3.18343 3.18461 3.18638

Beta virt. eigenvalues -- 3.21191 3.21723 3.22116 3.24682 3.25775

Beta virt. eigenvalues -- 3.25879 3.28795 3.29967 3.30883 3.31910

Beta virt. eigenvalues -- 3.32498 3.32544 3.33224 3.33953 3.35502

Beta virt. eigenvalues -- 3.36269 3.37589 3.37975 3.44792 3.48318

Beta virt. eigenvalues -- 3.51944 3.52047 3.52917 3.56890 3.57043

Beta virt. eigenvalues -- 3.57806 3.57808 3.59092 3.63078 3.65424

Beta virt. eigenvalues -- 3.65608 3.81948 3.82409 3.82623 3.84800

Beta virt. eigenvalues -- 3.86229 3.86258 3.86297 3.90025 3.93126

Beta virt. eigenvalues -- 3.93540 3.96750 4.00074 4.11524 4.20235

Beta virt. eigenvalues -- 4.20465 4.32579 4.33535 4.47014 4.51431

Beta virt. eigenvalues -- 4.51888 4.61599 4.65460 4.65493 4.66089

Beta virt. eigenvalues -- 5.14415 5.19317 5.19753 5.32115 7.78510

Beta virt. eigenvalues -- 7.78516 7.86606 7.92453 8.12821 11.11509

Beta virt. eigenvalues -- 23.26786 23.31875 23.31948 23.34715 23.51881

Beta virt. eigenvalues -- 23.54780 23.55905 23.57659 23.74784 23.76519

Beta virt. eigenvalues -- 23.76605 23.78444 23.91321 23.93747 23.93887

Beta virt. eigenvalues -- 23.96537 24.00323 24.01768 24.02164 24.03004

Beta virt. eigenvalues -- 24.13001 24.13099 24.14458 24.14775 24.93632

Beta virt. eigenvalues -- 24.93692 24.94006 24.94007 35.62424 35.63899

Beta virt. eigenvalues -- 35.65028 35.65123

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 5.178894 0.446208 -0.079224 -0.069209 0.504192 0.015237

2 C 0.446208 4.917587 0.433510 -0.159884 -0.069209 -0.000223

3 N -0.079224 0.433510 6.939022 0.433510 -0.079224 -0.012432

4 C -0.069209 -0.159884 0.433510 4.917587 0.446208 0.364003

5 C 0.504192 -0.069209 -0.079224 0.446208 5.178894 -0.079757

6 C 0.015237 -0.000223 -0.012432 0.364003 -0.079757 5.209292

7 C -0.001262 -0.000364 -0.021399 -0.104960 0.012978 0.410745

8 N 0.000048 0.000388 -0.013972 -0.019044 -0.000321 -0.017020

9 C -0.000005 0.000003 0.000478 -0.000453 0.000044 -0.000873

10 C 0.000001 -0.000005 0.000059 -0.001228 -0.000006 0.013654

11 C -0.000007 0.000043 -0.000378 0.012917 -0.000143 -0.074737

12 C -0.079757 0.364003 -0.012432 -0.000223 0.015237 -0.002536

13 C 0.012978 -0.104960 -0.021399 -0.000364 -0.001262 0.000223

14 C -0.000143 0.012917 -0.000378 0.000043 -0.000007 0.000001

15 C -0.000006 -0.001228 0.000059 -0.000005 0.000001 -0.000000

16 C 0.000044 -0.000453 0.000478 0.000003 -0.000005 0.000001

17 N -0.000321 -0.019044 -0.013972 0.000388 0.000048 -0.000168

18 C 0.000001 0.000210 -0.000179 0.000002 -0.000000 0.000002

19 C -0.000000 -0.000063 0.000175 -0.000006 0.000000 0.000002

20 C -0.000000 -0.000000 0.000002 0.000000 0.000000 -0.000000

21 C 0.000000 0.000000 0.000002 -0.000000 -0.000000 0.000001

22 C 0.000000 -0.000006 0.000175 -0.000063 -0.000000 0.000210

23 N 0.000002 0.000175 -0.001762 0.000175 0.000002 -0.000179

24 H 0.390420 -0.038942 0.005278 0.005789 -0.034782 -0.000169

25 H -0.034782 0.005789 0.005278 -0.038942 0.390420 -0.005749

26 H 0.000000 -0.000000 0.000002 0.000010 0.000000 -0.000160

27 H -0.000000 0.000001 -0.000003 -0.000022 0.000007 -0.005314

28 H 0.000007 -0.000022 -0.000003 0.000001 -0.000000 0.000000

29 H 0.000000 0.000010 0.000002 -0.000000 0.000000 0.000000

30 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

31 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

32 Zn 0.001886 -0.013895 0.125683 -0.013895 0.001886 -0.009078

33 C -0.000000 0.000002 -0.000179 0.000210 0.000001 -0.002325

34 C -0.000000 0.000000 -0.000000 0.000003 0.000000 -0.000055

35 C -0.017278 -0.075247 0.004260 -0.000441 0.002656 -0.000059

36 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000002

37 C -0.000617 -0.003979 -0.000069 -0.000053 0.000325 -0.000002

38 C 0.002656 -0.000441 0.004260 -0.075247 -0.017278 0.552310

39 C 0.000325 -0.000053 -0.000069 -0.003979 -0.000617 -0.104080

40 C 0.000000 0.000003 -0.000000 0.000000 -0.000000 0.000000

41 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

43 H -0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000002 -0.000000 0.000001 -0.000033 0.000093 0.001742

45 H 0.000093 -0.000033 0.000001 -0.000000 0.000002 -0.000000

7 8 9 10 11 12

1 C -0.001262 0.000048 -0.000005 0.000001 -0.000007 -0.079757

2 C -0.000364 0.000388 0.000003 -0.000005 0.000043 0.364003

3 N -0.021399 -0.013972 0.000478 0.000059 -0.000378 -0.012432

4 C -0.104960 -0.019044 -0.000453 -0.001228 0.012917 -0.000223

5 C 0.012978 -0.000321 0.000044 -0.000006 -0.000143 0.015237

6 C 0.410745 -0.017020 -0.000873 0.013654 -0.074737 -0.002536

7 C 4.883217 0.426061 -0.145591 -0.062824 0.402162 0.000223

8 N 0.426061 6.967264 0.426061 -0.076371 -0.076371 -0.000168

9 C -0.145591 0.426061 4.883217 0.402162 -0.062824 0.000001

10 C -0.062824 -0.076371 0.402162 5.146891 0.537680 -0.000000

11 C 0.402162 -0.076371 -0.062824 0.537680 5.146891 0.000001

12 C 0.000223 -0.000168 0.000001 -0.000000 0.000001 5.209292

13 C -0.000067 0.000175 -0.000005 0.000000 -0.000000 0.410745

14 C -0.000000 0.000002 0.000000 0.000000 -0.000000 -0.074737

15 C 0.000000 0.000002 -0.000000 -0.000000 0.000000 0.013654

16 C -0.000005 0.000175 -0.000067 -0.000000 0.000000 -0.000873

17 N 0.000175 -0.001798 0.000175 0.000002 0.000002 -0.017020

18 C 0.000001 -0.000168 0.000223 0.000001 -0.000000 -0.002325

19 C 0.000003 0.000388 -0.000364 0.000043 -0.000005 0.000210

20 C -0.000005 0.000048 -0.001262 -0.000007 0.000001 0.000001

21 C 0.000044 -0.000321 0.012978 -0.000143 -0.000006 -0.000000

22 C -0.000453 -0.019044 -0.104960 0.012917 -0.001228 0.000002

23 N 0.000478 -0.013972 -0.021399 -0.000378 0.000059 -0.000179

24 H 0.000013 0.000002 -0.000000 0.000000 0.000000 -0.005749

25 H -0.000059 -0.000002 0.000000 -0.000000 0.000009 -0.000169

26 H 0.005569 0.005113 -0.038091 0.388523 -0.032883 0.000000

27 H -0.038091 0.005113 0.005569 -0.032883 0.388523 0.000000

28 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.005314

29 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000160

30 H -0.000000 0.000002 0.000013 0.000000 0.000000 0.000000

31 H 0.000000 -0.000002 -0.000059 0.000009 -0.000000 0.000000

32 Zn -0.013811 0.122592 -0.013811 0.001814 0.001814 -0.009078

33 C -0.000873 -0.017020 0.410745 -0.074737 0.013654 0.000002

34 C -0.000511 0.004193 -0.076217 -0.015176 0.002583 0.000000

35 C 0.000003 -0.000000 0.000000 -0.000000 0.000000 0.552310

36 C -0.000051 -0.000055 -0.005130 -0.000531 0.000353 0.000000

37 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.104080

38 C -0.076217 0.004193 -0.000511 0.002583 -0.015176 -0.000059

39 C -0.005130 -0.000055 -0.000051 0.000353 -0.000531 -0.000002

40 C 0.000000 -0.000000 0.000003 0.000000 -0.000000 -0.000055

41 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000002

42 H 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

43 H -0.000000 0.000001 -0.000036 0.000095 0.000002 0.000000

44 H -0.000036 0.000001 -0.000000 0.000002 0.000095 -0.000000

45 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.001742

13 14 15 16 17 18

1 C 0.012978 -0.000143 -0.000006 0.000044 -0.000321 0.000001

2 C -0.104960 0.012917 -0.001228 -0.000453 -0.019044 0.000210

3 N -0.021399 -0.000378 0.000059 0.000478 -0.013972 -0.000179

4 C -0.000364 0.000043 -0.000005 0.000003 0.000388 0.000002

5 C -0.001262 -0.000007 0.000001 -0.000005 0.000048 -0.000000

6 C 0.000223 0.000001 -0.000000 0.000001 -0.000168 0.000002

7 C -0.000067 -0.000000 0.000000 -0.000005 0.000175 0.000001

8 N 0.000175 0.000002 0.000002 0.000175 -0.001798 -0.000168

9 C -0.000005 0.000000 -0.000000 -0.000067 0.000175 0.000223

10 C 0.000000 0.000000 -0.000000 -0.000000 0.000002 0.000001

11 C -0.000000 -0.000000 0.000000 0.000000 0.000002 -0.000000

12 C 0.410745 -0.074737 0.013654 -0.000873 -0.017020 -0.002325

13 C 4.883217 0.402162 -0.062824 -0.145591 0.426061 -0.000873

14 C 0.402162 5.146891 0.537680 -0.062824 -0.076371 0.013654

15 C -0.062824 0.537680 5.146891 0.402162 -0.076371 -0.074737

16 C -0.145591 -0.062824 0.402162 4.883217 0.426061 0.410745

17 N 0.426061 -0.076371 -0.076371 0.426061 6.967264 -0.017020

18 C -0.000873 0.013654 -0.074737 0.410745 -0.017020 5.209292

19 C -0.000453 -0.001228 0.012917 -0.104960 -0.019044 0.364003

20 C 0.000044 -0.000006 -0.000143 0.012978 -0.000321 -0.079757

21 C -0.000005 0.000001 -0.000007 -0.001262 0.000048 0.015237

22 C 0.000003 -0.000005 0.000043 -0.000364 0.000388 -0.000223

23 N 0.000478 0.000059 -0.000378 -0.021399 -0.013972 -0.012432

24 H -0.000059 0.000009 -0.000000 0.000000 -0.000002 0.000000

25 H 0.000013 0.000000 0.000000 -0.000000 0.000002 0.000000

26 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

27 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

28 H -0.038091 0.388523 -0.032883 0.005569 0.005113 -0.000160

29 H 0.005569 -0.032883 0.388523 -0.038091 0.005113 -0.005314

30 H 0.000000 -0.000000 0.000009 -0.000059 -0.000002 -0.005749

31 H -0.000000 0.000000 0.000000 0.000013 0.000002 -0.000169

32 Zn -0.013811 0.001814 0.001814 -0.013811 0.122592 -0.009078

33 C 0.000001 -0.000000 0.000001 0.000223 -0.000168 -0.002536

34 C 0.000000 -0.000000 0.000000 0.000003 -0.000000 -0.000059

35 C -0.076217 -0.015176 0.002583 -0.000511 0.004193 -0.000055

36 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000002

37 C -0.005130 -0.000531 0.000353 -0.000051 -0.000055 -0.000002

38 C 0.000003 0.000000 -0.000000 0.000000 -0.000000 0.000000

39 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

40 C -0.000511 0.002583 -0.015176 -0.076217 0.004193 0.552310

41 C -0.000051 0.000353 -0.000531 -0.005130 -0.000055 -0.104080

42 H -0.000000 0.000002 0.000095 -0.000036 0.000001 0.001742

43 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

45 H -0.000036 0.000095 0.000002 -0.000000 0.000001 -0.000000

19 20 21 22 23 24

1 C -0.000000 -0.000000 0.000000 0.000000 0.000002 0.390420

2 C -0.000063 -0.000000 0.000000 -0.000006 0.000175 -0.038942

3 N 0.000175 0.000002 0.000002 0.000175 -0.001762 0.005278

4 C -0.000006 0.000000 -0.000000 -0.000063 0.000175 0.005789

5 C 0.000000 0.000000 -0.000000 -0.000000 0.000002 -0.034782

6 C 0.000002 -0.000000 0.000001 0.000210 -0.000179 -0.000169

7 C 0.000003 -0.000005 0.000044 -0.000453 0.000478 0.000013

8 N 0.000388 0.000048 -0.000321 -0.019044 -0.013972 0.000002

9 C -0.000364 -0.001262 0.012978 -0.104960 -0.021399 -0.000000

10 C 0.000043 -0.000007 -0.000143 0.012917 -0.000378 0.000000

11 C -0.000005 0.000001 -0.000006 -0.001228 0.000059 0.000000

12 C 0.000210 0.000001 -0.000000 0.000002 -0.000179 -0.005749

13 C -0.000453 0.000044 -0.000005 0.000003 0.000478 -0.000059

14 C -0.001228 -0.000006 0.000001 -0.000005 0.000059 0.000009

15 C 0.012917 -0.000143 -0.000007 0.000043 -0.000378 -0.000000

16 C -0.104960 0.012978 -0.001262 -0.000364 -0.021399 0.000000

17 N -0.019044 -0.000321 0.000048 0.000388 -0.013972 -0.000002

18 C 0.364003 -0.079757 0.015237 -0.000223 -0.012432 0.000000

19 C 4.917587 0.446208 -0.069209 -0.159884 0.433510 -0.000000

20 C 0.446208 5.178894 0.504192 -0.069209 -0.079224 -0.000000

21 C -0.069209 0.504192 5.178894 0.446208 -0.079224 0.000000

22 C -0.159884 -0.069209 0.446208 4.917587 0.433510 -0.000000

23 N 0.433510 -0.079224 -0.079224 0.433510 6.939022 0.000000

24 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.440548

25 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.002391

26 H 0.000001 -0.000000 0.000007 -0.000022 -0.000003 -0.000000

27 H -0.000000 0.000000 0.000000 0.000010 0.000002 -0.000000

28 H 0.000010 0.000000 0.000000 -0.000000 0.000002 -0.000005

29 H -0.000022 0.000007 -0.000000 0.000001 -0.000003 -0.000000

30 H -0.038942 0.390420 -0.034782 0.005789 0.005278 -0.000000

31 H 0.005789 -0.034782 0.390420 -0.038942 0.005278 -0.000000

32 Zn -0.013895 0.001886 0.001886 -0.013895 0.125683 -0.000360

33 C -0.000223 0.015237 -0.079757 0.364003 -0.012432 0.000000

34 C -0.000441 0.002656 -0.017278 -0.075247 0.004260 -0.000000

35 C 0.000003 0.000000 -0.000000 0.000000 -0.000000 0.006199

36 C -0.000053 0.000325 -0.000617 -0.003979 -0.000069 -0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.003045

38 C 0.000000 -0.000000 0.000000 0.000003 -0.000000 -0.000096

39 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000010

40 C -0.075247 -0.017278 0.002656 -0.000441 0.004260 0.000000

41 C -0.003979 -0.000617 0.000325 -0.000053 -0.000069 -0.000000

42 H -0.000033 0.000093 0.000002 -0.000000 0.000001 -0.000000

43 H -0.000000 0.000002 0.000093 -0.000033 0.000001 -0.000000

44 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

45 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000061

25 26 27 28 29 30

1 C -0.034782 0.000000 -0.000000 0.000007 0.000000 -0.000000

2 C 0.005789 -0.000000 0.000001 -0.000022 0.000010 -0.000000

3 N 0.005278 0.000002 -0.000003 -0.000003 0.000002 0.000000

4 C -0.038942 0.000010 -0.000022 0.000001 -0.000000 -0.000000

5 C 0.390420 0.000000 0.000007 -0.000000 0.000000 0.000000

6 C -0.005749 -0.000160 -0.005314 0.000000 0.000000 0.000000

7 C -0.000059 0.005569 -0.038091 -0.000000 -0.000000 -0.000000

8 N -0.000002 0.005113 0.005113 0.000000 0.000000 0.000002

9 C 0.000000 -0.038091 0.005569 -0.000000 -0.000000 0.000013

10 C -0.000000 0.388523 -0.032883 0.000000 -0.000000 0.000000

11 C 0.000009 -0.032883 0.388523 -0.000000 0.000000 0.000000

12 C -0.000169 0.000000 0.000000 -0.005314 -0.000160 0.000000

13 C 0.000013 -0.000000 -0.000000 -0.038091 0.005569 0.000000

14 C 0.000000 0.000000 -0.000000 0.388523 -0.032883 -0.000000

15 C 0.000000 -0.000000 0.000000 -0.032883 0.388523 0.000009

16 C -0.000000 -0.000000 -0.000000 0.005569 -0.038091 -0.000059

17 N 0.000002 0.000000 0.000000 0.005113 0.005113 -0.000002

18 C 0.000000 0.000000 0.000000 -0.000160 -0.005314 -0.005749

19 C -0.000000 0.000001 -0.000000 0.000010 -0.000022 -0.038942

20 C 0.000000 -0.000000 0.000000 0.000000 0.000007 0.390420

21 C -0.000000 0.000007 0.000000 0.000000 -0.000000 -0.034782

22 C -0.000000 -0.000022 0.000010 -0.000000 0.000001 0.005789

23 N 0.000000 -0.000003 0.000002 0.000002 -0.000003 0.005278

24 H -0.002391 -0.000000 -0.000000 -0.000005 -0.000000 -0.000000

25 H 0.440548 -0.000000 -0.000005 -0.000000 -0.000000 -0.000000

26 H -0.000000 0.427385 -0.002204 -0.000000 -0.000000 -0.000000

27 H -0.000005 -0.002204 0.427385 -0.000000 -0.000000 -0.000000

28 H -0.000000 -0.000000 -0.000000 0.427385 -0.002204 -0.000000

29 H -0.000000 -0.000000 -0.000000 -0.002204 0.427385 -0.000005

30 H -0.000000 -0.000000 -0.000000 -0.000000 -0.000005 0.440548

31 H -0.000000 -0.000005 -0.000000 -0.000000 -0.000000 -0.002391

32 Zn -0.000360 -0.000350 -0.000350 -0.000350 -0.000350 -0.000360

33 C 0.000000 -0.005314 -0.000160 0.000000 0.000000 -0.000169

34 C 0.000000 0.006196 -0.000084 -0.000000 0.000000 -0.000096

35 C -0.000096 -0.000000 0.000000 0.006196 -0.000084 0.000000

36 C -0.000000 0.003092 -0.000008 -0.000000 -0.000000 -0.000010

37 C -0.000010 -0.000000 -0.000000 0.003092 -0.000008 -0.000000

38 C 0.006199 -0.000084 0.006196 0.000000 -0.000000 -0.000000

39 C 0.003045 -0.000008 0.003092 -0.000000 -0.000000 -0.000000

40 C -0.000000 0.000000 -0.000000 -0.000084 0.006196 0.006199

41 C -0.000000 -0.000000 -0.000000 -0.000008 0.003092 0.003045

42 H -0.000000 -0.000000 -0.000000 -0.000000 0.000053 0.000061

43 H -0.000000 0.000053 -0.000000 -0.000000 -0.000000 -0.000000

44 H 0.000061 -0.000000 0.000053 -0.000000 -0.000000 -0.000000

45 H -0.000000 -0.000000 -0.000000 0.000053 -0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000000 0.001886 -0.000000 -0.000000 -0.017278 -0.000000

2 C -0.000000 -0.013895 0.000002 0.000000 -0.075247 -0.000000

3 N 0.000000 0.125683 -0.000179 -0.000000 0.004260 -0.000000

4 C -0.000000 -0.013895 0.000210 0.000003 -0.000441 0.000000

5 C -0.000000 0.001886 0.000001 0.000000 0.002656 0.000000

6 C 0.000000 -0.009078 -0.002325 -0.000055 -0.000059 -0.000002

7 C 0.000000 -0.013811 -0.000873 -0.000511 0.000003 -0.000051

8 N -0.000002 0.122592 -0.017020 0.004193 -0.000000 -0.000055

9 C -0.000059 -0.013811 0.410745 -0.076217 0.000000 -0.005130

10 C 0.000009 0.001814 -0.074737 -0.015176 -0.000000 -0.000531

11 C -0.000000 0.001814 0.013654 0.002583 0.000000 0.000353

12 C 0.000000 -0.009078 0.000002 0.000000 0.552310 0.000000

13 C -0.000000 -0.013811 0.000001 0.000000 -0.076217 -0.000000

14 C 0.000000 0.001814 -0.000000 -0.000000 -0.015176 -0.000000

15 C 0.000000 0.001814 0.000001 0.000000 0.002583 0.000000

16 C 0.000013 -0.013811 0.000223 0.000003 -0.000511 0.000000

17 N 0.000002 0.122592 -0.000168 -0.000000 0.004193 -0.000000

18 C -0.000169 -0.009078 -0.002536 -0.000059 -0.000055 -0.000002

19 C 0.005789 -0.013895 -0.000223 -0.000441 0.000003 -0.000053

20 C -0.034782 0.001886 0.015237 0.002656 0.000000 0.000325

21 C 0.390420 0.001886 -0.079757 -0.017278 -0.000000 -0.000617

22 C -0.038942 -0.013895 0.364003 -0.075247 0.000000 -0.003979

23 N 0.005278 0.125683 -0.012432 0.004260 -0.000000 -0.000069

24 H -0.000000 -0.000360 0.000000 -0.000000 0.006199 -0.000000

25 H -0.000000 -0.000360 0.000000 0.000000 -0.000096 -0.000000

26 H -0.000005 -0.000350 -0.005314 0.006196 -0.000000 0.003092

27 H -0.000000 -0.000350 -0.000160 -0.000084 0.000000 -0.000008

28 H -0.000000 -0.000350 0.000000 -0.000000 0.006196 -0.000000

29 H -0.000000 -0.000350 0.000000 0.000000 -0.000084 -0.000000

30 H -0.002391 -0.000360 -0.000169 -0.000096 0.000000 -0.000010

31 H 0.440548 -0.000360 -0.005749 0.006199 -0.000000 0.003045

32 Zn -0.000360 10.216505 -0.009078 -0.000600 -0.000600 -0.000099

33 C -0.005749 -0.009078 5.209292 0.552310 0.000000 -0.104080

34 C 0.006199 -0.000600 0.552310 4.814641 0.000000 0.843448

35 C -0.000000 -0.000600 0.000000 0.000000 4.814641 0.000000

36 C 0.003045 -0.000099 -0.104080 0.843448 0.000000 5.168442

37 C -0.000000 -0.000099 0.000000 0.000000 0.843448 0.000000

38 C 0.000000 -0.000600 -0.000055 -0.000001 -0.000001 -0.000000

39 C -0.000000 -0.000099 -0.000002 -0.000000 -0.000000 -0.000000

40 C -0.000096 -0.000600 -0.000059 -0.000001 -0.000001 -0.000000

41 C -0.000010 -0.000099 -0.000002 -0.000000 -0.000000 -0.000000

42 H -0.000000 -0.000003 -0.000000 -0.000000 -0.000000 -0.000000

43 H 0.000061 -0.000003 0.001742 -0.019469 0.000000 0.369637

44 H -0.000000 -0.000003 -0.000000 -0.000000 -0.000000 -0.000000

45 H -0.000000 -0.000003 0.000000 0.000000 -0.019469 0.000000

37 38 39 40 41 42

1 C -0.000617 0.002656 0.000325 0.000000 0.000000 0.000000

2 C -0.003979 -0.000441 -0.000053 0.000003 0.000000 0.000000

3 N -0.000069 0.004260 -0.000069 -0.000000 -0.000000 0.000000

4 C -0.000053 -0.075247 -0.003979 0.000000 -0.000000 0.000000

5 C 0.000325 -0.017278 -0.000617 -0.000000 -0.000000 -0.000000

6 C -0.000002 0.552310 -0.104080 0.000000 0.000000 0.000000

7 C 0.000000 -0.076217 -0.005130 0.000000 -0.000000 0.000000

8 N -0.000000 0.004193 -0.000055 -0.000000 -0.000000 0.000000

9 C -0.000000 -0.000511 -0.000051 0.000003 0.000000 0.000000

10 C -0.000000 0.002583 0.000353 0.000000 0.000000 0.000000

11 C 0.000000 -0.015176 -0.000531 -0.000000 -0.000000 -0.000000

12 C -0.104080 -0.000059 -0.000002 -0.000055 -0.000002 -0.000000

13 C -0.005130 0.000003 0.000000 -0.000511 -0.000051 -0.000000

14 C -0.000531 0.000000 0.000000 0.002583 0.000353 0.000002

15 C 0.000353 -0.000000 -0.000000 -0.015176 -0.000531 0.000095

16 C -0.000051 0.000000 -0.000000 -0.076217 -0.005130 -0.000036

17 N -0.000055 -0.000000 -0.000000 0.004193 -0.000055 0.000001

18 C -0.000002 0.000000 0.000000 0.552310 -0.104080 0.001742

19 C 0.000000 0.000000 -0.000000 -0.075247 -0.003979 -0.000033

20 C 0.000000 -0.000000 -0.000000 -0.017278 -0.000617 0.000093

21 C -0.000000 0.000000 0.000000 0.002656 0.000325 0.000002

22 C -0.000000 0.000003 0.000000 -0.000441 -0.000053 -0.000000

23 N -0.000000 -0.000000 -0.000000 0.004260 -0.000069 0.000001

24 H 0.003045 -0.000096 -0.000010 0.000000 -0.000000 -0.000000

25 H -0.000010 0.006199 0.003045 -0.000000 -0.000000 -0.000000

26 H -0.000000 -0.000084 -0.000008 0.000000 -0.000000 -0.000000

27 H -0.000000 0.006196 0.003092 -0.000000 -0.000000 -0.000000

28 H 0.003092 0.000000 -0.000000 -0.000084 -0.000008 -0.000000

29 H -0.000008 -0.000000 -0.000000 0.006196 0.003092 0.000053

30 H -0.000000 -0.000000 -0.000000 0.006199 0.003045 0.000061

31 H -0.000000 0.000000 -0.000000 -0.000096 -0.000010 -0.000000

32 Zn -0.000099 -0.000600 -0.000099 -0.000600 -0.000099 -0.000003

33 C 0.000000 -0.000055 -0.000002 -0.000059 -0.000002 -0.000000

34 C 0.000000 -0.000001 -0.000000 -0.000001 -0.000000 -0.000000

35 C 0.843448 -0.000001 -0.000000 -0.000001 -0.000000 -0.000000

36 C 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

37 C 5.168442 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

38 C -0.000000 4.814641 0.843448 0.000000 0.000000 0.000000

39 C -0.000000 0.843448 5.168442 0.000000 0.000000 0.000000

40 C -0.000000 0.000000 0.000000 4.814641 0.843448 -0.019469

41 C -0.000000 0.000000 0.000000 0.843448 5.168442 0.369637

42 H -0.000000 0.000000 0.000000 -0.019469 0.369637 0.344762

43 H 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

44 H -0.000000 -0.019469 0.369637 0.000000 0.000000 0.000000

45 H 0.369637 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

43 44 45

1 C -0.000000 0.000002 0.000093

2 C 0.000000 -0.000000 -0.000033

3 N 0.000000 0.000001 0.000001

4 C 0.000000 -0.000033 -0.000000

5 C 0.000000 0.000093 0.000002

6 C -0.000000 0.001742 -0.000000

7 C -0.000000 -0.000036 0.000000

8 N 0.000001 0.000001 0.000000

9 C -0.000036 -0.000000 0.000000

10 C 0.000095 0.000002 -0.000000

11 C 0.000002 0.000095 0.000000

12 C 0.000000 -0.000000 0.001742

13 C 0.000000 0.000000 -0.000036

14 C -0.000000 0.000000 0.000095

15 C 0.000000 -0.000000 0.000002

16 C 0.000000 0.000000 -0.000000

17 N 0.000000 0.000000 0.000001

18 C -0.000000 0.000000 -0.000000

19 C -0.000000 0.000000 0.000000

20 C 0.000002 -0.000000 0.000000

21 C 0.000093 0.000000 -0.000000

22 C -0.000033 0.000000 0.000000

23 N 0.000001 0.000000 0.000000

24 H -0.000000 -0.000000 0.000061

25 H -0.000000 0.000061 -0.000000

26 H 0.000053 -0.000000 -0.000000

27 H -0.000000 0.000053 -0.000000

28 H -0.000000 -0.000000 0.000053

29 H -0.000000 -0.000000 -0.000000

30 H -0.000000 -0.000000 -0.000000

31 H 0.000061 -0.000000 -0.000000

32 Zn -0.000003 -0.000003 -0.000003

33 C 0.001742 -0.000000 0.000000

34 C -0.019469 -0.000000 0.000000

35 C 0.000000 -0.000000 -0.019469

36 C 0.369637 -0.000000 0.000000

37 C 0.000000 -0.000000 0.369637

38 C -0.000000 -0.019469 -0.000000

39 C -0.000000 0.369637 -0.000000

40 C -0.000000 0.000000 -0.000000

41 C -0.000000 0.000000 -0.000000

42 H -0.000000 0.000000 -0.000000

43 H 0.344762 -0.000000 0.000000

44 H -0.000000 0.344762 -0.000000

45 H 0.000000 -0.000000 0.344762

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.072672 0.034405 0.000866 -0.010716 -0.029438 0.000450

2 C 0.034405 0.072136 -0.002154 -0.012304 -0.010716 0.001173

3 N 0.000866 -0.002154 0.068407 -0.002154 0.000866 -0.005219

4 C -0.010716 -0.012304 -0.002154 0.072136 0.034405 -0.035045

5 C -0.029438 -0.010716 0.000866 0.034405 0.072672 -0.008923

6 C 0.000450 0.001173 -0.005219 -0.035045 -0.008923 0.333296

7 C 0.000043 0.000107 0.000716 -0.004241 -0.000766 0.030066

8 N -0.000009 -0.000122 0.000705 0.002272 0.000069 -0.010790

9 C 0.000000 0.000003 -0.000020 -0.000066 -0.000002 0.000840

10 C 0.000000 -0.000000 0.000001 0.000020 -0.000000 -0.000985

11 C -0.000001 -0.000000 0.000012 0.000304 0.000019 -0.002235

12 C -0.008923 -0.035045 -0.005219 0.001173 0.000450 0.000050

13 C -0.000766 -0.004241 0.000716 0.000107 0.000043 -0.000009

14 C 0.000019 0.000304 0.000012 -0.000000 -0.000001 0.000000

15 C -0.000000 0.000020 0.000001 -0.000000 0.000000 -0.000000

16 C -0.000002 -0.000066 -0.000020 0.000003 0.000000 -0.000000

17 N 0.000069 0.002272 0.000705 -0.000122 -0.000009 0.000010

18 C -0.000000 -0.000007 -0.000001 0.000000 -0.000000 0.000000

19 C 0.000000 0.000003 -0.000003 -0.000001 -0.000000 0.000000

20 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

21 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

22 C -0.000000 -0.000001 -0.000003 0.000003 0.000000 -0.000007

23 N -0.000000 -0.000003 0.000025 -0.000003 -0.000000 -0.000001

24 H -0.000065 -0.000202 -0.000032 -0.000013 0.000317 -0.000003

25 H 0.000317 -0.000013 -0.000032 -0.000202 -0.000065 0.000309

26 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000013

27 H -0.000000 0.000000 0.000000 -0.000019 0.000001 0.000001

28 H 0.000001 -0.000019 0.000000 0.000000 -0.000000 0.000000

29 H -0.000000 0.000000 -0.000000 0.000000 0.000000 -0.000000

30 H -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

31 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

32 Zn 0.000124 0.000291 0.002197 0.000291 0.000124 -0.001807

33 C -0.000000 0.000000 -0.000001 -0.000007 -0.000000 0.000160

34 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000002

35 C 0.000630 0.000494 -0.000059 -0.000029 0.000045 0.000001

36 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

37 C 0.000765 0.000916 0.000017 -0.000006 -0.000023 0.000000

38 C 0.000045 -0.000029 -0.000059 0.000494 0.000630 -0.004070

39 C -0.000023 -0.000006 0.000017 0.000916 0.000765 -0.008822

40 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

41 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

42 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

43 H -0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

44 H -0.000000 -0.000000 0.000000 -0.000003 0.000001 -0.000037

45 H 0.000001 -0.000003 0.000000 -0.000000 -0.000000 0.000000

7 8 9 10 11 12

1 C 0.000043 -0.000009 0.000000 0.000000 -0.000001 -0.008923

2 C 0.000107 -0.000122 0.000003 -0.000000 -0.000000 -0.035045

3 N 0.000716 0.000705 -0.000020 0.000001 0.000012 -0.005219

4 C -0.004241 0.002272 -0.000066 0.000020 0.000304 0.001173

5 C -0.000766 0.000069 -0.000002 -0.000000 0.000019 0.000450

6 C 0.030066 -0.010790 0.000840 -0.000985 -0.002235 0.000050

7 C -0.093108 -0.016023 0.007381 0.002024 -0.006362 -0.000009

8 N -0.016023 0.201554 -0.016023 0.002961 0.002961 0.000010

9 C 0.007381 -0.016023 -0.093108 -0.006362 0.002024 -0.000000

10 C 0.002024 0.002961 -0.006362 -0.013743 0.011861 -0.000000

11 C -0.006362 0.002961 0.002024 0.011861 -0.013743 0.000000

12 C -0.000009 0.000010 -0.000000 -0.000000 0.000000 0.333296

13 C 0.000001 -0.000004 0.000001 0.000000 -0.000000 0.030066

14 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.002235

15 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000985

16 C 0.000001 -0.000004 0.000001 -0.000000 0.000000 0.000840

17 N -0.000004 0.000002 -0.000004 -0.000000 -0.000000 -0.010790

18 C -0.000000 0.000010 -0.000009 0.000000 -0.000000 0.000160

19 C 0.000003 -0.000122 0.000107 -0.000000 -0.000000 -0.000007

20 C 0.000000 -0.000009 0.000043 -0.000001 0.000000 -0.000000

21 C -0.000002 0.000069 -0.000766 0.000019 -0.000000 -0.000000

22 C -0.000066 0.002272 -0.004241 0.000304 0.000020 0.000000

23 N -0.000020 0.000705 0.000716 0.000012 0.000001 -0.000001

24 H -0.000001 -0.000000 0.000000 0.000000 -0.000000 0.000309

25 H 0.000001 -0.000000 0.000000 -0.000000 0.000001 -0.000003

26 H -0.000078 -0.000005 0.000476 -0.000469 0.000252 -0.000000

27 H 0.000476 -0.000005 -0.000078 0.000252 -0.000469 0.000000

28 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000001

29 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000013

30 H 0.000000 -0.000000 -0.000001 -0.000000 0.000000 0.000000

31 H 0.000000 -0.000000 0.000001 0.000001 -0.000000 -0.000000

32 Zn 0.000100 0.000704 0.000100 0.000146 0.000146 -0.001807

33 C 0.000840 -0.010790 0.030066 -0.002235 -0.000985 0.000000

34 C 0.000010 0.000003 0.000176 0.000411 -0.000109 0.000000

35 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.004070

36 C 0.000001 0.000033 -0.000747 0.000340 -0.000002 -0.000000

37 C -0.000000 0.000000 0.000000 -0.000000 0.000000 -0.008822

38 C 0.000176 0.000003 0.000010 -0.000109 0.000411 0.000001

39 C -0.000747 0.000033 0.000001 -0.000002 0.000340 0.000000

40 C -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000002

41 C 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

42 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

43 H -0.000000 0.000000 -0.000009 0.000001 -0.000000 -0.000000

44 H -0.000009 0.000000 -0.000000 -0.000000 0.000001 0.000000

45 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000037

13 14 15 16 17 18

1 C -0.000766 0.000019 -0.000000 -0.000002 0.000069 -0.000000

2 C -0.004241 0.000304 0.000020 -0.000066 0.002272 -0.000007

3 N 0.000716 0.000012 0.000001 -0.000020 0.000705 -0.000001

4 C 0.000107 -0.000000 -0.000000 0.000003 -0.000122 0.000000

5 C 0.000043 -0.000001 0.000000 0.000000 -0.000009 -0.000000

6 C -0.000009 0.000000 -0.000000 -0.000000 0.000010 0.000000

7 C 0.000001 -0.000000 0.000000 0.000001 -0.000004 -0.000000

8 N -0.000004 -0.000000 -0.000000 -0.000004 0.000002 0.000010

9 C 0.000001 0.000000 -0.000000 0.000001 -0.000004 -0.000009

10 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

11 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

12 C 0.030066 -0.002235 -0.000985 0.000840 -0.010790 0.000160

13 C -0.093108 -0.006362 0.002024 0.007381 -0.016023 0.000840

14 C -0.006362 -0.013743 0.011861 0.002024 0.002961 -0.000985

15 C 0.002024 0.011861 -0.013743 -0.006362 0.002961 -0.002235

16 C 0.007381 0.002024 -0.006362 -0.093108 -0.016023 0.030066

17 N -0.016023 0.002961 0.002961 -0.016023 0.201554 -0.010790

18 C 0.000840 -0.000985 -0.002235 0.030066 -0.010790 0.333296

19 C -0.000066 0.000020 0.000304 -0.004241 0.002272 -0.035045

20 C -0.000002 -0.000000 0.000019 -0.000766 0.000069 -0.008923

21 C 0.000000 0.000000 -0.000001 0.000043 -0.000009 0.000450

22 C 0.000003 -0.000000 -0.000000 0.000107 -0.000122 0.001173

23 N -0.000020 0.000001 0.000012 0.000716 0.000705 -0.005219

24 H 0.000001 0.000001 -0.000000 0.000000 -0.000000 0.000000

25 H -0.000001 -0.000000 0.000000 0.000000 -0.000000 -0.000000

26 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

27 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

28 H 0.000476 -0.000469 0.000252 -0.000078 -0.000005 -0.000013

29 H -0.000078 0.000252 -0.000469 0.000476 -0.000005 0.000001

30 H 0.000000 -0.000000 0.000001 0.000001 -0.000000 0.000309

31 H 0.000000 0.000000 -0.000000 -0.000001 -0.000000 -0.000003

32 Zn 0.000100 0.000146 0.000146 0.000100 0.000704 -0.001807

33 C -0.000000 -0.000000 0.000000 -0.000009 0.000010 0.000050

34 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000001

35 C 0.000176 0.000411 -0.000109 0.000010 0.000003 0.000002

36 C 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

37 C -0.000747 0.000340 -0.000002 0.000001 0.000033 0.000000

38 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

39 C -0.000000 0.000000 -0.000000 0.000000 0.000000 -0.000000

40 C 0.000010 -0.000109 0.000411 0.000176 0.000003 -0.004070

41 C 0.000001 -0.000002 0.000340 -0.000747 0.000033 -0.008822

42 H -0.000000 -0.000000 0.000001 -0.000009 0.000000 -0.000037

43 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

44 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000000

45 H -0.000009 0.000001 -0.000000 -0.000000 0.000000 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000065

2 C 0.000003 0.000000 -0.000000 -0.000001 -0.000003 -0.000202

3 N -0.000003 -0.000000 -0.000000 -0.000003 0.000025 -0.000032

4 C -0.000001 -0.000000 0.000000 0.000003 -0.000003 -0.000013

5 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000317

6 C 0.000000 -0.000000 -0.000000 -0.000007 -0.000001 -0.000003

7 C 0.000003 0.000000 -0.000002 -0.000066 -0.000020 -0.000001

8 N -0.000122 -0.000009 0.000069 0.002272 0.000705 -0.000000

9 C 0.000107 0.000043 -0.000766 -0.004241 0.000716 0.000000

10 C -0.000000 -0.000001 0.000019 0.000304 0.000012 0.000000

11 C -0.000000 0.000000 -0.000000 0.000020 0.000001 -0.000000

12 C -0.000007 -0.000000 -0.000000 0.000000 -0.000001 0.000309

13 C -0.000066 -0.000002 0.000000 0.000003 -0.000020 0.000001

14 C 0.000020 -0.000000 0.000000 -0.000000 0.000001 0.000001

15 C 0.000304 0.000019 -0.000001 -0.000000 0.000012 -0.000000

16 C -0.004241 -0.000766 0.000043 0.000107 0.000716 0.000000

17 N 0.002272 0.000069 -0.000009 -0.000122 0.000705 -0.000000

18 C -0.035045 -0.008923 0.000450 0.001173 -0.005219 0.000000

19 C 0.072136 0.034405 -0.010716 -0.012304 -0.002154 -0.000000

20 C 0.034405 0.072672 -0.029438 -0.010716 0.000866 -0.000000

21 C -0.010716 -0.029438 0.072672 0.034405 0.000866 0.000000

22 C -0.012304 -0.010716 0.034405 0.072136 -0.002154 0.000000

23 N -0.002154 0.000866 0.000866 -0.002154 0.068407 -0.000000

24 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.004009

25 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000070

26 H 0.000000 -0.000000 0.000001 -0.000019 0.000000 0.000000

27 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000000

28 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000000

29 H -0.000019 0.000001 -0.000000 0.000000 0.000000 0.000000

30 H -0.000202 -0.000065 0.000317 -0.000013 -0.000032 -0.000000

31 H -0.000013 0.000317 -0.000065 -0.000202 -0.000032 0.000000

32 Zn 0.000291 0.000124 0.000124 0.000291 0.002197 -0.000004

33 C 0.001173 0.000450 -0.008923 -0.035045 -0.005219 -0.000000

34 C -0.000029 0.000045 0.000630 0.000494 -0.000059 -0.000000

35 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000238

36 C -0.000006 -0.000023 0.000765 0.000916 0.000017 -0.000000

37 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000143

38 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000004

39 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

40 C 0.000494 0.000630 0.000045 -0.000029 -0.000059 0.000000

41 C 0.000916 0.000765 -0.000023 -0.000006 0.000017 -0.000000

42 H -0.000003 0.000001 -0.000000 -0.000000 0.000000 0.000000

43 H -0.000000 -0.000000 0.000001 -0.000003 0.000000 -0.000000

44 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

45 H -0.000000 0.000000 -0.000000 0.000000 0.000000 -0.000005

25 26 27 28 29 30

1 C 0.000317 0.000000 -0.000000 0.000001 -0.000000 -0.000000

2 C -0.000013 0.000000 0.000000 -0.000019 0.000000 -0.000000

3 N -0.000032 -0.000000 0.000000 0.000000 -0.000000 -0.000000

4 C -0.000202 0.000000 -0.000019 0.000000 0.000000 0.000000

5 C -0.000065 -0.000000 0.000001 -0.000000 0.000000 0.000000

6 C 0.000309 -0.000013 0.000001 0.000000 -0.000000 -0.000000

7 C 0.000001 -0.000078 0.000476 -0.000000 0.000000 0.000000

8 N -0.000000 -0.000005 -0.000005 -0.000000 -0.000000 -0.000000

9 C 0.000000 0.000476 -0.000078 0.000000 -0.000000 -0.000001

10 C -0.000000 -0.000469 0.000252 0.000000 -0.000000 -0.000000

11 C 0.000001 0.000252 -0.000469 -0.000000 0.000000 0.000000

12 C -0.000003 -0.000000 0.000000 0.000001 -0.000013 0.000000

13 C -0.000001 0.000000 -0.000000 0.000476 -0.000078 0.000000

14 C -0.000000 0.000000 -0.000000 -0.000469 0.000252 -0.000000

15 C 0.000000 -0.000000 0.000000 0.000252 -0.000469 0.000001

16 C 0.000000 -0.000000 0.000000 -0.000078 0.000476 0.000001

17 N -0.000000 -0.000000 -0.000000 -0.000005 -0.000005 -0.000000

18 C -0.000000 0.000000 -0.000000 -0.000013 0.000001 0.000309

19 C 0.000000 0.000000 0.000000 0.000000 -0.000019 -0.000202

20 C 0.000000 -0.000000 0.000000 -0.000000 0.000001 -0.000065

21 C -0.000000 0.000001 -0.000000 0.000000 -0.000000 0.000317

22 C -0.000000 -0.000019 0.000000 0.000000 0.000000 -0.000013

23 N -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000032

24 H 0.000070 0.000000 -0.000000 0.000000 0.000000 -0.000000

25 H -0.004009 0.000000 0.000000 -0.000000 0.000000 0.000000

26 H 0.000000 0.000418 -0.000023 0.000000 -0.000000 -0.000000

27 H 0.000000 -0.000023 0.000418 -0.000000 0.000000 0.000000

28 H -0.000000 0.000000 -0.000000 0.000418 -0.000023 0.000000

29 H 0.000000 -0.000000 0.000000 -0.000023 0.000418 0.000000

30 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.004009

31 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000070

32 Zn -0.000004 -0.000001 -0.000001 -0.000001 -0.000001 -0.000004

33 C 0.000000 0.000001 -0.000013 -0.000000 0.000000 -0.000003

34 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000004

35 C 0.000004 -0.000000 0.000000 0.000000 -0.000000 0.000000

36 C -0.000000 0.000077 -0.000000 0.000000 0.000000 0.000000

37 C 0.000000 0.000000 0.000000 0.000077 -0.000000 -0.000000

38 C -0.000238 -0.000000 0.000000 0.000000 -0.000000 -0.000000

39 C -0.000143 -0.000000 0.000077 0.000000 0.000000 -0.000000

40 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000238

41 C -0.000000 0.000000 0.000000 -0.000000 0.000077 -0.000143

42 H -0.000000 0.000000 0.000000 -0.000000 0.000003 -0.000005

43 H 0.000000 0.000003 -0.000000 0.000000 0.000000 0.000000

44 H -0.000005 -0.000000 0.000003 0.000000 0.000000 -0.000000

45 H 0.000000 0.000000 0.000000 0.000003 -0.000000 0.000000

31 32 33 34 35 36

1 C 0.000000 0.000124 -0.000000 -0.000000 0.000630 -0.000000

2 C 0.000000 0.000291 0.000000 -0.000000 0.000494 -0.000000

3 N -0.000000 0.002197 -0.000001 0.000000 -0.000059 0.000000

4 C -0.000000 0.000291 -0.000007 -0.000000 -0.000029 -0.000000

5 C -0.000000 0.000124 -0.000000 0.000000 0.000045 0.000000

6 C 0.000000 -0.001807 0.000160 0.000002 0.000001 0.000000

7 C 0.000000 0.000100 0.000840 0.000010 -0.000000 0.000001

8 N -0.000000 0.000704 -0.010790 0.000003 0.000000 0.000033

9 C 0.000001 0.000100 0.030066 0.000176 -0.000000 -0.000747

10 C 0.000001 0.000146 -0.002235 0.000411 -0.000000 0.000340

11 C -0.000000 0.000146 -0.000985 -0.000109 0.000000 -0.000002

12 C -0.000000 -0.001807 0.000000 0.000000 -0.004070 -0.000000

13 C 0.000000 0.000100 -0.000000 -0.000000 0.000176 0.000000

14 C 0.000000 0.000146 -0.000000 -0.000000 0.000411 -0.000000

15 C -0.000000 0.000146 0.000000 0.000000 -0.000109 0.000000

16 C -0.000001 0.000100 -0.000009 -0.000000 0.000010 -0.000000

17 N -0.000000 0.000704 0.000010 0.000000 0.000003 0.000000

18 C -0.000003 -0.001807 0.000050 0.000001 0.000002 0.000000

19 C -0.000013 0.000291 0.001173 -0.000029 -0.000000 -0.000006

20 C 0.000317 0.000124 0.000450 0.000045 0.000000 -0.000023

21 C -0.000065 0.000124 -0.008923 0.000630 -0.000000 0.000765

22 C -0.000202 0.000291 -0.035045 0.000494 -0.000000 0.000916

23 N -0.000032 0.002197 -0.005219 -0.000059 0.000000 0.000017

24 H 0.000000 -0.000004 -0.000000 -0.000000 -0.000238 -0.000000

25 H -0.000000 -0.000004 0.000000 0.000000 0.000004 -0.000000

26 H 0.000000 -0.000001 0.000001 0.000000 -0.000000 0.000077

27 H 0.000000 -0.000001 -0.000013 -0.000000 0.000000 -0.000000

28 H 0.000000 -0.000001 -0.000000 -0.000000 0.000000 0.000000

29 H -0.000000 -0.000001 0.000000 0.000000 -0.000000 0.000000

30 H 0.000070 -0.000004 -0.000003 0.000004 0.000000 0.000000

31 H -0.004009 -0.000004 0.000309 -0.000238 -0.000000 -0.000143

32 Zn -0.000004 0.001827 -0.001807 -0.000027 -0.000027 0.000048

33 C 0.000309 -0.001807 0.333296 -0.004070 0.000000 -0.008822

34 C -0.000238 -0.000027 -0.004070 -0.096195 -0.000000 0.007426

35 C -0.000000 -0.000027 0.000000 -0.000000 -0.096195 -0.000000

36 C -0.000143 0.000048 -0.008822 0.007426 -0.000000 0.181992

37 C -0.000000 0.000048 -0.000000 -0.000000 0.007426 0.000000

38 C 0.000000 -0.000027 0.000002 0.000000 0.000000 0.000000

39 C -0.000000 0.000048 0.000000 0.000000 0.000000 0.000000

40 C 0.000004 -0.000027 0.000001 0.000000 0.000000 0.000000

41 C 0.000000 0.000048 0.000000 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H -0.000005 0.000000 -0.000037 -0.000785 -0.000000 -0.000859

44 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H -0.000000 0.000000 -0.000000 -0.000000 -0.000785 -0.000000

37 38 39 40 41 42

1 C 0.000765 0.000045 -0.000023 0.000000 0.000000 0.000000

2 C 0.000916 -0.000029 -0.000006 -0.000000 -0.000000 -0.000000

3 N 0.000017 -0.000059 0.000017 0.000000 0.000000 0.000000

4 C -0.000006 0.000494 0.000916 -0.000000 -0.000000 0.000000

5 C -0.000023 0.000630 0.000765 -0.000000 -0.000000 -0.000000

6 C 0.000000 -0.004070 -0.008822 0.000000 -0.000000 -0.000000

7 C -0.000000 0.000176 -0.000747 -0.000000 0.000000 -0.000000

8 N 0.000000 0.000003 0.000033 0.000000 0.000000 0.000000

9 C 0.000000 0.000010 0.000001 -0.000000 -0.000000 -0.000000

10 C -0.000000 -0.000109 -0.000002 0.000000 0.000000 0.000000

11 C 0.000000 0.000411 0.000340 -0.000000 -0.000000 -0.000000

12 C -0.008822 0.000001 0.000000 0.000002 0.000000 0.000000

13 C -0.000747 -0.000000 -0.000000 0.000010 0.000001 -0.000000

14 C 0.000340 0.000000 0.000000 -0.000109 -0.000002 -0.000000

15 C -0.000002 -0.000000 -0.000000 0.000411 0.000340 0.000001

16 C 0.000001 -0.000000 0.000000 0.000176 -0.000747 -0.000009

17 N 0.000033 0.000000 0.000000 0.000003 0.000033 0.000000

18 C 0.000000 0.000000 -0.000000 -0.004070 -0.008822 -0.000037

19 C -0.000000 -0.000000 -0.000000 0.000494 0.000916 -0.000003

20 C 0.000000 -0.000000 -0.000000 0.000630 0.000765 0.000001

21 C -0.000000 0.000000 0.000000 0.000045 -0.000023 -0.000000

22 C -0.000000 -0.000000 -0.000000 -0.000029 -0.000006 -0.000000

23 N 0.000000 0.000000 0.000000 -0.000059 0.000017 0.000000

24 H -0.000143 0.000004 0.000000 0.000000 -0.000000 0.000000

25 H 0.000000 -0.000238 -0.000143 -0.000000 -0.000000 -0.000000

26 H 0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000000 0.000077 -0.000000 0.000000 0.000000

28 H 0.000077 0.000000 0.000000 -0.000000 -0.000000 -0.000000

29 H -0.000000 -0.000000 0.000000 0.000000 0.000077 0.000003

30 H -0.000000 -0.000000 -0.000000 -0.000238 -0.000143 -0.000005

31 H -0.000000 0.000000 -0.000000 0.000004 0.000000 0.000000

32 Zn 0.000048 -0.000027 0.000048 -0.000027 0.000048 0.000000

33 C -0.000000 0.000002 0.000000 0.000001 0.000000 0.000000

34 C -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 C 0.007426 0.000000 0.000000 0.000000 0.000000 0.000000

36 C 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 C 0.181992 0.000000 0.000000 0.000000 0.000000 0.000000

38 C 0.000000 -0.096195 0.007426 -0.000000 -0.000000 -0.000000

39 C 0.000000 0.007426 0.181992 -0.000000 0.000000 -0.000000

40 C 0.000000 -0.000000 -0.000000 -0.096195 0.007426 -0.000785

41 C 0.000000 -0.000000 0.000000 0.007426 0.181992 -0.000859

42 H 0.000000 -0.000000 -0.000000 -0.000785 -0.000859 -0.005765

43 H -0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000000 -0.000785 -0.000859 -0.000000 -0.000000 -0.000000

45 H -0.000859 0.000000 0.000000 0.000000 0.000000 -0.000000

43 44 45

1 C -0.000000 -0.000000 0.000001

2 C 0.000000 -0.000000 -0.000003

3 N 0.000000 0.000000 0.000000

4 C -0.000000 -0.000003 -0.000000

5 C 0.000000 0.000001 -0.000000

6 C 0.000000 -0.000037 0.000000

7 C -0.000000 -0.000009 -0.000000

8 N 0.000000 0.000000 0.000000

9 C -0.000009 -0.000000 -0.000000

10 C 0.000001 -0.000000 -0.000000

11 C -0.000000 0.000001 0.000000

12 C -0.000000 0.000000 -0.000037

13 C -0.000000 -0.000000 -0.000009

14 C -0.000000 0.000000 0.000001

15 C 0.000000 -0.000000 -0.000000

16 C -0.000000 -0.000000 -0.000000

17 N 0.000000 0.000000 0.000000

18 C 0.000000 -0.000000 0.000000

19 C -0.000000 0.000000 -0.000000

20 C -0.000000 -0.000000 0.000000

21 C 0.000001 0.000000 -0.000000

22 C -0.000003 -0.000000 0.000000

23 N 0.000000 0.000000 0.000000

24 H -0.000000 0.000000 -0.000005

25 H 0.000000 -0.000005 0.000000

26 H 0.000003 -0.000000 0.000000

27 H -0.000000 0.000003 0.000000

28 H 0.000000 0.000000 0.000003

29 H 0.000000 0.000000 -0.000000

30 H 0.000000 -0.000000 0.000000

31 H -0.000005 0.000000 -0.000000

32 Zn 0.000000 0.000000 0.000000

33 C -0.000037 0.000000 -0.000000

34 C -0.000785 0.000000 -0.000000

35 C -0.000000 0.000000 -0.000785

36 C -0.000859 0.000000 -0.000000

37 C -0.000000 0.000000 -0.000859

38 C 0.000000 -0.000785 0.000000

39 C 0.000000 -0.000859 0.000000

40 C 0.000000 -0.000000 0.000000

41 C 0.000000 -0.000000 0.000000

42 H -0.000000 -0.000000 -0.000000

43 H -0.005765 -0.000000 -0.000000

44 H -0.000000 -0.005765 -0.000000

45 H -0.000000 -0.000000 -0.005765

Mulliken charges and spin densities:

1 2

1 C -0.270385 0.060463

2 C 0.307202 0.047194

3 N -0.695160 0.060286

4 C 0.307202 0.047194

5 C -0.270385 0.060463

6 C -0.252505 0.288392

7 C 0.330038 -0.079491

8 N -0.706113 0.160460

9 C 0.330038 -0.079491

10 C -0.242501 -0.005555

11 C -0.242501 -0.005555

12 C -0.252505 0.288392

13 C 0.330038 -0.079491

14 C -0.242501 -0.005555

15 C -0.242501 -0.005555

16 C 0.330038 -0.079491

17 N -0.706113 0.160460

18 C -0.252505 0.288392

19 C 0.307202 0.047194

20 C -0.270385 0.060463

21 C -0.270385 0.060463

22 C 0.307202 0.047194

23 N -0.695160 0.060286

24 H 0.231201 -0.004013

25 H 0.231201 -0.004013

26 H 0.243173 0.000618

27 H 0.243173 0.000618

28 H 0.243173 0.000618

29 H 0.243173 0.000618

30 H 0.231201 -0.004013

31 H 0.231201 -0.004013

32 Zn 1.424927 0.003110

33 C -0.252505 0.288392

34 C -0.031255 -0.092311

35 C -0.031255 -0.092311

36 C -0.273657 0.181012

37 C -0.273657 0.181012

38 C -0.031255 -0.092311

39 C -0.273657 0.181012

40 C -0.031255 -0.092311

41 C -0.273657 0.181012

42 H 0.303093 -0.007458

43 H 0.303093 -0.007458

44 H 0.303093 -0.007458

45 H 0.303093 -0.007458

Sum of Mulliken charges = -0.00000 2.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C -0.039183 0.056449

2 C 0.307202 0.047194

3 N -0.695160 0.060286

4 C 0.307202 0.047194

5 C -0.039183 0.056449

6 C -0.252505 0.288392

7 C 0.330038 -0.079491

8 N -0.706113 0.160460

9 C 0.330038 -0.079491

10 C 0.000672 -0.004937

11 C 0.000672 -0.004937

12 C -0.252505 0.288392

13 C 0.330038 -0.079491

14 C 0.000672 -0.004937

15 C 0.000672 -0.004937

16 C 0.330038 -0.079491

17 N -0.706113 0.160460

18 C -0.252505 0.288392

19 C 0.307202 0.047194

20 C -0.039183 0.056449

21 C -0.039183 0.056449

22 C 0.307202 0.047194

23 N -0.695160 0.060286

32 Zn 1.424927 0.003110

33 C -0.252505 0.288392

34 C -0.031255 -0.092311

35 C -0.031255 -0.092311

36 C 0.029436 0.173554

37 C 0.029436 0.173554

38 C -0.031255 -0.092311

39 C 0.029436 0.173554

40 C -0.031255 -0.092311

41 C 0.029436 0.173554

APT charges:

1

1 C 0.323506

2 C -1.669268

3 N 0.241330

4 C -1.669267

5 C 0.323506

6 C 1.348782

7 C -0.126955

8 N -0.909147

9 C -0.126955

10 C 0.234679

11 C 0.234680

12 C 1.348783

13 C -0.126954

14 C 0.234679

15 C 0.234680

16 C -0.126955

17 N -0.909147

18 C 1.348783

19 C -1.669268

20 C 0.323506

21 C 0.323506

22 C -1.669268

23 N 0.241331

24 H 0.088711

25 H 0.088711

26 H 0.097643

27 H 0.097642

28 H 0.097643

29 H 0.097642

30 H 0.088711

31 H 0.088711

32 Zn 1.389464

33 C 1.348783

34 C -0.099716

35 C -0.099717

36 C -0.549046

37 C -0.549045

38 C -0.099717

39 C -0.549045

40 C -0.099717

41 C -0.549045

42 H 0.338204

43 H 0.338204

44 H 0.338204

45 H 0.338204

Sum of APT charges = -0.00000

APT charges with hydrogens summed into heavy atoms:

1

1 C 0.412217

2 C -1.669268

3 N 0.241330

4 C -1.669267

5 C 0.412217

6 C 1.348782

7 C -0.126955

8 N -0.909147

9 C -0.126955

10 C 0.332322

11 C 0.332322

12 C 1.348783

13 C -0.126954

14 C 0.332322

15 C 0.332322

16 C -0.126955

17 N -0.909147

18 C 1.348783

19 C -1.669268

20 C 0.412217

21 C 0.412217

22 C -1.669268

23 N 0.241331

32 Zn 1.389464

33 C 1.348783

34 C -0.099716

35 C -0.099717

36 C -0.210842

37 C -0.210841

38 C -0.099717

39 C -0.210841

40 C -0.099717

41 C -0.210841

Electronic spatial extent (au): <R\*\*2>= 13450.7148

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -0.0000 Y= -0.0000 Z= 0.8406 Tot= 0.8406

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -146.5575 YY= -163.5829 ZZ= -200.0645

XY= -0.0000 XZ= -0.0000 YZ= -0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 23.5108 YY= 6.4854 ZZ= -29.9962

XY= -0.0000 XZ= -0.0000 YZ= -0.0000

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= -0.0000 YYY= 0.0000 ZZZ= 12.7387 XYY= 0.0000

XXY= -0.0000 XXZ= -5.7985 XZZ= -0.0000 YZZ= 0.0000

YYZ= -5.2975 XYZ= 0.0000

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -7682.7831 YYYY= -8058.7317 ZZZZ= -225.8464 XXXY= -0.0000

XXXZ= 0.0000 YYYX= -0.0000 YYYZ= 0.0000 ZZZX= 0.0000

ZZZY= -0.0000 XXYY= -1629.2320 XXZZ= -1788.4768 YYZZ= -1805.0464

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= -0.0000

N-N= 3.060485352020D+03 E-N=-9.363387603036D+03 KE= 1.403834754201D+03

Symmetry A1 KE= 4.222173701033D+02

Symmetry A2 KE= 2.911442126594D+02

Symmetry B1 KE= 3.459521407716D+02

Symmetry B2 KE= 3.445210306667D+02

Exact polarizability:1276.370 0.0001652.216 -0.000 0.000 181.240

Approx polarizability:1256.181 0.0001671.341 0.000 -0.000 214.859

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) -0.00026 -0.14877 -0.05309 -0.04963

2 C(13) -0.00800 -4.49828 -1.60510 -1.50047

3 N(14) 0.00166 0.26861 0.09585 0.08960

4 C(13) -0.00800 -4.49828 -1.60510 -1.50047

5 C(13) -0.00026 -0.14877 -0.05309 -0.04963

6 C(13) 0.01576 8.85979 3.16139 2.95531

7 C(13) -0.01679 -9.43809 -3.36775 -3.14821

8 N(14) 0.01668 2.69486 0.96159 0.89891

9 C(13) -0.01679 -9.43809 -3.36775 -3.14821

10 C(13) 0.00027 0.15343 0.05475 0.05118

11 C(13) 0.00027 0.15343 0.05475 0.05118

12 C(13) 0.01576 8.85979 3.16139 2.95531

13 C(13) -0.01679 -9.43809 -3.36775 -3.14821

14 C(13) 0.00027 0.15343 0.05475 0.05118

15 C(13) 0.00027 0.15343 0.05475 0.05118

16 C(13) -0.01679 -9.43809 -3.36775 -3.14821

17 N(14) 0.01668 2.69486 0.96159 0.89891

18 C(13) 0.01576 8.85979 3.16139 2.95531

19 C(13) -0.00800 -4.49828 -1.60510 -1.50047

20 C(13) -0.00026 -0.14877 -0.05309 -0.04963

21 C(13) -0.00026 -0.14877 -0.05309 -0.04963

22 C(13) -0.00800 -4.49828 -1.60510 -1.50047

23 N(14) 0.00166 0.26861 0.09585 0.08960

24 H(1) -0.00115 -2.57183 -0.91769 -0.85787

25 H(1) -0.00115 -2.57183 -0.91769 -0.85787

26 H(1) 0.00017 0.38630 0.13784 0.12886

27 H(1) 0.00017 0.38630 0.13784 0.12886

28 H(1) 0.00017 0.38630 0.13784 0.12886

29 H(1) 0.00017 0.38630 0.13784 0.12886

30 H(1) -0.00115 -2.57183 -0.91769 -0.85787

31 H(1) -0.00115 -2.57183 -0.91769 -0.85787

32 Zn(67) 0.00000 0.00000 0.00000 0.00000

33 C(13) 0.01576 8.85979 3.16139 2.95531

34 C(13) -0.02094 -11.77082 -4.20012 -3.92632

35 C(13) -0.02094 -11.77082 -4.20012 -3.92632

36 C(13) 0.00955 5.37060 1.91636 1.79144

37 C(13) 0.00955 5.37060 1.91636 1.79144

38 C(13) -0.02094 -11.77082 -4.20012 -3.92632

39 C(13) 0.00955 5.37060 1.91636 1.79144

40 C(13) -0.02094 -11.77082 -4.20012 -3.92632

41 C(13) 0.00955 5.37060 1.91636 1.79144

42 H(1) -0.00296 -6.62062 -2.36240 -2.20840

43 H(1) -0.00296 -6.62062 -2.36240 -2.20840

44 H(1) -0.00296 -6.62062 -2.36240 -2.20840

45 H(1) -0.00296 -6.62062 -2.36240 -2.20840

--------------------------------------------------------

Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

--------------------------------------------------------

1 Atom -0.038419 -0.037089 0.075508

2 Atom -0.034651 -0.045109 0.079760

3 Atom -0.073815 -0.079206 0.153021

4 Atom -0.034651 -0.045109 0.079760

5 Atom -0.038419 -0.037089 0.075508

6 Atom -0.171822 -0.173860 0.345682

7 Atom 0.028956 0.047502 -0.076458

8 Atom -0.188348 -0.178690 0.367038

9 Atom 0.028956 0.047502 -0.076458

10 Atom 0.008534 0.007841 -0.016374

11 Atom 0.008534 0.007841 -0.016374

12 Atom -0.171822 -0.173860 0.345682

13 Atom 0.028956 0.047502 -0.076458

14 Atom 0.008534 0.007841 -0.016374

15 Atom 0.008534 0.007841 -0.016374

16 Atom 0.028956 0.047502 -0.076458

17 Atom -0.188348 -0.178690 0.367038

18 Atom -0.171822 -0.173860 0.345682

19 Atom -0.034651 -0.045109 0.079760

20 Atom -0.038419 -0.037089 0.075508

21 Atom -0.038419 -0.037089 0.075508

22 Atom -0.034651 -0.045109 0.079760

23 Atom -0.073815 -0.079206 0.153021

24 Atom -0.001910 0.005550 -0.003640

25 Atom -0.001910 0.005550 -0.003640

26 Atom 0.001188 0.001153 -0.002342

27 Atom 0.001188 0.001153 -0.002342

28 Atom 0.001188 0.001153 -0.002342

29 Atom 0.001188 0.001153 -0.002342

30 Atom -0.001910 0.005550 -0.003640

31 Atom -0.001910 0.005550 -0.003640

32 Atom 0.008423 -0.006031 -0.002392

33 Atom -0.171822 -0.173860 0.345682

34 Atom 0.025664 0.024099 -0.049763

35 Atom 0.025664 0.024099 -0.049763

36 Atom -0.088324 -0.089646 0.177970

37 Atom -0.088324 -0.089646 0.177970

38 Atom 0.025664 0.024099 -0.049763

39 Atom -0.088324 -0.089646 0.177970

40 Atom 0.025664 0.024099 -0.049763

41 Atom -0.088324 -0.089646 0.177970

42 Atom 0.001636 0.000962 -0.002598

43 Atom 0.001636 0.000962 -0.002598

44 Atom 0.001636 0.000962 -0.002598

45 Atom 0.001636 0.000962 -0.002598

--------------------------------------------------------

XY XZ YZ

--------------------------------------------------------

1 Atom -0.000025 -0.000157 0.004213

2 Atom -0.002088 0.001133 0.002887

3 Atom 0.000000 -0.000000 0.009958

4 Atom 0.002088 -0.001133 0.002887

5 Atom 0.000025 0.000157 0.004213

6 Atom -0.000343 -0.006763 0.007702

7 Atom -0.001927 0.001720 -0.001367

8 Atom -0.000000 -0.024186 -0.000000

9 Atom 0.001927 0.001720 0.001367

10 Atom -0.001145 0.000131 0.000336

11 Atom 0.001145 0.000131 -0.000336

12 Atom 0.000343 0.006763 0.007702

13 Atom 0.001927 -0.001720 -0.001367

14 Atom -0.001145 -0.000131 -0.000336

15 Atom 0.001145 -0.000131 0.000336

16 Atom -0.001927 -0.001720 0.001367

17 Atom 0.000000 0.024186 0.000000

18 Atom -0.000343 0.006763 -0.007702

19 Atom 0.002088 0.001133 -0.002887

20 Atom 0.000025 -0.000157 -0.004213

21 Atom -0.000025 0.000157 -0.004213

22 Atom -0.002088 -0.001133 -0.002887

23 Atom 0.000000 -0.000000 -0.009958

24 Atom 0.005224 -0.000171 -0.000207

25 Atom -0.005224 0.000171 -0.000207

26 Atom -0.001673 0.000025 -0.000007

27 Atom 0.001673 0.000025 0.000007

28 Atom -0.001673 -0.000025 0.000007

29 Atom 0.001673 -0.000025 -0.000007

30 Atom -0.005224 -0.000171 0.000207

31 Atom 0.005224 0.000171 0.000207

32 Atom -0.000000 -0.000000 -0.000000

33 Atom 0.000343 -0.006763 -0.007702

34 Atom 0.029971 0.001601 0.001539

35 Atom 0.029971 -0.001601 -0.001539

36 Atom -0.011412 -0.004656 -0.004517

37 Atom -0.011412 0.004656 0.004517

38 Atom -0.029971 0.001601 -0.001539

39 Atom 0.011412 -0.004656 0.004517

40 Atom -0.029971 -0.001601 0.001539

41 Atom 0.011412 0.004656 -0.004517

42 Atom -0.012959 -0.000251 0.000249

43 Atom 0.012959 0.000251 0.000249

44 Atom -0.012959 0.000251 -0.000249

45 Atom 0.012959 -0.000251 -0.000249

--------------------------------------------------------

---------------------------------------------------------------------------------

Anisotropic Spin Dipole Couplings in Principal Axis System

---------------------------------------------------------------------------------

Atom a.u. MegaHertz Gauss 10(-4) cm-1 Axes

Baa -0.0384 -5.156 -1.840 -1.720 0.9999 0.0162 0.0008

1 C(13) Bbb -0.0372 -4.998 -1.783 -1.667 -0.0162 0.9992 -0.0374

Bcc 0.0757 10.154 3.623 3.387 -0.0014 0.0373 0.9993

Baa -0.0456 -6.117 -2.183 -2.040 0.1900 0.9815 -0.0243

2 C(13) Bbb -0.0343 -4.596 -1.640 -1.533 0.9817 -0.1902 -0.0049

Bcc 0.0798 10.713 3.823 3.574 0.0095 0.0229 0.9997

Baa -0.0796 -3.071 -1.096 -1.024 -0.0000 0.9991 -0.0428

3 N(14) Bbb -0.0738 -2.847 -1.016 -0.950 1.0000 0.0000 0.0000

Bcc 0.1534 5.918 2.112 1.974 -0.0000 0.0428 0.9991

Baa -0.0456 -6.117 -2.183 -2.040 -0.1900 0.9815 -0.0243

4 C(13) Bbb -0.0343 -4.596 -1.640 -1.533 0.9817 0.1902 0.0049

Bcc 0.0798 10.713 3.823 3.574 -0.0095 0.0229 0.9997

Baa -0.0384 -5.156 -1.840 -1.720 0.9999 -0.0162 -0.0008

5 C(13) Bbb -0.0372 -4.998 -1.783 -1.667 0.0162 0.9992 -0.0374

Bcc 0.0757 10.154 3.623 3.387 0.0014 0.0373 0.9993

Baa -0.1740 -23.349 -8.332 -7.789 0.1152 0.9932 -0.0132

6 C(13) Bbb -0.1719 -23.065 -8.230 -7.694 0.9933 -0.1150 0.0147

Bcc 0.3459 46.414 16.562 15.482 -0.0131 0.0148 0.9998

Baa -0.0765 -10.266 -3.663 -3.424 -0.0161 0.0108 0.9998

7 C(13) Bbb 0.0288 3.862 1.378 1.288 0.9945 0.1034 0.0149

Bcc 0.0477 6.403 2.285 2.136 -0.1033 0.9946 -0.0124

Baa -0.1894 -7.305 -2.606 -2.437 0.9991 0.0000 0.0434

8 N(14) Bbb -0.1787 -6.892 -2.459 -2.299 -0.0000 1.0000 -0.0000

Bcc 0.3681 14.196 5.066 4.735 -0.0434 0.0000 0.9991

Baa -0.0765 -10.266 -3.663 -3.424 -0.0161 -0.0108 0.9998

9 C(13) Bbb 0.0288 3.862 1.378 1.288 0.9945 -0.1034 0.0149

Bcc 0.0477 6.403 2.285 2.136 0.1033 0.9946 0.0124

Baa -0.0164 -2.198 -0.784 -0.733 -0.0059 -0.0142 0.9999

10 C(13) Bbb 0.0070 0.939 0.335 0.313 0.5964 0.8026 0.0149

Bcc 0.0094 1.259 0.449 0.420 0.8027 -0.5964 -0.0037

Baa -0.0164 -2.198 -0.784 -0.733 -0.0059 0.0142 0.9999

11 C(13) Bbb 0.0070 0.939 0.335 0.313 -0.5964 0.8026 -0.0149

Bcc 0.0094 1.259 0.449 0.420 0.8027 0.5964 -0.0037

Baa -0.1740 -23.349 -8.332 -7.789 -0.1152 0.9932 -0.0132

12 C(13) Bbb -0.1719 -23.065 -8.230 -7.694 0.9933 0.1150 -0.0147

Bcc 0.3459 46.414 16.562 15.482 0.0131 0.0148 0.9998

Baa -0.0765 -10.266 -3.663 -3.424 0.0161 0.0108 0.9998

13 C(13) Bbb 0.0288 3.862 1.378 1.288 0.9945 -0.1034 -0.0149

Bcc 0.0477 6.403 2.285 2.136 0.1033 0.9946 -0.0124

Baa -0.0164 -2.198 -0.784 -0.733 0.0059 0.0142 0.9999

14 C(13) Bbb 0.0070 0.939 0.335 0.313 0.5964 0.8026 -0.0149

Bcc 0.0094 1.259 0.449 0.420 0.8027 -0.5964 0.0037

Baa -0.0164 -2.198 -0.784 -0.733 0.0059 -0.0142 0.9999

15 C(13) Bbb 0.0070 0.939 0.335 0.313 -0.5964 0.8026 0.0149

Bcc 0.0094 1.259 0.449 0.420 0.8027 0.5964 0.0037

Baa -0.0765 -10.266 -3.663 -3.424 0.0161 -0.0108 0.9998

16 C(13) Bbb 0.0288 3.862 1.378 1.288 0.9945 0.1034 -0.0149

Bcc 0.0477 6.403 2.285 2.136 -0.1033 0.9946 0.0124

Baa -0.1894 -7.305 -2.606 -2.437 0.9991 -0.0000 -0.0434

17 N(14) Bbb -0.1787 -6.892 -2.459 -2.299 0.0000 1.0000 -0.0000

Bcc 0.3681 14.196 5.066 4.735 0.0434 0.0000 0.9991

Baa -0.1740 -23.349 -8.332 -7.789 0.1152 0.9932 0.0132

18 C(13) Bbb -0.1719 -23.065 -8.230 -7.694 0.9933 -0.1150 -0.0147

Bcc 0.3459 46.414 16.562 15.482 0.0131 -0.0148 0.9998

Baa -0.0456 -6.117 -2.183 -2.040 -0.1900 0.9815 0.0243

19 C(13) Bbb -0.0343 -4.596 -1.640 -1.533 0.9817 0.1902 -0.0049

Bcc 0.0798 10.713 3.823 3.574 0.0095 -0.0229 0.9997

Baa -0.0384 -5.156 -1.840 -1.720 0.9999 -0.0162 0.0008

20 C(13) Bbb -0.0372 -4.998 -1.783 -1.667 0.0162 0.9992 0.0374

Bcc 0.0757 10.154 3.623 3.387 -0.0014 -0.0373 0.9993

Baa -0.0384 -5.156 -1.840 -1.720 0.9999 0.0162 -0.0008

21 C(13) Bbb -0.0372 -4.998 -1.783 -1.667 -0.0162 0.9992 0.0374

Bcc 0.0757 10.154 3.623 3.387 0.0014 -0.0373 0.9993

Baa -0.0456 -6.117 -2.183 -2.040 0.1900 0.9815 0.0243

22 C(13) Bbb -0.0343 -4.596 -1.640 -1.533 0.9817 -0.1902 0.0049

Bcc 0.0798 10.713 3.823 3.574 -0.0095 -0.0229 0.9997

Baa -0.0796 -3.071 -1.096 -1.024 0.0000 0.9991 0.0428

23 N(14) Bbb -0.0738 -2.847 -1.016 -0.950 1.0000 -0.0000 0.0000

Bcc 0.1534 5.918 2.112 1.974 -0.0000 -0.0428 0.9991

Baa -0.0046 -2.456 -0.876 -0.819 0.8881 -0.4558 0.0601

24 H(1) Bbb -0.0036 -1.944 -0.694 -0.648 -0.0434 0.0471 0.9979

Bcc 0.0082 4.399 1.570 1.467 0.4577 0.8889 -0.0221

Baa -0.0046 -2.456 -0.876 -0.819 0.8881 0.4558 -0.0601

25 H(1) Bbb -0.0036 -1.944 -0.694 -0.648 0.0434 0.0471 0.9979

Bcc 0.0082 4.399 1.570 1.467 -0.4577 0.8889 -0.0221

Baa -0.0023 -1.250 -0.446 -0.417 -0.0079 -0.0018 1.0000

26 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 0.7033 0.7108 0.0068

Bcc 0.0028 1.517 0.541 0.506 0.7108 -0.7034 0.0043

Baa -0.0023 -1.250 -0.446 -0.417 -0.0079 0.0018 1.0000

27 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 -0.7033 0.7108 -0.0068

Bcc 0.0028 1.517 0.541 0.506 0.7108 0.7034 0.0043

Baa -0.0023 -1.250 -0.446 -0.417 0.0079 0.0018 1.0000

28 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 0.7033 0.7108 -0.0068

Bcc 0.0028 1.517 0.541 0.506 0.7108 -0.7034 -0.0043

Baa -0.0023 -1.250 -0.446 -0.417 0.0079 -0.0018 1.0000

29 H(1) Bbb -0.0005 -0.268 -0.096 -0.089 -0.7033 0.7108 0.0068

Bcc 0.0028 1.517 0.541 0.506 0.7108 0.7034 -0.0043

Baa -0.0046 -2.456 -0.876 -0.819 0.8881 0.4558 0.0601

30 H(1) Bbb -0.0036 -1.944 -0.694 -0.648 -0.0434 -0.0471 0.9979

Bcc 0.0082 4.399 1.570 1.467 -0.4577 0.8889 0.0221

Baa -0.0046 -2.456 -0.876 -0.819 0.8881 -0.4558 -0.0601

31 H(1) Bbb -0.0036 -1.944 -0.694 -0.648 0.0434 -0.0471 0.9979

Bcc 0.0082 4.399 1.570 1.467 0.4577 0.8889 0.0221

Baa -0.0060 -0.202 -0.072 -0.067 0.0000 1.0000 0.0000

32 Zn(67) Bbb -0.0024 -0.080 -0.029 -0.027 0.0000 -0.0000 1.0000

Bcc 0.0084 0.282 0.101 0.094 1.0000 -0.0000 -0.0000

Baa -0.1740 -23.349 -8.332 -7.789 -0.1152 0.9932 0.0132

33 C(13) Bbb -0.1719 -23.065 -8.230 -7.694 0.9933 0.1150 0.0147

Bcc 0.3459 46.414 16.562 15.482 -0.0131 -0.0148 0.9998

Baa -0.0498 -6.684 -2.385 -2.230 -0.0154 -0.0146 0.9998

34 C(13) Bbb -0.0051 -0.684 -0.244 -0.228 -0.6978 0.7163 -0.0003

Bcc 0.0549 7.368 2.629 2.458 0.7161 0.6977 0.0212

Baa -0.0498 -6.684 -2.385 -2.230 0.0154 0.0146 0.9998

35 C(13) Bbb -0.0051 -0.684 -0.244 -0.228 -0.6978 0.7163 0.0003

Bcc 0.0549 7.368 2.629 2.458 0.7161 0.6977 -0.0212

Baa -0.1006 -13.495 -4.815 -4.501 0.6864 0.7269 0.0233

36 C(13) Bbb -0.0776 -10.407 -3.713 -3.471 0.7270 -0.6866 0.0011

Bcc 0.1781 23.902 8.529 7.973 -0.0168 -0.0161 0.9997

Baa -0.1006 -13.495 -4.815 -4.501 0.6864 0.7269 -0.0233

37 C(13) Bbb -0.0776 -10.407 -3.713 -3.471 0.7270 -0.6866 -0.0011

Bcc 0.1781 23.902 8.529 7.973 0.0168 0.0161 0.9997

Baa -0.0498 -6.684 -2.385 -2.230 -0.0154 0.0146 0.9998

38 C(13) Bbb -0.0051 -0.684 -0.244 -0.228 0.6978 0.7163 0.0003

Bcc 0.0549 7.368 2.629 2.458 0.7161 -0.6977 0.0212

Baa -0.1006 -13.495 -4.815 -4.501 -0.6864 0.7269 -0.0233

39 C(13) Bbb -0.0776 -10.407 -3.713 -3.471 0.7270 0.6866 0.0011

Bcc 0.1781 23.902 8.529 7.973 -0.0168 0.0161 0.9997

Baa -0.0498 -6.684 -2.385 -2.230 0.0154 -0.0146 0.9998

40 C(13) Bbb -0.0051 -0.684 -0.244 -0.228 0.6978 0.7163 -0.0003

Bcc 0.0549 7.368 2.629 2.458 0.7161 -0.6977 -0.0212

Baa -0.1006 -13.495 -4.815 -4.501 -0.6864 0.7269 0.0233

41 C(13) Bbb -0.0776 -10.407 -3.713 -3.471 0.7270 0.6866 -0.0011

Bcc 0.1781 23.902 8.529 7.973 0.0168 -0.0161 0.9997

Baa -0.0117 -6.224 -2.221 -2.076 0.6979 0.7162 -0.0003

42 H(1) Bbb -0.0026 -1.390 -0.496 -0.464 0.0152 -0.0144 0.9998

Bcc 0.0143 7.614 2.717 2.540 0.7161 -0.6977 -0.0210

Baa -0.0117 -6.224 -2.221 -2.076 -0.6979 0.7162 -0.0003

43 H(1) Bbb -0.0026 -1.390 -0.496 -0.464 -0.0152 -0.0144 0.9998

Bcc 0.0143 7.614 2.717 2.540 0.7161 0.6977 0.0210

Baa -0.0117 -6.224 -2.221 -2.076 0.6979 0.7162 0.0003

44 H(1) Bbb -0.0026 -1.390 -0.496 -0.464 -0.0152 0.0144 0.9998

Bcc 0.0143 7.614 2.717 2.540 0.7161 -0.6977 0.0210

Baa -0.0117 -6.224 -2.221 -2.076 -0.6979 0.7162 0.0003

45 H(1) Bbb -0.0026 -1.390 -0.496 -0.464 0.0152 0.0144 0.9998

Bcc 0.0143 7.614 2.717 2.540 0.7161 0.6977 -0.0210

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Mon Jul 29 22:43:20 2019, MaxMem= 4294967296 cpu: 31.9

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

Density matrix has only Abelian symmetry.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

4 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16215 LenP2D= 44808.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 260

Leave Link 701 at Mon Jul 29 22:43:55 2019, MaxMem= 4294967296 cpu: 564.1

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Mon Jul 29 22:43:55 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Density matrix has only Abelian symmetry.

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 1.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 100127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Leave Link 703 at Mon Jul 29 22:46:02 2019, MaxMem= 4294967296 cpu: 2030.1

(Enter /home/kira/g09/l716.exe)

Dipole = 3.97744337D-13-8.30238656D-14 3.30714160D-01

Polarizability= 1.27637048D+03 3.32435407D-06 1.65221575D+03

-2.64424728D-06 1.44089610D-07 1.81239764D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.017899947 0.012088891 0.000238964

2 6 0.019226082 -0.021006560 -0.000172537

3 7 0.000000000 -0.002191909 -0.000290130

4 6 -0.019226082 -0.021006560 -0.000172537

5 6 0.017899947 0.012088891 0.000238964

6 6 0.019735576 0.006890175 -0.000110625

7 6 0.002230060 -0.004245263 -0.000110717

8 7 -0.001315531 0.000000000 -0.000191109

9 6 0.002230060 0.004245263 -0.000110717

10 6 0.001056283 -0.001688541 -0.000000675

11 6 0.001056283 0.001688541 -0.000000675

12 6 -0.019735576 0.006890175 -0.000110625

13 6 -0.002230060 -0.004245263 -0.000110717

14 6 -0.001056283 0.001688541 -0.000000675

15 6 -0.001056283 -0.001688541 -0.000000675

16 6 -0.002230060 0.004245263 -0.000110717

17 7 0.001315531 0.000000000 -0.000191109

18 6 -0.019735576 -0.006890175 -0.000110625

19 6 0.019226082 0.021006560 -0.000172537

20 6 -0.017899947 -0.012088891 0.000238964

21 6 0.017899947 -0.012088891 0.000238964

22 6 -0.019226082 0.021006560 -0.000172537

23 7 0.000000000 0.002191909 -0.000290130

24 1 -0.000316064 0.000003896 -0.000003844

25 1 0.000316064 0.000003896 -0.000003844

26 1 0.000004113 0.000027443 -0.000002126

27 1 0.000004113 -0.000027443 -0.000002126

28 1 -0.000004113 -0.000027443 -0.000002126

29 1 -0.000004113 0.000027443 -0.000002126

30 1 -0.000316064 -0.000003896 -0.000003844

31 1 0.000316064 -0.000003896 -0.000003844

32 30 0.000000000 0.000000000 0.000742902

33 6 0.019735576 -0.006890175 -0.000110625

34 6 -0.006523093 -0.007976155 0.000208311

35 6 0.006523093 0.007976155 0.000208311

36 6 0.002240125 0.002671886 0.000059288

37 6 -0.002240125 -0.002671886 0.000059288

38 6 -0.006523093 0.007976155 0.000208311

39 6 0.002240125 -0.002671886 0.000059288

40 6 0.006523093 -0.007976155 0.000208311

41 6 -0.002240125 0.002671886 0.000059288

42 1 -0.000106342 0.000124448 -0.000051145

43 1 0.000106342 0.000124448 -0.000051145

44 1 0.000106342 -0.000124448 -0.000051145

45 1 -0.000106342 -0.000124448 -0.000051145

-------------------------------------------------------------------

Cartesian Forces: Max 0.021006560 RMS 0.007430624

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Mon Jul 29 22:46:02 2019, MaxMem= 4294967296 cpu: 0.9

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.016626007 RMS 0.003166693

Search for a local minimum.

Step number 1 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .31667D-02 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- analytic derivatives used.

ITU= 0

Eigenvalues --- 0.00235 0.00254 0.00395 0.00491 0.00637

Eigenvalues --- 0.00784 0.00879 0.00948 0.01018 0.01053

Eigenvalues --- 0.01090 0.01170 0.01192 0.01280 0.01281

Eigenvalues --- 0.01469 0.01470 0.01573 0.01620 0.01702

Eigenvalues --- 0.01704 0.02009 0.02135 0.02147 0.02353

Eigenvalues --- 0.02685 0.02855 0.02855 0.02880 0.02883

Eigenvalues --- 0.02930 0.03178 0.03323 0.03786 0.04035

Eigenvalues --- 0.04166 0.04205 0.04252 0.04253 0.04257

Eigenvalues --- 0.04354 0.04408 0.04831 0.04861 0.06996

Eigenvalues --- 0.07016 0.08457 0.08465 0.08620 0.08632

Eigenvalues --- 0.08703 0.08738 0.08753 0.08973 0.09673

Eigenvalues --- 0.09685 0.09688 0.09712 0.10149 0.10458

Eigenvalues --- 0.10470 0.10486 0.10735 0.12646 0.12765

Eigenvalues --- 0.12923 0.14756 0.16604 0.17174 0.18551

Eigenvalues --- 0.19090 0.19429 0.20256 0.20289 0.20569

Eigenvalues --- 0.20789 0.21012 0.21866 0.21880 0.22089

Eigenvalues --- 0.22884 0.24442 0.25663 0.26509 0.28700

Eigenvalues --- 0.30224 0.30879 0.31115 0.31347 0.32277

Eigenvalues --- 0.32986 0.34087 0.34852 0.35270 0.35448

Eigenvalues --- 0.35648 0.36001 0.37123 0.37201 0.37237

Eigenvalues --- 0.37252 0.37344 0.37357 0.37413 0.37848

Eigenvalues --- 0.37898 0.38605 0.39721 0.40145 0.40146

Eigenvalues --- 0.40147 0.40154 0.41117 0.43599 0.43771

Eigenvalues --- 0.44179 0.44272 0.44605 0.45346 0.45737

Eigenvalues --- 0.52525 0.52583 0.52817 0.52924 0.97543

Eigenvalues --- 1.05216 1.05644 1.05723 1.64896

RFO step: Lambda=-8.74574464D-03 EMin= 2.34757225D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.01384727 RMS(Int)= 0.00006595

Iteration 2 RMS(Cart)= 0.00014573 RMS(Int)= 0.00002416

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00002416

ITry= 1 IFail=0 DXMaxC= 4.09D-02 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.73461 -0.01275 0.00000 -0.04877 -0.04879 2.68582

R2 2.57442 0.01416 0.00000 0.04045 0.04039 2.61481

R3 2.04039 0.00019 0.00000 0.00037 0.00037 2.04075

R4 2.58205 0.00101 0.00000 0.00472 0.00482 2.58687

R5 2.67450 0.01662 0.00000 0.04981 0.04980 2.72430

R6 2.58205 0.00101 0.00000 0.00473 0.00482 2.58687

R7 3.94732 0.00568 0.00000 0.01592 0.01603 3.96335

R8 2.73461 -0.01275 0.00000 -0.04877 -0.04879 2.68582

R9 2.67450 0.01663 0.00000 0.04981 0.04980 2.72430

R10 2.04039 0.00019 0.00000 0.00037 0.00037 2.04075

R11 2.67450 -0.00479 0.00000 -0.01152 -0.01157 2.66293

R12 2.69670 -0.00662 0.00000 -0.01851 -0.01851 2.67819

R13 2.58205 0.00216 0.00000 0.00294 0.00289 2.58494

R14 2.73461 0.00083 0.00000 0.00594 0.00594 2.74055

R15 2.58205 0.00216 0.00000 0.00294 0.00289 2.58494

R16 3.94732 0.00609 0.00000 0.02964 0.02962 3.97694

R17 2.73461 0.00083 0.00000 0.00594 0.00594 2.74055

R18 2.67450 -0.00479 0.00000 -0.01152 -0.01157 2.66293

R19 2.57442 -0.00228 0.00000 -0.00578 -0.00578 2.56864

R20 2.04039 0.00002 0.00000 0.00003 0.00003 2.04041

R21 2.04039 0.00002 0.00000 0.00003 0.00003 2.04041

R22 2.67450 -0.00479 0.00000 -0.01152 -0.01157 2.66293

R23 2.69670 -0.00662 0.00000 -0.01851 -0.01851 2.67819

R24 2.73461 0.00083 0.00000 0.00594 0.00594 2.74055

R25 2.58205 0.00216 0.00000 0.00294 0.00289 2.58494

R26 2.57442 -0.00228 0.00000 -0.00578 -0.00578 2.56864

R27 2.04039 0.00002 0.00000 0.00003 0.00003 2.04041

R28 2.73461 0.00083 0.00000 0.00594 0.00594 2.74055

R29 2.04039 0.00002 0.00000 0.00003 0.00003 2.04041

R30 2.58205 0.00216 0.00000 0.00294 0.00289 2.58494

R31 2.67450 -0.00479 0.00000 -0.01153 -0.01157 2.66293

R32 3.94732 0.00610 0.00000 0.02968 0.02966 3.97697

R33 2.67450 0.01662 0.00000 0.04981 0.04980 2.72430

R34 2.69670 -0.00662 0.00000 -0.01851 -0.01851 2.67819

R35 2.73461 -0.01275 0.00000 -0.04877 -0.04878 2.68582

R36 2.58205 0.00101 0.00000 0.00472 0.00482 2.58687

R37 2.57442 0.01416 0.00000 0.04045 0.04039 2.61481

R38 2.04039 0.00019 0.00000 0.00037 0.00037 2.04075

R39 2.73461 -0.01275 0.00000 -0.04877 -0.04878 2.68582

R40 2.04039 0.00019 0.00000 0.00037 0.00037 2.04075

R41 2.58205 0.00101 0.00000 0.00473 0.00482 2.58687

R42 2.67450 0.01662 0.00000 0.04981 0.04980 2.72430

R43 3.94732 0.00568 0.00000 0.01596 0.01606 3.96338

R44 2.69670 -0.00662 0.00000 -0.01851 -0.01851 2.67819

R45 2.27864 0.00364 0.00000 0.00404 0.00404 2.28268

R46 2.27864 0.00364 0.00000 0.00404 0.00404 2.28268

R47 2.01698 0.00016 0.00000 0.00047 0.00047 2.01744

R48 2.01698 0.00016 0.00000 0.00047 0.00047 2.01744

R49 2.27864 0.00364 0.00000 0.00404 0.00404 2.28268

R50 2.01698 0.00016 0.00000 0.00047 0.00047 2.01744

R51 2.27864 0.00364 0.00000 0.00404 0.00404 2.28268

R52 2.01698 0.00016 0.00000 0.00047 0.00047 2.01744

A1 1.86587 -0.00101 0.00000 -0.00334 -0.00337 1.86250

A2 2.19058 0.00025 0.00000 0.00742 0.00743 2.19801

A3 2.22672 0.00077 0.00000 -0.00407 -0.00406 2.22267

A4 1.90828 0.00107 0.00000 0.00761 0.00765 1.91592

A5 2.18404 0.00135 0.00000 0.00645 0.00636 2.19040

A6 2.19079 -0.00242 0.00000 -0.01405 -0.01399 2.17680

A7 1.87647 -0.00012 0.00000 -0.00853 -0.00854 1.86793

A8 2.20226 0.00006 0.00000 0.00425 0.00426 2.20651

A9 2.20226 0.00005 0.00000 0.00424 0.00424 2.20650

A10 1.90828 0.00107 0.00000 0.00761 0.00764 1.91592

A11 2.19079 -0.00242 0.00000 -0.01404 -0.01399 2.17680

A12 2.18404 0.00135 0.00000 0.00645 0.00636 2.19040

A13 1.86587 -0.00101 0.00000 -0.00334 -0.00337 1.86250

A14 2.22672 0.00077 0.00000 -0.00407 -0.00406 2.22267

A15 2.19058 0.00025 0.00000 0.00742 0.00743 2.19801

A16 2.20757 0.00156 0.00000 0.01077 0.01076 2.21833

A17 2.03777 -0.00020 0.00000 -0.01059 -0.01059 2.02718

A18 2.03777 -0.00136 0.00000 -0.00014 -0.00014 2.03763

A19 2.19079 -0.00092 0.00000 -0.00243 -0.00247 2.18831

A20 2.18404 -0.00079 0.00000 0.00169 0.00172 2.18576

A21 1.90828 0.00170 0.00000 0.00077 0.00078 1.90906

A22 1.87647 -0.00343 0.00000 -0.00267 -0.00267 1.87381

A23 2.20226 0.00171 0.00000 0.00126 0.00126 2.20351

A24 2.20226 0.00171 0.00000 0.00128 0.00127 2.20353

A25 1.90828 0.00170 0.00000 0.00077 0.00078 1.90906

A26 2.19079 -0.00092 0.00000 -0.00243 -0.00248 2.18831

A27 2.18404 -0.00079 0.00000 0.00169 0.00172 2.18576

A28 1.86587 0.00001 0.00000 0.00057 0.00055 1.86643

A29 2.19058 -0.00002 0.00000 -0.00129 -0.00129 2.18929

A30 2.22672 0.00002 0.00000 0.00073 0.00074 2.22746

A31 1.86587 0.00001 0.00000 0.00057 0.00055 1.86643

A32 2.19058 -0.00002 0.00000 -0.00129 -0.00129 2.18929

A33 2.22672 0.00002 0.00000 0.00073 0.00074 2.22746

A34 2.20757 0.00156 0.00000 0.01076 0.01076 2.21833

A35 2.03777 -0.00020 0.00000 -0.01059 -0.01059 2.02718

A36 2.03777 -0.00136 0.00000 -0.00014 -0.00014 2.03763

A37 2.18404 -0.00079 0.00000 0.00168 0.00172 2.18576

A38 2.19079 -0.00092 0.00000 -0.00243 -0.00247 2.18832

A39 1.90828 0.00171 0.00000 0.00077 0.00078 1.90906

A40 1.86587 0.00001 0.00000 0.00057 0.00055 1.86643

A41 2.19058 -0.00002 0.00000 -0.00129 -0.00129 2.18929

A42 2.22672 0.00002 0.00000 0.00073 0.00074 2.22746

A43 1.86587 0.00001 0.00000 0.00057 0.00055 1.86643

A44 2.22672 0.00002 0.00000 0.00073 0.00074 2.22746

A45 2.19058 -0.00002 0.00000 -0.00129 -0.00129 2.18929

A46 1.90828 0.00171 0.00000 0.00077 0.00078 1.90906

A47 2.18404 -0.00079 0.00000 0.00169 0.00172 2.18576

A48 2.19079 -0.00092 0.00000 -0.00243 -0.00248 2.18831

A49 1.87647 -0.00343 0.00000 -0.00267 -0.00267 1.87380

A50 2.20226 0.00171 0.00000 0.00126 0.00126 2.20352

A51 2.20226 0.00171 0.00000 0.00128 0.00127 2.20353

A52 2.20757 0.00156 0.00000 0.01076 0.01076 2.21833

A53 2.03777 -0.00136 0.00000 -0.00014 -0.00014 2.03763

A54 2.03777 -0.00020 0.00000 -0.01058 -0.01058 2.02718

A55 2.18404 0.00135 0.00000 0.00644 0.00636 2.19040

A56 2.19079 -0.00242 0.00000 -0.01404 -0.01399 2.17680

A57 1.90828 0.00108 0.00000 0.00761 0.00765 1.91593

A58 1.86587 -0.00101 0.00000 -0.00334 -0.00337 1.86250

A59 2.19058 0.00025 0.00000 0.00742 0.00743 2.19801

A60 2.22672 0.00077 0.00000 -0.00407 -0.00406 2.22267

A61 1.86587 -0.00101 0.00000 -0.00334 -0.00337 1.86250

A62 2.22672 0.00077 0.00000 -0.00407 -0.00406 2.22267

A63 2.19058 0.00025 0.00000 0.00742 0.00743 2.19801

A64 1.90828 0.00108 0.00000 0.00761 0.00765 1.91592

A65 2.18404 0.00135 0.00000 0.00644 0.00635 2.19040

A66 2.19079 -0.00242 0.00000 -0.01404 -0.01399 2.17680

A67 1.87647 -0.00012 0.00000 -0.00853 -0.00854 1.86793

A68 2.20226 0.00006 0.00000 0.00426 0.00426 2.20652

A69 2.20226 0.00006 0.00000 0.00424 0.00424 2.20650

A70 1.56397 0.00004 0.00000 0.00059 0.00058 1.56455

A71 1.56397 0.00003 0.00000 0.00058 0.00056 1.56454

A72 1.56397 0.00003 0.00000 0.00058 0.00057 1.56454

A73 1.56397 0.00003 0.00000 0.00056 0.00055 1.56453

A74 2.20757 0.00156 0.00000 0.01076 0.01076 2.21833

A75 2.03777 -0.00136 0.00000 -0.00014 -0.00014 2.03763

A76 2.03777 -0.00020 0.00000 -0.01058 -0.01058 2.02718

A77 3.12794 0.00006 0.00000 0.00114 0.00112 3.12906

A78 3.12794 0.00006 0.00000 0.00114 0.00112 3.12906

A79 3.14154 0.00075 0.00000 0.01204 0.01204 3.15359

A80 3.14154 -0.00075 0.00000 -0.01199 -0.01199 3.12956

A81 3.14162 0.00002 0.00000 -0.00328 -0.00328 3.13835

A82 3.14162 -0.00003 0.00000 0.00322 0.00322 3.14484

A83 3.14154 -0.00075 0.00000 -0.01199 -0.01199 3.12956

A84 3.14162 -0.00003 0.00000 0.00322 0.00322 3.14484

A85 3.14154 0.00075 0.00000 0.01204 0.01204 3.15359

A86 3.14162 0.00002 0.00000 -0.00328 -0.00328 3.13835

A87 3.30643 -0.00031 0.00000 -0.00654 -0.00654 3.29989

A88 2.97675 0.00045 0.00000 0.00732 0.00734 2.98409

A89 3.13776 0.00011 0.00000 0.00215 0.00215 3.13991

A90 3.14543 -0.00013 0.00000 -0.00247 -0.00247 3.14296

A91 3.14440 -0.00008 0.00000 -0.00243 -0.00243 3.14197

A92 3.13879 0.00008 0.00000 0.00255 0.00255 3.14133

A93 3.13776 0.00013 0.00000 0.00247 0.00247 3.14023

A94 3.14440 -0.00008 0.00000 -0.00255 -0.00255 3.14185

A95 3.14543 -0.00011 0.00000 -0.00215 -0.00215 3.14328

A96 3.13879 0.00008 0.00000 0.00243 0.00243 3.14121

D1 -0.00170 0.00007 0.00000 0.00151 0.00151 -0.00018

D2 3.12742 0.00006 0.00000 0.00269 0.00271 3.13013

D3 -3.13811 0.00003 0.00000 0.00082 0.00082 -3.13730

D4 -0.00899 0.00002 0.00000 0.00201 0.00201 -0.00698

D5 0.00000 -0.00000 0.00000 -0.00000 -0.00000 -0.00000

D6 -3.13628 -0.00004 0.00000 -0.00075 -0.00075 -3.13703

D7 3.13628 0.00004 0.00000 0.00075 0.00075 3.13703

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00274 -0.00011 0.00000 -0.00245 -0.00245 0.00030

D10 -3.07094 -0.00006 0.00000 -0.00192 -0.00193 -3.07286

D11 -3.12632 -0.00013 0.00000 -0.00382 -0.00381 -3.13013

D12 0.08319 -0.00008 0.00000 -0.00330 -0.00329 0.07990

D13 -3.11685 -0.00006 0.00000 -0.00012 -0.00012 -3.11697

D14 0.01114 0.00007 0.00000 0.00300 0.00300 0.01413

D15 0.01028 -0.00005 0.00000 0.00144 0.00143 0.01172

D16 3.13827 0.00009 0.00000 0.00456 0.00455 -3.14037

D17 -0.00274 0.00011 0.00000 0.00245 0.00245 -0.00030

D18 3.12632 0.00013 0.00000 0.00383 0.00381 3.13013

D19 3.07094 0.00006 0.00000 0.00192 0.00193 3.07287

D20 -0.08319 0.00008 0.00000 0.00330 0.00329 -0.07990

D21 -3.09930 -0.00025 0.00000 -0.00420 -0.00421 -3.10351

D22 -0.12255 0.00019 0.00000 0.00312 0.00313 -0.11942

D23 0.12255 -0.00019 0.00000 -0.00311 -0.00313 0.11943

D24 3.09930 0.00025 0.00000 0.00421 0.00421 3.10351

D25 0.00170 -0.00007 0.00000 -0.00151 -0.00151 0.00019

D26 3.13811 -0.00003 0.00000 -0.00082 -0.00082 3.13730

D27 -3.12742 -0.00006 0.00000 -0.00269 -0.00271 -3.13013

D28 0.00899 -0.00002 0.00000 -0.00201 -0.00202 0.00698

D29 -0.01028 0.00005 0.00000 -0.00144 -0.00144 -0.01172

D30 -3.13827 -0.00009 0.00000 -0.00456 -0.00455 3.14037

D31 3.11685 0.00006 0.00000 0.00012 0.00011 3.11696

D32 -0.01114 -0.00007 0.00000 -0.00300 -0.00300 -0.01414

D33 0.01028 -0.00002 0.00000 -0.00008 -0.00007 0.01021

D34 -3.11685 -0.00011 0.00000 -0.00259 -0.00258 -3.11943

D35 3.13827 0.00012 0.00000 0.00298 0.00299 3.14125

D36 0.01114 0.00004 0.00000 0.00047 0.00048 0.01161

D37 -3.12632 -0.00012 0.00000 -0.00305 -0.00305 -3.12936

D38 0.08319 -0.00005 0.00000 -0.00099 -0.00099 0.08220

D39 0.00274 -0.00006 0.00000 -0.00086 -0.00086 0.00188

D40 -3.07094 0.00001 0.00000 0.00119 0.00120 -3.06974

D41 3.12742 0.00009 0.00000 0.00267 0.00267 3.13010

D42 -0.00899 0.00005 0.00000 0.00207 0.00208 -0.00692

D43 -0.00170 0.00003 0.00000 0.00053 0.00053 -0.00117

D44 -3.13811 -0.00001 0.00000 -0.00007 -0.00007 -3.13818

D45 -0.00274 0.00006 0.00000 0.00086 0.00086 -0.00188

D46 3.12632 0.00012 0.00000 0.00305 0.00305 3.12936

D47 3.07094 -0.00001 0.00000 -0.00119 -0.00120 3.06974

D48 -0.08319 0.00005 0.00000 0.00099 0.00098 -0.08220

D49 -0.12255 0.00002 0.00000 0.00198 0.00198 -0.12057

D50 -3.09930 -0.00029 0.00000 -0.00456 -0.00456 -3.10387

D51 3.09930 0.00029 0.00000 0.00456 0.00456 3.10387

D52 0.12255 -0.00002 0.00000 -0.00198 -0.00198 0.12057

D53 0.00170 -0.00003 0.00000 -0.00053 -0.00053 0.00116

D54 3.13811 0.00001 0.00000 0.00006 0.00007 3.13818

D55 -3.12742 -0.00009 0.00000 -0.00267 -0.00267 -3.13010

D56 0.00899 -0.00005 0.00000 -0.00207 -0.00208 0.00692

D57 -0.01028 0.00002 0.00000 0.00008 0.00007 -0.01021

D58 -3.13827 -0.00012 0.00000 -0.00298 -0.00299 -3.14126

D59 3.11685 0.00011 0.00000 0.00258 0.00258 3.11943

D60 -0.01114 -0.00004 0.00000 -0.00047 -0.00048 -0.01161

D61 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D62 3.13628 0.00004 0.00000 0.00061 0.00061 3.13689

D63 -3.13628 -0.00004 0.00000 -0.00060 -0.00061 -3.13688

D64 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D65 3.11685 0.00011 0.00000 0.00258 0.00258 3.11943

D66 -0.01028 0.00002 0.00000 0.00008 0.00007 -0.01021

D67 -0.01114 -0.00004 0.00000 -0.00047 -0.00048 -0.01161

D68 -3.13827 -0.00012 0.00000 -0.00297 -0.00298 -3.14125

D69 -3.12742 -0.00009 0.00000 -0.00267 -0.00267 -3.13010

D70 0.00899 -0.00005 0.00000 -0.00207 -0.00207 0.00692

D71 0.00170 -0.00003 0.00000 -0.00053 -0.00053 0.00117

D72 3.13811 0.00001 0.00000 0.00007 0.00007 3.13818

D73 3.12632 0.00012 0.00000 0.00305 0.00304 3.12936

D74 -0.08319 0.00005 0.00000 0.00100 0.00099 -0.08220

D75 -0.00274 0.00006 0.00000 0.00086 0.00086 -0.00188

D76 3.07094 -0.00001 0.00000 -0.00119 -0.00119 3.06974

D77 -0.00000 -0.00000 0.00000 -0.00000 -0.00000 -0.00000

D78 3.13628 0.00004 0.00000 0.00060 0.00061 3.13688

D79 -3.13628 -0.00004 0.00000 -0.00060 -0.00061 -3.13689

D80 0.00000 -0.00000 0.00000 -0.00000 -0.00000 -0.00000

D81 -0.00170 0.00003 0.00000 0.00053 0.00053 -0.00117

D82 3.12742 0.00009 0.00000 0.00267 0.00267 3.13010

D83 -3.13811 -0.00001 0.00000 -0.00006 -0.00007 -3.13818

D84 -0.00899 0.00005 0.00000 0.00207 0.00208 -0.00692

D85 0.00274 -0.00006 0.00000 -0.00086 -0.00086 0.00188

D86 -3.07094 0.00001 0.00000 0.00119 0.00119 -3.06974

D87 -3.12632 -0.00012 0.00000 -0.00305 -0.00304 -3.12936

D88 0.08319 -0.00005 0.00000 -0.00099 -0.00099 0.08220

D89 -3.11685 -0.00011 0.00000 -0.00258 -0.00258 -3.11943

D90 0.01114 0.00004 0.00000 0.00047 0.00048 0.01161

D91 0.01028 -0.00002 0.00000 -0.00008 -0.00007 0.01021

D92 3.13827 0.00012 0.00000 0.00297 0.00299 3.14125

D93 0.12255 -0.00002 0.00000 -0.00198 -0.00198 0.12057

D94 3.09930 0.00029 0.00000 0.00455 0.00456 3.10386

D95 -3.09930 -0.00029 0.00000 -0.00455 -0.00456 -3.10386

D96 -0.12255 0.00002 0.00000 0.00199 0.00198 -0.12057

D97 3.11685 0.00006 0.00000 0.00012 0.00011 3.11696

D98 -0.01028 0.00005 0.00000 -0.00144 -0.00144 -0.01172

D99 -0.01114 -0.00007 0.00000 -0.00301 -0.00300 -0.01414

D100 -3.13827 -0.00009 0.00000 -0.00457 -0.00455 3.14037

D101 -3.12742 -0.00006 0.00000 -0.00269 -0.00271 -3.13013

D102 0.00899 -0.00002 0.00000 -0.00201 -0.00202 0.00698

D103 0.00170 -0.00007 0.00000 -0.00151 -0.00151 0.00018

D104 3.13811 -0.00003 0.00000 -0.00083 -0.00082 3.13729

D105 3.12632 0.00013 0.00000 0.00382 0.00381 3.13013

D106 -0.08319 0.00008 0.00000 0.00330 0.00330 -0.07989

D107 -0.00274 0.00011 0.00000 0.00245 0.00245 -0.00030

D108 3.07094 0.00006 0.00000 0.00193 0.00194 3.07287

D109 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D110 3.13628 0.00004 0.00000 0.00074 0.00075 3.13703

D111 -3.13628 -0.00004 0.00000 -0.00074 -0.00075 -3.13703

D112 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 -0.00170 0.00007 0.00000 0.00151 0.00151 -0.00018

D114 3.12742 0.00006 0.00000 0.00269 0.00271 3.13013

D115 -3.13811 0.00003 0.00000 0.00083 0.00082 -3.13729

D116 -0.00899 0.00002 0.00000 0.00201 0.00202 -0.00698

D117 0.00274 -0.00011 0.00000 -0.00245 -0.00245 0.00030

D118 -3.07094 -0.00006 0.00000 -0.00193 -0.00194 -3.07287

D119 -3.12632 -0.00013 0.00000 -0.00383 -0.00381 -3.13013

D120 0.08319 -0.00008 0.00000 -0.00330 -0.00330 0.07989

D121 -3.11685 -0.00006 0.00000 -0.00011 -0.00011 -3.11696

D122 0.01114 0.00007 0.00000 0.00301 0.00301 0.01414

D123 0.01028 -0.00005 0.00000 0.00145 0.00144 0.01172

D124 3.13827 0.00009 0.00000 0.00457 0.00455 -3.14036

D125 3.09930 0.00025 0.00000 0.00420 0.00420 3.10351

D126 0.12255 -0.00019 0.00000 -0.00312 -0.00313 0.11942

D127 -0.12255 0.00019 0.00000 0.00312 0.00313 -0.11942

D128 -3.09930 -0.00025 0.00000 -0.00420 -0.00421 -3.10351

Item Value Threshold Converged?

Maximum Force 0.016626 0.000450 NO

RMS Force 0.003167 0.000300 NO

Maximum Displacement 0.040930 0.001800 NO

RMS Displacement 0.013831 0.001200 NO

Predicted change in Energy=-4.510427D-03

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Mon Jul 29 22:46:02 2019, MaxMem= 4294967296 cpu: 1.3

(Enter /home/kira/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -0.691849 -4.265341 -0.046775

2 6 0 -1.100586 -2.904501 -0.014030

3 7 0 -0.000002 -2.090716 0.005789

4 6 0 1.100584 -2.904499 -0.014031

5 6 0 0.691849 -4.265340 -0.046775

6 6 0 2.465339 -2.439996 -0.016310

7 6 0 2.907928 -1.102148 -0.012256

8 7 0 2.097951 0.000002 0.006046

9 6 0 2.907930 1.102151 -0.012255

10 6 0 4.294954 0.679634 -0.041019

11 6 0 4.294953 -0.679634 -0.041019

12 6 0 -2.465340 -2.439997 -0.016307

13 6 0 -2.907926 -1.102148 -0.012251

14 6 0 -4.294952 -0.679634 -0.041015

15 6 0 -4.294953 0.679634 -0.041014

16 6 0 -2.907928 1.102150 -0.012250

17 7 0 -2.097949 0.000002 0.006052

18 6 0 -2.465341 2.439999 -0.016306

19 6 0 -1.100585 2.904500 -0.014030

20 6 0 -0.691849 4.265340 -0.046783

21 6 0 0.691849 4.265339 -0.046783

22 6 0 1.100584 2.904498 -0.014032

23 7 0 -0.000002 2.090714 0.005792

24 1 0 -1.347007 -5.123474 -0.071343

25 1 0 1.347009 -5.123472 -0.071344

26 1 0 5.149869 1.338790 -0.062775

27 1 0 5.149867 -1.338791 -0.062774

28 1 0 -5.149866 -1.338792 -0.062771

29 1 0 -5.149868 1.338791 -0.062772

30 1 0 -1.347008 5.123473 -0.071358

31 1 0 1.347009 5.123470 -0.071359

32 30 0 0.000010 -0.000009 0.172134

33 6 0 2.465339 2.439999 -0.016309

34 6 0 3.466442 3.442960 -0.036752

35 6 0 -3.466444 -3.442958 -0.036756

36 6 0 4.309353 4.307977 -0.056032

37 6 0 -4.309354 -4.307975 -0.056038

38 6 0 3.466441 -3.442958 -0.036755

39 6 0 4.309352 -4.307975 -0.056033

40 6 0 -3.466444 3.442960 -0.036753

41 6 0 -4.309355 4.307977 -0.056037

42 1 0 -5.056809 5.070060 -0.072769

43 1 0 5.056807 5.070060 -0.072760

44 1 0 5.056802 -5.070061 -0.072778

45 1 0 -5.056804 -5.070062 -0.072787

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.421275 0.000000

3 N 2.282632 1.368913 0.000000

4 C 2.250728 2.201170 1.368914 0.000000

5 C 1.383698 2.250728 2.282632 1.421275 0.000000

6 C 3.647005 3.596052 2.490058 1.441639 2.545205

7 C 4.792220 4.395072 3.071424 2.552442 3.862379

8 N 5.096953 4.320554 2.961842 3.071038 4.491442

9 C 6.462938 5.667580 4.318656 4.395423 5.807078

10 C 7.022892 6.477546 5.111133 4.801118 6.118428

11 C 6.142111 5.836318 4.521060 3.892910 5.083274

12 C 2.545207 1.441639 2.490056 3.596051 3.647005

13 C 3.862380 2.552442 3.071419 4.395069 4.792218

14 C 5.083275 3.892909 4.521055 5.836314 6.142109

15 C 6.118429 4.801118 5.111128 6.477543 7.022891

16 C 5.807078 4.395423 4.318651 5.667575 6.462935

17 N 4.491443 3.071038 2.961837 4.320549 5.096950

18 C 6.935978 5.515999 5.158077 6.424912 7.411501

19 C 7.181557 5.809001 5.115062 6.212054 7.390568

20 C 8.530681 7.181557 6.393814 7.390567 8.642171

21 C 8.642171 7.390568 6.393813 7.181553 8.530678

22 C 7.390567 6.212054 5.115060 5.808997 7.181553

23 N 6.393813 5.115061 4.181430 5.115060 6.393812

24 H 1.079921 2.233349 3.319337 3.304216 2.212224

25 H 2.212224 3.304215 3.319337 2.233350 1.079921

26 H 8.095197 7.554872 6.187680 5.865543 7.161038

27 H 6.533804 6.443756 5.204925 4.341717 5.332810

28 H 5.332810 4.341715 5.204919 6.443752 6.533802

29 H 7.161039 5.865542 6.187676 7.554868 8.095195

30 H 9.411677 8.031959 7.339270 8.392992 9.607671

31 H 9.607670 8.392993 7.339269 8.031955 9.411673

32 Zn 4.326620 3.111598 2.097314 3.111588 4.326616

33 C 7.411501 6.424913 5.158078 5.515996 6.935975

34 C 8.758390 7.819752 6.529902 6.774071 8.192457

35 C 2.893923 2.426465 3.721100 4.598717 4.238845

36 C 9.925416 9.016044 7.714767 7.894160 9.305277

37 C 3.617768 3.502527 4.846708 5.589181 5.001393

38 C 4.238843 4.598716 3.721102 2.426465 2.893920

39 C 5.001391 5.589180 4.846710 3.502528 3.617766

40 C 8.192459 6.774073 6.529900 7.819751 8.758389

41 C 9.305279 7.894163 7.714766 9.016042 9.925416

42 H 10.305496 8.902178 8.766651 10.075243 10.963459

43 H 10.963459 10.075245 8.766652 8.902176 10.305494

44 H 5.804760 6.527367 5.869748 4.510518 4.438588

45 H 4.438590 4.510517 5.869746 6.527368 5.804762

6 7 8 9 10

6 C 0.000000

7 C 1.409163 0.000000

8 N 2.467603 1.367893 0.000000

9 C 3.569693 2.204299 1.367893 0.000000

10 C 3.616656 2.258189 2.300204 1.450236 0.000000

11 C 2.539090 1.450236 2.300204 2.258189 1.359268

12 C 4.930679 5.537316 5.174720 6.435749 7.445421

13 C 5.537312 5.815854 5.125805 6.219575 7.420044

14 C 6.985772 7.215319 6.429100 7.420046 8.696787

15 C 7.445418 7.420045 6.429101 7.215322 8.589908

16 C 6.435745 6.219575 5.125806 5.815858 7.215321

17 N 5.174716 5.125804 4.195900 5.125806 6.429100

18 C 6.937288 6.435747 5.174720 5.537318 6.985778

19 C 6.424909 5.667575 4.320549 4.395072 5.836318

20 C 7.411498 6.462934 5.096948 4.792219 6.142111

21 C 6.935972 5.807074 4.491437 3.862378 5.083275

22 C 5.515993 4.395419 3.071032 2.552442 3.892910

23 N 5.158074 4.318651 2.961838 3.071425 4.521061

24 H 4.662410 5.854829 6.174443 7.540980 8.093746

25 H 2.907702 4.314047 5.178792 6.418593 6.509020

26 H 4.635525 3.314670 3.333361 2.254960 1.079741

27 H 2.901983 2.254960 3.333361 3.314669 2.192120

28 H 7.694553 8.061426 7.370750 8.419550 9.658113

29 H 8.501338 8.419549 7.370751 8.061430 9.467820

30 H 8.470129 7.540976 6.174438 5.854829 7.181947

31 H 7.645896 6.418589 5.178787 4.314044 5.332821

32 Zn 3.473743 3.115236 2.104505 3.115245 4.353607

33 C 4.879995 3.569692 2.467601 1.409163 2.539091

34 C 5.967563 4.579361 3.705207 2.406642 2.884861

35 C 6.016011 6.790626 6.543569 7.828873 8.788349

36 C 6.995506 5.588860 4.842809 3.499032 3.628402

37 C 7.027616 7.897367 7.721145 9.020009 9.945381

38 C 1.417235 2.406642 3.705208 4.579361 4.205023

39 C 2.625130 3.499033 4.842811 5.588860 4.987652

40 C 8.354378 7.828871 6.543568 6.790628 8.238646

41 C 9.562071 9.020008 7.721145 7.897369 9.338053

42 H 10.629526 10.076549 8.769395 8.898597 10.331133

43 H 7.944799 6.535862 5.870819 4.512830 4.456149

44 H 3.692711 4.512833 5.870822 6.535864 5.800036

45 H 7.968881 8.898592 8.769395 10.076549 10.977950

11 12 13 14 15

11 C 0.000000

12 C 6.985775 0.000000

13 C 7.215318 1.409163 0.000000

14 C 8.589905 2.539088 1.450237 0.000000

15 C 8.696787 3.616655 2.258189 1.359268 0.000000

16 C 7.420046 3.569693 2.204298 2.258189 1.450237

17 N 6.429099 2.467605 1.367893 2.300205 2.300205

18 C 7.445421 4.879996 3.569692 3.616655 2.539090

19 C 6.477544 5.515996 4.395419 4.801117 3.892909

20 C 7.022890 6.935975 5.807075 6.118427 5.083275

21 C 6.118427 7.411498 6.462932 7.022889 6.142110

22 C 4.801117 6.424908 5.667571 6.477541 5.836314

23 N 5.111131 5.158074 4.318647 5.111126 4.521055

24 H 7.181947 2.907705 4.314050 5.332824 6.509022

25 H 5.332822 4.662411 5.854828 7.181946 8.093744

26 H 2.192120 8.501342 8.419548 9.658114 9.467821

27 H 1.079741 7.694556 8.061426 9.467818 9.658113

28 H 9.467817 2.901980 2.254960 1.079741 2.192120

29 H 9.658113 4.635524 3.314670 2.192120 1.079741

30 H 8.093744 7.645899 6.418591 6.509020 5.332823

31 H 6.509018 8.470129 7.540974 8.093742 7.181946

32 Zn 4.353603 3.473760 3.115253 4.353622 4.353626

33 C 3.616656 6.937288 6.435744 7.445419 6.985775

34 C 4.205025 8.354379 7.828868 8.788346 8.238643

35 C 8.238644 1.417235 2.406644 2.884858 4.205022

36 C 4.987654 9.562071 9.020005 9.945379 9.338051

37 C 9.338051 2.625130 3.499035 3.628401 4.987653

38 C 2.884859 6.016010 6.790622 8.238641 8.788346

39 C 3.628401 7.027615 7.897363 9.338048 9.945378

40 C 8.788349 5.967563 4.579361 4.205024 2.884860

41 C 9.945381 6.995507 5.588861 4.987654 3.628402

42 H 10.977952 7.944800 6.535863 5.800035 4.456150

43 H 5.800035 10.629527 10.076546 10.977950 10.331131

44 H 4.456151 7.968880 8.898589 10.331126 10.977947

45 H 10.331129 3.692711 4.512835 4.456151 5.800037

16 17 18 19 20

16 C 0.000000

17 N 1.367893 0.000000

18 C 1.409163 2.467603 0.000000

19 C 2.552441 3.071033 1.441640 0.000000

20 C 3.862379 4.491438 2.545206 1.421276 0.000000

21 C 4.792218 5.096946 3.647005 2.250728 1.383698

22 C 4.395069 4.320545 3.596051 2.201169 2.250728

23 N 3.071419 2.961833 2.490057 1.368913 2.282633

24 H 6.418595 5.178794 7.645903 8.031960 9.411677

25 H 7.540978 6.174440 8.470132 8.392993 9.607670

26 H 8.061430 7.370750 7.694560 6.443757 6.533806

27 H 8.419549 7.370749 8.501342 7.554869 8.095195

28 H 3.314669 3.333362 4.635525 5.865541 7.161038

29 H 2.254960 3.333362 2.901982 4.341717 5.332812

30 H 4.314047 5.178789 2.907702 2.233350 1.079921

31 H 5.854828 6.174436 4.662410 3.304215 2.212224

32 Zn 3.115262 2.104523 3.473774 3.111614 4.326638

33 C 5.537315 5.174716 4.930681 3.596051 3.647004

34 C 6.790625 6.543564 6.016012 4.598716 4.238843

35 C 4.579360 3.705210 5.967563 6.774070 8.192456

36 C 7.897366 7.721141 7.027617 5.589181 5.001392

37 C 5.588861 4.842813 6.995507 7.894160 9.305276

38 C 7.828869 6.543565 8.354379 7.819748 8.758386

39 C 9.020005 7.721141 9.562071 9.016040 9.925413

40 C 2.406644 3.705209 1.417235 2.426467 2.893923

41 C 3.499034 4.842811 2.625130 3.502530 3.617770

42 H 4.512833 5.870822 3.692711 4.510521 4.438595

43 H 8.898594 8.769391 7.968884 6.527371 5.804764

44 H 10.076546 8.769391 10.629526 10.075242 10.963456

45 H 6.535865 5.870825 7.944802 8.902177 10.305495

21 22 23 24 25

21 C 0.000000

22 C 1.421276 0.000000

23 N 2.282633 1.368914 0.000000

24 H 9.607671 8.392992 7.339270 0.000000

25 H 9.411674 8.031955 7.339269 2.694016 0.000000

26 H 5.332812 4.341720 5.204927 9.163533 7.498176

27 H 7.161037 5.865541 6.187678 7.518861 5.365222

28 H 8.095194 7.554866 6.187673 5.365224 7.518860

29 H 6.533804 6.443753 5.204921 7.498179 9.163532

30 H 2.212224 3.304216 3.319338 10.246947 10.595169

31 H 1.079921 2.233350 3.319338 10.595169 10.246942

32 Zn 4.326634 3.111604 2.097330 5.303172 5.303165

33 C 2.545204 1.441639 2.490060 8.470132 7.645899

34 C 2.893920 2.426467 3.721104 9.826204 8.824792

35 C 8.758386 7.819747 6.529896 2.705059 5.098495

36 C 3.617767 3.502530 4.846712 10.997587 9.885744

37 C 9.925413 9.016039 7.714763 3.072584 5.714868

38 C 8.192454 6.774067 6.529897 5.098492 2.705054

39 C 9.305274 7.894157 7.714763 5.714864 3.072579

40 C 4.238845 4.598717 3.721102 8.824795 9.826204

41 C 5.001395 5.589182 4.846711 9.885748 10.997587

42 H 5.804767 6.527372 5.869750 10.847616 12.038147

43 H 4.438593 4.510522 5.869752 12.038147 10.847612

44 H 10.305493 8.902174 8.766649 6.404032 3.710177

45 H 10.963457 10.075241 8.766648 3.710181 6.404036

26 27 28 29 30

26 H 0.000000

27 H 2.677581 0.000000

28 H 10.642085 10.299733 0.000000

29 H 10.299737 10.642085 2.677582 0.000000

30 H 7.518864 9.163532 7.498177 5.365224 0.000000

31 H 5.365223 7.498175 9.163530 7.518862 2.694017

32 Zn 5.326220 5.326213 5.326231 5.326238 5.303189

33 C 2.901985 4.635526 8.501339 7.694556 4.662409

34 C 2.694836 5.069492 9.854267 8.869554 5.098491

35 C 9.854270 8.869555 2.694828 5.069488 8.824791

36 C 3.085868 5.708984 11.016481 9.914281 5.714866

37 C 11.016484 9.914281 3.085864 5.708982 9.885744

38 C 5.069489 2.694832 8.869551 9.854267 9.826201

39 C 5.708982 3.085865 9.914277 11.016480 10.997584

40 C 8.869558 9.854270 5.069491 2.694832 2.705056

41 C 9.914285 11.016484 5.708984 3.085866 3.072584

42 H 10.867325 12.051958 6.409535 3.732443 3.710186

43 H 3.732443 6.409534 12.051956 10.867321 6.404038

44 H 6.409535 3.732444 10.867315 12.051953 12.038144

45 H 12.051957 10.867318 3.732444 6.409536 10.847614

31 32 33 34 35

31 H 0.000000

32 Zn 5.303182 0.000000

33 C 2.907699 3.473758 0.000000

34 C 2.705052 4.890176 1.417235 0.000000

35 C 9.826201 4.890177 8.354379 9.771426 0.000000

36 C 3.072580 6.097642 2.625130 1.207943 10.979088

37 C 10.997584 6.097643 9.562071 10.979088 1.207943

38 C 8.824788 4.890161 5.967562 6.885918 6.932885

39 C 9.885741 6.097627 6.995506 7.796658 7.823786

40 C 5.098495 4.890192 6.016012 6.932886 6.885918

41 C 5.714869 6.097658 7.027618 7.823787 7.796657

42 H 6.404041 7.164984 7.968885 8.677243 8.660371

43 H 3.710182 7.164968 3.692711 2.275524 12.046517

44 H 10.847610 7.164953 7.944801 8.660374 8.677239

45 H 12.038144 7.164969 10.629526 12.046516 2.275524

36 37 38 39 40

36 C 0.000000

37 C 12.186745 0.000000

38 C 7.796657 7.823785 0.000000

39 C 8.615952 8.618706 1.207943 0.000000

40 C 7.823787 7.796658 9.771426 10.979088 0.000000

41 C 8.618709 8.615952 10.979088 12.186744 1.207943

42 H 9.397130 9.407790 12.046516 13.254161 2.275524

43 H 1.067585 13.254161 8.660371 9.407790 8.677243

44 H 9.407792 9.397123 2.275524 1.067585 12.046516

45 H 13.254161 1.067585 8.677238 9.397123 8.660374

41 42 43 44 45

41 C 0.000000

42 H 1.067585 0.000000

43 H 9.397130 10.113615 0.000000

44 H 13.254161 14.321563 10.140121 0.000000

45 H 9.407793 10.140122 14.321564 10.113605 0.000000

Stoichiometry C28H12N4Zn(3)

Framework group C1[X(C28H12N4Zn)]

Deg. of freedom 129

Full point group C1 NOp 1

Omega: Change in point group or standard orientation.

Old FWG=C04V [C4(Zn1),2SGV(N2),2SGD(C6H2),X(C16H8)]

New FWG=C01 [X(C28H12N4Zn1)]

RotChk: IX=3 Diff= 4.28D-06

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.691863 4.265338 -0.043186

2 6 0 1.100596 2.904497 -0.010441

3 7 0 0.000010 2.090715 0.009378

4 6 0 -1.100574 2.904502 -0.010443

5 6 0 -0.691835 4.265341 -0.043187

6 6 0 -2.465330 2.440003 -0.012721

7 6 0 -2.907923 1.102156 -0.008668

8 7 0 -2.097950 0.000003 0.009634

9 6 0 -2.907932 -1.102143 -0.008667

10 6 0 -4.294955 -0.679622 -0.037431

11 6 0 -4.294950 0.679646 -0.037431

12 6 0 2.465349 2.439989 -0.012719

13 6 0 2.907930 1.102138 -0.008662

14 6 0 4.294955 0.679620 -0.037426

15 6 0 4.294952 -0.679648 -0.037426

16 6 0 2.907926 -1.102159 -0.008661

17 7 0 2.097950 -0.000009 0.009641

18 6 0 2.465335 -2.440007 -0.012718

19 6 0 1.100577 -2.904504 -0.010442

20 6 0 0.691837 -4.265343 -0.043194

21 6 0 -0.691861 -4.265337 -0.043195

22 6 0 -1.100592 -2.904495 -0.010443

23 7 0 -0.000003 -2.090715 0.009381

24 1 0 1.347024 5.123469 -0.067754

25 1 0 -1.346993 5.123475 -0.067756

26 1 0 -5.149872 -1.338775 -0.059187

27 1 0 -5.149862 1.338806 -0.059186

28 1 0 5.149871 1.338775 -0.059182

29 1 0 5.149865 -1.338807 -0.059183

30 1 0 1.346993 -5.123478 -0.067769

31 1 0 -1.347024 -5.123467 -0.067771

32 30 0 -0.000009 0.000008 0.175723

33 6 0 -2.465346 -2.439992 -0.012720

34 6 0 -3.466451 -3.442951 -0.033164

35 6 0 3.466455 3.442946 -0.033168

36 6 0 -4.309365 -4.307964 -0.052444

37 6 0 4.309368 4.307961 -0.052450

38 6 0 -3.466430 3.442967 -0.033167

39 6 0 -4.309338 4.307987 -0.052444

40 6 0 3.466435 -3.442971 -0.033164

41 6 0 4.309343 -4.307990 -0.052449

42 1 0 5.056794 -5.070076 -0.069181

43 1 0 -5.056821 -5.070045 -0.069171

44 1 0 -5.056785 5.070076 -0.069190

45 1 0 5.056820 5.070046 -0.069199

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1466679 0.1454197 0.0730709

Leave Link 202 at Mon Jul 29 22:46:02 2019, MaxMem= 4294967296 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 671 symmetry adapted cartesian basis functions of A symmetry.

There are 636 symmetry adapted basis functions of A symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

111 alpha electrons 109 beta electrons

nuclear repulsion energy 3055.8110224214 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 45 NActive= 45 NUniq= 45 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1301804864 Hartrees.

Nuclear repulsion after empirical dispersion term = 3055.6808419351 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: York/Karplus (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3902

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.23D-09

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 136

GePol: Fraction of low-weight points (<1% of avg) = 3.49%

GePol: Cavity surface area = 415.616 Ang\*\*2

GePol: Cavity volume = 420.202 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = 0.0083019293 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3055.6891438644 Hartrees.

Leave Link 301 at Mon Jul 29 22:46:03 2019, MaxMem= 4294967296 cpu: 1.9

(Enter /home/kira/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16193 LenP2D= 44750.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 6.85D-05 NBF= 636

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 636

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Mon Jul 29 22:46:03 2019, MaxMem= 4294967296 cpu: 14.3

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Mon Jul 29 22:46:04 2019, MaxMem= 4294967296 cpu: 1.2

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "ZnTSPsim3.chk"

B after Tr= -0.000000 0.000000 -0.000000

Rot= 1.000000 -0.000000 0.000000 0.000002 Ang= -0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0541 S= 1.0179

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1359.39324019974

Leave Link 401 at Mon Jul 29 22:46:08 2019, MaxMem= 4294967296 cpu: 68.7

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1384965 IEndB= 1384965 NGot= 4294967296 MDV= 4294049884

LenX= 4294049884 LenY= 4293598972

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 660000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 45676812.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.88D-15 for 3879.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.02D-15 for 1063 835.

Iteration 1 A^-1\*A deviation from unit magnitude is 7.11D-15 for 3879.

Iteration 1 A^-1\*A deviation from orthogonality is 4.22D-14 for 1055 1005.

E= -1359.00776043969

DIIS: error= 2.05D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.00776043969 IErMin= 1 ErrMin= 2.05D-03

ErrMax= 2.05D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.12D-02 BMatP= 1.12D-02

IDIUse=3 WtCom= 9.79D-01 WtEn= 2.05D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.616 Goal= None Shift= 0.000

Gap= 0.677 Goal= None Shift= 0.000

GapD= 0.616 DampG=2.000 DampE=1.000 DampFc=2.0000 IDamp=-1.

RMSDP=1.70D-04 MaxDP=5.35D-03 OVMax= 3.05D-02

Cycle 2 Pass 1 IDiag 1:

RMSU= 1.69D-04 CP: 9.99D-01

E= -1359.01120370414 Delta-E= -0.003443264447 Rises=F Damp=F

DIIS: error= 5.23D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.01120370414 IErMin= 2 ErrMin= 5.23D-04

ErrMax= 5.23D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.39D-04 BMatP= 1.12D-02

IDIUse=3 WtCom= 9.95D-01 WtEn= 5.23D-03

Coeff-Com: 0.625D-01 0.938D+00

Coeff-En: 0.000D+00 0.100D+01

Coeff: 0.621D-01 0.938D+00

Gap= 0.038 Goal= None Shift= 0.000

Gap= 0.048 Goal= None Shift= 0.000

RMSDP=4.03D-05 MaxDP=1.56D-03 DE=-3.44D-03 OVMax= 6.06D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 4.03D-05 CP: 9.99D-01 9.97D-01

E= -1359.01114457571 Delta-E= 0.000059128429 Rises=F Damp=F

DIIS: error= 9.02D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1359.01120370414 IErMin= 2 ErrMin= 5.23D-04

ErrMax= 9.02D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.03D-03 BMatP= 7.39D-04

IDIUse=3 WtCom= 2.50D-01 WtEn= 7.50D-01

Coeff-Com: -0.818D-02 0.549D+00 0.459D+00

Coeff-En: 0.000D+00 0.572D+00 0.428D+00

Coeff: -0.204D-02 0.566D+00 0.436D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=2.49D-05 MaxDP=1.16D-03 DE= 5.91D-05 OVMax= 6.97D-03

Cycle 4 Pass 1 IDiag 1:

RMSU= 1.29D-05 CP: 9.99D-01 1.03D+00 4.90D-01

E= -1359.01137621918 Delta-E= -0.000231643467 Rises=F Damp=F

DIIS: error= 2.25D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.01137621918 IErMin= 4 ErrMin= 2.25D-04

ErrMax= 2.25D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.18D-05 BMatP= 7.39D-04

IDIUse=3 WtCom= 9.98D-01 WtEn= 2.25D-03

Coeff-Com: -0.840D-02 0.172D+00 0.232D+00 0.604D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.100D+01

Coeff: -0.838D-02 0.172D+00 0.231D+00 0.605D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=6.19D-06 MaxDP=3.30D-04 DE=-2.32D-04 OVMax= 1.32D-03

Cycle 5 Pass 1 IDiag 1:

RMSU= 5.62D-06 CP: 9.99D-01 1.03D+00 5.30D-01 8.66D-01

E= -1359.01138929293 Delta-E= -0.000013073748 Rises=F Damp=F

DIIS: error= 1.28D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.01138929293 IErMin= 5 ErrMin= 1.28D-04

ErrMax= 1.28D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.33D-05 BMatP= 6.18D-05

IDIUse=3 WtCom= 9.99D-01 WtEn= 1.28D-03

Coeff-Com: -0.413D-02 0.477D-01 0.100D+00 0.374D+00 0.482D+00

Coeff-En: 0.000D+00 0.000D+00 0.000D+00 0.806D-01 0.919D+00

Coeff: -0.413D-02 0.477D-01 0.999D-01 0.374D+00 0.483D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=2.50D-06 MaxDP=1.44D-04 DE=-1.31D-05 OVMax= 7.57D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 1.85D-06 CP: 9.99D-01 1.03D+00 5.48D-01 9.58D-01 8.38D-01

E= -1359.01139292677 Delta-E= -0.000003633847 Rises=F Damp=F

DIIS: error= 3.08D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.01139292677 IErMin= 6 ErrMin= 3.08D-05

ErrMax= 3.08D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.35D-07 BMatP= 1.33D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.645D-03-0.229D-01-0.130D-01-0.152D-01 0.952D-01 0.955D+00

Coeff: 0.645D-03-0.229D-01-0.130D-01-0.152D-01 0.952D-01 0.955D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=1.65D-06 MaxDP=8.97D-05 DE=-3.63D-06 OVMax= 8.94D-04

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.17D-06 CP: 9.99D-01 1.04D+00 5.60D-01 1.02D+00 9.45D-01

CP: 1.16D+00

E= -1359.01139352969 Delta-E= -0.000000602912 Rises=F Damp=F

DIIS: error= 1.95D-05 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.01139352969 IErMin= 7 ErrMin= 1.95D-05

ErrMax= 1.95D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.26D-07 BMatP= 6.35D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.121D-02-0.241D-01-0.275D-01-0.887D-01-0.470D-01 0.586D+00

Coeff-Com: 0.600D+00

Coeff: 0.121D-02-0.241D-01-0.275D-01-0.887D-01-0.470D-01 0.586D+00

Coeff: 0.600D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=8.83D-07 MaxDP=5.03D-05 DE=-6.03D-07 OVMax= 3.99D-04

Cycle 8 Pass 1 IDiag 1:

RMSU= 5.97D-07 CP: 9.99D-01 1.04D+00 5.68D-01 1.04D+00 9.97D-01

CP: 1.36D+00 1.16D+00

E= -1359.01139374477 Delta-E= -0.000000215085 Rises=F Damp=F

DIIS: error= 1.20D-05 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.01139374477 IErMin= 8 ErrMin= 1.20D-05

ErrMax= 1.20D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.39D-08 BMatP= 4.26D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.365D-03-0.203D-02-0.786D-02-0.424D-01-0.677D-01-0.101D+00

Coeff-Com: 0.335D+00 0.886D+00

Coeff: 0.365D-03-0.203D-02-0.786D-02-0.424D-01-0.677D-01-0.101D+00

Coeff: 0.335D+00 0.886D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=6.30D-07 MaxDP=4.05D-05 DE=-2.15D-07 OVMax= 3.21D-04

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.75D-07 CP: 9.99D-01 1.04D+00 5.70D-01 1.05D+00 1.04D+00

CP: 1.53D+00 1.46D+00 1.02D+00

E= -1359.01139382113 Delta-E= -0.000000076358 Rises=F Damp=F

DIIS: error= 4.67D-06 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.01139382113 IErMin= 9 ErrMin= 4.67D-06

ErrMax= 4.67D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.31D-08 BMatP= 9.39D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.563D-04 0.421D-02 0.156D-02-0.463D-02-0.239D-01-0.169D+00

Coeff-Com: 0.579D-01 0.472D+00 0.662D+00

Coeff: -0.563D-04 0.421D-02 0.156D-02-0.463D-02-0.239D-01-0.169D+00

Coeff: 0.579D-01 0.472D+00 0.662D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=1.95D-07 MaxDP=1.07D-05 DE=-7.64D-08 OVMax= 5.35D-05

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.26D-07 CP: 9.99D-01 1.04D+00 5.70D-01 1.06D+00 1.05D+00

CP: 1.56D+00 1.54D+00 1.12D+00 1.16D+00

E= -1359.01139383143 Delta-E= -0.000000010305 Rises=F Damp=F

DIIS: error= 1.83D-06 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.01139383143 IErMin=10 ErrMin= 1.83D-06

ErrMax= 1.83D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.53D-09 BMatP= 2.31D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.104D-03 0.225D-02 0.232D-02 0.765D-02 0.775D-02-0.492D-01

Coeff-Com: -0.549D-01 0.270D-02 0.289D+00 0.792D+00

Coeff: -0.104D-03 0.225D-02 0.232D-02 0.765D-02 0.775D-02-0.492D-01

Coeff: -0.549D-01 0.270D-02 0.289D+00 0.792D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=9.20D-08 MaxDP=3.69D-06 DE=-1.03D-08 OVMax= 1.90D-05

Cycle 11 Pass 1 IDiag 1:

RMSU= 5.97D-08 CP: 9.99D-01 1.04D+00 5.70D-01 1.05D+00 1.05D+00

CP: 1.56D+00 1.57D+00 1.18D+00 1.30D+00 1.08D+00

E= -1359.01139383353 Delta-E= -0.000000002098 Rises=F Damp=F

DIIS: error= 7.45D-07 at cycle 11 NSaved= 11.

NSaved=11 IEnMin=11 EnMin= -1359.01139383353 IErMin=11 ErrMin= 7.45D-07

ErrMax= 7.45D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 4.71D-10 BMatP= 3.53D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.177D-04-0.632D-04 0.281D-03 0.248D-02 0.531D-02 0.993D-02

Coeff-Com: -0.190D-01-0.676D-01-0.208D-01 0.175D+00 0.914D+00

Coeff: -0.177D-04-0.632D-04 0.281D-03 0.248D-02 0.531D-02 0.993D-02

Coeff: -0.190D-01-0.676D-01-0.208D-01 0.175D+00 0.914D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=4.53D-08 MaxDP=1.92D-06 DE=-2.10D-09 OVMax= 1.83D-05

Cycle 12 Pass 1 IDiag 1:

RMSU= 2.98D-08 CP: 9.99D-01 1.04D+00 5.70D-01 1.05D+00 1.05D+00

CP: 1.56D+00 1.57D+00 1.19D+00 1.38D+00 1.22D+00

CP: 1.27D+00

E= -1359.01139383403 Delta-E= -0.000000000497 Rises=F Damp=F

DIIS: error= 6.29D-07 at cycle 12 NSaved= 12.

NSaved=12 IEnMin=12 EnMin= -1359.01139383403 IErMin=12 ErrMin= 6.29D-07

ErrMax= 6.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.76D-10 BMatP= 4.71D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.215D-04-0.790D-03-0.532D-03-0.562D-03 0.143D-02 0.246D-01

Coeff-Com: 0.537D-02-0.493D-01-0.108D+00-0.139D+00 0.615D+00 0.652D+00

Coeff: 0.215D-04-0.790D-03-0.532D-03-0.562D-03 0.143D-02 0.246D-01

Coeff: 0.537D-02-0.493D-01-0.108D+00-0.139D+00 0.615D+00 0.652D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=2.74D-08 MaxDP=1.53D-06 DE=-4.97D-10 OVMax= 7.20D-06

Cycle 13 Pass 1 IDiag 1:

RMSU= 1.63D-08 CP: 9.99D-01 1.04D+00 5.70D-01 1.05D+00 1.05D+00

CP: 1.56D+00 1.57D+00 1.19D+00 1.41D+00 1.29D+00

CP: 1.57D+00 1.10D+00

E= -1359.01139383424 Delta-E= -0.000000000208 Rises=F Damp=F

DIIS: error= 2.80D-07 at cycle 13 NSaved= 13.

NSaved=13 IEnMin=13 EnMin= -1359.01139383424 IErMin=13 ErrMin= 2.80D-07

ErrMax= 2.80D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.31D-11 BMatP= 3.76D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.164D-04-0.382D-03-0.390D-03-0.123D-02-0.146D-02 0.821D-02

Coeff-Com: 0.882D-02-0.204D-02-0.458D-01-0.128D+00 0.513D-01 0.359D+00

Coeff-Com: 0.752D+00

Coeff: 0.164D-04-0.382D-03-0.390D-03-0.123D-02-0.146D-02 0.821D-02

Coeff: 0.882D-02-0.204D-02-0.458D-01-0.128D+00 0.513D-01 0.359D+00

Coeff: 0.752D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=1.46D-08 MaxDP=7.34D-07 DE=-2.08D-10 OVMax= 5.07D-06

Cycle 14 Pass 1 IDiag 1:

RMSU= 8.57D-09 CP: 9.99D-01 1.04D+00 5.70D-01 1.05D+00 1.05D+00

CP: 1.56D+00 1.57D+00 1.19D+00 1.42D+00 1.33D+00

CP: 1.68D+00 1.33D+00 1.12D+00

E= -1359.01139383429 Delta-E= -0.000000000056 Rises=F Damp=F

DIIS: error= 1.29D-07 at cycle 14 NSaved= 14.

NSaved=14 IEnMin=14 EnMin= -1359.01139383429 IErMin=14 ErrMin= 1.29D-07

ErrMax= 1.29D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.48D-11 BMatP= 7.31D-11

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.413D-05-0.349D-04-0.602D-04-0.370D-03-0.760D-03 0.196D-03

Coeff-Com: 0.263D-02 0.573D-02-0.316D-02-0.363D-01-0.953D-01 0.418D-01

Coeff-Com: 0.361D+00 0.724D+00

Coeff: 0.413D-05-0.349D-04-0.602D-04-0.370D-03-0.760D-03 0.196D-03

Coeff: 0.263D-02 0.573D-02-0.316D-02-0.363D-01-0.953D-01 0.418D-01

Coeff: 0.361D+00 0.724D+00

Gap= 0.039 Goal= None Shift= 0.000

Gap= 0.049 Goal= None Shift= 0.000

RMSDP=6.74D-09 MaxDP=3.52D-07 DE=-5.64D-11 OVMax= 1.69D-06

Error on total polarization charges = 0.06200

SCF Done: E(UB3LYP) = -1359.01139383 A.U. after 14 cycles

NFock= 14 Conv=0.67D-08 -V/T= 1.9681

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0582 S= 1.0193

<L.S>= 0.000000000000E+00

KE= 1.403759395131D+03 PE=-9.353820691916D+03 EE= 3.535360759086D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.21

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0582, after 2.0019

Leave Link 502 at Mon Jul 29 22:49:20 2019, MaxMem= 4294967296 cpu: 3035.8

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 109 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 109 NVA= 525 NVB= 527

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13976232D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.39178648D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13965943D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.49488357D-01

Leave Link 801 at Mon Jul 29 22:49:20 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16193 LenP2D= 44750.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Mon Jul 29 22:49:23 2019, MaxMem= 4294967296 cpu: 42.1

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Mon Jul 29 22:49:23 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 256

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Mon Jul 29 22:55:12 2019, MaxMem= 4294967296 cpu: 5579.3

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 660000000 NMat= 138 IRICut= 345 DoRegI=T DoRafI=T ISym2E= 2.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 138 NMatS0= 138 NMatT0= 0 NMatD0= 138 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 138 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

135 vectors produced by pass 0 Test12= 1.16D-13 1.00D-09 XBig12= 7.04D+03 5.72D+01.

AX will form 135 AO Fock derivatives at one time.

135 vectors produced by pass 1 Test12= 1.16D-13 1.00D-09 XBig12= 4.51D+02 3.32D+00.

135 vectors produced by pass 2 Test12= 1.16D-13 1.00D-09 XBig12= 1.61D+01 9.78D-01.

135 vectors produced by pass 3 Test12= 1.16D-13 1.00D-09 XBig12= 2.17D-01 9.10D-02.

135 vectors produced by pass 4 Test12= 1.16D-13 1.00D-09 XBig12= 1.25D-03 4.77D-03.

135 vectors produced by pass 5 Test12= 1.16D-13 1.00D-09 XBig12= 8.39D-06 2.21D-04.

133 vectors produced by pass 6 Test12= 1.16D-13 1.00D-09 XBig12= 4.71D-08 2.99D-05.

66 vectors produced by pass 7 Test12= 1.16D-13 1.00D-09 XBig12= 1.98D-10 1.19D-06.

3 vectors produced by pass 8 Test12= 1.16D-13 1.00D-09 XBig12= 1.05D-12 8.12D-08.

2 vectors produced by pass 9 Test12= 1.16D-13 1.00D-09 XBig12= 2.27D-14 1.30D-08.

InvSVY: IOpt=1 It= 1 EMax= 4.26D-14

Solved reduced A of dimension 1014 with 138 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1006.80 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Mon Jul 29 23:52:35 2019, MaxMem= 4294967296 cpu: 55081.3

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16193 LenP2D= 44750.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 256

Leave Link 701 at Mon Jul 29 23:53:10 2019, MaxMem= 4294967296 cpu: 562.6

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Mon Jul 29 23:53:10 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 100127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Tue Jul 30 00:00:33 2019, MaxMem= 4294967296 cpu: 7083.8

(Enter /home/kira/g09/l716.exe)

Dipole =-2.07219179D-05 2.53421523D-05 3.34074506D-01

Polarizability= 1.22441263D+03 1.19338256D-03 1.61462482D+03

-1.17297330D-06 7.73369522D-04 1.81356667D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.001473067 -0.000654730 -0.000022587

2 6 0.001575232 -0.000202934 -0.000013523

3 7 0.000000808 0.000136584 0.000111850

4 6 -0.001575744 -0.000203410 -0.000013525

5 6 0.001473012 -0.000654762 -0.000022608

6 6 0.001636076 0.000684067 0.000038437

7 6 0.000071384 -0.000042948 -0.000046061

8 7 0.000219292 -0.000000725 0.000025725

9 6 0.000070876 0.000043304 -0.000046130

10 6 0.000081448 -0.000067874 0.000026129

11 6 0.000081453 0.000067929 0.000026112

12 6 -0.001635699 0.000684203 0.000038447

13 6 -0.000071497 -0.000043386 -0.000046065

14 6 -0.000081398 0.000068206 0.000026095

15 6 -0.000081375 -0.000068154 0.000026113

16 6 -0.000070974 0.000043762 -0.000046132

17 7 -0.000218414 -0.000000625 0.000026101

18 6 -0.001635627 -0.000684551 0.000038372

19 6 0.001574859 0.000203119 -0.000013629

20 6 -0.001472823 0.000654624 -0.000022613

21 6 0.001472766 0.000654637 -0.000022635

22 6 -0.001575361 0.000203580 -0.000013628

23 7 0.000000870 -0.000137610 0.000112393

24 1 0.000022530 -0.000040391 -0.000010339

25 1 -0.000022525 -0.000040386 -0.000010343

26 1 -0.000005481 0.000006304 -0.000007671

27 1 -0.000005454 -0.000006307 -0.000007752

28 1 0.000005436 -0.000006297 -0.000007733

29 1 0.000005449 0.000006279 -0.000007652

30 1 0.000022533 0.000040433 -0.000010253

31 1 -0.000022533 0.000040438 -0.000010257

32 30 -0.000002092 0.000002098 -0.000278990

33 6 0.001635982 -0.000684387 0.000038361

34 6 -0.000025728 -0.000128751 0.000010987

35 6 0.000025600 0.000128776 0.000011231

36 6 0.000019454 0.000131785 0.000035956

37 6 -0.000019340 -0.000131851 0.000035319

38 6 -0.000025523 0.000128678 0.000011238

39 6 0.000019304 -0.000131831 0.000035311

40 6 0.000025784 -0.000128865 0.000010974

41 6 -0.000019488 0.000131824 0.000035966

42 1 -0.000011014 -0.000009000 -0.000010422

43 1 0.000011019 -0.000009004 -0.000010438

44 1 0.000011080 0.000009073 -0.000010072

45 1 -0.000011089 0.000009077 -0.000010059

-------------------------------------------------------------------

Cartesian Forces: Max 0.001636076 RMS 0.000498499

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Tue Jul 30 00:00:33 2019, MaxMem= 4294967296 cpu: 0.8

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.001620284 RMS 0.000265937

Search for a local minimum.

Step number 2 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .26594D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Second derivative matrix not updated -- analytic derivatives used.

DE= -4.57D-03 DEPred=-4.51D-03 R= 1.01D+00

TightC=F SS= 1.41D+00 RLast= 1.77D-01 DXNew= 5.0454D-01 5.3207D-01

Trust test= 1.01D+00 RLast= 1.77D-01 DXMaxT set to 5.05D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.00229 0.00243 0.00328 0.00413 0.00571

Eigenvalues --- 0.00846 0.00863 0.00924 0.01004 0.01045

Eigenvalues --- 0.01061 0.01160 0.01175 0.01254 0.01255

Eigenvalues --- 0.01350 0.01489 0.01492 0.01581 0.01690

Eigenvalues --- 0.01707 0.01944 0.02117 0.02160 0.02295

Eigenvalues --- 0.02335 0.02787 0.02790 0.02821 0.02828

Eigenvalues --- 0.02934 0.03177 0.03357 0.03775 0.04047

Eigenvalues --- 0.04159 0.04196 0.04208 0.04215 0.04217

Eigenvalues --- 0.04389 0.04462 0.04627 0.04703 0.06906

Eigenvalues --- 0.07207 0.08183 0.08310 0.08341 0.08384

Eigenvalues --- 0.08512 0.08631 0.08679 0.08812 0.09692

Eigenvalues --- 0.09703 0.09708 0.09728 0.10351 0.10409

Eigenvalues --- 0.10463 0.10485 0.10993 0.11348 0.12501

Eigenvalues --- 0.12603 0.12961 0.14432 0.16566 0.17178

Eigenvalues --- 0.19292 0.19480 0.19697 0.20296 0.20563

Eigenvalues --- 0.20578 0.20825 0.20978 0.21772 0.21798

Eigenvalues --- 0.21890 0.24491 0.25459 0.25889 0.28013

Eigenvalues --- 0.28086 0.29204 0.29526 0.31225 0.32609

Eigenvalues --- 0.33206 0.33376 0.33992 0.35814 0.35992

Eigenvalues --- 0.36060 0.36500 0.36688 0.37200 0.37299

Eigenvalues --- 0.37324 0.37580 0.37640 0.37868 0.38081

Eigenvalues --- 0.38131 0.38733 0.39264 0.39601 0.40087

Eigenvalues --- 0.40087 0.40087 0.40099 0.40912 0.41415

Eigenvalues --- 0.41472 0.42722 0.45301 0.45591 0.45749

Eigenvalues --- 0.46377 0.50784 0.50908 0.52876 0.53365

Eigenvalues --- 1.03263 1.03943 1.04351 1.04423

RFO step: Lambda=-4.73712268D-05 EMin= 2.28715007D-03

Quintic linear search produced a step of 0.05324.

Iteration 1 RMS(Cart)= 0.00757669 RMS(Int)= 0.00001280

Iteration 2 RMS(Cart)= 0.00003248 RMS(Int)= 0.00000449

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000449

ITry= 1 IFail=0 DXMaxC= 3.35D-02 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.68582 0.00063 -0.00260 0.00337 0.00077 2.68659

R2 2.61481 0.00132 0.00215 0.00144 0.00358 2.61839

R3 2.04075 0.00002 0.00002 -0.00005 -0.00003 2.04072

R4 2.58687 0.00026 0.00026 -0.00038 -0.00011 2.58676

R5 2.72430 0.00162 0.00265 0.00276 0.00540 2.72971

R6 2.58687 0.00026 0.00026 -0.00038 -0.00012 2.58676

R7 3.96335 0.00053 0.00085 0.00084 0.00171 3.96506

R8 2.68582 0.00063 -0.00260 0.00337 0.00077 2.68659

R9 2.72430 0.00162 0.00265 0.00276 0.00540 2.72971

R10 2.04075 0.00002 0.00002 -0.00005 -0.00003 2.04072

R11 2.66293 -0.00016 -0.00062 0.00036 -0.00026 2.66267

R12 2.67819 -0.00000 -0.00099 0.00068 -0.00031 2.67788

R13 2.58494 0.00016 0.00015 -0.00024 -0.00008 2.58486

R14 2.74055 0.00005 0.00032 0.00019 0.00050 2.74105

R15 2.58494 0.00016 0.00015 -0.00023 -0.00008 2.58487

R16 3.97694 0.00075 0.00158 0.00248 0.00407 3.98101

R17 2.74055 0.00005 0.00032 0.00019 0.00050 2.74105

R18 2.66293 -0.00016 -0.00062 0.00036 -0.00026 2.66267

R19 2.56864 -0.00015 -0.00031 0.00013 -0.00018 2.56846

R20 2.04041 -0.00000 0.00000 0.00002 0.00002 2.04044

R21 2.04041 -0.00000 0.00000 0.00002 0.00002 2.04044

R22 2.66293 -0.00016 -0.00062 0.00036 -0.00026 2.66267

R23 2.67819 -0.00000 -0.00099 0.00068 -0.00031 2.67788

R24 2.74055 0.00005 0.00032 0.00019 0.00050 2.74105

R25 2.58494 0.00016 0.00015 -0.00024 -0.00008 2.58486

R26 2.56864 -0.00015 -0.00031 0.00013 -0.00018 2.56846

R27 2.04041 -0.00000 0.00000 0.00002 0.00002 2.04044

R28 2.74055 0.00005 0.00032 0.00019 0.00050 2.74105

R29 2.04041 -0.00000 0.00000 0.00002 0.00002 2.04044

R30 2.58494 0.00016 0.00015 -0.00023 -0.00008 2.58486

R31 2.66293 -0.00016 -0.00062 0.00036 -0.00026 2.66267

R32 3.97697 0.00075 0.00158 0.00245 0.00404 3.98101

R33 2.72430 0.00162 0.00265 0.00276 0.00541 2.72971

R34 2.67819 -0.00000 -0.00099 0.00068 -0.00031 2.67788

R35 2.68582 0.00063 -0.00260 0.00337 0.00077 2.68659

R36 2.58687 0.00026 0.00026 -0.00038 -0.00012 2.58676

R37 2.61481 0.00132 0.00215 0.00144 0.00358 2.61839

R38 2.04075 0.00002 0.00002 -0.00005 -0.00003 2.04072

R39 2.68582 0.00063 -0.00260 0.00337 0.00077 2.68659

R40 2.04075 0.00002 0.00002 -0.00005 -0.00003 2.04072

R41 2.58687 0.00026 0.00026 -0.00038 -0.00012 2.58675

R42 2.72430 0.00162 0.00265 0.00276 0.00540 2.72971

R43 3.96338 0.00053 0.00086 0.00081 0.00168 3.96506

R44 2.67819 -0.00000 -0.00099 0.00068 -0.00031 2.67788

R45 2.28268 0.00011 0.00022 -0.00008 0.00014 2.28282

R46 2.28268 0.00011 0.00022 -0.00008 0.00014 2.28282

R47 2.01744 0.00000 0.00002 -0.00001 0.00001 2.01746

R48 2.01744 0.00000 0.00002 -0.00001 0.00001 2.01746

R49 2.28268 0.00011 0.00022 -0.00008 0.00014 2.28282

R50 2.01744 0.00000 0.00002 -0.00001 0.00001 2.01746

R51 2.28268 0.00011 0.00022 -0.00008 0.00014 2.28282

R52 2.01744 0.00000 0.00002 -0.00001 0.00001 2.01746

A1 1.86250 -0.00027 -0.00018 -0.00061 -0.00079 1.86171

A2 2.19801 0.00018 0.00040 0.00067 0.00107 2.19908

A3 2.22267 0.00009 -0.00022 -0.00006 -0.00028 2.22239

A4 1.91592 0.00030 0.00041 0.00033 0.00074 1.91667

A5 2.19040 -0.00012 0.00034 -0.00057 -0.00024 2.19017

A6 2.17680 -0.00018 -0.00074 0.00027 -0.00048 2.17631

A7 1.86793 -0.00007 -0.00045 0.00056 0.00009 1.86802

A8 2.20651 0.00004 0.00023 -0.00003 0.00018 2.20670

A9 2.20650 0.00003 0.00023 -0.00002 0.00020 2.20670

A10 1.91592 0.00030 0.00041 0.00033 0.00074 1.91667

A11 2.17680 -0.00018 -0.00074 0.00026 -0.00049 2.17631

A12 2.19040 -0.00012 0.00034 -0.00057 -0.00023 2.19017

A13 1.86250 -0.00027 -0.00018 -0.00061 -0.00079 1.86171

A14 2.22267 0.00009 -0.00022 -0.00006 -0.00028 2.22239

A15 2.19801 0.00018 0.00040 0.00067 0.00107 2.19908

A16 2.21833 0.00000 0.00057 0.00007 0.00063 2.21896

A17 2.02718 -0.00005 -0.00056 -0.00068 -0.00124 2.02594

A18 2.03763 0.00005 -0.00001 0.00063 0.00063 2.03825

A19 2.18831 0.00000 -0.00013 0.00008 -0.00005 2.18826

A20 2.18576 -0.00015 0.00009 0.00013 0.00021 2.18598

A21 1.90906 0.00014 0.00004 -0.00019 -0.00014 1.90892

A22 1.87381 -0.00027 -0.00014 0.00039 0.00024 1.87405

A23 2.20351 0.00014 0.00007 -0.00031 -0.00024 2.20328

A24 2.20353 0.00014 0.00007 -0.00032 -0.00025 2.20327

A25 1.90906 0.00014 0.00004 -0.00019 -0.00014 1.90891

A26 2.18831 0.00000 -0.00013 0.00008 -0.00005 2.18826

A27 2.18576 -0.00015 0.00009 0.00012 0.00021 2.18597

A28 1.86643 -0.00001 0.00003 -0.00000 0.00002 1.86645

A29 2.18929 -0.00000 -0.00007 -0.00009 -0.00015 2.18914

A30 2.22746 0.00001 0.00004 0.00009 0.00013 2.22759

A31 1.86643 -0.00001 0.00003 -0.00000 0.00002 1.86645

A32 2.18929 -0.00000 -0.00007 -0.00009 -0.00015 2.18914

A33 2.22746 0.00001 0.00004 0.00009 0.00013 2.22759

A34 2.21833 0.00000 0.00057 0.00007 0.00063 2.21896

A35 2.02718 -0.00005 -0.00056 -0.00068 -0.00124 2.02594

A36 2.03763 0.00005 -0.00001 0.00063 0.00062 2.03825

A37 2.18576 -0.00015 0.00009 0.00013 0.00022 2.18598

A38 2.18832 0.00000 -0.00013 0.00008 -0.00006 2.18826

A39 1.90906 0.00014 0.00004 -0.00019 -0.00015 1.90891

A40 1.86643 -0.00001 0.00003 -0.00000 0.00002 1.86645

A41 2.18929 -0.00000 -0.00007 -0.00009 -0.00015 2.18914

A42 2.22746 0.00001 0.00004 0.00009 0.00013 2.22759

A43 1.86643 -0.00001 0.00003 -0.00000 0.00003 1.86645

A44 2.22746 0.00001 0.00004 0.00009 0.00013 2.22759

A45 2.18929 -0.00000 -0.00007 -0.00009 -0.00015 2.18914

A46 1.90906 0.00014 0.00004 -0.00019 -0.00015 1.90891

A47 2.18576 -0.00015 0.00009 0.00013 0.00022 2.18598

A48 2.18831 0.00000 -0.00013 0.00008 -0.00005 2.18826

A49 1.87380 -0.00027 -0.00014 0.00039 0.00024 1.87405

A50 2.20352 0.00014 0.00007 -0.00031 -0.00024 2.20328

A51 2.20353 0.00014 0.00007 -0.00032 -0.00026 2.20327

A52 2.21833 0.00000 0.00057 0.00007 0.00064 2.21897

A53 2.03763 0.00005 -0.00001 0.00063 0.00062 2.03825

A54 2.02718 -0.00005 -0.00056 -0.00069 -0.00125 2.02594

A55 2.19040 -0.00012 0.00034 -0.00057 -0.00023 2.19017

A56 2.17680 -0.00018 -0.00074 0.00026 -0.00049 2.17631

A57 1.91593 0.00030 0.00041 0.00033 0.00074 1.91667

A58 1.86250 -0.00027 -0.00018 -0.00061 -0.00079 1.86171

A59 2.19801 0.00018 0.00040 0.00067 0.00107 2.19908

A60 2.22267 0.00009 -0.00022 -0.00006 -0.00028 2.22239

A61 1.86250 -0.00027 -0.00018 -0.00061 -0.00079 1.86171

A62 2.22267 0.00009 -0.00022 -0.00006 -0.00028 2.22239

A63 2.19801 0.00018 0.00040 0.00067 0.00107 2.19908

A64 1.91592 0.00030 0.00041 0.00033 0.00074 1.91667

A65 2.19040 -0.00012 0.00034 -0.00056 -0.00023 2.19017

A66 2.17680 -0.00018 -0.00074 0.00026 -0.00049 2.17631

A67 1.86793 -0.00007 -0.00045 0.00056 0.00010 1.86803

A68 2.20652 0.00004 0.00023 -0.00003 0.00018 2.20670

A69 2.20650 0.00004 0.00023 -0.00002 0.00020 2.20670

A70 1.56455 0.00001 0.00003 0.00056 0.00057 1.56511

A71 1.56454 0.00001 0.00003 0.00057 0.00058 1.56512

A72 1.56454 0.00001 0.00003 0.00057 0.00058 1.56512

A73 1.56453 0.00001 0.00003 0.00058 0.00060 1.56512

A74 2.21833 0.00000 0.00057 0.00007 0.00063 2.21896

A75 2.03763 0.00005 -0.00001 0.00063 0.00063 2.03825

A76 2.02718 -0.00005 -0.00056 -0.00069 -0.00125 2.02594

A77 3.12906 0.00002 0.00006 0.00114 0.00118 3.13024

A78 3.12906 0.00002 0.00006 0.00114 0.00118 3.13024

A79 3.15359 0.00012 0.00064 0.00159 0.00223 3.15582

A80 3.12956 -0.00012 -0.00064 -0.00156 -0.00220 3.12736

A81 3.13835 -0.00003 -0.00017 -0.00099 -0.00116 3.13719

A82 3.14484 0.00003 0.00017 0.00097 0.00115 3.14599

A83 3.12956 -0.00012 -0.00064 -0.00156 -0.00220 3.12736

A84 3.14484 0.00003 0.00017 0.00097 0.00115 3.14599

A85 3.15359 0.00012 0.00064 0.00159 0.00223 3.15582

A86 3.13835 -0.00003 -0.00017 -0.00099 -0.00116 3.13719

A87 3.29989 -0.00012 -0.00035 -0.00825 -0.00859 3.29130

A88 2.98409 0.00014 0.00039 0.00597 0.00637 2.99046

A89 3.13991 0.00004 0.00011 0.00121 0.00132 3.14123

A90 3.14296 -0.00004 -0.00013 -0.00129 -0.00142 3.14154

A91 3.14197 -0.00002 -0.00013 -0.00062 -0.00075 3.14123

A92 3.14133 0.00002 0.00014 0.00064 0.00077 3.14211

A93 3.14023 0.00004 0.00013 0.00129 0.00142 3.14165

A94 3.14185 -0.00002 -0.00014 -0.00064 -0.00077 3.14108

A95 3.14328 -0.00004 -0.00011 -0.00121 -0.00133 3.14195

A96 3.14121 0.00002 0.00013 0.00062 0.00074 3.14196

D1 -0.00018 0.00002 0.00008 0.00026 0.00034 0.00015

D2 3.13013 0.00004 0.00014 0.00262 0.00276 3.13289

D3 -3.13730 0.00001 0.00004 0.00017 0.00021 -3.13709

D4 -0.00698 0.00002 0.00011 0.00252 0.00263 -0.00435

D5 -0.00000 -0.00000 -0.00000 0.00000 0.00000 -0.00000

D6 -3.13703 -0.00002 -0.00004 -0.00009 -0.00013 -3.13716

D7 3.13703 0.00002 0.00004 0.00010 0.00013 3.13716

D8 0.00000 0.00000 0.00000 0.00000 0.00000 0.00000

D9 0.00030 -0.00003 -0.00013 -0.00042 -0.00054 -0.00025

D10 -3.07286 -0.00003 -0.00010 -0.00822 -0.00832 -3.08119

D11 -3.13013 -0.00005 -0.00020 -0.00274 -0.00294 -3.13307

D12 0.07990 -0.00005 -0.00018 -0.01055 -0.01072 0.06917

D13 -3.11697 -0.00003 -0.00001 0.00321 0.00321 -3.11376

D14 0.01413 0.00003 0.00016 0.00460 0.00476 0.01890

D15 0.01172 -0.00000 0.00008 0.00591 0.00599 0.01771

D16 -3.14037 0.00005 0.00024 0.00730 0.00754 -3.13283

D17 -0.00030 0.00003 0.00013 0.00042 0.00054 0.00025

D18 3.13013 0.00005 0.00020 0.00274 0.00294 3.13307

D19 3.07287 0.00003 0.00010 0.00822 0.00832 3.08119

D20 -0.07990 0.00005 0.00018 0.01055 0.01072 -0.06917

D21 -3.10351 -0.00007 -0.00022 0.00166 0.00144 -3.10207

D22 -0.11942 0.00006 0.00017 0.00764 0.00781 -0.11162

D23 0.11943 -0.00006 -0.00017 -0.00764 -0.00781 0.11162

D24 3.10351 0.00007 0.00022 -0.00166 -0.00144 3.10208

D25 0.00019 -0.00002 -0.00008 -0.00026 -0.00034 -0.00015

D26 3.13730 -0.00001 -0.00004 -0.00017 -0.00021 3.13709

D27 -3.13013 -0.00004 -0.00014 -0.00262 -0.00276 -3.13289

D28 0.00698 -0.00002 -0.00011 -0.00252 -0.00263 0.00435

D29 -0.01172 0.00000 -0.00008 -0.00591 -0.00599 -0.01771

D30 3.14037 -0.00005 -0.00024 -0.00730 -0.00754 3.13282

D31 3.11696 0.00003 0.00001 -0.00321 -0.00321 3.11375

D32 -0.01414 -0.00003 -0.00016 -0.00460 -0.00476 -0.01890

D33 0.01021 -0.00001 -0.00000 -0.00047 -0.00048 0.00973

D34 -3.11943 -0.00004 -0.00014 -0.00243 -0.00257 -3.12201

D35 3.14125 0.00004 0.00016 0.00092 0.00107 -3.14086

D36 0.01161 0.00001 0.00003 -0.00105 -0.00102 0.01059

D37 -3.12936 -0.00004 -0.00016 -0.00240 -0.00256 -3.13192

D38 0.08220 -0.00002 -0.00005 0.00118 0.00113 0.08333

D39 0.00188 -0.00002 -0.00005 -0.00070 -0.00074 0.00114

D40 -3.06974 0.00000 0.00006 0.00288 0.00295 -3.06679

D41 3.13010 0.00004 0.00014 0.00213 0.00227 3.13237

D42 -0.00692 0.00003 0.00011 0.00218 0.00229 -0.00463

D43 -0.00117 0.00001 0.00003 0.00043 0.00046 -0.00071

D44 -3.13818 -0.00000 -0.00000 0.00048 0.00048 -3.13771

D45 -0.00188 0.00002 0.00005 0.00070 0.00074 -0.00114

D46 3.12936 0.00004 0.00016 0.00240 0.00256 3.13192

D47 3.06974 -0.00000 -0.00006 -0.00288 -0.00295 3.06679

D48 -0.08220 0.00002 0.00005 -0.00118 -0.00113 -0.08333

D49 -0.12057 0.00004 0.00011 0.00202 0.00212 -0.11845

D50 -3.10387 -0.00008 -0.00024 -0.00623 -0.00647 -3.11034

D51 3.10387 0.00008 0.00024 0.00623 0.00647 3.11034

D52 0.12057 -0.00004 -0.00011 -0.00202 -0.00212 0.11845

D53 0.00116 -0.00001 -0.00003 -0.00043 -0.00046 0.00071

D54 3.13818 0.00000 0.00000 -0.00048 -0.00047 3.13771

D55 -3.13010 -0.00004 -0.00014 -0.00213 -0.00227 -3.13237

D56 0.00692 -0.00003 -0.00011 -0.00217 -0.00229 0.00463

D57 -0.01021 0.00001 0.00000 0.00048 0.00048 -0.00973

D58 -3.14126 -0.00004 -0.00016 -0.00091 -0.00107 3.14086

D59 3.11943 0.00004 0.00014 0.00244 0.00258 3.12201

D60 -0.01161 -0.00001 -0.00003 0.00105 0.00102 -0.01059

D61 0.00000 0.00000 0.00000 -0.00000 -0.00000 0.00000

D62 3.13689 0.00001 0.00003 -0.00005 -0.00002 3.13687

D63 -3.13688 -0.00001 -0.00003 0.00005 0.00002 -3.13687

D64 0.00000 0.00000 0.00000 -0.00000 -0.00000 -0.00000

D65 3.11943 0.00004 0.00014 0.00244 0.00257 3.12200

D66 -0.01021 0.00001 0.00000 0.00047 0.00048 -0.00973

D67 -0.01161 -0.00001 -0.00003 0.00105 0.00102 -0.01059

D68 -3.14125 -0.00004 -0.00016 -0.00092 -0.00108 3.14086

D69 -3.13010 -0.00004 -0.00014 -0.00213 -0.00227 -3.13237

D70 0.00692 -0.00003 -0.00011 -0.00218 -0.00229 0.00463

D71 0.00117 -0.00001 -0.00003 -0.00043 -0.00046 0.00071

D72 3.13818 0.00000 0.00000 -0.00048 -0.00048 3.13771

D73 3.12936 0.00004 0.00016 0.00240 0.00256 3.13192

D74 -0.08220 0.00002 0.00005 -0.00118 -0.00113 -0.08333

D75 -0.00188 0.00002 0.00005 0.00070 0.00074 -0.00114

D76 3.06974 -0.00000 -0.00006 -0.00288 -0.00295 3.06679

D77 -0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D78 3.13688 0.00001 0.00003 -0.00005 -0.00001 3.13687

D79 -3.13689 -0.00001 -0.00003 0.00005 0.00002 -3.13687

D80 -0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D81 -0.00117 0.00001 0.00003 0.00043 0.00046 -0.00071

D82 3.13010 0.00004 0.00014 0.00213 0.00227 3.13237

D83 -3.13818 -0.00000 -0.00000 0.00048 0.00047 -3.13771

D84 -0.00692 0.00003 0.00011 0.00217 0.00229 -0.00463

D85 0.00188 -0.00002 -0.00005 -0.00070 -0.00074 0.00114

D86 -3.06974 0.00000 0.00006 0.00288 0.00295 -3.06679

D87 -3.12936 -0.00004 -0.00016 -0.00240 -0.00256 -3.13192

D88 0.08220 -0.00002 -0.00005 0.00118 0.00113 0.08333

D89 -3.11943 -0.00004 -0.00014 -0.00244 -0.00258 -3.12201

D90 0.01161 0.00001 0.00003 -0.00105 -0.00102 0.01059

D91 0.01021 -0.00001 -0.00000 -0.00048 -0.00048 0.00973

D92 3.14125 0.00004 0.00016 0.00091 0.00107 -3.14086

D93 0.12057 -0.00004 -0.00011 -0.00202 -0.00212 0.11845

D94 3.10386 0.00008 0.00024 0.00623 0.00647 3.11034

D95 -3.10386 -0.00008 -0.00024 -0.00623 -0.00647 -3.11033

D96 -0.12057 0.00004 0.00011 0.00202 0.00212 -0.11845

D97 3.11696 0.00003 0.00001 -0.00321 -0.00320 3.11376

D98 -0.01172 0.00000 -0.00008 -0.00591 -0.00598 -0.01770

D99 -0.01414 -0.00003 -0.00016 -0.00460 -0.00476 -0.01890

D100 3.14037 -0.00005 -0.00024 -0.00730 -0.00754 3.13283

D101 -3.13013 -0.00004 -0.00014 -0.00261 -0.00276 -3.13289

D102 0.00698 -0.00002 -0.00011 -0.00252 -0.00263 0.00435

D103 0.00018 -0.00002 -0.00008 -0.00026 -0.00034 -0.00015

D104 3.13729 -0.00001 -0.00004 -0.00016 -0.00021 3.13709

D105 3.13013 0.00005 0.00020 0.00274 0.00294 3.13307

D106 -0.07989 0.00005 0.00018 0.01054 0.01072 -0.06917

D107 -0.00030 0.00003 0.00013 0.00041 0.00054 0.00025

D108 3.07287 0.00003 0.00010 0.00821 0.00832 3.08119

D109 0.00000 0.00000 0.00000 -0.00000 -0.00000 0.00000

D110 3.13703 0.00002 0.00004 0.00010 0.00014 3.13716

D111 -3.13703 -0.00002 -0.00004 -0.00010 -0.00014 -3.13716

D112 0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D113 -0.00018 0.00002 0.00008 0.00026 0.00034 0.00015

D114 3.13013 0.00004 0.00014 0.00261 0.00276 3.13289

D115 -3.13729 0.00001 0.00004 0.00016 0.00021 -3.13709

D116 -0.00698 0.00002 0.00011 0.00252 0.00263 -0.00435

D117 0.00030 -0.00003 -0.00013 -0.00041 -0.00054 -0.00025

D118 -3.07287 -0.00003 -0.00010 -0.00821 -0.00831 -3.08119

D119 -3.13013 -0.00005 -0.00020 -0.00274 -0.00294 -3.13307

D120 0.07989 -0.00005 -0.00018 -0.01054 -0.01072 0.06917

D121 -3.11696 -0.00003 -0.00001 0.00321 0.00320 -3.11375

D122 0.01414 0.00003 0.00016 0.00459 0.00476 0.01890

D123 0.01172 -0.00000 0.00008 0.00590 0.00598 0.01771

D124 -3.14036 0.00005 0.00024 0.00729 0.00753 -3.13283

D125 3.10351 0.00007 0.00022 -0.00166 -0.00143 3.10207

D126 0.11942 -0.00006 -0.00017 -0.00763 -0.00780 0.11162

D127 -0.11942 0.00006 0.00017 0.00763 0.00780 -0.11162

D128 -3.10351 -0.00007 -0.00022 0.00166 0.00143 -3.10207

Item Value Threshold Converged?

Maximum Force 0.001620 0.000450 NO

RMS Force 0.000266 0.000300 YES

Maximum Displacement 0.033489 0.001800 NO

RMS Displacement 0.007575 0.001200 NO

Predicted change in Energy=-3.708885D-05

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Jul 30 00:00:33 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -0.692796 -4.267432 -0.057448

2 6 0 -1.100573 -2.905964 -0.021328

3 7 0 0.000001 -2.092307 0.000061

4 6 0 1.100575 -2.905964 -0.021329

5 6 0 0.692798 -4.267432 -0.057448

6 6 0 2.467808 -2.439873 -0.019201

7 6 0 2.910529 -1.102213 -0.015344

8 7 0 2.100610 -0.000001 -0.002072

9 6 0 2.910529 1.102212 -0.015344

10 6 0 4.297935 0.679585 -0.036521

11 6 0 4.297935 -0.679586 -0.036521

12 6 0 -2.467808 -2.439873 -0.019200

13 6 0 -2.910532 -1.102214 -0.015342

14 6 0 -4.297939 -0.679587 -0.036519

15 6 0 -4.297939 0.679585 -0.036518

16 6 0 -2.910532 1.102213 -0.015341

17 7 0 -2.100615 -0.000001 -0.002068

18 6 0 -2.467809 2.439874 -0.019199

19 6 0 -1.100573 2.905968 -0.021325

20 6 0 -0.692796 4.267436 -0.057444

21 6 0 0.692798 4.267436 -0.057445

22 6 0 1.100575 2.905968 -0.021326

23 7 0 0.000001 2.092313 0.000064

24 1 0 -1.347706 -5.125673 -0.084022

25 1 0 1.347709 -5.125673 -0.084023

26 1 0 5.152879 1.338860 -0.053609

27 1 0 5.152879 -1.338861 -0.053609

28 1 0 -5.152883 -1.338862 -0.053609

29 1 0 -5.152883 1.338859 -0.053608

30 1 0 -1.347707 5.125677 -0.084017

31 1 0 1.347709 5.125677 -0.084019

32 30 0 -0.000003 0.000003 0.157420

33 6 0 2.467809 2.439873 -0.019201

34 6 0 3.468111 3.443521 -0.032616

35 6 0 -3.468107 -3.443524 -0.032614

36 6 0 4.308577 4.311148 -0.044331

37 6 0 -4.308569 -4.311156 -0.044328

38 6 0 3.468109 -3.443522 -0.032612

39 6 0 4.308571 -4.311153 -0.044323

40 6 0 -3.468109 3.443523 -0.032615

41 6 0 -4.308574 4.311152 -0.044331

42 1 0 -5.054709 5.074644 -0.055066

43 1 0 5.054714 5.074639 -0.055065

44 1 0 5.054704 -5.074647 -0.055058

45 1 0 -5.054701 -5.074651 -0.055066

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.421683 0.000000

3 N 2.283516 1.368853 0.000000

4 C 2.251905 2.201147 1.368853 0.000000

5 C 1.385594 2.251905 2.283516 1.421683 0.000000

6 C 3.651144 3.598693 2.492237 1.444498 2.547960

7 C 4.796283 4.398009 3.074360 2.555286 3.865063

8 N 5.100701 4.323490 2.964845 3.073282 4.493992

9 C 6.466746 5.670489 4.321615 4.397891 5.809749

10 C 7.027148 6.480762 5.114387 4.804113 6.121309

11 C 6.146582 5.839596 4.524307 3.896165 5.086265

12 C 2.547961 1.444499 2.492239 3.598694 3.651146

13 C 3.865066 2.555289 3.074366 4.398014 4.796287

14 C 5.086269 3.896170 4.524312 5.839600 6.146587

15 C 6.121313 4.804117 5.114392 6.480767 7.027152

16 C 5.809752 4.397894 4.321620 5.670493 6.466749

17 N 4.493995 3.073285 2.964850 4.323495 5.100705

18 C 6.938306 5.517909 5.160535 6.427390 7.414772

19 C 7.185072 5.811932 5.118054 6.214789 7.394265

20 C 8.534869 7.185072 6.397625 7.394265 8.646609

21 C 8.646609 7.394265 6.397625 7.185072 8.534868

22 C 7.394265 6.214790 5.118053 5.811932 7.185072

23 N 6.397627 5.118056 4.184619 5.118055 6.397627

24 H 1.079903 2.234304 3.320346 3.305317 2.213807

25 H 2.213807 3.305317 3.320346 2.234304 1.079903

26 H 8.099533 7.558124 6.190956 5.868623 7.163996

27 H 6.538231 6.446900 5.207947 4.344885 5.335623

28 H 5.335627 4.344890 5.207953 6.446905 6.538235

29 H 7.164000 5.868628 6.190961 7.558128 8.099538

30 H 9.415950 8.035687 7.343206 8.396742 9.612225

31 H 9.612225 8.396742 7.343206 8.035687 9.415950

32 Zn 4.328641 3.112531 2.098219 3.112534 4.328642

33 C 7.414771 6.427389 5.160533 5.517908 6.938304

34 C 8.761995 7.822337 6.532552 6.776527 8.195229

35 C 2.895133 2.427822 3.722181 4.600212 4.241766

36 C 9.930053 9.019210 7.718162 7.898007 9.309461

37 C 3.616061 3.502332 4.846549 5.588732 5.001575

38 C 4.241765 4.600212 3.722180 2.427821 2.895133

39 C 5.001576 5.588732 4.846548 3.502332 3.616061

40 C 8.195231 6.776529 6.532555 7.822339 8.761997

41 C 9.309464 7.898010 7.718165 9.019212 9.930055

42 H 10.310222 8.906539 8.770309 10.078629 10.968511

43 H 10.968508 10.078627 8.770306 8.906536 10.310218

44 H 5.803909 6.526236 5.869192 4.509930 4.435970

45 H 4.435969 4.509930 5.869193 6.526236 5.803908

6 7 8 9 10

6 C 0.000000

7 C 1.409024 0.000000

8 N 2.467408 1.367851 0.000000

9 C 3.569647 2.204426 1.367852 0.000000

10 C 3.616722 2.258351 2.300274 1.450503 0.000000

11 C 2.539345 1.450503 2.300274 2.258351 1.359171

12 C 4.935617 5.542189 5.179161 6.439945 7.450275

13 C 5.542192 5.821060 5.130944 6.224487 7.425446

14 C 6.991011 7.220877 6.434628 7.425447 8.702666

15 C 7.450279 7.425447 6.434629 7.220877 8.595874

16 C 6.439948 6.224487 5.130945 5.821061 7.220877

17 N 5.179166 5.130946 4.201225 5.130947 6.434631

18 C 6.940623 6.439946 5.179163 5.542190 6.991009

19 C 6.427392 5.670493 4.323494 4.398012 5.839598

20 C 7.414774 6.466750 5.100706 4.796287 6.146586

21 C 6.938308 5.809754 4.493998 3.865067 5.086269

22 C 5.517911 4.397896 3.073287 2.555289 3.896168

23 N 5.160537 4.321620 2.964850 3.074363 4.524309

24 H 4.666463 5.858798 6.178197 7.544789 8.097934

25 H 2.910730 4.316868 5.181321 6.421345 6.512074

26 H 4.635688 3.314881 3.333400 2.255128 1.079752

27 H 2.902243 2.255128 3.333399 3.314881 2.192109

28 H 7.699892 8.066974 7.376202 8.424898 9.663973

29 H 8.506171 8.424898 7.376202 8.066975 9.473801

30 H 8.473482 7.544793 6.178202 5.858802 7.186325

31 H 7.648292 6.421350 5.181327 4.316873 5.336087

32 Zn 3.474807 3.117038 2.106659 3.117035 4.355654

33 C 4.879746 3.569649 2.467410 1.409025 2.539346

34 C 5.967839 4.579836 3.705244 2.406849 2.885822

35 C 6.020182 6.794779 6.547472 7.832689 8.792693

36 C 6.997524 5.591052 4.843853 3.500378 3.631587

37 C 7.030051 7.900223 7.724339 9.023345 9.948842

38 C 1.417072 2.406848 3.705243 4.579835 4.205786

39 C 2.625020 3.500379 4.843853 5.591054 4.990755

40 C 8.357610 7.832690 6.547475 6.794782 8.243229

41 C 9.565371 9.023348 7.724342 7.900227 9.341325

42 H 10.632851 10.079690 8.772310 8.900944 10.333869

43 H 7.947405 6.538548 5.872096 4.514342 4.459771

44 H 3.692608 4.514343 5.872096 6.538552 5.803811

45 H 7.970664 8.900939 8.772306 10.079687 10.981046

11 12 13 14 15

11 C 0.000000

12 C 6.991008 0.000000

13 C 7.220877 1.409025 0.000000

14 C 8.595874 2.539348 1.450503 0.000000

15 C 8.702666 3.616725 2.258352 1.359171 0.000000

16 C 7.425447 3.569649 2.204427 2.258352 1.450503

17 N 6.434631 2.467408 1.367850 2.300272 2.300273

18 C 7.450277 4.879747 3.569650 3.616726 2.539349

19 C 6.480766 5.517912 4.397898 4.804121 3.896173

20 C 7.027152 6.938309 5.809756 6.121317 5.086273

21 C 6.121313 7.414776 6.466754 7.027157 6.146590

22 C 4.804117 6.427393 5.670497 6.480770 5.839603

23 N 5.114391 5.160539 4.321625 5.114397 4.524315

24 H 7.186321 2.910730 4.316870 5.336086 6.512077

25 H 5.336082 4.666465 5.858801 7.186326 8.097939

26 H 2.192109 8.506167 8.424898 9.663973 9.473801

27 H 1.079752 7.699889 8.066974 9.473800 9.663973

28 H 9.473800 2.902247 2.255128 1.079752 2.192110

29 H 9.663973 4.635691 3.314882 2.192110 1.079752

30 H 8.097939 7.648293 6.421352 6.512082 5.336090

31 H 6.512079 8.473484 7.544797 8.097943 7.186330

32 Zn 4.355655 3.474802 3.117035 4.355652 4.355651

33 C 3.616723 6.940622 6.439949 7.450280 6.991013

34 C 4.205786 8.357610 7.832693 8.792699 8.243233

35 C 8.243226 1.417072 2.406849 2.885825 4.205789

36 C 4.990752 9.565371 9.023351 9.948850 9.341329

37 C 9.341321 2.625020 3.500379 3.631593 4.990758

38 C 2.885822 6.020183 6.794783 8.243230 8.792697

39 C 3.631591 7.030053 7.900227 9.341325 9.948846

40 C 8.792695 5.967842 4.579838 4.205789 2.885825

41 C 9.948845 6.997527 5.591055 4.990756 3.631591

42 H 10.981050 7.947409 6.538551 5.803810 4.459775

43 H 5.803806 10.632851 10.079694 10.981055 10.333874

44 H 4.459776 7.970666 8.900943 10.333868 10.981050

45 H 10.333864 3.692608 4.514343 4.459778 5.803814

16 17 18 19 20

16 C 0.000000

17 N 1.367851 0.000000

18 C 1.409027 2.467410 0.000000

19 C 2.555293 3.073290 1.444501 0.000000

20 C 3.865070 4.494001 2.547963 1.421683 0.000000

21 C 4.796291 5.100710 3.651149 2.251906 1.385595

22 C 4.398017 4.323499 3.598696 2.201148 2.251906

23 N 3.074368 2.964856 2.492239 1.368852 2.283515

24 H 6.421347 5.181323 7.648289 8.035687 9.415950

25 H 7.544792 6.178201 8.473480 8.396742 9.612225

26 H 8.066974 7.376204 7.699890 6.446902 6.538234

27 H 8.424898 7.376204 8.506169 7.558127 8.099537

28 H 3.314882 3.333398 4.635693 5.868631 7.164005

29 H 2.255128 3.333398 2.902248 4.344892 5.335631

30 H 4.316874 5.181328 2.910733 2.234304 1.079903

31 H 5.858805 6.178206 4.666468 3.305318 2.213808

32 Zn 3.117033 2.106658 3.474799 3.112529 4.328639

33 C 5.542193 5.179168 4.935618 3.598694 3.651147

34 C 6.794785 6.547479 6.020185 4.600214 4.241769

35 C 4.579837 3.705242 5.967843 6.776533 8.195235

36 C 7.900231 7.724347 7.030058 5.588736 5.001582

37 C 5.591056 4.843852 6.997530 7.898015 9.309470

38 C 7.832692 6.547477 8.357610 7.822340 8.761999

39 C 9.023349 7.724344 9.565371 9.019213 9.930058

40 C 2.406850 3.705244 1.417072 2.427822 2.895136

41 C 3.500379 4.843852 2.625020 3.502334 3.616066

42 H 4.514342 5.872095 3.692608 4.509932 4.435975

43 H 8.900949 8.772315 7.970673 6.526242 5.803917

44 H 10.079691 8.772311 10.632851 10.078631 10.968514

45 H 6.538553 5.872095 7.947413 8.906545 10.310228

21 22 23 24 25

21 C 0.000000

22 C 1.421683 0.000000

23 N 2.283514 1.368852 0.000000

24 H 9.612225 8.396742 7.343208 0.000000

25 H 9.415950 8.035686 7.343208 2.695416 0.000000

26 H 5.335626 4.344887 5.207948 9.167809 7.501361

27 H 7.164001 5.868627 6.190960 7.523197 5.368444

28 H 8.099542 7.558132 6.190965 5.368448 7.523201

29 H 6.538239 6.446907 5.207955 7.501365 9.167813

30 H 2.213808 3.305318 3.320344 10.251350 10.599785

31 H 1.079903 2.234304 3.320344 10.599785 10.251350

32 Zn 4.328640 3.112532 2.098219 5.305389 5.305391

33 C 2.547962 1.444499 2.492237 8.473479 7.648288

34 C 2.895136 2.427821 3.722179 9.829844 8.827787

35 C 8.762001 7.822342 6.532559 2.707096 5.101407

36 C 3.616067 3.502333 4.846548 11.002214 9.890495

37 C 9.930060 9.019215 7.718171 3.071110 5.714761

38 C 8.195233 6.776530 6.532557 5.101407 2.707096

39 C 9.309467 7.898013 7.718168 5.714761 3.071111

40 C 4.241769 4.600214 3.722181 8.827790 9.829846

41 C 5.001581 5.588736 4.846549 9.890499 11.002217

42 H 5.803915 6.526241 5.869194 10.853072 12.043183

43 H 4.435977 4.509932 5.869193 12.043180 10.853068

44 H 10.310226 8.906542 8.770312 6.402680 3.707460

45 H 10.968516 10.078633 8.770315 3.707459 6.402679

26 27 28 29 30

26 H 0.000000

27 H 2.677720 0.000000

28 H 10.647954 10.305762 0.000000

29 H 10.305763 10.647954 2.677721 0.000000

30 H 7.523200 9.167813 7.501370 5.368452 0.000000

31 H 5.368448 7.501366 9.167818 7.523205 2.695416

32 Zn 5.328158 5.328160 5.328157 5.328156 5.305387

33 C 2.902244 4.635690 8.506172 7.699894 4.666466

34 C 2.696013 5.070509 9.858659 8.874209 5.101411

35 C 9.858653 8.874202 2.696018 5.070513 8.827794

36 C 3.089892 5.712752 11.020069 9.917350 5.714769

37 C 11.020062 9.917340 3.089901 5.712760 9.890505

38 C 5.070509 2.696014 8.874206 9.858657 9.829847

39 C 5.712756 3.089897 9.917344 11.020066 11.002219

40 C 8.874204 9.858655 5.070513 2.696018 2.707100

41 C 9.917344 11.020065 5.712757 3.089897 3.071117

42 H 10.869726 12.055202 6.414257 3.737075 3.707466

43 H 3.737069 6.414251 12.055207 10.869733 6.402690

44 H 6.414258 3.737076 10.869725 12.055203 12.043186

45 H 12.055199 10.869721 3.737079 6.414262 10.853079

31 32 33 34 35

31 H 0.000000

32 Zn 5.305389 0.000000

33 C 2.910733 3.474803 0.000000

34 C 2.707101 4.890986 1.417072 0.000000

35 C 9.829849 4.890985 8.357610 9.774585 0.000000

36 C 3.071119 6.098405 2.625020 1.208014 10.982345

37 C 11.002221 6.098404 9.565371 10.982345 1.208014

38 C 8.827792 4.890989 5.967840 6.887043 6.936216

39 C 9.890502 6.098408 6.997528 7.800095 7.824938

40 C 5.101411 4.890982 6.020184 6.936220 6.887047

41 C 5.714768 6.098401 7.030056 7.824944 7.800097

42 H 6.402687 7.165695 7.970670 8.677530 8.664698

43 H 3.707469 7.165699 3.692608 2.275601 12.049817

44 H 10.853076 7.165702 7.947410 8.664697 8.677522

45 H 12.043188 7.165698 10.632850 12.049816 2.275601

36 37 38 39 40

36 C 0.000000

37 C 12.190133 0.000000

38 C 7.800092 7.824937 0.000000

39 C 8.622301 8.617140 1.208014 0.000000

40 C 7.824945 7.800100 9.774585 10.982345 0.000000

41 C 8.617152 8.622308 10.982345 12.190133 1.208014

42 H 9.394369 9.415417 12.049817 13.257614 2.275601

43 H 1.067592 13.257614 8.664692 9.415409 8.677532

44 H 9.415411 9.394356 2.275601 1.067592 12.049817

45 H 13.257613 1.067592 8.677521 9.394355 8.664702

41 42 43 44 45

41 C 0.000000

42 H 1.067592 0.000000

43 H 9.394370 10.109423 0.000000

44 H 13.257614 14.325095 10.149286 0.000000

45 H 9.415419 10.149295 14.325095 10.109405 0.000000

Stoichiometry C28H12N4Zn(3)

Framework group C1[X(C28H12N4Zn)]

Deg. of freedom 129

Full point group C1 NOp 1

RotChk: IX=0 Diff= 5.60D-06

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.692791 4.267433 -0.051066

2 6 0 1.100570 2.905966 -0.014946

3 7 0 -0.000004 2.092307 0.006443

4 6 0 -1.100578 2.905963 -0.014946

5 6 0 -0.692803 4.267432 -0.051066

6 6 0 -2.467811 2.439871 -0.012819

7 6 0 -2.910530 1.102211 -0.008962

8 7 0 -2.100610 -0.000001 0.004310

9 6 0 -2.910528 -1.102214 -0.008962

10 6 0 -4.297935 -0.679588 -0.030139

11 6 0 -4.297936 0.679582 -0.030138

12 6 0 2.467806 2.439876 -0.012818

13 6 0 2.910530 1.102217 -0.008960

14 6 0 4.297938 0.679591 -0.030137

15 6 0 4.297939 -0.679580 -0.030136

16 6 0 2.910533 -1.102210 -0.008959

17 7 0 2.100615 0.000003 0.004314

18 6 0 2.467811 -2.439871 -0.012817

19 6 0 1.100576 -2.905967 -0.014943

20 6 0 0.692800 -4.267435 -0.051062

21 6 0 -0.692795 -4.267436 -0.051063

22 6 0 -1.100573 -2.905969 -0.014944

23 7 0 0.000000 -2.092312 0.006446

24 1 0 1.347701 5.125675 -0.077640

25 1 0 -1.347714 5.125672 -0.077641

26 1 0 -5.152879 -1.338864 -0.047227

27 1 0 -5.152881 1.338856 -0.047227

28 1 0 5.152881 1.338867 -0.047227

29 1 0 5.152884 -1.338854 -0.047226

30 1 0 1.347712 -5.125675 -0.077635

31 1 0 -1.347705 -5.125678 -0.077637

32 30 0 0.000003 -0.000003 0.163802

33 6 0 -2.467807 -2.439875 -0.012819

34 6 0 -3.468108 -3.443524 -0.026234

35 6 0 3.468104 3.443528 -0.026232

36 6 0 -4.308574 -4.311152 -0.037949

37 6 0 4.308564 4.311160 -0.037945

38 6 0 -3.468112 3.443519 -0.026230

39 6 0 -4.308576 4.311149 -0.037940

40 6 0 3.468112 -3.443519 -0.026233

41 6 0 4.308578 -4.311147 -0.037949

42 1 0 5.054714 -5.074639 -0.048684

43 1 0 -5.054709 -5.074643 -0.048683

44 1 0 -5.054710 5.074643 -0.048676

45 1 0 5.054696 5.074656 -0.048684

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1465458 0.1453001 0.0730033

Leave Link 202 at Tue Jul 30 00:00:33 2019, MaxMem= 4294967296 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 671 symmetry adapted cartesian basis functions of A symmetry.

There are 636 symmetry adapted basis functions of A symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

111 alpha electrons 109 beta electrons

nuclear repulsion energy 3054.5140301378 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 45 NActive= 45 NUniq= 45 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1301279856 Hartrees.

Nuclear repulsion after empirical dispersion term = 3054.3839021522 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: York/Karplus (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3890

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.21D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 132

GePol: Fraction of low-weight points (<1% of avg) = 3.39%

GePol: Cavity surface area = 415.755 Ang\*\*2

GePol: Cavity volume = 420.373 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = 0.0083158029 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3054.3922179550 Hartrees.

Leave Link 301 at Tue Jul 30 00:00:33 2019, MaxMem= 4294967296 cpu: 1.9

(Enter /home/kira/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16193 LenP2D= 44746.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 6.88D-05 NBF= 636

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 636

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Jul 30 00:00:34 2019, MaxMem= 4294967296 cpu: 14.5

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Tue Jul 30 00:00:34 2019, MaxMem= 4294967296 cpu: 1.3

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "ZnTSPsim3.chk"

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 0.000000 -0.000000 -0.000002 Ang= -0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0582 S= 1.0193

Generating alternative initial guess.

ExpMin= 3.51D-02 ExpMax= 6.29D+03 ExpMxC= 9.49D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Harris En= -1359.39231528045

Leave Link 401 at Tue Jul 30 00:00:38 2019, MaxMem= 4294967296 cpu: 66.7

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1384965 IEndB= 1384965 NGot= 4294967296 MDV= 4294049884

LenX= 4294049884 LenY= 4293598972

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 650000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 45396300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 6.55D-15 for 3870.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.77D-15 for 1952 1804.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.88D-15 for 3870.

Iteration 1 A^-1\*A deviation from orthogonality is 2.60D-14 for 1459 1369.

E= -1359.01115495418

DIIS: error= 6.96D-04 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.01115495418 IErMin= 1 ErrMin= 6.96D-04

ErrMax= 6.96D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.69D-04 BMatP= 7.69D-04

IDIUse=3 WtCom= 9.93D-01 WtEn= 6.96D-03

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.619 Goal= None Shift= 0.000

Gap= 0.679 Goal= None Shift= 0.000

RMSDP=3.66D-05 MaxDP=8.98D-04 OVMax= 3.02D-03

Cycle 2 Pass 1 IDiag 1:

RMSU= 3.65D-05 CP: 1.00D+00

E= -1359.01142660199 Delta-E= -0.000271647812 Rises=F Damp=F

DIIS: error= 6.84D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.01142660199 IErMin= 2 ErrMin= 6.84D-05

ErrMax= 6.84D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.28D-05 BMatP= 7.69D-04

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.348D-01 0.103D+01

Coeff: -0.348D-01 0.103D+01

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=5.56D-06 MaxDP=2.22D-04 DE=-2.72D-04 OVMax= 1.01D-03

Cycle 3 Pass 1 IDiag 1:

RMSU= 5.35D-06 CP: 1.00D+00 1.04D+00

E= -1359.01142728654 Delta-E= -0.000000684553 Rises=F Damp=F

DIIS: error= 1.26D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.01142728654 IErMin= 2 ErrMin= 6.84D-05

ErrMax= 1.26D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.97D-05 BMatP= 1.28D-05

IDIUse=3 WtCom= 4.72D-01 WtEn= 5.28D-01

Coeff-Com: -0.322D-01 0.599D+00 0.433D+00

Coeff-En: 0.000D+00 0.445D+00 0.555D+00

Coeff: -0.152D-01 0.517D+00 0.498D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=3.58D-06 MaxDP=2.34D-04 DE=-6.85D-07 OVMax= 9.88D-04

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.54D-06 CP: 1.00D+00 1.05D+00 5.36D-01

E= -1359.01143089072 Delta-E= -0.000003604174 Rises=F Damp=F

DIIS: error= 6.06D-05 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.01143089072 IErMin= 4 ErrMin= 6.06D-05

ErrMax= 6.06D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.64D-06 BMatP= 1.28D-05

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.955D-02 0.129D+00 0.310D+00 0.571D+00

Coeff: -0.955D-02 0.129D+00 0.310D+00 0.571D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=1.29D-06 MaxDP=9.81D-05 DE=-3.60D-06 OVMax= 3.07D-04

Cycle 5 Pass 1 IDiag 1:

RMSU= 8.63D-07 CP: 1.00D+00 1.05D+00 6.53D-01 7.20D-01

E= -1359.01143163887 Delta-E= -0.000000748150 Rises=F Damp=F

DIIS: error= 1.13D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.01143163887 IErMin= 5 ErrMin= 1.13D-05

ErrMax= 1.13D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.14D-07 BMatP= 3.64D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.222D-02 0.130D-01 0.136D+00 0.328D+00 0.526D+00

Coeff: -0.222D-02 0.130D-01 0.136D+00 0.328D+00 0.526D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=4.08D-07 MaxDP=2.07D-05 DE=-7.48D-07 OVMax= 1.22D-04

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.08D-07 CP: 1.00D+00 1.05D+00 6.72D-01 7.62D-01 7.43D-01

E= -1359.01143168975 Delta-E= -0.000000050886 Rises=F Damp=F

DIIS: error= 4.08D-06 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.01143168975 IErMin= 6 ErrMin= 4.08D-06

ErrMax= 4.08D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.68D-08 BMatP= 2.14D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.565D-03-0.189D-01 0.143D-01 0.662D-01 0.289D+00 0.649D+00

Coeff: 0.565D-03-0.189D-01 0.143D-01 0.662D-01 0.289D+00 0.649D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=1.64D-07 MaxDP=6.09D-06 DE=-5.09D-08 OVMax= 5.00D-05

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.22D-07 CP: 1.00D+00 1.05D+00 6.81D-01 7.85D-01 8.01D-01

CP: 7.95D-01

E= -1359.01143169769 Delta-E= -0.000000007931 Rises=F Damp=F

DIIS: error= 1.68D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.01143169769 IErMin= 7 ErrMin= 1.68D-06

ErrMax= 1.68D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.87D-09 BMatP= 2.68D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.501D-03-0.108D-01-0.620D-02-0.708D-03 0.917D-01 0.307D+00

Coeff-Com: 0.619D+00

Coeff: 0.501D-03-0.108D-01-0.620D-02-0.708D-03 0.917D-01 0.307D+00

Coeff: 0.619D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=6.67D-08 MaxDP=2.37D-06 DE=-7.93D-09 OVMax= 2.07D-05

Cycle 8 Pass 1 IDiag 1:

RMSU= 6.04D-08 CP: 1.00D+00 1.05D+00 6.83D-01 7.89D-01 8.17D-01

CP: 8.51D-01 9.74D-01

E= -1359.01143169895 Delta-E= -0.000000001265 Rises=F Damp=F

DIIS: error= 8.22D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -1359.01143169895 IErMin= 8 ErrMin= 8.22D-07

ErrMax= 8.22D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.36D-10 BMatP= 2.87D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.634D-04 0.573D-03-0.596D-02-0.179D-01-0.329D-01-0.530D-01

Coeff-Com: 0.256D+00 0.853D+00

Coeff: 0.634D-04 0.573D-03-0.596D-02-0.179D-01-0.329D-01-0.530D-01

Coeff: 0.256D+00 0.853D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=4.44D-08 MaxDP=2.38D-06 DE=-1.27D-09 OVMax= 2.18D-05

Cycle 9 Pass 1 IDiag 1:

RMSU= 2.33D-08 CP: 1.00D+00 1.05D+00 6.84D-01 7.93D-01 8.24D-01

CP: 8.99D-01 1.23D+00 1.11D+00

E= -1359.01143169939 Delta-E= -0.000000000441 Rises=F Damp=F

DIIS: error= 5.61D-07 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -1359.01143169939 IErMin= 9 ErrMin= 5.61D-07

ErrMax= 5.61D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.34D-10 BMatP= 6.36D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.110D-03 0.373D-02-0.181D-02-0.118D-01-0.493D-01-0.132D+00

Coeff-Com: -0.137D-01 0.571D+00 0.634D+00

Coeff: -0.110D-03 0.373D-02-0.181D-02-0.118D-01-0.493D-01-0.132D+00

Coeff: -0.137D-01 0.571D+00 0.634D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=2.44D-08 MaxDP=1.39D-06 DE=-4.41D-10 OVMax= 8.27D-06

Cycle 10 Pass 1 IDiag 1:

RMSU= 1.36D-08 CP: 1.00D+00 1.05D+00 6.84D-01 7.94D-01 8.35D-01

CP: 9.12D-01 1.35D+00 1.29D+00 9.52D-01

E= -1359.01143169951 Delta-E= -0.000000000119 Rises=F Damp=F

DIIS: error= 2.83D-07 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -1359.01143169951 IErMin=10 ErrMin= 2.83D-07

ErrMax= 2.83D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.85D-11 BMatP= 3.34D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.695D-04 0.190D-02 0.213D-03-0.307D-02-0.200D-01-0.610D-01

Coeff-Com: -0.581D-01 0.158D+00 0.364D+00 0.618D+00

Coeff: -0.695D-04 0.190D-02 0.213D-03-0.307D-02-0.200D-01-0.610D-01

Coeff: -0.581D-01 0.158D+00 0.364D+00 0.618D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=9.01D-09 MaxDP=5.52D-07 DE=-1.19D-10 OVMax= 3.94D-06

Error on total polarization charges = 0.06201

SCF Done: E(UB3LYP) = -1359.01143170 A.U. after 10 cycles

NFock= 10 Conv=0.90D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0585 S= 1.0194

<L.S>= 0.000000000000E+00

KE= 1.403719875520D+03 PE=-9.351187632429D+03 EE= 3.534064107255D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.22

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0585, after 2.0019

Leave Link 502 at Tue Jul 30 00:02:56 2019, MaxMem= 4294967296 cpu: 2173.8

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 109 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 109 NVA= 525 NVB= 527

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13959654D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.39723383D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13962006D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.49626218D-01

Leave Link 801 at Tue Jul 30 00:02:56 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16193 LenP2D= 44746.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Tue Jul 30 00:02:59 2019, MaxMem= 4294967296 cpu: 42.0

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Tue Jul 30 00:02:59 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 256

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Tue Jul 30 00:08:50 2019, MaxMem= 4294967296 cpu: 5603.8

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 650000000 NMat= 138 IRICut= 345 DoRegI=T DoRafI=T ISym2E= 2.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 138 NMatS0= 138 NMatT0= 0 NMatD0= 138 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 138 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

135 vectors produced by pass 0 Test12= 1.16D-13 1.00D-09 XBig12= 7.02D+03 5.70D+01.

AX will form 135 AO Fock derivatives at one time.

135 vectors produced by pass 1 Test12= 1.16D-13 1.00D-09 XBig12= 4.50D+02 3.30D+00.

135 vectors produced by pass 2 Test12= 1.16D-13 1.00D-09 XBig12= 1.60D+01 9.75D-01.

135 vectors produced by pass 3 Test12= 1.16D-13 1.00D-09 XBig12= 2.16D-01 9.06D-02.

135 vectors produced by pass 4 Test12= 1.16D-13 1.00D-09 XBig12= 1.24D-03 4.66D-03.

135 vectors produced by pass 5 Test12= 1.16D-13 1.00D-09 XBig12= 8.38D-06 2.22D-04.

133 vectors produced by pass 6 Test12= 1.16D-13 1.00D-09 XBig12= 4.68D-08 2.96D-05.

65 vectors produced by pass 7 Test12= 1.16D-13 1.00D-09 XBig12= 1.97D-10 1.19D-06.

3 vectors produced by pass 8 Test12= 1.16D-13 1.00D-09 XBig12= 1.05D-12 8.01D-08.

2 vectors produced by pass 9 Test12= 1.16D-13 1.00D-09 XBig12= 2.38D-14 1.31D-08.

InvSVY: IOpt=1 It= 1 EMax= 4.26D-14

Solved reduced A of dimension 1013 with 138 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1006.26 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Tue Jul 30 01:06:13 2019, MaxMem= 4294967296 cpu: 55080.9

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16193 LenP2D= 44746.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 256

Leave Link 701 at Tue Jul 30 01:06:48 2019, MaxMem= 4294967296 cpu: 561.8

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Tue Jul 30 01:06:48 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 100127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Tue Jul 30 01:14:02 2019, MaxMem= 4294967296 cpu: 6951.3

(Enter /home/kira/g09/l716.exe)

Dipole = 5.68437775D-06 1.43692777D-05 3.30911723D-01

Polarizability= 1.22311956D+03-5.60669183D-04 1.61430706D+03

1.16992796D-05 2.62524131D-04 1.81347787D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000040521 -0.000072532 -0.000001724

2 6 0.000047750 0.000050347 0.000000660

3 7 -0.000000589 -0.000011784 0.000034364

4 6 -0.000048281 0.000049808 0.000000656

5 6 0.000040428 -0.000072575 -0.000001723

6 6 0.000062322 0.000018979 -0.000000357

7 6 0.000004294 0.000010947 0.000001338

8 7 0.000008973 0.000000756 0.000019979

9 6 0.000003615 -0.000010389 0.000001299

10 6 0.000000228 0.000004326 -0.000000047

11 6 0.000000255 -0.000004260 -0.000000028

12 6 -0.000061994 0.000019262 -0.000000352

13 6 -0.000004423 0.000010353 0.000001328

14 6 -0.000000166 -0.000003865 -0.000000026

15 6 -0.000000161 0.000003941 -0.000000045

16 6 -0.000003766 -0.000009802 0.000001286

17 7 -0.000007384 0.000000652 0.000019887

18 6 -0.000061840 -0.000019668 -0.000000361

19 6 0.000047289 -0.000050116 0.000000634

20 6 -0.000040272 0.000072392 -0.000001723

21 6 0.000040186 0.000072462 -0.000001718

22 6 -0.000047846 -0.000049566 0.000000625

23 7 -0.000000684 0.000010104 0.000034312

24 1 -0.000001681 0.000000421 0.000000345

25 1 0.000001680 0.000000414 0.000000343

26 1 -0.000000078 -0.000000246 0.000000001

27 1 -0.000000077 0.000000222 0.000000014

28 1 0.000000034 0.000000261 0.000000016

29 1 0.000000055 -0.000000259 0.000000004

30 1 -0.000001661 -0.000000370 0.000000332

31 1 0.000001671 -0.000000378 0.000000331

32 30 0.000000342 -0.000000189 -0.000108714

33 6 0.000062208 -0.000019413 -0.000000366

34 6 0.000005295 0.000007852 -0.000001021

35 6 -0.000005276 -0.000007957 -0.000001044

36 6 0.000004834 0.000002493 -0.000000152

37 6 -0.000004870 -0.000002422 -0.000000322

38 6 0.000005359 -0.000008103 -0.000001044

39 6 0.000004817 -0.000002382 -0.000000326

40 6 -0.000005186 0.000007740 -0.000001017

41 6 -0.000004881 0.000002511 -0.000000150

42 1 0.000000756 -0.000000385 0.000001072

43 1 -0.000000763 -0.000000384 0.000001069

44 1 -0.000000746 0.000000404 0.000001181

45 1 0.000000754 0.000000399 0.000001186

-------------------------------------------------------------------

Cartesian Forces: Max 0.000108714 RMS 0.000024345

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Tue Jul 30 01:14:02 2019, MaxMem= 4294967296 cpu: 0.8

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000071259 RMS 0.000014320

Search for a local minimum.

Step number 3 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .14320D-04 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -3.79D-05 DEPred=-3.71D-05 R= 1.02D+00

TightC=F SS= 1.41D+00 RLast= 4.77D-02 DXNew= 8.4853D-01 1.4321D-01

Trust test= 1.02D+00 RLast= 4.77D-02 DXMaxT set to 5.05D-01

ITU= 1 1 0

Eigenvalues --- 0.00217 0.00224 0.00271 0.00321 0.00453

Eigenvalues --- 0.00800 0.00813 0.00838 0.00870 0.01042

Eigenvalues --- 0.01055 0.01156 0.01157 0.01158 0.01251

Eigenvalues --- 0.01252 0.01491 0.01493 0.01549 0.01675

Eigenvalues --- 0.01692 0.01872 0.02109 0.02150 0.02178

Eigenvalues --- 0.02321 0.02761 0.02765 0.02802 0.02812

Eigenvalues --- 0.02915 0.03175 0.03352 0.03754 0.04048

Eigenvalues --- 0.04158 0.04191 0.04202 0.04209 0.04211

Eigenvalues --- 0.04380 0.04456 0.04621 0.04698 0.06899

Eigenvalues --- 0.07810 0.08166 0.08235 0.08248 0.08328

Eigenvalues --- 0.08389 0.08486 0.08542 0.08719 0.09674

Eigenvalues --- 0.09685 0.09706 0.09726 0.10354 0.10439

Eigenvalues --- 0.10443 0.10484 0.11103 0.11375 0.12459

Eigenvalues --- 0.12588 0.12954 0.14384 0.16556 0.17162

Eigenvalues --- 0.19270 0.19511 0.19690 0.20230 0.20521

Eigenvalues --- 0.20538 0.20720 0.20939 0.21703 0.21737

Eigenvalues --- 0.21823 0.24518 0.25439 0.25894 0.27851

Eigenvalues --- 0.27908 0.29200 0.29317 0.31176 0.32568

Eigenvalues --- 0.33197 0.33374 0.33962 0.35792 0.35959

Eigenvalues --- 0.36005 0.36491 0.36673 0.37202 0.37295

Eigenvalues --- 0.37318 0.37572 0.37615 0.37862 0.38066

Eigenvalues --- 0.38085 0.38645 0.39148 0.39518 0.40079

Eigenvalues --- 0.40079 0.40079 0.40088 0.40782 0.41104

Eigenvalues --- 0.41192 0.42512 0.45284 0.45566 0.45713

Eigenvalues --- 0.46349 0.50568 0.50699 0.52886 0.53382

Eigenvalues --- 1.03266 1.03901 1.04308 1.04379

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-1.49677031D-07.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 3.79D-05 SmlDif= 1.00D-05

RMS Error= 0.5931822890D-04 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.07075 -0.07075

Iteration 1 RMS(Cart)= 0.00068422 RMS(Int)= 0.00000106

Iteration 2 RMS(Cart)= 0.00000118 RMS(Int)= 0.00000089

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000089

ITry= 1 IFail=0 DXMaxC= 7.98D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.68659 0.00007 0.00005 0.00016 0.00021 2.68680

R2 2.61839 0.00005 0.00025 -0.00012 0.00013 2.61852

R3 2.04072 0.00000 -0.00000 0.00000 0.00000 2.04072

R4 2.58676 0.00001 -0.00001 -0.00008 -0.00008 2.58668

R5 2.72971 0.00007 0.00038 -0.00011 0.00028 2.72998

R6 2.58676 0.00001 -0.00001 -0.00007 -0.00008 2.58667

R7 3.96506 0.00003 0.00012 -0.00001 0.00011 3.96517

R8 2.68659 0.00007 0.00005 0.00016 0.00021 2.68680

R9 2.72971 0.00007 0.00038 -0.00010 0.00028 2.72998

R10 2.04072 0.00000 -0.00000 0.00000 0.00000 2.04072

R11 2.66267 0.00000 -0.00002 0.00011 0.00009 2.66276

R12 2.67788 0.00001 -0.00002 0.00004 0.00002 2.67790

R13 2.58486 0.00001 -0.00001 -0.00003 -0.00003 2.58483

R14 2.74105 -0.00000 0.00004 -0.00001 0.00002 2.74108

R15 2.58487 0.00001 -0.00001 -0.00003 -0.00003 2.58483

R16 3.98101 0.00003 0.00029 -0.00023 0.00006 3.98107

R17 2.74105 -0.00000 0.00004 -0.00001 0.00002 2.74108

R18 2.66267 0.00000 -0.00002 0.00011 0.00009 2.66276

R19 2.56846 -0.00000 -0.00001 0.00004 0.00003 2.56849

R20 2.04044 -0.00000 0.00000 -0.00000 0.00000 2.04044

R21 2.04044 -0.00000 0.00000 -0.00000 0.00000 2.04044

R22 2.66267 0.00000 -0.00002 0.00011 0.00009 2.66276

R23 2.67788 0.00001 -0.00002 0.00004 0.00002 2.67790

R24 2.74105 -0.00000 0.00004 -0.00001 0.00002 2.74108

R25 2.58486 0.00001 -0.00001 -0.00003 -0.00003 2.58483

R26 2.56846 -0.00000 -0.00001 0.00004 0.00003 2.56849

R27 2.04044 -0.00000 0.00000 -0.00000 0.00000 2.04044

R28 2.74105 -0.00000 0.00004 -0.00001 0.00002 2.74108

R29 2.04044 -0.00000 0.00000 -0.00000 0.00000 2.04044

R30 2.58486 0.00001 -0.00001 -0.00003 -0.00003 2.58483

R31 2.66267 0.00000 -0.00002 0.00011 0.00009 2.66276

R32 3.98101 0.00003 0.00029 -0.00022 0.00007 3.98107

R33 2.72971 0.00006 0.00038 -0.00011 0.00027 2.72998

R34 2.67788 0.00001 -0.00002 0.00004 0.00002 2.67790

R35 2.68659 0.00007 0.00005 0.00016 0.00021 2.68680

R36 2.58676 0.00001 -0.00001 -0.00007 -0.00008 2.58667

R37 2.61839 0.00005 0.00025 -0.00012 0.00013 2.61852

R38 2.04072 0.00000 -0.00000 0.00000 0.00000 2.04072

R39 2.68659 0.00007 0.00005 0.00016 0.00021 2.68680

R40 2.04072 0.00000 -0.00000 0.00000 0.00000 2.04072

R41 2.58675 0.00001 -0.00001 -0.00007 -0.00008 2.58667

R42 2.72971 0.00007 0.00038 -0.00010 0.00028 2.72998

R43 3.96506 0.00003 0.00012 -0.00001 0.00011 3.96517

R44 2.67788 0.00001 -0.00002 0.00004 0.00002 2.67790

R45 2.28282 0.00000 0.00001 -0.00000 0.00001 2.28282

R46 2.28282 0.00000 0.00001 -0.00000 0.00001 2.28282

R47 2.01746 -0.00000 0.00000 -0.00000 -0.00000 2.01746

R48 2.01746 -0.00000 0.00000 -0.00000 -0.00000 2.01746

R49 2.28282 0.00000 0.00001 -0.00000 0.00001 2.28282

R50 2.01746 -0.00000 0.00000 -0.00000 -0.00000 2.01746

R51 2.28282 0.00000 0.00001 -0.00000 0.00001 2.28282

R52 2.01746 -0.00000 0.00000 -0.00000 -0.00000 2.01746

A1 1.86171 -0.00001 -0.00006 0.00004 -0.00002 1.86169

A2 2.19908 0.00000 0.00008 -0.00008 -0.00000 2.19908

A3 2.22239 0.00001 -0.00002 0.00004 0.00002 2.22241

A4 1.91667 0.00001 0.00005 -0.00012 -0.00007 1.91660

A5 2.19017 -0.00001 -0.00002 0.00007 0.00005 2.19022

A6 2.17631 -0.00000 -0.00003 0.00005 0.00002 2.17633

A7 1.86802 0.00000 0.00001 0.00018 0.00018 1.86820

A8 2.20670 -0.00000 0.00001 -0.00005 -0.00004 2.20666

A9 2.20670 -0.00000 0.00001 -0.00006 -0.00005 2.20666

A10 1.91667 0.00001 0.00005 -0.00013 -0.00007 1.91660

A11 2.17631 -0.00000 -0.00003 0.00005 0.00002 2.17633

A12 2.19017 -0.00001 -0.00002 0.00007 0.00005 2.19022

A13 1.86171 -0.00001 -0.00006 0.00004 -0.00002 1.86169

A14 2.22239 0.00001 -0.00002 0.00004 0.00002 2.22241

A15 2.19908 0.00000 0.00008 -0.00008 -0.00000 2.19908

A16 2.21896 -0.00001 0.00004 0.00006 0.00010 2.21907

A17 2.02594 0.00000 -0.00009 0.00001 -0.00008 2.02586

A18 2.03825 0.00000 0.00004 -0.00007 -0.00003 2.03823

A19 2.18826 0.00000 -0.00000 0.00003 0.00003 2.18829

A20 2.18598 -0.00001 0.00002 0.00004 0.00006 2.18603

A21 1.90892 0.00001 -0.00001 -0.00007 -0.00008 1.90883

A22 1.87405 -0.00001 0.00002 0.00011 0.00012 1.87417

A23 2.20328 0.00001 -0.00002 -0.00001 -0.00002 2.20325

A24 2.20327 0.00001 -0.00002 -0.00000 -0.00002 2.20325

A25 1.90891 0.00001 -0.00001 -0.00007 -0.00008 1.90883

A26 2.18826 0.00000 -0.00000 0.00003 0.00003 2.18829

A27 2.18597 -0.00001 0.00001 0.00004 0.00006 2.18603

A28 1.86645 -0.00000 0.00000 0.00002 0.00002 1.86647

A29 2.18914 0.00000 -0.00001 0.00002 0.00001 2.18914

A30 2.22759 0.00000 0.00001 -0.00003 -0.00002 2.22756

A31 1.86645 -0.00000 0.00000 0.00002 0.00002 1.86647

A32 2.18914 0.00000 -0.00001 0.00002 0.00001 2.18914

A33 2.22759 0.00000 0.00001 -0.00003 -0.00002 2.22756

A34 2.21896 -0.00001 0.00004 0.00006 0.00010 2.21907

A35 2.02594 0.00000 -0.00009 0.00001 -0.00008 2.02586

A36 2.03825 0.00000 0.00004 -0.00007 -0.00002 2.03823

A37 2.18598 -0.00001 0.00002 0.00004 0.00005 2.18603

A38 2.18826 0.00000 -0.00000 0.00003 0.00003 2.18829

A39 1.90891 0.00001 -0.00001 -0.00007 -0.00008 1.90883

A40 1.86645 -0.00000 0.00000 0.00002 0.00002 1.86647

A41 2.18914 0.00000 -0.00001 0.00002 0.00001 2.18914

A42 2.22759 0.00000 0.00001 -0.00003 -0.00002 2.22756

A43 1.86645 -0.00000 0.00000 0.00002 0.00002 1.86647

A44 2.22759 0.00000 0.00001 -0.00003 -0.00002 2.22756

A45 2.18914 0.00000 -0.00001 0.00002 0.00001 2.18914

A46 1.90891 0.00001 -0.00001 -0.00007 -0.00008 1.90883

A47 2.18598 -0.00001 0.00002 0.00004 0.00005 2.18603

A48 2.18826 0.00000 -0.00000 0.00003 0.00003 2.18829

A49 1.87405 -0.00001 0.00002 0.00011 0.00012 1.87417

A50 2.20328 0.00001 -0.00002 -0.00000 -0.00002 2.20325

A51 2.20327 0.00001 -0.00002 0.00000 -0.00002 2.20325

A52 2.21897 -0.00001 0.00005 0.00006 0.00010 2.21907

A53 2.03825 0.00000 0.00004 -0.00007 -0.00002 2.03823

A54 2.02594 0.00000 -0.00009 0.00001 -0.00008 2.02586

A55 2.19017 -0.00001 -0.00002 0.00007 0.00005 2.19022

A56 2.17631 -0.00000 -0.00003 0.00005 0.00002 2.17633

A57 1.91667 0.00001 0.00005 -0.00012 -0.00007 1.91660

A58 1.86171 -0.00001 -0.00006 0.00004 -0.00002 1.86169

A59 2.19908 0.00000 0.00008 -0.00008 -0.00000 2.19908

A60 2.22239 0.00001 -0.00002 0.00004 0.00002 2.22241

A61 1.86171 -0.00001 -0.00006 0.00004 -0.00002 1.86169

A62 2.22239 0.00001 -0.00002 0.00004 0.00002 2.22241

A63 2.19908 0.00000 0.00008 -0.00008 -0.00000 2.19908

A64 1.91667 0.00001 0.00005 -0.00012 -0.00007 1.91660

A65 2.19017 -0.00001 -0.00002 0.00007 0.00005 2.19022

A66 2.17631 -0.00000 -0.00003 0.00005 0.00002 2.17633

A67 1.86803 0.00000 0.00001 0.00017 0.00018 1.86821

A68 2.20670 -0.00000 0.00001 -0.00005 -0.00004 2.20666

A69 2.20670 -0.00000 0.00001 -0.00006 -0.00004 2.20666

A70 1.56511 0.00000 0.00004 0.00021 0.00024 1.56536

A71 1.56512 0.00000 0.00004 0.00020 0.00024 1.56536

A72 1.56512 0.00000 0.00004 0.00020 0.00024 1.56536

A73 1.56512 0.00000 0.00004 0.00020 0.00024 1.56536

A74 2.21896 -0.00001 0.00004 0.00006 0.00010 2.21907

A75 2.03825 0.00000 0.00004 -0.00007 -0.00002 2.03823

A76 2.02594 0.00000 -0.00009 0.00001 -0.00008 2.02586

A77 3.13024 0.00000 0.00008 0.00040 0.00048 3.13072

A78 3.13024 0.00000 0.00008 0.00040 0.00048 3.13072

A79 3.15582 -0.00000 0.00016 -0.00019 -0.00003 3.15579

A80 3.12736 0.00000 -0.00016 0.00019 0.00003 3.12739

A81 3.13719 0.00000 -0.00008 0.00011 0.00003 3.13721

A82 3.14599 -0.00000 0.00008 -0.00011 -0.00003 3.14596

A83 3.12736 0.00000 -0.00016 0.00019 0.00003 3.12739

A84 3.14599 -0.00000 0.00008 -0.00011 -0.00003 3.14596

A85 3.15582 -0.00000 0.00016 -0.00019 -0.00003 3.15579

A86 3.13719 0.00000 -0.00008 0.00011 0.00003 3.13721

A87 3.29130 -0.00003 -0.00061 -0.00285 -0.00346 3.28784

A88 2.99046 0.00002 0.00045 0.00250 0.00295 2.99341

A89 3.14123 0.00000 0.00009 -0.00003 0.00007 3.14130

A90 3.14154 -0.00000 -0.00010 0.00004 -0.00006 3.14148

A91 3.14123 0.00000 -0.00005 0.00009 0.00004 3.14127

A92 3.14211 -0.00000 0.00005 -0.00010 -0.00005 3.14206

A93 3.14165 0.00000 0.00010 -0.00004 0.00006 3.14171

A94 3.14108 0.00000 -0.00005 0.00010 0.00005 3.14113

A95 3.14195 -0.00000 -0.00009 0.00003 -0.00007 3.14189

A96 3.14196 -0.00000 0.00005 -0.00009 -0.00004 3.14192

D1 0.00015 0.00000 0.00002 -0.00008 -0.00006 0.00010

D2 3.13289 0.00000 0.00020 -0.00013 0.00007 3.13296

D3 -3.13709 -0.00000 0.00001 -0.00014 -0.00012 -3.13721

D4 -0.00435 0.00000 0.00019 -0.00018 0.00000 -0.00434

D5 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13716 -0.00000 -0.00001 -0.00006 -0.00007 -3.13723

D7 3.13716 0.00000 0.00001 0.00006 0.00007 3.13723

D8 0.00000 0.00000 0.00000 -0.00000 -0.00000 -0.00000

D9 -0.00025 -0.00000 -0.00004 0.00013 0.00009 -0.00016

D10 -3.08119 -0.00001 -0.00059 -0.00096 -0.00155 -3.08274

D11 -3.13307 -0.00000 -0.00021 0.00017 -0.00003 -3.13310

D12 0.06917 -0.00001 -0.00076 -0.00091 -0.00167 0.06750

D13 -3.11376 -0.00001 0.00023 -0.00058 -0.00036 -3.11411

D14 0.01890 -0.00000 0.00034 -0.00046 -0.00012 0.01878

D15 0.01771 -0.00001 0.00042 -0.00064 -0.00022 0.01749

D16 -3.13283 0.00000 0.00053 -0.00051 0.00002 -3.13280

D17 0.00025 0.00000 0.00004 -0.00013 -0.00009 0.00016

D18 3.13307 0.00000 0.00021 -0.00017 0.00003 3.13310

D19 3.08119 0.00001 0.00059 0.00096 0.00155 3.08274

D20 -0.06917 0.00001 0.00076 0.00091 0.00167 -0.06750

D21 -3.10207 -0.00001 0.00010 -0.00060 -0.00050 -3.10257

D22 -0.11162 0.00001 0.00055 0.00190 0.00245 -0.10916

D23 0.11162 -0.00001 -0.00055 -0.00190 -0.00245 0.10916

D24 3.10208 0.00001 -0.00010 0.00060 0.00050 3.10257

D25 -0.00015 -0.00000 -0.00002 0.00008 0.00006 -0.00010

D26 3.13709 0.00000 -0.00001 0.00014 0.00012 3.13721

D27 -3.13289 -0.00000 -0.00020 0.00013 -0.00007 -3.13296

D28 0.00435 -0.00000 -0.00019 0.00018 -0.00000 0.00434

D29 -0.01771 0.00001 -0.00042 0.00064 0.00022 -0.01749

D30 3.13282 -0.00000 -0.00053 0.00051 -0.00002 3.13280

D31 3.11375 0.00001 -0.00023 0.00059 0.00036 3.11411

D32 -0.01890 0.00000 -0.00034 0.00046 0.00012 -0.01878

D33 0.00973 -0.00001 -0.00003 -0.00019 -0.00023 0.00951

D34 -3.12201 -0.00001 -0.00018 -0.00040 -0.00058 -3.12258

D35 -3.14086 0.00000 0.00008 -0.00006 0.00001 -3.14084

D36 0.01059 -0.00000 -0.00007 -0.00027 -0.00034 0.01025

D37 -3.13192 -0.00001 -0.00018 -0.00027 -0.00045 -3.13237

D38 0.08333 -0.00001 0.00008 -0.00173 -0.00164 0.08169

D39 0.00114 -0.00001 -0.00005 -0.00009 -0.00014 0.00100

D40 -3.06679 -0.00001 0.00021 -0.00155 -0.00134 -3.06813

D41 3.13237 0.00001 0.00016 0.00023 0.00039 3.13276

D42 -0.00463 0.00000 0.00016 0.00010 0.00026 -0.00437

D43 -0.00071 0.00000 0.00003 0.00005 0.00009 -0.00062

D44 -3.13771 0.00000 0.00003 -0.00008 -0.00005 -3.13775

D45 -0.00114 0.00001 0.00005 0.00009 0.00014 -0.00100

D46 3.13192 0.00001 0.00018 0.00027 0.00045 3.13237

D47 3.06679 0.00001 -0.00021 0.00155 0.00134 3.06813

D48 -0.08333 0.00001 -0.00008 0.00172 0.00164 -0.08169

D49 -0.11845 0.00001 0.00015 0.00229 0.00244 -0.11601

D50 -3.11034 -0.00001 -0.00046 -0.00056 -0.00102 -3.11136

D51 3.11034 0.00001 0.00046 0.00056 0.00102 3.11136

D52 0.11845 -0.00001 -0.00015 -0.00229 -0.00244 0.11601

D53 0.00071 -0.00000 -0.00003 -0.00005 -0.00009 0.00062

D54 3.13771 -0.00000 -0.00003 0.00008 0.00005 3.13775

D55 -3.13237 -0.00001 -0.00016 -0.00023 -0.00039 -3.13276

D56 0.00463 -0.00000 -0.00016 -0.00010 -0.00026 0.00437

D57 -0.00973 0.00001 0.00003 0.00019 0.00022 -0.00951

D58 3.14086 -0.00000 -0.00008 0.00006 -0.00002 3.14084

D59 3.12201 0.00001 0.00018 0.00039 0.00058 3.12258

D60 -0.01059 0.00000 0.00007 0.00026 0.00034 -0.01025

D61 0.00000 0.00000 -0.00000 -0.00000 -0.00000 0.00000

D62 3.13687 0.00000 -0.00000 0.00014 0.00014 3.13701

D63 -3.13687 -0.00000 0.00000 -0.00014 -0.00014 -3.13701

D64 -0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D65 3.12200 0.00001 0.00018 0.00040 0.00058 3.12258

D66 -0.00973 0.00001 0.00003 0.00019 0.00023 -0.00951

D67 -0.01059 0.00000 0.00007 0.00027 0.00034 -0.01025

D68 3.14086 -0.00000 -0.00008 0.00006 -0.00001 3.14084

D69 -3.13237 -0.00001 -0.00016 -0.00023 -0.00039 -3.13276

D70 0.00463 -0.00000 -0.00016 -0.00010 -0.00026 0.00437

D71 0.00071 -0.00000 -0.00003 -0.00006 -0.00009 0.00062

D72 3.13771 -0.00000 -0.00003 0.00008 0.00005 3.13775

D73 3.13192 0.00001 0.00018 0.00027 0.00045 3.13237

D74 -0.08333 0.00001 -0.00008 0.00172 0.00164 -0.08169

D75 -0.00114 0.00001 0.00005 0.00009 0.00014 -0.00100

D76 3.06679 0.00001 -0.00021 0.00155 0.00134 3.06813

D77 -0.00000 -0.00000 0.00000 -0.00000 -0.00000 -0.00000

D78 3.13687 0.00000 -0.00000 0.00014 0.00014 3.13701

D79 -3.13687 -0.00000 0.00000 -0.00014 -0.00014 -3.13701

D80 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D81 -0.00071 0.00000 0.00003 0.00006 0.00009 -0.00062

D82 3.13237 0.00001 0.00016 0.00023 0.00039 3.13276

D83 -3.13771 0.00000 0.00003 -0.00008 -0.00005 -3.13775

D84 -0.00463 0.00000 0.00016 0.00010 0.00026 -0.00437

D85 0.00114 -0.00001 -0.00005 -0.00009 -0.00014 0.00100

D86 -3.06679 -0.00001 0.00021 -0.00155 -0.00134 -3.06813

D87 -3.13192 -0.00001 -0.00018 -0.00027 -0.00045 -3.13237

D88 0.08333 -0.00001 0.00008 -0.00172 -0.00164 0.08169

D89 -3.12201 -0.00001 -0.00018 -0.00040 -0.00058 -3.12258

D90 0.01059 -0.00000 -0.00007 -0.00026 -0.00034 0.01025

D91 0.00973 -0.00001 -0.00003 -0.00019 -0.00022 0.00951

D92 -3.14086 0.00000 0.00008 -0.00006 0.00002 -3.14084

D93 0.11845 -0.00001 -0.00015 -0.00229 -0.00244 0.11601

D94 3.11034 0.00001 0.00046 0.00056 0.00102 3.11135

D95 -3.11033 -0.00001 -0.00046 -0.00056 -0.00102 -3.11135

D96 -0.11845 0.00001 0.00015 0.00229 0.00244 -0.11601

D97 3.11376 0.00001 -0.00023 0.00058 0.00036 3.11411

D98 -0.01770 0.00001 -0.00042 0.00064 0.00021 -0.01749

D99 -0.01890 0.00000 -0.00034 0.00045 0.00012 -0.01878

D100 3.13283 -0.00000 -0.00053 0.00051 -0.00003 3.13280

D101 -3.13289 -0.00000 -0.00020 0.00012 -0.00007 -3.13296

D102 0.00435 -0.00000 -0.00019 0.00018 -0.00000 0.00434

D103 -0.00015 -0.00000 -0.00002 0.00008 0.00006 -0.00010

D104 3.13709 0.00000 -0.00001 0.00014 0.00012 3.13721

D105 3.13307 0.00000 0.00021 -0.00017 0.00004 3.13310

D106 -0.06917 0.00001 0.00076 0.00091 0.00167 -0.06750

D107 0.00025 0.00000 0.00004 -0.00013 -0.00009 0.00016

D108 3.08119 0.00001 0.00059 0.00096 0.00155 3.08274

D109 0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D110 3.13716 0.00000 0.00001 0.00006 0.00007 3.13723

D111 -3.13716 -0.00000 -0.00001 -0.00006 -0.00007 -3.13723

D112 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D113 0.00015 0.00000 0.00002 -0.00008 -0.00006 0.00010

D114 3.13289 0.00000 0.00020 -0.00013 0.00007 3.13296

D115 -3.13709 -0.00000 0.00001 -0.00014 -0.00012 -3.13721

D116 -0.00435 0.00000 0.00019 -0.00018 0.00000 -0.00434

D117 -0.00025 -0.00000 -0.00004 0.00013 0.00009 -0.00016

D118 -3.08119 -0.00001 -0.00059 -0.00096 -0.00155 -3.08274

D119 -3.13307 -0.00000 -0.00021 0.00017 -0.00004 -3.13310

D120 0.06917 -0.00001 -0.00076 -0.00091 -0.00167 0.06750

D121 -3.11375 -0.00001 0.00023 -0.00058 -0.00036 -3.11411

D122 0.01890 -0.00000 0.00034 -0.00045 -0.00012 0.01878

D123 0.01771 -0.00001 0.00042 -0.00064 -0.00021 0.01749

D124 -3.13283 0.00000 0.00053 -0.00051 0.00002 -3.13280

D125 3.10207 0.00001 -0.00010 0.00060 0.00050 3.10257

D126 0.11162 -0.00001 -0.00055 -0.00190 -0.00245 0.10916

D127 -0.11162 0.00001 0.00055 0.00190 0.00245 -0.10916

D128 -3.10207 -0.00001 0.00010 -0.00060 -0.00050 -3.10257

Item Value Threshold Converged?

Maximum Force 0.000071 0.000450 YES

RMS Force 0.000014 0.000300 YES

Maximum Displacement 0.007982 0.001800 NO

RMS Displacement 0.000684 0.001200 YES

Predicted change in Energy=-4.836161D-07

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Jul 30 01:14:02 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -0.692831 -4.267782 -0.056982

2 6 0 -1.100613 -2.906180 -0.021560

3 7 0 0.000000 -2.092640 -0.000521

4 6 0 1.100613 -2.906180 -0.021560

5 6 0 0.692832 -4.267782 -0.056982

6 6 0 2.467952 -2.439941 -0.019588

7 6 0 2.910728 -1.102249 -0.016013

8 7 0 2.100882 -0.000000 -0.003168

9 6 0 2.910728 1.102249 -0.016012

10 6 0 4.298148 0.679592 -0.036652

11 6 0 4.298147 -0.679593 -0.036652

12 6 0 -2.467952 -2.439941 -0.019588

13 6 0 -2.910729 -1.102249 -0.016011

14 6 0 -4.298148 -0.679593 -0.036651

15 6 0 -4.298148 0.679592 -0.036651

16 6 0 -2.910729 1.102249 -0.016011

17 7 0 -2.100883 -0.000000 -0.003166

18 6 0 -2.467952 2.439941 -0.019588

19 6 0 -1.100613 2.906181 -0.021559

20 6 0 -0.692831 4.267783 -0.056981

21 6 0 0.692832 4.267782 -0.056981

22 6 0 1.100613 2.906181 -0.021559

23 7 0 0.000000 2.092641 -0.000520

24 1 0 -1.347760 -5.126024 -0.083057

25 1 0 1.347761 -5.126024 -0.083057

26 1 0 5.153116 1.338847 -0.053292

27 1 0 5.153116 -1.338847 -0.053293

28 1 0 -5.153117 -1.338847 -0.053292

29 1 0 -5.153117 1.338847 -0.053292

30 1 0 -1.347760 5.126025 -0.083057

31 1 0 1.347761 5.126025 -0.083057

32 30 0 -0.000001 0.000001 0.153196

33 6 0 2.467952 2.439941 -0.019588

34 6 0 3.468256 3.443606 -0.032549

35 6 0 -3.468255 -3.443606 -0.032549

36 6 0 4.308746 4.311220 -0.043799

37 6 0 -4.308745 -4.311221 -0.043799

38 6 0 3.468256 -3.443606 -0.032550

39 6 0 4.308745 -4.311220 -0.043799

40 6 0 -3.468256 3.443606 -0.032550

41 6 0 -4.308746 4.311220 -0.043800

42 1 0 -5.054881 5.074718 -0.054087

43 1 0 5.054882 5.074717 -0.054084

44 1 0 5.054880 -5.074718 -0.054085

45 1 0 -5.054879 -5.074719 -0.054085

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.421794 0.000000

3 N 2.283516 1.368810 0.000000

4 C 2.252034 2.201226 1.368809 0.000000

5 C 1.385663 2.252034 2.283516 1.421794 0.000000

6 C 3.651431 3.598894 2.492342 1.444645 2.548225

7 C 4.796657 4.398301 3.074646 2.555526 3.865402

8 N 5.101145 4.323862 2.965274 3.073558 4.494381

9 C 6.467190 5.670837 4.322024 4.398187 5.810161

10 C 7.027574 6.481096 5.114748 4.804396 6.121701

11 C 6.146982 5.839908 4.524608 3.896427 5.086631

12 C 2.548225 1.444645 2.492342 3.598894 3.651432

13 C 3.865403 2.555527 3.074648 4.398302 4.796658

14 C 5.086632 3.896429 4.524609 5.839910 6.146983

15 C 6.121702 4.804397 5.114749 6.481097 7.027575

16 C 5.810161 4.398188 4.322025 5.670838 6.467191

17 N 4.494381 3.073558 2.965275 4.323864 5.101146

18 C 6.938731 5.518209 5.160954 6.427727 7.415220

19 C 7.185630 5.812362 5.118594 6.215219 7.394825

20 C 8.535564 7.185630 6.398295 7.394825 8.647307

21 C 8.647307 7.394825 6.398295 7.185630 8.535564

22 C 7.394825 6.215219 5.118594 5.812362 7.185630

23 N 6.398295 5.118595 4.185281 5.118595 6.398295

24 H 1.079904 2.234406 3.320345 3.305453 2.213883

25 H 2.213883 3.305453 3.320345 2.234406 1.079904

26 H 8.099963 7.558465 6.191324 5.868905 7.164386

27 H 6.538637 6.447221 5.208224 4.345149 5.335991

28 H 5.335993 4.345151 5.208225 6.447223 6.538638

29 H 7.164387 5.868906 6.191325 7.558466 8.099964

30 H 9.416646 8.036242 7.343868 8.397300 9.612924

31 H 9.612924 8.397300 7.343868 8.036242 9.416646

32 Zn 4.328759 3.112519 2.098279 3.112520 4.328759

33 C 7.415220 6.427727 5.160953 5.518209 6.938731

34 C 8.762462 7.822689 6.532981 6.776846 8.195674

35 C 2.895313 2.427896 3.722222 4.600381 4.241993

36 C 9.930519 9.019563 7.718587 7.898321 9.309902

37 C 3.616198 3.502391 4.846572 5.588898 5.001783

38 C 4.241993 4.600381 3.722221 2.427896 2.895313

39 C 5.001783 5.588899 4.846572 3.502391 3.616198

40 C 8.195674 6.776846 6.532981 7.822689 8.762462

41 C 9.309903 7.898322 7.718588 9.019564 9.930520

42 H 10.310663 8.906853 8.770730 10.078983 10.968979

43 H 10.968979 10.078983 8.770730 8.906852 10.310663

44 H 5.804080 6.526385 5.869197 4.509972 4.436059

45 H 4.436059 4.509971 5.869197 6.526385 5.804080

6 7 8 9 10

6 C 0.000000

7 C 1.409071 0.000000

8 N 2.467452 1.367834 0.000000

9 C 3.569758 2.204498 1.367834 0.000000

10 C 3.616821 2.258388 2.300205 1.450516 0.000000

11 C 2.539435 1.450516 2.300205 2.258388 1.359185

12 C 4.935904 5.542529 5.179558 6.440289 7.450630

13 C 5.542530 5.821457 5.131409 6.224884 7.425853

14 C 6.991368 7.221285 6.435103 7.425853 8.703085

15 C 7.450630 7.425853 6.435103 7.221286 8.596296

16 C 6.440289 6.224883 5.131409 5.821457 7.221286

17 N 5.179559 5.131409 4.201764 5.131410 6.435104

18 C 6.940922 6.440289 5.179558 5.542530 6.991368

19 C 6.427727 5.670838 4.323863 4.398302 5.839909

20 C 7.415221 6.467191 5.101147 4.796658 6.146983

21 C 6.938732 5.810162 4.494382 3.865404 5.086632

22 C 5.518210 4.398188 3.073559 2.555527 3.896428

23 N 5.160954 4.322025 2.965275 3.074647 4.524609

24 H 4.666769 5.859179 6.178643 7.545237 8.098371

25 H 2.910997 4.317190 5.181669 6.421740 6.512459

26 H 4.635783 3.314913 3.333341 2.255144 1.079752

27 H 2.902353 2.255144 3.333341 3.314913 2.192110

28 H 7.700275 8.067402 7.376688 8.425316 9.664408

29 H 8.506531 8.425316 7.376688 8.067402 9.474244

30 H 8.473932 7.545238 6.178645 5.859180 7.186737

31 H 7.648706 6.421741 5.181671 4.317191 5.336450

32 Zn 3.474760 3.117039 2.106693 3.117038 4.355682

33 C 4.879882 3.569758 2.467453 1.409072 2.539436

34 C 5.967989 4.579946 3.705266 2.406878 2.885915

35 C 6.020471 6.795120 6.547868 7.833039 8.793054

36 C 6.997662 5.591142 4.843855 3.500389 3.631650

37 C 7.030355 7.900573 7.724739 9.023703 9.949214

38 C 1.417081 2.406878 3.705266 4.579946 4.205889

39 C 2.625032 3.500389 4.843855 5.591142 4.990829

40 C 8.357922 7.833040 6.547868 6.795120 8.243592

41 C 9.565688 9.023704 7.724739 7.900574 9.341701

42 H 10.633170 10.080044 8.772701 8.901286 10.334243

43 H 7.947545 6.538636 5.872092 4.514349 4.459829

44 H 3.692620 4.514349 5.872092 6.538636 5.803881

45 H 7.970962 8.901284 8.772701 10.080044 10.981417

11 12 13 14 15

11 C 0.000000

12 C 6.991367 0.000000

13 C 7.221285 1.409072 0.000000

14 C 8.596296 2.539436 1.450516 0.000000

15 C 8.703085 3.616822 2.258389 1.359185 0.000000

16 C 7.425852 3.569758 2.204498 2.258389 1.450516

17 N 6.435104 2.467452 1.367834 2.300205 2.300205

18 C 7.450630 4.879882 3.569759 3.616822 2.539436

19 C 6.481097 5.518210 4.398189 4.804398 3.896429

20 C 7.027575 6.938732 5.810163 6.121703 5.086633

21 C 6.121702 7.415221 6.467192 7.027576 6.146984

22 C 4.804397 6.427728 5.670839 6.481098 5.839910

23 N 5.114749 5.160955 4.322026 5.114750 4.524610

24 H 7.186736 2.910997 4.317190 5.336450 6.512460

25 H 5.336449 4.666769 5.859180 7.186737 8.098372

26 H 2.192110 8.506530 8.425316 9.664408 9.474244

27 H 1.079752 7.700274 8.067402 9.474244 9.664408

28 H 9.474244 2.902354 2.255144 1.079752 2.192110

29 H 9.664408 4.635783 3.314913 2.192110 1.079752

30 H 8.098372 7.648706 6.421742 6.512461 5.336451

31 H 6.512460 8.473933 7.545239 8.098373 7.186738

32 Zn 4.355682 3.474759 3.117038 4.355682 4.355681

33 C 3.616821 6.940922 6.440290 7.450631 6.991369

34 C 4.205889 8.357922 7.833040 8.793055 8.243593

35 C 8.243591 1.417081 2.406878 2.885916 4.205890

36 C 4.990829 9.565688 9.023705 9.949216 9.341702

37 C 9.341701 2.625032 3.500389 3.631651 4.990830

38 C 2.885915 6.020471 6.795121 8.243592 8.793055

39 C 3.631650 7.030356 7.900575 9.341702 9.949215

40 C 8.793054 5.967990 4.579947 4.205890 2.885916

41 C 9.949215 6.997663 5.591143 4.990830 3.631651

42 H 10.981418 7.947546 6.538636 5.803881 4.459829

43 H 5.803881 10.633170 10.080045 10.981419 10.334244

44 H 4.459829 7.970963 8.901286 10.334243 10.981418

45 H 10.334242 3.692620 4.514349 4.459830 5.803882

16 17 18 19 20

16 C 0.000000

17 N 1.367834 0.000000

18 C 1.409072 2.467453 0.000000

19 C 2.555528 3.073560 1.444646 0.000000

20 C 3.865404 4.494383 2.548226 1.421794 0.000000

21 C 4.796659 5.101148 3.651432 2.252034 1.385664

22 C 4.398303 4.323865 3.598895 2.201226 2.252034

23 N 3.074648 2.965277 2.492342 1.368809 2.283515

24 H 6.421741 5.181669 7.648705 8.036242 9.416646

25 H 7.545238 6.178644 8.473932 8.397300 9.612924

26 H 8.067402 7.376688 7.700275 6.447222 6.538638

27 H 8.425316 7.376688 8.506530 7.558466 8.099964

28 H 3.314913 3.333340 4.635784 5.868907 7.164388

29 H 2.255144 3.333341 2.902354 4.345151 5.335993

30 H 4.317191 5.181671 2.910998 2.234406 1.079904

31 H 5.859181 6.178646 4.666770 3.305453 2.213883

32 Zn 3.117037 2.106693 3.474758 3.112518 4.328758

33 C 5.542530 5.179559 4.935904 3.598894 3.651432

34 C 6.795121 6.547869 6.020472 4.600381 4.241994

35 C 4.579947 3.705266 5.967990 6.776847 8.195675

36 C 7.900575 7.724741 7.030356 5.588899 5.001784

37 C 5.591143 4.843855 6.997664 7.898323 9.309904

38 C 7.833040 6.547869 8.357922 7.822690 8.762463

39 C 9.023704 7.724740 9.565688 9.019564 9.930520

40 C 2.406878 3.705266 1.417081 2.427896 2.895314

41 C 3.500389 4.843855 2.625032 3.502392 3.616199

42 H 4.514349 5.872092 3.692620 4.509972 4.436060

43 H 8.901287 8.772703 7.970964 6.526386 5.804081

44 H 10.080045 8.772702 10.633170 10.078983 10.968980

45 H 6.538636 5.872092 7.947547 8.906854 10.310665

21 22 23 24 25

21 C 0.000000

22 C 1.421794 0.000000

23 N 2.283515 1.368809 0.000000

24 H 9.612924 8.397300 7.343869 0.000000

25 H 9.416646 8.036242 7.343869 2.695521 0.000000

26 H 5.335992 4.345150 5.208224 9.168252 7.501745

27 H 7.164387 5.868906 6.191325 7.523629 5.368829

28 H 8.099965 7.558467 6.191326 5.368830 7.523630

29 H 6.538639 6.447223 5.208225 7.501746 9.168253

30 H 2.213883 3.305453 3.320345 10.252050 10.600488

31 H 1.079904 2.234406 3.320344 10.600488 10.252049

32 Zn 4.328759 3.112519 2.098279 5.305507 5.305508

33 C 2.548226 1.444645 2.492342 8.473932 7.648705

34 C 2.895314 2.427896 3.722221 9.830316 8.828228

35 C 8.762463 7.822690 6.532983 2.707320 5.101675

36 C 3.616199 3.502391 4.846571 11.002690 9.890933

37 C 9.930521 9.019565 7.718589 3.071298 5.715024

38 C 8.195675 6.776846 6.532982 5.101675 2.707320

39 C 9.309903 7.898322 7.718588 5.715024 3.071299

40 C 4.241994 4.600381 3.722221 8.828228 9.830317

41 C 5.001784 5.588899 4.846572 9.890933 11.002690

42 H 5.804081 6.526386 5.869197 10.853512 12.043662

43 H 4.436060 4.509972 5.869197 12.043661 10.853511

44 H 10.310664 8.906853 8.770731 6.402912 3.707588

45 H 10.968980 10.078984 8.770732 3.707587 6.402911

26 27 28 29 30

26 H 0.000000

27 H 2.677694 0.000000

28 H 10.648404 10.306234 0.000000

29 H 10.306234 10.648404 2.677694 0.000000

30 H 7.523630 9.168253 7.501747 5.368831 0.000000

31 H 5.368830 7.501746 9.168254 7.523631 2.695521

32 Zn 5.328205 5.328205 5.328204 5.328204 5.305506

33 C 2.902353 4.635783 8.506531 7.700275 4.666770

34 C 2.696144 5.070606 9.859025 8.874600 5.101676

35 C 9.859023 8.874598 2.696146 5.070607 8.828230

36 C 3.089992 5.712820 11.020445 9.917759 5.715025

37 C 11.020444 9.917757 3.089994 5.712821 9.890935

38 C 5.070605 2.696144 8.874599 9.859024 9.830317

39 C 5.712820 3.089993 9.917759 11.020445 11.002691

40 C 8.874599 9.859024 5.070606 2.696145 2.707321

41 C 9.917758 11.020444 5.712821 3.089993 3.071300

42 H 10.870140 12.055581 6.414317 3.737162 3.707589

43 H 3.737162 6.414317 12.055582 10.870141 6.402913

44 H 6.414317 3.737162 10.870140 12.055581 12.043663

45 H 12.055580 10.870138 3.737163 6.414319 10.853514

31 32 33 34 35

31 H 0.000000

32 Zn 5.305507 0.000000

33 C 2.910997 3.474759 0.000000

34 C 2.707321 4.890984 1.417081 0.000000

35 C 9.830318 4.890984 8.357922 9.774911 0.000000

36 C 3.071300 6.098419 2.625032 1.208017 10.982678

37 C 11.002691 6.098419 9.565688 10.982678 1.208017

38 C 8.828229 4.890985 5.967989 6.887211 6.936511

39 C 9.890934 6.098420 6.997663 7.800248 7.825255

40 C 5.101676 4.890983 6.020471 6.936512 6.887212

41 C 5.715025 6.098418 7.030356 7.825257 7.800249

42 H 6.402913 7.165719 7.970963 8.677837 8.664854

43 H 3.707589 7.165720 3.692620 2.275603 12.050152

44 H 10.853513 7.165721 7.947546 8.664853 8.677836

45 H 12.043663 7.165720 10.633170 12.050152 2.275603

36 37 38 39 40

36 C 0.000000

37 C 12.190473 0.000000

38 C 7.800248 7.825255 0.000000

39 C 8.622440 8.617490 1.208017 0.000000

40 C 7.825257 7.800250 9.774911 10.982678 0.000000

41 C 8.617492 8.622442 10.982678 12.190473 1.208017

42 H 9.394709 9.415555 12.050152 13.257958 2.275603

43 H 1.067591 13.257958 8.664853 9.415553 8.677837

44 H 9.415554 9.394706 2.275603 1.067591 12.050152

45 H 13.257958 1.067591 8.677835 9.394706 8.664855

41 42 43 44 45

41 C 0.000000

42 H 1.067591 0.000000

43 H 9.394709 10.109762 0.000000

44 H 13.257958 14.325443 10.149435 0.000000

45 H 9.415556 10.149437 14.325443 10.109760 0.000000

Stoichiometry C28H12N4Zn(3)

Framework group C1[X(C28H12N4Zn)]

Deg. of freedom 129

Full point group C1 NOp 1

RotChk: IX=0 Diff= 1.68D-06

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.692832 4.267781 -0.049970

2 6 0 1.100613 2.906180 -0.014548

3 7 0 0.000000 2.092640 0.006491

4 6 0 -1.100612 2.906181 -0.014548

5 6 0 -0.692831 4.267782 -0.049970

6 6 0 -2.467951 2.439942 -0.012576

7 6 0 -2.910728 1.102250 -0.009001

8 7 0 -2.100882 0.000001 0.003844

9 6 0 -2.910729 -1.102248 -0.009000

10 6 0 -4.298148 -0.679591 -0.029640

11 6 0 -4.298147 0.679594 -0.029640

12 6 0 2.467952 2.439940 -0.012576

13 6 0 2.910729 1.102249 -0.008999

14 6 0 4.298149 0.679592 -0.029639

15 6 0 4.298148 -0.679593 -0.029639

16 6 0 2.910729 -1.102250 -0.008999

17 7 0 2.100883 -0.000000 0.003846

18 6 0 2.467951 -2.439941 -0.012576

19 6 0 1.100612 -2.906181 -0.014547

20 6 0 0.692830 -4.267783 -0.049969

21 6 0 -0.692833 -4.267782 -0.049969

22 6 0 -1.100614 -2.906181 -0.014547

23 7 0 -0.000001 -2.092641 0.006492

24 1 0 1.347761 5.126024 -0.076045

25 1 0 -1.347759 5.126025 -0.076045

26 1 0 -5.153117 -1.338845 -0.046280

27 1 0 -5.153116 1.338849 -0.046281

28 1 0 5.153118 1.338846 -0.046280

29 1 0 5.153117 -1.338848 -0.046280

30 1 0 1.347759 -5.126026 -0.076045

31 1 0 -1.347762 -5.126025 -0.076045

32 30 0 0.000001 -0.000001 0.160208

33 6 0 -2.467953 -2.439940 -0.012576

34 6 0 -3.468257 -3.443605 -0.025537

35 6 0 3.468256 3.443606 -0.025537

36 6 0 -4.308748 -4.311219 -0.036787

37 6 0 4.308746 4.311220 -0.036787

38 6 0 -3.468255 3.443607 -0.025538

39 6 0 -4.308744 4.311222 -0.036787

40 6 0 3.468255 -3.443607 -0.025538

41 6 0 4.308744 -4.311221 -0.036788

42 1 0 5.054879 -5.074719 -0.047075

43 1 0 -5.054883 -5.074716 -0.047072

44 1 0 -5.054879 5.074719 -0.047073

45 1 0 5.054880 5.074718 -0.047073

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1465354 0.1452891 0.0729961

Leave Link 202 at Tue Jul 30 01:14:02 2019, MaxMem= 4294967296 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 671 symmetry adapted cartesian basis functions of A symmetry.

There are 636 symmetry adapted basis functions of A symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

111 alpha electrons 109 beta electrons

nuclear repulsion energy 3054.3969147723 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 45 NActive= 45 NUniq= 45 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1301245592 Hartrees.

Nuclear repulsion after empirical dispersion term = 3054.2667902131 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: York/Karplus (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3890

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.14D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 128

GePol: Fraction of low-weight points (<1% of avg) = 3.29%

GePol: Cavity surface area = 415.768 Ang\*\*2

GePol: Cavity volume = 420.392 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = 0.0083168201 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3054.2751070332 Hartrees.

Leave Link 301 at Tue Jul 30 01:14:03 2019, MaxMem= 4294967296 cpu: 1.8

(Enter /home/kira/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16189 LenP2D= 44742.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 6.88D-05 NBF= 636

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 636

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Jul 30 01:14:04 2019, MaxMem= 4294967296 cpu: 14.5

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Tue Jul 30 01:14:04 2019, MaxMem= 4294967296 cpu: 1.2

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "ZnTSPsim3.chk"

B after Tr= -0.000000 0.000000 -0.000000

Rot= 1.000000 0.000000 -0.000000 0.000001 Ang= 0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0585 S= 1.0194

Leave Link 401 at Tue Jul 30 01:14:05 2019, MaxMem= 4294967296 cpu: 16.0

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1384965 IEndB= 1384965 NGot= 4294967296 MDV= 4294049884

LenX= 4294049884 LenY= 4293598972

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 650000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 45396300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 8.77D-15 for 3884.

Iteration 1 A\*A^-1 deviation from orthogonality is 3.77D-15 for 3884 830.

Iteration 1 A^-1\*A deviation from unit magnitude is 9.10D-15 for 3884.

Iteration 1 A^-1\*A deviation from orthogonality is 2.15D-14 for 3494 3443.

E= -1359.01142979309

DIIS: error= 5.90D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.01142979309 IErMin= 1 ErrMin= 5.90D-05

ErrMax= 5.90D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.85D-06 BMatP= 6.85D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.619 Goal= None Shift= 0.000

Gap= 0.679 Goal= None Shift= 0.000

RMSDP=6.63D-06 MaxDP=3.22D-04 OVMax= 3.41D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 6.63D-06 CP: 1.00D+00

E= -1359.01143217306 Delta-E= -0.000002379968 Rises=F Damp=F

DIIS: error= 1.33D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.01143217306 IErMin= 2 ErrMin= 1.33D-05

ErrMax= 1.33D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.61D-07 BMatP= 6.85D-06

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.122D-01 0.101D+01

Coeff: -0.122D-01 0.101D+01

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=7.81D-07 MaxDP=2.41D-05 DE=-2.38D-06 OVMax= 9.69D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 7.21D-07 CP: 1.00D+00 1.04D+00

E= -1359.01143216750 Delta-E= 0.000000005563 Rises=F Damp=F

DIIS: error= 1.82D-05 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 2 EnMin= -1359.01143217306 IErMin= 2 ErrMin= 1.33D-05

ErrMax= 1.82D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.94D-07 BMatP= 1.61D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.266D-01 0.603D+00 0.423D+00

Coeff: -0.266D-01 0.603D+00 0.423D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=3.87D-07 MaxDP=2.14D-05 DE= 5.56D-09 OVMax= 7.40D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 2.68D-07 CP: 1.00D+00 1.05D+00 6.14D-01

E= -1359.01143222095 Delta-E= -0.000000053447 Rises=F Damp=F

DIIS: error= 3.86D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.01143222095 IErMin= 4 ErrMin= 3.86D-06

ErrMax= 3.86D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.54D-08 BMatP= 1.61D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.107D-01 0.183D+00 0.217D+00 0.611D+00

Coeff: -0.107D-01 0.183D+00 0.217D+00 0.611D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=1.18D-07 MaxDP=5.95D-06 DE=-5.34D-08 OVMax= 1.95D-05

Cycle 5 Pass 1 IDiag 1:

RMSU= 9.34D-08 CP: 1.00D+00 1.04D+00 6.40D-01 7.45D-01

E= -1359.01143222411 Delta-E= -0.000000003164 Rises=F Damp=F

DIIS: error= 2.21D-06 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.01143222411 IErMin= 5 ErrMin= 2.21D-06

ErrMax= 2.21D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.38D-09 BMatP= 1.54D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.254D-02 0.241D-01 0.664D-01 0.340D+00 0.572D+00

Coeff: -0.254D-02 0.241D-01 0.664D-01 0.340D+00 0.572D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=3.89D-08 MaxDP=1.27D-06 DE=-3.16D-09 OVMax= 4.74D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 3.36D-08 CP: 1.00D+00 1.05D+00 6.35D-01 7.88D-01 8.53D-01

E= -1359.01143222451 Delta-E= -0.000000000398 Rises=F Damp=F

DIIS: error= 3.51D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.01143222451 IErMin= 6 ErrMin= 3.51D-07

ErrMax= 3.51D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.90D-10 BMatP= 2.38D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.264D-03-0.154D-01-0.214D-05 0.732D-01 0.267D+00 0.675D+00

Coeff: 0.264D-03-0.154D-01-0.214D-05 0.732D-01 0.267D+00 0.675D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=1.48D-08 MaxDP=4.99D-07 DE=-3.98D-10 OVMax= 2.80D-06

Cycle 7 Pass 1 IDiag 1:

RMSU= 1.05D-08 CP: 1.00D+00 1.05D+00 6.43D-01 8.09D-01 8.72D-01

CP: 8.03D-01

E= -1359.01143222452 Delta-E= -0.000000000012 Rises=F Damp=F

DIIS: error= 2.30D-07 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -1359.01143222452 IErMin= 7 ErrMin= 2.30D-07

ErrMax= 2.30D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.80D-11 BMatP= 1.90D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.421D-03-0.125D-01-0.670D-02 0.136D-01 0.114D+00 0.433D+00

Coeff-Com: 0.458D+00

Coeff: 0.421D-03-0.125D-01-0.670D-02 0.136D-01 0.114D+00 0.433D+00

Coeff: 0.458D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=5.68D-09 MaxDP=2.87D-07 DE=-1.18D-11 OVMax= 1.34D-06

Error on total polarization charges = 0.06201

SCF Done: E(UB3LYP) = -1359.01143222 A.U. after 7 cycles

NFock= 7 Conv=0.57D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0585 S= 1.0194

<L.S>= 0.000000000000E+00

KE= 1.403716658040D+03 PE=-9.350949213495D+03 EE= 3.533946016198D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.22

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0585, after 2.0019

Leave Link 502 at Tue Jul 30 01:15:43 2019, MaxMem= 4294967296 cpu: 1542.9

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 109 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 109 NVA= 525 NVB= 527

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13972341D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.39729999D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13962961D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.49630624D-01

Leave Link 801 at Tue Jul 30 01:15:43 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16189 LenP2D= 44742.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Tue Jul 30 01:15:46 2019, MaxMem= 4294967296 cpu: 41.6

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Tue Jul 30 01:15:46 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 256

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Tue Jul 30 01:21:37 2019, MaxMem= 4294967296 cpu: 5609.3

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 650000000 NMat= 138 IRICut= 345 DoRegI=T DoRafI=T ISym2E= 2.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 138 NMatS0= 138 NMatT0= 0 NMatD0= 138 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 138 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

135 vectors produced by pass 0 Test12= 1.16D-13 1.00D-09 XBig12= 7.02D+03 5.70D+01.

AX will form 135 AO Fock derivatives at one time.

135 vectors produced by pass 1 Test12= 1.16D-13 1.00D-09 XBig12= 4.50D+02 3.30D+00.

135 vectors produced by pass 2 Test12= 1.16D-13 1.00D-09 XBig12= 1.60D+01 9.75D-01.

135 vectors produced by pass 3 Test12= 1.16D-13 1.00D-09 XBig12= 2.16D-01 9.07D-02.

135 vectors produced by pass 4 Test12= 1.16D-13 1.00D-09 XBig12= 1.24D-03 4.64D-03.

135 vectors produced by pass 5 Test12= 1.16D-13 1.00D-09 XBig12= 8.37D-06 2.22D-04.

133 vectors produced by pass 6 Test12= 1.16D-13 1.00D-09 XBig12= 4.67D-08 2.94D-05.

65 vectors produced by pass 7 Test12= 1.16D-13 1.00D-09 XBig12= 1.97D-10 1.19D-06.

3 vectors produced by pass 8 Test12= 1.16D-13 1.00D-09 XBig12= 1.05D-12 7.98D-08.

2 vectors produced by pass 9 Test12= 1.16D-13 1.00D-09 XBig12= 2.31D-14 1.32D-08.

InvSVY: IOpt=1 It= 1 EMax= 7.11D-14

Solved reduced A of dimension 1013 with 138 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1006.37 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Tue Jul 30 02:18:54 2019, MaxMem= 4294967296 cpu: 54992.6

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16189 LenP2D= 44742.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 256

Leave Link 701 at Tue Jul 30 02:19:29 2019, MaxMem= 4294967296 cpu: 561.6

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Tue Jul 30 02:19:29 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 100127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Tue Jul 30 02:26:44 2019, MaxMem= 4294967296 cpu: 6959.1

(Enter /home/kira/g09/l716.exe)

Dipole = 1.56254027D-06 3.58958318D-06 3.24036276D-01

Polarizability= 1.22329229D+03 1.62048344D-04 1.61447706D+03

4.34142532D-06 7.40026308D-06 1.81336315D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 -0.000000812 -0.000000032 0.000000014

2 6 0.000001068 -0.000000225 -0.000000036

3 7 -0.000000170 -0.000002900 0.000007559

4 6 -0.000001218 -0.000000356 -0.000000037

5 6 0.000000790 -0.000000051 0.000000015

6 6 0.000001382 -0.000000056 0.000000012

7 6 0.000000160 0.000000248 0.000000006

8 7 0.000002805 0.000000169 0.000005499

9 6 -0.000000001 -0.000000124 0.000000002

10 6 0.000000072 0.000000231 0.000000024

11 6 0.000000074 -0.000000211 0.000000027

12 6 -0.000001280 0.000000013 0.000000013

13 6 -0.000000202 0.000000096 0.000000003

14 6 -0.000000058 -0.000000117 0.000000027

15 6 -0.000000050 0.000000132 0.000000024

16 6 -0.000000027 0.000000013 0.000000000

17 7 -0.000002412 0.000000214 0.000005476

18 6 -0.000001275 -0.000000118 0.000000015

19 6 0.000000981 0.000000293 -0.000000041

20 6 -0.000000756 0.000000004 0.000000015

21 6 0.000000733 0.000000013 0.000000016

22 6 -0.000001094 0.000000426 -0.000000041

23 7 -0.000000150 0.000002492 0.000007541

24 1 -0.000000007 0.000000017 0.000000009

25 1 0.000000009 0.000000020 0.000000008

26 1 -0.000000038 0.000000011 -0.000000012

27 1 -0.000000034 -0.000000007 -0.000000011

28 1 0.000000029 -0.000000006 -0.000000010

29 1 0.000000026 0.000000000 -0.000000011

30 1 -0.000000004 -0.000000011 0.000000009

31 1 0.000000003 -0.000000009 0.000000008

32 30 0.000000092 -0.000000081 -0.000026284

33 6 0.000001343 -0.000000049 0.000000013

34 6 -0.000000199 -0.000000170 -0.000000044

35 6 0.000000184 0.000000154 -0.000000046

36 6 0.000000125 0.000000130 0.000000044

37 6 -0.000000122 -0.000000112 0.000000036

38 6 -0.000000162 0.000000135 -0.000000048

39 6 0.000000113 -0.000000111 0.000000035

40 6 0.000000222 -0.000000213 -0.000000044

41 6 -0.000000142 0.000000145 0.000000046

42 1 0.000000000 -0.000000013 0.000000040

43 1 0.000000003 -0.000000013 0.000000038

44 1 0.000000002 0.000000013 0.000000044

45 1 -0.000000004 0.000000013 0.000000044

-------------------------------------------------------------------

Cartesian Forces: Max 0.000026284 RMS 0.000002595

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Tue Jul 30 02:26:45 2019, MaxMem= 4294967296 cpu: 0.8

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000006212 RMS 0.000001130

Search for a local minimum.

Step number 4 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .11299D-05 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -5.25D-07 DEPred=-4.84D-07 R= 1.09D+00

Trust test= 1.09D+00 RLast= 1.09D-02 DXMaxT set to 5.05D-01

ITU= 0 1 1 0

Eigenvalues --- 0.00211 0.00224 0.00241 0.00273 0.00338

Eigenvalues --- 0.00750 0.00803 0.00803 0.00823 0.01042

Eigenvalues --- 0.01055 0.01118 0.01152 0.01155 0.01251

Eigenvalues --- 0.01252 0.01491 0.01493 0.01540 0.01670

Eigenvalues --- 0.01685 0.01855 0.02108 0.02149 0.02159

Eigenvalues --- 0.02320 0.02759 0.02764 0.02801 0.02810

Eigenvalues --- 0.02906 0.03175 0.03352 0.03748 0.04048

Eigenvalues --- 0.04158 0.04191 0.04201 0.04208 0.04210

Eigenvalues --- 0.04381 0.04455 0.04626 0.04700 0.06901

Eigenvalues --- 0.07811 0.08167 0.08228 0.08238 0.08318

Eigenvalues --- 0.08380 0.08469 0.08525 0.08710 0.09673

Eigenvalues --- 0.09685 0.09706 0.09726 0.10353 0.10439

Eigenvalues --- 0.10442 0.10484 0.11097 0.11375 0.12458

Eigenvalues --- 0.12592 0.12957 0.14384 0.16556 0.17162

Eigenvalues --- 0.19269 0.19509 0.19689 0.20227 0.20517

Eigenvalues --- 0.20536 0.20712 0.20937 0.21697 0.21732

Eigenvalues --- 0.21818 0.24516 0.25438 0.25887 0.27839

Eigenvalues --- 0.27897 0.29197 0.29307 0.31171 0.32564

Eigenvalues --- 0.33197 0.33370 0.33962 0.35790 0.35952

Eigenvalues --- 0.36001 0.36491 0.36669 0.37202 0.37294

Eigenvalues --- 0.37318 0.37570 0.37612 0.37863 0.38066

Eigenvalues --- 0.38079 0.38638 0.39136 0.39515 0.40078

Eigenvalues --- 0.40078 0.40079 0.40087 0.40769 0.41084

Eigenvalues --- 0.41174 0.42492 0.45276 0.45560 0.45703

Eigenvalues --- 0.46340 0.50558 0.50688 0.52884 0.53380

Eigenvalues --- 1.03265 1.03899 1.04306 1.04377

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3 2

RFO step: Lambda=-4.25120223D-09.

NNeg= 0 NP= 3 Switch= 2.50D-03 Rises=F DC= 3.79D-05 SmlDif= 1.00D-05

RMS Error= 0.1547697474D-04 NUsed= 3 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.30985 -0.31914 0.00928

Iteration 1 RMS(Cart)= 0.00019826 RMS(Int)= 0.00000020

Iteration 2 RMS(Cart)= 0.00000013 RMS(Int)= 0.00000019

ITry= 1 IFail=0 DXMaxC= 2.47D-03 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.68680 0.00000 0.00006 -0.00005 0.00001 2.68681

R2 2.61852 0.00000 0.00001 0.00000 0.00001 2.61853

R3 2.04072 -0.00000 0.00000 0.00000 0.00000 2.04072

R4 2.58668 -0.00000 -0.00002 0.00001 -0.00002 2.58666

R5 2.72998 0.00000 0.00004 -0.00000 0.00003 2.73002

R6 2.58667 0.00000 -0.00002 0.00001 -0.00002 2.58666

R7 3.96517 0.00000 0.00002 -0.00001 0.00001 3.96518

R8 2.68680 0.00000 0.00006 -0.00005 0.00001 2.68681

R9 2.72998 0.00000 0.00004 -0.00000 0.00003 2.73002

R10 2.04072 -0.00000 0.00000 0.00000 0.00000 2.04072

R11 2.66276 0.00000 0.00003 -0.00000 0.00003 2.66279

R12 2.67790 -0.00000 0.00001 -0.00001 -0.00000 2.67789

R13 2.58483 0.00000 -0.00001 -0.00001 -0.00001 2.58482

R14 2.74108 0.00000 0.00000 0.00001 0.00001 2.74109

R15 2.58483 0.00000 -0.00001 -0.00001 -0.00001 2.58482

R16 3.98107 0.00000 -0.00002 0.00001 -0.00001 3.98107

R17 2.74108 0.00000 0.00000 0.00001 0.00001 2.74109

R18 2.66276 0.00000 0.00003 -0.00000 0.00003 2.66279

R19 2.56849 0.00000 0.00001 -0.00000 0.00001 2.56850

R20 2.04044 -0.00000 -0.00000 0.00000 0.00000 2.04044

R21 2.04044 -0.00000 -0.00000 0.00000 0.00000 2.04044

R22 2.66276 0.00000 0.00003 -0.00000 0.00003 2.66279

R23 2.67790 -0.00000 0.00001 -0.00001 -0.00000 2.67789

R24 2.74108 0.00000 0.00000 0.00001 0.00001 2.74109

R25 2.58483 0.00000 -0.00001 -0.00000 -0.00001 2.58482

R26 2.56849 0.00000 0.00001 -0.00000 0.00001 2.56850

R27 2.04044 -0.00000 -0.00000 0.00000 0.00000 2.04044

R28 2.74108 0.00000 0.00000 0.00001 0.00001 2.74109

R29 2.04044 -0.00000 -0.00000 0.00000 0.00000 2.04044

R30 2.58483 0.00000 -0.00001 -0.00001 -0.00001 2.58482

R31 2.66276 0.00000 0.00003 -0.00000 0.00003 2.66279

R32 3.98107 0.00000 -0.00002 0.00001 -0.00001 3.98107

R33 2.72998 0.00000 0.00003 -0.00000 0.00003 2.73002

R34 2.67790 -0.00000 0.00001 -0.00001 -0.00000 2.67789

R35 2.68680 0.00000 0.00006 -0.00005 0.00001 2.68681

R36 2.58667 0.00000 -0.00002 0.00001 -0.00002 2.58666

R37 2.61852 0.00000 0.00001 0.00000 0.00001 2.61853

R38 2.04072 -0.00000 0.00000 0.00000 0.00000 2.04072

R39 2.68680 0.00000 0.00006 -0.00005 0.00001 2.68681

R40 2.04072 -0.00000 0.00000 0.00000 0.00000 2.04072

R41 2.58667 0.00000 -0.00002 0.00001 -0.00002 2.58666

R42 2.72998 0.00000 0.00004 -0.00000 0.00003 2.73002

R43 3.96517 0.00000 0.00002 -0.00001 0.00001 3.96518

R44 2.67790 -0.00000 0.00001 -0.00001 -0.00000 2.67789

R45 2.28282 0.00000 0.00000 0.00000 0.00000 2.28282

R46 2.28282 0.00000 0.00000 0.00000 0.00000 2.28282

R47 2.01746 -0.00000 -0.00000 0.00000 0.00000 2.01746

R48 2.01746 -0.00000 -0.00000 0.00000 0.00000 2.01746

R49 2.28282 0.00000 0.00000 0.00000 0.00000 2.28282

R50 2.01746 -0.00000 -0.00000 0.00000 0.00000 2.01746

R51 2.28282 0.00000 0.00000 0.00000 0.00000 2.28282

R52 2.01746 -0.00000 -0.00000 0.00000 0.00000 2.01746

A1 1.86169 -0.00000 0.00000 0.00000 0.00001 1.86169

A2 2.19908 -0.00000 -0.00001 0.00001 0.00000 2.19908

A3 2.22241 0.00000 0.00001 -0.00002 -0.00001 2.22240

A4 1.91660 -0.00000 -0.00003 -0.00000 -0.00003 1.91657

A5 2.19022 0.00000 0.00002 0.00001 0.00003 2.19025

A6 2.17633 0.00000 0.00001 -0.00001 -0.00000 2.17633

A7 1.86820 0.00000 0.00006 -0.00001 0.00005 1.86825

A8 2.20666 -0.00000 -0.00001 0.00001 -0.00001 2.20665

A9 2.20666 -0.00000 -0.00002 0.00001 -0.00001 2.20665

A10 1.91660 -0.00000 -0.00003 -0.00000 -0.00003 1.91657

A11 2.17633 0.00000 0.00001 -0.00001 -0.00000 2.17633

A12 2.19022 0.00000 0.00002 0.00001 0.00003 2.19025

A13 1.86169 -0.00000 0.00000 0.00000 0.00001 1.86169

A14 2.22241 0.00000 0.00001 -0.00002 -0.00001 2.22240

A15 2.19908 -0.00000 -0.00001 0.00001 0.00000 2.19908

A16 2.21907 0.00000 0.00003 0.00002 0.00004 2.21911

A17 2.02586 -0.00000 -0.00001 -0.00001 -0.00002 2.02584

A18 2.03823 -0.00000 -0.00001 -0.00001 -0.00002 2.03821

A19 2.18829 0.00000 0.00001 -0.00000 0.00001 2.18829

A20 2.18603 0.00000 0.00002 0.00001 0.00003 2.18606

A21 1.90883 -0.00000 -0.00002 -0.00001 -0.00003 1.90880

A22 1.87417 0.00000 0.00004 0.00001 0.00005 1.87422

A23 2.20325 -0.00000 -0.00000 -0.00000 -0.00001 2.20325

A24 2.20325 -0.00000 -0.00000 -0.00000 -0.00001 2.20325

A25 1.90883 -0.00000 -0.00002 -0.00001 -0.00003 1.90880

A26 2.18829 0.00000 0.00001 -0.00000 0.00001 2.18829

A27 2.18603 0.00000 0.00002 0.00001 0.00003 2.18606

A28 1.86647 0.00000 0.00001 0.00000 0.00001 1.86648

A29 2.18914 -0.00000 0.00000 -0.00000 0.00000 2.18914

A30 2.22756 0.00000 -0.00001 0.00000 -0.00001 2.22756

A31 1.86647 0.00000 0.00001 0.00000 0.00001 1.86648

A32 2.18914 -0.00000 0.00000 -0.00000 0.00000 2.18914

A33 2.22756 0.00000 -0.00001 0.00000 -0.00001 2.22756

A34 2.21907 0.00000 0.00003 0.00002 0.00004 2.21911

A35 2.02586 -0.00000 -0.00001 -0.00001 -0.00002 2.02584

A36 2.03823 -0.00000 -0.00001 -0.00001 -0.00002 2.03821

A37 2.18603 0.00000 0.00001 0.00001 0.00003 2.18606

A38 2.18829 0.00000 0.00001 -0.00000 0.00001 2.18829

A39 1.90883 -0.00000 -0.00002 -0.00001 -0.00003 1.90880

A40 1.86647 0.00000 0.00001 0.00000 0.00001 1.86648

A41 2.18914 -0.00000 0.00000 -0.00000 0.00000 2.18914

A42 2.22756 0.00000 -0.00001 0.00000 -0.00001 2.22756

A43 1.86647 0.00000 0.00001 0.00000 0.00001 1.86648

A44 2.22756 -0.00000 -0.00001 0.00000 -0.00001 2.22756

A45 2.18914 -0.00000 0.00000 -0.00000 0.00000 2.18914

A46 1.90883 -0.00000 -0.00002 -0.00001 -0.00003 1.90880

A47 2.18603 0.00000 0.00001 0.00001 0.00003 2.18606

A48 2.18829 0.00000 0.00001 -0.00000 0.00001 2.18829

A49 1.87417 0.00000 0.00004 0.00001 0.00005 1.87422

A50 2.20325 -0.00000 -0.00000 -0.00000 -0.00001 2.20325

A51 2.20325 0.00000 -0.00000 -0.00000 -0.00001 2.20325

A52 2.21907 0.00000 0.00003 0.00002 0.00004 2.21911

A53 2.03823 -0.00000 -0.00001 -0.00001 -0.00002 2.03821

A54 2.02586 -0.00000 -0.00001 -0.00001 -0.00002 2.02584

A55 2.19022 0.00000 0.00002 0.00001 0.00003 2.19025

A56 2.17633 0.00000 0.00001 -0.00001 -0.00000 2.17633

A57 1.91660 -0.00000 -0.00003 -0.00000 -0.00003 1.91657

A58 1.86169 -0.00000 0.00000 0.00000 0.00001 1.86169

A59 2.19908 -0.00000 -0.00001 0.00001 0.00000 2.19908

A60 2.22241 0.00000 0.00001 -0.00002 -0.00001 2.22240

A61 1.86169 -0.00000 0.00000 0.00000 0.00001 1.86169

A62 2.22241 0.00000 0.00001 -0.00002 -0.00001 2.22240

A63 2.19908 -0.00000 -0.00001 0.00001 0.00000 2.19908

A64 1.91660 -0.00000 -0.00003 -0.00000 -0.00003 1.91657

A65 2.19022 0.00000 0.00002 0.00001 0.00003 2.19025

A66 2.17633 0.00000 0.00001 -0.00001 -0.00000 2.17633

A67 1.86821 0.00000 0.00005 -0.00001 0.00005 1.86825

A68 2.20666 -0.00000 -0.00001 0.00001 -0.00001 2.20665

A69 2.20666 -0.00000 -0.00002 0.00001 -0.00001 2.20665

A70 1.56536 0.00000 0.00007 0.00001 0.00008 1.56543

A71 1.56536 0.00000 0.00007 0.00001 0.00008 1.56543

A72 1.56536 0.00000 0.00007 0.00001 0.00008 1.56543

A73 1.56536 0.00000 0.00007 0.00001 0.00007 1.56543

A74 2.21907 0.00000 0.00003 0.00002 0.00004 2.21911

A75 2.03823 -0.00000 -0.00001 -0.00001 -0.00002 2.03821

A76 2.02586 -0.00000 -0.00001 -0.00001 -0.00002 2.02584

A77 3.13072 0.00000 0.00014 0.00001 0.00015 3.13087

A78 3.13072 0.00000 0.00014 0.00001 0.00015 3.13087

A79 3.15579 -0.00000 -0.00003 0.00003 0.00000 3.15579

A80 3.12739 0.00000 0.00003 -0.00003 -0.00000 3.12739

A81 3.13721 -0.00000 0.00002 -0.00002 -0.00000 3.13721

A82 3.14596 0.00000 -0.00002 0.00002 0.00000 3.14596

A83 3.12739 0.00000 0.00003 -0.00003 -0.00000 3.12739

A84 3.14596 0.00000 -0.00002 0.00002 0.00000 3.14596

A85 3.15579 -0.00000 -0.00003 0.00003 0.00000 3.15579

A86 3.13721 -0.00000 0.00002 -0.00002 -0.00000 3.13721

A87 3.28784 -0.00001 -0.00099 -0.00009 -0.00108 3.28675

A88 2.99341 0.00001 0.00086 0.00011 0.00096 2.99437

A89 3.14130 0.00000 0.00001 -0.00000 0.00001 3.14131

A90 3.14148 -0.00000 -0.00001 -0.00000 -0.00001 3.14147

A91 3.14127 0.00000 0.00002 -0.00002 0.00000 3.14127

A92 3.14206 -0.00000 -0.00002 0.00002 -0.00000 3.14206

A93 3.14171 0.00000 0.00000 0.00000 0.00001 3.14171

A94 3.14113 0.00000 0.00002 -0.00002 0.00000 3.14113

A95 3.14189 -0.00000 -0.00001 0.00000 -0.00001 3.14188

A96 3.14192 -0.00000 -0.00002 0.00002 -0.00000 3.14192

D1 0.00010 0.00000 -0.00002 0.00001 -0.00001 0.00008

D2 3.13296 0.00000 -0.00000 0.00002 0.00002 3.13298

D3 -3.13721 0.00000 -0.00004 0.00001 -0.00003 -3.13724

D4 -0.00434 0.00000 -0.00002 0.00002 -0.00000 -0.00434

D5 0.00000 -0.00000 0.00000 -0.00000 -0.00000 0.00000

D6 -3.13723 -0.00000 -0.00002 -0.00000 -0.00002 -3.13725

D7 3.13723 0.00000 0.00002 0.00000 0.00002 3.13725

D8 -0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D9 -0.00016 -0.00000 0.00003 -0.00001 0.00002 -0.00013

D10 -3.08274 -0.00000 -0.00040 -0.00008 -0.00048 -3.08322

D11 -3.13310 -0.00000 0.00002 -0.00003 -0.00001 -3.13311

D12 0.06750 -0.00000 -0.00042 -0.00010 -0.00051 0.06699

D13 -3.11411 -0.00000 -0.00014 0.00001 -0.00013 -3.11424

D14 0.01878 -0.00000 -0.00008 0.00002 -0.00007 0.01871

D15 0.01749 -0.00000 -0.00012 0.00003 -0.00009 0.01740

D16 -3.13280 0.00000 -0.00006 0.00004 -0.00003 -3.13283

D17 0.00016 0.00000 -0.00003 0.00001 -0.00002 0.00013

D18 3.13310 0.00000 -0.00002 0.00003 0.00001 3.13311

D19 3.08274 0.00000 0.00040 0.00008 0.00048 3.08322

D20 -0.06750 0.00000 0.00042 0.00010 0.00051 -0.06699

D21 -3.10257 -0.00000 -0.00017 -0.00001 -0.00018 -3.10275

D22 -0.10916 0.00000 0.00069 0.00009 0.00078 -0.10838

D23 0.10916 -0.00000 -0.00069 -0.00009 -0.00078 0.10838

D24 3.10257 0.00000 0.00017 0.00001 0.00018 3.10275

D25 -0.00010 -0.00000 0.00002 -0.00001 0.00001 -0.00008

D26 3.13721 -0.00000 0.00004 -0.00001 0.00003 3.13724

D27 -3.13296 -0.00000 0.00000 -0.00002 -0.00002 -3.13298

D28 0.00434 -0.00000 0.00002 -0.00002 0.00000 0.00434

D29 -0.01749 0.00000 0.00012 -0.00004 0.00009 -0.01740

D30 3.13280 -0.00000 0.00006 -0.00004 0.00003 3.13283

D31 3.11411 0.00000 0.00014 -0.00001 0.00013 3.11424

D32 -0.01878 0.00000 0.00008 -0.00002 0.00007 -0.01871

D33 0.00951 -0.00000 -0.00007 0.00000 -0.00006 0.00944

D34 -3.12258 -0.00000 -0.00016 -0.00001 -0.00016 -3.12275

D35 -3.14084 0.00000 -0.00001 0.00000 -0.00000 -3.14084

D36 0.01025 -0.00000 -0.00010 -0.00001 -0.00010 0.01015

D37 -3.13237 -0.00000 -0.00011 -0.00000 -0.00012 -3.13249

D38 0.08169 -0.00000 -0.00052 -0.00003 -0.00055 0.08114

D39 0.00100 -0.00000 -0.00004 0.00000 -0.00003 0.00097

D40 -3.06813 -0.00000 -0.00044 -0.00002 -0.00047 -3.06860

D41 3.13276 0.00000 0.00010 0.00001 0.00011 3.13287

D42 -0.00437 0.00000 0.00006 0.00001 0.00007 -0.00431

D43 -0.00062 0.00000 0.00002 -0.00000 0.00002 -0.00060

D44 -3.13775 0.00000 -0.00002 0.00000 -0.00002 -3.13777

D45 -0.00100 0.00000 0.00004 -0.00000 0.00003 -0.00097

D46 3.13237 0.00000 0.00011 0.00000 0.00012 3.13249

D47 3.06813 0.00000 0.00044 0.00002 0.00047 3.06860

D48 -0.08169 0.00000 0.00052 0.00003 0.00055 -0.08114

D49 -0.11601 0.00000 0.00074 0.00006 0.00080 -0.11521

D50 -3.11136 -0.00000 -0.00025 -0.00003 -0.00028 -3.11164

D51 3.11136 0.00000 0.00026 0.00003 0.00028 3.11164

D52 0.11601 -0.00000 -0.00074 -0.00006 -0.00080 0.11521

D53 0.00062 -0.00000 -0.00002 0.00000 -0.00002 0.00060

D54 3.13775 -0.00000 0.00002 -0.00000 0.00002 3.13777

D55 -3.13276 -0.00000 -0.00010 -0.00001 -0.00011 -3.13287

D56 0.00437 -0.00000 -0.00006 -0.00001 -0.00007 0.00431

D57 -0.00951 0.00000 0.00006 -0.00000 0.00006 -0.00944

D58 3.14084 -0.00000 0.00000 -0.00000 0.00000 3.14085

D59 3.12258 0.00000 0.00015 0.00001 0.00016 3.12275

D60 -0.01025 0.00000 0.00009 0.00001 0.00010 -0.01015

D61 -0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D62 3.13701 0.00000 0.00004 -0.00000 0.00004 3.13705

D63 -3.13701 -0.00000 -0.00004 0.00000 -0.00004 -3.13705

D64 -0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D65 3.12258 0.00000 0.00016 0.00001 0.00017 3.12275

D66 -0.00951 0.00000 0.00007 -0.00000 0.00006 -0.00944

D67 -0.01025 0.00000 0.00010 0.00001 0.00010 -0.01015

D68 3.14084 -0.00000 0.00001 -0.00000 0.00000 3.14085

D69 -3.13276 -0.00000 -0.00010 -0.00001 -0.00011 -3.13287

D70 0.00437 -0.00000 -0.00006 -0.00001 -0.00007 0.00431

D71 0.00062 -0.00000 -0.00002 0.00000 -0.00002 0.00060

D72 3.13775 -0.00000 0.00002 -0.00000 0.00002 3.13777

D73 3.13237 0.00000 0.00011 0.00000 0.00012 3.13249

D74 -0.08169 0.00000 0.00052 0.00003 0.00055 -0.08114

D75 -0.00100 0.00000 0.00004 -0.00000 0.00003 -0.00097

D76 3.06813 0.00000 0.00044 0.00002 0.00047 3.06860

D77 -0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D78 3.13701 0.00000 0.00004 -0.00000 0.00004 3.13705

D79 -3.13701 -0.00000 -0.00004 0.00000 -0.00004 -3.13705

D80 0.00000 0.00000 -0.00000 0.00000 -0.00000 0.00000

D81 -0.00062 0.00000 0.00002 -0.00000 0.00002 -0.00060

D82 3.13276 0.00000 0.00010 0.00001 0.00011 3.13287

D83 -3.13775 0.00000 -0.00002 -0.00000 -0.00002 -3.13777

D84 -0.00437 0.00000 0.00006 0.00001 0.00007 -0.00431

D85 0.00100 -0.00000 -0.00004 0.00000 -0.00003 0.00097

D86 -3.06813 -0.00000 -0.00044 -0.00002 -0.00047 -3.06860

D87 -3.13237 -0.00000 -0.00012 -0.00000 -0.00012 -3.13249

D88 0.08169 -0.00000 -0.00052 -0.00003 -0.00055 0.08114

D89 -3.12258 -0.00000 -0.00016 -0.00001 -0.00016 -3.12275

D90 0.01025 -0.00000 -0.00009 -0.00001 -0.00010 0.01015

D91 0.00951 -0.00000 -0.00007 0.00000 -0.00006 0.00944

D92 -3.14084 0.00000 -0.00000 0.00000 -0.00000 -3.14085

D93 0.11601 -0.00000 -0.00074 -0.00006 -0.00080 0.11521

D94 3.11135 0.00000 0.00026 0.00003 0.00028 3.11164

D95 -3.11135 -0.00000 -0.00026 -0.00003 -0.00029 -3.11164

D96 -0.11601 0.00000 0.00074 0.00006 0.00080 -0.11521

D97 3.11411 0.00000 0.00014 -0.00001 0.00013 3.11424

D98 -0.01749 0.00000 0.00012 -0.00003 0.00009 -0.01740

D99 -0.01878 0.00000 0.00008 -0.00002 0.00007 -0.01871

D100 3.13280 -0.00000 0.00006 -0.00004 0.00003 3.13283

D101 -3.13296 -0.00000 0.00000 -0.00002 -0.00002 -3.13298

D102 0.00434 -0.00000 0.00002 -0.00002 -0.00000 0.00434

D103 -0.00010 -0.00000 0.00002 -0.00001 0.00001 -0.00008

D104 3.13721 -0.00000 0.00004 -0.00001 0.00003 3.13724

D105 3.13310 0.00000 -0.00002 0.00003 0.00001 3.13311

D106 -0.06750 0.00000 0.00042 0.00009 0.00051 -0.06699

D107 0.00016 0.00000 -0.00003 0.00001 -0.00002 0.00013

D108 3.08274 0.00000 0.00040 0.00008 0.00048 3.08322

D109 0.00000 0.00000 0.00000 -0.00000 -0.00000 -0.00000

D110 3.13723 0.00000 0.00002 0.00000 0.00002 3.13725

D111 -3.13723 -0.00000 -0.00002 -0.00000 -0.00002 -3.13725

D112 -0.00000 -0.00000 -0.00000 0.00000 0.00000 0.00000

D113 0.00010 0.00000 -0.00002 0.00001 -0.00001 0.00008

D114 3.13296 0.00000 -0.00000 0.00002 0.00002 3.13298

D115 -3.13721 0.00000 -0.00004 0.00001 -0.00003 -3.13724

D116 -0.00434 0.00000 -0.00002 0.00002 0.00000 -0.00434

D117 -0.00016 -0.00000 0.00003 -0.00001 0.00002 -0.00013

D118 -3.08274 -0.00000 -0.00040 -0.00008 -0.00048 -3.08322

D119 -3.13310 -0.00000 0.00002 -0.00003 -0.00001 -3.13311

D120 0.06750 -0.00000 -0.00042 -0.00009 -0.00051 0.06699

D121 -3.11411 -0.00000 -0.00014 0.00001 -0.00013 -3.11424

D122 0.01878 -0.00000 -0.00008 0.00002 -0.00007 0.01871

D123 0.01749 -0.00000 -0.00012 0.00003 -0.00009 0.01740

D124 -3.13280 0.00000 -0.00006 0.00004 -0.00003 -3.13283

D125 3.10257 0.00000 0.00017 0.00001 0.00018 3.10275

D126 0.10916 -0.00000 -0.00069 -0.00009 -0.00078 0.10838

D127 -0.10916 0.00000 0.00069 0.00009 0.00078 -0.10838

D128 -3.10257 -0.00000 -0.00017 -0.00001 -0.00018 -3.10275

Item Value Threshold Converged?

Maximum Force 0.000006 0.000450 YES

RMS Force 0.000001 0.000300 YES

Maximum Displacement 0.002470 0.001800 NO

RMS Displacement 0.000198 0.001200 YES

Predicted change in Energy=-3.231675D-08

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Tue Jul 30 02:26:45 2019, MaxMem= 4294967296 cpu: 1.0

(Enter /home/kira/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -0.692834 -4.267848 -0.056805

2 6 0 -1.100625 -2.906239 -0.021607

3 7 0 0.000000 -2.092728 -0.000684

4 6 0 1.100625 -2.906239 -0.021607

5 6 0 0.692835 -4.267848 -0.056805

6 6 0 2.467968 -2.439959 -0.019688

7 6 0 2.910772 -1.102262 -0.016189

8 7 0 2.100954 -0.000000 -0.003455

9 6 0 2.910772 1.102262 -0.016190

10 6 0 4.298195 0.679595 -0.036685

11 6 0 4.298195 -0.679595 -0.036685

12 6 0 -2.467968 -2.439959 -0.019688

13 6 0 -2.910772 -1.102262 -0.016189

14 6 0 -4.298196 -0.679595 -0.036685

15 6 0 -4.298196 0.679595 -0.036685

16 6 0 -2.910772 1.102262 -0.016189

17 7 0 -2.100954 -0.000000 -0.003455

18 6 0 -2.467969 2.439959 -0.019688

19 6 0 -1.100625 2.906239 -0.021607

20 6 0 -0.692834 4.267849 -0.056805

21 6 0 0.692835 4.267849 -0.056805

22 6 0 1.100625 2.906239 -0.021607

23 7 0 0.000000 2.092728 -0.000684

24 1 0 -1.347756 -5.126102 -0.082721

25 1 0 1.347756 -5.126102 -0.082721

26 1 0 5.153172 1.338842 -0.053203

27 1 0 5.153172 -1.338842 -0.053203

28 1 0 -5.153173 -1.338842 -0.053203

29 1 0 -5.153173 1.338842 -0.053203

30 1 0 -1.347756 5.126102 -0.082721

31 1 0 1.347756 5.126102 -0.082721

32 30 0 -0.000000 0.000000 0.151889

33 6 0 2.467968 2.439959 -0.019688

34 6 0 3.468275 3.443623 -0.032543

35 6 0 -3.468275 -3.443623 -0.032543

36 6 0 4.308766 4.311238 -0.043693

37 6 0 -4.308765 -4.311239 -0.043693

38 6 0 3.468275 -3.443623 -0.032543

39 6 0 4.308765 -4.311238 -0.043692

40 6 0 -3.468275 3.443623 -0.032543

41 6 0 -4.308765 4.311238 -0.043693

42 1 0 -5.054901 5.074736 -0.053889

43 1 0 5.054902 5.074736 -0.053889

44 1 0 5.054901 -5.074736 -0.053888

45 1 0 -5.054901 -5.074736 -0.053890

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.421799 0.000000

3 N 2.283489 1.368800 0.000000

4 C 2.252047 2.201250 1.368800 0.000000

5 C 1.385669 2.252047 2.283489 1.421799 0.000000

6 C 3.651470 3.598928 2.492348 1.444662 2.548265

7 C 4.796724 4.398371 3.074712 2.555581 3.865467

8 N 5.101238 4.323964 2.965388 3.073632 4.494461

9 C 6.467280 5.670927 4.322128 4.398266 5.810248

10 C 7.027658 6.481180 5.114836 4.804465 6.121783

11 C 6.147060 5.839986 4.524679 3.896489 5.086708

12 C 2.548265 1.444662 2.492348 3.598928 3.651470

13 C 3.865467 2.555581 3.074712 4.398371 4.796724

14 C 5.086708 3.896489 4.524680 5.839986 6.147060

15 C 6.121783 4.804465 5.114836 6.481180 7.027658

16 C 5.810248 4.398266 4.322128 5.670927 6.467280

17 N 4.494461 3.073632 2.965388 4.323964 5.101238

18 C 6.938816 5.518285 5.161054 6.427807 7.415304

19 C 7.185754 5.812478 5.118738 6.215336 7.394949

20 C 8.535697 7.185754 6.398445 7.394949 8.647439

21 C 8.647439 7.394949 6.398445 7.185754 8.535697

22 C 7.394949 6.215336 5.118738 5.812478 7.185754

23 N 6.398445 5.118738 4.185455 5.118738 6.398445

24 H 1.079904 2.234413 3.320322 3.305464 2.213883

25 H 2.213883 3.305464 3.320322 2.234413 1.079904

26 H 8.100049 7.558551 6.191414 5.868974 7.164468

27 H 6.538722 6.447303 5.208290 4.345212 5.336076

28 H 5.336076 4.345213 5.208290 6.447303 6.538722

29 H 7.164468 5.868974 6.191415 7.558551 8.100049

30 H 9.416788 8.036374 7.344023 8.397429 9.613063

31 H 9.613063 8.397429 7.344023 8.036374 9.416788

32 Zn 4.328753 3.112507 2.098282 3.112508 4.328753

33 C 7.415304 6.427807 5.161054 5.518285 6.938816

34 C 8.762546 7.822769 6.533079 6.776919 8.195758

35 C 2.895342 2.427893 3.722212 4.600407 4.242024

36 C 9.930604 9.019644 7.718684 7.898394 9.309987

37 C 3.616215 3.502381 4.846555 5.588919 5.001805

38 C 4.242024 4.600407 3.722212 2.427893 2.895342

39 C 5.001805 5.588919 4.846555 3.502381 3.616215

40 C 8.195758 6.776919 6.533079 7.822769 8.762546

41 C 9.309987 7.898394 7.718684 9.019644 9.930604

42 H 10.310748 8.906925 8.770826 10.079063 10.969064

43 H 10.969064 10.079063 8.770826 8.906925 10.310748

44 H 5.804097 6.526402 5.869176 4.509958 4.436068

45 H 4.436068 4.509958 5.869177 6.526402 5.804097

6 7 8 9 10

6 C 0.000000

7 C 1.409085 0.000000

8 N 2.467461 1.367826 0.000000

9 C 3.569792 2.204524 1.367826 0.000000

10 C 3.616854 2.258402 2.300179 1.450521 0.000000

11 C 2.539469 1.450521 2.300179 2.258402 1.359189

12 C 4.935937 5.542589 5.179645 6.440356 7.450697

13 C 5.542589 5.821544 5.131524 6.224974 7.425944

14 C 6.991434 7.221376 6.435221 7.425944 8.703179

15 C 7.450697 7.425944 6.435221 7.221376 8.596391

16 C 6.440357 6.224974 5.131524 5.821544 7.221376

17 N 5.179645 5.131524 4.201909 5.131524 6.435221

18 C 6.940971 6.440356 5.179645 5.542589 6.991434

19 C 6.427807 5.670927 4.323964 4.398371 5.839986

20 C 7.415305 6.467280 5.101238 4.796725 6.147060

21 C 6.938816 5.810248 4.494461 3.865467 5.086708

22 C 5.518285 4.398266 3.073632 2.555581 3.896489

23 N 5.161054 4.322128 2.965388 3.074712 4.524679

24 H 4.666807 5.859247 6.178738 7.545330 8.098456

25 H 2.911050 4.317260 5.181748 6.421835 6.512551

26 H 4.635815 3.314924 3.333318 2.255150 1.079753

27 H 2.902396 2.255150 3.333318 3.314924 2.192110

28 H 7.700349 8.067499 7.376810 8.425411 9.664508

29 H 8.506601 8.425411 7.376810 8.067499 9.474346

30 H 8.474020 7.545330 6.178738 5.859247 7.186815

31 H 7.648800 6.421835 5.181748 4.317260 5.336538

32 Zn 3.474725 3.117022 2.106690 3.117022 4.355674

33 C 4.879919 3.569793 2.467461 1.409085 2.539469

34 C 5.968024 4.579972 3.705260 2.406875 2.885938

35 C 6.020506 6.795180 6.547953 7.833107 8.793122

36 C 6.997698 5.591165 4.843844 3.500382 3.631666

37 C 7.030390 7.900633 7.724823 9.023772 9.949283

38 C 1.417081 2.406875 3.705260 4.579972 4.205913

39 C 2.625032 3.500382 4.843844 5.591165 4.990849

40 C 8.357972 7.833107 6.547954 6.795180 8.243660

41 C 9.565739 9.023772 7.724824 7.900633 9.341769

42 H 10.633221 10.080113 8.772785 8.901344 10.334311

43 H 7.947581 6.538656 5.872078 4.514340 4.459839

44 H 3.692620 4.514340 5.872077 6.538656 5.803897

45 H 7.970997 8.901343 8.772785 10.080113 10.981486

11 12 13 14 15

11 C 0.000000

12 C 6.991434 0.000000

13 C 7.221376 1.409085 0.000000

14 C 8.596391 2.539469 1.450521 0.000000

15 C 8.703179 3.616855 2.258402 1.359189 0.000000

16 C 7.425944 3.569793 2.204524 2.258402 1.450521

17 N 6.435221 2.467461 1.367826 2.300179 2.300179

18 C 7.450697 4.879919 3.569793 3.616855 2.539469

19 C 6.481180 5.518285 4.398266 4.804466 3.896490

20 C 7.027658 6.938816 5.810248 6.121783 5.086708

21 C 6.121783 7.415305 6.467281 7.027658 6.147061

22 C 4.804465 6.427807 5.670927 6.481180 5.839986

23 N 5.114836 5.161054 4.322128 5.114837 4.524680

24 H 7.186815 2.911050 4.317260 5.336538 6.512552

25 H 5.336538 4.666807 5.859247 7.186815 8.098457

26 H 2.192110 8.506600 8.425411 9.664508 9.474346

27 H 1.079753 7.700349 8.067499 9.474346 9.664508

28 H 9.474346 2.902396 2.255150 1.079753 2.192110

29 H 9.664508 4.635815 3.314924 2.192110 1.079753

30 H 8.098457 7.648800 6.421835 6.512552 5.336539

31 H 6.512552 8.474020 7.545330 8.098457 7.186816

32 Zn 4.355674 3.474724 3.117022 4.355674 4.355674

33 C 3.616855 6.940971 6.440357 7.450697 6.991434

34 C 4.205913 8.357972 7.833108 8.793122 8.243660

35 C 8.243660 1.417081 2.406875 2.885938 4.205914

36 C 4.990849 9.565739 9.023772 9.949283 9.341770

37 C 9.341769 2.625032 3.500382 3.631666 4.990849

38 C 2.885938 6.020506 6.795180 8.243660 8.793122

39 C 3.631666 7.030390 7.900633 9.341770 9.949283

40 C 8.793122 5.968025 4.579972 4.205914 2.885938

41 C 9.949283 6.997698 5.591165 4.990849 3.631666

42 H 10.981486 7.947581 6.538656 5.803897 4.459840

43 H 5.803897 10.633221 10.080113 10.981486 10.334311

44 H 4.459840 7.970997 8.901344 10.334311 10.981486

45 H 10.334311 3.692620 4.514340 4.459840 5.803897

16 17 18 19 20

16 C 0.000000

17 N 1.367826 0.000000

18 C 1.409085 2.467461 0.000000

19 C 2.555581 3.073632 1.444662 0.000000

20 C 3.865467 4.494461 2.548266 1.421799 0.000000

21 C 4.796725 5.101239 3.651470 2.252047 1.385669

22 C 4.398371 4.323964 3.598928 2.201250 2.252047

23 N 3.074712 2.965388 2.492348 1.368800 2.283488

24 H 6.421835 5.181748 7.648800 8.036374 9.416788

25 H 7.545330 6.178738 8.474020 8.397429 9.613063

26 H 8.067499 7.376810 7.700349 6.447303 6.538722

27 H 8.425411 7.376810 8.506600 7.558551 8.100049

28 H 3.314924 3.333318 4.635815 5.868974 7.164469

29 H 2.255150 3.333318 2.902396 4.345213 5.336076

30 H 4.317260 5.181748 2.911050 2.234413 1.079904

31 H 5.859247 6.178739 4.666807 3.305464 2.213883

32 Zn 3.117022 2.106689 3.474724 3.112507 4.328753

33 C 5.542589 5.179645 4.935937 3.598928 3.651470

34 C 6.795180 6.547954 6.020506 4.600407 4.242024

35 C 4.579972 3.705260 5.968025 6.776919 8.195758

36 C 7.900633 7.724824 7.030390 5.588919 5.001805

37 C 5.591165 4.843844 6.997698 7.898395 9.309987

38 C 7.833107 6.547954 8.357972 7.822769 8.762546

39 C 9.023772 7.724824 9.565739 9.019644 9.930605

40 C 2.406875 3.705260 1.417081 2.427893 2.895342

41 C 3.500382 4.843844 2.625032 3.502381 3.616215

42 H 4.514340 5.872077 3.692620 4.509958 4.436068

43 H 8.901344 8.772785 7.970997 6.526402 5.804097

44 H 10.080113 8.772785 10.633221 10.079063 10.969064

45 H 6.538656 5.872077 7.947581 8.906925 10.310748

21 22 23 24 25

21 C 0.000000

22 C 1.421799 0.000000

23 N 2.283488 1.368800 0.000000

24 H 9.613063 8.397429 7.344023 0.000000

25 H 9.416788 8.036374 7.344023 2.695512 0.000000

26 H 5.336076 4.345212 5.208290 9.168339 7.501838

27 H 7.164468 5.868974 6.191415 7.523714 5.368929

28 H 8.100049 7.558551 6.191415 5.368930 7.523714

29 H 6.538723 6.447303 5.208291 7.501838 9.168339

30 H 2.213883 3.305464 3.320322 10.252204 10.600635

31 H 1.079904 2.234413 3.320322 10.600636 10.252204

32 Zn 4.328753 3.112507 2.098282 5.305508 5.305508

33 C 2.548266 1.444662 2.492348 8.474020 7.648799

34 C 2.895342 2.427893 3.722212 9.830404 8.828324

35 C 8.762546 7.822769 6.533079 2.707370 5.101706

36 C 3.616215 3.502381 4.846555 11.002779 9.891031

37 C 9.930605 9.019644 7.718685 3.071336 5.715046

38 C 8.195758 6.776919 6.533079 5.101706 2.707370

39 C 9.309987 7.898394 7.718685 5.715046 3.071336

40 C 4.242024 4.600407 3.722212 8.828324 9.830404

41 C 5.001805 5.588919 4.846555 9.891031 11.002779

42 H 5.804097 6.526402 5.869176 10.853610 12.043751

43 H 4.436068 4.509958 5.869176 12.043751 10.853610

44 H 10.310748 8.906925 8.770827 6.402928 3.707613

45 H 10.969064 10.079063 8.770827 3.707613 6.402928

26 27 28 29 30

26 H 0.000000

27 H 2.677684 0.000000

28 H 10.648509 10.306345 0.000000

29 H 10.306345 10.648509 2.677684 0.000000

30 H 7.523714 9.168339 7.501838 5.368930 0.000000

31 H 5.368930 7.501838 9.168339 7.523715 2.695512

32 Zn 5.328203 5.328203 5.328203 5.328203 5.305507

33 C 2.902396 4.635815 8.506601 7.700349 4.666807

34 C 2.696184 5.070629 9.859095 8.874677 5.101706

35 C 9.859095 8.874676 2.696184 5.070629 8.828324

36 C 3.090025 5.712838 11.020516 9.917838 5.715047

37 C 11.020515 9.917837 3.090025 5.712839 9.891031

38 C 5.070629 2.696184 8.874676 9.859095 9.830405

39 C 5.712838 3.090025 9.917837 11.020516 11.002779

40 C 8.874676 9.859095 5.070629 2.696184 2.707370

41 C 9.917837 11.020516 5.712839 3.090025 3.071336

42 H 10.870219 12.055652 6.414331 3.737187 3.707613

43 H 3.737186 6.414331 12.055653 10.870220 6.402928

44 H 6.414331 3.737187 10.870219 12.055652 12.043752

45 H 12.055652 10.870219 3.737186 6.414331 10.853611

31 32 33 34 35

31 H 0.000000

32 Zn 5.305507 0.000000

33 C 2.911050 3.474724 0.000000

34 C 2.707371 4.890959 1.417081 0.000000

35 C 9.830405 4.890959 8.357972 9.774961 0.000000

36 C 3.071336 6.098400 2.625032 1.208017 10.982730

37 C 11.002779 6.098400 9.565739 10.982730 1.208017

38 C 8.828324 4.890960 5.968025 6.887246 6.936549

39 C 9.891031 6.098401 6.997698 7.800283 7.825294

40 C 5.101706 4.890959 6.020506 6.936550 6.887246

41 C 5.715047 6.098400 7.030390 7.825294 7.800284

42 H 6.402928 7.165704 7.970997 8.677875 8.664888

43 H 3.707614 7.165704 3.692620 2.275603 12.050204

44 H 10.853611 7.165705 7.947581 8.664888 8.677875

45 H 12.043752 7.165704 10.633221 12.050204 2.275603

36 37 38 39 40

36 C 0.000000

37 C 12.190527 0.000000

38 C 7.800283 7.825294 0.000000

39 C 8.622477 8.617530 1.208017 0.000000

40 C 7.825295 7.800284 9.774961 10.982730 0.000000

41 C 8.617531 8.622477 10.982730 12.190527 1.208017

42 H 9.394748 9.415591 12.050204 13.258012 2.275603

43 H 1.067592 13.258012 8.664888 9.415590 8.677875

44 H 9.415590 9.394747 2.275603 1.067592 12.050204

45 H 13.258012 1.067592 8.677875 9.394747 8.664888

41 42 43 44 45

41 C 0.000000

42 H 1.067592 0.000000

43 H 9.394748 10.109803 0.000000

44 H 13.258012 14.325498 10.149472 0.000000

45 H 9.415591 10.149473 14.325498 10.109802 0.000000

Stoichiometry C28H12N4Zn(3)

Framework group C1[X(C28H12N4Zn)]

Deg. of freedom 129

Full point group C1 NOp 1

RotChk: IX=0 Diff= 4.87D-08

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.692835 4.267848 -0.049605

2 6 0 1.100626 2.906239 -0.014407

3 7 0 0.000000 2.092728 0.006516

4 6 0 -1.100624 2.906239 -0.014407

5 6 0 -0.692834 4.267849 -0.049605

6 6 0 -2.467968 2.439960 -0.012488

7 6 0 -2.910771 1.102263 -0.008990

8 7 0 -2.100954 0.000001 0.003745

9 6 0 -2.910772 -1.102261 -0.008990

10 6 0 -4.298196 -0.679594 -0.029485

11 6 0 -4.298195 0.679596 -0.029485

12 6 0 2.467969 2.439959 -0.012488

13 6 0 2.910772 1.102261 -0.008990

14 6 0 4.298196 0.679594 -0.029485

15 6 0 4.298195 -0.679595 -0.029485

16 6 0 2.910772 -1.102263 -0.008989

17 7 0 2.100954 -0.000000 0.003745

18 6 0 2.467968 -2.439960 -0.012488

19 6 0 1.100624 -2.906239 -0.014407

20 6 0 0.692833 -4.267849 -0.049605

21 6 0 -0.692836 -4.267848 -0.049605

22 6 0 -1.100626 -2.906239 -0.014407

23 7 0 -0.000001 -2.092728 0.006516

24 1 0 1.347757 5.126102 -0.075521

25 1 0 -1.347755 5.126102 -0.075521

26 1 0 -5.153173 -1.338841 -0.046003

27 1 0 -5.153172 1.338843 -0.046003

28 1 0 5.153173 1.338841 -0.046003

29 1 0 5.153172 -1.338843 -0.046003

30 1 0 1.347755 -5.126102 -0.075521

31 1 0 -1.347757 -5.126102 -0.075521

32 30 0 0.000000 -0.000000 0.159089

33 6 0 -2.467969 -2.439959 -0.012488

34 6 0 -3.468276 -3.443622 -0.025343

35 6 0 3.468275 3.443622 -0.025343

36 6 0 -4.308766 -4.311237 -0.036493

37 6 0 4.308766 4.311238 -0.036494

38 6 0 -3.468274 3.443624 -0.025343

39 6 0 -4.308764 4.311239 -0.036493

40 6 0 3.468274 -3.443624 -0.025343

41 6 0 4.308764 -4.311239 -0.036493

42 1 0 5.054900 -5.074737 -0.046689

43 1 0 -5.054903 -5.074735 -0.046689

44 1 0 -5.054900 5.074737 -0.046688

45 1 0 5.054902 5.074735 -0.046690

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1465333 0.1452876 0.0729946

Leave Link 202 at Tue Jul 30 02:26:45 2019, MaxMem= 4294967296 cpu: 0.1

(Enter /home/kira/g09/l301.exe)

Basis read from rwf: (5D, 7F)

Pseudo-potential data read from rwf file.

There are 671 symmetry adapted cartesian basis functions of A symmetry.

There are 636 symmetry adapted basis functions of A symmetry.

636 basis functions, 1123 primitive gaussians, 671 cartesian basis functions

111 alpha electrons 109 beta electrons

nuclear repulsion energy 3054.3766505968 Hartrees.

IExCor= 402 DFT=T Ex+Corr=B3LYP ExCW=0 ScaHFX= 0.200000

ScaDFX= 0.800000 0.720000 1.000000 0.810000 ScalE2= 1.000000 1.000000

IRadAn= 0 IRanWt= -1 IRanGd= 0 ICorTp=0 IEmpDi=141

NAtoms= 45 NActive= 45 NUniq= 45 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

R6Disp: Grimme-D3(BJ) Dispersion energy= -0.1301240356 Hartrees.

Nuclear repulsion after empirical dispersion term = 3054.2465265612 Hartrees.

No density basis found on file 724.

Force inversion solution in PCM.

------------------------------------------------------------------------------

Polarizable Continuum Model (PCM)

=================================

Model : PCM (using non-symmetric T matrix).

Atomic radii : SMD-Coulomb.

Polarization charges : Total charges.

Charge compensation : None.

Solution method : Matrix inversion.

Cavity type : VdW (van der Waals Surface) (Alpha=1.000).

Cavity algorithm : GePol (No added spheres)

Default sphere list used, NSphG= 45.

Lebedev-Laikov grids with approx. 5.0 points / Ang\*\*2.

Smoothing algorithm: York/Karplus (Gamma=1.0000).

Polarization charges: spherical gaussians, with

point-specific exponents (IZeta= 3).

Self-potential: point-specific (ISelfS= 7).

Self-field : sphere-specific E.n sum rule (ISelfD= 2).

1st derivatives : Analytical E(r).r(x)/FMM algorithm (CHGder, D1EAlg=3).

Cavity 1st derivative terms included.

2nd derivatives : Analytical E(r).r(xy)/FMM algorithm (CHGder, D2EAlg=3).

Cavity 2nd derivative terms included.

Solvent : DiMethylSulfoxide, Eps= 46.826000 Eps(inf)= 2.007889

------------------------------------------------------------------------------

GePol: Number of generator spheres = 45

GePol: Total number of spheres = 45

GePol: Number of exposed spheres = 45 (100.00%)

GePol: Number of points = 3890

GePol: Average weight of points = 0.11

GePol: Minimum weight of points = 0.13D-07

GePol: Maximum weight of points = 0.18390

GePol: Number of points with low weight = 128

GePol: Fraction of low-weight points (<1% of avg) = 3.29%

GePol: Cavity surface area = 415.770 Ang\*\*2

GePol: Cavity volume = 420.395 Ang\*\*3

------------------------------------------------------------------------------

Atomic radii for non-electrostatic terms: SMD-CDS.

------------------------------------------------------------------------------

PCM non-electrostatic energy = 0.0083168984 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 3054.2548434596 Hartrees.

Leave Link 301 at Tue Jul 30 02:26:45 2019, MaxMem= 4294967296 cpu: 1.9

(Enter /home/kira/g09/l302.exe)

NPDir=0 NMtPBC= 1 NCelOv= 1 NCel= 1 NClECP= 1 NCelD= 1

NCelK= 1 NCelE2= 1 NClLst= 1 CellRange= 0.0.

One-electron integrals computed using PRISM.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16189 LenP2D= 44742.

LDataN: DoStor=T MaxTD1= 5 Len= 102

NBasis= 636 RedAO= T EigKep= 6.88D-05 NBF= 636

NBsUse= 636 1.00D-06 EigRej= -1.00D+00 NBFU= 636

Precomputing XC quadrature grid using

IXCGrd= 4 IRadAn= 0 IRanWt= -1 IRanGd= 0 AccXCQ= 0.00D+00.

Generated NRdTot= 0 NPtTot= 0 NUsed= 0 NTot= 32

NSgBfM= 654 654 654 654 654 MxSgAt= 45 MxSgA2= 45.

Leave Link 302 at Tue Jul 30 02:26:46 2019, MaxMem= 4294967296 cpu: 14.3

(Enter /home/kira/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Tue Jul 30 02:26:46 2019, MaxMem= 4294967296 cpu: 1.2

(Enter /home/kira/g09/l401.exe)

Initial guess from the checkpoint file: "ZnTSPsim3.chk"

B after Tr= 0.000000 -0.000000 0.000000

Rot= 1.000000 -0.000000 -0.000000 -0.000000 Ang= -0.00 deg.

Guess basis will be translated and rotated to current coordinates.

JPrj=2 DoOrth=T DoCkMO=T.

Initial guess <Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0585 S= 1.0194

Leave Link 401 at Tue Jul 30 02:26:47 2019, MaxMem= 4294967296 cpu: 15.6

(Enter /home/kira/g09/l502.exe)

UHF open shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

IVT= 1384965 IEndB= 1384965 NGot= 4294967296 MDV= 4294049884

LenX= 4294049884 LenY= 4293598972

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

Fock matrices will be formed incrementally for 20 cycles.

Cycle 1 Pass 1 IDiag 1:

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 650000000 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Inv3: Mode=1 IEnd= 45396300.

Iteration 1 A\*A^-1 deviation from unit magnitude is 5.55D-15 for 3864.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.69D-15 for 3443 3219.

Iteration 1 A^-1\*A deviation from unit magnitude is 5.55D-15 for 3864.

Iteration 1 A^-1\*A deviation from orthogonality is 2.72D-14 for 3476 3443.

E= -1359.01143205789

DIIS: error= 1.90D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -1359.01143205789 IErMin= 1 ErrMin= 1.90D-05

ErrMax= 1.90D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.64D-07 BMatP= 5.64D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.619 Goal= None Shift= 0.000

Gap= 0.679 Goal= None Shift= 0.000

RMSDP=2.06D-06 MaxDP=1.01D-04 OVMax= 1.10D-04

Cycle 2 Pass 1 IDiag 1:

RMSU= 2.06D-06 CP: 1.00D+00

E= -1359.01143225437 Delta-E= -0.000000196473 Rises=F Damp=F

DIIS: error= 4.51D-06 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -1359.01143225437 IErMin= 2 ErrMin= 4.51D-06

ErrMax= 4.51D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.23D-08 BMatP= 5.64D-07

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.133D-01 0.101D+01

Coeff: -0.133D-01 0.101D+01

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=2.29D-07 MaxDP=5.55D-06 DE=-1.96D-07 OVMax= 2.83D-05

Cycle 3 Pass 1 IDiag 1:

RMSU= 2.08D-07 CP: 1.00D+00 1.05D+00

E= -1359.01143225516 Delta-E= -0.000000000795 Rises=F Damp=F

DIIS: error= 6.19D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -1359.01143225516 IErMin= 2 ErrMin= 4.51D-06

ErrMax= 6.19D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.85D-08 BMatP= 1.23D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.245D-01 0.576D+00 0.448D+00

Coeff: -0.245D-01 0.576D+00 0.448D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=1.01D-07 MaxDP=5.12D-06 DE=-7.95D-10 OVMax= 2.20D-05

Cycle 4 Pass 1 IDiag 1:

RMSU= 7.17D-08 CP: 1.00D+00 1.05D+00 6.62D-01

E= -1359.01143225797 Delta-E= -0.000000002812 Rises=F Damp=F

DIIS: error= 1.20D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -1359.01143225797 IErMin= 4 ErrMin= 1.20D-06

ErrMax= 1.20D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.25D-09 BMatP= 1.23D-08

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.997D-02 0.175D+00 0.234D+00 0.601D+00

Coeff: -0.997D-02 0.175D+00 0.234D+00 0.601D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=3.36D-08 MaxDP=1.67D-06 DE=-2.81D-09 OVMax= 7.06D-06

Cycle 5 Pass 1 IDiag 1:

RMSU= 2.69D-08 CP: 1.00D+00 1.04D+00 6.85D-01 7.31D-01

E= -1359.01143225826 Delta-E= -0.000000000286 Rises=F Damp=F

DIIS: error= 6.43D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -1359.01143225826 IErMin= 5 ErrMin= 6.43D-07

ErrMax= 6.43D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.01D-10 BMatP= 1.25D-09

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: -0.235D-02 0.206D-01 0.723D-01 0.343D+00 0.567D+00

Coeff: -0.235D-02 0.206D-01 0.723D-01 0.343D+00 0.567D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=1.19D-08 MaxDP=3.97D-07 DE=-2.86D-10 OVMax= 1.72D-06

Cycle 6 Pass 1 IDiag 1:

RMSU= 9.74D-09 CP: 1.00D+00 1.05D+00 6.74D-01 7.86D-01 8.30D-01

E= -1359.01143225829 Delta-E= -0.000000000028 Rises=F Damp=F

DIIS: error= 1.35D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -1359.01143225829 IErMin= 6 ErrMin= 1.35D-07

ErrMax= 1.35D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 9.74D-12 BMatP= 2.01D-10

IDIUse=1 WtCom= 1.00D+00 WtEn= 0.00D+00

Coeff-Com: 0.493D-03-0.186D-01-0.671D-02 0.454D-01 0.218D+00 0.762D+00

Coeff: 0.493D-03-0.186D-01-0.671D-02 0.454D-01 0.218D+00 0.762D+00

Gap= 0.040 Goal= None Shift= 0.000

Gap= 0.050 Goal= None Shift= 0.000

RMSDP=3.94D-09 MaxDP=1.02D-07 DE=-2.82D-11 OVMax= 6.78D-07

Error on total polarization charges = 0.06201

SCF Done: E(UB3LYP) = -1359.01143226 A.U. after 6 cycles

NFock= 6 Conv=0.39D-08 -V/T= 1.9682

<Sx>= 0.0000 <Sy>= 0.0000 <Sz>= 1.0000 <S\*\*2>= 2.0585 S= 1.0194

<L.S>= 0.000000000000E+00

KE= 1.403716296051D+03 PE=-9.350907882113D+03 EE= 3.533925310345D+03

SMD-CDS (non-electrostatic) energy (kcal/mol) = 5.22

(included in total energy above)

Annihilation of the first spin contaminant:

S\*\*2 before annihilation 2.0585, after 2.0019

Leave Link 502 at Tue Jul 30 02:28:12 2019, MaxMem= 4294967296 cpu: 1333.0

(Enter /home/kira/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 636

NBasis= 636 NAE= 111 NBE= 109 NFC= 0 NFV= 0

NROrb= 636 NOA= 111 NOB= 109 NVA= 525 NVB= 527

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.13973051D+02

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.39730190D-01

\*\*\*\* Warning!!: The largest beta MO coefficient is 0.13963603D+02

\*\*\*\* Warning!!: The smallest beta delta epsilon is 0.49633856D-01

Leave Link 801 at Tue Jul 30 02:28:12 2019, MaxMem= 4294967296 cpu: 0.5

(Enter /home/kira/g09/l1101.exe)

Using compressed storage, NAtomX= 45.

Will process 46 centers per pass.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16189 LenP2D= 44742.

LDataN: DoStor=T MaxTD1= 6 Len= 172

Number of processors reduced to 11 by ecpmxn.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Tue Jul 30 02:28:15 2019, MaxMem= 4294967296 cpu: 42.0

(Enter /home/kira/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Tue Jul 30 02:28:15 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 45.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 4294966832.

G2DrvN: will do 46 centers at a time, making 1 passes.

Calling FoFCou, ICntrl= 3107 FMM=F I1Cent= 0 AccDes= 0.00D+00.

FoFJK: IHMeth= 1 ICntrl= 3107 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 3107 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

G2PCM: DoFxE=T DoFxN=T DoGrad=T DoDP/DQ/DG/TGxP=FFFF NFrqRd= 0 IEInf=0 SqF1=F DoCFld=F IF1Alg=4.

GePol: Maximum number of non-zero 1st derivatives = 256

End of G2Drv F.D. properties file 721 does not exist.

End of G2Drv F.D. properties file 722 does not exist.

End of G2Drv F.D. properties file 788 does not exist.

Leave Link 1110 at Tue Jul 30 02:34:06 2019, MaxMem= 4294967296 cpu: 5602.7

(Enter /home/kira/g09/l1002.exe)

Minotr: UHF open shell wavefunction.

IDoAtm=111111111111111111111111111111111111111111111

NEqPCM: Using equilibrium solvation (IEInf=0, Eps= 46.8260, EpsInf= 2.0079)

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Differentiating once with respect to nuclear coordinates.

Requested convergence is 1.0D-08 RMS, and 1.0D-07 maximum.

Secondary convergence is 1.0D-12 RMS, and 1.0D-12 maximum.

NewPWx=T KeepS1=F KeepF1=F KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 4294965570 using IRadAn= 2.

Generate precomputed XC quadrature information.

Solving linear equations simultaneously, MaxMat= 0.

FoFJK: IHMeth= 1 ICntrl= 0 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 650000000 NMat= 138 IRICut= 345 DoRegI=T DoRafI=T ISym2E= 2.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 0 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 138 NMatS0= 138 NMatT0= 0 NMatD0= 138 NMtDS0= 0 NMtDT0= 0

Integrals replicated using symmetry in FoFCou.

There are 138 degrees of freedom in the 1st order CPHF. IDoFFX=6 NUNeed= 3.

135 vectors produced by pass 0 Test12= 1.16D-13 1.00D-09 XBig12= 7.02D+03 5.70D+01.

AX will form 135 AO Fock derivatives at one time.

135 vectors produced by pass 1 Test12= 1.16D-13 1.00D-09 XBig12= 4.50D+02 3.30D+00.

135 vectors produced by pass 2 Test12= 1.16D-13 1.00D-09 XBig12= 1.60D+01 9.75D-01.

135 vectors produced by pass 3 Test12= 1.16D-13 1.00D-09 XBig12= 2.16D-01 9.07D-02.

135 vectors produced by pass 4 Test12= 1.16D-13 1.00D-09 XBig12= 1.24D-03 4.63D-03.

135 vectors produced by pass 5 Test12= 1.16D-13 1.00D-09 XBig12= 8.37D-06 2.22D-04.

133 vectors produced by pass 6 Test12= 1.16D-13 1.00D-09 XBig12= 4.67D-08 2.94D-05.

65 vectors produced by pass 7 Test12= 1.16D-13 1.00D-09 XBig12= 1.97D-10 1.19D-06.

3 vectors produced by pass 8 Test12= 1.16D-13 1.00D-09 XBig12= 1.04D-12 7.97D-08.

2 vectors produced by pass 9 Test12= 1.16D-13 1.00D-09 XBig12= 2.28D-14 1.30D-08.

InvSVY: IOpt=1 It= 1 EMax= 8.53D-14

Solved reduced A of dimension 1013 with 138 vectors.

FullF1: Do perturbations 1 to 3.

Isotropic polarizability for W= 0.000000 1006.39 Bohr\*\*3.

End of Minotr F.D. properties file 721 does not exist.

End of Minotr F.D. properties file 722 does not exist.

End of Minotr F.D. properties file 788 does not exist.

Leave Link 1002 at Tue Jul 30 03:31:20 2019, MaxMem= 4294967296 cpu: 54940.5

(Enter /home/kira/g09/l701.exe)

Compute integral second derivatives.

... and contract with generalized density number 0.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 2nd derivatives to the Hessian.

1 Symmetry operations used in ECPInt.

ECPInt: NShTT= 20910 NPrTT= 103900 LenC2= 16189 LenP2D= 44742.

LDataN: DoStor=T MaxTD1= 7 Len= 274

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 256

Leave Link 701 at Tue Jul 30 03:31:55 2019, MaxMem= 4294967296 cpu: 561.7

(Enter /home/kira/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Tue Jul 30 03:31:55 2019, MaxMem= 4294967296 cpu: 0.3

(Enter /home/kira/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 1 NMat=1 NMatS=1 NMatT=0.

FoFJK: IHMeth= 1 ICntrl= 100127 DoSepK=F KAlg= 0 I1Cent= 0 FoldK=F

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0.

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 800

NFxFlg= 0 DoJE=F BraDBF=F KetDBF=F FulRan=T

wScrn= 0.000000 ICntrl= 100127 IOpCl= 1 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Symmetry not used in FoFCou.

Leave Link 703 at Tue Jul 30 03:39:13 2019, MaxMem= 4294967296 cpu: 7004.8

(Enter /home/kira/g09/l716.exe)

Dipole = 4.24278762D-07 9.95524792D-07 3.21707658D-01

Polarizability= 1.22330807D+03-1.54031080D-04 1.61451938D+03

1.31824202D-06-2.25026142D-06 1.81332168D+02

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000000014 -0.000000015 -0.000000008

2 6 -0.000000055 0.000000068 0.000000007

3 7 -0.000000049 -0.000000554 0.000001666

4 6 0.000000054 0.000000028 0.000000007

5 6 -0.000000017 -0.000000015 -0.000000007

6 6 -0.000000172 -0.000000064 0.000000007

7 6 0.000000132 0.000000044 0.000000010

8 7 0.000000492 0.000000058 0.000001303

9 6 0.000000085 -0.000000021 0.000000010

10 6 -0.000000029 0.000000035 -0.000000002

11 6 -0.000000028 -0.000000033 -0.000000000

12 6 0.000000167 -0.000000062 0.000000008

13 6 -0.000000130 0.000000030 0.000000010

14 6 0.000000032 -0.000000008 -0.000000001

15 6 0.000000034 0.000000015 -0.000000001

16 6 -0.000000099 0.000000035 0.000000010

17 7 -0.000000402 0.000000025 0.000001297

18 6 0.000000195 0.000000014 0.000000008

19 6 -0.000000117 -0.000000048 0.000000007

20 6 0.000000031 0.000000006 -0.000000008

21 6 -0.000000037 0.000000013 -0.000000007

22 6 0.000000050 -0.000000023 0.000000006

23 7 -0.000000029 0.000000460 0.000001661

24 1 -0.000000007 0.000000008 -0.000000005

25 1 0.000000007 0.000000007 -0.000000005

26 1 -0.000000005 0.000000009 0.000000003

27 1 -0.000000006 -0.000000011 0.000000003

28 1 0.000000003 -0.000000007 0.000000003

29 1 0.000000004 0.000000009 0.000000004

30 1 -0.000000005 -0.000000005 -0.000000005

31 1 0.000000006 -0.000000006 -0.000000005

32 30 0.000000025 -0.000000026 -0.000005961

33 6 -0.000000150 0.000000041 0.000000008

34 6 0.000000143 0.000000145 0.000000009

35 6 -0.000000145 -0.000000143 0.000000009

36 6 -0.000000022 -0.000000023 -0.000000011

37 6 0.000000020 0.000000024 -0.000000010

38 6 0.000000163 -0.000000166 0.000000008

39 6 -0.000000030 0.000000033 -0.000000010

40 6 -0.000000148 0.000000152 0.000000009

41 6 0.000000027 -0.000000030 -0.000000011

42 1 0.000000029 -0.000000029 -0.000000003

43 1 -0.000000030 -0.000000030 -0.000000003

44 1 -0.000000031 0.000000030 -0.000000004

45 1 0.000000031 0.000000030 -0.000000004

-------------------------------------------------------------------

Cartesian Forces: Max 0.000005961 RMS 0.000000582

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Leave Link 716 at Tue Jul 30 03:39:13 2019, MaxMem= 4294967296 cpu: 0.8

(Enter /home/kira/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000001353 RMS 0.000000244

Search for a local minimum.

Step number 5 out of a maximum of 270

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .24431D-06 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -3.38D-08 DEPred=-3.23D-08 R= 1.04D+00

Trust test= 1.04D+00 RLast= 3.49D-03 DXMaxT set to 5.05D-01

ITU= 0 0 1 1 0

Eigenvalues --- 0.00209 0.00224 0.00231 0.00257 0.00289

Eigenvalues --- 0.00734 0.00793 0.00800 0.00812 0.01042

Eigenvalues --- 0.01055 0.01110 0.01151 0.01155 0.01251

Eigenvalues --- 0.01252 0.01491 0.01492 0.01538 0.01668

Eigenvalues --- 0.01683 0.01850 0.02107 0.02149 0.02155

Eigenvalues --- 0.02320 0.02759 0.02764 0.02800 0.02810

Eigenvalues --- 0.02904 0.03175 0.03352 0.03747 0.04048

Eigenvalues --- 0.04158 0.04191 0.04201 0.04208 0.04210

Eigenvalues --- 0.04381 0.04456 0.04628 0.04701 0.06901

Eigenvalues --- 0.07810 0.08167 0.08226 0.08235 0.08315

Eigenvalues --- 0.08379 0.08465 0.08522 0.08709 0.09673

Eigenvalues --- 0.09685 0.09706 0.09726 0.10353 0.10439

Eigenvalues --- 0.10442 0.10484 0.11095 0.11376 0.12458

Eigenvalues --- 0.12593 0.12959 0.14385 0.16556 0.17162

Eigenvalues --- 0.19269 0.19508 0.19689 0.20227 0.20517

Eigenvalues --- 0.20536 0.20711 0.20937 0.21696 0.21732

Eigenvalues --- 0.21817 0.24516 0.25437 0.25886 0.27837

Eigenvalues --- 0.27896 0.29196 0.29306 0.31170 0.32563

Eigenvalues --- 0.33197 0.33369 0.33962 0.35790 0.35952

Eigenvalues --- 0.36001 0.36492 0.36669 0.37202 0.37294

Eigenvalues --- 0.37318 0.37570 0.37612 0.37863 0.38066

Eigenvalues --- 0.38079 0.38638 0.39135 0.39516 0.40078

Eigenvalues --- 0.40078 0.40078 0.40087 0.40768 0.41081

Eigenvalues --- 0.41172 0.42489 0.45274 0.45558 0.45701

Eigenvalues --- 0.46338 0.50557 0.50688 0.52883 0.53380

Eigenvalues --- 1.03265 1.03899 1.04306 1.04377

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4 3 2

RFO step: Lambda=-2.26029266D-10.

NNeg= 0 NP= 4 Switch= 2.50D-03 Rises=F DC= 3.79D-05 SmlDif= 1.00D-05

RMS Error= 0.3799893881D-05 NUsed= 4 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.28758 -0.28644 -0.00143 0.00030

Iteration 1 RMS(Cart)= 0.00005392 RMS(Int)= 0.00000002

Iteration 2 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000002

ITry= 1 IFail=0 DXMaxC= 7.00D-04 DCOld= 1.00D+10 DXMaxT= 5.05D-01 DXLimC= 3.00D+00 Rises=F

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.68681 0.00000 0.00000 0.00000 0.00000 2.68681

R2 2.61853 0.00000 0.00000 0.00000 0.00000 2.61854

R3 2.04072 -0.00000 0.00000 -0.00000 0.00000 2.04072

R4 2.58666 -0.00000 -0.00001 0.00000 -0.00001 2.58665

R5 2.73002 0.00000 0.00001 0.00000 0.00001 2.73002

R6 2.58666 0.00000 -0.00001 0.00000 -0.00000 2.58665

R7 3.96518 0.00000 0.00000 -0.00000 0.00000 3.96518

R8 2.68681 0.00000 0.00000 0.00000 0.00000 2.68681

R9 2.73002 0.00000 0.00001 -0.00000 0.00001 2.73002

R10 2.04072 -0.00000 0.00000 -0.00000 0.00000 2.04072

R11 2.66279 0.00000 0.00001 -0.00000 0.00001 2.66279

R12 2.67789 0.00000 -0.00000 0.00000 0.00000 2.67790

R13 2.58482 0.00000 -0.00000 0.00000 -0.00000 2.58481

R14 2.74109 -0.00000 0.00000 -0.00000 0.00000 2.74109

R15 2.58482 0.00000 -0.00000 0.00000 -0.00000 2.58481

R16 3.98107 0.00000 -0.00000 0.00000 -0.00000 3.98106

R17 2.74109 -0.00000 0.00000 -0.00000 0.00000 2.74109

R18 2.66279 0.00000 0.00001 0.00000 0.00001 2.66279

R19 2.56850 0.00000 0.00000 -0.00000 0.00000 2.56850

R20 2.04044 0.00000 0.00000 0.00000 0.00000 2.04044

R21 2.04044 0.00000 0.00000 0.00000 0.00000 2.04044

R22 2.66279 0.00000 0.00001 0.00000 0.00001 2.66279

R23 2.67789 0.00000 -0.00000 0.00000 0.00000 2.67790

R24 2.74109 -0.00000 0.00000 -0.00000 0.00000 2.74109

R25 2.58482 0.00000 -0.00000 -0.00000 -0.00000 2.58481

R26 2.56850 0.00000 0.00000 -0.00000 0.00000 2.56850

R27 2.04044 0.00000 0.00000 0.00000 0.00000 2.04044

R28 2.74109 -0.00000 0.00000 -0.00000 0.00000 2.74109

R29 2.04044 0.00000 0.00000 0.00000 0.00000 2.04044

R30 2.58482 0.00000 -0.00000 0.00000 -0.00000 2.58481

R31 2.66279 0.00000 0.00001 -0.00000 0.00001 2.66279

R32 3.98107 0.00000 -0.00000 0.00000 -0.00000 3.98106

R33 2.73002 -0.00000 0.00001 -0.00000 0.00001 2.73002

R34 2.67789 0.00000 -0.00000 0.00000 0.00000 2.67790

R35 2.68681 0.00000 0.00000 0.00000 0.00000 2.68681

R36 2.58666 0.00000 -0.00001 0.00000 -0.00000 2.58665

R37 2.61853 0.00000 0.00000 0.00000 0.00000 2.61854

R38 2.04072 -0.00000 0.00000 -0.00000 0.00000 2.04072

R39 2.68681 0.00000 0.00000 0.00000 0.00000 2.68681

R40 2.04072 -0.00000 0.00000 -0.00000 0.00000 2.04072

R41 2.58666 0.00000 -0.00000 0.00000 -0.00000 2.58665

R42 2.73002 0.00000 0.00001 0.00000 0.00001 2.73002

R43 3.96518 0.00000 0.00000 -0.00000 0.00000 3.96518

R44 2.67789 0.00000 -0.00000 0.00000 0.00000 2.67790

R45 2.28282 -0.00000 0.00000 -0.00000 0.00000 2.28282

R46 2.28282 -0.00000 0.00000 -0.00000 0.00000 2.28282

R47 2.01746 -0.00000 0.00000 -0.00000 -0.00000 2.01746

R48 2.01746 -0.00000 0.00000 -0.00000 -0.00000 2.01746

R49 2.28282 -0.00000 0.00000 -0.00000 -0.00000 2.28282

R50 2.01746 -0.00000 0.00000 -0.00000 -0.00000 2.01746

R51 2.28282 -0.00000 0.00000 -0.00000 -0.00000 2.28282

R52 2.01746 -0.00000 0.00000 -0.00000 -0.00000 2.01746

A1 1.86169 0.00000 0.00000 -0.00000 0.00000 1.86170

A2 2.19908 -0.00000 0.00000 0.00000 0.00000 2.19908

A3 2.22240 0.00000 -0.00000 0.00000 -0.00000 2.22240

A4 1.91657 -0.00000 -0.00001 0.00000 -0.00001 1.91656

A5 2.19025 0.00000 0.00001 -0.00000 0.00001 2.19026

A6 2.17633 0.00000 -0.00000 0.00000 -0.00000 2.17633

A7 1.86825 0.00000 0.00001 -0.00000 0.00001 1.86827

A8 2.20665 -0.00000 -0.00000 0.00000 -0.00000 2.20665

A9 2.20665 -0.00000 -0.00000 0.00000 -0.00000 2.20664

A10 1.91657 -0.00000 -0.00001 0.00000 -0.00001 1.91656

A11 2.17633 0.00000 -0.00000 -0.00000 -0.00000 2.17633

A12 2.19025 0.00000 0.00001 -0.00000 0.00001 2.19026

A13 1.86169 0.00000 0.00000 -0.00000 0.00000 1.86170

A14 2.22240 0.00000 -0.00000 -0.00000 -0.00000 2.22240

A15 2.19908 -0.00000 0.00000 0.00000 0.00000 2.19908

A16 2.21911 0.00000 0.00001 0.00000 0.00001 2.21912

A17 2.02584 -0.00000 -0.00001 -0.00000 -0.00001 2.02583

A18 2.03821 -0.00000 -0.00001 -0.00000 -0.00001 2.03820

A19 2.18829 -0.00000 0.00000 -0.00000 0.00000 2.18829

A20 2.18606 0.00000 0.00001 0.00000 0.00001 2.18606

A21 1.90880 -0.00000 -0.00001 -0.00000 -0.00001 1.90880

A22 1.87422 0.00000 0.00001 -0.00000 0.00001 1.87423

A23 2.20325 -0.00000 -0.00000 0.00000 -0.00000 2.20324

A24 2.20325 -0.00000 -0.00000 0.00000 -0.00000 2.20324

A25 1.90880 -0.00000 -0.00001 -0.00000 -0.00001 1.90880

A26 2.18829 -0.00000 0.00000 -0.00000 0.00000 2.18829

A27 2.18606 0.00000 0.00001 0.00000 0.00001 2.18606

A28 1.86648 0.00000 0.00000 0.00000 0.00000 1.86648

A29 2.18914 -0.00000 0.00000 -0.00000 0.00000 2.18914

A30 2.22756 -0.00000 -0.00000 0.00000 -0.00000 2.22755

A31 1.86648 0.00000 0.00000 0.00000 0.00000 1.86648

A32 2.18914 -0.00000 0.00000 -0.00000 0.00000 2.18914

A33 2.22756 0.00000 -0.00000 0.00000 -0.00000 2.22755

A34 2.21911 0.00000 0.00001 0.00000 0.00001 2.21912

A35 2.02584 -0.00000 -0.00001 -0.00000 -0.00001 2.02583

A36 2.03821 -0.00000 -0.00001 -0.00000 -0.00001 2.03820

A37 2.18606 0.00000 0.00001 0.00000 0.00001 2.18606

A38 2.18829 -0.00000 0.00000 -0.00000 0.00000 2.18829

A39 1.90880 -0.00000 -0.00001 -0.00000 -0.00001 1.90880

A40 1.86648 0.00000 0.00000 0.00000 0.00000 1.86648

A41 2.18914 -0.00000 0.00000 -0.00000 0.00000 2.18914

A42 2.22756 -0.00000 -0.00000 0.00000 -0.00000 2.22755

A43 1.86648 0.00000 0.00000 0.00000 0.00000 1.86648

A44 2.22756 -0.00000 -0.00000 0.00000 -0.00000 2.22755

A45 2.18914 -0.00000 0.00000 -0.00000 0.00000 2.18914

A46 1.90880 -0.00000 -0.00001 -0.00000 -0.00001 1.90880

A47 2.18606 0.00000 0.00001 0.00000 0.00001 2.18606

A48 2.18829 -0.00000 0.00000 -0.00000 0.00000 2.18829

A49 1.87422 0.00000 0.00001 -0.00000 0.00001 1.87423

A50 2.20325 -0.00000 -0.00000 0.00000 -0.00000 2.20324

A51 2.20325 -0.00000 -0.00000 0.00000 -0.00000 2.20324

A52 2.21911 0.00000 0.00001 0.00000 0.00001 2.21912

A53 2.03821 -0.00000 -0.00001 -0.00000 -0.00001 2.03820

A54 2.02584 -0.00000 -0.00001 -0.00000 -0.00001 2.02583

A55 2.19025 0.00000 0.00001 -0.00000 0.00001 2.19026

A56 2.17633 0.00000 -0.00000 -0.00000 -0.00000 2.17633

A57 1.91657 -0.00000 -0.00001 0.00000 -0.00001 1.91656

A58 1.86169 0.00000 0.00000 -0.00000 0.00000 1.86170

A59 2.19908 -0.00000 0.00000 0.00000 0.00000 2.19908

A60 2.22240 -0.00000 -0.00000 -0.00000 -0.00000 2.22240

A61 1.86169 0.00000 0.00000 -0.00000 0.00000 1.86170

A62 2.22240 -0.00000 -0.00000 0.00000 -0.00000 2.22240

A63 2.19908 -0.00000 0.00000 0.00000 0.00000 2.19908

A64 1.91657 -0.00000 -0.00001 0.00000 -0.00001 1.91656

A65 2.19025 0.00000 0.00001 -0.00000 0.00001 2.19026

A66 2.17633 0.00000 -0.00000 0.00000 -0.00000 2.17633

A67 1.86825 0.00000 0.00001 -0.00000 0.00001 1.86827

A68 2.20665 -0.00000 -0.00000 0.00000 -0.00000 2.20664

A69 2.20665 -0.00000 -0.00000 0.00000 -0.00000 2.20665

A70 1.56543 0.00000 0.00002 0.00000 0.00002 1.56546

A71 1.56543 0.00000 0.00002 0.00000 0.00002 1.56546

A72 1.56543 0.00000 0.00002 0.00000 0.00002 1.56546

A73 1.56543 0.00000 0.00002 0.00000 0.00002 1.56546

A74 2.21911 0.00000 0.00001 0.00000 0.00001 2.21912

A75 2.03821 -0.00000 -0.00001 -0.00000 -0.00001 2.03820

A76 2.02584 -0.00000 -0.00001 -0.00000 -0.00001 2.02583

A77 3.13087 0.00000 0.00004 0.00000 0.00004 3.13091

A78 3.13087 0.00000 0.00004 0.00000 0.00004 3.13091

A79 3.15579 0.00000 -0.00000 0.00000 0.00000 3.15579

A80 3.12739 -0.00000 0.00000 -0.00000 -0.00000 3.12739

A81 3.13721 0.00000 0.00000 -0.00000 -0.00000 3.13721

A82 3.14596 -0.00000 -0.00000 0.00000 0.00000 3.14596

A83 3.12739 0.00000 0.00000 -0.00000 -0.00000 3.12739

A84 3.14596 -0.00000 -0.00000 0.00000 0.00000 3.14596

A85 3.15579 -0.00000 0.00000 0.00000 0.00000 3.15579

A86 3.13721 0.00000 0.00000 -0.00000 -0.00000 3.13721

A87 3.28675 -0.00000 -0.00031 0.00000 -0.00031 3.28644

A88 2.99437 0.00000 0.00028 0.00000 0.00028 2.99465

A89 3.14131 -0.00000 0.00000 -0.00000 -0.00000 3.14131

A90 3.14147 0.00000 -0.00000 0.00000 0.00000 3.14147

A91 3.14127 -0.00000 0.00000 -0.00000 0.00000 3.14127

A92 3.14206 0.00000 -0.00000 0.00000 -0.00000 3.14206

A93 3.14171 -0.00000 0.00000 -0.00000 -0.00000 3.14171

A94 3.14113 -0.00000 0.00000 -0.00000 0.00000 3.14113

A95 3.14188 0.00000 -0.00000 0.00000 0.00000 3.14188

A96 3.14192 0.00000 -0.00000 0.00000 -0.00000 3.14192

D1 0.00008 0.00000 -0.00000 0.00000 -0.00000 0.00008

D2 3.13298 0.00000 0.00000 0.00000 0.00001 3.13299

D3 -3.13724 0.00000 -0.00001 0.00000 -0.00001 -3.13725

D4 -0.00434 0.00000 -0.00000 0.00000 0.00000 -0.00434

D5 -0.00000 -0.00000 0.00000 0.00000 0.00000 0.00000

D6 -3.13725 -0.00000 -0.00001 -0.00000 -0.00001 -3.13726

D7 3.13725 0.00000 0.00001 0.00000 0.00001 3.13726

D8 -0.00000 0.00000 -0.00000 -0.00000 0.00000 0.00000

D9 -0.00013 -0.00000 0.00001 -0.00000 0.00001 -0.00013

D10 -3.08322 -0.00000 -0.00014 -0.00000 -0.00014 -3.08336

D11 -3.13311 -0.00000 -0.00000 -0.00000 -0.00000 -3.13312

D12 0.06699 -0.00000 -0.00015 -0.00000 -0.00015 0.06683

D13 -3.11424 -0.00000 -0.00004 0.00000 -0.00004 -3.11428

D14 0.01871 -0.00000 -0.00002 -0.00000 -0.00002 0.01869

D15 0.01740 -0.00000 -0.00003 0.00000 -0.00003 0.01738

D16 -3.13283 0.00000 -0.00001 -0.00000 -0.00001 -3.13284

D17 0.00013 0.00000 -0.00001 0.00000 -0.00001 0.00013

D18 3.13311 0.00000 0.00000 0.00000 0.00000 3.13312

D19 3.08322 0.00000 0.00014 0.00000 0.00014 3.08336

D20 -0.06699 0.00000 0.00015 0.00000 0.00015 -0.06683

D21 -3.10275 -0.00000 -0.00005 -0.00000 -0.00005 -3.10281

D22 -0.10838 0.00000 0.00023 0.00000 0.00023 -0.10815

D23 0.10838 -0.00000 -0.00023 -0.00000 -0.00023 0.10815

D24 3.10275 0.00000 0.00005 0.00000 0.00005 3.10281

D25 -0.00008 -0.00000 0.00000 -0.00000 0.00000 -0.00008

D26 3.13724 -0.00000 0.00001 -0.00000 0.00001 3.13725

D27 -3.13298 -0.00000 -0.00000 -0.00000 -0.00001 -3.13299

D28 0.00434 -0.00000 0.00000 -0.00000 -0.00000 0.00434

D29 -0.01740 0.00000 0.00003 -0.00000 0.00003 -0.01738

D30 3.13283 -0.00000 0.00001 0.00000 0.00001 3.13284

D31 3.11424 0.00000 0.00004 -0.00000 0.00004 3.11428

D32 -0.01871 0.00000 0.00002 0.00000 0.00002 -0.01869

D33 0.00944 -0.00000 -0.00002 -0.00000 -0.00002 0.00942

D34 -3.12275 -0.00000 -0.00005 0.00000 -0.00005 -3.12279

D35 -3.14084 0.00000 -0.00000 -0.00000 -0.00001 -3.14085

D36 0.01015 -0.00000 -0.00003 -0.00000 -0.00003 0.01012

D37 -3.13249 -0.00000 -0.00003 0.00001 -0.00003 -3.13252

D38 0.08114 -0.00000 -0.00016 0.00000 -0.00016 0.08098

D39 0.00097 -0.00000 -0.00001 0.00000 -0.00001 0.00096

D40 -3.06860 -0.00000 -0.00014 -0.00000 -0.00014 -3.06873

D41 3.13287 0.00000 0.00003 -0.00000 0.00003 3.13289

D42 -0.00431 0.00000 0.00002 -0.00000 0.00002 -0.00429

D43 -0.00060 0.00000 0.00001 -0.00000 0.00000 -0.00059

D44 -3.13777 0.00000 -0.00001 -0.00000 -0.00001 -3.13778

D45 -0.00097 0.00000 0.00001 -0.00000 0.00001 -0.00096

D46 3.13249 0.00000 0.00003 -0.00001 0.00003 3.13252

D47 3.06860 0.00000 0.00014 0.00000 0.00014 3.06873

D48 -0.08114 0.00000 0.00016 -0.00000 0.00016 -0.08098

D49 -0.11521 0.00000 0.00023 0.00000 0.00023 -0.11497

D50 -3.11164 -0.00000 -0.00008 0.00000 -0.00008 -3.11172

D51 3.11164 0.00000 0.00008 -0.00000 0.00008 3.11172

D52 0.11521 -0.00000 -0.00023 -0.00000 -0.00023 0.11497

D53 0.00060 -0.00000 -0.00001 0.00000 -0.00000 0.00059

D54 3.13777 -0.00000 0.00001 0.00000 0.00001 3.13778

D55 -3.13287 -0.00000 -0.00003 0.00000 -0.00003 -3.13289

D56 0.00431 -0.00000 -0.00002 0.00000 -0.00002 0.00429

D57 -0.00944 0.00000 0.00002 0.00000 0.00002 -0.00942

D58 3.14085 -0.00000 0.00000 0.00000 0.00001 3.14085

D59 3.12275 0.00000 0.00005 -0.00000 0.00005 3.12279

D60 -0.01015 0.00000 0.00003 0.00000 0.00003 -0.01012

D61 0.00000 0.00000 0.00000 -0.00000 -0.00000 0.00000

D62 3.13705 0.00000 0.00001 -0.00000 0.00001 3.13706

D63 -3.13705 -0.00000 -0.00001 0.00000 -0.00001 -3.13706

D64 0.00000 -0.00000 0.00000 -0.00000 -0.00000 -0.00000

D65 3.12275 0.00000 0.00005 -0.00000 0.00005 3.12279

D66 -0.00944 0.00000 0.00002 0.00000 0.00002 -0.00942

D67 -0.01015 0.00000 0.00003 0.00000 0.00003 -0.01012

D68 3.14085 -0.00000 0.00000 0.00000 0.00001 3.14085

D69 -3.13287 -0.00000 -0.00003 0.00000 -0.00003 -3.13289

D70 0.00431 -0.00000 -0.00002 0.00000 -0.00002 0.00429

D71 0.00060 -0.00000 -0.00001 0.00000 -0.00000 0.00059

D72 3.13777 -0.00000 0.00001 0.00000 0.00001 3.13778

D73 3.13249 0.00000 0.00003 -0.00001 0.00003 3.13252

D74 -0.08114 0.00000 0.00016 -0.00000 0.00016 -0.08098

D75 -0.00097 0.00000 0.00001 -0.00000 0.00001 -0.00096

D76 3.06860 0.00000 0.00014 0.00000 0.00014 3.06873

D77 0.00000 0.00000 0.00000 -0.00000 0.00000 0.00000

D78 3.13705 0.00000 0.00001 -0.00000 0.00001 3.13706

D79 -3.13705 -0.00000 -0.00001 0.00000 -0.00001 -3.13706

D80 -0.00000 0.00000 -0.00000 0.00000 0.00000 0.00000

D81 -0.00060 0.00000 0.00001 -0.00000 0.00000 -0.00059

D82 3.13287 0.00000 0.00003 -0.00000 0.00003 3.13289

D83 -3.13777 0.00000 -0.00001 -0.00000 -0.00001 -3.13778

D84 -0.00431 0.00000 0.00002 -0.00000 0.00002 -0.00429

D85 0.00097 -0.00000 -0.00001 0.00000 -0.00001 0.00096

D86 -3.06860 -0.00000 -0.00014 -0.00000 -0.00014 -3.06873

D87 -3.13249 -0.00000 -0.00003 0.00001 -0.00003 -3.13252

D88 0.08114 -0.00000 -0.00016 0.00000 -0.00016 0.08098

D89 -3.12275 -0.00000 -0.00005 0.00000 -0.00005 -3.12279

D90 0.01015 -0.00000 -0.00003 -0.00000 -0.00003 0.01012

D91 0.00944 -0.00000 -0.00002 -0.00000 -0.00002 0.00942

D92 -3.14085 0.00000 -0.00000 -0.00000 -0.00001 -3.14085

D93 0.11521 -0.00000 -0.00023 -0.00000 -0.00023 0.11497

D94 3.11164 0.00000 0.00008 -0.00000 0.00008 3.11172

D95 -3.11164 -0.00000 -0.00008 0.00000 -0.00008 -3.11172

D96 -0.11521 0.00000 0.00023 0.00000 0.00023 -0.11497

D97 3.11424 0.00000 0.00004 -0.00000 0.00004 3.11428

D98 -0.01740 0.00000 0.00003 -0.00000 0.00003 -0.01738

D99 -0.01871 0.00000 0.00002 0.00000 0.00002 -0.01869

D100 3.13283 -0.00000 0.00001 0.00000 0.00001 3.13284

D101 -3.13298 -0.00000 -0.00000 -0.00000 -0.00001 -3.13299

D102 0.00434 -0.00000 0.00000 -0.00000 -0.00000 0.00434

D103 -0.00008 -0.00000 0.00000 -0.00000 0.00000 -0.00008

D104 3.13724 -0.00000 0.00001 -0.00000 0.00001 3.13725

D105 3.13311 0.00000 0.00000 0.00000 0.00000 3.13312

D106 -0.06699 0.00000 0.00015 0.00000 0.00015 -0.06683

D107 0.00013 0.00000 -0.00001 0.00000 -0.00001 0.00013

D108 3.08322 0.00000 0.00014 0.00000 0.00014 3.08336

D109 -0.00000 0.00000 -0.00000 0.00000 0.00000 -0.00000

D110 3.13725 0.00000 0.00001 0.00000 0.00001 3.13726

D111 -3.13725 -0.00000 -0.00001 -0.00000 -0.00001 -3.13726

D112 0.00000 -0.00000 0.00000 -0.00000 0.00000 0.00000

D113 0.00008 0.00000 -0.00000 0.00000 -0.00000 0.00008

D114 3.13298 0.00000 0.00000 0.00000 0.00001 3.13299

D115 -3.13724 0.00000 -0.00001 0.00000 -0.00001 -3.13725

D116 -0.00434 0.00000 -0.00000 0.00000 0.00000 -0.00434

D117 -0.00013 -0.00000 0.00001 -0.00000 0.00001 -0.00013

D118 -3.08322 -0.00000 -0.00014 -0.00000 -0.00014 -3.08336

D119 -3.13311 -0.00000 -0.00000 -0.00000 -0.00000 -3.13312

D120 0.06699 -0.00000 -0.00015 -0.00000 -0.00015 0.06683

D121 -3.11424 -0.00000 -0.00004 0.00000 -0.00004 -3.11428

D122 0.01871 -0.00000 -0.00002 -0.00000 -0.00002 0.01869

D123 0.01740 -0.00000 -0.00003 0.00000 -0.00003 0.01738

D124 -3.13283 0.00000 -0.00001 -0.00000 -0.00001 -3.13284

D125 3.10275 0.00000 0.00005 0.00000 0.00005 3.10281

D126 0.10838 -0.00000 -0.00022 -0.00000 -0.00023 0.10815

D127 -0.10838 0.00000 0.00023 0.00000 0.00023 -0.10815

D128 -3.10275 -0.00000 -0.00005 -0.00000 -0.00005 -3.10281

Item Value Threshold Converged?

Maximum Force 0.000001 0.000450 YES

RMS Force 0.000000 0.000300 YES

Maximum Displacement 0.000700 0.001800 YES

RMS Displacement 0.000054 0.001200 YES

Predicted change in Energy=-1.976649D-09

Optimization completed.

-- Stationary point found.

----------------------------

! Optimized Parameters !

! (Angstroms and Degrees) !

-------------------------- --------------------------

! Name Definition Value Derivative Info. !

--------------------------------------------------------------------------------

! R1 R(1,2) 1.4218 -DE/DX = 0.0 !

! R2 R(1,5) 1.3857 -DE/DX = 0.0 !

! R3 R(1,24) 1.0799 -DE/DX = 0.0 !

! R4 R(2,3) 1.3688 -DE/DX = 0.0 !

! R5 R(2,12) 1.4447 -DE/DX = 0.0 !

! R6 R(3,4) 1.3688 -DE/DX = 0.0 !

! R7 R(3,32) 2.0983 -DE/DX = 0.0 !

! R8 R(4,5) 1.4218 -DE/DX = 0.0 !

! R9 R(4,6) 1.4447 -DE/DX = 0.0 !

! R10 R(5,25) 1.0799 -DE/DX = 0.0 !

! R11 R(6,7) 1.4091 -DE/DX = 0.0 !

! R12 R(6,38) 1.4171 -DE/DX = 0.0 !

! R13 R(7,8) 1.3678 -DE/DX = 0.0 !

! R14 R(7,11) 1.4505 -DE/DX = 0.0 !

! R15 R(8,9) 1.3678 -DE/DX = 0.0 !

! R16 R(8,32) 2.1067 -DE/DX = 0.0 !

! R17 R(9,10) 1.4505 -DE/DX = 0.0 !

! R18 R(9,33) 1.4091 -DE/DX = 0.0 !

! R19 R(10,11) 1.3592 -DE/DX = 0.0 !

! R20 R(10,26) 1.0798 -DE/DX = 0.0 !

! R21 R(11,27) 1.0798 -DE/DX = 0.0 !

! R22 R(12,13) 1.4091 -DE/DX = 0.0 !

! R23 R(12,35) 1.4171 -DE/DX = 0.0 !

! R24 R(13,14) 1.4505 -DE/DX = 0.0 !

! R25 R(13,17) 1.3678 -DE/DX = 0.0 !

! R26 R(14,15) 1.3592 -DE/DX = 0.0 !

! R27 R(14,28) 1.0798 -DE/DX = 0.0 !

! R28 R(15,16) 1.4505 -DE/DX = 0.0 !

! R29 R(15,29) 1.0798 -DE/DX = 0.0 !

! R30 R(16,17) 1.3678 -DE/DX = 0.0 !

! R31 R(16,18) 1.4091 -DE/DX = 0.0 !

! R32 R(17,32) 2.1067 -DE/DX = 0.0 !

! R33 R(18,19) 1.4447 -DE/DX = 0.0 !

! R34 R(18,40) 1.4171 -DE/DX = 0.0 !

! R35 R(19,20) 1.4218 -DE/DX = 0.0 !

! R36 R(19,23) 1.3688 -DE/DX = 0.0 !

! R37 R(20,21) 1.3857 -DE/DX = 0.0 !

! R38 R(20,30) 1.0799 -DE/DX = 0.0 !

! R39 R(21,22) 1.4218 -DE/DX = 0.0 !

! R40 R(21,31) 1.0799 -DE/DX = 0.0 !

! R41 R(22,23) 1.3688 -DE/DX = 0.0 !

! R42 R(22,33) 1.4447 -DE/DX = 0.0 !

! R43 R(23,32) 2.0983 -DE/DX = 0.0 !

! R44 R(33,34) 1.4171 -DE/DX = 0.0 !

! R45 R(34,36) 1.208 -DE/DX = 0.0 !

! R46 R(35,37) 1.208 -DE/DX = 0.0 !

! R47 R(36,43) 1.0676 -DE/DX = 0.0 !

! R48 R(37,45) 1.0676 -DE/DX = 0.0 !

! R49 R(38,39) 1.208 -DE/DX = 0.0 !

! R50 R(39,44) 1.0676 -DE/DX = 0.0 !

! R51 R(40,41) 1.208 -DE/DX = 0.0 !

! R52 R(41,42) 1.0676 -DE/DX = 0.0 !

! A1 A(2,1,5) 106.6673 -DE/DX = 0.0 !

! A2 A(2,1,24) 125.9981 -DE/DX = 0.0 !

! A3 A(5,1,24) 127.3342 -DE/DX = 0.0 !

! A4 A(1,2,3) 109.8112 -DE/DX = 0.0 !

! A5 A(1,2,12) 125.4922 -DE/DX = 0.0 !

! A6 A(3,2,12) 124.6945 -DE/DX = 0.0 !

! A7 A(2,3,4) 107.043 -DE/DX = 0.0 !

! A8 A(2,3,32) 126.4316 -DE/DX = 0.0 !

! A9 A(4,3,32) 126.4316 -DE/DX = 0.0 !

! A10 A(3,4,5) 109.8112 -DE/DX = 0.0 !

! A11 A(3,4,6) 124.6945 -DE/DX = 0.0 !

! A12 A(5,4,6) 125.4922 -DE/DX = 0.0 !

! A13 A(1,5,4) 106.6673 -DE/DX = 0.0 !

! A14 A(1,5,25) 127.3342 -DE/DX = 0.0 !

! A15 A(4,5,25) 125.9981 -DE/DX = 0.0 !

! A16 A(4,6,7) 127.1455 -DE/DX = 0.0 !

! A17 A(4,6,38) 116.0721 -DE/DX = 0.0 !

! A18 A(7,6,38) 116.7806 -DE/DX = 0.0 !

! A19 A(6,7,8) 125.38 -DE/DX = 0.0 !

! A20 A(6,7,11) 125.2518 -DE/DX = 0.0 !

! A21 A(8,7,11) 109.3664 -DE/DX = 0.0 !

! A22 A(7,8,9) 107.3848 -DE/DX = 0.0 !

! A23 A(7,8,32) 126.2367 -DE/DX = 0.0 !

! A24 A(9,8,32) 126.2367 -DE/DX = 0.0 !

! A25 A(8,9,10) 109.3664 -DE/DX = 0.0 !

! A26 A(8,9,33) 125.38 -DE/DX = 0.0 !

! A27 A(10,9,33) 125.2518 -DE/DX = 0.0 !

! A28 A(9,10,11) 106.9412 -DE/DX = 0.0 !

! A29 A(9,10,26) 125.4287 -DE/DX = 0.0 !

! A30 A(11,10,26) 127.6296 -DE/DX = 0.0 !

! A31 A(7,11,10) 106.9412 -DE/DX = 0.0 !

! A32 A(7,11,27) 125.4287 -DE/DX = 0.0 !

! A33 A(10,11,27) 127.6296 -DE/DX = 0.0 !

! A34 A(2,12,13) 127.1456 -DE/DX = 0.0 !

! A35 A(2,12,35) 116.0721 -DE/DX = 0.0 !

! A36 A(13,12,35) 116.7806 -DE/DX = 0.0 !

! A37 A(12,13,14) 125.2518 -DE/DX = 0.0 !

! A38 A(12,13,17) 125.38 -DE/DX = 0.0 !

! A39 A(14,13,17) 109.3664 -DE/DX = 0.0 !

! A40 A(13,14,15) 106.9412 -DE/DX = 0.0 !

! A41 A(13,14,28) 125.4287 -DE/DX = 0.0 !

! A42 A(15,14,28) 127.6296 -DE/DX = 0.0 !

! A43 A(14,15,16) 106.9412 -DE/DX = 0.0 !

! A44 A(14,15,29) 127.6296 -DE/DX = 0.0 !

! A45 A(16,15,29) 125.4287 -DE/DX = 0.0 !

! A46 A(15,16,17) 109.3664 -DE/DX = 0.0 !

! A47 A(15,16,18) 125.2518 -DE/DX = 0.0 !

! A48 A(17,16,18) 125.38 -DE/DX = 0.0 !

! A49 A(13,17,16) 107.3848 -DE/DX = 0.0 !

! A50 A(13,17,32) 126.2367 -DE/DX = 0.0 !

! A51 A(16,17,32) 126.2367 -DE/DX = 0.0 !

! A52 A(16,18,19) 127.1456 -DE/DX = 0.0 !

! A53 A(16,18,40) 116.7806 -DE/DX = 0.0 !

! A54 A(19,18,40) 116.0721 -DE/DX = 0.0 !

! A55 A(18,19,20) 125.4922 -DE/DX = 0.0 !

! A56 A(18,19,23) 124.6945 -DE/DX = 0.0 !

! A57 A(20,19,23) 109.8112 -DE/DX = 0.0 !

! A58 A(19,20,21) 106.6673 -DE/DX = 0.0 !

! A59 A(19,20,30) 125.9981 -DE/DX = 0.0 !

! A60 A(21,20,30) 127.3342 -DE/DX = 0.0 !

! A61 A(20,21,22) 106.6673 -DE/DX = 0.0 !

! A62 A(20,21,31) 127.3342 -DE/DX = 0.0 !

! A63 A(22,21,31) 125.9981 -DE/DX = 0.0 !

! A64 A(21,22,23) 109.8112 -DE/DX = 0.0 !

! A65 A(21,22,33) 125.4922 -DE/DX = 0.0 !

! A66 A(23,22,33) 124.6945 -DE/DX = 0.0 !

! A67 A(19,23,22) 107.043 -DE/DX = 0.0 !

! A68 A(19,23,32) 126.4316 -DE/DX = 0.0 !

! A69 A(22,23,32) 126.4316 -DE/DX = 0.0 !

! A70 A(3,32,8) 89.6928 -DE/DX = 0.0 !

! A71 A(3,32,17) 89.6928 -DE/DX = 0.0 !

! A72 A(8,32,23) 89.6928 -DE/DX = 0.0 !

! A73 A(17,32,23) 89.6928 -DE/DX = 0.0 !

! A74 A(9,33,22) 127.1456 -DE/DX = 0.0 !

! A75 A(9,33,34) 116.7806 -DE/DX = 0.0 !

! A76 A(22,33,34) 116.0721 -DE/DX = 0.0 !

! A77 L(3,32,23,17,-1) 179.3856 -DE/DX = 0.0 !

! A78 L(8,32,17,23,-1) 179.3856 -DE/DX = 0.0 !

! A79 L(33,34,36,26,-1) 180.8137 -DE/DX = 0.0 !

! A80 L(12,35,37,24,-1) 179.1862 -DE/DX = 0.0 !

! A81 L(34,36,43,26,-1) 179.749 -DE/DX = 0.0 !

! A82 L(35,37,45,24,-1) 180.2505 -DE/DX = 0.0 !

! A83 L(6,38,39,25,-1) 179.1862 -DE/DX = 0.0 !

! A84 L(38,39,44,25,-1) 180.2504 -DE/DX = 0.0 !

! A85 L(18,40,41,29,-1) 180.8137 -DE/DX = 0.0 !

! A86 L(40,41,42,29,-1) 179.749 -DE/DX = 0.0 !

! A87 L(3,32,23,17,-2) 188.3171 -DE/DX = 0.0 !

! A88 L(8,32,17,23,-2) 171.5648 -DE/DX = 0.0 !

! A89 L(33,34,36,26,-2) 179.9836 -DE/DX = 0.0 !

! A90 L(12,35,37,24,-2) 179.9931 -DE/DX = 0.0 !

! A91 L(34,36,43,26,-2) 179.9814 -DE/DX = 0.0 !

! A92 L(35,37,45,24,-2) 180.0266 -DE/DX = 0.0 !

! A93 L(6,38,39,25,-2) 180.0069 -DE/DX = 0.0 !

! A94 L(38,39,44,25,-2) 179.9734 -DE/DX = 0.0 !

! A95 L(18,40,41,29,-2) 180.0164 -DE/DX = 0.0 !

! A96 L(40,41,42,29,-2) 180.0186 -DE/DX = 0.0 !

! D1 D(5,1,2,3) 0.0047 -DE/DX = 0.0 !

! D2 D(5,1,2,12) 179.5065 -DE/DX = 0.0 !

! D3 D(24,1,2,3) -179.7507 -DE/DX = 0.0 !

! D4 D(24,1,2,12) -0.2489 -DE/DX = 0.0 !

! D5 D(2,1,5,4) 0.0 -DE/DX = 0.0 !

! D6 D(2,1,5,25) -179.7511 -DE/DX = 0.0 !

! D7 D(24,1,5,4) 179.7511 -DE/DX = 0.0 !

! D8 D(24,1,5,25) 0.0 -DE/DX = 0.0 !

! D9 D(1,2,3,4) -0.0076 -DE/DX = 0.0 !

! D10 D(1,2,3,32) -176.6554 -DE/DX = 0.0 !

! D11 D(12,2,3,4) -179.5142 -DE/DX = 0.0 !

! D12 D(12,2,3,32) 3.838 -DE/DX = 0.0 !

! D13 D(1,2,12,13) -178.4328 -DE/DX = 0.0 !

! D14 D(1,2,12,35) 1.0722 -DE/DX = 0.0 !

! D15 D(3,2,12,13) 0.9971 -DE/DX = 0.0 !

! D16 D(3,2,12,35) -179.4979 -DE/DX = 0.0 !

! D17 D(2,3,4,5) 0.0076 -DE/DX = 0.0 !

! D18 D(2,3,4,6) 179.5142 -DE/DX = 0.0 !

! D19 D(32,3,4,5) 176.6554 -DE/DX = 0.0 !

! D20 D(32,3,4,6) -3.838 -DE/DX = 0.0 !

! D21 D(2,3,32,8) -177.7747 -DE/DX = 0.0 !

! D22 D(2,3,32,17) -6.2098 -DE/DX = 0.0 !

! D23 D(4,3,32,8) 6.2098 -DE/DX = 0.0 !

! D24 D(4,3,32,17) 177.7747 -DE/DX = 0.0 !

! D25 D(3,4,5,1) -0.0047 -DE/DX = 0.0 !

! D26 D(3,4,5,25) 179.7507 -DE/DX = 0.0 !

! D27 D(6,4,5,1) -179.5065 -DE/DX = 0.0 !

! D28 D(6,4,5,25) 0.2489 -DE/DX = 0.0 !

! D29 D(3,4,6,7) -0.9971 -DE/DX = 0.0 !

! D30 D(3,4,6,38) 179.4979 -DE/DX = 0.0 !

! D31 D(5,4,6,7) 178.4328 -DE/DX = 0.0 !

! D32 D(5,4,6,38) -1.0722 -DE/DX = 0.0 !

! D33 D(4,6,7,8) 0.5409 -DE/DX = 0.0 !

! D34 D(4,6,7,11) -178.9203 -DE/DX = 0.0 !

! D35 D(38,6,7,8) -179.9572 -DE/DX = 0.0 !

! D36 D(38,6,7,11) 0.5816 -DE/DX = 0.0 !

! D37 D(6,7,8,9) -179.4783 -DE/DX = 0.0 !

! D38 D(6,7,8,32) 4.6488 -DE/DX = 0.0 !

! D39 D(11,7,8,9) 0.0553 -DE/DX = 0.0 !

! D40 D(11,7,8,32) -175.8176 -DE/DX = 0.0 !

! D41 D(6,7,11,10) 179.5001 -DE/DX = 0.0 !

! D42 D(6,7,11,27) -0.2467 -DE/DX = 0.0 !

! D43 D(8,7,11,10) -0.0343 -DE/DX = 0.0 !

! D44 D(8,7,11,27) -179.7811 -DE/DX = 0.0 !

! D45 D(7,8,9,10) -0.0553 -DE/DX = 0.0 !

! D46 D(7,8,9,33) 179.4783 -DE/DX = 0.0 !

! D47 D(32,8,9,10) 175.8176 -DE/DX = 0.0 !

! D48 D(32,8,9,33) -4.6488 -DE/DX = 0.0 !

! D49 D(7,8,32,3) -6.6009 -DE/DX = 0.0 !

! D50 D(7,8,32,23) -178.2838 -DE/DX = 0.0 !

! D51 D(9,8,32,3) 178.2838 -DE/DX = 0.0 !

! D52 D(9,8,32,23) 6.6009 -DE/DX = 0.0 !

! D53 D(8,9,10,11) 0.0343 -DE/DX = 0.0 !

! D54 D(8,9,10,26) 179.7811 -DE/DX = 0.0 !

! D55 D(33,9,10,11) -179.5001 -DE/DX = 0.0 !

! D56 D(33,9,10,26) 0.2467 -DE/DX = 0.0 !

! D57 D(8,9,33,22) -0.5409 -DE/DX = 0.0 !

! D58 D(8,9,33,34) 179.9572 -DE/DX = 0.0 !

! D59 D(10,9,33,22) 178.9203 -DE/DX = 0.0 !

! D60 D(10,9,33,34) -0.5816 -DE/DX = 0.0 !

! D61 D(9,10,11,7) 0.0 -DE/DX = 0.0 !

! D62 D(9,10,11,27) 179.7395 -DE/DX = 0.0 !

! D63 D(26,10,11,7) -179.7395 -DE/DX = 0.0 !

! D64 D(26,10,11,27) 0.0 -DE/DX = 0.0 !

! D65 D(2,12,13,14) 178.9203 -DE/DX = 0.0 !

! D66 D(2,12,13,17) -0.5409 -DE/DX = 0.0 !

! D67 D(35,12,13,14) -0.5816 -DE/DX = 0.0 !

! D68 D(35,12,13,17) 179.9572 -DE/DX = 0.0 !

! D69 D(12,13,14,15) -179.5001 -DE/DX = 0.0 !

! D70 D(12,13,14,28) 0.2467 -DE/DX = 0.0 !

! D71 D(17,13,14,15) 0.0343 -DE/DX = 0.0 !

! D72 D(17,13,14,28) 179.7811 -DE/DX = 0.0 !

! D73 D(12,13,17,16) 179.4783 -DE/DX = 0.0 !

! D74 D(12,13,17,32) -4.6488 -DE/DX = 0.0 !

! D75 D(14,13,17,16) -0.0554 -DE/DX = 0.0 !

! D76 D(14,13,17,32) 175.8176 -DE/DX = 0.0 !

! D77 D(13,14,15,16) 0.0 -DE/DX = 0.0 !

! D78 D(13,14,15,29) 179.7395 -DE/DX = 0.0 !

! D79 D(28,14,15,16) -179.7395 -DE/DX = 0.0 !

! D80 D(28,14,15,29) 0.0 -DE/DX = 0.0 !

! D81 D(14,15,16,17) -0.0343 -DE/DX = 0.0 !

! D82 D(14,15,16,18) 179.5001 -DE/DX = 0.0 !

! D83 D(29,15,16,17) -179.7811 -DE/DX = 0.0 !

! D84 D(29,15,16,18) -0.2467 -DE/DX = 0.0 !

! D85 D(15,16,17,13) 0.0554 -DE/DX = 0.0 !

! D86 D(15,16,17,32) -175.8176 -DE/DX = 0.0 !

! D87 D(18,16,17,13) -179.4783 -DE/DX = 0.0 !

! D88 D(18,16,17,32) 4.6488 -DE/DX = 0.0 !

! D89 D(15,16,18,19) -178.9203 -DE/DX = 0.0 !

! D90 D(15,16,18,40) 0.5816 -DE/DX = 0.0 !

! D91 D(17,16,18,19) 0.5409 -DE/DX = 0.0 !

! D92 D(17,16,18,40) -179.9572 -DE/DX = 0.0 !

! D93 D(13,17,32,3) 6.6009 -DE/DX = 0.0 !

! D94 D(13,17,32,23) 178.2838 -DE/DX = 0.0 !

! D95 D(16,17,32,3) -178.2838 -DE/DX = 0.0 !

! D96 D(16,17,32,23) -6.6009 -DE/DX = 0.0 !

! D97 D(16,18,19,20) 178.4328 -DE/DX = 0.0 !

! D98 D(16,18,19,23) -0.9971 -DE/DX = 0.0 !

! D99 D(40,18,19,20) -1.0722 -DE/DX = 0.0 !

! D100 D(40,18,19,23) 179.4979 -DE/DX = 0.0 !

! D101 D(18,19,20,21) -179.5065 -DE/DX = 0.0 !

! D102 D(18,19,20,30) 0.2489 -DE/DX = 0.0 !

! D103 D(23,19,20,21) -0.0047 -DE/DX = 0.0 !

! D104 D(23,19,20,30) 179.7507 -DE/DX = 0.0 !

! D105 D(18,19,23,22) 179.5142 -DE/DX = 0.0 !

! D106 D(18,19,23,32) -3.838 -DE/DX = 0.0 !

! D107 D(20,19,23,22) 0.0076 -DE/DX = 0.0 !

! D108 D(20,19,23,32) 176.6554 -DE/DX = 0.0 !

! D109 D(19,20,21,22) 0.0 -DE/DX = 0.0 !

! D110 D(19,20,21,31) 179.7511 -DE/DX = 0.0 !

! D111 D(30,20,21,22) -179.7511 -DE/DX = 0.0 !

! D112 D(30,20,21,31) 0.0 -DE/DX = 0.0 !

! D113 D(20,21,22,23) 0.0047 -DE/DX = 0.0 !

! D114 D(20,21,22,33) 179.5065 -DE/DX = 0.0 !

! D115 D(31,21,22,23) -179.7507 -DE/DX = 0.0 !

! D116 D(31,21,22,33) -0.2489 -DE/DX = 0.0 !

! D117 D(21,22,23,19) -0.0076 -DE/DX = 0.0 !

! D118 D(21,22,23,32) -176.6554 -DE/DX = 0.0 !

! D119 D(33,22,23,19) -179.5142 -DE/DX = 0.0 !

! D120 D(33,22,23,32) 3.838 -DE/DX = 0.0 !

! D121 D(21,22,33,9) -178.4328 -DE/DX = 0.0 !

! D122 D(21,22,33,34) 1.0722 -DE/DX = 0.0 !

! D123 D(23,22,33,9) 0.9971 -DE/DX = 0.0 !

! D124 D(23,22,33,34) -179.4979 -DE/DX = 0.0 !

! D125 D(19,23,32,8) 177.7747 -DE/DX = 0.0 !

! D126 D(19,23,32,17) 6.2098 -DE/DX = 0.0 !

! D127 D(22,23,32,8) -6.2098 -DE/DX = 0.0 !

! D128 D(22,23,32,17) -177.7747 -DE/DX = 0.0 !

--------------------------------------------------------------------------------

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 44 0.049 Angstoms.

Leave Link 103 at Tue Jul 30 03:39:13 2019, MaxMem= 4294967296 cpu: 1.1

(Enter /home/kira/g09/l202.exe)

Input orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 -0.692834 -4.267848 -0.056805

2 6 0 -1.100625 -2.906239 -0.021607

3 7 0 0.000000 -2.092728 -0.000684

4 6 0 1.100625 -2.906239 -0.021607

5 6 0 0.692835 -4.267848 -0.056805

6 6 0 2.467968 -2.439959 -0.019688

7 6 0 2.910772 -1.102262 -0.016189

8 7 0 2.100954 -0.000000 -0.003455

9 6 0 2.910772 1.102262 -0.016190

10 6 0 4.298195 0.679595 -0.036685

11 6 0 4.298195 -0.679595 -0.036685

12 6 0 -2.467968 -2.439959 -0.019688

13 6 0 -2.910772 -1.102262 -0.016189

14 6 0 -4.298196 -0.679595 -0.036685

15 6 0 -4.298196 0.679595 -0.036685

16 6 0 -2.910772 1.102262 -0.016189

17 7 0 -2.100954 -0.000000 -0.003455

18 6 0 -2.467969 2.439959 -0.019688

19 6 0 -1.100625 2.906239 -0.021607

20 6 0 -0.692834 4.267849 -0.056805

21 6 0 0.692835 4.267849 -0.056805

22 6 0 1.100625 2.906239 -0.021607

23 7 0 0.000000 2.092728 -0.000684

24 1 0 -1.347756 -5.126102 -0.082721

25 1 0 1.347756 -5.126102 -0.082721

26 1 0 5.153172 1.338842 -0.053203

27 1 0 5.153172 -1.338842 -0.053203

28 1 0 -5.153173 -1.338842 -0.053203

29 1 0 -5.153173 1.338842 -0.053203

30 1 0 -1.347756 5.126102 -0.082721

31 1 0 1.347756 5.126102 -0.082721

32 30 0 -0.000000 0.000000 0.151889

33 6 0 2.467968 2.439959 -0.019688

34 6 0 3.468275 3.443623 -0.032543

35 6 0 -3.468275 -3.443623 -0.032543

36 6 0 4.308766 4.311238 -0.043693

37 6 0 -4.308765 -4.311239 -0.043693

38 6 0 3.468275 -3.443623 -0.032543

39 6 0 4.308765 -4.311238 -0.043692

40 6 0 -3.468275 3.443623 -0.032543

41 6 0 -4.308765 4.311238 -0.043693

42 1 0 -5.054901 5.074736 -0.053889

43 1 0 5.054902 5.074736 -0.053889

44 1 0 5.054901 -5.074736 -0.053888

45 1 0 -5.054901 -5.074736 -0.053890

---------------------------------------------------------------------

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.421799 0.000000

3 N 2.283489 1.368800 0.000000

4 C 2.252047 2.201250 1.368800 0.000000

5 C 1.385669 2.252047 2.283489 1.421799 0.000000

6 C 3.651470 3.598928 2.492348 1.444662 2.548265

7 C 4.796724 4.398371 3.074712 2.555581 3.865467

8 N 5.101238 4.323964 2.965388 3.073632 4.494461

9 C 6.467280 5.670927 4.322128 4.398266 5.810248

10 C 7.027658 6.481180 5.114836 4.804465 6.121783

11 C 6.147060 5.839986 4.524679 3.896489 5.086708

12 C 2.548265 1.444662 2.492348 3.598928 3.651470

13 C 3.865467 2.555581 3.074712 4.398371 4.796724

14 C 5.086708 3.896489 4.524680 5.839986 6.147060

15 C 6.121783 4.804465 5.114836 6.481180 7.027658

16 C 5.810248 4.398266 4.322128 5.670927 6.467280

17 N 4.494461 3.073632 2.965388 4.323964 5.101238

18 C 6.938816 5.518285 5.161054 6.427807 7.415304

19 C 7.185754 5.812478 5.118738 6.215336 7.394949

20 C 8.535697 7.185754 6.398445 7.394949 8.647439

21 C 8.647439 7.394949 6.398445 7.185754 8.535697

22 C 7.394949 6.215336 5.118738 5.812478 7.185754

23 N 6.398445 5.118738 4.185455 5.118738 6.398445

24 H 1.079904 2.234413 3.320322 3.305464 2.213883

25 H 2.213883 3.305464 3.320322 2.234413 1.079904

26 H 8.100049 7.558551 6.191414 5.868974 7.164468

27 H 6.538722 6.447303 5.208290 4.345212 5.336076

28 H 5.336076 4.345213 5.208290 6.447303 6.538722

29 H 7.164468 5.868974 6.191415 7.558551 8.100049

30 H 9.416788 8.036374 7.344023 8.397429 9.613063

31 H 9.613063 8.397429 7.344023 8.036374 9.416788

32 Zn 4.328753 3.112507 2.098282 3.112508 4.328753

33 C 7.415304 6.427807 5.161054 5.518285 6.938816

34 C 8.762546 7.822769 6.533079 6.776919 8.195758

35 C 2.895342 2.427893 3.722212 4.600407 4.242024

36 C 9.930604 9.019644 7.718684 7.898394 9.309987

37 C 3.616215 3.502381 4.846555 5.588919 5.001805

38 C 4.242024 4.600407 3.722212 2.427893 2.895342

39 C 5.001805 5.588919 4.846555 3.502381 3.616215

40 C 8.195758 6.776919 6.533079 7.822769 8.762546

41 C 9.309987 7.898394 7.718684 9.019644 9.930604

42 H 10.310748 8.906925 8.770826 10.079063 10.969064

43 H 10.969064 10.079063 8.770826 8.906925 10.310748

44 H 5.804097 6.526402 5.869176 4.509958 4.436068

45 H 4.436068 4.509958 5.869177 6.526402 5.804097

6 7 8 9 10

6 C 0.000000

7 C 1.409085 0.000000

8 N 2.467461 1.367826 0.000000

9 C 3.569792 2.204524 1.367826 0.000000

10 C 3.616854 2.258402 2.300179 1.450521 0.000000

11 C 2.539469 1.450521 2.300179 2.258402 1.359189

12 C 4.935937 5.542589 5.179645 6.440356 7.450697

13 C 5.542589 5.821544 5.131524 6.224974 7.425944

14 C 6.991434 7.221376 6.435221 7.425944 8.703179

15 C 7.450697 7.425944 6.435221 7.221376 8.596391

16 C 6.440357 6.224974 5.131524 5.821544 7.221376

17 N 5.179645 5.131524 4.201909 5.131524 6.435221

18 C 6.940971 6.440356 5.179645 5.542589 6.991434

19 C 6.427807 5.670927 4.323964 4.398371 5.839986

20 C 7.415305 6.467280 5.101238 4.796725 6.147060

21 C 6.938816 5.810248 4.494461 3.865467 5.086708

22 C 5.518285 4.398266 3.073632 2.555581 3.896489

23 N 5.161054 4.322128 2.965388 3.074712 4.524679

24 H 4.666807 5.859247 6.178738 7.545330 8.098456

25 H 2.911050 4.317260 5.181748 6.421835 6.512551

26 H 4.635815 3.314924 3.333318 2.255150 1.079753

27 H 2.902396 2.255150 3.333318 3.314924 2.192110

28 H 7.700349 8.067499 7.376810 8.425411 9.664508

29 H 8.506601 8.425411 7.376810 8.067499 9.474346

30 H 8.474020 7.545330 6.178738 5.859247 7.186815

31 H 7.648800 6.421835 5.181748 4.317260 5.336538

32 Zn 3.474725 3.117022 2.106690 3.117022 4.355674

33 C 4.879919 3.569793 2.467461 1.409085 2.539469

34 C 5.968024 4.579972 3.705260 2.406875 2.885938

35 C 6.020506 6.795180 6.547953 7.833107 8.793122

36 C 6.997698 5.591165 4.843844 3.500382 3.631666

37 C 7.030390 7.900633 7.724823 9.023772 9.949283

38 C 1.417081 2.406875 3.705260 4.579972 4.205913

39 C 2.625032 3.500382 4.843844 5.591165 4.990849

40 C 8.357972 7.833107 6.547954 6.795180 8.243660

41 C 9.565739 9.023772 7.724824 7.900633 9.341769

42 H 10.633221 10.080113 8.772785 8.901344 10.334311

43 H 7.947581 6.538656 5.872078 4.514340 4.459839

44 H 3.692620 4.514340 5.872077 6.538656 5.803897

45 H 7.970997 8.901343 8.772785 10.080113 10.981486

11 12 13 14 15

11 C 0.000000

12 C 6.991434 0.000000

13 C 7.221376 1.409085 0.000000

14 C 8.596391 2.539469 1.450521 0.000000

15 C 8.703179 3.616855 2.258402 1.359189 0.000000

16 C 7.425944 3.569793 2.204524 2.258402 1.450521

17 N 6.435221 2.467461 1.367826 2.300179 2.300179

18 C 7.450697 4.879919 3.569793 3.616855 2.539469

19 C 6.481180 5.518285 4.398266 4.804466 3.896490

20 C 7.027658 6.938816 5.810248 6.121783 5.086708

21 C 6.121783 7.415305 6.467281 7.027658 6.147061

22 C 4.804465 6.427807 5.670927 6.481180 5.839986

23 N 5.114836 5.161054 4.322128 5.114837 4.524680

24 H 7.186815 2.911050 4.317260 5.336538 6.512552

25 H 5.336538 4.666807 5.859247 7.186815 8.098457

26 H 2.192110 8.506600 8.425411 9.664508 9.474346

27 H 1.079753 7.700349 8.067499 9.474346 9.664508

28 H 9.474346 2.902396 2.255150 1.079753 2.192110

29 H 9.664508 4.635815 3.314924 2.192110 1.079753

30 H 8.098457 7.648800 6.421835 6.512552 5.336539

31 H 6.512552 8.474020 7.545330 8.098457 7.186816

32 Zn 4.355674 3.474724 3.117022 4.355674 4.355674

33 C 3.616855 6.940971 6.440357 7.450697 6.991434

34 C 4.205913 8.357972 7.833108 8.793122 8.243660

35 C 8.243660 1.417081 2.406875 2.885938 4.205914

36 C 4.990849 9.565739 9.023772 9.949283 9.341770

37 C 9.341769 2.625032 3.500382 3.631666 4.990849

38 C 2.885938 6.020506 6.795180 8.243660 8.793122

39 C 3.631666 7.030390 7.900633 9.341770 9.949283

40 C 8.793122 5.968025 4.579972 4.205914 2.885938

41 C 9.949283 6.997698 5.591165 4.990849 3.631666

42 H 10.981486 7.947581 6.538656 5.803897 4.459840

43 H 5.803897 10.633221 10.080113 10.981486 10.334311

44 H 4.459840 7.970997 8.901344 10.334311 10.981486

45 H 10.334311 3.692620 4.514340 4.459840 5.803897

16 17 18 19 20

16 C 0.000000

17 N 1.367826 0.000000

18 C 1.409085 2.467461 0.000000

19 C 2.555581 3.073632 1.444662 0.000000

20 C 3.865467 4.494461 2.548266 1.421799 0.000000

21 C 4.796725 5.101239 3.651470 2.252047 1.385669

22 C 4.398371 4.323964 3.598928 2.201250 2.252047

23 N 3.074712 2.965388 2.492348 1.368800 2.283488

24 H 6.421835 5.181748 7.648800 8.036374 9.416788

25 H 7.545330 6.178738 8.474020 8.397429 9.613063

26 H 8.067499 7.376810 7.700349 6.447303 6.538722

27 H 8.425411 7.376810 8.506600 7.558551 8.100049

28 H 3.314924 3.333318 4.635815 5.868974 7.164469

29 H 2.255150 3.333318 2.902396 4.345213 5.336076

30 H 4.317260 5.181748 2.911050 2.234413 1.079904

31 H 5.859247 6.178739 4.666807 3.305464 2.213883

32 Zn 3.117022 2.106689 3.474724 3.112507 4.328753

33 C 5.542589 5.179645 4.935937 3.598928 3.651470

34 C 6.795180 6.547954 6.020506 4.600407 4.242024

35 C 4.579972 3.705260 5.968025 6.776919 8.195758

36 C 7.900633 7.724824 7.030390 5.588919 5.001805

37 C 5.591165 4.843844 6.997698 7.898395 9.309987

38 C 7.833107 6.547954 8.357972 7.822769 8.762546

39 C 9.023772 7.724824 9.565739 9.019644 9.930605

40 C 2.406875 3.705260 1.417081 2.427893 2.895342

41 C 3.500382 4.843844 2.625032 3.502381 3.616215

42 H 4.514340 5.872077 3.692620 4.509958 4.436068

43 H 8.901344 8.772785 7.970997 6.526402 5.804097

44 H 10.080113 8.772785 10.633221 10.079063 10.969064

45 H 6.538656 5.872077 7.947581 8.906925 10.310748

21 22 23 24 25

21 C 0.000000

22 C 1.421799 0.000000

23 N 2.283488 1.368800 0.000000

24 H 9.613063 8.397429 7.344023 0.000000

25 H 9.416788 8.036374 7.344023 2.695512 0.000000

26 H 5.336076 4.345212 5.208290 9.168339 7.501838

27 H 7.164468 5.868974 6.191415 7.523714 5.368929

28 H 8.100049 7.558551 6.191415 5.368930 7.523714

29 H 6.538723 6.447303 5.208291 7.501838 9.168339

30 H 2.213883 3.305464 3.320322 10.252204 10.600635

31 H 1.079904 2.234413 3.320322 10.600636 10.252204

32 Zn 4.328753 3.112507 2.098282 5.305508 5.305508

33 C 2.548266 1.444662 2.492348 8.474020 7.648799

34 C 2.895342 2.427893 3.722212 9.830404 8.828324

35 C 8.762546 7.822769 6.533079 2.707370 5.101706

36 C 3.616215 3.502381 4.846555 11.002779 9.891031

37 C 9.930605 9.019644 7.718685 3.071336 5.715046

38 C 8.195758 6.776919 6.533079 5.101706 2.707370

39 C 9.309987 7.898394 7.718685 5.715046 3.071336

40 C 4.242024 4.600407 3.722212 8.828324 9.830404

41 C 5.001805 5.588919 4.846555 9.891031 11.002779

42 H 5.804097 6.526402 5.869176 10.853610 12.043751

43 H 4.436068 4.509958 5.869176 12.043751 10.853610

44 H 10.310748 8.906925 8.770827 6.402928 3.707613

45 H 10.969064 10.079063 8.770827 3.707613 6.402928

26 27 28 29 30

26 H 0.000000

27 H 2.677684 0.000000

28 H 10.648509 10.306345 0.000000

29 H 10.306345 10.648509 2.677684 0.000000

30 H 7.523714 9.168339 7.501838 5.368930 0.000000

31 H 5.368930 7.501838 9.168339 7.523715 2.695512

32 Zn 5.328203 5.328203 5.328203 5.328203 5.305507

33 C 2.902396 4.635815 8.506601 7.700349 4.666807

34 C 2.696184 5.070629 9.859095 8.874677 5.101706

35 C 9.859095 8.874676 2.696184 5.070629 8.828324

36 C 3.090025 5.712838 11.020516 9.917838 5.715047

37 C 11.020515 9.917837 3.090025 5.712839 9.891031

38 C 5.070629 2.696184 8.874676 9.859095 9.830405

39 C 5.712838 3.090025 9.917837 11.020516 11.002779

40 C 8.874676 9.859095 5.070629 2.696184 2.707370

41 C 9.917837 11.020516 5.712839 3.090025 3.071336

42 H 10.870219 12.055652 6.414331 3.737187 3.707613

43 H 3.737186 6.414331 12.055653 10.870220 6.402928

44 H 6.414331 3.737187 10.870219 12.055652 12.043752

45 H 12.055652 10.870219 3.737186 6.414331 10.853611

31 32 33 34 35

31 H 0.000000

32 Zn 5.305507 0.000000

33 C 2.911050 3.474724 0.000000

34 C 2.707371 4.890959 1.417081 0.000000

35 C 9.830405 4.890959 8.357972 9.774961 0.000000

36 C 3.071336 6.098400 2.625032 1.208017 10.982730

37 C 11.002779 6.098400 9.565739 10.982730 1.208017

38 C 8.828324 4.890960 5.968025 6.887246 6.936549

39 C 9.891031 6.098401 6.997698 7.800283 7.825294

40 C 5.101706 4.890959 6.020506 6.936550 6.887246

41 C 5.715047 6.098400 7.030390 7.825294 7.800284

42 H 6.402928 7.165704 7.970997 8.677875 8.664888

43 H 3.707614 7.165704 3.692620 2.275603 12.050204

44 H 10.853611 7.165705 7.947581 8.664888 8.677875

45 H 12.043752 7.165704 10.633221 12.050204 2.275603

36 37 38 39 40

36 C 0.000000

37 C 12.190527 0.000000

38 C 7.800283 7.825294 0.000000

39 C 8.622477 8.617530 1.208017 0.000000

40 C 7.825295 7.800284 9.774961 10.982730 0.000000

41 C 8.617531 8.622477 10.982730 12.190527 1.208017

42 H 9.394748 9.415591 12.050204 13.258012 2.275603

43 H 1.067592 13.258012 8.664888 9.415590 8.677875

44 H 9.415590 9.394747 2.275603 1.067592 12.050204

45 H 13.258012 1.067592 8.677875 9.394747 8.664888

41 42 43 44 45

41 C 0.000000

42 H 1.067592 0.000000

43 H 9.394748 10.109803 0.000000

44 H 13.258012 14.325498 10.149472 0.000000

45 H 9.415591 10.149473 14.325498 10.109802 0.000000

Stoichiometry C28H12N4Zn(3)

Framework group C1[X(C28H12N4Zn)]

Deg. of freedom 129

Full point group C1 NOp 1

RotChk: IX=0 Diff= 2.98D-14

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

---------------------------------------------------------------------

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

---------------------------------------------------------------------

1 6 0 0.692835 4.267848 -0.049605

2 6 0 1.100626 2.906239 -0.014407

3 7 0 0.000000 2.092728 0.006516

4 6 0 -1.100624 2.906239 -0.014407

5 6 0 -0.692834 4.267849 -0.049605

6 6 0 -2.467968 2.439960 -0.012488

7 6 0 -2.910771 1.102263 -0.008990

8 7 0 -2.100954 0.000001 0.003745

9 6 0 -2.910772 -1.102261 -0.008990

10 6 0 -4.298196 -0.679594 -0.029485

11 6 0 -4.298195 0.679596 -0.029485

12 6 0 2.467969 2.439959 -0.012488

13 6 0 2.910772 1.102261 -0.008990

14 6 0 4.298196 0.679594 -0.029485

15 6 0 4.298195 -0.679595 -0.029485

16 6 0 2.910772 -1.102263 -0.008989

17 7 0 2.100954 -0.000000 0.003745

18 6 0 2.467968 -2.439960 -0.012488

19 6 0 1.100624 -2.906239 -0.014407

20 6 0 0.692833 -4.267849 -0.049605

21 6 0 -0.692836 -4.267848 -0.049605

22 6 0 -1.100626 -2.906239 -0.014407

23 7 0 -0.000001 -2.092728 0.006516

24 1 0 1.347757 5.126102 -0.075521

25 1 0 -1.347755 5.126102 -0.075521

26 1 0 -5.153173 -1.338841 -0.046003

27 1 0 -5.153172 1.338843 -0.046003

28 1 0 5.153173 1.338841 -0.046003

29 1 0 5.153172 -1.338843 -0.046003

30 1 0 1.347755 -5.126102 -0.075521

31 1 0 -1.347757 -5.126102 -0.075521

32 30 0 0.000000 -0.000000 0.159089

33 6 0 -2.467969 -2.439959 -0.012488

34 6 0 -3.468276 -3.443622 -0.025343

35 6 0 3.468275 3.443622 -0.025343

36 6 0 -4.308766 -4.311237 -0.036493

37 6 0 4.308766 4.311238 -0.036494

38 6 0 -3.468274 3.443624 -0.025343

39 6 0 -4.308764 4.311239 -0.036493

40 6 0 3.468274 -3.443624 -0.025343

41 6 0 4.308764 -4.311239 -0.036493

42 1 0 5.054900 -5.074737 -0.046689

43 1 0 -5.054903 -5.074735 -0.046689

44 1 0 -5.054900 5.074737 -0.046688

45 1 0 5.054902 5.074735 -0.046690

---------------------------------------------------------------------

Rotational constants (GHZ): 0.1465333 0.1452876 0.0729946

Leave Link 202 at Tue Jul 30 03:39:13 2019, MaxMem= 4294967296 cpu: 0.2

(Enter /home/kira/g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 1 IROHF=0.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Population analysis using the SCF density.

\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Orbital symmetries:

Alpha Orbitals:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A)

Beta Orbitals:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

The electronic state is 3-A.

Alpha occ. eigenvalues -- -14.31982 -14.31982 -14.31374 -14.31373 -10.22859

Alpha occ. eigenvalues -- -10.22859 -10.22859 -10.22859 -10.22229 -10.22228

Alpha occ. eigenvalues -- -10.22228 -10.22228 -10.20870 -10.20870 -10.20870

Alpha occ. eigenvalues -- -10.20870 -10.18820 -10.18819 -10.18819 -10.18819

Alpha occ. eigenvalues -- -10.18185 -10.18185 -10.18185 -10.18185 -10.17742

Alpha occ. eigenvalues -- -10.17742 -10.17674 -10.17674 -10.16234 -10.16234

Alpha occ. eigenvalues -- -10.16178 -10.16178 -0.97591 -0.97098 -0.96170

Alpha occ. eigenvalues -- -0.95622 -0.85477 -0.83715 -0.83391 -0.81718

Alpha occ. eigenvalues -- -0.77791 -0.77621 -0.76741 -0.76232 -0.75940

Alpha occ. eigenvalues -- -0.75157 -0.75129 -0.73613 -0.72890 -0.68244

Alpha occ. eigenvalues -- -0.67578 -0.63245 -0.60150 -0.59795 -0.59411

Alpha occ. eigenvalues -- -0.58912 -0.58274 -0.57362 -0.56401 -0.56363

Alpha occ. eigenvalues -- -0.56142 -0.55594 -0.55515 -0.55302 -0.54905

Alpha occ. eigenvalues -- -0.53142 -0.52692 -0.52616 -0.52200 -0.51754

Alpha occ. eigenvalues -- -0.51526 -0.50352 -0.49802 -0.45995 -0.45181

Alpha occ. eigenvalues -- -0.44963 -0.44631 -0.43406 -0.43308 -0.42827

Alpha occ. eigenvalues -- -0.42593 -0.41283 -0.40946 -0.40334 -0.39868

Alpha occ. eigenvalues -- -0.38506 -0.38459 -0.38409 -0.38148 -0.38004

Alpha occ. eigenvalues -- -0.37906 -0.35031 -0.34863 -0.33350 -0.32927

Alpha occ. eigenvalues -- -0.32399 -0.30068 -0.29733 -0.29692 -0.29368

Alpha occ. eigenvalues -- -0.28305 -0.27457 -0.27293 -0.27238 -0.26983

Alpha occ. eigenvalues -- -0.25997 -0.25240 -0.24947 -0.21725 -0.21545

Alpha occ. eigenvalues -- -0.14931

Alpha virt. eigenvalues -- -0.10958 -0.07214 0.02242 0.02424 0.02721

Alpha virt. eigenvalues -- 0.02852 0.02941 0.03324 0.03374 0.03538

Alpha virt. eigenvalues -- 0.03770 0.04352 0.05063 0.05082 0.05107

Alpha virt. eigenvalues -- 0.05654 0.05762 0.06668 0.07800 0.08382

Alpha virt. eigenvalues -- 0.08419 0.08455 0.09664 0.09753 0.09865

Alpha virt. eigenvalues -- 0.09943 0.11440 0.12389 0.12588 0.13637

Alpha virt. eigenvalues -- 0.13647 0.15612 0.15695 0.15715 0.15740

Alpha virt. eigenvalues -- 0.17127 0.18286 0.18817 0.19721 0.21847

Alpha virt. eigenvalues -- 0.22456 0.22874 0.23849 0.24125 0.24201

Alpha virt. eigenvalues -- 0.24693 0.24939 0.25470 0.25523 0.26067

Alpha virt. eigenvalues -- 0.26277 0.26526 0.27912 0.29194 0.29840

Alpha virt. eigenvalues -- 0.30867 0.31010 0.32485 0.32531 0.32718

Alpha virt. eigenvalues -- 0.35002 0.35178 0.35188 0.35286 0.35381

Alpha virt. eigenvalues -- 0.35786 0.35940 0.36170 0.36340 0.36616

Alpha virt. eigenvalues -- 0.36717 0.37971 0.38158 0.39559 0.40029

Alpha virt. eigenvalues -- 0.40188 0.40427 0.40449 0.40794 0.41238

Alpha virt. eigenvalues -- 0.41398 0.42029 0.42357 0.43125 0.43191

Alpha virt. eigenvalues -- 0.43790 0.43875 0.44275 0.44433 0.44854

Alpha virt. eigenvalues -- 0.45083 0.45515 0.46931 0.47439 0.47677

Alpha virt. eigenvalues -- 0.48167 0.48711 0.48875 0.49125 0.49388

Alpha virt. eigenvalues -- 0.50481 0.51058 0.51453 0.51542 0.51881

Alpha virt. eigenvalues -- 0.51905 0.52012 0.52020 0.54700 0.55992

Alpha virt. eigenvalues -- 0.56264 0.56906 0.57045 0.57160 0.57405

Alpha virt. eigenvalues -- 0.57470 0.57597 0.57941 0.58440 0.58542

Alpha virt. eigenvalues -- 0.61173 0.61580 0.61861 0.62045 0.62277

Alpha virt. eigenvalues -- 0.62397 0.63181 0.63188 0.63703 0.64099

Alpha virt. eigenvalues -- 0.64681 0.64765 0.64960 0.65317 0.65352

Alpha virt. eigenvalues -- 0.68345 0.68392 0.68968 0.69026 0.70052

Alpha virt. eigenvalues -- 0.70111 0.70260 0.70521 0.71726 0.71764

Alpha virt. eigenvalues -- 0.73125 0.73544 0.73553 0.74047 0.74207

Alpha virt. eigenvalues -- 0.74562 0.74689 0.75075 0.75077 0.75436

Alpha virt. eigenvalues -- 0.76953 0.77120 0.78848 0.81216 0.81282

Alpha virt. eigenvalues -- 0.81924 0.82052 0.83425 0.84122 0.84705

Alpha virt. eigenvalues -- 0.85489 0.85564 0.85744 0.88239 0.89709

Alpha virt. eigenvalues -- 0.90354 0.90833 0.90939 0.92513 0.92590

Alpha virt. eigenvalues -- 0.94650 0.95091 0.95718 0.95835 0.97444

Alpha virt. eigenvalues -- 0.97612 0.99512 1.00028 1.00188 1.00492

Alpha virt. eigenvalues -- 1.00900 1.01465 1.01791 1.01858 1.03227

Alpha virt. eigenvalues -- 1.05007 1.05470 1.05799 1.05906 1.06399

Alpha virt. eigenvalues -- 1.06972 1.08487 1.08626 1.11330 1.12227

Alpha virt. eigenvalues -- 1.12261 1.12345 1.12359 1.13130 1.13167

Alpha virt. eigenvalues -- 1.13616 1.13713 1.14002 1.14844 1.15354

Alpha virt. eigenvalues -- 1.16039 1.16365 1.16901 1.17135 1.17786

Alpha virt. eigenvalues -- 1.18470 1.18484 1.18829 1.19056 1.20628

Alpha virt. eigenvalues -- 1.21129 1.21164 1.21178 1.21663 1.23767

Alpha virt. eigenvalues -- 1.24228 1.24562 1.24920 1.25350 1.25462

Alpha virt. eigenvalues -- 1.27786 1.28075 1.28387 1.29052 1.31534

Alpha virt. eigenvalues -- 1.31660 1.33241 1.33565 1.33944 1.37168

Alpha virt. eigenvalues -- 1.42158 1.42498 1.42883 1.47013 1.47449

Alpha virt. eigenvalues -- 1.47932 1.48075 1.49032 1.51456 1.51937

Alpha virt. eigenvalues -- 1.52785 1.54611 1.54627 1.54715 1.54728

Alpha virt. eigenvalues -- 1.54943 1.55063 1.56789 1.57490 1.58081

Alpha virt. eigenvalues -- 1.58383 1.58529 1.58635 1.59148 1.59261

Alpha virt. eigenvalues -- 1.60721 1.60815 1.61362 1.62488 1.62662

Alpha virt. eigenvalues -- 1.62725 1.64809 1.64912 1.65414 1.65689

Alpha virt. eigenvalues -- 1.66034 1.67111 1.69758 1.69800 1.71829

Alpha virt. eigenvalues -- 1.72435 1.73691 1.75297 1.76596 1.76706

Alpha virt. eigenvalues -- 1.76744 1.78415 1.78853 1.79307 1.79668

Alpha virt. eigenvalues -- 1.79748 1.80458 1.80744 1.81243 1.83733

Alpha virt. eigenvalues -- 1.84627 1.85875 1.85949 1.87457 1.88311

Alpha virt. eigenvalues -- 1.88399 1.88494 1.88561 1.89467 1.89750

Alpha virt. eigenvalues -- 1.90174 1.90622 1.93188 1.93975 1.94406

Alpha virt. eigenvalues -- 1.94419 1.94623 1.94640 1.95297 1.96020

Alpha virt. eigenvalues -- 1.96784 1.97046 1.99013 1.99562 2.00567

Alpha virt. eigenvalues -- 2.02858 2.03121 2.03941 2.04062 2.04422

Alpha virt. eigenvalues -- 2.09014 2.09743 2.10953 2.11967 2.14098

Alpha virt. eigenvalues -- 2.17716 2.19548 2.25160 2.26374 2.27657

Alpha virt. eigenvalues -- 2.27869 2.28023 2.30698 2.30768 2.33097

Alpha virt. eigenvalues -- 2.33464 2.34573 2.35196 2.36022 2.36371

Alpha virt. eigenvalues -- 2.36505 2.37590 2.40475 2.40618 2.40924

Alpha virt. eigenvalues -- 2.40979 2.41238 2.41253 2.43537 2.45378

Alpha virt. eigenvalues -- 2.47872 2.47988 2.48819 2.49373 2.51378

Alpha virt. eigenvalues -- 2.52530 2.53068 2.53254 2.55723 2.56110

Alpha virt. eigenvalues -- 2.56691 2.56695 2.57529 2.57657 2.58228

Alpha virt. eigenvalues -- 2.59557 2.59577 2.61618 2.62330 2.62342

Alpha virt. eigenvalues -- 2.64040 2.64118 2.64583 2.66324 2.66607

Alpha virt. eigenvalues -- 2.70692 2.70852 2.72347 2.76803 2.77558

Alpha virt. eigenvalues -- 2.77925 2.79976 2.80533 2.82513 2.83058

Alpha virt. eigenvalues -- 2.83420 2.84547 2.86201 2.86880 2.87830

Alpha virt. eigenvalues -- 2.87879 2.87888 2.87904 2.91818 2.94985

Alpha virt. eigenvalues -- 2.95343 2.95688 2.95846 2.95908 2.95965

Alpha virt. eigenvalues -- 2.97424 2.98534 2.98626 2.99567 3.00675

Alpha virt. eigenvalues -- 3.01429 3.02543 3.03288 3.03375 3.03875

Alpha virt. eigenvalues -- 3.04192 3.05136 3.05385 3.06930 3.07003

Alpha virt. eigenvalues -- 3.07938 3.08183 3.09342 3.16855 3.17555

Alpha virt. eigenvalues -- 3.18640 3.19093 3.19407 3.20495 3.21241

Alpha virt. eigenvalues -- 3.23684 3.24975 3.25788 3.25947 3.27456

Alpha virt. eigenvalues -- 3.29909 3.30253 3.30722 3.31030 3.31598

Alpha virt. eigenvalues -- 3.32032 3.33922 3.34722 3.35096 3.37531

Alpha virt. eigenvalues -- 3.37607 3.45171 3.47547 3.51624 3.51813

Alpha virt. eigenvalues -- 3.52573 3.56353 3.56550 3.57730 3.58519

Alpha virt. eigenvalues -- 3.60030 3.62818 3.64561 3.64782 3.81058

Alpha virt. eigenvalues -- 3.81648 3.81709 3.83753 3.84844 3.85009

Alpha virt. eigenvalues -- 3.85394 3.88932 3.92383 3.94564 3.96080

Alpha virt. eigenvalues -- 4.00069 4.10999 4.19665 4.20386 4.32208

Alpha virt. eigenvalues -- 4.32546 4.46674 4.51133 4.51347 4.61006

Alpha virt. eigenvalues -- 4.65215 4.65527 4.65875 5.13970 5.18513

Alpha virt. eigenvalues -- 5.18514 5.30201 7.77794 7.77852 7.86395

Alpha virt. eigenvalues -- 7.92016 8.11780 11.09563 23.26447 23.31558

Alpha virt. eigenvalues -- 23.31881 23.34614 23.52450 23.54551 23.57887

Alpha virt. eigenvalues -- 23.58657 23.75483 23.77188 23.77949 23.80119

Alpha virt. eigenvalues -- 23.87568 23.88604 23.96300 23.96809 23.98581

Alpha virt. eigenvalues -- 23.98948 24.01276 24.01328 24.10669 24.10686

Alpha virt. eigenvalues -- 24.13715 24.13930 24.93531 24.93572 24.93888

Alpha virt. eigenvalues -- 24.93902 35.61871 35.63339 35.64380 35.64828

Beta occ. eigenvalues -- -14.31628 -14.31628 -14.31271 -14.31271 -10.22431

Beta occ. eigenvalues -- -10.22431 -10.22431 -10.22431 -10.22349 -10.22349

Beta occ. eigenvalues -- -10.22348 -10.22348 -10.20804 -10.20803 -10.20803

Beta occ. eigenvalues -- -10.20803 -10.18932 -10.18932 -10.18932 -10.18932

Beta occ. eigenvalues -- -10.17939 -10.17939 -10.17939 -10.17939 -10.17756

Beta occ. eigenvalues -- -10.17756 -10.17688 -10.17688 -10.16144 -10.16144

Beta occ. eigenvalues -- -10.16088 -10.16088 -0.97256 -0.96779 -0.95842

Beta occ. eigenvalues -- -0.95319 -0.84855 -0.83149 -0.82731 -0.81119

Beta occ. eigenvalues -- -0.77630 -0.77467 -0.76476 -0.75937 -0.75585

Beta occ. eigenvalues -- -0.74769 -0.74687 -0.72883 -0.72747 -0.67679

Beta occ. eigenvalues -- -0.67353 -0.62838 -0.60003 -0.59627 -0.59312

Beta occ. eigenvalues -- -0.58672 -0.58202 -0.57331 -0.56349 -0.56348

Beta occ. eigenvalues -- -0.56127 -0.55406 -0.55337 -0.55092 -0.54721

Beta occ. eigenvalues -- -0.53050 -0.52496 -0.52461 -0.51978 -0.51540

Beta occ. eigenvalues -- -0.51374 -0.50261 -0.49576 -0.45758 -0.44934

Beta occ. eigenvalues -- -0.44726 -0.43703 -0.43082 -0.42649 -0.42522

Beta occ. eigenvalues -- -0.41713 -0.41197 -0.40903 -0.39814 -0.39666

Beta occ. eigenvalues -- -0.38387 -0.38318 -0.38078 -0.37964 -0.37741

Beta occ. eigenvalues -- -0.36817 -0.33821 -0.33633 -0.32634 -0.32242

Beta occ. eigenvalues -- -0.32177 -0.29960 -0.29606 -0.29565 -0.29231

Beta occ. eigenvalues -- -0.26986 -0.26964 -0.26466 -0.26297 -0.26137

Beta occ. eigenvalues -- -0.24418 -0.24265 -0.24116 -0.21056

Beta virt. eigenvalues -- -0.16093 -0.09828 -0.09707 -0.05181 0.02433

Beta virt. eigenvalues -- 0.02499 0.02798 0.02913 0.03432 0.03774

Beta virt. eigenvalues -- 0.03895 0.04239 0.04343 0.04652 0.05478

Beta virt. eigenvalues -- 0.05574 0.05688 0.05820 0.05900 0.07042

Beta virt. eigenvalues -- 0.07874 0.08464 0.08525 0.08549 0.09714

Beta virt. eigenvalues -- 0.09805 0.09942 0.10016 0.11479 0.12403

Beta virt. eigenvalues -- 0.12669 0.13686 0.14669 0.15774 0.16958

Beta virt. eigenvalues -- 0.16959 0.16996 0.17278 0.18389 0.18992

Beta virt. eigenvalues -- 0.19933 0.22402 0.22805 0.23162 0.24007

Beta virt. eigenvalues -- 0.24305 0.24371 0.24799 0.25150 0.25678

Beta virt. eigenvalues -- 0.25752 0.26471 0.26538 0.26643 0.27977

Beta virt. eigenvalues -- 0.29523 0.30020 0.31059 0.31131 0.32582

Beta virt. eigenvalues -- 0.32597 0.32833 0.35411 0.35476 0.35508

Beta virt. eigenvalues -- 0.35604 0.35713 0.36038 0.36162 0.36424

Beta virt. eigenvalues -- 0.36657 0.36794 0.37166 0.38193 0.38285

Beta virt. eigenvalues -- 0.39674 0.40299 0.40427 0.40618 0.40709

Beta virt. eigenvalues -- 0.41124 0.41481 0.41824 0.42225 0.42458

Beta virt. eigenvalues -- 0.43282 0.43419 0.44032 0.44083 0.44604

Beta virt. eigenvalues -- 0.44743 0.45401 0.45521 0.45831 0.47178

Beta virt. eigenvalues -- 0.47829 0.47848 0.48441 0.49169 0.49210

Beta virt. eigenvalues -- 0.49400 0.49651 0.50653 0.51207 0.51551

Beta virt. eigenvalues -- 0.51640 0.52118 0.52138 0.52265 0.52266

Beta virt. eigenvalues -- 0.55064 0.56189 0.56387 0.57152 0.57307

Beta virt. eigenvalues -- 0.57332 0.57705 0.57818 0.57887 0.58197

Beta virt. eigenvalues -- 0.58698 0.58704 0.61179 0.61890 0.62180

Beta virt. eigenvalues -- 0.62275 0.62493 0.62514 0.63218 0.63322

Beta virt. eigenvalues -- 0.63841 0.64195 0.64702 0.64898 0.65070

Beta virt. eigenvalues -- 0.65375 0.65388 0.68404 0.68493 0.69013

Beta virt. eigenvalues -- 0.69119 0.70241 0.70648 0.70732 0.70920

Beta virt. eigenvalues -- 0.71911 0.71976 0.73651 0.73742 0.73777

Beta virt. eigenvalues -- 0.74147 0.74287 0.74693 0.74802 0.75184

Beta virt. eigenvalues -- 0.75189 0.75553 0.77043 0.77856 0.79707

Beta virt. eigenvalues -- 0.81256 0.81413 0.81979 0.82164 0.83518

Beta virt. eigenvalues -- 0.84173 0.84851 0.85632 0.85831 0.86087

Beta virt. eigenvalues -- 0.88370 0.89948 0.90407 0.91028 0.91132

Beta virt. eigenvalues -- 0.92650 0.92663 0.94776 0.95401 0.96080

Beta virt. eigenvalues -- 0.96239 0.97683 0.97705 0.99599 1.00640

Beta virt. eigenvalues -- 1.00864 1.00925 1.01239 1.01566 1.02060

Beta virt. eigenvalues -- 1.02202 1.03416 1.05823 1.05883 1.06245

Beta virt. eigenvalues -- 1.06324 1.07132 1.07599 1.08774 1.09016

Beta virt. eigenvalues -- 1.11495 1.12409 1.12482 1.12497 1.12630

Beta virt. eigenvalues -- 1.13351 1.13393 1.13730 1.13998 1.14323

Beta virt. eigenvalues -- 1.15073 1.15546 1.16144 1.16679 1.17250

Beta virt. eigenvalues -- 1.17253 1.18261 1.18618 1.18793 1.19273

Beta virt. eigenvalues -- 1.19273 1.21002 1.21300 1.21358 1.21534

Beta virt. eigenvalues -- 1.21757 1.23837 1.24628 1.24924 1.25050

Beta virt. eigenvalues -- 1.25531 1.25733 1.28013 1.28284 1.28746

Beta virt. eigenvalues -- 1.29390 1.31913 1.32261 1.33618 1.33967

Beta virt. eigenvalues -- 1.34347 1.37202 1.42390 1.42760 1.43099

Beta virt. eigenvalues -- 1.47412 1.47703 1.48403 1.48474 1.49529

Beta virt. eigenvalues -- 1.51775 1.52151 1.52914 1.55032 1.55045

Beta virt. eigenvalues -- 1.55097 1.55110 1.55125 1.55139 1.57605

Beta virt. eigenvalues -- 1.57619 1.58375 1.58459 1.58750 1.59064

Beta virt. eigenvalues -- 1.59556 1.59754 1.60853 1.61071 1.61649

Beta virt. eigenvalues -- 1.62729 1.62861 1.63595 1.65008 1.65038

Beta virt. eigenvalues -- 1.65457 1.65720 1.66241 1.67322 1.69862

Beta virt. eigenvalues -- 1.69962 1.71940 1.72897 1.73842 1.75627

Beta virt. eigenvalues -- 1.76842 1.76877 1.76907 1.78904 1.79274

Beta virt. eigenvalues -- 1.79321 1.79805 1.80172 1.80552 1.80760

Beta virt. eigenvalues -- 1.81241 1.83760 1.84931 1.86013 1.86396

Beta virt. eigenvalues -- 1.87829 1.88760 1.88892 1.88918 1.89102

Beta virt. eigenvalues -- 1.89949 1.90123 1.90723 1.90974 1.93499

Beta virt. eigenvalues -- 1.94593 1.94643 1.94741 1.94808 1.94949

Beta virt. eigenvalues -- 1.95852 1.96673 1.97032 1.97087 1.99160

Beta virt. eigenvalues -- 1.99623 2.00997 2.03183 2.03520 2.04347

Beta virt. eigenvalues -- 2.04413 2.05175 2.09129 2.09805 2.11036

Beta virt. eigenvalues -- 2.12523 2.14133 2.17758 2.19622 2.25930

Beta virt. eigenvalues -- 2.27191 2.27750 2.28025 2.28538 2.31415

Beta virt. eigenvalues -- 2.31478 2.33516 2.33690 2.34599 2.35903

Beta virt. eigenvalues -- 2.36494 2.36594 2.37231 2.37633 2.40469

Beta virt. eigenvalues -- 2.40654 2.40976 2.41030 2.41317 2.41375

Beta virt. eigenvalues -- 2.43620 2.45928 2.48006 2.48309 2.49013

Beta virt. eigenvalues -- 2.49616 2.52088 2.53124 2.53695 2.53838

Beta virt. eigenvalues -- 2.56096 2.56734 2.57015 2.57411 2.57842

Beta virt. eigenvalues -- 2.57846 2.58560 2.59749 2.60199 2.61797

Beta virt. eigenvalues -- 2.62667 2.62861 2.64353 2.64687 2.64769

Beta virt. eigenvalues -- 2.66754 2.67095 2.70841 2.70990 2.72553

Beta virt. eigenvalues -- 2.76975 2.77834 2.78190 2.80158 2.80922

Beta virt. eigenvalues -- 2.82626 2.83205 2.83768 2.84812 2.86287

Beta virt. eigenvalues -- 2.86990 2.88282 2.88300 2.88302 2.88310

Beta virt. eigenvalues -- 2.91988 2.95447 2.95554 2.95909 2.96094

Beta virt. eigenvalues -- 2.96739 2.97393 2.97523 2.98473 2.98546

Beta virt. eigenvalues -- 2.99557 3.00910 3.01570 3.02573 3.03970

Beta virt. eigenvalues -- 3.04166 3.04401 3.04531 3.05280 3.05581

Beta virt. eigenvalues -- 3.07096 3.08028 3.08315 3.08346 3.09418

Beta virt. eigenvalues -- 3.16875 3.17607 3.18670 3.19226 3.19457

Beta virt. eigenvalues -- 3.20570 3.21289 3.23821 3.25121 3.25888

Beta virt. eigenvalues -- 3.26088 3.27633 3.30032 3.30355 3.30865

Beta virt. eigenvalues -- 3.31112 3.31743 3.32120 3.34009 3.34952

Beta virt. eigenvalues -- 3.35126 3.37596 3.37737 3.45263 3.47768

Beta virt. eigenvalues -- 3.51774 3.51943 3.52688 3.56499 3.56558

Beta virt. eigenvalues -- 3.57732 3.58693 3.60180 3.62926 3.64673

Beta virt. eigenvalues -- 3.64931 3.81267 3.81779 3.81928 3.83785

Beta virt. eigenvalues -- 3.85876 3.85999 3.86081 3.89858 3.92631

Beta virt. eigenvalues -- 3.94849 3.96398 4.00329 4.11388 4.20017

Beta virt. eigenvalues -- 4.20761 4.32442 4.32886 4.46890 4.51263

Beta virt. eigenvalues -- 4.51690 4.61324 4.65557 4.65725 4.66111

Beta virt. eigenvalues -- 5.14139 5.18702 5.18721 5.30440 7.77822

Beta virt. eigenvalues -- 7.77857 7.86399 7.92020 8.11785 11.09579

Beta virt. eigenvalues -- 23.26568 23.31678 23.32010 23.34744 23.52510

Beta virt. eigenvalues -- 23.54561 23.58009 23.58728 23.75637 23.77360

Beta virt. eigenvalues -- 23.78085 23.80297 23.87632 23.88712 23.96359

Beta virt. eigenvalues -- 23.96881 23.98809 23.99186 24.01421 24.01489

Beta virt. eigenvalues -- 24.10765 24.10786 24.13696 24.13916 24.93582

Beta virt. eigenvalues -- 24.93623 24.93940 24.93954 35.62137 35.63555

Beta virt. eigenvalues -- 35.64752 35.64938

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 5.189365 0.452349 -0.082809 -0.068348 0.493660 0.014633

2 C 0.452349 4.899574 0.435470 -0.157004 -0.068348 -0.000124

3 N -0.082809 0.435470 6.938614 0.435470 -0.082809 -0.014596

4 C -0.068348 -0.157004 0.435470 4.899573 0.452349 0.369698

5 C 0.493660 -0.068348 -0.082809 0.452349 5.189365 -0.078186

6 C 0.014633 -0.000124 -0.014596 0.369698 -0.078186 5.204521

7 C -0.001189 -0.000345 -0.019800 -0.104428 0.013176 0.409549

8 N 0.000045 0.000347 -0.013201 -0.016378 -0.000294 -0.020435

9 C -0.000005 0.000004 0.000447 -0.000480 0.000045 -0.001146

10 C 0.000001 -0.000005 0.000052 -0.001111 -0.000007 0.013508

11 C -0.000006 0.000039 -0.000353 0.011834 -0.000120 -0.074485

12 C -0.078186 0.369698 -0.014596 -0.000124 0.014633 -0.002184

13 C 0.013176 -0.104428 -0.019800 -0.000345 -0.001189 0.000190

14 C -0.000120 0.011834 -0.000353 0.000039 -0.000006 0.000001

15 C -0.000007 -0.001111 0.000052 -0.000005 0.000001 -0.000000

16 C 0.000045 -0.000480 0.000447 0.000004 -0.000005 0.000001

17 N -0.000294 -0.016378 -0.013201 0.000347 0.000045 -0.000138

18 C 0.000001 0.000184 -0.000156 0.000001 -0.000000 0.000002

19 C -0.000000 -0.000053 0.000155 -0.000005 0.000000 0.000001

20 C -0.000000 -0.000000 0.000002 0.000000 0.000000 -0.000000

21 C 0.000000 0.000000 0.000002 -0.000000 -0.000000 0.000001

22 C 0.000000 -0.000005 0.000155 -0.000053 -0.000000 0.000184

23 N 0.000002 0.000155 -0.001631 0.000155 0.000002 -0.000156

24 H 0.390602 -0.039264 0.005576 0.005312 -0.034319 -0.000158

25 H -0.034319 0.005312 0.005576 -0.039264 0.390602 -0.005845

26 H 0.000000 0.000000 0.000002 0.000009 -0.000000 -0.000156

27 H -0.000000 0.000000 -0.000003 -0.000027 0.000006 -0.005543

28 H 0.000006 -0.000027 -0.000003 0.000000 -0.000000 0.000000

29 H -0.000000 0.000009 0.000002 0.000000 0.000000 0.000000

30 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

31 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

32 Zn 0.001710 -0.013155 0.129313 -0.013155 0.001710 -0.009167

33 C -0.000000 0.000001 -0.000156 0.000184 0.000001 -0.002318

34 C -0.000000 0.000000 -0.000000 0.000002 0.000000 -0.000056

35 C -0.016508 -0.071267 0.003940 -0.000415 0.002409 -0.000049

36 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.000709 -0.003720 -0.000075 -0.000051 0.000305 -0.000002

38 C 0.002409 -0.000415 0.003940 -0.071267 -0.016508 0.554457

39 C 0.000305 -0.000051 -0.000075 -0.003720 -0.000709 -0.106092

40 C 0.000000 0.000002 -0.000000 0.000000 -0.000000 0.000000

41 C 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 -0.000000 0.000000

43 H -0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000001 -0.000000 0.000001 -0.000004 0.000090 0.001767

45 H 0.000090 -0.000004 0.000001 -0.000000 0.000001 -0.000000

7 8 9 10 11 12

1 C -0.001189 0.000045 -0.000005 0.000001 -0.000006 -0.078186

2 C -0.000345 0.000347 0.000004 -0.000005 0.000039 0.369698

3 N -0.019800 -0.013201 0.000447 0.000052 -0.000353 -0.014596

4 C -0.104428 -0.016378 -0.000480 -0.001111 0.011834 -0.000124

5 C 0.013176 -0.000294 0.000045 -0.000007 -0.000120 0.014633

6 C 0.409549 -0.020435 -0.001146 0.013508 -0.074485 -0.002184

7 C 4.887057 0.429142 -0.147143 -0.061350 0.397759 0.000190

8 N 0.429142 6.949142 0.429142 -0.075276 -0.075276 -0.000138

9 C -0.147143 0.429142 4.887057 0.397759 -0.061350 0.000001

10 C -0.061350 -0.075276 0.397759 5.142167 0.539721 -0.000000

11 C 0.397759 -0.075276 -0.061350 0.539721 5.142167 0.000001

12 C 0.000190 -0.000138 0.000001 -0.000000 0.000001 5.204521

13 C -0.000057 0.000149 -0.000004 0.000000 -0.000000 0.409549

14 C -0.000000 0.000001 0.000000 0.000000 -0.000000 -0.074485

15 C 0.000000 0.000001 -0.000000 -0.000000 0.000000 0.013508

16 C -0.000004 0.000149 -0.000057 -0.000000 0.000000 -0.001146

17 N 0.000149 -0.001515 0.000149 0.000001 0.000001 -0.020435

18 C 0.000001 -0.000138 0.000190 0.000001 -0.000000 -0.002318

19 C 0.000004 0.000347 -0.000345 0.000039 -0.000005 0.000184

20 C -0.000005 0.000045 -0.001189 -0.000006 0.000001 0.000001

21 C 0.000045 -0.000294 0.013176 -0.000120 -0.000007 -0.000000

22 C -0.000480 -0.016378 -0.104428 0.011834 -0.001111 0.000001

23 N 0.000447 -0.013201 -0.019800 -0.000353 0.000052 -0.000156

24 H 0.000012 0.000002 -0.000000 0.000000 0.000000 -0.005845

25 H -0.000083 -0.000001 0.000000 -0.000000 0.000007 -0.000158

26 H 0.005627 0.005048 -0.037822 0.388260 -0.032791 0.000000

27 H -0.037822 0.005048 0.005627 -0.032791 0.388260 0.000000

28 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.005543

29 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000156

30 H -0.000000 0.000002 0.000012 0.000000 0.000000 0.000000

31 H 0.000000 -0.000001 -0.000083 0.000007 -0.000000 0.000000

32 Zn -0.013192 0.121170 -0.013192 0.001844 0.001844 -0.009167

33 C -0.001146 -0.020435 0.409549 -0.074485 0.013508 0.000002

34 C -0.000502 0.003600 -0.075455 -0.014536 0.002620 0.000000

35 C 0.000002 -0.000000 0.000000 -0.000000 0.000000 0.554457

36 C -0.000051 -0.000085 -0.004790 -0.000305 0.000350 0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.106092

38 C -0.075456 0.003600 -0.000502 0.002620 -0.014536 -0.000049

39 C -0.004790 -0.000085 -0.000051 0.000350 -0.000305 -0.000002

40 C 0.000000 -0.000000 0.000002 0.000000 -0.000000 -0.000056

41 C -0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000002

42 H 0.000000 0.000000 0.000000 0.000000 -0.000000 -0.000000

43 H -0.000000 0.000001 -0.000057 0.000100 0.000002 0.000000

44 H -0.000057 0.000001 -0.000000 0.000002 0.000100 -0.000000

45 H 0.000000 0.000000 0.000000 -0.000000 0.000000 0.001767

13 14 15 16 17 18

1 C 0.013176 -0.000120 -0.000007 0.000045 -0.000294 0.000001

2 C -0.104428 0.011834 -0.001111 -0.000480 -0.016378 0.000184

3 N -0.019800 -0.000353 0.000052 0.000447 -0.013201 -0.000156

4 C -0.000345 0.000039 -0.000005 0.000004 0.000347 0.000001

5 C -0.001189 -0.000006 0.000001 -0.000005 0.000045 -0.000000

6 C 0.000190 0.000001 -0.000000 0.000001 -0.000138 0.000002

7 C -0.000057 -0.000000 0.000000 -0.000004 0.000149 0.000001

8 N 0.000149 0.000001 0.000001 0.000149 -0.001515 -0.000138

9 C -0.000004 0.000000 -0.000000 -0.000057 0.000149 0.000190

10 C 0.000000 0.000000 -0.000000 -0.000000 0.000001 0.000001

11 C -0.000000 -0.000000 0.000000 0.000000 0.000001 -0.000000

12 C 0.409549 -0.074485 0.013508 -0.001146 -0.020435 -0.002318

13 C 4.887057 0.397759 -0.061350 -0.147143 0.429142 -0.001146

14 C 0.397759 5.142167 0.539721 -0.061350 -0.075276 0.013508

15 C -0.061350 0.539721 5.142167 0.397759 -0.075276 -0.074485

16 C -0.147143 -0.061350 0.397759 4.887057 0.429142 0.409549

17 N 0.429142 -0.075276 -0.075276 0.429142 6.949142 -0.020435

18 C -0.001146 0.013508 -0.074485 0.409549 -0.020435 5.204521

19 C -0.000480 -0.001111 0.011834 -0.104428 -0.016378 0.369698

20 C 0.000045 -0.000007 -0.000120 0.013176 -0.000294 -0.078186

21 C -0.000005 0.000001 -0.000006 -0.001189 0.000045 0.014633

22 C 0.000004 -0.000005 0.000039 -0.000345 0.000347 -0.000124

23 N 0.000447 0.000052 -0.000353 -0.019800 -0.013201 -0.014596

24 H -0.000083 0.000007 -0.000000 0.000000 -0.000001 0.000000

25 H 0.000012 0.000000 0.000000 -0.000000 0.000002 0.000000

26 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

27 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

28 H -0.037822 0.388260 -0.032791 0.005627 0.005048 -0.000156

29 H 0.005627 -0.032791 0.388260 -0.037822 0.005048 -0.005543

30 H 0.000000 -0.000000 0.000007 -0.000083 -0.000001 -0.005844

31 H -0.000000 0.000000 0.000000 0.000012 0.000002 -0.000158

32 Zn -0.013192 0.001844 0.001844 -0.013192 0.121170 -0.009167

33 C 0.000001 -0.000000 0.000001 0.000190 -0.000138 -0.002184

34 C 0.000000 -0.000000 0.000000 0.000002 -0.000000 -0.000049

35 C -0.075456 -0.014536 0.002620 -0.000502 0.003600 -0.000056

36 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000002

37 C -0.004790 -0.000305 0.000350 -0.000051 -0.000085 -0.000002

38 C 0.000002 0.000000 -0.000000 0.000000 -0.000000 0.000000

39 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

40 C -0.000502 0.002620 -0.014536 -0.075455 0.003600 0.554457

41 C -0.000051 0.000350 -0.000305 -0.004790 -0.000085 -0.106092

42 H -0.000000 0.000002 0.000100 -0.000057 0.000001 0.001767

43 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000000

45 H -0.000057 0.000100 0.000002 -0.000000 0.000001 -0.000000

19 20 21 22 23 24

1 C -0.000000 -0.000000 0.000000 0.000000 0.000002 0.390602

2 C -0.000053 -0.000000 0.000000 -0.000005 0.000155 -0.039264

3 N 0.000155 0.000002 0.000002 0.000155 -0.001631 0.005576

4 C -0.000005 0.000000 -0.000000 -0.000053 0.000155 0.005312

5 C 0.000000 0.000000 -0.000000 -0.000000 0.000002 -0.034319

6 C 0.000001 -0.000000 0.000001 0.000184 -0.000156 -0.000158

7 C 0.000004 -0.000005 0.000045 -0.000480 0.000447 0.000012

8 N 0.000347 0.000045 -0.000294 -0.016378 -0.013201 0.000002

9 C -0.000345 -0.001189 0.013176 -0.104428 -0.019800 -0.000000

10 C 0.000039 -0.000006 -0.000120 0.011834 -0.000353 0.000000

11 C -0.000005 0.000001 -0.000007 -0.001111 0.000052 0.000000

12 C 0.000184 0.000001 -0.000000 0.000001 -0.000156 -0.005845

13 C -0.000480 0.000045 -0.000005 0.000004 0.000447 -0.000083

14 C -0.001111 -0.000007 0.000001 -0.000005 0.000052 0.000007

15 C 0.011834 -0.000120 -0.000006 0.000039 -0.000353 -0.000000

16 C -0.104428 0.013176 -0.001189 -0.000345 -0.019800 0.000000

17 N -0.016378 -0.000294 0.000045 0.000347 -0.013201 -0.000001

18 C 0.369698 -0.078186 0.014633 -0.000124 -0.014596 0.000000

19 C 4.899573 0.452349 -0.068348 -0.157004 0.435470 -0.000000

20 C 0.452349 5.189365 0.493660 -0.068348 -0.082809 -0.000000

21 C -0.068348 0.493660 5.189365 0.452349 -0.082809 0.000000

22 C -0.157004 -0.068348 0.452349 4.899573 0.435470 -0.000000

23 N 0.435470 -0.082809 -0.082809 0.435470 6.938614 0.000000

24 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.441390

25 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.001915

26 H 0.000000 -0.000000 0.000006 -0.000027 -0.000003 -0.000000

27 H 0.000000 0.000000 -0.000000 0.000009 0.000002 -0.000000

28 H 0.000009 -0.000000 0.000000 0.000000 0.000002 -0.000005

29 H -0.000027 0.000006 -0.000000 0.000000 -0.000003 -0.000000

30 H -0.039264 0.390602 -0.034319 0.005312 0.005576 -0.000000

31 H 0.005312 -0.034319 0.390602 -0.039264 0.005576 -0.000000

32 Zn -0.013155 0.001710 0.001710 -0.013155 0.129313 -0.000395

33 C -0.000124 0.014633 -0.078186 0.369698 -0.014596 0.000000

34 C -0.000415 0.002409 -0.016508 -0.071267 0.003940 -0.000000

35 C 0.000002 0.000000 -0.000000 0.000000 -0.000000 0.006154

36 C -0.000051 0.000305 -0.000709 -0.003720 -0.000075 -0.000000

37 C 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.002903

38 C 0.000000 -0.000000 0.000000 0.000002 -0.000000 -0.000087

39 C -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000010

40 C -0.071267 -0.016508 0.002409 -0.000415 0.003940 0.000000

41 C -0.003720 -0.000709 0.000305 -0.000051 -0.000075 -0.000000

42 H -0.000004 0.000090 0.000001 -0.000000 0.000001 -0.000000

43 H -0.000000 0.000001 0.000090 -0.000004 0.000001 -0.000000

44 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

45 H 0.000000 0.000000 -0.000000 0.000000 0.000000 0.000052

25 26 27 28 29 30

1 C -0.034319 0.000000 -0.000000 0.000006 -0.000000 -0.000000

2 C 0.005312 0.000000 0.000000 -0.000027 0.000009 -0.000000

3 N 0.005576 0.000002 -0.000003 -0.000003 0.000002 0.000000

4 C -0.039264 0.000009 -0.000027 0.000000 0.000000 -0.000000

5 C 0.390602 -0.000000 0.000006 -0.000000 0.000000 0.000000

6 C -0.005845 -0.000156 -0.005543 0.000000 0.000000 0.000000

7 C -0.000083 0.005627 -0.037822 -0.000000 -0.000000 -0.000000

8 N -0.000001 0.005048 0.005048 0.000000 0.000000 0.000002

9 C 0.000000 -0.037822 0.005627 -0.000000 -0.000000 0.000012

10 C -0.000000 0.388260 -0.032791 0.000000 -0.000000 0.000000

11 C 0.000007 -0.032791 0.388260 -0.000000 0.000000 0.000000

12 C -0.000158 0.000000 0.000000 -0.005543 -0.000156 0.000000

13 C 0.000012 -0.000000 -0.000000 -0.037822 0.005627 0.000000

14 C 0.000000 0.000000 -0.000000 0.388260 -0.032791 -0.000000

15 C 0.000000 -0.000000 0.000000 -0.032791 0.388260 0.000007

16 C -0.000000 -0.000000 -0.000000 0.005627 -0.037822 -0.000083

17 N 0.000002 0.000000 0.000000 0.005048 0.005048 -0.000001

18 C 0.000000 0.000000 0.000000 -0.000156 -0.005543 -0.005844

19 C -0.000000 0.000000 0.000000 0.000009 -0.000027 -0.039264

20 C 0.000000 -0.000000 0.000000 -0.000000 0.000006 0.390602

21 C -0.000000 0.000006 -0.000000 0.000000 -0.000000 -0.034319

22 C -0.000000 -0.000027 0.000009 0.000000 0.000000 0.005312

23 N 0.000000 -0.000003 0.000002 0.000002 -0.000003 0.005576

24 H -0.001915 -0.000000 -0.000000 -0.000005 -0.000000 -0.000000

25 H 0.441390 -0.000000 -0.000005 -0.000000 -0.000000 -0.000000

26 H -0.000000 0.425998 -0.002242 -0.000000 -0.000000 -0.000000

27 H -0.000005 -0.002242 0.425998 -0.000000 -0.000000 -0.000000

28 H -0.000000 -0.000000 -0.000000 0.425998 -0.002242 -0.000000

29 H -0.000000 -0.000000 -0.000000 -0.002242 0.425998 -0.000005

30 H -0.000000 -0.000000 -0.000000 -0.000000 -0.000005 0.441390

31 H -0.000000 -0.000005 -0.000000 -0.000000 -0.000000 -0.001915

32 Zn -0.000395 -0.000338 -0.000338 -0.000338 -0.000338 -0.000395

33 C 0.000000 -0.005543 -0.000156 0.000000 0.000000 -0.000158

34 C 0.000000 0.006361 -0.000082 -0.000000 -0.000000 -0.000087

35 C -0.000087 -0.000000 -0.000000 0.006361 -0.000082 0.000000

36 C -0.000000 0.003118 -0.000007 -0.000000 -0.000000 -0.000010

37 C -0.000010 -0.000000 -0.000000 0.003118 -0.000007 -0.000000

38 C 0.006154 -0.000082 0.006361 -0.000000 -0.000000 -0.000000

39 C 0.002903 -0.000007 0.003118 -0.000000 -0.000000 -0.000000

40 C -0.000000 -0.000000 -0.000000 -0.000082 0.006361 0.006154

41 C -0.000000 -0.000000 -0.000000 -0.000007 0.003118 0.002903

42 H -0.000000 -0.000000 -0.000000 -0.000000 0.000057 0.000052

43 H -0.000000 0.000057 -0.000000 -0.000000 -0.000000 -0.000000

44 H 0.000052 -0.000000 0.000057 -0.000000 -0.000000 -0.000000

45 H -0.000000 -0.000000 -0.000000 0.000057 -0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000000 0.001710 -0.000000 -0.000000 -0.016508 -0.000000

2 C -0.000000 -0.013155 0.000001 0.000000 -0.071267 -0.000000

3 N 0.000000 0.129313 -0.000156 -0.000000 0.003940 0.000000

4 C -0.000000 -0.013155 0.000184 0.000002 -0.000415 0.000000

5 C -0.000000 0.001710 0.000001 0.000000 0.002409 0.000000

6 C 0.000000 -0.009167 -0.002318 -0.000056 -0.000049 -0.000002

7 C 0.000000 -0.013192 -0.001146 -0.000502 0.000002 -0.000051

8 N -0.000001 0.121170 -0.020435 0.003600 -0.000000 -0.000085

9 C -0.000083 -0.013192 0.409549 -0.075455 0.000000 -0.004790

10 C 0.000007 0.001844 -0.074485 -0.014536 -0.000000 -0.000305

11 C -0.000000 0.001844 0.013508 0.002620 0.000000 0.000350

12 C 0.000000 -0.009167 0.000002 0.000000 0.554457 0.000000

13 C -0.000000 -0.013192 0.000001 0.000000 -0.075456 -0.000000

14 C 0.000000 0.001844 -0.000000 -0.000000 -0.014536 -0.000000

15 C 0.000000 0.001844 0.000001 0.000000 0.002620 0.000000

16 C 0.000012 -0.013192 0.000190 0.000002 -0.000502 0.000000

17 N 0.000002 0.121170 -0.000138 -0.000000 0.003600 0.000000

18 C -0.000158 -0.009167 -0.002184 -0.000049 -0.000056 -0.000002

19 C 0.005312 -0.013155 -0.000124 -0.000415 0.000002 -0.000051

20 C -0.034319 0.001710 0.014633 0.002409 0.000000 0.000305

21 C 0.390602 0.001710 -0.078186 -0.016508 -0.000000 -0.000709

22 C -0.039264 -0.013155 0.369698 -0.071267 0.000000 -0.003720

23 N 0.005576 0.129313 -0.014596 0.003940 -0.000000 -0.000075

24 H -0.000000 -0.000395 0.000000 -0.000000 0.006154 -0.000000

25 H -0.000000 -0.000395 0.000000 0.000000 -0.000087 -0.000000

26 H -0.000005 -0.000338 -0.005543 0.006361 -0.000000 0.003118

27 H -0.000000 -0.000338 -0.000156 -0.000082 -0.000000 -0.000007

28 H -0.000000 -0.000338 0.000000 -0.000000 0.006361 -0.000000

29 H -0.000000 -0.000338 0.000000 -0.000000 -0.000082 -0.000000

30 H -0.001915 -0.000395 -0.000158 -0.000087 0.000000 -0.000010

31 H 0.441390 -0.000395 -0.005844 0.006154 -0.000000 0.002903

32 Zn -0.000395 10.216923 -0.009167 -0.000748 -0.000748 -0.000128

33 C -0.005844 -0.009167 5.204521 0.554457 0.000000 -0.106092

34 C 0.006154 -0.000748 0.554457 4.808191 0.000000 0.839488

35 C -0.000000 -0.000748 0.000000 0.000000 4.808191 0.000000

36 C 0.002903 -0.000128 -0.106092 0.839488 0.000000 5.174203

37 C -0.000000 -0.000128 0.000000 0.000000 0.839488 0.000000

38 C 0.000000 -0.000748 -0.000056 -0.000001 -0.000001 -0.000000

39 C -0.000000 -0.000128 -0.000002 -0.000000 -0.000000 -0.000000

40 C -0.000087 -0.000748 -0.000049 -0.000001 -0.000001 -0.000000

41 C -0.000010 -0.000128 -0.000002 -0.000000 -0.000000 -0.000000

42 H -0.000000 -0.000004 -0.000000 -0.000000 -0.000000 -0.000000

43 H 0.000052 -0.000004 0.001767 -0.019487 0.000000 0.369532

44 H -0.000000 -0.000004 -0.000000 -0.000000 -0.000000 0.000000

45 H -0.000000 -0.000004 0.000000 0.000000 -0.019487 0.000000

37 38 39 40 41 42

1 C -0.000709 0.002409 0.000305 0.000000 0.000000 0.000000

2 C -0.003720 -0.000415 -0.000051 0.000002 0.000000 0.000000

3 N -0.000075 0.003940 -0.000075 -0.000000 0.000000 0.000000

4 C -0.000051 -0.071267 -0.003720 0.000000 -0.000000 0.000000

5 C 0.000305 -0.016508 -0.000709 -0.000000 -0.000000 -0.000000

6 C -0.000002 0.554457 -0.106092 0.000000 0.000000 0.000000

7 C 0.000000 -0.075456 -0.004790 0.000000 -0.000000 0.000000

8 N 0.000000 0.003600 -0.000085 -0.000000 0.000000 0.000000

9 C -0.000000 -0.000502 -0.000051 0.000002 0.000000 0.000000

10 C -0.000000 0.002620 0.000350 0.000000 0.000000 0.000000

11 C 0.000000 -0.014536 -0.000305 -0.000000 -0.000000 -0.000000

12 C -0.106092 -0.000049 -0.000002 -0.000056 -0.000002 -0.000000

13 C -0.004790 0.000002 0.000000 -0.000502 -0.000051 -0.000000

14 C -0.000305 0.000000 0.000000 0.002620 0.000350 0.000002

15 C 0.000350 -0.000000 -0.000000 -0.014536 -0.000305 0.000100

16 C -0.000051 0.000000 -0.000000 -0.075455 -0.004790 -0.000057

17 N -0.000085 -0.000000 0.000000 0.003600 -0.000085 0.000001

18 C -0.000002 0.000000 0.000000 0.554457 -0.106092 0.001767

19 C 0.000000 0.000000 -0.000000 -0.071267 -0.003720 -0.000004

20 C 0.000000 -0.000000 -0.000000 -0.016508 -0.000709 0.000090

21 C -0.000000 0.000000 0.000000 0.002409 0.000305 0.000001

22 C -0.000000 0.000002 0.000000 -0.000415 -0.000051 -0.000000

23 N 0.000000 -0.000000 0.000000 0.003940 -0.000075 0.000001

24 H 0.002903 -0.000087 -0.000010 0.000000 -0.000000 -0.000000

25 H -0.000010 0.006154 0.002903 -0.000000 -0.000000 -0.000000

26 H -0.000000 -0.000082 -0.000007 -0.000000 -0.000000 -0.000000

27 H -0.000000 0.006361 0.003118 -0.000000 -0.000000 -0.000000

28 H 0.003118 -0.000000 -0.000000 -0.000082 -0.000007 -0.000000

29 H -0.000007 -0.000000 -0.000000 0.006361 0.003118 0.000057

30 H -0.000000 -0.000000 -0.000000 0.006154 0.002903 0.000052

31 H -0.000000 0.000000 -0.000000 -0.000087 -0.000010 -0.000000

32 Zn -0.000128 -0.000748 -0.000128 -0.000748 -0.000128 -0.000004

33 C 0.000000 -0.000056 -0.000002 -0.000049 -0.000002 -0.000000

34 C 0.000000 -0.000001 -0.000000 -0.000001 -0.000000 -0.000000

35 C 0.839488 -0.000001 -0.000000 -0.000001 -0.000000 -0.000000

36 C 0.000000 -0.000000 -0.000000 -0.000000 -0.000000 -0.000000

37 C 5.174203 -0.000000 -0.000000 -0.000000 -0.000000 0.000000

38 C -0.000000 4.808191 0.839488 0.000000 0.000000 0.000000

39 C -0.000000 0.839488 5.174203 0.000000 0.000000 0.000000

40 C -0.000000 0.000000 0.000000 4.808191 0.839488 -0.019487

41 C -0.000000 0.000000 0.000000 0.839488 5.174203 0.369532

42 H 0.000000 0.000000 0.000000 -0.019487 0.369532 0.344472

43 H 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

44 H -0.000000 -0.019487 0.369532 0.000000 0.000000 0.000000

45 H 0.369532 -0.000000 -0.000000 -0.000000 0.000000 0.000000

43 44 45

1 C -0.000000 0.000001 0.000090

2 C 0.000000 -0.000000 -0.000004

3 N 0.000000 0.000001 0.000001

4 C 0.000000 -0.000004 -0.000000

5 C 0.000000 0.000090 0.000001

6 C -0.000000 0.001767 -0.000000

7 C -0.000000 -0.000057 0.000000

8 N 0.000001 0.000001 0.000000

9 C -0.000057 -0.000000 0.000000

10 C 0.000100 0.000002 -0.000000

11 C 0.000002 0.000100 0.000000

12 C 0.000000 -0.000000 0.001767

13 C 0.000000 0.000000 -0.000057

14 C -0.000000 0.000000 0.000100

15 C 0.000000 -0.000000 0.000002

16 C 0.000000 0.000000 -0.000000

17 N 0.000000 0.000000 0.000001

18 C -0.000000 0.000000 -0.000000

19 C -0.000000 0.000000 0.000000

20 C 0.000001 -0.000000 0.000000

21 C 0.000090 0.000000 -0.000000

22 C -0.000004 0.000000 0.000000

23 N 0.000001 0.000000 0.000000

24 H -0.000000 -0.000000 0.000052

25 H -0.000000 0.000052 -0.000000

26 H 0.000057 -0.000000 -0.000000

27 H -0.000000 0.000057 -0.000000

28 H -0.000000 -0.000000 0.000057

29 H -0.000000 -0.000000 -0.000000

30 H -0.000000 -0.000000 -0.000000

31 H 0.000052 -0.000000 -0.000000

32 Zn -0.000004 -0.000004 -0.000004

33 C 0.001767 -0.000000 0.000000

34 C -0.019487 -0.000000 0.000000

35 C 0.000000 -0.000000 -0.019487

36 C 0.369532 0.000000 0.000000

37 C 0.000000 -0.000000 0.369532

38 C -0.000000 -0.019487 -0.000000

39 C 0.000000 0.369532 -0.000000

40 C -0.000000 0.000000 -0.000000

41 C -0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000

43 H 0.344472 0.000000 0.000000

44 H 0.000000 0.344472 0.000000

45 H 0.000000 0.000000 0.344472

Atomic-Atomic Spin Densities.

1 2 3 4 5 6

1 C 0.073142 0.032764 0.000877 -0.009973 -0.027872 0.000463

2 C 0.032764 0.061813 -0.001549 -0.010779 -0.009973 0.001041

3 N 0.000877 -0.001549 0.055662 -0.001549 0.000877 -0.004595

4 C -0.009973 -0.010779 -0.001549 0.061813 0.032764 -0.032988

5 C -0.027872 -0.009973 0.000877 0.032764 0.073142 -0.008878

6 C 0.000463 0.001041 -0.004595 -0.032988 -0.008878 0.340863

7 C 0.000037 0.000093 0.000601 -0.003294 -0.000730 0.029613

8 N -0.000008 -0.000107 0.000642 0.002112 0.000069 -0.011123

9 C 0.000000 0.000002 -0.000016 -0.000054 -0.000001 0.000812

10 C 0.000000 -0.000000 0.000001 0.000019 -0.000000 -0.000963

11 C -0.000001 0.000000 0.000010 0.000246 0.000018 -0.002153

12 C -0.008878 -0.032988 -0.004595 0.001041 0.000463 0.000040

13 C -0.000730 -0.003294 0.000601 0.000093 0.000037 -0.000008

14 C 0.000018 0.000246 0.000010 0.000000 -0.000001 0.000000

15 C -0.000000 0.000019 0.000001 -0.000000 0.000000 -0.000000

16 C -0.000001 -0.000054 -0.000016 0.000002 0.000000 -0.000000

17 N 0.000069 0.002112 0.000642 -0.000107 -0.000008 0.000008

18 C -0.000000 -0.000007 -0.000001 0.000000 -0.000000 0.000000

19 C 0.000000 0.000002 -0.000002 -0.000000 -0.000000 0.000000

20 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000000

21 C -0.000000 -0.000000 -0.000000 0.000000 0.000000 -0.000000

22 C -0.000000 -0.000000 -0.000002 0.000002 0.000000 -0.000007

23 N -0.000000 -0.000002 0.000017 -0.000002 -0.000000 -0.000001

24 H -0.000060 -0.000203 -0.000032 -0.000009 0.000279 -0.000002

25 H 0.000279 -0.000009 -0.000032 -0.000203 -0.000060 0.000273

26 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000013

27 H -0.000000 0.000000 0.000000 -0.000021 0.000001 -0.000021

28 H 0.000001 -0.000021 0.000000 0.000000 -0.000000 0.000000

29 H -0.000000 0.000000 -0.000000 0.000000 0.000000 -0.000000

30 H -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.000000

31 H 0.000000 0.000000 0.000000 -0.000000 -0.000000 0.000000

32 Zn 0.000125 0.000301 0.002019 0.000301 0.000125 -0.001719

33 C -0.000000 0.000000 -0.000001 -0.000007 -0.000000 0.000162

34 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000003

35 C 0.000710 0.000772 -0.000031 -0.000028 0.000030 0.000001

36 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

37 C 0.000792 0.000887 0.000018 -0.000006 -0.000023 0.000000

38 C 0.000030 -0.000028 -0.000031 0.000772 0.000710 -0.005238

39 C -0.000023 -0.000006 0.000018 0.000887 0.000792 -0.009098

40 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 0.000000

41 C 0.000000 -0.000000 0.000000 -0.000000 -0.000000 -0.000000

42 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

43 H -0.000000 0.000000 0.000000 -0.000000 0.000000 0.000000

44 H -0.000000 -0.000000 0.000000 -0.000003 0.000001 -0.000041

45 H 0.000001 -0.000003 0.000000 -0.000000 -0.000000 0.000000

7 8 9 10 11 12

1 C 0.000037 -0.000008 0.000000 0.000000 -0.000001 -0.008878

2 C 0.000093 -0.000107 0.000002 -0.000000 0.000000 -0.032988

3 N 0.000601 0.000642 -0.000016 0.000001 0.000010 -0.004595

4 C -0.003294 0.002112 -0.000054 0.000019 0.000246 0.001041

5 C -0.000730 0.000069 -0.000001 -0.000000 0.000018 0.000463

6 C 0.029613 -0.011123 0.000812 -0.000963 -0.002153 0.000040

7 C -0.100955 -0.015801 0.007413 0.002385 -0.005800 -0.000008

8 N -0.015801 0.213209 -0.015801 0.002829 0.002829 0.000008

9 C 0.007413 -0.015801 -0.100955 -0.005800 0.002385 -0.000000

10 C 0.002385 0.002829 -0.005800 -0.015100 0.011449 -0.000000

11 C -0.005800 0.002829 0.002385 0.011449 -0.015100 0.000000

12 C -0.000008 0.000008 -0.000000 -0.000000 0.000000 0.340863

13 C 0.000001 -0.000003 0.000000 0.000000 -0.000000 0.029613

14 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.002153

15 C 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000963

16 C 0.000000 -0.000003 0.000001 -0.000000 0.000000 0.000812

17 N -0.000003 0.000003 -0.000003 -0.000000 -0.000000 -0.011123

18 C -0.000000 0.000008 -0.000008 0.000000 -0.000000 0.000162

19 C 0.000002 -0.000107 0.000093 0.000000 -0.000000 -0.000007

20 C 0.000000 -0.000008 0.000037 -0.000001 0.000000 -0.000000

21 C -0.000001 0.000069 -0.000730 0.000018 -0.000000 -0.000000

22 C -0.000054 0.002112 -0.003294 0.000246 0.000019 0.000000

23 N -0.000016 0.000642 0.000601 0.000010 0.000001 -0.000001

24 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000273

25 H -0.000000 -0.000000 0.000000 -0.000000 0.000001 -0.000002

26 H -0.000077 -0.000004 0.000499 -0.000491 0.000255 -0.000000

27 H 0.000499 -0.000004 -0.000077 0.000255 -0.000491 0.000000

28 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000021

29 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 -0.000013

30 H 0.000000 -0.000000 -0.000000 -0.000000 0.000000 0.000000

31 H 0.000000 -0.000000 -0.000000 0.000001 -0.000000 -0.000000

32 Zn 0.000125 0.000386 0.000125 0.000138 0.000138 -0.001719

33 C 0.000812 -0.011123 0.029613 -0.002153 -0.000963 0.000000

34 C 0.000010 0.000009 -0.000045 0.000471 -0.000116 0.000000

35 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.005238

36 C 0.000001 0.000035 -0.000785 0.000346 -0.000003 -0.000000

37 C -0.000000 0.000000 0.000000 -0.000000 0.000000 -0.009098

38 C -0.000045 0.000009 0.000010 -0.000116 0.000471 0.000001

39 C -0.000785 0.000035 0.000001 -0.000003 0.000346 0.000000

40 C -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000003

41 C 0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

42 H -0.000000 0.000000 -0.000000 0.000000 -0.000000 0.000000

43 H -0.000000 0.000000 -0.000009 0.000001 -0.000000 -0.000000

44 H -0.000009 0.000000 -0.000000 -0.000000 0.000001 0.000000

45 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000041

13 14 15 16 17 18

1 C -0.000730 0.000018 -0.000000 -0.000001 0.000069 -0.000000

2 C -0.003294 0.000246 0.000019 -0.000054 0.002112 -0.000007

3 N 0.000601 0.000010 0.000001 -0.000016 0.000642 -0.000001

4 C 0.000093 0.000000 -0.000000 0.000002 -0.000107 0.000000

5 C 0.000037 -0.000001 0.000000 0.000000 -0.000008 -0.000000

6 C -0.000008 0.000000 -0.000000 -0.000000 0.000008 0.000000

7 C 0.000001 -0.000000 0.000000 0.000000 -0.000003 -0.000000

8 N -0.000003 -0.000000 -0.000000 -0.000003 0.000003 0.000008

9 C 0.000000 0.000000 -0.000000 0.000001 -0.000003 -0.000008

10 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

11 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

12 C 0.029613 -0.002153 -0.000963 0.000812 -0.011123 0.000162

13 C -0.100955 -0.005800 0.002385 0.007413 -0.015801 0.000812

14 C -0.005800 -0.015100 0.011449 0.002385 0.002829 -0.000963

15 C 0.002385 0.011449 -0.015100 -0.005800 0.002829 -0.002153

16 C 0.007413 0.002385 -0.005800 -0.100955 -0.015801 0.029613

17 N -0.015801 0.002829 0.002829 -0.015801 0.213209 -0.011123

18 C 0.000812 -0.000963 -0.002153 0.029613 -0.011123 0.340864

19 C -0.000054 0.000019 0.000246 -0.003294 0.002112 -0.032988

20 C -0.000001 -0.000000 0.000018 -0.000730 0.000069 -0.008878

21 C 0.000000 0.000000 -0.000001 0.000037 -0.000008 0.000463

22 C 0.000002 -0.000000 0.000000 0.000093 -0.000107 0.001041

23 N -0.000016 0.000001 0.000010 0.000601 0.000642 -0.004595

24 H -0.000000 0.000001 -0.000000 0.000000 -0.000000 0.000000

25 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

26 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 0.000000

27 H -0.000000 -0.000000 0.000000 0.000000 -0.000000 -0.000000

28 H 0.000499 -0.000491 0.000255 -0.000077 -0.000004 -0.000013

29 H -0.000077 0.000255 -0.000491 0.000499 -0.000004 -0.000021

30 H 0.000000 -0.000000 0.000001 -0.000000 -0.000000 0.000273

31 H 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000002

32 Zn 0.000125 0.000138 0.000138 0.000125 0.000386 -0.001719

33 C -0.000000 -0.000000 0.000000 -0.000008 0.000008 0.000040

34 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000001

35 C -0.000045 0.000471 -0.000116 0.000010 0.000009 0.000003

36 C 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

37 C -0.000785 0.000346 -0.000003 0.000001 0.000035 0.000000

38 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000000

39 C -0.000000 0.000000 -0.000000 0.000000 0.000000 -0.000000

40 C 0.000010 -0.000116 0.000471 -0.000045 0.000009 -0.005238

41 C 0.000001 -0.000003 0.000346 -0.000785 0.000035 -0.009098

42 H -0.000000 -0.000000 0.000001 -0.000009 0.000000 -0.000041

43 H -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

44 H -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000000

45 H -0.000009 0.000001 -0.000000 -0.000000 0.000000 0.000000

19 20 21 22 23 24

1 C 0.000000 0.000000 -0.000000 -0.000000 -0.000000 -0.000060

2 C 0.000002 0.000000 -0.000000 -0.000000 -0.000002 -0.000203

3 N -0.000002 -0.000000 -0.000000 -0.000002 0.000017 -0.000032

4 C -0.000000 -0.000000 0.000000 0.000002 -0.000002 -0.000009

5 C -0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000279

6 C 0.000000 -0.000000 -0.000000 -0.000007 -0.000001 -0.000002

7 C 0.000002 0.000000 -0.000001 -0.000054 -0.000016 -0.000000

8 N -0.000107 -0.000008 0.000069 0.002112 0.000642 -0.000000

9 C 0.000093 0.000037 -0.000730 -0.003294 0.000601 0.000000

10 C 0.000000 -0.000001 0.000018 0.000246 0.000010 0.000000

11 C -0.000000 0.000000 -0.000000 0.000019 0.000001 -0.000000

12 C -0.000007 -0.000000 -0.000000 0.000000 -0.000001 0.000273

13 C -0.000054 -0.000001 0.000000 0.000002 -0.000016 -0.000000

14 C 0.000019 -0.000000 0.000000 -0.000000 0.000001 0.000001

15 C 0.000246 0.000018 -0.000001 0.000000 0.000010 -0.000000

16 C -0.003294 -0.000730 0.000037 0.000093 0.000601 0.000000

17 N 0.002112 0.000069 -0.000008 -0.000107 0.000642 -0.000000

18 C -0.032988 -0.008878 0.000463 0.001041 -0.004595 0.000000

19 C 0.061813 0.032764 -0.009973 -0.010779 -0.001549 -0.000000

20 C 0.032764 0.073142 -0.027872 -0.009973 0.000877 -0.000000

21 C -0.009973 -0.027872 0.073142 0.032764 0.000877 0.000000

22 C -0.010779 -0.009973 0.032764 0.061813 -0.001549 0.000000

23 N -0.001549 0.000877 0.000877 -0.001549 0.055662 0.000000

24 H -0.000000 -0.000000 0.000000 0.000000 0.000000 -0.003999

25 H 0.000000 0.000000 -0.000000 -0.000000 0.000000 0.000060

26 H 0.000000 -0.000000 0.000001 -0.000021 0.000000 0.000000

27 H 0.000000 0.000000 -0.000000 0.000000 -0.000000 -0.000000

28 H 0.000000 -0.000000 0.000000 0.000000 -0.000000 0.000000

29 H -0.000021 0.000001 -0.000000 0.000000 0.000000 0.000000

30 H -0.000203 -0.000060 0.000279 -0.000009 -0.000032 -0.000000

31 H -0.000009 0.000279 -0.000060 -0.000203 -0.000032 0.000000

32 Zn 0.000301 0.000125 0.000125 0.000301 0.002019 -0.000004

33 C 0.001041 0.000463 -0.008878 -0.032988 -0.004595 -0.000000

34 C -0.000028 0.000030 0.000710 0.000772 -0.000031 -0.000000

35 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000233

36 C -0.000006 -0.000023 0.000792 0.000887 0.000018 -0.000000

37 C -0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000134

38 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000003

39 C -0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

40 C 0.000772 0.000710 0.000030 -0.000028 -0.000031 -0.000000

41 C 0.000887 0.000792 -0.000023 -0.000006 0.000018 -0.000000

42 H -0.000003 0.000001 -0.000000 -0.000000 0.000000 -0.000000

43 H -0.000000 -0.000000 0.000001 -0.000003 0.000000 -0.000000

44 H 0.000000 -0.000000 0.000000 -0.000000 0.000000 0.000000

45 H -0.000000 0.000000 -0.000000 0.000000 0.000000 -0.000005

25 26 27 28 29 30

1 C 0.000279 0.000000 -0.000000 0.000001 -0.000000 -0.000000

2 C -0.000009 0.000000 0.000000 -0.000021 0.000000 -0.000000

3 N -0.000032 -0.000000 0.000000 0.000000 -0.000000 0.000000

4 C -0.000203 0.000000 -0.000021 0.000000 0.000000 0.000000

5 C -0.000060 -0.000000 0.000001 -0.000000 0.000000 0.000000

6 C 0.000273 -0.000013 -0.000021 0.000000 -0.000000 -0.000000

7 C -0.000000 -0.000077 0.000499 -0.000000 0.000000 0.000000

8 N -0.000000 -0.000004 -0.000004 -0.000000 -0.000000 -0.000000

9 C 0.000000 0.000499 -0.000077 0.000000 -0.000000 -0.000000

10 C -0.000000 -0.000491 0.000255 0.000000 -0.000000 -0.000000

11 C 0.000001 0.000255 -0.000491 -0.000000 0.000000 0.000000

12 C -0.000002 -0.000000 0.000000 -0.000021 -0.000013 0.000000

13 C -0.000000 0.000000 -0.000000 0.000499 -0.000077 0.000000

14 C -0.000000 0.000000 -0.000000 -0.000491 0.000255 -0.000000

15 C 0.000000 -0.000000 0.000000 0.000255 -0.000491 0.000001

16 C 0.000000 -0.000000 0.000000 -0.000077 0.000499 -0.000000

17 N -0.000000 -0.000000 -0.000000 -0.000004 -0.000004 -0.000000

18 C -0.000000 0.000000 -0.000000 -0.000013 -0.000021 0.000273

19 C 0.000000 0.000000 0.000000 0.000000 -0.000021 -0.000203

20 C 0.000000 -0.000000 0.000000 -0.000000 0.000001 -0.000060

21 C -0.000000 0.000001 -0.000000 0.000000 -0.000000 0.000279

22 C -0.000000 -0.000021 0.000000 0.000000 0.000000 -0.000009

23 N 0.000000 0.000000 -0.000000 -0.000000 0.000000 -0.000032

24 H 0.000060 0.000000 -0.000000 0.000000 0.000000 -0.000000

25 H -0.003999 0.000000 0.000000 -0.000000 0.000000 0.000000

26 H 0.000000 0.000485 -0.000026 0.000000 -0.000000 -0.000000

27 H 0.000000 -0.000026 0.000485 -0.000000 0.000000 0.000000

28 H -0.000000 0.000000 -0.000000 0.000485 -0.000026 0.000000

29 H 0.000000 -0.000000 0.000000 -0.000026 0.000485 0.000000

30 H 0.000000 -0.000000 0.000000 0.000000 0.000000 -0.003999

31 H -0.000000 0.000000 0.000000 0.000000 -0.000000 0.000060

32 Zn -0.000004 -0.000001 -0.000001 -0.000001 -0.000001 -0.000004

33 C 0.000000 -0.000021 -0.000013 -0.000000 0.000000 -0.000002

34 C -0.000000 0.000005 -0.000000 -0.000000 0.000000 0.000003

35 C 0.000003 -0.000000 0.000000 0.000005 -0.000000 -0.000000

36 C -0.000000 0.000081 -0.000000 0.000000 0.000000 0.000000

37 C 0.000000 0.000000 0.000000 0.000081 -0.000000 -0.000000

38 C -0.000233 -0.000000 0.000005 0.000000 -0.000000 -0.000000

39 C -0.000134 -0.000000 0.000081 0.000000 0.000000 -0.000000

40 C -0.000000 0.000000 -0.000000 -0.000000 0.000005 -0.000233

41 C -0.000000 0.000000 0.000000 -0.000000 0.000081 -0.000134

42 H -0.000000 0.000000 0.000000 -0.000000 0.000003 -0.000005

43 H -0.000000 0.000003 -0.000000 0.000000 0.000000 0.000000

44 H -0.000005 -0.000000 0.000003 0.000000 0.000000 -0.000000

45 H 0.000000 0.000000 0.000000 0.000003 -0.000000 -0.000000

31 32 33 34 35 36

1 C 0.000000 0.000125 -0.000000 -0.000000 0.000710 -0.000000

2 C 0.000000 0.000301 0.000000 -0.000000 0.000772 -0.000000

3 N 0.000000 0.002019 -0.000001 0.000000 -0.000031 0.000000

4 C -0.000000 0.000301 -0.000007 -0.000000 -0.000028 -0.000000

5 C -0.000000 0.000125 -0.000000 0.000000 0.000030 0.000000

6 C 0.000000 -0.001719 0.000162 0.000003 0.000001 0.000000

7 C 0.000000 0.000125 0.000812 0.000010 -0.000000 0.000001

8 N -0.000000 0.000386 -0.011123 0.000009 0.000000 0.000035

9 C -0.000000 0.000125 0.029613 -0.000045 -0.000000 -0.000785

10 C 0.000001 0.000138 -0.002153 0.000471 -0.000000 0.000346

11 C -0.000000 0.000138 -0.000963 -0.000116 0.000000 -0.000003

12 C -0.000000 -0.001719 0.000000 0.000000 -0.005238 -0.000000

13 C 0.000000 0.000125 -0.000000 -0.000000 -0.000045 0.000000

14 C 0.000000 0.000138 -0.000000 -0.000000 0.000471 -0.000000

15 C -0.000000 0.000138 0.000000 0.000000 -0.000116 0.000000

16 C -0.000000 0.000125 -0.000008 -0.000000 0.000010 -0.000000

17 N -0.000000 0.000386 0.000008 0.000000 0.000009 0.000000

18 C -0.000002 -0.001719 0.000040 0.000001 0.000003 0.000000

19 C -0.000009 0.000301 0.001041 -0.000028 -0.000000 -0.000006

20 C 0.000279 0.000125 0.000463 0.000030 0.000000 -0.000023

21 C -0.000060 0.000125 -0.008878 0.000710 -0.000000 0.000792

22 C -0.000203 0.000301 -0.032988 0.000772 -0.000000 0.000887

23 N -0.000032 0.002019 -0.004595 -0.000031 0.000000 0.000018

24 H 0.000000 -0.000004 -0.000000 -0.000000 -0.000233 -0.000000

25 H -0.000000 -0.000004 0.000000 -0.000000 0.000003 -0.000000

26 H 0.000000 -0.000001 -0.000021 0.000005 -0.000000 0.000081

27 H 0.000000 -0.000001 -0.000013 -0.000000 0.000000 -0.000000

28 H 0.000000 -0.000001 -0.000000 -0.000000 0.000005 0.000000

29 H -0.000000 -0.000001 0.000000 0.000000 -0.000000 0.000000

30 H 0.000060 -0.000004 -0.000002 0.000003 -0.000000 0.000000

31 H -0.003999 -0.000004 0.000273 -0.000233 -0.000000 -0.000134

32 Zn -0.000004 0.001337 -0.001719 -0.000028 -0.000028 0.000048

33 C 0.000273 -0.001719 0.340863 -0.005238 0.000000 -0.009098

34 C -0.000233 -0.000028 -0.005238 -0.101190 -0.000000 0.008110

35 C -0.000000 -0.000028 0.000000 -0.000000 -0.101190 -0.000000

36 C -0.000134 0.000048 -0.009098 0.008110 -0.000000 0.191993

37 C -0.000000 0.000048 -0.000000 -0.000000 0.008110 -0.000000

38 C -0.000000 -0.000028 0.000003 0.000000 0.000000 0.000000

39 C -0.000000 0.000048 0.000000 0.000000 0.000000 0.000000

40 C 0.000003 -0.000028 0.000001 0.000000 0.000000 0.000000

41 C 0.000000 0.000048 0.000000 0.000000 0.000000 0.000000

42 H 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

43 H -0.000005 0.000000 -0.000041 -0.000820 -0.000000 -0.000919

44 H -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

45 H -0.000000 0.000000 -0.000000 -0.000000 -0.000820 -0.000000

37 38 39 40 41 42

1 C 0.000792 0.000030 -0.000023 0.000000 0.000000 0.000000

2 C 0.000887 -0.000028 -0.000006 -0.000000 -0.000000 -0.000000

3 N 0.000018 -0.000031 0.000018 0.000000 0.000000 0.000000

4 C -0.000006 0.000772 0.000887 -0.000000 -0.000000 0.000000

5 C -0.000023 0.000710 0.000792 -0.000000 -0.000000 -0.000000

6 C 0.000000 -0.005238 -0.009098 0.000000 -0.000000 -0.000000

7 C -0.000000 -0.000045 -0.000785 -0.000000 0.000000 -0.000000

8 N 0.000000 0.000009 0.000035 0.000000 0.000000 0.000000

9 C 0.000000 0.000010 0.000001 -0.000000 -0.000000 -0.000000

10 C -0.000000 -0.000116 -0.000003 0.000000 0.000000 0.000000

11 C 0.000000 0.000471 0.000346 -0.000000 -0.000000 -0.000000

12 C -0.009098 0.000001 0.000000 0.000003 0.000000 0.000000

13 C -0.000785 -0.000000 -0.000000 0.000010 0.000001 -0.000000

14 C 0.000346 0.000000 0.000000 -0.000116 -0.000003 -0.000000

15 C -0.000003 -0.000000 -0.000000 0.000471 0.000346 0.000001

16 C 0.000001 -0.000000 0.000000 -0.000045 -0.000785 -0.000009

17 N 0.000035 0.000000 0.000000 0.000009 0.000035 0.000000

18 C 0.000000 0.000000 -0.000000 -0.005238 -0.009098 -0.000041

19 C -0.000000 -0.000000 -0.000000 0.000772 0.000887 -0.000003

20 C 0.000000 -0.000000 -0.000000 0.000710 0.000792 0.000001

21 C -0.000000 0.000000 0.000000 0.000030 -0.000023 -0.000000

22 C -0.000000 -0.000000 -0.000000 -0.000028 -0.000006 -0.000000

23 N 0.000000 0.000000 0.000000 -0.000031 0.000018 0.000000

24 H -0.000134 0.000003 0.000000 -0.000000 -0.000000 -0.000000

25 H 0.000000 -0.000233 -0.000134 -0.000000 -0.000000 -0.000000

26 H 0.000000 -0.000000 -0.000000 0.000000 0.000000 0.000000

27 H 0.000000 0.000005 0.000081 -0.000000 0.000000 0.000000

28 H 0.000081 0.000000 0.000000 -0.000000 -0.000000 -0.000000

29 H -0.000000 -0.000000 0.000000 0.000005 0.000081 0.000003

30 H -0.000000 -0.000000 -0.000000 -0.000233 -0.000134 -0.000005

31 H -0.000000 -0.000000 -0.000000 0.000003 0.000000 0.000000

32 Zn 0.000048 -0.000028 0.000048 -0.000028 0.000048 0.000000

33 C -0.000000 0.000003 0.000000 0.000001 0.000000 0.000000

34 C -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

35 C 0.008110 0.000000 0.000000 0.000000 0.000000 0.000000

36 C -0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

37 C 0.191993 0.000000 0.000000 0.000000 0.000000 0.000000

38 C 0.000000 -0.101190 0.008110 -0.000000 -0.000000 -0.000000

39 C 0.000000 0.008110 0.191993 -0.000000 -0.000000 -0.000000

40 C 0.000000 -0.000000 -0.000000 -0.101190 0.008110 -0.000820

41 C 0.000000 -0.000000 -0.000000 0.008110 0.191993 -0.000919

42 H 0.000000 -0.000000 -0.000000 -0.000820 -0.000919 -0.006079

43 H -0.000000 0.000000 0.000000 0.000000 0.000000 -0.000000

44 H 0.000000 -0.000820 -0.000919 -0.000000 -0.000000 -0.000000

45 H -0.000919 0.000000 0.000000 0.000000 0.000000 -0.000000

43 44 45

1 C -0.000000 -0.000000 0.000001

2 C 0.000000 -0.000000 -0.000003

3 N 0.000000 0.000000 0.000000

4 C -0.000000 -0.000003 -0.000000

5 C 0.000000 0.000001 -0.000000

6 C 0.000000 -0.000041 0.000000

7 C -0.000000 -0.000009 -0.000000

8 N 0.000000 0.000000 0.000000

9 C -0.000009 -0.000000 -0.000000

10 C 0.000001 -0.000000 -0.000000

11 C -0.000000 0.000001 0.000000

12 C -0.000000 0.000000 -0.000041

13 C -0.000000 -0.000000 -0.000009

14 C -0.000000 0.000000 0.000001

15 C 0.000000 -0.000000 -0.000000

16 C -0.000000 -0.000000 -0.000000

17 N 0.000000 0.000000 0.000000

18 C 0.000000 -0.000000 0.000000

19 C -0.000000 0.000000 -0.000000

20 C -0.000000 -0.000000 0.000000

21 C 0.000001 0.000000 -0.000000

22 C -0.000003 -0.000000 0.000000

23 N 0.000000 0.000000 0.000000

24 H -0.000000 0.000000 -0.000005

25 H -0.000000 -0.000005 0.000000

26 H 0.000003 -0.000000 0.000000

27 H -0.000000 0.000003 0.000000

28 H 0.000000 0.000000 0.000003

29 H 0.000000 0.000000 -0.000000

30 H 0.000000 -0.000000 -0.000000

31 H -0.000005 -0.000000 -0.000000

32 Zn 0.000000 0.000000 0.000000

33 C -0.000041 0.000000 -0.000000

34 C -0.000820 0.000000 -0.000000

35 C -0.000000 0.000000 -0.000820

36 C -0.000919 0.000000 -0.000000

37 C -0.000000 0.000000 -0.000919

38 C 0.000000 -0.000820 0.000000

39 C 0.000000 -0.000919 0.000000

40 C 0.000000 -0.000000 0.000000

41 C 0.000000 -0.000000 0.000000

42 H -0.000000 -0.000000 -0.000000

43 H -0.006079 -0.000000 -0.000000

44 H -0.000000 -0.006079 -0.000000

45 H -0.000000 -0.000000 -0.006079

Mulliken charges and spin densities:

1 2

1 C -0.275902 0.061759

2 C 0.301203 0.041030

3 N -0.695597 0.049542

4 C 0.301203 0.041030

5 C -0.275902 0.061760

6 C -0.247676 0.296432

7 C 0.324739 -0.085989

8 N -0.693852 0.170915

9 C 0.324739 -0.085989

10 C -0.237919 -0.006458

11 C -0.237919 -0.006458

12 C -0.247676 0.296432

13 C 0.324739 -0.085989

14 C -0.237919 -0.006458

15 C -0.237919 -0.006458

16 C 0.324739 -0.085990

17 N -0.693852 0.170915

18 C -0.247676 0.296433

19 C 0.301203 0.041030

20 C -0.275902 0.061760

21 C -0.275902 0.061760

22 C 0.301203 0.041030

23 N -0.695598 0.049542

24 H 0.230074 -0.004065

25 H 0.230074 -0.004065

26 H 0.244530 0.000674

27 H 0.244530 0.000674

28 H 0.244530 0.000674

29 H 0.244530 0.000674

30 H 0.230074 -0.004065

31 H 0.230074 -0.004065

32 Zn 1.416398 0.002087

33 C -0.247676 0.296432

34 C -0.028030 -0.097606

35 C -0.028030 -0.097606

36 C -0.273873 0.191342

37 C -0.273873 0.191342

38 C -0.028030 -0.097606

39 C -0.273873 0.191342

40 C -0.028030 -0.097606

41 C -0.273873 0.191343

42 H 0.303480 -0.007870

43 H 0.303480 -0.007870

44 H 0.303480 -0.007870

45 H 0.303480 -0.007870

Sum of Mulliken charges = -0.00000 2.00000

Mulliken charges and spin densities with hydrogens summed into heavy atoms:

1 2

1 C -0.045828 0.057694

2 C 0.301203 0.041030

3 N -0.695597 0.049542

4 C 0.301203 0.041030

5 C -0.045828 0.057694

6 C -0.247676 0.296432

7 C 0.324739 -0.085989

8 N -0.693852 0.170915

9 C 0.324739 -0.085989

10 C 0.006610 -0.005784

11 C 0.006610 -0.005784

12 C -0.247676 0.296432

13 C 0.324739 -0.085989

14 C 0.006610 -0.005784

15 C 0.006610 -0.005784

16 C 0.324739 -0.085990

17 N -0.693852 0.170915

18 C -0.247676 0.296433

19 C 0.301203 0.041030

20 C -0.045828 0.057694

21 C -0.045828 0.057694

22 C 0.301203 0.041030

23 N -0.695598 0.049542

32 Zn 1.416398 0.002087

33 C -0.247676 0.296432

34 C -0.028030 -0.097606

35 C -0.028030 -0.097606

36 C 0.029607 0.183472

37 C 0.029607 0.183472

38 C -0.028030 -0.097606

39 C 0.029607 0.183472

40 C -0.028030 -0.097606

41 C 0.029607 0.183472

APT charges:

1

1 C 0.286992

2 C -1.521548

3 N 0.103581

4 C -1.521548

5 C 0.286991

6 C 1.295802

7 C -0.085745

8 N -0.880318

9 C -0.085745

10 C 0.186712

11 C 0.186712

12 C 1.295803

13 C -0.085745

14 C 0.186713

15 C 0.186711

16 C -0.085743

17 N -0.880319

18 C 1.295800

19 C -1.521546

20 C 0.286991

21 C 0.286992

22 C -1.521547

23 N 0.103580

24 H 0.088827

25 H 0.088827

26 H 0.099239

27 H 0.099239

28 H 0.099239

29 H 0.099239

30 H 0.088827

31 H 0.088827

32 Zn 1.466606

33 C 1.295802

34 C -0.139100

35 C -0.139100

36 C -0.528114

37 C -0.528114

38 C -0.139100

39 C -0.528114

40 C -0.139100

41 C -0.528114

42 H 0.338653

43 H 0.338653

44 H 0.338653

45 H 0.338653

Sum of APT charges = 0.00000

APT charges with hydrogens summed into heavy atoms:

1

1 C 0.375819

2 C -1.521548

3 N 0.103581

4 C -1.521548

5 C 0.375818

6 C 1.295802

7 C -0.085745

8 N -0.880318

9 C -0.085745

10 C 0.285951

11 C 0.285951

12 C 1.295803

13 C -0.085745

14 C 0.285952

15 C 0.285951

16 C -0.085743

17 N -0.880319

18 C 1.295800

19 C -1.521546

20 C 0.375818

21 C 0.375819

22 C -1.521547

23 N 0.103580

32 Zn 1.466606

33 C 1.295802

34 C -0.139100

35 C -0.139100

36 C -0.189461

37 C -0.189461

38 C -0.139100

39 C -0.189461

40 C -0.139100

41 C -0.189461

Electronic spatial extent (au): <R\*\*2>= 13505.7645

Charge= -0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 0.8177 Tot= 0.8177

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -144.2251 YY= -164.5664 ZZ= -200.2648

XY= -0.0000 XZ= -0.0000 YZ= 0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 25.4604 YY= 5.1191 ZZ= -30.5794

XY= -0.0000 XZ= -0.0000 YZ= 0.0000

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= -0.0000 YYY= 0.0001 ZZZ= 10.7010 XYY= 0.0000

XXY= 0.0000 XXZ= -2.3132 XZZ= 0.0000 YZZ= 0.0000

YYZ= -2.7944 XYZ= -0.0000

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -7722.2625 YYYY= -8058.4295 ZZZZ= -224.9886 XXXY= 0.0008

XXXZ= -0.0001 YYYX= -0.0008 YYYZ= 0.0001 ZZZX= -0.0000

ZZZY= 0.0000 XXYY= -1628.1691 XXZZ= -1801.1272 YYZZ= -1808.0974

XXYZ= 0.0000 YYXZ= -0.0001 ZZXY= 0.0000

N-N= 3.054254843460D+03 E-N=-9.350907896667D+03 KE= 1.403716296051D+03

Exact polarizability:1223.308 -0.0001614.519 0.000 -0.000 181.332

Approx polarizability:1181.846 -0.0001636.822 0.000 -0.000 214.789

Isotropic Fermi Contact Couplings

Atom a.u. MegaHertz Gauss 10(-4) cm-1

1 C(13) -0.00014 -0.08087 -0.02886 -0.02698

2 C(13) -0.00828 -4.65477 -1.66094 -1.55266

3 N(14) 0.00054 0.08785 0.03135 0.02930

4 C(13) -0.00828 -4.65477 -1.66094 -1.55266

5 C(13) -0.00014 -0.08087 -0.02886 -0.02697

6 C(13) 0.01697 9.53614 3.40273 3.18091

7 C(13) -0.01760 -9.89313 -3.53012 -3.29999

8 N(14) 0.01816 2.93435 1.04705 0.97879

9 C(13) -0.01760 -9.89314 -3.53012 -3.30000

10 C(13) 0.00035 0.19813 0.07070 0.06609

11 C(13) 0.00035 0.19812 0.07070 0.06609

12 C(13) 0.01697 9.53614 3.40273 3.18091

13 C(13) -0.01760 -9.89313 -3.53011 -3.29999

14 C(13) 0.00035 0.19812 0.07069 0.06609

15 C(13) 0.00035 0.19813 0.07070 0.06609

16 C(13) -0.01760 -9.89314 -3.53012 -3.30000

17 N(14) 0.01816 2.93435 1.04705 0.97879

18 C(13) 0.01697 9.53616 3.40274 3.18092

19 C(13) -0.00828 -4.65477 -1.66094 -1.55267

20 C(13) -0.00014 -0.08087 -0.02886 -0.02698

21 C(13) -0.00014 -0.08087 -0.02886 -0.02697

22 C(13) -0.00828 -4.65477 -1.66094 -1.55267

23 N(14) 0.00054 0.08785 0.03135 0.02930

24 H(1) -0.00116 -2.59584 -0.92626 -0.86588

25 H(1) -0.00116 -2.59584 -0.92626 -0.86588

26 H(1) 0.00019 0.43528 0.15532 0.14519

27 H(1) 0.00019 0.43528 0.15532 0.14520

28 H(1) 0.00019 0.43528 0.15532 0.14520

29 H(1) 0.00019 0.43528 0.15532 0.14519

30 H(1) -0.00116 -2.59584 -0.92626 -0.86588

31 H(1) -0.00116 -2.59584 -0.92626 -0.86588

32 Zn(67) 0.00000 0.00000 0.00000 0.00000

33 C(13) 0.01697 9.53615 3.40274 3.18092

34 C(13) -0.02166 -12.17597 -4.34469 -4.06147

35 C(13) -0.02166 -12.17596 -4.34469 -4.06146

36 C(13) 0.01026 5.76975 2.05879 1.92458

37 C(13) 0.01026 5.76974 2.05879 1.92458

38 C(13) -0.02166 -12.17596 -4.34469 -4.06146

39 C(13) 0.01026 5.76974 2.05879 1.92458

40 C(13) -0.02166 -12.17598 -4.34469 -4.06147

41 C(13) 0.01026 5.76975 2.05879 1.92458

42 H(1) -0.00313 -6.98513 -2.49247 -2.32999

43 H(1) -0.00313 -6.98512 -2.49246 -2.32999

44 H(1) -0.00313 -6.98512 -2.49246 -2.32998

45 H(1) -0.00313 -6.98512 -2.49246 -2.32998

--------------------------------------------------------

Center ---- Spin Dipole Couplings ----

3XX-RR 3YY-RR 3ZZ-RR

--------------------------------------------------------

1 Atom -0.039628 -0.038522 0.078150

2 Atom -0.032544 -0.041079 0.073623

3 Atom -0.060292 -0.065520 0.125811

4 Atom -0.032544 -0.041079 0.073623

5 Atom -0.039628 -0.038522 0.078150

6 Atom -0.176430 -0.178283 0.354712

7 Atom 0.032043 0.051346 -0.083390

8 Atom -0.200842 -0.190768 0.391610

9 Atom 0.032043 0.051346 -0.083390

10 Atom 0.009372 0.008545 -0.017918

11 Atom 0.009372 0.008545 -0.017918

12 Atom -0.176430 -0.178282 0.354712

13 Atom 0.032043 0.051346 -0.083390

14 Atom 0.009372 0.008545 -0.017918

15 Atom 0.009372 0.008545 -0.017918

16 Atom 0.032044 0.051346 -0.083390

17 Atom -0.200842 -0.190768 0.391610

18 Atom -0.176430 -0.178283 0.354712

19 Atom -0.032544 -0.041079 0.073623

20 Atom -0.039628 -0.038522 0.078150

21 Atom -0.039628 -0.038522 0.078150

22 Atom -0.032544 -0.041079 0.073623

23 Atom -0.060292 -0.065520 0.125812

24 Atom -0.001742 0.005412 -0.003669

25 Atom -0.001742 0.005412 -0.003669

26 Atom 0.001115 0.001196 -0.002311

27 Atom 0.001115 0.001196 -0.002311

28 Atom 0.001115 0.001196 -0.002311

29 Atom 0.001115 0.001196 -0.002311

30 Atom -0.001742 0.005412 -0.003669

31 Atom -0.001742 0.005412 -0.003669

32 Atom 0.009570 -0.006866 -0.002704

33 Atom -0.176430 -0.178283 0.354712

34 Atom 0.027152 0.026681 -0.053833

35 Atom 0.027152 0.026681 -0.053833

36 Atom -0.092978 -0.095031 0.188009

37 Atom -0.092978 -0.095031 0.188009

38 Atom 0.027152 0.026681 -0.053833

39 Atom -0.092978 -0.095031 0.188009

40 Atom 0.027152 0.026681 -0.053833

41 Atom -0.092978 -0.095031 0.188010

42 Atom 0.001389 0.001317 -0.002705

43 Atom 0.001389 0.001317 -0.002705

44 Atom 0.001389 0.001317 -0.002705

45 Atom 0.001389 0.001317 -0.002705

--------------------------------------------------------

XY XZ YZ

--------------------------------------------------------

1 Atom -0.000150 -0.000223 0.004461

2 Atom -0.002293 0.000596 0.002608

3 Atom -0.000000 -0.000000 0.008995

4 Atom 0.002293 -0.000596 0.002608

5 Atom 0.000150 0.000223 0.004461

6 Atom -0.000478 -0.002471 0.004581

7 Atom -0.002179 0.000882 -0.000940

8 Atom 0.000000 -0.017706 0.000000

9 Atom 0.002179 0.000882 0.000940

10 Atom -0.001118 -0.000017 0.000319

11 Atom 0.001118 -0.000017 -0.000319

12 Atom 0.000478 0.002471 0.004581

13 Atom 0.002179 -0.000882 -0.000940

14 Atom -0.001118 0.000017 -0.000319

15 Atom 0.001118 0.000017 0.000319

16 Atom -0.002179 -0.000882 0.000940

17 Atom 0.000000 0.017706 0.000000

18 Atom -0.000478 0.002471 -0.004581

19 Atom 0.002293 0.000596 -0.002608

20 Atom 0.000150 -0.000223 -0.004461

21 Atom -0.000150 0.000223 -0.004461

22 Atom -0.002293 -0.000596 -0.002608

23 Atom -0.000000 -0.000000 -0.008995

24 Atom 0.005262 -0.000162 -0.000213

25 Atom -0.005262 0.000162 -0.000213

26 Atom -0.001786 0.000003 -0.000009

27 Atom 0.001786 0.000003 0.000009

28 Atom -0.001786 -0.000003 0.000009

29 Atom 0.001786 -0.000003 -0.000009

30 Atom -0.005262 -0.000162 0.000213

31 Atom 0.005262 0.000162 0.000213

32 Atom -0.000000 -0.000000 0.000000

33 Atom 0.000478 -0.002471 -0.004581

34 Atom 0.031651 0.000767 0.000684

35 Atom 0.031651 -0.000767 -0.000684

36 Atom -0.012418 -0.001923 -0.001885

37 Atom -0.012418 0.001923 0.001885

38 Atom -0.031651 0.000767 -0.000684

39 Atom 0.012418 -0.001923 0.001885

40 Atom -0.031651 -0.000767 0.000684

41 Atom 0.012418 0.001923 -0.001885

42 Atom -0.013595 -0.000110 0.000114

43 Atom 0.013595 0.000110 0.000114

44 Atom -0.013595 0.000110 -0.000114

45 Atom 0.013595 -0.000110 -0.000114

--------------------------------------------------------

---------------------------------------------------------------------------------

Anisotropic Spin Dipole Couplings in Principal Axis System

---------------------------------------------------------------------------------

Atom a.u. MegaHertz Gauss 10(-4) cm-1 Axes

Baa -0.0396 -5.321 -1.898 -1.775 0.9893 0.1459 -0.0037

1 C(13) Bbb -0.0387 -5.189 -1.852 -1.731 -0.1459 0.9886 -0.0380

Bcc 0.0783 10.510 3.750 3.506 -0.0019 0.0382 0.9993

Baa -0.0417 -5.598 -1.998 -1.867 0.2439 0.9695 -0.0232

2 C(13) Bbb -0.0320 -4.290 -1.531 -1.431 0.9698 -0.2439 0.0006

Bcc 0.0737 9.888 3.528 3.298 0.0051 0.0226 0.9997

Baa -0.0659 -2.543 -0.907 -0.848 0.0000 0.9989 -0.0469

3 N(14) Bbb -0.0603 -2.325 -0.830 -0.776 1.0000 -0.0000 0.0000

Bcc 0.1262 4.869 1.737 1.624 -0.0000 0.0469 0.9989

Baa -0.0417 -5.598 -1.998 -1.867 -0.2439 0.9695 -0.0232

4 C(13) Bbb -0.0320 -4.290 -1.531 -1.431 0.9698 0.2439 -0.0006

Bcc 0.0737 9.888 3.528 3.298 -0.0051 0.0226 0.9997

Baa -0.0396 -5.321 -1.899 -1.775 0.9893 -0.1459 0.0037

5 C(13) Bbb -0.0387 -5.189 -1.852 -1.731 0.1459 0.9886 -0.0380

Bcc 0.0783 10.510 3.750 3.506 0.0019 0.0382 0.9993

Baa -0.1784 -23.943 -8.544 -7.987 0.2241 0.9745 -0.0073

6 C(13) Bbb -0.1763 -23.663 -8.443 -7.893 0.9745 -0.2241 0.0065

Bcc 0.3548 47.606 16.987 15.880 -0.0047 0.0086 1.0000

Baa -0.0834 -11.192 -3.994 -3.733 -0.0075 0.0069 0.9999

7 C(13) Bbb 0.0318 4.268 1.523 1.424 0.9938 0.1112 0.0067

Bcc 0.0516 6.924 2.471 2.310 -0.1111 0.9938 -0.0076

Baa -0.2014 -7.766 -2.771 -2.591 0.9996 -0.0000 0.0298

8 N(14) Bbb -0.1908 -7.357 -2.625 -2.454 0.0000 1.0000 0.0000

Bcc 0.3921 15.124 5.397 5.045 -0.0298 0.0000 0.9996

Baa -0.0834 -11.192 -3.994 -3.733 -0.0075 -0.0069 0.9999

9 C(13) Bbb 0.0318 4.268 1.523 1.424 0.9938 -0.1112 0.0067

Bcc 0.0516 6.924 2.471 2.310 0.1111 0.9938 0.0076

Baa -0.0179 -2.405 -0.858 -0.802 0.0001 -0.0121 0.9999

10 C(13) Bbb 0.0078 1.043 0.372 0.348 0.5721 0.8201 0.0098

Bcc 0.0102 1.362 0.486 0.454 0.8202 -0.5720 -0.0070

Baa -0.0179 -2.405 -0.858 -0.802 0.0001 0.0121 0.9999

11 C(13) Bbb 0.0078 1.043 0.372 0.348 -0.5721 0.8201 -0.0098

Bcc 0.0102 1.362 0.486 0.454 0.8202 0.5720 -0.0070

Baa -0.1784 -23.943 -8.544 -7.987 -0.2241 0.9745 -0.0073

12 C(13) Bbb -0.1763 -23.663 -8.443 -7.893 0.9745 0.2241 -0.0065

Bcc 0.3548 47.606 16.987 15.880 0.0047 0.0086 1.0000

Baa -0.0834 -11.192 -3.994 -3.733 0.0075 0.0069 0.9999

13 C(13) Bbb 0.0318 4.268 1.523 1.424 0.9938 -0.1112 -0.0067

Bcc 0.0516 6.924 2.471 2.310 0.1111 0.9938 -0.0076

Baa -0.0179 -2.405 -0.858 -0.802 -0.0001 0.0121 0.9999

14 C(13) Bbb 0.0078 1.043 0.372 0.348 0.5721 0.8201 -0.0098

Bcc 0.0102 1.362 0.486 0.454 0.8202 -0.5720 0.0070

Baa -0.0179 -2.405 -0.858 -0.802 -0.0001 -0.0121 0.9999

15 C(13) Bbb 0.0078 1.043 0.372 0.348 -0.5721 0.8201 0.0098

Bcc 0.0102 1.362 0.486 0.454 0.8202 0.5720 0.0070

Baa -0.0834 -11.192 -3.994 -3.733 0.0075 -0.0069 0.9999

16 C(13) Bbb 0.0318 4.268 1.523 1.424 0.9938 0.1112 -0.0067

Bcc 0.0516 6.924 2.471 2.310 -0.1111 0.9938 0.0076

Baa -0.2014 -7.766 -2.771 -2.591 0.9996 -0.0000 -0.0298

17 N(14) Bbb -0.1908 -7.357 -2.625 -2.454 0.0000 1.0000 -0.0000

Bcc 0.3921 15.124 5.397 5.045 0.0298 0.0000 0.9996

Baa -0.1784 -23.943 -8.544 -7.987 0.2241 0.9745 0.0073

18 C(13) Bbb -0.1763 -23.663 -8.443 -7.893 0.9745 -0.2241 -0.0065

Bcc 0.3548 47.606 16.987 15.880 0.0047 -0.0086 1.0000

Baa -0.0417 -5.598 -1.998 -1.867 -0.2439 0.9695 0.0232

19 C(13) Bbb -0.0320 -4.290 -1.531 -1.431 0.9698 0.2439 0.0006

Bcc 0.0737 9.888 3.528 3.298 0.0051 -0.0226 0.9997

Baa -0.0396 -5.321 -1.899 -1.775 0.9893 -0.1459 -0.0037

20 C(13) Bbb -0.0387 -5.189 -1.852 -1.731 0.1459 0.9886 0.0380

Bcc 0.0783 10.510 3.750 3.506 -0.0019 -0.0382 0.9993

Baa -0.0396 -5.321 -1.899 -1.775 0.9893 0.1459 0.0037

21 C(13) Bbb -0.0387 -5.189 -1.852 -1.731 -0.1459 0.9886 0.0380

Bcc 0.0783 10.510 3.750 3.506 0.0019 -0.0382 0.9993

Baa -0.0417 -5.598 -1.998 -1.867 0.2439 0.9695 0.0232

22 C(13) Bbb -0.0320 -4.290 -1.531 -1.431 0.9698 -0.2439 -0.0006

Bcc 0.0737 9.888 3.528 3.298 -0.0051 -0.0226 0.9997

Baa -0.0659 -2.543 -0.907 -0.848 0.0000 0.9989 0.0469

23 N(14) Bbb -0.0603 -2.325 -0.830 -0.776 1.0000 -0.0000 0.0000

Bcc 0.1262 4.869 1.737 1.624 -0.0000 -0.0469 0.9989

Baa -0.0045 -2.417 -0.863 -0.806 0.8832 -0.4663 0.0507

24 H(1) Bbb -0.0037 -1.960 -0.699 -0.654 -0.0344 0.0434 0.9985

Bcc 0.0082 4.377 1.562 1.460 0.4678 0.8835 -0.0223

Baa -0.0045 -2.417 -0.863 -0.806 0.8832 0.4663 -0.0507

25 H(1) Bbb -0.0037 -1.960 -0.699 -0.654 0.0344 0.0434 0.9985

Bcc 0.0082 4.377 1.562 1.460 -0.4678 0.8835 -0.0223

Baa -0.0023 -1.233 -0.440 -0.411 0.0008 0.0030 1.0000

26 H(1) Bbb -0.0006 -0.336 -0.120 -0.112 0.7151 0.6990 -0.0027

Bcc 0.0029 1.570 0.560 0.524 -0.6991 0.7151 -0.0016

Baa -0.0023 -1.233 -0.440 -0.411 0.0008 -0.0030 1.0000

27 H(1) Bbb -0.0006 -0.336 -0.120 -0.112 0.7151 -0.6990 -0.0027

Bcc 0.0029 1.570 0.560 0.524 0.6991 0.7151 0.0016

Baa -0.0023 -1.233 -0.440 -0.411 -0.0008 -0.0030 1.0000

28 H(1) Bbb -0.0006 -0.336 -0.120 -0.112 0.7151 0.6990 0.0027

Bcc 0.0029 1.570 0.560 0.524 -0.6990 0.7151 0.0016

Baa -0.0023 -1.233 -0.440 -0.411 -0.0008 0.0030 1.0000

29 H(1) Bbb -0.0006 -0.336 -0.120 -0.112 0.7151 -0.6990 0.0027

Bcc 0.0029 1.570 0.560 0.524 0.6991 0.7151 -0.0016

Baa -0.0045 -2.417 -0.863 -0.806 0.8832 0.4663 0.0507

30 H(1) Bbb -0.0037 -1.960 -0.699 -0.654 -0.0344 -0.0434 0.9985

Bcc 0.0082 4.377 1.562 1.460 -0.4678 0.8835 0.0223

Baa -0.0045 -2.417 -0.863 -0.806 0.8832 -0.4663 -0.0507

31 H(1) Bbb -0.0037 -1.960 -0.699 -0.654 0.0344 -0.0434 0.9985

Bcc 0.0082 4.377 1.562 1.460 0.4678 0.8835 0.0223

Baa -0.0069 -0.230 -0.082 -0.077 0.0000 1.0000 -0.0000

32 Zn(67) Bbb -0.0027 -0.090 -0.032 -0.030 0.0000 0.0000 1.0000

Bcc 0.0096 0.320 0.114 0.107 1.0000 -0.0000 -0.0000

Baa -0.1784 -23.943 -8.544 -7.987 -0.2241 0.9745 0.0073

33 C(13) Bbb -0.1763 -23.663 -8.443 -7.893 0.9745 0.2241 0.0065

Bcc 0.3548 47.606 16.987 15.880 -0.0047 -0.0086 1.0000

Baa -0.0538 -7.225 -2.578 -2.410 -0.0073 -0.0056 1.0000

34 C(13) Bbb -0.0047 -0.635 -0.227 -0.212 -0.7045 0.7097 -0.0011

Bcc 0.0586 7.861 2.805 2.622 0.7097 0.7044 0.0091

Baa -0.0538 -7.225 -2.578 -2.410 0.0073 0.0056 1.0000

35 C(13) Bbb -0.0047 -0.635 -0.227 -0.212 -0.7045 0.7097 0.0011

Bcc 0.0586 7.861 2.805 2.622 0.7097 0.7044 -0.0091

Baa -0.1065 -14.290 -5.099 -4.767 0.6774 0.7356 0.0091

36 C(13) Bbb -0.0815 -10.942 -3.905 -3.650 0.7356 -0.6774 0.0005

Bcc 0.1880 25.232 9.004 8.417 -0.0066 -0.0064 1.0000

Baa -0.1065 -14.290 -5.099 -4.767 0.6774 0.7356 -0.0091

37 C(13) Bbb -0.0815 -10.942 -3.905 -3.650 0.7356 -0.6774 -0.0005

Bcc 0.1880 25.232 9.004 8.417 0.0066 0.0064 1.0000

Baa -0.0538 -7.225 -2.578 -2.410 -0.0073 0.0056 1.0000

38 C(13) Bbb -0.0047 -0.635 -0.227 -0.212 0.7045 0.7097 0.0011

Bcc 0.0586 7.861 2.805 2.622 0.7097 -0.7044 0.0091

Baa -0.1065 -14.290 -5.099 -4.767 -0.6774 0.7356 -0.0091

39 C(13) Bbb -0.0815 -10.942 -3.905 -3.650 0.7356 0.6774 0.0005

Bcc 0.1880 25.232 9.004 8.417 -0.0066 0.0064 1.0000

Baa -0.0538 -7.225 -2.578 -2.410 0.0073 -0.0056 1.0000

40 C(13) Bbb -0.0047 -0.635 -0.227 -0.212 0.7045 0.7097 -0.0011

Bcc 0.0586 7.861 2.805 2.622 0.7097 -0.7044 -0.0091

Baa -0.1065 -14.290 -5.099 -4.767 -0.6774 0.7356 0.0091

41 C(13) Bbb -0.0815 -10.942 -3.905 -3.650 0.7356 0.6774 -0.0005

Bcc 0.1880 25.232 9.004 8.417 0.0066 -0.0064 1.0000

Baa -0.0122 -6.532 -2.331 -2.179 0.7062 0.7080 -0.0003

42 H(1) Bbb -0.0027 -1.444 -0.515 -0.482 0.0066 -0.0061 1.0000

Bcc 0.0149 7.976 2.846 2.661 0.7080 -0.7061 -0.0090

Baa -0.0122 -6.532 -2.331 -2.179 -0.7062 0.7080 -0.0003

43 H(1) Bbb -0.0027 -1.444 -0.515 -0.482 -0.0066 -0.0061 1.0000

Bcc 0.0149 7.976 2.846 2.661 0.7080 0.7061 0.0090

Baa -0.0122 -6.532 -2.331 -2.179 0.7062 0.7080 0.0003

44 H(1) Bbb -0.0027 -1.444 -0.515 -0.482 -0.0066 0.0061 1.0000

Bcc 0.0149 7.976 2.846 2.661 0.7080 -0.7061 0.0090

Baa -0.0122 -6.532 -2.331 -2.179 -0.7062 0.7080 0.0003

45 H(1) Bbb -0.0027 -1.444 -0.515 -0.482 0.0066 0.0061 1.0000

Bcc 0.0149 7.976 2.846 2.661 0.7080 0.7061 -0.0090

---------------------------------------------------------------------------------

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Tue Jul 30 03:39:14 2019, MaxMem= 4294967296 cpu: 17.5

(Enter /home/kira/g09/l716.exe)

Rotating derivatives to standard orientation.

Dipole = 4.24278762D-07 9.95524792D-07 3.21707658D-01

Polarizability= 1.22330807D+03-1.54031071D-04 1.61451938D+03

1.31824202D-06-2.25026142D-06 1.81332168D+02

Full mass-weighted force constant matrix:

Low frequencies --- -27.1280 -25.6837 -12.1930 -0.0004 0.0009 0.0010

Low frequencies --- 16.2237 41.3214 42.8008

Diagonal vibrational polarizability:

182.8867325 131.1340114 262.3490323

Harmonic frequencies (cm\*\*-1), IR intensities (KM/Mole), Raman scattering

activities (A\*\*4/AMU), depolarization ratios for plane and unpolarized

incident light, reduced masses (AMU), force constants (mDyne/A),

and normal coordinates:

1 2 3

A A A

Frequencies -- 16.2117 41.3214 42.8008

Red. masses -- 6.2961 7.6725 5.6085

Frc consts -- 0.0010 0.0077 0.0061

IR Inten -- 0.0000 0.0213 1.8166

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.03 -0.00 -0.01 0.01 0.00 0.01 0.24

2 6 0.00 0.00 0.05 -0.00 -0.01 0.04 0.00 0.01 0.09

3 7 0.00 -0.00 0.00 -0.00 -0.01 0.07 0.00 0.01 0.02

4 6 0.00 -0.00 -0.05 0.00 -0.01 0.04 -0.00 0.01 0.09

5 6 0.00 -0.00 -0.03 0.00 -0.01 0.01 -0.00 0.01 0.24

6 6 0.00 -0.00 -0.09 0.00 -0.00 0.01 0.00 0.00 0.00

7 6 0.00 -0.00 -0.05 0.00 -0.00 0.03 0.00 0.00 -0.07

8 7 -0.00 -0.00 0.00 0.01 0.00 0.10 0.00 0.00 -0.04

9 6 -0.00 -0.00 0.05 0.00 0.00 0.03 0.00 -0.00 -0.07

10 6 -0.00 -0.00 0.03 0.01 0.00 -0.06 0.00 -0.00 -0.16

11 6 0.00 -0.00 -0.03 0.01 -0.00 -0.06 0.00 0.00 -0.16

12 6 0.00 0.00 0.09 -0.00 -0.00 0.01 -0.00 0.00 0.00

13 6 0.00 0.00 0.05 -0.00 -0.00 0.03 -0.00 0.00 -0.07

14 6 0.00 0.00 0.03 -0.01 -0.00 -0.06 -0.00 0.00 -0.16

15 6 -0.00 0.00 -0.03 -0.01 0.00 -0.06 -0.00 -0.00 -0.16

16 6 -0.00 0.00 -0.05 -0.00 0.00 0.03 -0.00 -0.00 -0.07

17 7 -0.00 0.00 -0.00 -0.01 0.00 0.10 -0.00 -0.00 -0.04

18 6 -0.00 0.00 -0.09 -0.00 0.00 0.01 -0.00 -0.00 0.00

19 6 -0.00 0.00 -0.05 -0.00 0.01 0.04 0.00 -0.01 0.09

20 6 -0.00 0.00 -0.03 -0.00 0.01 0.01 0.00 -0.01 0.24

21 6 -0.00 -0.00 0.03 0.00 0.01 0.01 -0.00 -0.01 0.24

22 6 -0.00 -0.00 0.05 0.00 0.01 0.04 -0.00 -0.01 0.09

23 7 -0.00 -0.00 -0.00 -0.00 0.01 0.07 0.00 -0.01 0.02

24 1 0.00 0.00 0.06 0.00 -0.01 -0.01 -0.00 0.01 0.32

25 1 0.00 -0.00 -0.06 -0.00 -0.01 -0.01 0.00 0.01 0.32

26 1 -0.00 -0.00 0.07 0.01 -0.00 -0.12 0.00 0.00 -0.21

27 1 0.00 -0.00 -0.07 0.01 0.00 -0.12 0.00 -0.00 -0.21

28 1 0.00 0.00 0.07 -0.01 0.00 -0.12 -0.00 -0.00 -0.21

29 1 -0.00 0.00 -0.07 -0.01 -0.00 -0.12 -0.00 0.00 -0.21

30 1 -0.00 0.00 -0.06 0.00 0.01 -0.01 -0.00 -0.01 0.32

31 1 -0.00 -0.00 0.06 -0.00 0.01 -0.01 0.00 -0.01 0.32

32 30 0.00 -0.00 0.00 0.00 -0.00 0.21 -0.00 0.00 -0.06

33 6 -0.00 -0.00 0.09 0.00 0.00 0.01 0.00 -0.00 0.00

34 6 -0.00 -0.00 0.18 0.00 0.00 -0.12 -0.00 -0.00 -0.00

35 6 0.00 0.00 0.18 -0.00 -0.00 -0.12 0.00 0.00 -0.00

36 6 -0.00 -0.00 0.27 0.00 0.01 -0.25 -0.00 0.00 -0.01

37 6 0.00 0.00 0.27 -0.00 -0.01 -0.25 0.00 -0.00 -0.01

38 6 0.00 -0.00 -0.18 0.00 -0.00 -0.12 -0.00 0.00 -0.00

39 6 0.00 -0.00 -0.27 0.00 -0.01 -0.25 -0.00 -0.00 -0.01

40 6 -0.00 0.00 -0.18 -0.00 0.00 -0.12 0.00 -0.00 -0.00

41 6 -0.00 0.00 -0.27 -0.00 0.01 -0.25 0.00 0.00 -0.01

42 1 -0.00 0.00 -0.35 -0.00 0.01 -0.37 0.00 0.00 -0.01

43 1 -0.00 -0.00 0.35 0.00 0.01 -0.37 -0.00 0.00 -0.01

44 1 0.00 -0.00 -0.35 0.00 -0.01 -0.37 -0.00 -0.00 -0.01

45 1 0.00 0.00 0.35 -0.00 -0.01 -0.37 0.00 -0.00 -0.01

4 5 6

A A A

Frequencies -- 51.8090 56.6851 64.4588

Red. masses -- 5.8565 5.3085 7.4951

Frc consts -- 0.0093 0.0100 0.0183

IR Inten -- 0.5181 0.0505 14.2484

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 0.00 -0.01 -0.00 0.01 0.18 -0.00 -0.01 -0.08

2 6 -0.00 0.00 -0.02 -0.00 0.00 0.11 -0.00 -0.01 -0.03

3 7 -0.00 0.00 -0.00 -0.00 0.00 0.08 0.00 -0.01 0.00

4 6 -0.00 -0.00 0.02 0.00 0.00 0.11 0.00 -0.01 -0.03

5 6 -0.01 -0.00 0.01 0.00 0.01 0.18 0.00 -0.01 -0.08

6 6 -0.00 -0.00 0.05 0.00 0.00 0.02 0.01 -0.00 -0.04

7 6 -0.01 -0.00 0.13 0.00 0.00 0.00 0.02 -0.00 -0.11

8 7 -0.01 -0.00 0.16 0.00 0.00 -0.00 0.02 0.00 -0.08

9 6 -0.01 0.00 0.13 -0.00 0.00 -0.00 0.02 0.00 -0.11

10 6 -0.01 0.00 0.14 -0.00 0.00 0.00 0.02 0.00 -0.18

11 6 -0.01 -0.00 0.14 0.00 0.00 -0.00 0.02 -0.00 -0.18

12 6 -0.00 0.00 -0.05 -0.00 0.00 0.02 -0.01 -0.00 -0.04

13 6 -0.01 0.00 -0.13 -0.00 0.00 0.00 -0.02 -0.00 -0.11

14 6 -0.01 0.00 -0.14 -0.00 0.00 -0.00 -0.02 -0.00 -0.18

15 6 -0.01 -0.00 -0.14 0.00 0.00 0.00 -0.02 0.00 -0.18

16 6 -0.01 -0.00 -0.13 0.00 0.00 -0.00 -0.02 0.00 -0.11

17 7 -0.01 -0.00 -0.16 -0.00 0.00 -0.00 -0.02 -0.00 -0.08

18 6 -0.00 -0.00 -0.05 0.00 0.00 -0.02 -0.01 0.00 -0.04

19 6 -0.00 -0.00 -0.02 0.00 0.00 -0.11 -0.00 0.01 -0.03

20 6 -0.01 -0.00 -0.01 0.00 0.01 -0.18 -0.00 0.01 -0.08

21 6 -0.01 0.00 0.01 -0.00 0.01 -0.18 0.00 0.01 -0.08

22 6 -0.00 0.00 0.02 -0.00 0.00 -0.11 0.00 0.01 -0.03

23 7 -0.00 0.00 -0.00 -0.00 0.00 -0.08 0.00 0.01 0.00

24 1 -0.01 0.00 -0.02 -0.00 0.01 0.22 0.00 -0.01 -0.12

25 1 -0.01 -0.00 0.02 0.00 0.01 0.22 -0.00 -0.01 -0.12

26 1 -0.01 0.00 0.14 -0.00 0.00 0.01 0.02 -0.00 -0.24

27 1 -0.01 -0.00 0.14 0.00 0.00 -0.01 0.02 0.00 -0.24

28 1 -0.01 0.00 -0.14 -0.00 0.00 -0.01 -0.02 0.00 -0.24

29 1 -0.01 -0.00 -0.14 0.00 0.00 0.01 -0.02 -0.00 -0.24

30 1 -0.01 -0.00 -0.02 0.00 0.01 -0.22 0.00 0.01 -0.12

31 1 -0.01 0.00 0.02 -0.00 0.01 -0.22 -0.00 0.01 -0.12

32 30 0.03 0.00 0.00 -0.00 -0.02 0.00 -0.00 -0.00 0.20

33 6 -0.00 0.00 0.05 -0.00 0.00 -0.02 0.01 0.00 -0.04

34 6 -0.00 0.00 -0.08 -0.00 0.00 0.08 0.00 0.00 0.05

35 6 -0.00 0.00 0.08 -0.00 0.00 -0.08 -0.00 -0.00 0.05

36 6 -0.01 0.01 -0.22 0.00 -0.00 0.21 0.00 0.00 0.17

37 6 -0.01 0.01 0.22 0.00 -0.00 -0.21 -0.00 -0.00 0.17

38 6 -0.00 -0.00 -0.08 0.00 0.00 -0.08 0.00 -0.00 0.05

39 6 -0.01 -0.01 -0.22 -0.00 -0.00 -0.21 0.00 -0.00 0.17

40 6 -0.00 -0.00 0.08 0.00 0.00 0.08 -0.00 0.00 0.05

41 6 -0.01 -0.01 0.22 -0.00 -0.00 0.21 -0.00 0.00 0.17

42 1 -0.01 -0.01 0.35 -0.00 -0.00 0.33 -0.00 0.00 0.28

43 1 -0.01 0.01 -0.35 0.00 -0.00 0.33 0.00 0.00 0.28

44 1 -0.01 -0.01 -0.35 -0.00 -0.00 -0.33 0.00 -0.00 0.28

45 1 -0.01 0.01 0.35 0.00 -0.00 -0.33 -0.00 -0.00 0.28

7 8 9

A A A

Frequencies -- 96.9530 110.7251 112.8096

Red. masses -- 5.9226 5.3400 4.4822

Frc consts -- 0.0328 0.0386 0.0336

IR Inten -- 1.0184 1.2554 1.1250

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 0.17 0.01 -0.00 0.05 0.00 0.03 -0.03

2 6 0.00 -0.01 -0.10 0.00 -0.00 0.08 0.00 0.03 0.03

3 7 0.00 -0.01 -0.28 0.00 -0.00 0.00 -0.00 0.03 0.08

4 6 -0.00 -0.01 -0.10 0.00 0.00 -0.08 -0.00 0.03 0.03

5 6 -0.00 -0.00 0.17 0.01 0.00 -0.05 -0.00 0.03 -0.03

6 6 -0.00 -0.01 -0.10 0.00 0.00 -0.08 0.01 0.01 0.01

7 6 -0.00 -0.01 -0.07 -0.00 0.00 -0.06 0.03 0.00 -0.02

8 7 0.00 -0.01 -0.00 0.00 0.00 -0.22 0.03 0.00 -0.05

9 6 0.00 -0.01 0.07 -0.00 -0.00 -0.06 0.03 -0.00 -0.02

10 6 0.00 -0.01 0.04 -0.00 -0.00 0.20 0.03 0.00 0.00

11 6 -0.00 -0.01 -0.04 -0.00 0.00 0.20 0.03 -0.00 0.00

12 6 0.00 -0.01 -0.10 0.00 -0.00 0.08 -0.01 0.01 0.01

13 6 0.00 -0.01 -0.07 -0.00 -0.00 0.06 -0.03 0.00 -0.02

14 6 0.00 -0.01 -0.04 -0.00 -0.00 -0.20 -0.03 -0.00 0.00

15 6 -0.00 -0.01 0.04 -0.00 0.00 -0.20 -0.03 0.00 0.00

16 6 -0.00 -0.01 0.07 -0.00 0.00 0.06 -0.03 -0.00 -0.02

17 7 -0.00 -0.01 -0.00 0.00 0.00 0.22 -0.03 -0.00 -0.05

18 6 -0.00 -0.01 0.10 0.00 0.00 0.08 -0.01 -0.01 0.01

19 6 -0.00 -0.01 0.10 0.00 0.00 0.08 0.00 -0.03 0.03

20 6 -0.00 -0.00 -0.17 0.01 0.00 0.05 0.00 -0.03 -0.03

21 6 0.00 -0.00 -0.17 0.01 -0.00 -0.05 -0.00 -0.03 -0.03

22 6 0.00 -0.01 0.10 0.00 -0.00 -0.08 -0.00 -0.03 0.03

23 7 0.00 -0.01 0.28 0.00 0.00 0.00 0.00 -0.03 0.08

24 1 0.00 0.01 0.36 0.01 -0.00 0.10 0.00 0.03 -0.07

25 1 -0.00 0.01 0.36 0.01 0.00 -0.10 -0.00 0.03 -0.07

26 1 0.00 -0.01 0.09 -0.01 -0.00 0.37 0.03 0.00 0.03

27 1 -0.00 -0.01 -0.09 -0.01 0.00 0.37 0.03 -0.00 0.03

28 1 0.00 -0.01 -0.09 -0.01 -0.00 -0.37 -0.03 -0.00 0.03

29 1 -0.00 -0.01 0.09 -0.01 0.00 -0.37 -0.03 0.00 0.03

30 1 -0.00 0.01 -0.36 0.01 0.00 0.10 0.00 -0.03 -0.07

31 1 0.00 0.01 -0.36 0.01 -0.00 -0.10 -0.00 -0.03 -0.07

32 30 -0.00 0.06 0.00 -0.06 -0.00 0.00 -0.00 -0.00 -0.01

33 6 0.00 -0.01 0.10 0.00 -0.00 -0.08 0.01 -0.01 0.01

34 6 0.01 -0.01 0.04 0.01 -0.01 -0.04 -0.04 0.04 0.00

35 6 0.01 -0.01 -0.04 0.01 -0.01 0.04 0.04 -0.04 0.00

36 6 0.02 -0.02 -0.05 0.05 -0.05 -0.01 -0.18 0.18 -0.01

37 6 0.02 -0.02 0.05 0.05 -0.05 0.01 0.18 -0.18 -0.01

38 6 -0.01 -0.01 -0.04 0.01 0.01 -0.04 -0.04 -0.04 0.00

39 6 -0.02 -0.02 0.05 0.05 0.05 -0.01 -0.18 -0.18 -0.01

40 6 -0.01 -0.01 0.04 0.01 0.01 0.04 0.04 0.04 0.00

41 6 -0.02 -0.02 -0.05 0.05 0.05 0.01 0.18 0.18 -0.01

42 1 -0.02 -0.03 -0.12 0.08 0.08 -0.01 0.29 0.28 -0.02

43 1 0.02 -0.03 -0.12 0.08 -0.08 0.01 -0.29 0.28 -0.02

44 1 -0.02 -0.03 0.12 0.08 0.08 0.01 -0.29 -0.28 -0.02

45 1 0.02 -0.03 0.12 0.08 -0.08 -0.01 0.29 -0.28 -0.02

10 11 12

A A A

Frequencies -- 116.9800 118.2108 125.0336

Red. masses -- 4.3753 4.3721 7.1108

Frc consts -- 0.0353 0.0360 0.0655

IR Inten -- 6.6785 0.6692 25.7482

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.03 -0.01 -0.02 -0.00 -0.01 -0.00 0.03 -0.11

2 6 0.00 0.04 0.01 -0.02 0.00 -0.02 -0.00 0.04 0.14

3 7 -0.00 0.04 0.02 -0.02 -0.00 -0.00 -0.00 0.05 0.33

4 6 -0.00 0.04 0.01 -0.02 -0.00 0.02 0.00 0.04 0.14

5 6 -0.00 0.03 -0.01 -0.02 0.00 0.01 0.00 0.03 -0.11

6 6 -0.00 0.02 0.01 -0.02 0.00 0.02 0.01 0.01 0.06

7 6 0.00 0.01 0.01 -0.04 0.00 0.02 0.02 0.00 -0.05

8 7 -0.00 0.02 0.00 -0.04 -0.00 0.06 0.02 0.00 -0.11

9 6 -0.00 0.01 -0.01 -0.04 -0.00 0.02 0.02 -0.00 -0.05

10 6 0.00 0.01 -0.00 -0.04 -0.00 -0.04 0.02 -0.00 -0.04

11 6 -0.00 0.01 0.00 -0.04 0.00 -0.04 0.02 0.00 -0.04

12 6 0.00 0.02 0.01 -0.02 -0.00 -0.02 -0.01 0.01 0.06

13 6 -0.00 0.01 0.01 -0.04 -0.00 -0.02 -0.02 0.00 -0.05

14 6 0.00 0.01 0.00 -0.04 -0.00 0.04 -0.02 0.00 -0.04

15 6 -0.00 0.01 -0.00 -0.04 0.00 0.04 -0.02 -0.00 -0.04

16 6 0.00 0.01 -0.01 -0.04 0.00 -0.02 -0.02 -0.00 -0.05

17 7 -0.00 0.02 -0.00 -0.04 -0.00 -0.06 -0.02 -0.00 -0.11

18 6 -0.00 0.02 -0.01 -0.02 0.00 -0.02 -0.01 -0.01 0.06

19 6 -0.00 0.04 -0.01 -0.02 -0.00 -0.02 -0.00 -0.04 0.14

20 6 -0.00 0.03 0.01 -0.02 0.00 -0.01 -0.00 -0.03 -0.11

21 6 0.00 0.03 0.01 -0.02 -0.00 0.01 0.00 -0.03 -0.11

22 6 0.00 0.04 -0.01 -0.02 0.00 0.02 0.00 -0.04 0.14

23 7 -0.00 0.04 -0.02 -0.02 -0.00 0.00 0.00 -0.05 0.33

24 1 0.00 0.03 -0.03 -0.01 -0.00 -0.03 -0.00 0.03 -0.30

25 1 -0.00 0.03 -0.03 -0.01 0.00 0.03 0.00 0.03 -0.30

26 1 0.00 0.01 -0.01 -0.04 -0.00 -0.09 0.02 0.00 -0.01

27 1 -0.00 0.01 0.01 -0.04 0.00 -0.09 0.02 -0.00 -0.01

28 1 0.00 0.01 0.01 -0.04 -0.00 0.09 -0.02 -0.00 -0.01

29 1 -0.00 0.01 -0.01 -0.04 0.00 0.09 -0.02 0.00 -0.01

30 1 -0.00 0.03 0.03 -0.01 0.00 -0.03 -0.00 -0.03 -0.30

31 1 0.00 0.03 0.03 -0.01 -0.00 0.03 0.00 -0.03 -0.30

32 30 -0.00 0.04 0.00 -0.03 -0.00 0.00 0.00 -0.00 -0.07

33 6 0.00 0.02 -0.01 -0.02 -0.00 0.02 0.01 -0.01 0.06

34 6 0.05 -0.02 -0.01 0.02 -0.05 0.01 0.02 -0.02 0.02

35 6 0.05 -0.02 0.01 0.02 -0.05 -0.01 -0.02 0.02 0.02

36 6 0.20 -0.17 0.00 0.17 -0.19 -0.00 0.08 -0.08 -0.03

37 6 0.20 -0.17 -0.00 0.17 -0.19 0.00 -0.08 0.08 -0.03

38 6 -0.05 -0.02 0.01 0.02 0.05 0.01 0.02 0.02 0.02

39 6 -0.20 -0.17 -0.00 0.17 0.19 -0.00 0.08 0.08 -0.03

40 6 -0.05 -0.02 -0.01 0.02 0.05 -0.01 -0.02 -0.02 0.02

41 6 -0.20 -0.17 0.00 0.17 0.19 0.00 -0.08 -0.08 -0.03

42 1 -0.31 -0.28 0.01 0.28 0.30 0.01 -0.12 -0.12 -0.07

43 1 0.31 -0.28 0.01 0.28 -0.30 -0.01 0.12 -0.12 -0.07

44 1 -0.31 -0.28 -0.01 0.28 0.30 -0.01 0.12 0.12 -0.07

45 1 0.31 -0.28 -0.01 0.28 -0.30 0.01 -0.12 0.12 -0.07

13 14 15

A A A

Frequencies -- 140.8821 142.3200 143.8675

Red. masses -- 5.1205 6.1675 4.2861

Frc consts -- 0.0599 0.0736 0.0523

IR Inten -- 0.0000 42.0904 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.03 0.01 0.08 0.00 -0.02 -0.09 -0.08 0.01 -0.03

2 6 -0.01 0.02 0.11 0.00 -0.02 -0.00 -0.05 0.02 -0.04

3 7 -0.00 -0.00 0.00 -0.00 -0.01 0.02 -0.03 0.00 -0.00

4 6 -0.01 -0.02 -0.11 -0.00 -0.02 -0.00 -0.05 -0.02 0.04

5 6 -0.03 -0.01 -0.08 -0.00 -0.02 -0.09 -0.08 -0.01 0.03

6 6 -0.01 -0.03 -0.15 -0.02 -0.01 0.06 -0.05 -0.04 0.05

7 6 -0.01 -0.03 -0.10 -0.04 0.00 0.11 -0.03 -0.04 0.04

8 7 -0.00 -0.02 0.00 -0.05 -0.00 0.29 0.00 -0.03 -0.00

9 6 0.01 -0.03 0.10 -0.04 -0.00 0.11 0.03 -0.04 -0.04

10 6 0.00 -0.04 0.07 -0.04 -0.00 -0.16 0.02 -0.07 -0.03

11 6 -0.00 -0.04 -0.07 -0.04 0.00 -0.16 -0.02 -0.07 0.03

12 6 -0.01 0.03 0.15 0.02 -0.01 0.06 -0.05 0.04 -0.05

13 6 -0.01 0.03 0.10 0.04 0.00 0.11 -0.03 0.04 -0.04

14 6 -0.00 0.04 0.07 0.04 0.00 -0.16 -0.02 0.07 -0.03

15 6 0.00 0.04 -0.07 0.04 -0.00 -0.16 0.02 0.07 0.03

16 6 0.01 0.03 -0.10 0.04 -0.00 0.11 0.03 0.04 0.04

17 7 0.00 0.02 0.00 0.05 0.00 0.29 -0.00 0.03 -0.00

18 6 0.01 0.03 -0.15 0.02 0.01 0.06 0.05 0.04 0.05

19 6 0.01 0.02 -0.11 0.00 0.02 -0.00 0.05 0.02 0.04

20 6 0.03 0.01 -0.08 0.00 0.02 -0.09 0.08 0.01 0.03

21 6 0.03 -0.01 0.08 -0.00 0.02 -0.09 0.08 -0.01 -0.03

22 6 0.01 -0.02 0.11 -0.00 0.02 -0.00 0.05 -0.02 -0.04

23 7 0.00 0.00 0.00 -0.00 0.01 0.02 0.03 -0.00 -0.00

24 1 -0.03 0.02 0.15 -0.00 -0.02 -0.13 -0.09 0.03 -0.05

25 1 -0.03 -0.02 -0.15 0.00 -0.02 -0.13 -0.09 -0.03 0.05

26 1 0.01 -0.04 0.14 -0.04 0.00 -0.36 0.03 -0.09 -0.05

27 1 -0.01 -0.04 -0.14 -0.04 -0.00 -0.36 -0.03 -0.09 0.05

28 1 -0.01 0.04 0.14 0.04 -0.00 -0.36 -0.03 0.09 -0.05

29 1 0.01 0.04 -0.14 0.04 0.00 -0.36 0.03 0.09 0.05

30 1 0.03 0.02 -0.15 -0.00 0.02 -0.13 0.09 0.03 0.05

31 1 0.03 -0.02 0.15 0.00 0.02 -0.13 0.09 -0.03 -0.05

32 30 -0.00 -0.00 -0.00 0.00 -0.00 -0.08 -0.00 0.00 0.00

33 6 0.01 -0.03 0.15 -0.02 0.01 0.06 0.05 -0.04 -0.05

34 6 -0.00 -0.02 0.07 -0.01 -0.00 0.02 0.01 -0.01 -0.02

35 6 0.00 0.02 0.07 0.01 0.00 0.02 -0.01 0.01 -0.02

36 6 -0.07 0.05 -0.13 -0.03 0.02 0.03 -0.15 0.14 0.05

37 6 0.07 -0.05 -0.13 0.03 -0.02 0.03 0.15 -0.14 0.05

38 6 0.00 -0.02 -0.07 -0.01 0.00 0.02 -0.01 -0.01 0.02

39 6 0.07 0.05 0.13 -0.03 -0.02 0.03 0.15 0.14 -0.05

40 6 -0.00 0.02 -0.07 0.01 -0.00 0.02 0.01 0.01 0.02

41 6 -0.07 -0.05 0.13 0.03 0.02 0.03 -0.15 -0.14 -0.05

42 1 -0.12 -0.11 0.29 0.04 0.03 0.03 -0.27 -0.26 -0.11

43 1 -0.12 0.11 -0.29 -0.04 0.03 0.03 -0.27 0.26 0.11

44 1 0.12 0.11 0.29 -0.04 -0.03 0.03 0.27 0.26 -0.11

45 1 0.12 -0.11 -0.29 0.04 -0.03 0.03 0.27 -0.26 0.11

16 17 18

A A A

Frequencies -- 163.5604 196.4877 208.4180

Red. masses -- 9.6773 8.8611 8.1183

Frc consts -- 0.1525 0.2016 0.2078

IR Inten -- 0.0000 0.0369 7.6288

Atom AN X Y Z X Y Z X Y Z

1 6 0.04 0.04 -0.01 0.00 0.18 0.00 -0.05 0.01 0.14

2 6 0.12 0.07 -0.01 -0.01 0.16 -0.05 -0.04 0.01 0.17

3 7 0.16 0.00 0.00 -0.00 0.16 -0.09 -0.04 0.00 0.00

4 6 0.12 -0.07 0.01 0.01 0.16 -0.05 -0.04 -0.01 -0.17

5 6 0.04 -0.04 0.01 -0.00 0.18 0.00 -0.05 -0.01 -0.14

6 6 0.14 -0.13 0.02 0.06 0.06 -0.00 -0.04 -0.01 -0.13

7 6 0.08 -0.12 0.01 0.16 0.01 0.06 -0.02 -0.01 0.06

8 7 0.00 -0.16 -0.00 0.16 0.00 0.12 0.00 -0.00 0.16

9 6 -0.08 -0.12 -0.01 0.16 -0.01 0.06 -0.02 0.01 0.06

10 6 -0.04 -0.03 -0.01 0.18 -0.00 -0.02 -0.02 0.00 0.02

11 6 0.04 -0.03 0.01 0.18 0.00 -0.02 -0.02 -0.00 0.02

12 6 0.14 0.13 -0.02 -0.06 0.06 -0.00 -0.04 0.01 0.13

13 6 0.08 0.12 -0.01 -0.16 0.01 0.06 -0.02 0.01 -0.06

14 6 0.04 0.03 -0.01 -0.18 0.00 -0.02 -0.02 0.00 -0.02

15 6 -0.04 0.03 0.01 -0.18 -0.00 -0.02 -0.02 -0.00 -0.02

16 6 -0.08 0.12 0.01 -0.16 -0.01 0.06 -0.02 -0.01 -0.06

17 7 -0.00 0.16 -0.00 -0.16 -0.00 0.12 0.00 -0.00 -0.16

18 6 -0.14 0.13 0.02 -0.06 -0.06 -0.00 -0.04 -0.01 0.13

19 6 -0.12 0.07 0.01 -0.01 -0.16 -0.05 -0.04 -0.01 0.17

20 6 -0.04 0.04 0.01 0.00 -0.18 0.00 -0.05 -0.01 0.14

21 6 -0.04 -0.04 -0.01 -0.00 -0.18 0.00 -0.05 0.01 -0.14

22 6 -0.12 -0.07 -0.01 0.01 -0.16 -0.05 -0.04 0.01 -0.17

23 7 -0.16 -0.00 0.00 0.00 -0.16 -0.09 -0.04 -0.00 -0.00

24 1 -0.01 0.08 -0.02 0.00 0.18 0.05 -0.06 0.02 0.24

25 1 -0.01 -0.08 0.02 -0.00 0.18 0.05 -0.06 -0.02 -0.24

26 1 -0.08 0.02 -0.02 0.18 0.00 -0.08 -0.01 -0.00 -0.04

27 1 0.08 0.02 0.02 0.18 -0.00 -0.08 -0.01 0.00 -0.04

28 1 0.08 -0.02 -0.02 -0.18 -0.00 -0.08 -0.01 -0.00 0.04

29 1 -0.08 -0.02 0.02 -0.18 0.00 -0.08 -0.01 0.00 0.04

30 1 0.01 0.08 0.02 0.00 -0.18 0.05 -0.06 -0.02 0.24

31 1 0.01 -0.08 -0.02 -0.00 -0.18 0.05 -0.06 0.02 -0.24

32 30 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.18 0.00 -0.00

33 6 -0.14 -0.13 -0.02 0.06 -0.06 -0.00 -0.04 0.01 -0.13

34 6 -0.14 -0.14 -0.01 0.01 -0.00 -0.01 -0.04 0.00 -0.10

35 6 0.14 0.14 -0.01 -0.01 0.00 -0.01 -0.04 0.00 0.10

36 6 -0.14 -0.15 0.01 0.04 -0.03 0.01 -0.00 -0.04 0.10

37 6 0.14 0.15 0.01 -0.04 0.03 0.01 -0.00 -0.04 -0.10

38 6 0.14 -0.14 0.01 0.01 0.00 -0.01 -0.04 -0.00 -0.10

39 6 0.14 -0.15 -0.01 0.04 0.03 0.01 -0.00 0.04 0.10

40 6 -0.14 0.14 0.01 -0.01 -0.00 -0.01 -0.04 -0.00 0.10

41 6 -0.14 0.15 -0.01 -0.04 -0.03 0.01 -0.00 0.04 -0.10

42 1 -0.13 0.16 -0.04 -0.05 -0.04 0.02 0.03 0.07 -0.25

43 1 -0.13 -0.16 0.04 0.05 -0.04 0.02 0.03 -0.07 0.25

44 1 0.13 -0.16 -0.04 0.05 0.04 0.02 0.03 0.07 0.25

45 1 0.13 0.16 0.04 -0.05 0.04 0.02 0.03 -0.07 -0.25

19 20 21

A A A

Frequencies -- 212.3244 234.6252 237.0183

Red. masses -- 7.9965 10.2691 11.6159

Frc consts -- 0.2124 0.3331 0.3845

IR Inten -- 0.9863 0.0069 14.8515

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.02 -0.02 0.01 0.01 -0.01 -0.10 0.00 -0.10

2 6 0.01 -0.01 -0.05 0.02 0.01 0.11 -0.09 0.00 -0.12

3 7 0.00 0.01 -0.13 0.00 0.05 0.22 -0.08 0.00 0.00

4 6 -0.01 -0.01 -0.05 -0.02 0.01 0.11 -0.09 -0.00 0.12

5 6 -0.00 -0.02 -0.02 -0.01 0.01 -0.01 -0.10 -0.00 0.10

6 6 -0.01 -0.04 0.12 -0.01 -0.07 -0.06 -0.08 -0.00 0.06

7 6 -0.01 -0.05 0.16 -0.00 -0.08 -0.13 0.01 -0.02 -0.11

8 7 0.00 -0.04 0.00 -0.00 -0.07 0.00 0.05 -0.00 -0.24

9 6 0.01 -0.05 -0.16 0.00 -0.08 0.13 0.01 0.02 -0.11

10 6 0.01 -0.06 -0.14 0.00 -0.10 0.12 0.00 0.01 0.03

11 6 -0.01 -0.06 0.14 -0.00 -0.10 -0.12 0.00 -0.01 0.03

12 6 0.01 -0.04 0.12 0.01 -0.07 -0.06 -0.08 0.00 -0.06

13 6 0.01 -0.05 0.16 0.00 -0.08 -0.13 0.01 0.02 0.11

14 6 0.01 -0.06 0.14 0.00 -0.10 -0.12 0.00 0.01 -0.03

15 6 -0.01 -0.06 -0.14 -0.00 -0.10 0.12 0.00 -0.01 -0.03

16 6 -0.01 -0.05 -0.16 -0.00 -0.08 0.13 0.01 -0.02 0.11

17 7 -0.00 -0.04 -0.00 -0.00 -0.07 -0.00 0.05 -0.00 0.24

18 6 -0.01 -0.04 -0.12 -0.01 -0.07 0.06 -0.08 -0.00 -0.06

19 6 -0.01 -0.01 0.05 -0.02 0.01 -0.11 -0.09 -0.00 -0.12

20 6 -0.00 -0.02 0.02 -0.01 0.01 0.01 -0.10 -0.00 -0.10

21 6 0.00 -0.02 0.02 0.01 0.01 0.01 -0.10 0.00 0.10

22 6 0.01 -0.01 0.05 0.02 0.01 -0.11 -0.09 0.00 0.12

23 7 0.00 0.01 0.13 0.00 0.05 -0.22 -0.08 0.00 -0.00

24 1 -0.00 -0.01 0.03 -0.00 0.01 -0.13 -0.11 0.01 -0.18

25 1 0.00 -0.01 0.03 0.00 0.01 -0.13 -0.11 -0.01 0.18

26 1 0.02 -0.07 -0.26 0.01 -0.11 0.23 0.01 -0.01 0.16

27 1 -0.02 -0.07 0.26 -0.01 -0.11 -0.23 0.01 0.01 0.16

28 1 0.02 -0.07 0.26 0.01 -0.11 -0.23 0.01 -0.01 -0.16

29 1 -0.02 -0.07 -0.26 -0.01 -0.11 0.23 0.01 0.01 -0.16

30 1 0.00 -0.01 -0.03 0.00 0.01 0.13 -0.11 -0.01 -0.18

31 1 -0.00 -0.01 -0.03 -0.00 0.01 0.13 -0.11 0.01 0.18

32 30 -0.00 0.19 0.00 -0.00 0.25 -0.00 0.28 0.00 0.00

33 6 0.01 -0.04 -0.12 0.01 -0.07 0.06 -0.08 0.00 0.06

34 6 0.01 -0.05 -0.10 0.01 -0.08 0.08 -0.09 0.01 0.08

35 6 0.01 -0.05 0.10 0.01 -0.08 -0.08 -0.09 0.01 -0.08

36 6 -0.04 -0.00 0.09 -0.06 -0.01 -0.05 -0.01 -0.07 -0.05

37 6 -0.04 -0.00 -0.09 -0.06 -0.01 0.05 -0.01 -0.07 0.05

38 6 -0.01 -0.05 0.10 -0.01 -0.08 -0.08 -0.09 -0.01 0.08

39 6 0.04 -0.00 -0.09 0.06 -0.01 0.05 -0.01 0.07 -0.05

40 6 -0.01 -0.05 -0.10 -0.01 -0.08 0.08 -0.09 -0.01 -0.08

41 6 0.04 -0.00 0.09 0.06 -0.01 -0.05 -0.01 0.07 0.05

42 1 0.08 0.03 0.24 0.12 0.05 -0.15 0.05 0.13 0.15

43 1 -0.08 0.03 0.24 -0.12 0.05 -0.15 0.05 -0.13 -0.15

44 1 0.08 0.03 -0.24 0.12 0.05 0.15 0.05 0.13 -0.15

45 1 -0.08 0.03 -0.24 -0.12 0.05 0.15 0.05 -0.13 0.15

22 23 24

A A A

Frequencies -- 275.6679 307.2961 312.5067

Red. masses -- 5.3030 6.2667 6.7352

Frc consts -- 0.2374 0.3487 0.3875

IR Inten -- 0.0000 2.6087 47.5800

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.15 -0.00 -0.04 -0.03 0.00 -0.11 -0.00

2 6 0.00 0.00 0.16 -0.01 -0.04 -0.04 0.03 -0.08 0.01

3 7 -0.00 0.00 0.00 0.00 -0.05 -0.11 -0.00 -0.08 0.02

4 6 0.00 -0.00 -0.16 0.01 -0.04 -0.04 -0.03 -0.08 0.01

5 6 0.00 -0.00 -0.15 0.00 -0.04 -0.03 -0.00 -0.11 -0.00

6 6 -0.00 -0.00 0.00 0.03 -0.02 0.13 -0.12 0.04 0.00

7 6 -0.00 0.00 0.15 0.04 -0.01 -0.01 -0.13 0.04 -0.01

8 7 0.00 0.00 -0.00 0.05 -0.00 -0.09 0.00 0.12 0.00

9 6 0.00 0.00 -0.15 0.04 0.01 -0.01 0.13 0.04 0.01

10 6 0.00 0.00 -0.16 0.04 0.00 -0.04 0.09 -0.13 0.01

11 6 -0.00 0.00 0.16 0.04 -0.00 -0.04 -0.09 -0.13 -0.01

12 6 -0.00 0.00 -0.00 -0.03 -0.02 0.13 0.12 0.04 0.00

13 6 -0.00 -0.00 -0.15 -0.04 -0.01 -0.01 0.13 0.04 -0.01

14 6 -0.00 -0.00 -0.16 -0.04 -0.00 -0.04 0.09 -0.13 -0.01

15 6 0.00 -0.00 0.16 -0.04 0.00 -0.04 -0.09 -0.13 0.01

16 6 0.00 -0.00 0.15 -0.04 0.01 -0.01 -0.13 0.04 0.01

17 7 0.00 -0.00 0.00 -0.05 -0.00 -0.09 0.00 0.12 -0.00

18 6 0.00 0.00 0.00 -0.03 0.02 0.13 -0.12 0.04 -0.00

19 6 -0.00 0.00 -0.16 -0.01 0.04 -0.04 -0.03 -0.08 -0.01

20 6 -0.00 0.00 -0.15 -0.00 0.04 -0.03 -0.00 -0.11 0.00

21 6 -0.00 -0.00 0.15 0.00 0.04 -0.03 0.00 -0.11 0.00

22 6 -0.00 -0.00 0.16 0.01 0.04 -0.04 0.03 -0.08 -0.01

23 7 0.00 0.00 -0.00 0.00 0.05 -0.11 -0.00 -0.08 -0.02

24 1 0.00 0.01 0.26 0.00 -0.05 0.00 -0.01 -0.10 -0.01

25 1 0.00 -0.01 -0.26 -0.00 -0.05 0.00 0.01 -0.10 -0.01

26 1 0.01 -0.00 -0.29 0.05 -0.00 -0.06 0.18 -0.25 0.02

27 1 -0.01 -0.00 0.29 0.05 0.00 -0.06 -0.18 -0.25 -0.02

28 1 -0.01 0.00 -0.29 -0.05 0.00 -0.06 0.18 -0.25 -0.02

29 1 0.01 0.00 0.29 -0.05 -0.00 -0.06 -0.18 -0.25 0.02

30 1 -0.00 0.01 -0.26 0.00 0.05 0.00 0.01 -0.10 0.01

31 1 -0.00 -0.01 0.26 -0.00 0.05 0.00 -0.01 -0.10 0.01

32 30 0.00 0.00 -0.00 0.00 -0.00 -0.01 0.00 0.02 0.00

33 6 0.00 -0.00 -0.00 0.03 0.02 0.13 0.12 0.04 -0.00

34 6 0.00 0.00 -0.02 0.03 0.03 0.25 0.09 0.10 0.00

35 6 -0.00 -0.00 -0.02 -0.03 -0.03 0.25 0.09 0.10 -0.00

36 6 0.00 -0.00 0.01 0.03 0.03 -0.10 0.10 0.10 0.00

37 6 -0.00 0.00 0.01 -0.03 -0.03 -0.10 0.10 0.10 -0.00

38 6 -0.00 0.00 0.02 0.03 -0.03 0.25 -0.09 0.10 -0.00

39 6 -0.00 -0.00 -0.01 0.03 -0.03 -0.10 -0.10 0.10 -0.00

40 6 0.00 -0.00 0.02 -0.03 0.03 0.25 -0.09 0.10 0.00

41 6 0.00 0.00 -0.01 -0.03 0.03 -0.10 -0.10 0.10 0.00

42 1 0.00 0.00 -0.03 -0.03 0.04 -0.35 -0.10 0.10 0.00

43 1 0.00 -0.00 0.03 0.03 0.04 -0.35 0.10 0.10 0.00

44 1 -0.00 -0.00 -0.03 0.03 -0.04 -0.35 -0.10 0.10 -0.00

45 1 -0.00 0.00 0.03 -0.03 -0.04 -0.35 0.10 0.10 -0.00

25 26 27

A A A

Frequencies -- 321.1915 324.6075 347.0453

Red. masses -- 6.7765 8.3017 5.4927

Frc consts -- 0.4119 0.5154 0.3898

IR Inten -- 30.9399 0.2212 0.1245

Atom AN X Y Z X Y Z X Y Z

1 6 -0.12 0.09 -0.00 0.00 0.13 -0.01 -0.00 0.00 0.15

2 6 0.05 0.13 -0.00 0.04 0.12 -0.03 -0.00 0.00 0.13

3 7 0.13 -0.00 0.00 0.00 0.13 -0.06 -0.00 -0.00 0.00

4 6 0.05 -0.13 0.00 -0.04 0.12 -0.03 -0.00 -0.00 -0.13

5 6 -0.12 -0.09 0.00 -0.00 0.13 -0.01 -0.00 -0.00 -0.15

6 6 0.04 -0.11 0.00 -0.09 0.08 0.04 -0.00 0.00 0.07

7 6 -0.09 -0.03 -0.01 -0.11 0.04 -0.02 0.00 -0.00 0.00

8 7 -0.09 0.00 -0.02 -0.12 0.00 -0.05 0.01 -0.00 -0.03

9 6 -0.09 0.03 -0.01 -0.11 -0.04 -0.02 0.00 0.00 0.00

10 6 -0.11 0.00 0.00 -0.13 -0.00 -0.01 0.01 0.00 -0.03

11 6 -0.11 -0.00 0.00 -0.13 0.00 -0.01 0.01 -0.00 -0.03

12 6 0.04 0.11 -0.00 0.09 0.08 0.04 -0.00 -0.00 -0.07

13 6 -0.09 0.03 0.01 0.11 0.04 -0.02 0.00 0.00 -0.00

14 6 -0.11 0.00 -0.00 0.13 0.00 -0.01 0.01 0.00 0.03

15 6 -0.11 -0.00 -0.00 0.13 -0.00 -0.01 0.01 -0.00 0.03

16 6 -0.09 -0.03 0.01 0.11 -0.04 -0.02 0.00 -0.00 -0.00

17 7 -0.09 0.00 0.02 0.12 -0.00 -0.05 0.01 0.00 0.03

18 6 0.04 -0.11 -0.00 0.09 -0.08 0.04 -0.00 0.00 -0.07

19 6 0.05 -0.13 -0.00 0.04 -0.12 -0.03 -0.00 -0.00 0.13

20 6 -0.12 -0.09 -0.00 0.00 -0.13 -0.01 -0.00 -0.00 0.15

21 6 -0.12 0.09 0.00 -0.00 -0.13 -0.01 -0.00 0.00 -0.15

22 6 0.05 0.13 0.00 -0.04 -0.12 -0.03 -0.00 0.00 -0.13

23 7 0.13 0.00 0.00 0.00 -0.13 -0.06 -0.00 -0.00 0.00

24 1 -0.24 0.18 -0.01 -0.01 0.15 0.02 -0.00 0.01 0.25

25 1 -0.24 -0.18 0.01 0.01 0.15 0.02 -0.00 -0.01 -0.25

26 1 -0.11 -0.01 0.02 -0.14 0.01 0.00 0.01 -0.00 -0.08

27 1 -0.11 0.01 0.02 -0.14 -0.01 0.00 0.01 0.00 -0.08

28 1 -0.11 -0.01 -0.02 0.14 -0.01 0.00 0.01 -0.00 0.08

29 1 -0.11 0.01 -0.02 0.14 0.01 0.00 0.01 0.00 0.08

30 1 -0.24 -0.18 -0.01 -0.01 -0.15 0.02 -0.00 -0.01 0.25

31 1 -0.24 0.18 0.01 0.01 -0.15 0.02 -0.00 0.01 -0.25

32 30 0.03 -0.00 -0.00 0.00 0.00 0.04 0.00 0.00 0.00

33 6 0.04 0.11 0.00 -0.09 -0.08 0.04 -0.00 -0.00 0.07

34 6 0.11 0.08 0.01 -0.11 -0.11 0.10 -0.01 -0.00 0.22

35 6 0.11 0.08 -0.01 0.11 0.11 0.10 -0.01 -0.00 -0.22

36 6 0.09 0.10 -0.00 -0.11 -0.12 -0.04 0.00 -0.00 -0.08

37 6 0.09 0.10 0.00 0.11 0.12 -0.04 0.00 -0.00 0.08

38 6 0.11 -0.08 0.01 -0.11 0.11 0.10 -0.01 0.00 0.22

39 6 0.09 -0.10 -0.00 -0.11 0.12 -0.04 0.00 0.00 -0.08

40 6 0.11 -0.08 -0.01 0.11 -0.11 0.10 -0.01 0.00 -0.22

41 6 0.09 -0.10 0.00 0.11 -0.12 -0.04 0.00 0.00 0.08

42 1 0.08 -0.11 0.01 0.11 -0.12 -0.14 0.00 0.00 0.28

43 1 0.08 0.11 -0.01 -0.11 -0.12 -0.14 0.00 -0.00 -0.28

44 1 0.08 -0.11 -0.01 -0.11 0.12 -0.14 0.00 0.00 -0.28

45 1 0.08 0.11 0.01 0.11 0.12 -0.14 0.00 -0.00 0.28

28 29 30

A A A

Frequencies -- 359.1077 366.3007 372.1946

Red. masses -- 5.3446 7.3998 7.1330

Frc consts -- 0.4061 0.5850 0.5822

IR Inten -- 8.2690 119.5846 0.1846

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.04 0.02 -0.01 -0.16 0.00 0.17 -0.03 -0.00

2 6 0.01 0.03 0.01 -0.03 -0.14 0.03 0.07 -0.03 -0.00

3 7 0.00 0.04 0.05 -0.00 -0.15 0.04 0.04 -0.00 0.00

4 6 -0.01 0.03 0.01 0.03 -0.14 0.03 0.07 0.03 0.00

5 6 -0.00 0.04 0.02 0.01 -0.16 0.00 0.17 0.03 0.00

6 6 -0.01 -0.00 -0.06 0.05 0.01 -0.02 0.01 0.06 -0.00

7 6 -0.01 -0.02 0.12 0.02 0.06 0.03 -0.13 0.04 -0.02

8 7 0.00 -0.01 -0.00 0.00 0.04 0.00 -0.15 -0.00 -0.03

9 6 0.01 -0.02 -0.12 -0.02 0.06 -0.03 -0.13 -0.04 -0.02

10 6 0.01 -0.04 -0.15 -0.02 0.15 -0.04 -0.16 -0.01 0.01

11 6 -0.01 -0.04 0.15 0.02 0.15 0.04 -0.16 0.01 0.01

12 6 0.01 -0.00 -0.06 -0.05 0.01 -0.02 0.01 -0.06 0.00

13 6 0.01 -0.02 0.12 -0.02 0.06 0.03 -0.13 -0.04 0.02

14 6 0.01 -0.04 0.15 -0.02 0.15 0.04 -0.16 -0.01 -0.01

15 6 -0.01 -0.04 -0.15 0.02 0.15 -0.04 -0.16 0.01 -0.01

16 6 -0.01 -0.02 -0.12 0.02 0.06 -0.03 -0.13 0.04 0.02

17 7 0.00 -0.01 -0.00 0.00 0.04 -0.00 -0.15 0.00 0.03

18 6 -0.01 -0.00 0.06 0.05 0.01 0.02 0.01 0.06 0.00

19 6 -0.01 0.03 -0.01 0.03 -0.14 -0.03 0.07 0.03 -0.00

20 6 -0.00 0.04 -0.02 0.01 -0.16 -0.00 0.17 0.03 -0.00

21 6 0.00 0.04 -0.02 -0.01 -0.16 -0.00 0.17 -0.03 0.00

22 6 0.01 0.03 -0.01 -0.03 -0.14 -0.03 0.07 -0.03 0.00

23 7 0.00 0.04 -0.05 -0.00 -0.15 -0.04 0.04 -0.00 -0.00

24 1 -0.00 0.04 0.03 0.01 -0.18 -0.02 0.22 -0.08 -0.01

25 1 0.00 0.04 0.03 -0.01 -0.18 -0.02 0.22 0.08 0.01

26 1 0.02 -0.05 -0.27 -0.06 0.20 -0.07 -0.18 0.01 0.03

27 1 -0.02 -0.05 0.27 0.06 0.20 0.07 -0.18 -0.01 0.03

28 1 0.02 -0.05 0.27 -0.06 0.20 0.07 -0.18 0.01 -0.03

29 1 -0.02 -0.05 -0.27 0.06 0.20 -0.07 -0.18 -0.01 -0.03

30 1 0.00 0.04 -0.03 -0.01 -0.18 0.02 0.22 0.08 -0.01

31 1 -0.00 0.04 -0.03 0.01 -0.18 0.02 0.22 -0.08 0.01

32 30 -0.00 -0.02 -0.00 -0.00 0.10 -0.00 0.09 0.00 0.00

33 6 0.01 -0.00 0.06 -0.05 0.01 0.02 0.01 -0.06 -0.00

34 6 0.03 -0.02 0.21 -0.13 0.08 0.08 0.08 -0.14 0.02

35 6 0.03 -0.02 -0.21 -0.13 0.08 -0.08 0.08 -0.14 -0.02

36 6 0.00 0.01 -0.07 -0.00 -0.05 -0.03 -0.06 -0.01 -0.00

37 6 0.00 0.01 0.07 -0.00 -0.05 0.03 -0.06 -0.01 0.00

38 6 -0.03 -0.02 -0.21 0.13 0.08 -0.08 0.08 0.14 0.02

39 6 -0.00 0.01 0.07 0.00 -0.05 0.03 -0.06 0.01 -0.00

40 6 -0.03 -0.02 0.21 0.13 0.08 0.08 0.08 0.14 -0.02

41 6 -0.00 0.01 -0.07 0.00 -0.05 -0.03 -0.06 0.01 0.00

42 1 0.02 0.04 -0.26 -0.09 -0.14 -0.10 -0.16 -0.08 0.02

43 1 -0.02 0.04 -0.26 0.09 -0.14 -0.10 -0.16 0.08 -0.02

44 1 0.02 0.04 0.26 -0.09 -0.14 0.10 -0.16 -0.08 -0.02

45 1 -0.02 0.04 0.26 0.09 -0.14 0.10 -0.16 0.08 0.02

31 32 33

A A A

Frequencies -- 372.7357 385.7860 402.1002

Red. masses -- 5.3628 4.9932 5.6961

Frc consts -- 0.4390 0.4378 0.5426

IR Inten -- 0.0000 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 0.01 -0.08 0.18 -0.05 -0.03 -0.07 0.08 -0.00

2 6 -0.03 0.01 -0.07 0.06 -0.04 -0.03 0.06 0.11 -0.00

3 7 0.01 -0.00 0.00 -0.02 0.00 -0.00 0.13 0.00 0.00

4 6 -0.03 -0.01 0.07 0.06 0.04 0.03 0.06 -0.11 0.00

5 6 -0.07 -0.01 0.08 0.18 0.05 0.03 -0.07 -0.08 0.00

6 6 0.01 -0.01 -0.04 -0.03 0.02 -0.01 0.00 0.00 -0.00

7 6 0.01 0.02 0.09 -0.04 -0.05 0.03 -0.11 0.05 -0.00

8 7 0.00 -0.01 0.00 -0.00 0.02 -0.00 0.00 0.12 0.00

9 6 -0.01 0.02 -0.09 0.04 -0.05 -0.03 0.11 0.05 0.00

10 6 -0.02 0.07 -0.11 0.04 -0.17 -0.04 0.08 -0.09 0.00

11 6 0.02 0.07 0.11 -0.04 -0.17 0.04 -0.08 -0.09 -0.00

12 6 0.01 0.01 0.04 -0.03 -0.02 0.01 0.00 -0.00 0.00

13 6 0.01 -0.02 -0.09 -0.04 0.05 -0.03 -0.11 -0.05 0.00

14 6 0.02 -0.07 -0.11 -0.04 0.17 -0.04 -0.08 0.09 0.00

15 6 -0.02 -0.07 0.11 0.04 0.17 0.04 0.08 0.09 -0.00

16 6 -0.01 -0.02 0.09 0.04 0.05 0.03 0.11 -0.05 -0.00

17 7 0.00 0.01 -0.00 -0.00 -0.02 0.00 -0.00 -0.12 0.00

18 6 -0.01 0.01 -0.04 0.03 -0.02 -0.01 -0.00 -0.00 -0.00

19 6 0.03 0.01 0.07 -0.06 -0.04 0.03 -0.06 0.11 0.00

20 6 0.07 0.01 0.08 -0.18 -0.05 0.03 0.07 0.08 0.00

21 6 0.07 -0.01 -0.08 -0.18 0.05 -0.03 0.07 -0.08 -0.00

22 6 0.03 -0.01 -0.07 -0.06 0.04 -0.03 -0.06 -0.11 -0.00

23 7 -0.01 -0.00 0.00 0.02 0.00 0.00 -0.13 0.00 0.00

24 1 -0.10 0.03 -0.15 0.25 -0.10 -0.06 -0.18 0.16 -0.01

25 1 -0.10 -0.03 0.15 0.25 0.10 0.06 -0.18 -0.16 0.01

26 1 -0.04 0.10 -0.20 0.10 -0.24 -0.07 0.17 -0.19 0.00

27 1 0.04 0.10 0.20 -0.10 -0.24 0.07 -0.17 -0.19 -0.00

28 1 0.04 -0.10 -0.20 -0.10 0.24 -0.07 -0.17 0.19 0.00

29 1 -0.04 -0.10 0.20 0.10 0.24 0.07 0.17 0.19 -0.00

30 1 0.10 0.03 0.15 -0.25 -0.10 0.06 0.18 0.16 0.01

31 1 0.10 -0.03 -0.15 -0.25 0.10 -0.06 0.18 -0.16 -0.01

32 30 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

33 6 -0.01 -0.01 0.04 0.03 0.02 0.01 -0.00 0.00 0.00

34 6 -0.01 -0.00 0.22 0.01 -0.01 0.08 -0.12 0.12 0.01

35 6 0.01 0.00 0.22 -0.01 0.01 0.08 0.12 -0.12 0.01

36 6 -0.01 -0.01 -0.07 0.01 0.01 -0.03 0.02 -0.02 -0.00

37 6 0.01 0.01 -0.07 -0.01 -0.01 -0.03 -0.02 0.02 -0.00

38 6 0.01 -0.00 -0.22 -0.01 -0.01 -0.08 0.12 0.12 -0.01

39 6 0.01 -0.01 0.07 -0.01 0.01 0.03 -0.02 -0.02 0.00

40 6 -0.01 0.00 -0.22 0.01 0.01 -0.08 -0.12 -0.12 -0.01

41 6 -0.01 0.01 0.07 0.01 -0.01 0.03 0.02 0.02 0.00

42 1 -0.01 0.00 0.26 0.01 -0.02 0.09 0.11 0.10 0.01

43 1 -0.01 -0.00 -0.26 0.01 0.02 -0.09 0.11 -0.10 -0.01

44 1 0.01 -0.00 0.26 -0.01 0.02 0.09 -0.11 -0.10 0.01

45 1 0.01 0.00 -0.26 -0.01 -0.02 -0.09 -0.11 0.10 -0.01

34 35 36

A A A

Frequencies -- 451.9085 456.3088 475.0287

Red. masses -- 8.3705 7.0024 6.0935

Frc consts -- 1.0072 0.8590 0.8101

IR Inten -- 0.1380 0.0004 5.2201

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.13 -0.00 -0.01 0.01 -0.00 0.13 -0.06 -0.00

2 6 -0.02 0.09 -0.01 -0.04 -0.01 0.00 0.00 -0.07 -0.00

3 7 0.00 0.12 -0.00 0.00 -0.01 0.00 -0.05 0.00 0.00

4 6 0.02 0.09 -0.01 0.04 -0.01 0.00 0.00 0.07 0.00

5 6 -0.00 0.13 -0.00 0.01 0.01 -0.00 0.13 0.06 0.00

6 6 0.08 -0.08 -0.01 0.06 0.06 -0.00 0.00 -0.06 -0.00

7 6 -0.09 -0.02 -0.01 -0.01 0.04 -0.00 -0.03 -0.03 -0.01

8 7 -0.12 -0.00 -0.01 -0.03 0.00 -0.00 -0.05 0.00 -0.00

9 6 -0.09 0.02 -0.01 -0.01 -0.04 -0.00 -0.03 0.03 -0.01

10 6 -0.14 -0.00 0.00 -0.00 -0.01 0.00 -0.07 0.00 0.00

11 6 -0.14 0.00 0.00 -0.00 0.01 0.00 -0.07 -0.00 0.00

12 6 -0.08 -0.08 -0.01 -0.06 0.06 -0.00 0.00 0.06 0.00

13 6 0.09 -0.02 -0.01 0.01 0.04 -0.00 -0.03 0.03 0.01

14 6 0.14 0.00 0.00 0.00 0.01 0.00 -0.07 0.00 -0.00

15 6 0.14 -0.00 0.00 0.00 -0.01 0.00 -0.07 -0.00 -0.00

16 6 0.09 0.02 -0.01 0.01 -0.04 -0.00 -0.03 -0.03 0.01

17 7 0.12 -0.00 -0.01 0.03 -0.00 -0.00 -0.05 0.00 0.00

18 6 -0.08 0.08 -0.01 -0.06 -0.06 -0.00 0.00 -0.06 0.00

19 6 -0.02 -0.09 -0.01 -0.04 0.01 0.00 0.00 0.07 -0.00

20 6 0.00 -0.13 -0.00 -0.01 -0.01 -0.00 0.13 0.06 -0.00

21 6 -0.00 -0.13 -0.00 0.01 -0.01 -0.00 0.13 -0.06 0.00

22 6 0.02 -0.09 -0.01 0.04 0.01 0.00 0.00 -0.07 0.00

23 7 0.00 -0.12 -0.00 -0.00 0.01 0.00 -0.05 0.00 0.00

24 1 0.00 0.14 0.01 0.01 -0.01 -0.00 0.23 -0.14 -0.00

25 1 -0.00 0.14 0.01 -0.01 -0.01 -0.00 0.23 0.14 0.00

26 1 -0.14 -0.00 0.01 -0.02 0.01 0.00 -0.07 -0.00 0.01

27 1 -0.14 0.00 0.01 -0.02 -0.01 0.00 -0.07 0.00 0.01

28 1 0.14 0.00 0.01 0.02 -0.01 0.00 -0.07 -0.00 -0.01

29 1 0.14 -0.00 0.01 0.02 0.01 0.00 -0.07 0.00 -0.01

30 1 0.00 -0.14 0.01 0.01 0.01 -0.00 0.23 0.14 -0.00

31 1 -0.00 -0.14 0.01 -0.01 0.01 -0.00 0.23 -0.14 0.00

32 30 0.00 -0.00 0.02 -0.00 -0.00 0.00 0.01 -0.00 0.00

33 6 0.08 0.08 -0.01 0.06 -0.06 -0.00 0.00 0.06 -0.00

34 6 0.13 0.14 0.02 0.25 -0.24 -0.00 -0.11 0.23 0.01

35 6 -0.13 -0.14 0.02 -0.25 0.24 -0.00 -0.11 0.23 -0.01

36 6 0.15 0.15 -0.00 -0.03 0.03 0.00 0.08 0.06 -0.00

37 6 -0.15 -0.15 -0.00 0.03 -0.03 0.00 0.08 0.06 0.00

38 6 0.13 -0.14 0.02 0.25 0.24 -0.00 -0.11 -0.23 0.01

39 6 0.15 -0.15 -0.00 -0.03 -0.03 0.00 0.08 -0.06 -0.00

40 6 -0.13 0.14 0.02 -0.25 -0.24 -0.00 -0.11 -0.23 -0.01

41 6 -0.15 0.15 -0.00 0.03 0.03 0.00 0.08 -0.06 0.00

42 1 -0.15 0.15 -0.01 0.24 0.24 -0.00 0.22 0.08 0.00

43 1 0.15 0.15 -0.01 -0.24 0.24 -0.00 0.22 -0.08 -0.00

44 1 0.15 -0.15 -0.01 -0.24 -0.24 -0.00 0.22 0.08 -0.00

45 1 -0.15 -0.15 -0.01 0.24 -0.24 -0.00 0.22 -0.08 0.00

37 38 39

A A A

Frequencies -- 478.2673 552.5100 557.8853

Red. masses -- 5.9402 6.0860 6.9037

Frc consts -- 0.8006 1.0946 1.2660

IR Inten -- 0.9322 0.0000 0.0773

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.07 0.00 0.00 0.01 0.14 -0.00 -0.01 0.03

2 6 -0.03 0.03 -0.01 0.01 0.01 -0.03 0.00 -0.01 -0.03

3 7 0.00 0.05 0.00 0.00 0.00 -0.00 -0.00 0.00 0.13

4 6 0.03 0.03 -0.01 0.01 -0.01 0.03 -0.00 -0.01 -0.03

5 6 0.00 0.07 0.00 0.00 -0.01 -0.14 0.00 -0.01 0.03

6 6 0.06 -0.00 -0.00 -0.00 0.00 0.22 -0.00 -0.00 -0.24

7 6 -0.07 0.00 -0.00 0.00 -0.00 0.05 0.00 0.00 -0.06

8 7 0.00 0.05 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

9 6 0.07 0.00 0.00 -0.00 -0.00 -0.05 -0.00 0.00 0.06

10 6 0.07 -0.14 -0.00 -0.00 0.00 0.13 0.00 0.01 -0.14

11 6 -0.07 -0.14 0.00 0.00 0.00 -0.13 -0.00 0.01 0.14

12 6 -0.06 -0.00 -0.00 -0.00 -0.00 -0.22 0.00 -0.00 -0.24

13 6 0.07 0.00 -0.00 0.00 0.00 -0.05 -0.00 0.00 -0.06

14 6 0.07 -0.14 0.00 0.00 -0.00 0.13 0.00 0.01 0.14

15 6 -0.07 -0.14 -0.00 -0.00 -0.00 -0.13 -0.00 0.01 -0.14

16 6 -0.07 0.00 0.00 -0.00 0.00 0.05 0.00 0.00 0.06

17 7 0.00 0.05 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

18 6 0.06 -0.00 0.00 0.00 -0.00 0.22 -0.00 -0.00 0.24

19 6 0.03 0.03 0.01 -0.01 0.01 0.03 -0.00 -0.01 0.03

20 6 0.00 0.07 -0.00 -0.00 0.01 -0.14 0.00 -0.01 -0.03

21 6 -0.00 0.07 -0.00 -0.00 -0.01 0.14 -0.00 -0.01 -0.03

22 6 -0.03 0.03 0.01 -0.01 -0.01 -0.03 0.00 -0.01 0.03

23 7 0.00 0.05 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.13

24 1 -0.00 0.07 0.01 -0.01 0.02 0.23 -0.00 -0.01 0.01

25 1 0.00 0.07 0.01 -0.01 -0.02 -0.23 0.00 -0.01 0.01

26 1 0.14 -0.24 -0.00 -0.01 0.01 0.24 0.00 0.01 -0.27

27 1 -0.14 -0.24 0.00 0.01 0.01 -0.24 -0.00 0.01 0.27

28 1 0.14 -0.24 0.00 0.01 -0.01 0.24 0.00 0.01 0.27

29 1 -0.14 -0.24 -0.00 -0.01 -0.01 -0.24 -0.00 0.01 -0.27

30 1 0.00 0.07 -0.01 0.01 0.02 -0.23 0.00 -0.01 -0.01

31 1 -0.00 0.07 -0.01 0.01 -0.02 0.23 -0.00 -0.01 -0.01

32 30 -0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.00 0.01 -0.00

33 6 -0.06 -0.00 0.00 0.00 0.00 -0.22 0.00 -0.00 0.24

34 6 -0.23 0.11 -0.00 0.01 -0.01 0.15 0.00 0.00 -0.17

35 6 -0.23 0.11 0.00 -0.01 0.01 0.15 0.00 0.00 0.17

36 6 -0.05 -0.08 -0.00 0.00 0.00 -0.07 0.00 -0.00 0.08

37 6 -0.05 -0.08 0.00 -0.00 -0.00 -0.07 0.00 -0.00 -0.08

38 6 0.23 0.11 0.00 -0.01 -0.01 -0.15 -0.00 0.00 0.17

39 6 0.05 -0.08 0.00 -0.00 0.00 0.07 -0.00 -0.00 -0.08

40 6 0.23 0.11 -0.00 0.01 0.01 -0.15 -0.00 0.00 -0.17

41 6 0.05 -0.08 -0.00 0.00 -0.00 0.07 -0.00 -0.00 0.08

42 1 -0.09 -0.22 0.00 -0.00 -0.00 -0.15 0.01 0.01 -0.22

43 1 0.09 -0.22 0.00 -0.00 0.00 0.15 -0.01 0.01 -0.22

44 1 -0.09 -0.22 -0.00 0.00 0.00 -0.15 0.01 0.01 0.22

45 1 0.09 -0.22 -0.00 0.00 -0.00 0.15 -0.01 0.01 0.22

40 41 42

A A A

Frequencies -- 560.4483 567.9221 568.4211

Red. masses -- 6.9011 6.2565 7.0633

Frc consts -- 1.2771 1.1889 1.3446

IR Inten -- 0.7472 5.6539 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.01 -0.01 -0.15 0.00 0.01 -0.03 0.06 0.08 -0.01

2 6 -0.00 -0.00 0.04 0.00 0.01 0.03 0.11 0.08 -0.00

3 7 -0.01 -0.00 -0.00 0.00 0.00 -0.12 0.16 -0.00 0.00

4 6 -0.00 0.00 -0.04 -0.00 0.01 0.03 0.11 -0.08 0.00

5 6 -0.01 0.01 0.15 -0.00 0.01 -0.03 0.06 -0.08 0.01

6 6 0.00 -0.00 -0.24 -0.00 0.00 0.23 -0.02 -0.01 -0.01

7 6 0.01 0.00 -0.05 -0.01 0.00 0.05 -0.06 0.08 -0.00

8 7 -0.00 -0.00 0.14 -0.00 0.00 -0.13 0.00 0.11 0.00

9 6 0.01 -0.00 -0.05 -0.01 -0.00 0.05 0.06 0.08 0.00

10 6 0.01 -0.00 0.03 -0.01 -0.00 -0.03 0.05 0.07 -0.00

11 6 0.01 0.00 0.03 -0.01 0.00 -0.03 -0.05 0.07 0.00

12 6 0.00 0.00 0.24 0.00 0.00 0.23 -0.02 0.01 0.01

13 6 0.01 -0.00 0.05 0.01 0.00 0.05 -0.06 -0.08 0.00

14 6 0.01 -0.00 -0.03 0.01 0.00 -0.03 -0.05 -0.07 -0.00

15 6 0.01 0.00 -0.03 0.01 -0.00 -0.03 0.05 -0.07 0.00

16 6 0.01 0.00 0.05 0.01 -0.00 0.05 0.06 -0.08 -0.00

17 7 -0.00 -0.00 -0.14 0.00 -0.00 -0.13 -0.00 -0.11 0.00

18 6 0.00 -0.00 0.24 0.00 -0.00 0.23 0.02 0.01 -0.01

19 6 -0.00 0.00 0.04 0.00 -0.01 0.03 -0.11 0.08 0.00

20 6 -0.01 0.01 -0.15 0.00 -0.01 -0.03 -0.06 0.08 0.01

21 6 -0.01 -0.01 0.15 -0.00 -0.01 -0.03 -0.06 -0.08 -0.01

22 6 -0.00 -0.00 -0.04 -0.00 -0.01 0.03 -0.11 -0.08 -0.00

23 7 -0.01 -0.00 0.00 -0.00 -0.00 -0.12 -0.16 0.00 0.00

24 1 -0.01 -0.01 -0.25 0.00 0.01 0.00 -0.03 0.15 -0.01

25 1 -0.01 0.01 0.25 -0.00 0.01 0.00 -0.03 -0.15 0.01

26 1 0.01 0.00 0.05 -0.01 -0.00 -0.05 0.09 0.02 -0.01

27 1 0.01 -0.00 0.05 -0.01 0.00 -0.05 -0.09 0.02 0.01

28 1 0.01 0.00 -0.05 0.01 0.00 -0.05 -0.09 -0.02 -0.01

29 1 0.01 -0.00 -0.05 0.01 -0.00 -0.05 0.09 -0.02 0.01

30 1 -0.01 0.01 -0.25 0.00 -0.01 0.00 0.03 0.15 0.01

31 1 -0.01 -0.01 0.25 -0.00 -0.01 0.00 0.03 -0.15 -0.01

32 30 -0.01 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

33 6 0.00 0.00 -0.24 -0.00 -0.00 0.23 0.02 -0.01 0.01

34 6 0.01 -0.00 0.18 0.00 0.00 -0.18 0.20 -0.17 -0.01

35 6 0.01 -0.00 -0.18 -0.00 -0.00 -0.18 -0.20 0.17 -0.01

36 6 0.00 0.00 -0.09 0.00 0.00 0.10 0.01 0.02 0.01

37 6 0.00 0.00 0.09 -0.00 -0.00 0.10 -0.01 -0.02 0.01

38 6 0.01 0.00 0.18 0.00 -0.00 -0.18 -0.20 -0.17 0.01

39 6 0.00 -0.00 -0.09 0.00 -0.00 0.10 -0.01 0.02 -0.01

40 6 0.01 0.00 -0.18 -0.00 0.00 -0.18 0.20 0.17 0.01

41 6 0.00 -0.00 0.09 -0.00 0.00 0.10 0.01 -0.02 -0.01

42 1 0.00 0.00 -0.23 0.00 0.01 -0.36 -0.19 -0.22 0.03

43 1 0.00 -0.00 0.23 -0.00 0.01 -0.36 -0.19 0.22 -0.03

44 1 0.00 0.00 0.23 -0.00 -0.01 -0.36 0.19 0.22 0.03

45 1 0.00 -0.00 -0.23 0.00 -0.01 -0.36 0.19 -0.22 -0.03

43 44 45

A A A

Frequencies -- 590.6504 591.6672 592.4536

Red. masses -- 5.5386 1.2758 1.2949

Frc consts -- 1.1384 0.2632 0.2678

IR Inten -- 13.2269 0.0000 0.2727

Atom AN X Y Z X Y Z X Y Z

1 6 0.06 0.10 0.01 0.00 -0.00 -0.02 -0.00 -0.00 0.00

2 6 0.10 0.10 -0.01 0.00 0.00 0.01 0.00 -0.00 -0.01

3 7 0.20 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.02

4 6 0.10 -0.10 0.01 0.00 -0.00 -0.01 -0.00 -0.00 -0.01

5 6 0.06 -0.10 -0.01 0.00 0.00 0.02 0.00 -0.00 0.00

6 6 -0.02 0.02 0.01 0.00 -0.00 -0.02 -0.00 -0.00 -0.03

7 6 0.00 0.01 0.01 -0.00 0.00 -0.01 0.00 -0.00 -0.02

8 7 0.00 0.00 -0.01 -0.00 0.00 -0.00 0.00 -0.00 0.00

9 6 0.00 -0.01 0.01 0.00 0.00 0.01 -0.00 -0.00 0.02

10 6 0.00 0.00 -0.00 0.00 0.00 -0.02 -0.00 0.00 -0.02

11 6 0.00 -0.00 -0.00 -0.00 0.00 0.02 0.00 0.00 0.02

12 6 -0.02 -0.02 -0.01 0.00 0.00 0.02 0.00 -0.00 -0.03

13 6 0.00 -0.01 -0.01 -0.00 -0.00 0.01 -0.00 -0.00 -0.02

14 6 0.00 0.00 0.00 -0.00 -0.00 -0.02 -0.00 0.00 0.02

15 6 0.00 -0.00 0.00 0.00 -0.00 0.02 0.00 0.00 -0.02

16 6 0.00 0.01 -0.01 0.00 -0.00 -0.01 0.00 -0.00 0.02

17 7 0.00 -0.00 0.01 -0.00 -0.00 0.00 0.00 -0.00 -0.00

18 6 -0.02 0.02 -0.01 -0.00 0.00 -0.02 -0.00 -0.00 0.03

19 6 0.10 -0.10 -0.01 -0.00 0.00 -0.01 -0.00 -0.00 0.01

20 6 0.06 -0.10 0.01 -0.00 -0.00 0.02 0.00 -0.00 -0.00

21 6 0.06 0.10 -0.01 -0.00 0.00 -0.02 -0.00 -0.00 -0.00

22 6 0.10 0.10 0.01 -0.00 -0.00 0.01 0.00 -0.00 0.01

23 7 0.20 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.02

24 1 -0.04 0.17 0.01 0.00 -0.00 -0.04 -0.00 -0.00 0.01

25 1 -0.04 -0.17 -0.01 0.00 0.00 0.04 0.00 -0.00 0.01

26 1 -0.00 0.01 -0.01 0.00 -0.00 -0.04 -0.00 0.00 -0.05

27 1 -0.00 -0.01 -0.01 -0.00 -0.00 0.04 0.00 0.00 0.05

28 1 -0.00 0.01 0.01 -0.00 0.00 -0.04 -0.00 0.00 0.05

29 1 -0.00 -0.01 0.01 0.00 0.00 0.04 0.00 0.00 -0.05

30 1 -0.04 -0.17 0.01 -0.00 -0.00 0.04 0.00 -0.00 -0.01

31 1 -0.04 0.17 -0.01 -0.00 0.00 -0.04 -0.00 -0.00 -0.01

32 30 -0.01 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

33 6 -0.02 -0.02 0.01 -0.00 -0.00 0.02 0.00 -0.00 0.03

34 6 -0.17 0.03 0.00 0.00 -0.00 0.01 0.00 0.00 0.01

35 6 -0.17 0.03 -0.00 -0.00 0.00 0.01 0.00 0.00 -0.01

36 6 -0.08 -0.08 -0.04 -0.00 0.00 -0.07 -0.00 0.00 -0.07

37 6 -0.08 -0.08 0.04 0.00 -0.00 -0.07 -0.00 0.00 0.07

38 6 -0.17 -0.03 0.00 -0.00 -0.00 -0.01 -0.00 0.00 -0.01

39 6 -0.08 0.08 -0.04 0.00 0.00 0.07 0.00 0.00 0.07

40 6 -0.17 -0.03 -0.00 0.00 0.00 -0.01 -0.00 0.00 0.01

41 6 -0.08 0.08 0.04 -0.00 -0.00 0.07 0.00 0.00 -0.07

42 1 0.05 0.22 -0.26 0.01 0.01 -0.49 -0.01 -0.01 0.49

43 1 0.05 -0.22 0.26 0.01 -0.01 0.49 0.01 -0.01 0.49

44 1 0.05 0.22 0.26 -0.01 -0.01 -0.49 -0.01 -0.01 -0.49

45 1 0.05 -0.22 -0.26 -0.01 0.01 0.49 0.01 -0.01 -0.49

46 47 48

A A A

Frequencies -- 592.8913 594.9409 601.0086

Red. masses -- 1.3762 1.3939 7.2142

Frc consts -- 0.2850 0.2907 1.5353

IR Inten -- 0.9776 290.3476 0.3394

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.01 -0.02 0.00 0.00 -0.01 0.00 -0.00 0.00

2 6 0.01 0.01 0.01 -0.00 0.00 0.01 -0.01 -0.00 -0.00

3 7 0.03 -0.00 -0.00 0.00 -0.00 -0.03 0.00 -0.00 0.00

4 6 0.01 -0.01 -0.01 0.00 0.00 0.01 0.01 -0.00 -0.00

5 6 0.01 -0.01 0.02 -0.00 0.00 -0.01 -0.00 -0.00 0.00

6 6 -0.00 0.00 -0.03 -0.00 0.00 0.05 0.02 -0.01 -0.00

7 6 0.00 0.00 -0.01 -0.00 0.00 0.02 -0.12 0.12 -0.00

8 7 0.00 0.00 0.02 0.00 0.00 -0.04 0.00 0.23 0.00

9 6 0.00 -0.00 -0.01 -0.00 -0.00 0.02 0.12 0.12 0.00

10 6 0.00 0.00 0.00 -0.00 -0.00 -0.01 0.12 0.07 0.00

11 6 0.00 -0.00 0.00 -0.00 0.00 -0.01 -0.12 0.07 -0.00

12 6 -0.00 -0.00 0.03 0.00 0.00 0.05 -0.02 -0.01 -0.00

13 6 0.00 -0.00 0.01 0.00 0.00 0.02 0.12 0.12 -0.00

14 6 0.00 0.00 -0.00 0.00 0.00 -0.01 0.12 0.07 -0.00

15 6 0.00 -0.00 -0.00 0.00 -0.00 -0.01 -0.12 0.07 0.00

16 6 0.00 0.00 0.01 0.00 -0.00 0.02 -0.12 0.12 0.00

17 7 0.00 0.00 -0.02 -0.00 0.00 -0.04 0.00 0.23 -0.00

18 6 -0.00 0.00 0.03 0.00 -0.00 0.05 0.02 -0.01 0.00

19 6 0.01 -0.01 0.01 -0.00 -0.00 0.01 0.01 -0.00 0.00

20 6 0.01 -0.01 -0.02 0.00 -0.00 -0.01 -0.00 -0.00 -0.00

21 6 0.01 0.01 0.02 -0.00 -0.00 -0.01 0.00 -0.00 -0.00

22 6 0.01 0.01 -0.01 0.00 -0.00 0.01 -0.01 -0.00 0.00

23 7 0.03 -0.00 0.00 0.00 0.00 -0.03 -0.00 -0.00 -0.00

24 1 -0.01 0.02 -0.05 -0.00 0.00 -0.01 0.01 -0.01 0.01

25 1 -0.01 -0.02 0.05 0.00 0.00 -0.01 -0.01 -0.01 0.01

26 1 0.00 0.00 0.02 -0.00 0.00 -0.03 0.21 -0.05 0.01

27 1 0.00 -0.00 0.02 -0.00 -0.00 -0.03 -0.21 -0.05 -0.01

28 1 0.00 0.00 -0.02 0.00 -0.00 -0.03 0.21 -0.05 -0.01

29 1 0.00 -0.00 -0.02 0.00 0.00 -0.03 -0.21 -0.05 0.01

30 1 -0.01 -0.02 -0.05 -0.00 -0.00 -0.01 -0.01 -0.01 -0.01

31 1 -0.01 0.02 0.05 0.00 -0.00 -0.01 0.01 -0.01 -0.01

32 30 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.01 -0.00

33 6 -0.00 -0.00 -0.03 -0.00 -0.00 0.05 -0.02 -0.01 0.00

34 6 -0.02 0.00 -0.00 0.00 -0.00 -0.01 0.03 -0.20 -0.00

35 6 -0.02 0.00 0.00 -0.00 0.00 -0.01 0.03 -0.20 0.00

36 6 -0.01 -0.01 0.06 -0.00 0.00 -0.06 -0.10 -0.10 -0.01

37 6 -0.01 -0.01 -0.06 0.00 -0.00 -0.06 -0.10 -0.10 0.01

38 6 -0.02 -0.00 -0.00 0.00 0.00 -0.01 -0.03 -0.20 0.00

39 6 -0.01 0.01 0.06 -0.00 -0.00 -0.06 0.10 -0.10 0.01

40 6 -0.02 -0.00 0.00 -0.00 -0.00 -0.01 -0.03 -0.20 -0.00

41 6 -0.01 0.01 -0.06 0.00 0.00 -0.06 0.10 -0.10 -0.01

42 1 -0.00 0.01 0.49 -0.01 -0.01 0.49 0.25 0.04 0.03

43 1 -0.00 -0.01 -0.49 0.01 -0.01 0.49 -0.25 0.04 0.03

44 1 -0.00 0.01 -0.49 0.01 0.01 0.49 0.25 0.04 -0.03

45 1 -0.00 -0.01 0.49 -0.01 0.01 0.49 -0.25 0.04 -0.03

49 50 51

A A A

Frequencies -- 610.6242 657.9992 658.1091

Red. masses -- 7.0333 1.2902 1.3070

Frc consts -- 1.5451 0.3291 0.3335

IR Inten -- 0.0000 0.2941 163.9523

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.08 0.01 0.00 0.00 -0.00 -0.00 0.00 -0.00

2 6 -0.08 -0.09 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

3 7 -0.12 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

4 6 -0.08 0.09 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

5 6 -0.02 0.08 -0.01 -0.00 0.00 -0.00 0.00 0.00 -0.00

6 6 0.03 -0.02 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

7 6 -0.11 0.10 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00

8 7 0.00 0.16 -0.00 0.00 -0.00 0.00 0.00 -0.01 -0.00

9 6 0.11 0.10 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00

10 6 0.11 0.03 0.01 0.00 -0.00 0.00 -0.00 -0.00 -0.00

11 6 -0.11 0.03 -0.01 0.00 0.00 0.00 0.00 -0.00 0.00

12 6 0.03 0.02 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

13 6 -0.11 -0.10 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00

14 6 -0.11 -0.03 0.01 -0.00 0.00 0.00 -0.00 -0.00 0.00

15 6 0.11 -0.03 -0.01 -0.00 -0.00 0.00 0.00 -0.00 -0.00

16 6 0.11 -0.10 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

17 7 -0.00 -0.16 -0.00 -0.00 -0.00 0.00 0.00 -0.01 0.00

18 6 -0.03 0.02 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

19 6 0.08 -0.09 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

20 6 0.02 -0.08 -0.01 0.00 -0.00 -0.00 0.00 0.00 0.00

21 6 0.02 0.08 0.01 -0.00 -0.00 -0.00 -0.00 0.00 0.00

22 6 0.08 0.09 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

23 7 0.12 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

24 1 0.08 -0.16 0.01 0.00 0.00 0.00 -0.00 0.00 0.00

25 1 0.08 0.16 -0.01 -0.00 0.00 0.00 0.00 0.00 0.00

26 1 0.20 -0.09 0.02 0.00 -0.00 0.00 -0.01 0.00 -0.00

27 1 -0.20 -0.09 -0.02 0.00 0.00 0.00 0.01 0.00 0.00

28 1 -0.20 0.09 0.02 -0.00 0.00 0.00 -0.01 0.00 0.00

29 1 0.20 0.09 -0.02 -0.00 -0.00 0.00 0.01 0.00 -0.00

30 1 -0.08 -0.16 -0.01 0.00 -0.00 0.00 0.00 0.00 -0.00

31 1 -0.08 0.16 0.01 -0.00 -0.00 0.00 -0.00 0.00 -0.00

32 30 0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 -0.00

33 6 -0.03 -0.02 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

34 6 -0.08 -0.13 -0.00 0.02 -0.02 -0.00 -0.02 0.03 0.00

35 6 0.08 0.13 -0.00 -0.02 0.02 -0.00 -0.02 0.03 -0.00

36 6 -0.13 -0.13 -0.00 -0.05 0.05 0.00 0.06 -0.05 -0.00

37 6 0.13 0.13 -0.00 0.05 -0.05 0.00 0.06 -0.05 0.00

38 6 0.08 -0.13 0.00 0.02 0.02 -0.00 0.02 0.03 -0.00

39 6 0.13 -0.13 0.00 -0.05 -0.05 0.00 -0.06 -0.05 0.00

40 6 -0.08 0.13 0.00 -0.02 -0.02 -0.00 0.02 0.03 0.00

41 6 -0.13 0.13 0.00 0.05 0.05 0.00 -0.06 -0.05 -0.00

42 1 -0.15 0.11 0.01 -0.35 -0.34 -0.02 0.35 0.35 0.02

43 1 -0.15 -0.11 -0.01 0.35 -0.34 -0.02 -0.35 0.35 0.02

44 1 0.15 -0.11 0.01 0.35 0.34 -0.02 0.35 0.35 -0.02

45 1 0.15 0.11 -0.01 -0.35 0.34 -0.02 -0.35 0.35 -0.02

52 53 54

A A A

Frequencies -- 658.1578 658.1845 665.8175

Red. masses -- 1.3116 1.3074 3.6582

Frc consts -- 0.3347 0.3337 0.9555

IR Inten -- 0.0000 153.7258 0.3332

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.10

2 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.14

3 7 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00 -0.00 -0.00 -0.00

4 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.14

5 6 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.10

6 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.02

7 6 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 0.13

8 7 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.01 -0.00 -0.14

9 6 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.13

10 6 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.01

11 6 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.01

12 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.02

13 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.13

14 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 0.01

15 6 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.01

16 6 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.13

17 7 0.00 0.00 0.00 0.00 0.00 0.00 0.01 -0.00 0.14

18 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.02

19 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.14

20 6 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.10

21 6 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.10

22 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.14

23 7 0.00 -0.00 0.00 -0.01 -0.00 0.00 -0.00 0.00 -0.00

24 1 0.00 -0.01 -0.00 0.00 -0.01 -0.00 0.00 -0.01 -0.27

25 1 0.00 0.01 0.00 0.00 0.01 0.00 0.00 0.01 0.27

26 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.34

27 1 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.34

28 1 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.34

29 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.34

30 1 -0.00 -0.01 0.00 0.00 0.01 -0.00 0.00 0.01 -0.27

31 1 -0.00 0.01 -0.00 0.00 -0.01 0.00 0.00 -0.01 0.27

32 30 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

33 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.02

34 6 -0.03 0.03 0.00 0.03 -0.02 -0.00 0.00 -0.00 -0.02

35 6 0.03 -0.03 0.00 0.03 -0.02 0.00 0.00 -0.00 0.02

36 6 0.05 -0.05 -0.00 -0.05 0.05 0.00 0.00 -0.00 0.00

37 6 -0.05 0.05 -0.00 -0.05 0.05 -0.00 0.00 -0.00 -0.00

38 6 0.03 0.03 -0.00 0.03 0.02 -0.00 0.00 0.00 -0.02

39 6 -0.05 -0.05 0.00 -0.05 -0.05 0.00 0.00 0.00 0.00

40 6 -0.03 -0.03 -0.00 0.03 0.02 0.00 0.00 0.00 0.02

41 6 0.05 0.05 0.00 -0.05 -0.05 -0.00 0.00 0.00 -0.00

42 1 -0.35 -0.34 -0.02 0.35 0.34 0.02 -0.01 -0.01 -0.02

43 1 -0.35 0.34 0.02 0.36 -0.34 -0.02 -0.01 0.01 0.02

44 1 0.35 0.34 -0.02 0.35 0.34 -0.02 -0.01 -0.01 0.02

45 1 0.35 -0.34 0.02 0.35 -0.34 0.02 -0.01 0.01 -0.02

55 56 57

A A A

Frequencies -- 668.0375 670.4751 686.8798

Red. masses -- 4.3581 3.1989 3.9431

Frc consts -- 1.1459 0.8473 1.0961

IR Inten -- 0.0000 2.0223 0.0196

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 -0.12 -0.00 0.00 -0.01 -0.00 -0.00 0.01

2 6 0.00 0.00 0.17 -0.00 0.00 0.11 0.00 -0.01 -0.14

3 7 0.00 -0.00 -0.00 -0.00 -0.01 -0.12 0.00 0.01 0.16

4 6 0.00 -0.00 -0.17 0.00 0.00 0.11 -0.00 -0.01 -0.14

5 6 0.00 0.00 0.12 0.00 0.00 -0.01 0.00 -0.00 0.01

6 6 -0.00 -0.00 0.01 0.00 0.00 0.03 -0.00 -0.00 -0.04

7 6 -0.00 -0.00 0.14 0.00 0.00 -0.13 -0.00 -0.00 0.15

8 7 -0.00 0.00 0.00 -0.01 0.00 0.13 0.00 -0.00 -0.00

9 6 0.00 -0.00 -0.14 0.00 -0.00 -0.13 0.00 -0.00 -0.15

10 6 -0.00 0.00 0.11 0.00 -0.00 -0.00 -0.00 0.00 0.10

11 6 0.00 0.00 -0.11 0.00 0.00 -0.00 0.00 0.00 -0.10

12 6 -0.00 0.00 -0.01 -0.00 0.00 0.03 0.00 -0.00 -0.04

13 6 -0.00 0.00 -0.14 -0.00 0.00 -0.13 0.00 -0.00 0.15

14 6 0.00 -0.00 0.11 -0.00 0.00 -0.00 -0.00 0.00 -0.10

15 6 -0.00 -0.00 -0.11 -0.00 -0.00 -0.00 0.00 0.00 0.10

16 6 0.00 0.00 0.14 -0.00 -0.00 -0.13 -0.00 -0.00 -0.15

17 7 0.00 -0.00 0.00 0.01 -0.00 0.13 0.00 -0.00 -0.00

18 6 0.00 0.00 0.01 -0.00 -0.00 0.03 -0.00 -0.00 0.04

19 6 -0.00 0.00 -0.17 -0.00 -0.00 0.11 -0.00 -0.01 0.14

20 6 -0.00 -0.00 0.12 -0.00 -0.00 -0.01 0.00 -0.00 -0.01

21 6 -0.00 0.00 -0.12 0.00 -0.00 -0.01 -0.00 -0.00 -0.01

22 6 -0.00 -0.00 0.17 0.00 -0.00 0.11 0.00 -0.01 0.14

23 7 -0.00 0.00 -0.00 0.00 0.01 -0.12 0.00 0.01 -0.16

24 1 -0.00 -0.01 -0.34 0.00 -0.01 -0.25 -0.00 0.01 0.36

25 1 -0.00 0.01 0.34 -0.00 -0.01 -0.25 0.00 0.01 0.36

26 1 -0.01 0.00 0.25 -0.01 0.00 0.37 -0.01 0.01 0.23

27 1 0.01 0.00 -0.25 -0.01 -0.00 0.37 0.01 0.01 -0.23

28 1 0.01 -0.00 0.25 0.01 -0.00 0.37 -0.01 0.01 -0.23

29 1 -0.01 -0.00 -0.25 0.01 0.00 0.37 0.01 0.01 0.23

30 1 0.00 -0.01 0.34 0.00 0.01 -0.25 0.00 0.01 -0.36

31 1 0.00 0.01 -0.34 -0.00 0.01 -0.25 -0.00 0.01 -0.36

32 30 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

33 6 0.00 -0.00 -0.01 0.00 -0.00 0.03 0.00 -0.00 0.04

34 6 0.00 -0.00 0.01 -0.00 0.00 -0.01 -0.00 0.00 -0.02

35 6 -0.00 0.00 0.01 0.00 -0.00 -0.01 -0.00 0.00 0.02

36 6 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

37 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

38 6 -0.00 -0.00 -0.01 -0.00 -0.00 -0.01 0.00 0.00 0.02

39 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

40 6 0.00 0.00 -0.01 0.00 0.00 -0.01 0.00 0.00 -0.02

41 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

42 1 0.01 0.01 0.01 -0.00 -0.00 0.03 -0.00 -0.00 0.03

43 1 0.01 -0.01 -0.01 0.00 -0.00 0.03 0.00 -0.00 0.03

44 1 -0.01 -0.01 0.01 0.00 0.00 0.03 -0.00 -0.00 -0.03

45 1 -0.01 0.01 -0.01 -0.00 0.00 0.03 0.00 -0.00 -0.03

58 59 60

A A A

Frequencies -- 714.5465 717.1380 719.2168

Red. masses -- 3.0788 2.0577 2.7465

Frc consts -- 0.9262 0.6235 0.8371

IR Inten -- 0.0164 107.7502 0.1510

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 -0.05 -0.00 -0.00 -0.02 -0.00 0.00 0.03

2 6 0.00 0.00 0.13 0.00 -0.00 -0.09 -0.00 0.00 0.08

3 7 -0.00 -0.00 -0.00 -0.00 0.00 0.08 0.00 -0.00 -0.07

4 6 0.00 -0.00 -0.13 -0.00 -0.00 -0.09 0.00 0.00 0.08

5 6 -0.00 0.00 0.05 0.00 -0.00 -0.02 0.00 0.00 0.03

6 6 0.00 0.00 0.11 -0.00 0.00 0.07 0.00 -0.00 -0.10

7 6 0.00 0.00 -0.10 0.00 -0.00 -0.07 -0.00 0.00 0.12

8 7 -0.00 -0.00 0.08 -0.00 0.00 0.06 0.00 -0.00 -0.00

9 6 0.00 -0.00 -0.10 0.00 0.00 -0.07 0.00 0.00 -0.12

10 6 0.00 0.00 -0.02 0.00 0.00 -0.01 -0.00 -0.00 0.06

11 6 0.00 -0.00 -0.02 0.00 -0.00 -0.01 0.00 -0.00 -0.06

12 6 0.00 -0.00 -0.11 0.00 0.00 0.07 -0.00 -0.00 -0.10

13 6 0.00 -0.00 0.10 -0.00 -0.00 -0.07 0.00 0.00 0.12

14 6 0.00 0.00 0.02 -0.00 -0.00 -0.01 -0.00 -0.00 -0.06

15 6 0.00 -0.00 0.02 -0.00 0.00 -0.01 0.00 -0.00 0.06

16 6 0.00 0.00 0.10 -0.00 0.00 -0.07 -0.00 0.00 -0.12

17 7 -0.00 0.00 -0.08 0.00 -0.00 0.06 -0.00 -0.00 -0.00

18 6 0.00 0.00 -0.11 0.00 -0.00 0.07 0.00 -0.00 0.10

19 6 0.00 -0.00 0.13 0.00 0.00 -0.09 0.00 0.00 -0.08

20 6 -0.00 0.00 -0.05 -0.00 0.00 -0.02 0.00 0.00 -0.03

21 6 -0.00 -0.00 0.05 0.00 0.00 -0.02 -0.00 0.00 -0.03

22 6 0.00 0.00 -0.13 -0.00 0.00 -0.09 -0.00 0.00 -0.08

23 7 -0.00 0.00 -0.00 0.00 -0.00 0.08 -0.00 -0.00 0.07

24 1 -0.00 -0.01 -0.23 0.00 0.01 0.40 -0.00 -0.01 -0.42

25 1 -0.00 0.01 0.23 -0.00 0.01 0.40 0.00 -0.01 -0.42

26 1 -0.00 -0.00 0.38 -0.00 -0.00 0.25 -0.00 -0.00 0.17

27 1 -0.00 0.00 0.38 -0.00 0.00 0.25 0.00 -0.00 -0.17

28 1 -0.00 -0.00 -0.38 0.00 0.00 0.25 -0.00 -0.00 -0.17

29 1 -0.00 0.00 -0.38 0.00 -0.00 0.25 0.00 -0.00 0.17

30 1 -0.00 0.01 -0.23 0.00 -0.01 0.40 0.00 -0.01 0.42

31 1 -0.00 -0.01 0.23 -0.00 -0.01 0.40 -0.00 -0.01 0.42

32 30 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

33 6 0.00 -0.00 0.11 -0.00 -0.00 0.07 -0.00 -0.00 0.10

34 6 -0.00 0.00 -0.03 -0.00 -0.00 -0.01 0.00 0.00 -0.03

35 6 -0.00 0.00 0.03 0.00 0.00 -0.01 0.00 0.00 0.03

36 6 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00

37 6 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

38 6 -0.00 -0.00 -0.03 -0.00 0.00 -0.01 -0.00 0.00 0.03

39 6 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

40 6 -0.00 -0.00 0.03 0.00 -0.00 -0.01 -0.00 0.00 -0.03

41 6 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

42 1 -0.00 -0.00 -0.07 0.00 0.00 0.04 0.00 0.00 0.06

43 1 -0.00 0.00 0.07 -0.00 0.00 0.04 -0.00 0.00 0.06

44 1 -0.00 -0.00 0.07 -0.00 -0.00 0.04 0.00 0.00 -0.06

45 1 -0.00 0.00 -0.07 0.00 -0.00 0.04 -0.00 0.00 -0.06

61 62 63

A A A

Frequencies -- 726.3387 770.1058 770.4846

Red. masses -- 5.5598 1.9375 2.0611

Frc consts -- 1.7282 0.6770 0.7209

IR Inten -- 0.0000 78.9517 0.9892

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 0.05 -0.00 -0.00 -0.09 -0.00 -0.00 -0.09

2 6 -0.00 -0.00 -0.15 -0.00 0.00 0.10 -0.00 0.00 0.11

3 7 0.01 -0.00 -0.00 0.00 -0.00 -0.05 -0.00 -0.00 -0.06

4 6 -0.00 0.00 0.15 0.00 0.00 0.10 0.00 0.00 0.11

5 6 0.00 -0.00 -0.05 0.00 -0.00 -0.09 0.00 -0.00 -0.09

6 6 0.00 -0.01 -0.17 0.00 0.00 -0.04 0.00 0.00 -0.05

7 6 -0.00 0.00 0.20 -0.00 0.00 0.00 0.00 0.00 0.02

8 7 0.00 -0.01 -0.00 -0.00 -0.00 -0.01 -0.00 -0.00 -0.00

9 6 0.00 0.00 -0.20 -0.00 -0.00 0.00 -0.00 0.00 -0.02

10 6 -0.00 -0.00 0.09 -0.00 -0.00 0.02 -0.00 -0.00 0.00

11 6 0.00 -0.00 -0.09 -0.00 0.00 0.02 0.00 -0.00 -0.00

12 6 0.00 0.01 0.17 -0.00 0.00 -0.04 -0.00 0.00 -0.05

13 6 -0.00 -0.00 -0.20 0.00 0.00 0.00 -0.00 0.00 0.02

14 6 0.00 0.00 0.09 0.00 0.00 0.02 -0.00 -0.00 -0.00

15 6 -0.00 0.00 -0.09 0.00 -0.00 0.02 0.00 -0.00 0.00

16 6 0.00 -0.00 0.20 0.00 -0.00 0.00 0.00 0.00 -0.02

17 7 -0.00 0.01 0.00 0.00 0.00 -0.01 0.00 -0.00 -0.00

18 6 -0.00 0.01 -0.17 -0.00 -0.00 -0.04 0.00 0.00 0.05

19 6 0.00 -0.00 0.15 -0.00 -0.00 0.10 0.00 0.00 -0.11

20 6 -0.00 0.00 -0.05 -0.00 0.00 -0.09 0.00 -0.00 0.09

21 6 -0.00 -0.00 0.05 0.00 0.00 -0.09 -0.00 -0.00 0.09

22 6 0.00 0.00 -0.15 0.00 -0.00 0.10 -0.00 0.00 -0.11

23 7 -0.01 -0.00 -0.00 -0.00 0.00 -0.05 -0.00 -0.00 0.06

24 1 0.01 0.01 0.27 0.00 0.01 0.46 0.00 0.01 0.47

25 1 0.01 -0.01 -0.27 -0.00 0.01 0.46 -0.00 0.01 0.47

26 1 -0.00 -0.01 0.25 0.00 0.00 -0.14 -0.00 -0.00 0.03

27 1 0.00 -0.01 -0.25 0.00 -0.00 -0.14 0.00 -0.00 -0.03

28 1 0.00 0.01 0.25 -0.00 -0.00 -0.14 -0.00 -0.00 -0.03

29 1 -0.00 0.01 -0.25 -0.00 0.00 -0.14 0.00 -0.00 0.03

30 1 -0.01 0.01 -0.27 0.00 -0.01 0.46 -0.00 0.01 -0.47

31 1 -0.01 -0.01 0.27 -0.00 -0.01 0.46 0.00 0.01 -0.47

32 30 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00

33 6 -0.00 -0.01 0.17 0.00 -0.00 -0.04 -0.00 0.00 0.05

34 6 0.00 0.00 -0.05 -0.00 0.00 0.01 0.00 -0.00 -0.01

35 6 -0.00 -0.00 -0.05 0.00 -0.00 0.01 0.00 -0.00 0.01

36 6 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

37 6 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00

38 6 -0.00 0.00 0.05 -0.00 -0.00 0.01 -0.00 -0.00 0.01

39 6 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00

40 6 0.00 -0.00 0.05 0.00 0.00 0.01 -0.00 -0.00 -0.01

41 6 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

42 1 0.00 -0.00 -0.10 -0.00 -0.00 -0.01 0.00 0.00 0.02

43 1 0.00 0.00 0.10 0.00 -0.00 -0.01 -0.00 0.00 0.02

44 1 -0.00 0.00 -0.10 0.00 0.00 -0.01 0.00 0.00 -0.02

45 1 -0.00 -0.00 0.10 -0.00 0.00 -0.01 -0.00 0.00 -0.02

64 65 66

A A A

Frequencies -- 791.5470 799.2396 799.6378

Red. masses -- 8.9378 1.8251 1.8729

Frc consts -- 3.2994 0.6869 0.7056

IR Inten -- 0.0000 0.4949 181.8711

Atom AN X Y Z X Y Z X Y Z

1 6 -0.13 -0.05 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.01

2 6 0.00 -0.07 0.00 0.00 -0.00 0.01 0.00 0.00 0.02

3 7 0.11 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.01

4 6 0.00 0.07 -0.00 0.00 0.00 -0.01 -0.00 0.00 0.02

5 6 -0.13 0.05 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.01

6 6 0.17 0.19 -0.00 0.00 0.00 0.03 -0.00 -0.00 -0.04

7 6 0.13 0.01 0.00 0.00 0.00 -0.09 -0.00 -0.00 0.09

8 7 0.00 0.20 -0.00 -0.00 -0.00 0.04 0.00 -0.00 -0.05

9 6 -0.13 0.01 -0.00 0.00 -0.00 -0.09 -0.00 0.00 0.09

10 6 -0.09 -0.16 -0.00 0.00 -0.00 0.09 -0.00 0.00 -0.09

11 6 0.09 -0.16 0.00 0.00 0.00 0.09 -0.00 -0.00 -0.09

12 6 0.17 -0.19 0.00 0.00 -0.00 -0.03 0.00 -0.00 -0.04

13 6 0.13 -0.01 -0.00 0.00 -0.00 0.09 0.00 -0.00 0.09

14 6 0.09 0.16 -0.00 0.00 -0.00 -0.09 0.00 -0.00 -0.09

15 6 -0.09 0.16 0.00 0.00 0.00 -0.09 0.00 0.00 -0.09

16 6 -0.13 -0.01 0.00 0.00 0.00 0.09 0.00 0.00 0.09

17 7 0.00 -0.20 -0.00 -0.00 -0.00 -0.04 -0.00 0.00 -0.05

18 6 -0.17 -0.19 -0.00 0.00 0.00 -0.03 0.00 0.00 -0.04

19 6 -0.00 -0.07 -0.00 0.00 0.00 0.01 0.00 -0.00 0.02

20 6 0.13 -0.05 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.01

21 6 0.13 0.05 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.01

22 6 -0.00 0.07 0.00 0.00 -0.00 -0.01 -0.00 -0.00 0.02

23 7 -0.11 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.01

24 1 -0.17 -0.02 0.01 -0.00 -0.00 -0.04 -0.00 0.00 0.05

25 1 -0.17 0.02 -0.01 -0.00 0.00 0.04 0.00 0.00 0.05

26 1 -0.10 -0.15 -0.01 0.01 0.00 -0.48 -0.01 -0.00 0.48

27 1 0.10 -0.15 0.01 0.01 -0.00 -0.48 -0.01 0.00 0.48

28 1 0.10 0.15 -0.01 0.01 0.00 0.48 0.01 0.00 0.48

29 1 -0.10 0.15 0.01 0.01 -0.00 0.48 0.01 -0.00 0.48

30 1 0.17 -0.02 -0.01 -0.00 0.00 -0.04 -0.00 -0.00 0.05

31 1 0.17 0.02 0.01 -0.00 -0.00 0.04 0.00 -0.00 0.05

32 30 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

33 6 -0.17 0.19 0.00 0.00 -0.00 0.03 -0.00 0.00 -0.04

34 6 0.05 -0.07 -0.00 -0.00 0.00 -0.01 0.00 -0.00 0.01

35 6 -0.05 0.07 -0.00 -0.00 0.00 0.01 -0.00 0.00 0.01

36 6 -0.01 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

37 6 0.01 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

38 6 -0.05 -0.07 0.00 -0.00 -0.00 -0.01 0.00 0.00 0.01

39 6 0.01 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

40 6 0.05 0.07 0.00 -0.00 -0.00 0.01 -0.00 -0.00 0.01

41 6 -0.01 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00

42 1 -0.08 -0.07 -0.00 0.00 0.00 -0.01 0.00 0.00 -0.01

43 1 -0.08 0.07 0.00 0.00 -0.00 0.01 -0.00 0.00 -0.01

44 1 0.08 0.07 -0.00 0.00 0.00 0.01 -0.00 -0.00 -0.01

45 1 0.08 -0.07 0.00 0.00 -0.00 -0.01 0.00 -0.00 -0.01

67 68 69

A A A

Frequencies -- 851.3349 860.4114 865.9054

Red. masses -- 8.1566 5.9262 7.6322

Frc consts -- 3.4831 2.5849 3.3717

IR Inten -- 101.1933 0.0000 481.6224

Atom AN X Y Z X Y Z X Y Z

1 6 0.01 0.00 -0.00 0.05 0.10 -0.02 0.17 0.11 -0.02

2 6 0.11 -0.00 0.01 0.03 0.09 -0.01 -0.09 0.11 0.00

3 7 0.00 0.14 -0.01 -0.20 -0.00 -0.00 -0.08 -0.00 -0.00

4 6 -0.11 -0.00 0.01 0.03 -0.09 0.01 -0.09 -0.11 -0.00

5 6 -0.01 0.00 -0.00 0.05 -0.10 0.02 0.17 -0.11 0.02

6 6 -0.14 -0.17 0.00 -0.12 0.07 -0.01 -0.16 -0.14 0.00

7 6 -0.14 -0.09 -0.00 0.05 -0.07 0.01 -0.00 -0.13 -0.01

8 7 -0.00 -0.11 -0.00 0.00 0.20 0.00 0.16 -0.00 0.01

9 6 0.14 -0.09 0.00 -0.05 -0.07 -0.01 -0.00 0.13 -0.01

10 6 0.13 0.18 0.00 -0.08 -0.00 -0.00 -0.02 0.02 0.00

11 6 -0.13 0.18 -0.00 0.08 -0.00 0.00 -0.02 -0.02 0.00

12 6 0.14 -0.17 0.00 -0.12 -0.07 0.01 -0.16 0.14 -0.00

13 6 0.14 -0.09 -0.00 0.05 0.07 -0.01 -0.00 0.13 0.01

14 6 0.13 0.18 -0.00 0.08 0.00 -0.00 -0.02 0.02 -0.00

15 6 -0.13 0.18 0.00 -0.08 0.00 0.00 -0.02 -0.02 -0.00

16 6 -0.14 -0.09 0.00 -0.05 0.07 0.01 -0.00 -0.13 0.01

17 7 0.00 -0.11 0.00 0.00 -0.20 -0.00 0.16 0.00 -0.01

18 6 -0.14 -0.17 -0.00 0.12 -0.07 -0.01 -0.16 -0.14 -0.00

19 6 -0.11 -0.00 -0.01 -0.03 0.09 0.01 -0.09 -0.11 0.00

20 6 -0.01 0.00 0.00 -0.05 0.10 0.02 0.17 -0.11 -0.02

21 6 0.01 0.00 0.00 -0.05 -0.10 -0.02 0.17 0.11 0.02

22 6 0.11 -0.00 -0.01 -0.03 -0.09 -0.01 -0.09 0.11 -0.00

23 7 -0.00 0.14 0.01 0.20 0.00 0.00 -0.08 0.00 0.00

24 1 -0.14 0.12 0.00 -0.09 0.21 0.06 0.20 0.10 0.10

25 1 0.14 0.12 0.00 -0.09 -0.21 -0.06 0.20 -0.10 -0.10

26 1 0.13 0.19 0.00 -0.23 0.18 -0.00 0.12 -0.16 -0.01

27 1 -0.13 0.19 -0.00 0.23 0.18 0.00 0.12 0.16 -0.01

28 1 0.13 0.19 -0.00 0.23 -0.18 -0.00 0.12 -0.16 0.01

29 1 -0.13 0.19 0.00 -0.23 -0.18 0.00 0.12 0.16 0.01

30 1 0.14 0.12 -0.00 0.09 0.21 -0.06 0.20 -0.10 0.10

31 1 -0.14 0.12 -0.00 0.09 -0.21 0.06 0.20 0.10 -0.10

32 30 -0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.02 0.00 -0.00

33 6 0.14 -0.17 -0.00 0.12 0.07 0.01 -0.16 0.14 0.00

34 6 -0.05 0.06 0.00 -0.06 -0.04 -0.00 0.06 -0.05 -0.00

35 6 -0.05 0.06 -0.00 0.06 0.04 -0.00 0.06 -0.05 0.00

36 6 0.01 0.00 -0.00 -0.04 -0.05 -0.00 -0.00 0.01 -0.00

37 6 0.01 0.00 0.00 0.04 0.05 -0.00 -0.00 0.01 0.00

38 6 0.05 0.06 -0.00 0.06 -0.04 0.00 0.06 0.05 -0.00

39 6 -0.01 0.00 0.00 0.04 -0.05 0.00 -0.00 -0.01 -0.00

40 6 0.05 0.06 0.00 -0.06 0.04 0.00 0.06 0.05 0.00

41 6 -0.01 0.00 -0.00 -0.04 0.05 0.00 -0.00 -0.01 0.00

42 1 -0.06 -0.05 -0.00 -0.04 0.06 -0.00 -0.05 -0.05 -0.00

43 1 0.06 -0.05 -0.00 -0.04 -0.06 0.00 -0.05 0.05 0.00

44 1 -0.06 -0.05 0.00 0.04 -0.06 -0.00 -0.05 -0.05 0.00

45 1 0.06 -0.05 0.00 0.04 0.06 0.00 -0.05 0.05 -0.00

70 71 72

A A A

Frequencies -- 866.9223 866.9295 874.2414

Red. masses -- 1.3754 1.3818 7.4404

Frc consts -- 0.6090 0.6119 3.3505

IR Inten -- 0.0002 4.6653 0.0025

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.01 0.09 -0.01 -0.01 -0.09 0.01 -0.03 -0.00

2 6 0.00 0.00 -0.02 0.00 -0.00 0.02 0.14 -0.01 0.01

3 7 -0.01 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.16 -0.01

4 6 0.00 -0.00 0.02 0.00 0.00 -0.02 -0.14 -0.01 0.01

5 6 0.00 -0.01 -0.09 -0.01 0.01 0.09 -0.01 -0.03 -0.00

6 6 -0.00 0.00 -0.01 0.01 0.01 0.01 -0.17 -0.17 0.00

7 6 0.00 -0.00 0.00 0.00 0.00 -0.01 -0.01 -0.15 -0.01

8 7 -0.00 0.01 0.00 -0.01 -0.00 0.00 0.18 0.00 0.01

9 6 -0.00 -0.00 -0.00 0.00 -0.00 -0.01 -0.01 0.15 -0.01

10 6 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.04 0.01 0.00

11 6 0.00 -0.00 0.00 0.00 0.00 0.00 -0.04 -0.01 0.00

12 6 -0.00 -0.00 0.01 0.01 -0.01 -0.01 0.17 -0.17 0.00

13 6 0.00 0.00 -0.00 0.00 -0.00 0.01 0.01 -0.15 -0.01

14 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.04 -0.01 0.00

15 6 -0.00 0.00 0.00 0.00 0.00 -0.00 0.04 0.01 0.00

16 6 -0.00 0.00 0.00 0.00 0.00 0.01 0.01 0.15 -0.01

17 7 -0.00 -0.01 -0.00 -0.01 0.00 -0.00 -0.18 -0.00 0.01

18 6 0.00 -0.00 -0.01 0.01 0.01 -0.01 0.17 0.17 0.00

19 6 -0.00 0.00 0.02 0.00 0.00 0.02 0.14 0.01 0.01

20 6 -0.00 0.01 -0.09 -0.01 0.01 -0.09 0.01 0.03 -0.00

21 6 -0.00 -0.01 0.09 -0.01 -0.01 0.09 -0.01 0.03 -0.00

22 6 -0.00 -0.00 -0.02 0.00 -0.00 -0.02 -0.14 0.01 0.01

23 7 0.01 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.16 -0.01

24 1 -0.00 -0.01 -0.49 -0.01 0.01 0.49 -0.18 0.13 0.00

25 1 -0.00 0.01 0.49 -0.01 -0.01 -0.49 0.18 0.13 0.00

26 1 -0.01 0.00 0.02 -0.00 0.01 -0.01 0.13 -0.19 -0.01

27 1 0.01 0.00 -0.02 -0.00 -0.01 -0.01 0.13 0.19 -0.01

28 1 0.01 -0.00 0.02 -0.00 0.01 0.01 -0.13 0.19 -0.01

29 1 -0.01 -0.00 -0.02 -0.00 -0.01 0.01 -0.13 -0.19 -0.01

30 1 0.00 -0.01 0.49 -0.01 -0.01 0.49 -0.18 -0.13 0.00

31 1 0.00 0.01 -0.49 -0.01 0.01 -0.49 0.18 -0.13 0.00

32 30 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

33 6 0.00 0.00 0.01 0.01 -0.01 0.01 -0.17 0.17 0.00

34 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.07 -0.07 -0.00

35 6 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.07 0.07 -0.00

36 6 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.01 0.00 -0.00

37 6 0.00 0.00 0.00 0.00 -0.00 -0.00 0.01 -0.00 -0.00

38 6 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.07 0.07 -0.00

39 6 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.01 -0.00 -0.00

40 6 -0.00 0.00 0.00 -0.00 -0.00 0.00 -0.07 -0.07 -0.00

41 6 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.01 0.00 -0.00

42 1 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.06 0.06 0.00

43 1 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.06 0.06 0.00

44 1 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.06 -0.06 0.00

45 1 0.00 0.00 0.00 0.00 -0.00 -0.00 0.06 -0.06 0.00

73 74 75

A A A

Frequencies -- 925.8974 925.9174 960.2820

Red. masses -- 1.3315 1.3316 4.4747

Frc consts -- 0.6725 0.6726 2.4312

IR Inten -- 0.0444 0.0000 167.0116

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.08 0.00

2 6 0.00 0.00 0.00 0.00 -0.00 0.00 0.10 0.01 0.00

3 7 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.13 -0.01

4 6 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.10 0.01 0.00

5 6 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.08 0.00

6 6 -0.00 0.00 -0.01 -0.00 0.00 0.01 -0.11 0.01 -0.00

7 6 -0.00 -0.00 0.01 0.00 0.00 -0.01 0.00 0.01 -0.00

8 7 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.15 -0.00

9 6 0.00 -0.00 -0.01 -0.00 0.00 0.01 -0.00 0.01 0.00

10 6 -0.00 -0.00 0.08 0.00 -0.00 -0.08 -0.14 -0.05 -0.00

11 6 0.00 -0.00 -0.08 -0.00 -0.00 0.08 0.14 -0.05 0.00

12 6 0.00 0.00 -0.01 -0.00 -0.00 -0.01 0.11 0.01 -0.00

13 6 0.00 -0.00 0.01 0.00 -0.00 0.01 -0.00 0.01 -0.00

14 6 -0.00 -0.00 -0.08 -0.00 0.00 -0.08 -0.14 -0.05 0.00

15 6 0.00 -0.00 0.08 0.00 0.00 0.08 0.14 -0.05 -0.00

16 6 -0.00 -0.00 -0.01 -0.00 -0.00 -0.01 0.00 0.01 0.00

17 7 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.15 0.00

18 6 -0.00 0.00 0.01 0.00 -0.00 0.01 -0.11 0.01 0.00

19 6 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.10 0.01 -0.00

20 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.08 -0.00

21 6 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00 -0.08 -0.00

22 6 0.00 0.00 -0.00 -0.00 0.00 0.00 0.10 0.01 -0.00

23 7 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.13 0.01

24 1 -0.00 0.00 0.00 -0.00 0.00 0.02 -0.19 0.06 0.00

25 1 0.00 0.00 0.00 -0.00 -0.00 -0.02 0.19 0.06 0.00

26 1 0.01 0.00 -0.49 -0.01 -0.00 0.49 -0.32 0.17 -0.00

27 1 -0.01 0.00 0.49 0.01 -0.00 -0.49 0.32 0.17 0.00

28 1 0.01 0.00 0.49 0.01 0.00 0.49 -0.32 0.17 0.00

29 1 -0.01 0.00 -0.49 -0.01 0.00 -0.49 0.32 0.17 -0.00

30 1 0.00 0.00 -0.00 0.00 0.00 -0.02 0.19 0.06 -0.00

31 1 -0.00 0.00 -0.00 0.00 -0.00 0.02 -0.19 0.06 -0.00

32 30 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 -0.01 -0.00

33 6 0.00 0.00 0.01 0.00 0.00 -0.01 0.11 0.01 0.00

34 6 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.04 -0.01 -0.00

35 6 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.04 -0.01 0.00

36 6 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.04 -0.04 -0.00

37 6 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.04 -0.04 0.00

38 6 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.04 -0.01 0.00

39 6 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.04 -0.04 0.00

40 6 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.04 -0.01 -0.00

41 6 0.00 -0.00 0.00 0.00 0.00 0.00 0.04 -0.04 -0.00

42 1 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.03 -0.06 -0.00

43 1 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.03 -0.06 -0.00

44 1 0.00 -0.00 -0.00 0.00 0.00 0.00 0.03 -0.06 0.00

45 1 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.03 -0.06 0.00

76 77 78

A A A

Frequencies -- 961.1450 989.7276 1016.9873

Red. masses -- 6.0402 6.3046 4.6238

Frc consts -- 3.2876 3.6386 2.8176

IR Inten -- 74.0526 0.0759 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.08 -0.15 0.00 0.01 0.10 -0.00 -0.07 -0.04 0.00

2 6 0.05 -0.04 0.00 -0.10 -0.01 -0.00 0.20 -0.04 -0.00

3 7 0.13 0.00 -0.00 0.00 -0.14 0.01 -0.17 -0.00 0.00

4 6 0.05 0.04 -0.00 0.10 -0.01 -0.00 0.20 0.04 0.00

5 6 -0.08 0.15 -0.00 -0.01 0.10 -0.00 -0.07 0.04 -0.00

6 6 0.02 -0.09 0.00 0.08 -0.03 0.00 -0.01 0.04 -0.00

7 6 0.04 -0.10 -0.00 0.07 -0.07 -0.00 0.05 0.02 0.00

8 7 0.20 0.00 0.01 0.22 -0.00 0.01 0.00 -0.10 0.00

9 6 0.04 0.10 -0.00 0.07 0.07 -0.00 -0.05 0.02 -0.00

10 6 -0.15 0.01 -0.00 -0.19 -0.00 -0.00 0.08 0.02 0.00

11 6 -0.15 -0.01 -0.00 -0.19 0.00 -0.00 -0.08 0.02 -0.00

12 6 0.02 0.09 -0.00 -0.08 -0.03 0.00 -0.01 -0.04 0.00

13 6 0.04 0.10 0.00 -0.07 -0.07 -0.00 0.05 -0.02 -0.00

14 6 -0.15 0.01 0.00 0.19 0.00 -0.00 -0.08 -0.02 0.00

15 6 -0.15 -0.01 0.00 0.19 -0.00 -0.00 0.08 -0.02 -0.00

16 6 0.04 -0.10 0.00 -0.07 0.07 -0.00 -0.05 -0.02 0.00

17 7 0.20 0.00 -0.01 -0.22 -0.00 0.01 0.00 0.10 -0.00

18 6 0.02 -0.09 -0.00 -0.08 0.03 0.00 0.01 -0.04 -0.00

19 6 0.05 0.04 0.00 -0.10 0.01 -0.00 -0.20 -0.04 0.00

20 6 -0.08 0.15 0.00 0.01 -0.10 -0.00 0.07 -0.04 -0.00

21 6 -0.08 -0.15 -0.00 -0.01 -0.10 -0.00 0.07 0.04 0.00

22 6 0.05 -0.04 -0.00 0.10 0.01 -0.00 -0.20 0.04 -0.00

23 7 0.13 0.00 0.00 0.00 0.14 0.01 0.17 0.00 0.00

24 1 0.09 -0.28 0.01 0.27 -0.09 0.00 -0.29 0.12 -0.00

25 1 0.09 0.28 -0.01 -0.27 -0.09 0.00 -0.29 -0.12 0.00

26 1 0.01 -0.22 -0.00 -0.04 -0.22 -0.00 0.22 -0.16 0.00

27 1 0.01 0.22 -0.00 -0.04 0.22 -0.00 -0.22 -0.16 -0.00

28 1 0.01 -0.22 0.00 0.04 0.22 -0.00 -0.22 0.16 0.00

29 1 0.01 0.22 0.00 0.04 -0.22 -0.00 0.22 0.16 -0.00

30 1 0.09 0.28 0.01 0.27 0.09 0.00 0.29 0.12 0.00

31 1 0.09 -0.28 -0.01 -0.27 0.09 0.00 0.29 -0.12 -0.00

32 30 -0.01 -0.00 0.00 0.00 0.00 -0.01 -0.00 -0.00 0.00

33 6 0.02 0.09 0.00 0.08 0.03 0.00 0.01 0.04 0.00

34 6 -0.01 -0.04 -0.00 -0.03 -0.02 -0.00 0.00 -0.01 0.00

35 6 -0.01 -0.04 0.00 0.03 0.02 -0.00 -0.00 0.01 0.00

36 6 -0.04 -0.04 -0.00 -0.04 -0.04 -0.00 0.01 0.01 0.00

37 6 -0.04 -0.04 0.00 0.04 0.04 -0.00 -0.01 -0.01 0.00

38 6 -0.01 0.04 -0.00 -0.03 0.02 -0.00 -0.00 -0.01 -0.00

39 6 -0.04 0.04 -0.00 -0.04 0.04 -0.00 -0.01 0.01 -0.00

40 6 -0.01 0.04 0.00 0.03 -0.02 -0.00 0.00 0.01 -0.00

41 6 -0.04 0.04 0.00 0.04 -0.04 -0.00 0.01 -0.01 -0.00

42 1 -0.06 0.04 0.00 0.04 -0.05 -0.00 0.00 -0.01 -0.00

43 1 -0.06 -0.04 -0.00 -0.04 -0.05 -0.00 0.00 0.01 0.00

44 1 -0.06 0.04 -0.00 -0.04 0.05 -0.00 -0.00 0.01 -0.00

45 1 -0.06 -0.04 0.00 0.04 0.05 -0.00 -0.00 -0.01 0.00

79 80 81

A A A

Frequencies -- 1023.9096 1034.4116 1051.3196

Red. masses -- 4.2207 3.9958 5.4678

Frc consts -- 2.6071 2.5190 3.5607

IR Inten -- 0.0000 269.2990 0.0017

Atom AN X Y Z X Y Z X Y Z

1 6 0.08 0.15 -0.00 0.02 0.09 -0.00 0.02 0.18 -0.00

2 6 -0.09 -0.02 0.00 0.02 -0.04 0.00 -0.01 -0.05 0.00

3 7 -0.08 0.00 -0.00 -0.12 -0.00 -0.00 0.00 -0.19 0.01

4 6 -0.09 0.02 -0.00 0.02 0.04 -0.00 0.01 -0.05 0.00

5 6 0.08 -0.15 0.00 0.02 -0.09 0.00 -0.02 0.18 -0.00

6 6 0.06 0.04 0.00 0.05 0.08 -0.00 -0.06 -0.10 0.00

7 6 0.04 0.12 -0.00 0.07 0.03 0.00 -0.07 -0.06 -0.00

8 7 -0.00 -0.12 -0.00 0.14 -0.00 0.01 -0.13 -0.00 -0.00

9 6 -0.04 0.12 0.00 0.07 -0.03 0.00 -0.07 0.06 -0.00

10 6 -0.01 -0.04 0.00 -0.14 0.01 -0.00 0.12 -0.01 0.00

11 6 0.01 -0.04 -0.00 -0.14 -0.01 -0.00 0.12 0.01 0.00

12 6 0.06 -0.04 -0.00 0.05 -0.08 0.00 0.06 -0.10 0.00

13 6 0.04 -0.12 0.00 0.07 -0.03 -0.00 0.07 -0.06 -0.00

14 6 0.01 0.04 0.00 -0.14 0.01 0.00 -0.12 0.01 0.00

15 6 -0.01 0.04 -0.00 -0.14 -0.01 0.00 -0.12 -0.01 0.00

16 6 -0.04 -0.12 -0.00 0.07 0.03 -0.00 0.07 0.06 -0.00

17 7 -0.00 0.12 0.00 0.14 0.00 -0.01 0.13 -0.00 -0.00

18 6 -0.06 -0.04 0.00 0.05 0.08 0.00 0.06 0.10 0.00

19 6 0.09 -0.02 -0.00 0.02 0.04 0.00 -0.01 0.05 0.00

20 6 -0.08 0.15 0.00 0.02 -0.09 -0.00 0.02 -0.18 -0.00

21 6 -0.08 -0.15 -0.00 0.02 0.09 0.00 -0.02 -0.18 -0.00

22 6 0.09 0.02 0.00 0.02 -0.04 -0.00 0.01 0.05 0.00

23 7 0.08 -0.00 -0.00 -0.12 0.00 0.00 -0.00 0.19 0.01

24 1 -0.12 0.31 -0.01 -0.24 0.30 -0.01 0.17 0.08 -0.00

25 1 -0.12 -0.31 0.01 -0.24 -0.30 0.01 -0.17 0.08 -0.00

26 1 0.13 -0.22 0.00 -0.19 0.05 -0.00 0.28 -0.20 0.00

27 1 -0.13 -0.22 -0.00 -0.19 -0.05 -0.00 0.28 0.20 0.00

28 1 -0.13 0.22 0.00 -0.19 0.05 0.00 -0.28 0.20 0.00

29 1 0.13 0.22 -0.00 -0.19 -0.05 0.00 -0.28 -0.20 0.00

30 1 0.12 0.31 0.01 -0.24 -0.30 -0.01 0.17 -0.08 -0.00

31 1 0.12 -0.31 -0.01 -0.24 0.30 0.01 -0.17 -0.08 -0.00

32 30 0.00 -0.00 0.00 -0.01 0.00 -0.00 0.00 -0.00 -0.00

33 6 -0.06 0.04 -0.00 0.05 -0.08 -0.00 -0.06 0.10 0.00

34 6 0.01 -0.01 -0.00 -0.00 0.01 -0.00 0.01 -0.02 -0.00

35 6 -0.01 0.01 -0.00 -0.00 0.01 0.00 -0.01 0.02 -0.00

36 6 -0.02 -0.02 -0.00 0.01 0.01 -0.00 -0.01 -0.01 -0.00

37 6 0.02 0.02 -0.00 0.01 0.01 0.00 0.01 0.01 -0.00

38 6 -0.01 -0.01 0.00 -0.00 -0.01 -0.00 0.01 0.02 -0.00

39 6 0.02 -0.02 0.00 0.01 -0.01 -0.00 -0.01 0.01 -0.00

40 6 0.01 0.01 0.00 -0.00 -0.01 0.00 -0.01 -0.02 -0.00

41 6 -0.02 0.02 0.00 0.01 -0.01 0.00 0.01 -0.01 -0.00

42 1 -0.03 0.01 0.00 0.02 0.00 0.00 0.03 0.00 -0.00

43 1 -0.03 -0.01 -0.00 0.02 -0.00 -0.00 -0.03 0.00 -0.00

44 1 0.03 -0.01 0.00 0.02 0.00 -0.00 -0.03 -0.00 -0.00

45 1 0.03 0.01 -0.00 0.02 -0.00 0.00 0.03 -0.00 -0.00

82 83 84

A A A

Frequencies -- 1051.8880 1054.3090 1074.6031

Red. masses -- 4.1776 6.3631 1.2614

Frc consts -- 2.7234 4.1673 0.8582

IR Inten -- 104.7183 0.0000 942.9073

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.16 0.00 0.03 0.05 -0.00 -0.06 0.02 -0.00

2 6 0.02 0.05 -0.00 -0.09 0.01 -0.00 0.00 -0.02 0.00

3 7 0.00 0.18 -0.01 0.00 0.00 -0.00 0.00 -0.05 0.00

4 6 -0.02 0.05 -0.00 -0.09 -0.01 0.00 -0.00 -0.02 0.00

5 6 0.02 -0.16 0.00 0.03 -0.05 0.00 0.06 0.02 -0.00

6 6 0.06 0.06 -0.00 0.09 0.07 -0.00 0.01 0.00 0.00

7 6 0.07 0.04 0.00 0.07 -0.21 0.00 0.00 0.00 -0.00

8 7 0.00 -0.09 -0.00 -0.00 0.07 -0.00 -0.00 -0.00 0.00

9 6 -0.07 0.04 -0.00 -0.07 -0.21 -0.00 -0.00 0.00 0.00

10 6 0.06 0.01 0.00 0.19 0.10 0.00 0.00 -0.00 -0.00

11 6 -0.06 0.01 -0.00 -0.19 0.10 -0.00 -0.00 -0.00 0.00

12 6 -0.06 0.06 -0.00 0.09 -0.07 0.00 -0.01 0.00 0.00

13 6 -0.07 0.04 0.00 0.07 0.21 -0.00 -0.00 0.00 -0.00

14 6 0.06 0.01 -0.00 -0.19 -0.10 0.00 0.00 -0.00 0.00

15 6 -0.06 0.01 0.00 0.19 -0.10 -0.00 -0.00 -0.00 -0.00

16 6 0.07 0.04 -0.00 -0.07 0.21 0.00 0.00 0.00 0.00

17 7 -0.00 -0.09 0.00 0.00 -0.07 -0.00 -0.00 -0.00 -0.00

18 6 0.06 0.06 0.00 -0.09 -0.07 -0.00 0.01 0.00 -0.00

19 6 -0.02 0.05 0.00 0.09 0.01 0.00 -0.00 -0.02 -0.00

20 6 0.02 -0.16 -0.00 -0.03 0.05 0.00 0.06 0.02 0.00

21 6 -0.02 -0.16 -0.00 -0.03 -0.05 -0.00 -0.06 0.02 0.00

22 6 0.02 0.05 0.00 0.09 -0.01 -0.00 0.00 -0.02 -0.00

23 7 0.00 0.18 0.01 -0.00 0.00 0.00 -0.00 -0.05 -0.00

24 1 -0.21 -0.03 0.00 -0.02 0.10 -0.00 -0.41 0.28 -0.01

25 1 0.21 -0.03 0.00 -0.02 -0.10 0.00 0.41 0.28 -0.01

26 1 0.27 -0.25 0.00 0.33 -0.08 0.01 0.01 -0.01 0.00

27 1 -0.27 -0.25 -0.00 -0.33 -0.08 -0.01 -0.01 -0.01 -0.00

28 1 0.27 -0.25 -0.00 -0.33 0.08 0.01 0.01 -0.01 -0.00

29 1 -0.27 -0.25 0.00 0.33 0.08 -0.01 -0.01 -0.01 0.00

30 1 0.21 -0.03 -0.00 0.02 0.10 0.00 0.41 0.28 0.01

31 1 -0.21 -0.03 -0.00 0.02 -0.10 -0.00 -0.41 0.28 0.01

32 30 -0.00 -0.01 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

33 6 -0.06 0.06 0.00 -0.09 0.07 0.00 -0.01 0.00 -0.00

34 6 0.01 -0.01 -0.00 0.00 0.00 -0.00 0.01 -0.00 0.00

35 6 0.01 -0.01 0.00 -0.00 -0.00 -0.00 0.01 -0.00 -0.00

36 6 -0.00 -0.00 -0.00 0.02 0.02 0.00 0.00 0.00 0.00

37 6 -0.00 -0.00 0.00 -0.02 -0.02 0.00 0.00 0.00 -0.00

38 6 -0.01 -0.01 0.00 -0.00 0.00 0.00 -0.01 -0.00 -0.00

39 6 0.00 -0.00 0.00 -0.02 0.02 -0.00 -0.00 0.00 -0.00

40 6 -0.01 -0.01 -0.00 0.00 -0.00 0.00 -0.01 -0.00 0.00

41 6 0.00 -0.00 -0.00 0.02 -0.02 -0.00 -0.00 0.00 0.00

42 1 0.01 0.01 -0.00 0.01 -0.03 -0.00 -0.00 0.00 0.00

43 1 -0.01 0.01 -0.00 0.01 0.03 0.00 0.00 0.00 0.00

44 1 0.01 0.01 0.00 -0.01 0.03 -0.00 -0.00 0.00 -0.00

45 1 -0.01 0.01 0.00 -0.01 -0.03 0.00 0.00 0.00 -0.00

85 86 87

A A A

Frequencies -- 1082.5232 1096.0212 1100.5344

Red. masses -- 1.2669 1.1780 1.3012

Frc consts -- 0.8747 0.8338 0.9285

IR Inten -- 0.0904 246.6832 0.0476

Atom AN X Y Z X Y Z X Y Z

1 6 0.05 -0.01 0.00 -0.00 -0.01 0.00 0.01 0.03 -0.00

2 6 -0.00 0.01 0.00 -0.01 0.02 -0.00 0.01 -0.01 0.00

3 7 -0.00 0.06 -0.00 0.02 0.00 -0.00 0.00 -0.04 0.00

4 6 0.00 0.01 0.00 -0.01 -0.02 0.00 -0.01 -0.01 0.00

5 6 -0.05 -0.01 0.00 -0.00 0.01 -0.00 -0.01 0.03 -0.00

6 6 -0.01 -0.01 -0.00 -0.02 -0.01 -0.00 -0.03 -0.02 0.00

7 6 -0.01 -0.00 0.00 0.00 0.01 -0.00 -0.00 0.00 -0.00

8 7 -0.01 0.00 -0.00 0.04 -0.00 0.00 0.04 0.00 0.00

9 6 -0.01 0.00 0.00 0.00 -0.01 -0.00 -0.00 -0.00 -0.00

10 6 0.01 0.00 0.00 0.01 0.04 0.00 0.01 0.04 0.00

11 6 0.01 -0.00 0.00 0.01 -0.04 0.00 0.01 -0.04 0.00

12 6 0.01 -0.01 -0.00 -0.02 0.01 0.00 0.03 -0.02 0.00

13 6 0.01 -0.00 0.00 0.00 -0.01 0.00 0.00 0.00 -0.00

14 6 -0.01 -0.00 0.00 0.01 0.04 -0.00 -0.01 -0.04 0.00

15 6 -0.01 0.00 0.00 0.01 -0.04 -0.00 -0.01 0.04 0.00

16 6 0.01 0.00 0.00 0.00 0.01 0.00 0.00 -0.00 -0.00

17 7 0.01 -0.00 -0.00 0.04 0.00 -0.00 -0.04 -0.00 0.00

18 6 0.01 0.01 -0.00 -0.02 -0.01 0.00 0.03 0.02 0.00

19 6 -0.00 -0.01 0.00 -0.01 -0.02 -0.00 0.01 0.01 0.00

20 6 0.05 0.01 0.00 -0.00 0.01 0.00 0.01 -0.03 -0.00

21 6 -0.05 0.01 0.00 -0.00 -0.01 -0.00 -0.01 -0.03 -0.00

22 6 0.00 -0.01 0.00 -0.01 0.02 0.00 -0.01 0.01 0.00

23 7 0.00 -0.06 -0.00 0.02 -0.00 -0.00 0.00 0.04 0.00

24 1 0.41 -0.28 0.01 0.07 -0.07 0.00 0.04 0.02 -0.00

25 1 -0.41 -0.28 0.01 0.07 0.07 -0.00 -0.04 0.02 -0.00

26 1 0.01 0.01 0.00 -0.27 0.41 -0.00 -0.27 0.41 -0.00

27 1 0.01 -0.01 0.00 -0.27 -0.41 -0.00 -0.27 -0.41 -0.00

28 1 -0.01 -0.01 0.00 -0.27 0.41 0.00 0.27 -0.41 -0.00

29 1 -0.01 0.01 0.00 -0.27 -0.41 0.00 0.27 0.41 -0.00

30 1 0.41 0.28 0.01 0.07 0.07 0.00 0.04 -0.02 -0.00

31 1 -0.41 0.28 0.01 0.07 -0.07 -0.00 -0.04 -0.02 -0.00

32 30 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

33 6 -0.01 0.01 -0.00 -0.02 0.01 -0.00 -0.03 0.02 0.00

34 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.01 -0.00 0.00

35 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.01 0.00 0.00

36 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00

37 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

38 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.01 0.00 0.00

39 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

40 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.01 -0.00 0.00

41 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00

42 1 0.00 0.00 0.00 -0.00 -0.01 0.00 -0.00 0.01 0.00

43 1 -0.00 0.00 0.00 -0.00 0.01 -0.00 0.00 0.01 0.00

44 1 -0.00 -0.00 0.00 -0.00 -0.01 -0.00 0.00 -0.01 0.00

45 1 0.00 -0.00 0.00 -0.00 0.01 0.00 -0.00 -0.01 0.00

88 89 90

A A A

Frequencies -- 1144.4619 1163.5477 1165.4876

Red. masses -- 6.8950 6.5013 5.9903

Frc consts -- 5.3209 5.1858 4.7942

IR Inten -- 0.1444 0.0035 15.7448

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 0.03 -0.00 -0.04 -0.04 0.00 -0.02 -0.00 0.00

2 6 0.07 0.03 -0.00 -0.09 -0.05 0.00 -0.06 0.03 -0.00

3 7 -0.00 -0.14 0.01 0.00 0.18 -0.01 0.16 -0.00 0.00

4 6 -0.07 0.03 -0.00 0.09 -0.05 0.00 -0.06 -0.03 0.00

5 6 -0.03 0.03 -0.00 0.04 -0.04 0.00 -0.02 0.00 -0.00

6 6 -0.19 0.20 -0.00 0.19 -0.15 0.00 -0.15 0.18 -0.00

7 6 -0.02 0.08 -0.00 -0.07 -0.03 -0.00 -0.04 0.10 -0.00

8 7 0.13 0.00 0.01 0.00 0.12 0.00 0.14 -0.00 0.01

9 6 -0.02 -0.08 -0.00 0.07 -0.03 0.00 -0.04 -0.10 -0.00

10 6 -0.04 -0.03 -0.00 -0.02 -0.03 -0.00 -0.03 -0.04 -0.00

11 6 -0.04 0.03 -0.00 0.02 -0.03 0.00 -0.03 0.04 -0.00

12 6 0.19 0.20 -0.00 -0.19 -0.15 0.00 -0.15 -0.18 0.00

13 6 0.02 0.08 -0.00 0.07 -0.03 -0.00 -0.04 -0.10 0.00

14 6 0.04 0.03 -0.00 -0.02 -0.03 0.00 -0.03 -0.04 0.00

15 6 0.04 -0.03 -0.00 0.02 -0.03 -0.00 -0.03 0.04 0.00

16 6 0.02 -0.08 -0.00 -0.07 -0.03 0.00 -0.04 0.10 0.00

17 7 -0.13 -0.00 0.01 0.00 0.12 -0.00 0.14 -0.00 -0.01

18 6 0.19 -0.20 -0.00 0.19 -0.15 -0.00 -0.15 0.18 0.00

19 6 0.07 -0.03 -0.00 0.09 -0.05 -0.00 -0.06 -0.03 -0.00

20 6 0.03 -0.03 -0.00 0.04 -0.04 -0.00 -0.02 0.00 0.00

21 6 -0.03 -0.03 -0.00 -0.04 -0.04 -0.00 -0.02 -0.00 -0.00

22 6 -0.07 -0.03 -0.00 -0.09 -0.05 -0.00 -0.06 0.03 0.00

23 7 0.00 0.14 0.01 0.00 0.18 0.01 0.16 -0.00 -0.00

24 1 0.14 -0.04 0.00 -0.07 -0.03 0.00 0.21 -0.19 0.01

25 1 -0.14 -0.04 0.00 0.07 -0.03 0.00 0.21 0.19 -0.01

26 1 0.12 -0.25 0.00 -0.23 0.23 -0.00 0.08 -0.19 0.00

27 1 0.12 0.25 0.00 0.23 0.23 0.00 0.08 0.19 0.00

28 1 -0.12 0.25 0.00 -0.23 0.23 0.00 0.08 -0.19 -0.00

29 1 -0.12 -0.25 0.00 0.23 0.23 -0.00 0.08 0.19 -0.00

30 1 0.14 0.04 0.00 0.07 -0.03 -0.00 0.21 0.19 0.01

31 1 -0.14 0.04 0.00 -0.07 -0.03 -0.00 0.21 -0.19 -0.01

32 30 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

33 6 -0.19 -0.20 -0.00 -0.19 -0.15 -0.00 -0.15 -0.18 -0.00

34 6 0.04 0.04 0.00 0.05 0.02 0.00 0.02 0.04 0.00

35 6 -0.04 -0.04 0.00 0.05 0.02 -0.00 0.02 0.04 -0.00

36 6 0.09 0.09 0.00 0.07 0.08 0.00 0.08 0.08 0.00

37 6 -0.09 -0.09 0.00 0.07 0.08 -0.00 0.08 0.08 -0.00

38 6 0.04 -0.04 0.00 -0.05 0.02 -0.00 0.02 -0.04 0.00

39 6 0.09 -0.09 0.00 -0.07 0.08 -0.00 0.08 -0.08 0.00

40 6 -0.04 0.04 0.00 -0.05 0.02 0.00 0.02 -0.04 -0.00

41 6 -0.09 0.09 0.00 -0.07 0.08 0.00 0.08 -0.08 -0.00

42 1 -0.11 0.11 0.00 -0.08 0.10 0.00 0.09 -0.09 -0.00

43 1 0.11 0.11 0.00 0.08 0.10 0.00 0.09 0.09 0.00

44 1 0.11 -0.11 0.00 -0.08 0.10 -0.00 0.09 -0.09 0.00

45 1 -0.11 -0.11 0.00 0.08 0.10 -0.00 0.09 0.09 -0.00

91 92 93

A A A

Frequencies -- 1191.4515 1234.6622 1239.1010

Red. masses -- 2.1987 5.0310 2.3863

Frc consts -- 1.8390 4.5186 2.1587

IR Inten -- 0.0000 0.0000 900.5009

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.01 0.00 0.01 -0.00 0.00 -0.02 0.03 -0.00

2 6 -0.02 0.08 -0.00 -0.02 -0.13 0.00 -0.04 0.11 -0.00

3 7 0.04 -0.00 0.00 0.17 0.00 0.00 -0.06 0.00 -0.00

4 6 -0.02 -0.08 0.00 -0.02 0.13 -0.00 -0.04 -0.11 0.00

5 6 -0.02 0.01 -0.00 0.01 0.00 -0.00 -0.02 -0.03 0.00

6 6 -0.08 0.06 -0.00 -0.15 0.14 -0.00 0.09 0.01 -0.00

7 6 0.08 0.03 0.00 -0.04 -0.04 -0.00 0.06 0.04 0.00

8 7 0.00 -0.04 -0.00 -0.00 -0.09 -0.00 -0.03 -0.00 -0.00

9 6 -0.08 0.03 -0.00 0.04 -0.04 0.00 0.06 -0.04 0.00

10 6 0.00 0.02 0.00 0.02 0.01 0.00 -0.03 -0.02 -0.00

11 6 -0.00 0.02 -0.00 -0.02 0.01 -0.00 -0.03 0.02 -0.00

12 6 -0.08 -0.06 0.00 -0.15 -0.14 0.00 0.09 -0.01 0.00

13 6 0.08 -0.03 -0.00 -0.04 0.04 0.00 0.06 -0.04 -0.00

14 6 -0.00 -0.02 0.00 -0.02 -0.01 0.00 -0.03 -0.02 0.00

15 6 0.00 -0.02 -0.00 0.02 -0.01 -0.00 -0.03 0.02 0.00

16 6 -0.08 -0.03 0.00 0.04 0.04 -0.00 0.06 0.04 -0.00

17 7 -0.00 0.04 -0.00 -0.00 0.09 -0.00 -0.03 -0.00 0.00

18 6 0.08 -0.06 -0.00 0.15 -0.14 -0.00 0.09 0.01 0.00

19 6 0.02 0.08 0.00 0.02 -0.13 -0.00 -0.04 -0.11 -0.00

20 6 0.02 -0.01 -0.00 -0.01 -0.00 -0.00 -0.02 -0.03 -0.00

21 6 0.02 0.01 0.00 -0.01 0.00 0.00 -0.02 0.03 0.00

22 6 0.02 -0.08 -0.00 0.02 0.13 0.00 -0.04 0.11 0.00

23 7 -0.04 -0.00 -0.00 -0.17 0.00 0.00 -0.06 0.00 0.00

24 1 0.27 -0.24 0.01 -0.29 0.23 -0.00 0.38 -0.27 0.01

25 1 0.27 0.24 -0.01 -0.29 -0.23 0.00 0.38 0.27 -0.01

26 1 0.20 -0.23 0.00 -0.06 0.12 0.00 -0.02 -0.05 -0.00

27 1 -0.20 -0.23 -0.00 0.06 0.12 -0.00 -0.02 0.05 -0.00

28 1 -0.20 0.23 0.00 0.06 -0.12 0.00 -0.02 -0.05 0.00

29 1 0.20 0.23 -0.00 -0.06 -0.12 -0.00 -0.02 0.05 0.00

30 1 -0.27 -0.24 -0.01 0.29 0.23 0.00 0.38 0.27 0.01

31 1 -0.27 0.24 0.01 0.29 -0.23 -0.00 0.38 -0.27 -0.01

32 30 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00

33 6 0.08 0.06 0.00 0.15 0.14 0.00 0.09 -0.01 -0.00

34 6 -0.01 -0.01 -0.00 -0.03 -0.01 -0.00 -0.01 0.00 -0.00

35 6 0.01 0.01 -0.00 0.03 0.01 -0.00 -0.01 0.00 0.00

36 6 -0.02 -0.03 -0.00 -0.05 -0.05 -0.00 -0.01 -0.01 -0.00

37 6 0.02 0.03 -0.00 0.05 0.05 -0.00 -0.01 -0.01 0.00

38 6 0.01 -0.01 0.00 0.03 -0.01 0.00 -0.01 -0.00 -0.00

39 6 0.02 -0.03 0.00 0.05 -0.05 0.00 -0.01 0.01 -0.00

40 6 -0.01 0.01 0.00 -0.03 0.01 0.00 -0.01 -0.00 0.00

41 6 -0.02 0.03 0.00 -0.05 0.05 0.00 -0.01 0.01 0.00

42 1 -0.03 0.03 0.00 -0.06 0.07 0.00 -0.01 0.02 0.00

43 1 -0.03 -0.03 -0.00 -0.06 -0.07 -0.00 -0.01 -0.02 -0.00

44 1 0.03 -0.03 0.00 0.06 -0.07 0.00 -0.01 0.02 -0.00

45 1 0.03 0.03 -0.00 0.06 0.07 -0.00 -0.01 -0.02 0.00

94 95 96

A A A

Frequencies -- 1240.0430 1274.4087 1306.2067

Red. masses -- 8.9079 2.9778 10.8890

Frc consts -- 8.0705 2.8495 10.9462

IR Inten -- 154.5134 0.4945 3968.7809

Atom AN X Y Z X Y Z X Y Z

1 6 0.02 -0.01 0.00 -0.02 -0.06 0.00 0.03 0.12 -0.00

2 6 0.03 0.02 -0.00 -0.04 0.10 -0.00 -0.31 -0.18 0.01

3 7 0.00 -0.05 0.00 0.00 -0.05 0.00 0.30 0.00 -0.00

4 6 -0.03 0.02 -0.00 0.04 0.10 -0.00 -0.31 0.18 -0.01

5 6 -0.02 -0.01 0.00 0.02 -0.06 0.00 0.03 -0.12 0.00

6 6 0.00 -0.02 -0.00 0.01 0.10 -0.00 0.11 -0.03 0.00

7 6 0.21 -0.24 0.00 -0.07 -0.09 -0.00 0.08 -0.04 0.00

8 7 -0.00 0.32 0.00 -0.00 -0.02 -0.00 -0.07 0.00 -0.00

9 6 -0.21 -0.24 -0.00 0.07 -0.09 0.00 0.08 0.04 0.00

10 6 0.10 0.05 0.00 0.07 -0.02 0.00 -0.04 -0.03 -0.00

11 6 -0.10 0.05 -0.00 -0.07 -0.02 -0.00 -0.04 0.03 -0.00

12 6 -0.00 -0.02 -0.00 -0.01 0.10 -0.00 0.11 0.03 -0.00

13 6 -0.21 -0.24 0.00 0.07 -0.09 -0.00 0.08 0.04 -0.00

14 6 0.10 0.05 -0.00 0.07 -0.02 -0.00 -0.04 -0.03 0.00

15 6 -0.10 0.05 0.00 -0.07 -0.02 0.00 -0.04 0.03 0.00

16 6 0.21 -0.24 -0.00 -0.07 -0.09 0.00 0.08 -0.04 -0.00

17 7 -0.00 0.32 -0.00 0.00 -0.02 -0.00 -0.07 -0.00 0.00

18 6 0.00 -0.02 0.00 0.01 0.10 0.00 0.11 -0.03 -0.00

19 6 -0.03 0.02 0.00 0.04 0.10 0.00 -0.31 0.18 0.01

20 6 -0.02 -0.01 -0.00 0.02 -0.06 -0.00 0.03 -0.12 -0.00

21 6 0.02 -0.01 -0.00 -0.02 -0.06 -0.00 0.03 0.12 0.00

22 6 0.03 0.02 0.00 -0.04 0.10 0.00 -0.31 -0.18 -0.01

23 7 -0.00 -0.05 -0.00 -0.00 -0.05 -0.00 0.30 -0.00 -0.00

24 1 0.00 0.01 0.00 -0.07 -0.04 0.00 0.04 0.12 -0.00

25 1 -0.00 0.01 0.00 0.07 -0.04 0.00 0.04 -0.12 0.00

26 1 0.25 -0.13 0.00 -0.23 0.38 -0.00 -0.12 0.06 -0.00

27 1 -0.25 -0.13 -0.00 0.23 0.38 0.00 -0.12 -0.06 -0.00

28 1 0.25 -0.13 -0.00 -0.23 0.38 0.00 -0.12 0.06 0.00

29 1 -0.25 -0.13 0.00 0.23 0.38 -0.00 -0.12 -0.06 0.00

30 1 -0.00 0.01 -0.00 0.07 -0.04 -0.00 0.04 -0.12 -0.00

31 1 0.00 0.01 -0.00 -0.07 -0.04 -0.00 0.04 0.12 0.00

32 30 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

33 6 -0.00 -0.02 0.00 -0.01 0.10 0.00 0.11 0.03 0.00

34 6 -0.02 0.01 0.00 -0.00 -0.01 -0.00 0.00 -0.02 -0.00

35 6 -0.02 0.01 -0.00 -0.00 -0.01 0.00 0.00 -0.02 0.00

36 6 0.03 0.02 0.00 -0.01 -0.01 -0.00 -0.01 -0.01 -0.00

37 6 0.03 0.02 -0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

38 6 0.02 0.01 -0.00 0.00 -0.01 0.00 0.00 0.02 -0.00

39 6 -0.03 0.02 -0.00 0.01 -0.01 0.00 -0.01 0.01 -0.00

40 6 0.02 0.01 0.00 0.00 -0.01 -0.00 0.00 0.02 0.00

41 6 -0.03 0.02 0.00 0.01 -0.01 -0.00 -0.01 0.01 0.00

42 1 -0.03 0.02 0.00 0.02 -0.00 -0.00 -0.01 0.01 0.00

43 1 0.03 0.02 0.00 -0.02 -0.00 -0.00 -0.01 -0.01 -0.00

44 1 -0.03 0.02 -0.00 0.02 -0.00 0.00 -0.01 0.01 -0.00

45 1 0.03 0.02 -0.00 -0.02 -0.00 0.00 -0.01 -0.01 0.00

97 98 99

A A A

Frequencies -- 1307.5162 1313.8076 1356.4104

Red. masses -- 2.6299 12.0669 12.1123

Frc consts -- 2.6490 12.2718 13.1298

IR Inten -- 0.0000 0.0021 1030.2151

Atom AN X Y Z X Y Z X Y Z

1 6 0.03 -0.03 0.00 -0.12 0.07 -0.00 -0.01 -0.03 0.00

2 6 -0.01 -0.06 0.00 -0.14 -0.21 0.01 0.06 0.00 -0.00

3 7 0.05 0.00 -0.00 -0.00 0.22 -0.01 0.04 0.00 -0.00

4 6 -0.01 0.06 -0.00 0.14 -0.21 0.01 0.06 -0.00 0.00

5 6 0.03 0.03 -0.00 0.12 0.07 -0.00 -0.01 0.03 -0.00

6 6 -0.05 -0.11 0.00 0.01 0.03 -0.00 -0.21 0.04 -0.00

7 6 0.08 0.00 0.00 -0.28 0.09 -0.01 0.35 -0.06 0.01

8 7 0.00 0.09 0.00 0.27 -0.00 0.01 -0.31 0.00 -0.01

9 6 -0.08 0.00 -0.00 -0.28 -0.09 -0.01 0.35 0.06 0.01

10 6 -0.05 0.03 -0.00 0.08 -0.05 0.00 -0.09 0.11 -0.00

11 6 0.05 0.03 0.00 0.08 0.05 0.00 -0.09 -0.11 -0.00

12 6 -0.05 0.11 -0.00 -0.01 0.03 -0.00 -0.21 -0.04 0.00

13 6 0.08 -0.00 -0.00 0.28 0.09 -0.01 0.35 0.06 -0.01

14 6 0.05 -0.03 -0.00 -0.08 0.05 0.00 -0.09 0.11 0.00

15 6 -0.05 -0.03 0.00 -0.08 -0.05 0.00 -0.09 -0.11 0.00

16 6 -0.08 -0.00 0.00 0.28 -0.09 -0.01 0.35 -0.06 -0.01

17 7 0.00 -0.09 -0.00 -0.27 0.00 0.01 -0.31 0.00 0.01

18 6 0.05 0.11 0.00 -0.01 -0.03 -0.00 -0.21 0.04 0.00

19 6 0.01 -0.06 -0.00 -0.14 0.21 0.01 0.06 -0.00 -0.00

20 6 -0.03 -0.03 -0.00 -0.12 -0.07 -0.00 -0.01 0.03 0.00

21 6 -0.03 0.03 0.00 0.12 -0.07 -0.00 -0.01 -0.03 -0.00

22 6 0.01 0.06 0.00 0.14 0.21 0.01 0.06 0.00 0.00

23 7 -0.05 -0.00 -0.00 -0.00 -0.22 -0.01 0.04 0.00 -0.00

24 1 -0.21 0.15 -0.00 0.03 -0.05 -0.00 -0.04 -0.00 0.00

25 1 -0.21 -0.15 0.00 -0.03 -0.05 -0.00 -0.04 0.00 -0.00

26 1 0.21 -0.32 0.00 0.07 -0.03 0.00 0.01 -0.03 -0.00

27 1 -0.21 -0.32 -0.00 0.07 0.03 0.00 0.01 0.03 -0.00

28 1 -0.21 0.32 0.00 -0.07 0.03 0.00 0.01 -0.03 0.00

29 1 0.21 0.32 -0.00 -0.07 -0.03 0.00 0.01 0.03 0.00

30 1 0.21 0.15 0.00 0.03 0.05 -0.00 -0.04 0.00 0.00

31 1 0.21 -0.15 -0.00 -0.03 0.05 -0.00 -0.04 -0.00 -0.00

32 30 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00

33 6 0.05 -0.11 -0.00 0.01 -0.03 -0.00 -0.21 -0.04 -0.00

34 6 -0.01 0.02 0.00 -0.02 0.03 0.00 0.03 -0.01 0.00

35 6 0.01 -0.02 0.00 0.02 -0.03 0.00 0.03 -0.01 -0.00

36 6 0.01 0.01 0.00 0.00 0.00 0.00 0.03 0.03 0.00

37 6 -0.01 -0.01 0.00 -0.00 -0.00 0.00 0.03 0.03 -0.00

38 6 0.01 0.02 -0.00 -0.02 -0.03 0.00 0.03 0.01 0.00

39 6 -0.01 0.01 -0.00 0.00 -0.00 0.00 0.03 -0.03 0.00

40 6 -0.01 -0.02 -0.00 0.02 0.03 0.00 0.03 0.01 -0.00

41 6 0.01 -0.01 -0.00 -0.00 0.00 0.00 0.03 -0.03 -0.00

42 1 0.02 -0.00 -0.00 -0.01 -0.01 -0.00 0.02 -0.05 -0.00

43 1 0.02 0.00 0.00 0.01 -0.01 -0.00 0.02 0.05 0.00

44 1 -0.02 0.00 -0.00 0.01 0.01 -0.00 0.02 -0.05 0.00

45 1 -0.02 -0.00 0.00 -0.01 0.01 -0.00 0.02 0.05 -0.00

100 101 102

A A A

Frequencies -- 1364.8574 1389.3084 1417.5063

Red. masses -- 8.8145 10.8077 3.3526

Frc consts -- 9.6743 12.2908 3.9690

IR Inten -- 836.8652 0.1285 35.9776

Atom AN X Y Z X Y Z X Y Z

1 6 0.20 -0.09 0.00 -0.02 -0.14 0.00 0.09 0.03 -0.00

2 6 0.07 0.23 -0.01 -0.08 0.31 -0.01 0.08 -0.07 0.00

3 7 0.00 -0.21 0.01 0.00 -0.17 0.01 -0.00 0.01 -0.00

4 6 -0.07 0.23 -0.01 0.08 0.31 -0.01 -0.08 -0.07 0.00

5 6 -0.20 -0.09 0.00 0.02 -0.14 0.00 -0.09 0.03 -0.00

6 6 0.08 -0.16 0.00 0.04 -0.03 0.00 0.04 -0.00 -0.00

7 6 -0.03 0.07 -0.00 -0.23 -0.10 -0.00 0.08 0.07 0.00

8 7 -0.00 0.02 0.00 0.13 -0.00 0.00 -0.00 -0.02 -0.00

9 6 0.03 0.07 0.00 -0.23 0.10 -0.00 -0.08 0.07 -0.00

10 6 -0.05 -0.00 -0.00 0.08 0.02 0.00 0.12 -0.06 0.00

11 6 0.05 -0.00 0.00 0.08 -0.02 0.00 -0.12 -0.06 -0.00

12 6 -0.08 -0.16 0.00 -0.04 -0.03 0.00 -0.04 -0.00 -0.00

13 6 0.03 0.07 -0.00 0.23 -0.10 -0.00 -0.08 0.07 0.00

14 6 -0.05 -0.00 0.00 -0.08 -0.02 0.00 0.12 -0.06 -0.00

15 6 0.05 -0.00 -0.00 -0.08 0.02 0.00 -0.12 -0.06 0.00

16 6 -0.03 0.07 0.00 0.23 0.10 -0.00 0.08 0.07 -0.00

17 7 -0.00 0.02 0.00 -0.13 -0.00 0.00 0.00 -0.02 -0.00

18 6 0.08 -0.16 -0.00 -0.04 0.03 0.00 0.04 -0.00 0.00

19 6 -0.07 0.23 0.01 -0.08 -0.31 -0.01 -0.08 -0.07 -0.00

20 6 -0.20 -0.09 -0.00 -0.02 0.14 0.00 -0.09 0.03 0.00

21 6 0.20 -0.09 -0.00 0.02 0.14 0.00 0.09 0.03 0.00

22 6 0.07 0.23 0.01 0.08 -0.31 -0.01 0.08 -0.07 -0.00

23 7 0.00 -0.21 -0.01 0.00 0.17 0.01 0.00 0.01 0.00

24 1 -0.15 0.19 -0.00 -0.08 -0.12 0.00 -0.00 0.12 -0.00

25 1 0.15 0.19 -0.00 0.08 -0.12 0.00 0.00 0.12 -0.00

26 1 0.03 -0.12 0.00 0.07 0.07 0.00 -0.20 0.37 -0.00

27 1 -0.03 -0.12 -0.00 0.07 -0.07 0.00 0.20 0.37 0.00

28 1 0.03 -0.12 -0.00 -0.07 -0.07 0.00 -0.20 0.37 0.00

29 1 -0.03 -0.12 0.00 -0.07 0.07 0.00 0.20 0.37 -0.00

30 1 0.15 0.19 0.00 -0.08 0.12 0.00 0.00 0.12 0.00

31 1 -0.15 0.19 0.00 0.08 0.12 0.00 -0.00 0.12 0.00

32 30 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

33 6 -0.08 -0.16 -0.00 0.04 0.03 0.00 -0.04 -0.00 0.00

34 6 -0.00 0.02 0.00 0.00 0.00 -0.00 0.01 0.00 0.00

35 6 -0.00 0.02 -0.00 -0.00 -0.00 -0.00 0.01 0.00 -0.00

36 6 0.03 0.03 0.00 -0.01 -0.01 -0.00 -0.00 0.00 0.00

37 6 0.03 0.03 -0.00 0.01 0.01 -0.00 -0.00 0.00 -0.00

38 6 0.00 0.02 -0.00 0.00 -0.00 -0.00 -0.01 0.00 -0.00

39 6 -0.03 0.03 -0.00 -0.01 0.01 -0.00 0.00 0.00 -0.00

40 6 0.00 0.02 0.00 -0.00 0.00 -0.00 -0.01 0.00 0.00

41 6 -0.03 0.03 0.00 0.01 -0.01 -0.00 0.00 0.00 0.00

42 1 -0.04 0.03 0.00 0.01 -0.01 -0.00 0.00 0.00 0.00

43 1 0.04 0.03 0.00 -0.01 -0.01 -0.00 -0.00 0.00 0.00

44 1 -0.04 0.03 -0.00 -0.01 0.01 -0.00 0.00 0.00 -0.00

45 1 0.04 0.03 -0.00 0.01 0.01 -0.00 -0.00 0.00 -0.00

103 104 105

A A A

Frequencies -- 1423.9147 1429.5248 1454.7620

Red. masses -- 7.1471 3.5236 3.4461

Frc consts -- 8.5379 4.2425 4.2969

IR Inten -- 0.0751 0.0000 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 0.27 -0.00 -0.00 -0.01 0.03 -0.00 -0.07 0.16 -0.00

2 6 0.12 -0.02 0.00 0.00 -0.04 0.00 0.06 -0.13 0.00

3 7 -0.00 -0.04 0.00 0.03 -0.00 0.00 0.00 -0.00 0.00

4 6 -0.12 -0.02 0.00 0.00 0.04 -0.00 0.06 0.13 -0.00

5 6 -0.27 -0.00 -0.00 -0.01 -0.03 0.00 -0.07 -0.16 0.00

6 6 0.12 -0.05 0.00 -0.04 -0.06 0.00 -0.01 -0.02 0.00

7 6 -0.08 0.12 -0.00 0.14 0.07 0.00 -0.03 -0.03 -0.00

8 7 0.09 -0.00 0.00 0.00 0.03 0.00 -0.00 0.02 -0.00

9 6 -0.08 -0.12 -0.00 -0.14 0.07 -0.00 0.03 -0.03 0.00

10 6 0.01 -0.08 0.00 0.14 -0.07 0.00 -0.04 0.02 -0.00

11 6 0.01 0.08 0.00 -0.14 -0.07 -0.00 0.04 0.02 0.00

12 6 -0.12 -0.05 0.00 -0.04 0.06 -0.00 -0.01 0.02 -0.00

13 6 0.08 0.12 -0.00 0.14 -0.07 -0.00 -0.03 0.03 0.00

14 6 -0.01 0.08 0.00 -0.14 0.07 0.00 0.04 -0.02 -0.00

15 6 -0.01 -0.08 0.00 0.14 0.07 -0.00 -0.04 -0.02 0.00

16 6 0.08 -0.12 -0.00 -0.14 -0.07 0.00 0.03 0.03 -0.00

17 7 -0.09 -0.00 0.00 -0.00 -0.03 0.00 -0.00 -0.02 0.00

18 6 -0.12 0.05 0.00 0.04 0.06 0.00 0.01 0.02 0.00

19 6 0.12 0.02 0.00 -0.00 -0.04 -0.00 -0.06 -0.13 -0.00

20 6 0.27 0.00 -0.00 0.01 0.03 0.00 0.07 0.16 0.00

21 6 -0.27 0.00 -0.00 0.01 -0.03 -0.00 0.07 -0.16 -0.00

22 6 -0.12 0.02 0.00 -0.00 0.04 0.00 -0.06 0.13 0.00

23 7 0.00 0.04 0.00 -0.03 0.00 0.00 -0.00 -0.00 -0.00

24 1 -0.10 0.31 -0.01 0.08 -0.03 0.00 0.39 -0.17 0.00

25 1 0.10 0.31 -0.01 0.08 0.03 -0.00 0.39 0.17 -0.00

26 1 -0.02 -0.05 0.00 -0.19 0.39 -0.00 0.06 -0.11 0.00

27 1 -0.02 0.05 0.00 0.19 0.39 0.00 -0.06 -0.11 -0.00

28 1 0.02 0.05 0.00 0.19 -0.39 -0.00 -0.06 0.11 0.00

29 1 0.02 -0.05 0.00 -0.19 -0.39 0.00 0.06 0.11 -0.00

30 1 -0.10 -0.31 -0.01 -0.08 -0.03 -0.00 -0.39 -0.17 -0.00

31 1 0.10 -0.31 -0.01 -0.08 0.03 0.00 -0.39 0.17 0.00

32 30 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

33 6 0.12 0.05 0.00 0.04 -0.06 -0.00 0.01 -0.02 -0.00

34 6 -0.01 0.00 -0.00 -0.00 0.01 0.00 -0.01 0.00 0.00

35 6 0.01 -0.00 -0.00 0.00 -0.01 0.00 0.01 -0.00 0.00

36 6 -0.02 -0.02 -0.00 0.00 -0.00 0.00 0.01 0.00 0.00

37 6 0.02 0.02 -0.00 -0.00 0.00 0.00 -0.01 -0.00 0.00

38 6 -0.01 -0.00 -0.00 0.00 0.01 -0.00 0.01 0.00 -0.00

39 6 -0.02 0.02 -0.00 -0.00 -0.00 -0.00 -0.01 0.00 -0.00

40 6 0.01 0.00 -0.00 -0.00 -0.01 -0.00 -0.01 -0.00 -0.00

41 6 0.02 -0.02 -0.00 0.00 0.00 -0.00 0.01 -0.00 -0.00

42 1 0.02 -0.03 -0.00 0.01 0.01 0.00 0.01 -0.01 -0.00

43 1 -0.02 -0.03 -0.00 0.01 -0.01 -0.00 0.01 0.01 0.00

44 1 -0.02 0.03 -0.00 -0.01 -0.01 0.00 -0.01 0.01 -0.00

45 1 0.02 0.03 -0.00 -0.01 0.01 -0.00 -0.01 -0.01 0.00

106 107 108

A A A

Frequencies -- 1455.6817 1477.7512 1503.3582

Red. masses -- 3.5722 5.1828 5.9226

Frc consts -- 4.4598 6.6683 7.8866

IR Inten -- 337.5942 206.4320 0.0533

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 0.15 -0.00 0.22 0.00 -0.00 -0.18 0.03 -0.00

2 6 0.09 -0.12 0.00 -0.07 -0.10 0.00 0.19 0.03 -0.00

3 7 -0.02 0.00 -0.00 -0.00 0.07 -0.00 0.00 -0.06 0.00

4 6 0.09 0.12 -0.00 0.07 -0.10 0.00 -0.19 0.03 -0.00

5 6 -0.07 -0.15 0.00 -0.22 0.00 -0.00 0.18 0.03 -0.00

6 6 -0.02 0.02 -0.00 0.03 0.11 -0.00 0.07 -0.06 0.00

7 6 -0.03 -0.06 -0.00 -0.07 -0.09 -0.00 0.00 0.05 -0.00

8 7 0.00 0.00 0.00 0.00 -0.00 -0.00 0.03 -0.00 0.00

9 6 -0.03 0.06 -0.00 0.07 -0.09 0.00 0.00 -0.05 -0.00

10 6 0.01 0.05 0.00 -0.05 0.04 -0.00 0.01 -0.17 -0.00

11 6 0.01 -0.05 0.00 0.05 0.04 0.00 0.01 0.17 -0.00

12 6 -0.02 -0.02 0.00 -0.03 0.11 -0.00 -0.07 -0.06 0.00

13 6 -0.03 0.06 0.00 0.07 -0.09 -0.00 -0.00 0.05 -0.00

14 6 0.01 0.05 -0.00 -0.05 0.04 0.00 -0.01 0.17 -0.00

15 6 0.01 -0.05 -0.00 0.05 0.04 -0.00 -0.01 -0.17 -0.00

16 6 -0.03 -0.06 0.00 -0.07 -0.09 0.00 -0.00 -0.05 -0.00

17 7 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.03 0.00 0.00

18 6 -0.02 0.02 0.00 0.03 0.11 0.00 -0.07 0.06 0.00

19 6 0.09 0.12 0.00 0.07 -0.10 -0.00 0.19 -0.03 -0.00

20 6 -0.07 -0.15 -0.00 -0.22 0.00 0.00 -0.18 -0.03 -0.00

21 6 -0.07 0.15 0.00 0.22 0.00 0.00 0.18 -0.03 -0.00

22 6 0.09 -0.12 -0.00 -0.07 -0.10 -0.00 -0.19 -0.03 -0.00

23 7 -0.02 0.00 0.00 0.00 0.07 0.00 0.00 0.06 0.00

24 1 0.39 -0.19 0.00 -0.15 0.32 -0.01 0.19 -0.27 0.01

25 1 0.39 0.19 -0.00 0.15 0.32 -0.01 -0.19 -0.27 0.01

26 1 0.05 0.02 0.00 0.08 -0.15 0.00 -0.17 0.03 -0.00

27 1 0.05 -0.02 0.00 -0.08 -0.15 -0.00 -0.17 -0.03 -0.00

28 1 0.05 0.02 -0.00 0.08 -0.15 -0.00 0.17 -0.03 -0.00

29 1 0.05 -0.02 -0.00 -0.08 -0.15 0.00 0.17 0.03 -0.00

30 1 0.39 0.19 0.00 0.15 0.32 0.01 0.19 0.27 0.01

31 1 0.39 -0.19 -0.00 -0.15 0.32 0.01 -0.19 0.27 0.01

32 30 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

33 6 -0.02 -0.02 -0.00 -0.03 0.11 0.00 0.07 0.06 0.00

34 6 0.00 0.00 -0.00 0.00 -0.01 -0.00 -0.00 -0.00 -0.00

35 6 0.00 0.00 0.00 0.00 -0.01 0.00 0.00 0.00 -0.00

36 6 -0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.01 -0.01 -0.00

37 6 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.01 0.01 -0.00

38 6 0.00 -0.00 -0.00 -0.00 -0.01 0.00 -0.00 0.00 -0.00

39 6 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.01 0.01 -0.00

40 6 0.00 -0.00 0.00 -0.00 -0.01 -0.00 0.00 -0.00 -0.00

41 6 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.01 -0.01 -0.00

42 1 -0.00 -0.00 -0.00 0.01 0.00 -0.00 0.02 -0.02 -0.00

43 1 -0.00 0.00 0.00 -0.01 0.00 -0.00 -0.02 -0.02 -0.00

44 1 -0.00 -0.00 0.00 0.01 0.00 0.00 -0.02 0.02 -0.00

45 1 -0.00 0.00 -0.00 -0.01 0.00 0.00 0.02 0.02 -0.00

109 110 111

A A A

Frequencies -- 1508.3031 1543.0835 1548.8656

Red. masses -- 8.6532 10.0110 5.7963

Frc consts -- 11.5986 14.0445 8.1928

IR Inten -- 935.1549 711.6911 123.9044

Atom AN X Y Z X Y Z X Y Z

1 6 -0.06 0.04 -0.00 0.02 -0.06 0.00 0.01 -0.00 -0.00

2 6 0.30 -0.04 -0.00 -0.07 0.09 -0.00 -0.03 -0.01 0.00

3 7 0.00 -0.05 0.00 0.00 0.00 0.00 0.02 0.00 -0.00

4 6 -0.30 -0.04 -0.00 -0.07 -0.09 0.00 -0.03 0.01 -0.00

5 6 0.06 0.04 -0.00 0.02 0.06 -0.00 0.01 0.00 0.00

6 6 0.20 0.11 0.00 0.11 0.23 -0.00 0.02 -0.07 0.00

7 6 -0.11 -0.08 -0.00 -0.08 -0.27 -0.00 -0.02 0.17 -0.00

8 7 0.00 -0.01 0.00 -0.02 -0.00 -0.00 0.03 -0.00 0.00

9 6 0.11 -0.08 0.00 -0.08 0.27 -0.00 -0.02 -0.17 -0.00

10 6 -0.06 0.03 -0.00 0.01 0.20 0.00 -0.02 0.27 -0.00

11 6 0.06 0.03 0.00 0.01 -0.20 0.00 -0.02 -0.27 -0.00

12 6 -0.20 0.11 0.00 0.11 -0.23 0.00 0.02 0.07 -0.00

13 6 0.11 -0.08 -0.00 -0.08 0.27 0.00 -0.02 -0.17 0.00

14 6 -0.06 0.03 0.00 0.01 0.20 -0.00 -0.02 0.27 0.00

15 6 0.06 0.03 -0.00 0.01 -0.20 -0.00 -0.02 -0.27 0.00

16 6 -0.11 -0.08 0.00 -0.08 -0.27 0.00 -0.02 0.17 0.00

17 7 -0.00 -0.01 0.00 -0.02 0.00 0.00 0.03 -0.00 -0.00

18 6 0.20 0.11 -0.00 0.11 0.23 0.00 0.02 -0.07 -0.00

19 6 -0.30 -0.04 0.00 -0.07 -0.09 -0.00 -0.03 0.01 0.00

20 6 0.06 0.04 0.00 0.02 0.06 0.00 0.01 0.00 -0.00

21 6 -0.06 0.04 0.00 0.02 -0.06 -0.00 0.01 -0.00 0.00

22 6 0.30 -0.04 0.00 -0.07 0.09 0.00 -0.03 -0.01 -0.00

23 7 0.00 -0.05 -0.00 0.00 0.00 0.00 0.02 -0.00 -0.00

24 1 0.18 -0.14 0.00 -0.11 0.04 -0.00 -0.01 0.02 -0.00

25 1 -0.18 -0.14 0.00 -0.11 -0.04 0.00 -0.01 -0.02 0.00

26 1 0.06 -0.13 0.00 0.16 0.07 0.00 0.34 -0.15 0.01

27 1 -0.06 -0.13 -0.00 0.16 -0.07 0.00 0.34 0.15 0.01

28 1 0.06 -0.13 -0.00 0.16 0.07 -0.00 0.34 -0.15 -0.01

29 1 -0.06 -0.13 0.00 0.16 -0.07 -0.00 0.34 0.15 -0.01

30 1 -0.18 -0.14 -0.00 -0.11 -0.04 -0.00 -0.01 -0.02 -0.00

31 1 0.18 -0.14 -0.00 -0.11 0.04 0.00 -0.01 0.02 0.00

32 30 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00

33 6 -0.20 0.11 -0.00 0.11 -0.23 -0.00 0.02 0.07 0.00

34 6 0.01 -0.01 -0.00 -0.01 0.01 0.00 -0.00 -0.00 -0.00

35 6 0.01 -0.01 0.00 -0.01 0.01 -0.00 -0.00 -0.00 0.00

36 6 0.01 0.01 0.00 0.01 0.01 0.00 -0.00 -0.00 -0.00

37 6 0.01 0.01 -0.00 0.01 0.01 -0.00 -0.00 -0.00 0.00

38 6 -0.01 -0.01 0.00 -0.01 -0.01 0.00 -0.00 0.00 -0.00

39 6 -0.01 0.01 -0.00 0.01 -0.01 0.00 -0.00 0.00 -0.00

40 6 -0.01 -0.01 -0.00 -0.01 -0.01 -0.00 -0.00 0.00 0.00

41 6 -0.01 0.01 0.00 0.01 -0.01 -0.00 -0.00 0.00 0.00

42 1 0.00 0.02 0.00 0.03 -0.00 -0.00 -0.01 0.00 0.00

43 1 -0.00 0.02 0.00 0.03 0.00 0.00 -0.01 -0.00 -0.00

44 1 0.00 0.02 -0.00 0.03 -0.00 0.00 -0.01 0.00 -0.00

45 1 -0.00 0.02 -0.00 0.03 0.00 -0.00 -0.01 -0.00 0.00

112 113 114

A A A

Frequencies -- 1558.5379 1568.4309 2135.0089

Red. masses -- 5.9331 11.0681 6.1595

Frc consts -- 8.4912 16.0419 16.5421

IR Inten -- 0.0050 0.0065 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.07 0.02 -0.00 -0.03 -0.03 0.00 0.00 -0.00 -0.00

2 6 0.12 -0.00 -0.00 -0.16 0.10 -0.00 -0.03 -0.00 0.00

3 7 0.00 -0.03 0.00 -0.00 -0.02 0.00 0.02 -0.00 0.00

4 6 -0.12 -0.00 -0.00 0.16 0.10 -0.00 -0.03 0.00 -0.00

5 6 0.07 0.02 -0.00 0.03 -0.03 0.00 0.00 0.00 0.00

6 6 0.07 -0.02 0.00 -0.16 -0.25 0.00 -0.02 0.02 -0.00

7 6 -0.04 0.10 -0.00 0.08 0.31 -0.00 -0.00 0.03 -0.00

8 7 0.03 -0.00 0.00 0.01 0.00 0.00 0.00 -0.02 -0.00

9 6 -0.04 -0.10 -0.00 0.08 -0.31 -0.00 0.00 0.03 0.00

10 6 -0.02 0.27 -0.00 -0.03 -0.02 -0.00 -0.00 -0.00 -0.00

11 6 -0.02 -0.27 -0.00 -0.03 0.02 -0.00 0.00 -0.00 0.00

12 6 -0.07 -0.02 0.00 0.16 -0.25 0.00 -0.02 -0.02 0.00

13 6 0.04 0.10 -0.00 -0.08 0.31 -0.00 -0.00 -0.03 0.00

14 6 0.02 -0.27 -0.00 0.03 0.02 -0.00 0.00 0.00 -0.00

15 6 0.02 0.27 -0.00 0.03 -0.02 -0.00 -0.00 0.00 0.00

16 6 0.04 -0.10 -0.00 -0.08 -0.31 -0.00 0.00 -0.03 -0.00

17 7 -0.03 -0.00 0.00 -0.01 -0.00 0.00 0.00 0.02 -0.00

18 6 -0.07 0.02 0.00 0.16 0.25 0.00 0.02 -0.02 -0.00

19 6 0.12 0.00 -0.00 -0.16 -0.10 -0.00 0.03 -0.00 -0.00

20 6 -0.07 -0.02 -0.00 -0.03 0.03 0.00 -0.00 -0.00 0.00

21 6 0.07 -0.02 -0.00 0.03 0.03 0.00 -0.00 0.00 -0.00

22 6 -0.12 0.00 -0.00 0.16 -0.10 -0.00 0.03 0.00 0.00

23 7 0.00 0.03 0.00 0.00 0.02 0.00 -0.02 0.00 -0.00

24 1 0.08 -0.10 0.00 -0.05 -0.03 0.00 -0.00 0.00 -0.00

25 1 -0.08 -0.10 0.00 0.05 -0.03 0.00 -0.00 -0.00 0.00

26 1 0.33 -0.12 0.00 0.03 -0.13 0.00 -0.00 0.00 -0.00

27 1 0.33 0.12 0.00 0.03 0.13 0.00 0.00 0.00 0.00

28 1 -0.33 0.12 0.00 -0.03 0.13 0.00 0.00 -0.00 -0.00

29 1 -0.33 -0.12 0.00 -0.03 -0.13 0.00 -0.00 -0.00 0.00

30 1 0.08 0.10 0.00 -0.05 0.03 0.00 0.00 0.00 0.00

31 1 -0.08 0.10 0.00 0.05 0.03 0.00 0.00 -0.00 -0.00

32 30 -0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

33 6 0.07 0.02 0.00 -0.16 0.25 0.00 0.02 0.02 0.00

34 6 -0.00 0.00 0.00 0.01 -0.02 -0.00 -0.19 -0.20 -0.00

35 6 0.00 -0.00 0.00 -0.01 0.02 -0.00 0.19 0.20 -0.00

36 6 -0.01 -0.01 -0.00 -0.01 -0.00 -0.00 0.14 0.14 0.00

37 6 0.01 0.01 -0.00 0.01 0.00 -0.00 -0.14 -0.14 0.00

38 6 -0.00 -0.00 0.00 0.01 0.02 -0.00 0.19 -0.20 0.00

39 6 -0.01 0.01 -0.00 -0.01 0.00 -0.00 -0.14 0.14 -0.00

40 6 0.00 0.00 0.00 -0.01 -0.02 -0.00 -0.19 0.20 0.00

41 6 0.01 -0.01 -0.00 0.01 -0.00 -0.00 0.14 -0.14 -0.00

42 1 0.01 -0.01 -0.00 0.02 0.01 -0.00 0.25 -0.26 -0.00

43 1 -0.01 -0.01 -0.00 -0.02 0.01 -0.00 0.25 0.26 0.00

44 1 -0.01 0.01 -0.00 -0.02 -0.01 -0.00 -0.25 0.26 -0.00

45 1 0.01 0.01 -0.00 0.02 -0.01 -0.00 -0.25 -0.26 0.00

115 116 117

A A A

Frequencies -- 2150.1099 2157.5165 2162.9574

Red. masses -- 6.1067 6.0715 6.0828

Frc consts -- 16.6333 16.6516 16.7667

IR Inten -- 138.1393 375.7234 0.0015

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

2 6 -0.01 0.00 -0.00 -0.01 0.00 -0.00 -0.00 0.00 -0.00

3 7 -0.00 -0.00 0.00 0.01 -0.00 -0.00 0.00 0.00 -0.00

4 6 0.01 0.00 -0.00 -0.01 -0.00 0.00 0.00 0.00 -0.00

5 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

6 6 0.03 -0.02 0.00 -0.03 0.03 -0.00 0.04 -0.03 0.00

7 6 0.00 -0.02 0.00 0.00 0.01 0.00 -0.00 -0.01 0.00

8 7 -0.00 0.02 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

9 6 -0.00 -0.02 -0.00 0.00 -0.01 0.00 -0.00 0.01 0.00

10 6 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

11 6 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

12 6 -0.03 -0.02 0.00 -0.03 -0.03 0.00 -0.04 -0.03 0.00

13 6 -0.00 -0.02 0.00 0.00 -0.01 -0.00 0.00 -0.01 0.00

14 6 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

15 6 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

16 6 0.00 -0.02 -0.00 0.00 0.01 -0.00 0.00 0.01 0.00

17 7 -0.00 0.02 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

18 6 0.03 -0.02 -0.00 -0.03 0.03 0.00 -0.04 0.03 0.00

19 6 0.01 0.00 0.00 -0.01 -0.00 -0.00 -0.00 -0.00 -0.00

20 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00

21 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00

22 6 -0.01 0.00 0.00 -0.01 0.00 0.00 0.00 -0.00 -0.00

23 7 -0.00 -0.00 -0.00 0.01 -0.00 -0.00 -0.00 -0.00 -0.00

24 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00

25 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

26 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

27 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

28 1 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

29 1 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

30 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00

31 1 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 -0.00

32 30 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00

33 6 -0.03 -0.02 -0.00 -0.03 -0.03 -0.00 0.04 0.03 0.00

34 6 0.19 0.20 0.00 0.19 0.20 0.00 -0.19 -0.20 -0.00

35 6 0.19 0.20 -0.00 0.19 0.20 -0.00 0.19 0.20 -0.00

36 6 -0.14 -0.14 -0.00 -0.14 -0.14 -0.00 0.13 0.14 0.00

37 6 -0.14 -0.14 0.00 -0.14 -0.14 0.00 -0.13 -0.14 0.00

38 6 -0.19 0.20 -0.00 0.19 -0.20 0.00 -0.19 0.20 -0.00

39 6 0.14 -0.14 0.00 -0.14 0.14 -0.00 0.13 -0.14 0.00

40 6 -0.19 0.20 0.00 0.19 -0.20 -0.00 0.19 -0.20 -0.00

41 6 0.14 -0.14 -0.00 -0.14 0.14 0.00 -0.13 0.14 0.00

42 1 0.25 -0.26 -0.00 -0.26 0.26 0.00 -0.26 0.26 0.00

43 1 -0.25 -0.26 -0.00 -0.26 -0.26 -0.00 0.26 0.26 0.00

44 1 0.25 -0.26 0.00 -0.26 0.26 -0.00 0.26 -0.26 0.00

45 1 -0.25 -0.26 0.00 -0.26 -0.26 0.00 -0.26 -0.26 0.00

118 119 120

A A A

Frequencies -- 3237.0549 3237.0761 3243.6584

Red. masses -- 1.0908 1.0908 1.0904

Frc consts -- 6.7345 6.7347 6.7597

IR Inten -- 0.0000 6.3882 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.02 -0.04 0.00 0.02 0.04 -0.00 0.00 0.00 -0.00

2 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

3 7 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

4 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

5 6 -0.02 0.04 -0.00 0.02 -0.04 0.00 0.00 -0.00 0.00

6 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

7 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00

8 7 -0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

9 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00

10 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.04 -0.03 -0.00

11 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.04 -0.03 0.00

12 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00

13 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00

14 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.04 0.03 -0.00

15 6 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.04 0.03 0.00

16 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00

17 7 -0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

18 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00

19 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

20 6 0.02 -0.04 -0.00 0.02 -0.04 -0.00 -0.00 0.00 0.00

21 6 0.02 0.04 0.00 0.02 0.04 0.00 -0.00 -0.00 -0.00

22 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

23 7 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00

24 1 0.30 0.40 -0.01 -0.30 -0.40 0.01 -0.01 -0.01 0.00

25 1 0.30 -0.40 0.01 -0.30 0.40 -0.01 -0.01 0.01 -0.00

26 1 0.01 0.01 0.00 0.00 0.00 0.00 0.40 0.30 0.01

27 1 -0.01 0.01 -0.00 0.00 -0.00 0.00 -0.40 0.30 -0.01

28 1 -0.01 -0.01 0.00 0.00 0.00 -0.00 -0.40 -0.30 0.01

29 1 0.01 -0.01 -0.00 0.00 -0.00 -0.00 0.40 -0.30 -0.01

30 1 -0.30 0.40 0.01 -0.30 0.40 0.01 0.01 -0.01 -0.00

31 1 -0.30 -0.40 -0.01 -0.30 -0.40 -0.01 0.01 0.01 0.00

32 30 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00

33 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

34 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00

35 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00

36 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

37 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00

38 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00

39 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00

40 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

41 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00

42 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

43 1 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00

44 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

45 1 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

121 122 123

A A A

Frequencies -- 3243.7060 3252.0583 3252.1019

Red. masses -- 1.0905 1.1020 1.1020

Frc consts -- 6.7601 6.8666 6.8666

IR Inten -- 0.0157 30.9724 0.0043

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 0.00 -0.00 -0.03 -0.04 0.00 -0.03 -0.04 0.00

2 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

3 7 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

4 6 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

5 6 -0.00 0.00 -0.00 0.03 -0.04 0.00 0.03 -0.04 0.00

6 6 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

7 6 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

8 7 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 0.00

9 6 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

10 6 -0.04 -0.03 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

11 6 0.04 -0.03 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

12 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

13 6 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

14 6 -0.04 -0.03 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

15 6 0.04 -0.03 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

16 6 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

17 7 0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 0.00

18 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

19 6 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

20 6 -0.00 0.00 0.00 0.03 -0.04 -0.00 -0.03 0.04 0.00

21 6 0.00 0.00 0.00 -0.03 -0.04 -0.00 0.03 0.04 0.00

22 6 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

23 7 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

24 1 -0.01 -0.01 0.00 0.30 0.39 -0.01 0.30 0.39 -0.01

25 1 0.01 -0.01 0.00 -0.30 0.39 -0.01 -0.30 0.39 -0.01

26 1 0.40 0.30 0.01 0.01 0.01 0.00 0.01 0.01 0.00

27 1 -0.40 0.30 -0.01 -0.01 0.01 -0.00 0.01 -0.01 0.00

28 1 0.40 0.30 -0.01 0.01 0.01 -0.00 -0.01 -0.01 0.00

29 1 -0.40 0.30 0.01 -0.01 0.01 0.00 -0.01 0.01 0.00

30 1 0.01 -0.01 -0.00 -0.30 0.39 0.01 0.30 -0.39 -0.01

31 1 -0.01 -0.01 -0.00 0.30 0.39 0.01 -0.30 -0.39 -0.01

32 30 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00 -0.00

33 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

34 6 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

35 6 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

36 6 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

37 6 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

38 6 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

39 6 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

40 6 -0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

41 6 -0.00 -0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

42 1 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

43 1 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

44 1 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

45 1 -0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

124 125 126

A A A

Frequencies -- 3260.1153 3260.1579 3425.1340

Red. masses -- 1.1045 1.1045 1.1563

Frc consts -- 6.9163 6.9164 7.9924

IR Inten -- 12.9274 0.0001 0.0000

Atom AN X Y Z X Y Z X Y Z

1 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

2 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 0.00 0.00

3 7 0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

4 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00

5 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

6 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

7 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00

8 7 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00

9 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00

10 6 -0.04 -0.03 -0.00 -0.04 -0.03 -0.00 0.00 0.00 0.00

11 6 -0.04 0.03 -0.00 -0.04 0.03 -0.00 -0.00 0.00 -0.00

12 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

13 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 0.00 0.00

14 6 -0.04 -0.03 0.00 0.04 0.03 -0.00 -0.00 -0.00 0.00

15 6 -0.04 0.03 0.00 0.04 -0.03 -0.00 0.00 -0.00 -0.00

16 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.00 0.00 -0.00

17 7 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

18 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

19 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00

20 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 -0.00

21 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

22 6 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 0.00

23 7 0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00

24 1 0.00 0.00 -0.00 -0.01 -0.01 0.00 0.00 0.00 -0.00

25 1 0.00 -0.00 0.00 0.01 -0.01 0.00 0.00 -0.00 0.00

26 1 0.39 0.31 0.01 0.39 0.31 0.01 -0.00 -0.00 -0.00

27 1 0.39 -0.31 0.01 0.39 -0.31 0.01 0.00 -0.00 0.00

28 1 0.39 0.31 -0.01 -0.39 -0.31 0.01 0.00 0.00 -0.00

29 1 0.39 -0.31 -0.01 -0.39 0.31 0.01 -0.00 0.00 0.00

30 1 0.00 -0.00 -0.00 -0.01 0.01 0.00 -0.00 0.00 0.00

31 1 0.00 0.00 0.00 0.01 0.01 0.00 -0.00 -0.00 -0.00

32 30 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00

33 6 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00

34 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.01 0.01 0.00

35 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.01 -0.01 0.00

36 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.04 -0.04 -0.00

37 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.04 0.04 -0.00

38 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.01 0.01 -0.00

39 6 0.00 0.00 0.00 0.00 0.00 0.00 0.04 -0.04 0.00

40 6 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.01 -0.01 -0.00

41 6 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.04 0.04 0.00

42 1 0.00 -0.00 -0.00 -0.00 0.00 0.00 0.35 -0.36 -0.00

43 1 0.00 0.00 0.00 0.00 0.00 0.00 0.35 0.36 0.00

44 1 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.35 0.36 -0.00

45 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 -0.35 -0.36 0.00

127 128 129

A A A

Frequencies -- 3426.7213 3427.6778 3427.7658

Red. masses -- 1.1586 1.1599 1.1600

Frc consts -- 8.0154 8.0291 8.0303

IR Inten -- 837.1417 298.7134 0.0460

Atom AN X Y Z X Y Z X Y Z

1 6 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

2 6 -0.00 0.00 -0.00 0.00 -0.00 0.00 0.00 -0.00 0.00

3 7 0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

4 6 0.00 0.00 -0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00

5 6 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00

6 6 0.00 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

7 6 0.00 -0.00 0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00

8 7 0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00

9 6 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00

10 6 0.00 -0.00 0.00 0.00 -0.00 0.00 -0.00 0.00 0.00

11 6 -0.00 -0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00

12 6 -0.00 0.00 0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

13 6 -0.00 -0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00

14 6 0.00 -0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 0.00

15 6 -0.00 -0.00 0.00 0.00 0.00 -0.00 0.00 0.00 0.00

16 6 0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00

17 7 0.00 0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

18 6 0.00 0.00 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

19 6 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00

20 6 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00 0.00

21 6 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00 0.00

22 6 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00

23 7 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

24 1 0.00 0.00 -0.00 -0.00 -0.00 0.00 0.00 -0.00 0.00

25 1 -0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00 -0.00 0.00

26 1 0.00 0.00 0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

27 1 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00 0.00 -0.00

28 1 0.00 0.00 -0.00 0.00 0.00 -0.00 0.00 0.00 -0.00

29 1 -0.00 0.00 0.00 0.00 -0.00 -0.00 0.00 -0.00 -0.00

30 1 -0.00 0.00 0.00 -0.00 0.00 0.00 0.00 0.00 0.00

31 1 0.00 0.00 0.00 -0.00 -0.00 -0.00 -0.00 0.00 0.00

32 30 -0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 -0.00

33 6 -0.00 0.00 -0.00 0.00 0.00 0.00 -0.00 -0.00 -0.00

34 6 0.01 0.01 0.00 -0.01 -0.01 -0.00 0.01 0.01 0.00

35 6 0.01 0.01 -0.00 -0.01 -0.01 0.00 -0.01 -0.01 0.00

36 6 -0.04 -0.04 -0.00 0.04 0.04 0.00 -0.04 -0.04 -0.00

37 6 -0.04 -0.04 0.00 0.04 0.04 -0.00 0.04 0.04 -0.00

38 6 -0.01 0.01 -0.00 -0.01 0.01 -0.00 0.01 -0.01 0.00

39 6 0.04 -0.04 0.00 0.04 -0.04 0.00 -0.04 0.04 -0.00

40 6 -0.01 0.01 0.00 -0.01 0.01 0.00 -0.01 0.01 0.00

41 6 0.04 -0.04 -0.00 0.04 -0.04 -0.00 0.04 -0.04 -0.00

42 1 -0.35 0.36 0.00 -0.35 0.36 0.00 -0.35 0.36 0.00

43 1 0.35 0.36 0.00 -0.35 -0.36 -0.00 0.35 0.36 0.00

44 1 -0.35 0.36 -0.00 -0.35 0.36 -0.00 0.35 -0.36 0.00

45 1 0.35 0.36 -0.00 -0.35 -0.36 0.00 -0.35 -0.36 0.00

-------------------

- Thermochemistry -

-------------------

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 6 and mass 12.00000

Atom 2 has atomic number 6 and mass 12.00000

Atom 3 has atomic number 7 and mass 14.00307

Atom 4 has atomic number 6 and mass 12.00000

Atom 5 has atomic number 6 and mass 12.00000

Atom 6 has atomic number 6 and mass 12.00000

Atom 7 has atomic number 6 and mass 12.00000

Atom 8 has atomic number 7 and mass 14.00307

Atom 9 has atomic number 6 and mass 12.00000

Atom 10 has atomic number 6 and mass 12.00000

Atom 11 has atomic number 6 and mass 12.00000

Atom 12 has atomic number 6 and mass 12.00000

Atom 13 has atomic number 6 and mass 12.00000

Atom 14 has atomic number 6 and mass 12.00000

Atom 15 has atomic number 6 and mass 12.00000

Atom 16 has atomic number 6 and mass 12.00000

Atom 17 has atomic number 7 and mass 14.00307

Atom 18 has atomic number 6 and mass 12.00000

Atom 19 has atomic number 6 and mass 12.00000

Atom 20 has atomic number 6 and mass 12.00000

Atom 21 has atomic number 6 and mass 12.00000

Atom 22 has atomic number 6 and mass 12.00000

Atom 23 has atomic number 7 and mass 14.00307

Atom 24 has atomic number 1 and mass 1.00783

Atom 25 has atomic number 1 and mass 1.00783

Atom 26 has atomic number 1 and mass 1.00783

Atom 27 has atomic number 1 and mass 1.00783

Atom 28 has atomic number 1 and mass 1.00783

Atom 29 has atomic number 1 and mass 1.00783

Atom 30 has atomic number 1 and mass 1.00783

Atom 31 has atomic number 1 and mass 1.00783

Atom 32 has atomic number 30 and mass 63.92915

Atom 33 has atomic number 6 and mass 12.00000

Atom 34 has atomic number 6 and mass 12.00000

Atom 35 has atomic number 6 and mass 12.00000

Atom 36 has atomic number 6 and mass 12.00000

Atom 37 has atomic number 6 and mass 12.00000

Atom 38 has atomic number 6 and mass 12.00000

Atom 39 has atomic number 6 and mass 12.00000

Atom 40 has atomic number 6 and mass 12.00000

Atom 41 has atomic number 6 and mass 12.00000

Atom 42 has atomic number 1 and mass 1.00783

Atom 43 has atomic number 1 and mass 1.00783

Atom 44 has atomic number 1 and mass 1.00783

Atom 45 has atomic number 1 and mass 1.00783

Molecular mass: 468.03534 amu.

Principal axes and moments of inertia in atomic units:

1 2 3

Eigenvalues -- \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

X 1.00000 0.00000 -0.00000

Y -0.00000 1.00000 0.00000

Z 0.00000 -0.00000 1.00000

This molecule is an asymmetric top.

Rotational symmetry number 1.

Warning -- assumption of classical behavior for rotation

may cause significant error

Rotational temperatures (Kelvin) 0.00703 0.00697 0.00350

Rotational constants (GHZ): 0.14653 0.14529 0.07299

Zero-point vibrational energy 790551.7 (Joules/Mol)

188.94639 (Kcal/Mol)

Warning -- explicit consideration of 49 degrees of freedom as

vibrations may cause significant error

Vibrational temperatures: 23.32 59.45 61.58 74.54 81.56

(Kelvin) 92.74 139.49 159.31 162.31 168.31

170.08 179.90 202.70 204.77 206.99

235.33 282.70 299.87 305.49 337.57

341.02 396.62 442.13 449.63 462.12

467.04 499.32 516.68 527.02 535.50

536.28 555.06 578.53 650.19 656.53

683.46 688.12 794.94 802.67 806.36

817.11 817.83 849.81 851.28 852.41

853.04 855.99 864.72 878.55 946.71

946.87 946.94 946.98 957.96 961.16

964.66 988.27 1028.07 1031.80 1034.79

1045.04 1108.01 1108.55 1138.86 1149.93

1150.50 1224.88 1237.94 1245.84 1247.31

1247.32 1257.84 1332.16 1332.19 1381.63

1382.87 1424.00 1463.22 1473.18 1488.29

1512.61 1513.43 1516.91 1546.11 1557.51

1576.93 1583.42 1646.62 1674.08 1676.87

1714.23 1776.40 1782.79 1784.14 1833.59

1879.34 1881.22 1890.27 1951.57 1963.72

1998.90 2039.47 2048.69 2056.76 2093.08

2094.40 2126.15 2162.99 2170.11 2220.15

2228.47 2242.39 2256.62 3071.80 3093.52

3104.18 3112.01 4657.39 4657.42 4666.90

4666.96 4678.98 4679.04 4690.57 4690.63

4928.00 4930.28 4931.66 4931.78

Zero-point correction= 0.301105 (Hartree/Particle)

Thermal correction to Energy= 0.328983

Thermal correction to Enthalpy= 0.329927

Thermal correction to Gibbs Free Energy= 0.241916

Sum of electronic and zero-point Energies= -1358.710327

Sum of electronic and thermal Energies= -1358.682449

Sum of electronic and thermal Enthalpies= -1358.681505

Sum of electronic and thermal Free Energies= -1358.769517

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 206.440 109.032 185.236

Electronic 0.000 0.000 2.183

Translational 0.889 2.981 44.319

Rotational 0.889 2.981 36.579

Vibrational 204.662 103.071 102.155

Vibration 1 0.593 1.986 7.051

Vibration 2 0.594 1.981 5.195

Vibration 3 0.595 1.980 5.125

Vibration 4 0.596 1.977 4.747

Vibration 5 0.596 1.975 4.569

Vibration 6 0.597 1.971 4.316

Vibration 7 0.603 1.951 3.515

Vibration 8 0.607 1.941 3.256

Vibration 9 0.607 1.939 3.220

Vibration 10 0.608 1.935 3.150

Vibration 11 0.608 1.934 3.129

Vibration 12 0.610 1.928 3.021

Vibration 13 0.615 1.912 2.792

Vibration 14 0.616 1.911 2.772

Vibration 15 0.616 1.909 2.752

Vibration 16 0.623 1.887 2.508

Vibration 17 0.636 1.845 2.166

Vibration 18 0.642 1.828 2.057

Vibration 19 0.643 1.822 2.024

Vibration 20 0.654 1.788 1.843

Vibration 21 0.656 1.784 1.825

Vibration 22 0.677 1.718 1.560

Vibration 23 0.697 1.660 1.377

Vibration 24 0.701 1.650 1.349

Vibration 25 0.707 1.633 1.304

Vibration 26 0.709 1.626 1.287

Vibration 27 0.725 1.581 1.180

Vibration 28 0.734 1.557 1.126

Vibration 29 0.739 1.542 1.095

Vibration 30 0.744 1.529 1.071

Vibration 31 0.744 1.528 1.069

Vibration 32 0.754 1.501 1.016

Vibration 33 0.768 1.466 0.955

Vibration 34 0.811 1.357 0.790

Vibration 35 0.815 1.347 0.777

Vibration 36 0.832 1.305 0.724

Vibration 37 0.835 1.298 0.715

Vibration 38 0.908 1.134 0.539

Vibration 39 0.913 1.122 0.528

Vibration 40 0.916 1.117 0.523

Vibration 41 0.924 1.101 0.508

Vibration 42 0.924 1.100 0.507

Vibration 43 0.948 1.052 0.466

Vibration 44 0.949 1.050 0.464

Vibration 45 0.950 1.048 0.463

Vibration 46 0.950 1.047 0.462

Vibration 47 0.953 1.043 0.458

Vibration 48 0.959 1.030 0.448

Vibration 49 0.970 1.009 0.432

Q Log10(Q) Ln(Q)

Total Bot 0.533090-111 -111.273200 -256.216011

Total V=0 0.167998D+28 27.225304 62.688579

Vib (Bot) 0.202799-127 -127.692935 -294.023849

Vib (Bot) 1 0.127792D+02 1.106503 2.547816

Vib (Bot) 2 0.500666D+01 0.699548 1.610768

Vib (Bot) 3 0.483302D+01 0.684218 1.575471

Vib (Bot) 4 0.398939D+01 0.600906 1.383638

Vib (Bot) 5 0.364434D+01 0.561619 1.293177

Vib (Bot) 6 0.320192D+01 0.505410 1.163750

Vib (Bot) 7 0.211800D+01 0.325927 0.750474

Vib (Bot) 8 0.184945D+01 0.267042 0.614886

Vib (Bot) 9 0.181445D+01 0.258746 0.595785

Vib (Bot) 10 0.174815D+01 0.242579 0.558559

Vib (Bot) 11 0.172947D+01 0.237912 0.547813

Vib (Bot) 12 0.163248D+01 0.212847 0.490099

Vib (Bot) 13 0.144296D+01 0.159254 0.366697

Vib (Bot) 14 0.142782D+01 0.154674 0.356150

Vib (Bot) 15 0.141186D+01 0.149792 0.344909

Vib (Bot) 16 0.123466D+01 0.091548 0.210798

Vib (Bot) 17 0.101615D+01 0.006958 0.016021

Vib (Bot) 18 0.953573D+00 -0.020646 -0.047539

Vib (Bot) 19 0.934562D+00 -0.029392 -0.067677

Vib (Bot) 20 0.837747D+00 -0.076887 -0.177040

Vib (Bot) 21 0.828400D+00 -0.081760 -0.188260

Vib (Bot) 22 0.699024D+00 -0.155508 -0.358070

Vib (Bot) 23 0.616307D+00 -0.210203 -0.484011

Vib (Bot) 24 0.604202D+00 -0.218818 -0.503847

Vib (Bot) 25 0.584849D+00 -0.232956 -0.536402

Vib (Bot) 26 0.577504D+00 -0.238445 -0.549040

Vib (Bot) 27 0.532646D+00 -0.273561 -0.629898

Vib (Bot) 28 0.510709D+00 -0.291827 -0.671956

Vib (Bot) 29 0.498272D+00 -0.302534 -0.696610

Vib (Bot) 30 0.488416D+00 -0.311210 -0.716588

Vib (Bot) 31 0.487526D+00 -0.312002 -0.718412

Vib (Bot) 32 0.466763D+00 -0.330903 -0.761933

Vib (Bot) 33 0.442581D+00 -0.354007 -0.815131

Vib (Bot) 34 0.378885D+00 -0.421492 -0.970522

Vib (Bot) 35 0.373883D+00 -0.427264 -0.983811

Vib (Bot) 36 0.353574D+00 -0.451519 -1.039661

Vib (Bot) 37 0.350212D+00 -0.455669 -1.049217

Vib (Bot) 38 0.283351D+00 -0.547675 -1.261069

Vib (Bot) 39 0.279166D+00 -0.554138 -1.275950

Vib (Bot) 40 0.277197D+00 -0.557211 -1.283027

Vib (Bot) 41 0.271553D+00 -0.566145 -1.303596

Vib (Bot) 42 0.271182D+00 -0.566740 -1.304967

Vib (Bot) 43 0.255234D+00 -0.593062 -1.365576

Vib (Bot) 44 0.254532D+00 -0.594258 -1.368330

Vib (Bot) 45 0.253990D+00 -0.595183 -1.370459

Vib (Bot) 46 0.253690D+00 -0.595697 -1.371643

Vib (Bot) 47 0.252288D+00 -0.598104 -1.377186

Vib (Bot) 48 0.248191D+00 -0.605214 -1.393557

Vib (Bot) 49 0.241861D+00 -0.616435 -1.419394

Vib (V=0) 0.639099D+11 10.805568 24.880741

Vib (V=0) 1 0.132889D+02 1.123490 2.586932

Vib (V=0) 2 0.553156D+01 0.742848 1.710470

Vib (V=0) 3 0.535881D+01 0.729069 1.678742

Vib (V=0) 4 0.452060D+01 0.655196 1.508645

Vib (V=0) 5 0.417848D+01 0.621019 1.429949

Vib (V=0) 6 0.374072D+01 0.572956 1.319279

Vib (V=0) 7 0.267622D+01 0.427522 0.984406

Vib (V=0) 8 0.241584D+01 0.383069 0.882048

Vib (V=0) 9 0.238209D+01 0.376957 0.867976

Vib (V=0) 10 0.231825D+01 0.365160 0.840813

Vib (V=0) 11 0.230029D+01 0.361783 0.833037

Vib (V=0) 12 0.220733D+01 0.343868 0.791784

Vib (V=0) 13 0.202713D+01 0.306882 0.706622

Vib (V=0) 14 0.201284D+01 0.303808 0.699545

Vib (V=0) 15 0.199778D+01 0.300548 0.692038

Vib (V=0) 16 0.183206D+01 0.262941 0.605443

Vib (V=0) 17 0.163250D+01 0.212854 0.490114

Vib (V=0) 18 0.157671D+01 0.197751 0.455340

Vib (V=0) 19 0.155991D+01 0.193099 0.444627

Vib (V=0) 20 0.147561D+01 0.168972 0.389073

Vib (V=0) 21 0.146760D+01 0.166607 0.383627

Vib (V=0) 22 0.135944D+01 0.133360 0.307072

Vib (V=0) 23 0.129362D+01 0.111807 0.257445

Vib (V=0) 24 0.128426D+01 0.108652 0.250181

Vib (V=0) 25 0.126945D+01 0.103614 0.238581

Vib (V=0) 26 0.126388D+01 0.101705 0.234186

Vib (V=0) 27 0.123056D+01 0.090101 0.207466

Vib (V=0) 28 0.121472D+01 0.084476 0.194513

Vib (V=0) 29 0.120589D+01 0.081306 0.187214

Vib (V=0) 30 0.119896D+01 0.078806 0.181458

Vib (V=0) 31 0.119834D+01 0.078581 0.180939

Vib (V=0) 32 0.118401D+01 0.073355 0.168906

Vib (V=0) 33 0.116774D+01 0.067347 0.155071

Vib (V=0) 34 0.112734D+01 0.052054 0.119860

Vib (V=0) 35 0.112433D+01 0.050894 0.117188

Vib (V=0) 36 0.111238D+01 0.046255 0.106506

Vib (V=0) 37 0.111045D+01 0.045499 0.104765

Vib (V=0) 38 0.107471D+01 0.031290 0.072048

Vib (V=0) 39 0.107265D+01 0.030460 0.070137

Vib (V=0) 40 0.107170D+01 0.030072 0.069244

Vib (V=0) 41 0.106898D+01 0.028971 0.066707

Vib (V=0) 42 0.106881D+01 0.028899 0.066541

Vib (V=0) 43 0.106138D+01 0.025870 0.059567

Vib (V=0) 44 0.106106D+01 0.025739 0.059267

Vib (V=0) 45 0.106081D+01 0.025639 0.059036

Vib (V=0) 46 0.106068D+01 0.025583 0.058907

Vib (V=0) 47 0.106004D+01 0.025324 0.058310

Vib (V=0) 48 0.105821D+01 0.024572 0.056579

Vib (V=0) 49 0.105542D+01 0.023427 0.053943

Electronic 0.300000D+01 0.477121 1.098612

Translational 0.397991D+09 8.599873 19.801940

Rotational 0.220161D+08 7.342741 16.907286

ZnTSPsim3

IR Spectrum

33333333333 2222111111111111111111111111111111111111

44442222222 1111555555444444333333222211111000000000999988888887777777766666666665555555555444443333333333222221111111111

22226655433 65536544007553218651007433966409875553219662766665099772111876655551099999666557755087765422107331096444211119655441

88750022477 38058993838650489564864095154416354214470106477601092006975708688881153221880838562263269751376752864421587317472316

XX X X X XX XXXXXX XXXXX XXXX X X XXX X X XXX X X XXX XX XX X XX XX XXXX X XXX XX X XXXXXXXX X XX X XXXXXXXXXX

XX X XX X XX X X X X

X XX XX X X X

X XX XX X X X

X X X X X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

X

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

-------------------------------------------------------------------

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

-------------------------------------------------------------------

1 6 0.000000014 -0.000000015 -0.000000008

2 6 -0.000000055 0.000000068 0.000000007

3 7 -0.000000049 -0.000000554 0.000001666

4 6 0.000000054 0.000000028 0.000000007

5 6 -0.000000017 -0.000000015 -0.000000007

6 6 -0.000000172 -0.000000064 0.000000007

7 6 0.000000132 0.000000044 0.000000010

8 7 0.000000492 0.000000058 0.000001303

9 6 0.000000085 -0.000000021 0.000000010

10 6 -0.000000029 0.000000035 -0.000000002

11 6 -0.000000028 -0.000000033 -0.000000000

12 6 0.000000167 -0.000000062 0.000000008

13 6 -0.000000130 0.000000030 0.000000010

14 6 0.000000032 -0.000000008 -0.000000001

15 6 0.000000034 0.000000015 -0.000000001

16 6 -0.000000099 0.000000035 0.000000010

17 7 -0.000000402 0.000000025 0.000001297

18 6 0.000000195 0.000000014 0.000000008

19 6 -0.000000117 -0.000000048 0.000000007

20 6 0.000000031 0.000000006 -0.000000008

21 6 -0.000000037 0.000000013 -0.000000007

22 6 0.000000050 -0.000000023 0.000000006

23 7 -0.000000029 0.000000460 0.000001661

24 1 -0.000000007 0.000000008 -0.000000005

25 1 0.000000007 0.000000007 -0.000000005

26 1 -0.000000005 0.000000009 0.000000003

27 1 -0.000000006 -0.000000011 0.000000003

28 1 0.000000003 -0.000000007 0.000000003

29 1 0.000000004 0.000000009 0.000000004

30 1 -0.000000005 -0.000000005 -0.000000005

31 1 0.000000006 -0.000000006 -0.000000005

32 30 0.000000025 -0.000000026 -0.000005961

33 6 -0.000000150 0.000000041 0.000000008

34 6 0.000000143 0.000000145 0.000000009

35 6 -0.000000145 -0.000000143 0.000000009

36 6 -0.000000022 -0.000000023 -0.000000011

37 6 0.000000020 0.000000024 -0.000000010

38 6 0.000000163 -0.000000166 0.000000008

39 6 -0.000000030 0.000000033 -0.000000010

40 6 -0.000000148 0.000000152 0.000000009

41 6 0.000000027 -0.000000030 -0.000000011

42 1 0.000000029 -0.000000029 -0.000000003

43 1 -0.000000030 -0.000000030 -0.000000003

44 1 -0.000000031 0.000000030 -0.000000004

45 1 0.000000031 0.000000030 -0.000000004

-------------------------------------------------------------------

Cartesian Forces: Max 0.000005961 RMS 0.000000582

Red2BG is reusing G-inverse.

Leave Link 716 at Tue Jul 30 03:39:14 2019, MaxMem= 4294967296 cpu: 1.2

(Enter /home/kira/g09/l9999.exe)

1\1\ WCSS.PL-BEM-LOCALHOST\Freq\UB3LYP\GenECP\C28H12N4Zn1(3)\KIRA\30-J

ul-2019\0\\#p opt=calcall b3lyp/genecp scrf=(solvent=dmso,smd) empiric

aldispersion=gd3bj\\ZnTSPsim3\\0,3\C,-0.6928344159,-4.2678484554,-0.05

68045703\C,-1.1006249016,-2.9062390522,-0.0216070583\N,0.0000000829,-2

.0927275112,-0.0006841455\C,1.1006249951,-2.9062390132,-0.0216070219\C

,0.6928345532,-4.2678484372,-0.0568045397\C,2.4679684966,-2.4399593219

,-0.0196881081\C,2.9107717059,-1.1022620304,-0.0161894774\N,2.10095410

21,-0.0000000908,-0.0034549102\C,2.9107716828,1.1022619457,-0.01618955

38\C,4.2981953525,0.6795946362,-0.0366850727\C,4.2981953739,-0.6795946

833,-0.0366850145\C,-2.4679684433,-2.4399593674,-0.0196881942\C,-2.910

771884,-1.1022621012,-0.0161893406\C,-4.298195569,-0.6795948017,-0.036

6849343\C,-4.2981956066,0.6795945651,-0.0366848336\C,-2.9107719266,1.1

022619313,-0.0161891882\N,-2.1009544467,-0.0000000587,-0.003454554\C,-

2.4679685355,2.4399593609,-0.0196878925\C,-1.1006249153,2.9062392533,-

0.021606839\C,-0.6928344586,4.2678486764,-0.0568045095\C,0.6928345668,

4.2678486806,-0.0568046298\C,1.1006250433,2.9062392688,-0.0216070217\N

,0.0000000723,2.0927278731,-0.0006839402\H,-1.3477557276,-5.126101973,

-0.0827211222\H,1.3477559018,-5.1261019256,-0.0827210617\H,5.153172296

1,1.3388420755,-0.0532030025\H,5.1531723521,-1.3388420799,-0.053202878

\H,-5.1531725042,-1.3388422496,-0.0532029586\H,-5.1531725877,1.3388419

56,-0.0532027686\H,-1.3477558009,5.1261021681,-0.0827210937\H,1.347755

8853,5.1261021892,-0.0827213171\Zn,-0.0000001994,0.0000002383,0.151889

0368\C,2.4679684753,2.439959342,-0.0196882492\C,3.4682748016,3.4436227

683,-0.0325431201\C,-3.4682745794,-3.4436229915,-0.0325431675\C,4.3087

655036,4.3112381573,-0.0436932169\C,-4.3087651276,-4.311238524,-0.0436

933713\C,3.468274692,-3.4436228538,-0.0325427048\C,4.3087652421,-4.311

2384028,-0.0436924919\C,-3.4682747382,3.4436228726,-0.0325426827\C,-4.

3087652834,4.3112384294,-0.0436927037\H,-5.0549011509,5.0747363311,-0.

0538887148\H,5.0549015236,5.0747359118,-0.053889296\H,5.0549011189,-5.

0747363008,-0.05388825\H,-5.0549010176,-5.0747364056,-0.0538895155\\Ve

rsion=ES64L-G09RevE.01\State=3-A\HF=-1359.0114323\S2=2.058475\S2-1=0.\

S2A=2.001899\RMSD=3.942e-09\RMSF=5.825e-07\ZeroPoint=0.3011052\Thermal

=0.3289829\Dipole=-0.0000004,-0.000001,0.3217077\DipoleDeriv=-0.004909

5,-1.9679029,0.0016221,0.0076101,1.1269002,0.0027309,0.0202413,0.03336

86,-0.2610141,-3.2016619,0.6912875,0.0113719,-0.1938179,-1.40261,0.009

9805,0.0030879,-0.0408021,0.0396268,1.9775842,-0.0000009,-0.0000002,0.

,-1.2563225,-0.0213631,0.,-0.0014364,-0.41052,-3.2016604,-0.6912846,-0

.0113717,0.1938199,-1.4026105,0.0099805,-0.0030882,-0.0408022,0.039626

9,-0.004912,1.967903,-0.0016221,-0.0076118,1.1269,0.0027309,-0.0202414

,0.0333686,-0.2610142,3.0919764,1.1605645,-0.0010471,0.7546412,0.77720

09,0.0021524,0.0141658,0.0276094,0.0182292,-0.535954,-0.1575665,-0.006

4498,-0.4134996,0.1681468,0.0098819,-0.0027928,-0.0143341,0.1105709,-1

.3698852,0.0000001,0.0106139,-0.0000009,-0.8362208,0.0000001,0.0095908

,0.,-0.4348492,-0.535953,0.1575663,-0.0064499,0.4135008,0.168147,-0.00

98822,-0.0027927,0.0143341,0.1105708,0.6569031,-0.0359888,0.0007981,-0

.9824561,0.1123357,-0.0052559,-0.014172,-0.0026201,-0.2091031,0.656903

3,0.0359888,0.0007981,0.9824563,0.1123357,0.0052558,-0.0141721,0.00262

01,-0.2091031,3.0919782,-1.1605664,0.0010471,-0.7546421,0.7772012,0.00

21523,-0.0141655,0.0276095,0.0182293,-0.5359543,0.1575686,0.00645,0.41

35009,0.1681477,0.0098823,0.0027927,-0.0143341,0.1105708,0.6569038,-0.

0359901,-0.0007981,-0.9824566,0.1123376,0.0052559,0.014172,0.0026202,-

0.2091031,0.6569031,0.0359878,-0.0007981,0.9824563,0.1123343,-0.005255

9,0.0141722,-0.0026202,-0.2091031,-0.535953,-0.1575657,0.0064499,-0.41

34999,0.1681516,-0.009882,0.0027928,0.0143342,0.1105709,-1.3698852,0.0

000003,-0.0106139,0.,-0.8362229,-0.0000002,-0.0095907,-0.0000001,-0.43

48492,3.091973,1.1605642,0.0010471,0.754641,0.7771974,-0.0021525,-0.01

41657,-0.0276098,0.0182292,-3.2016563,-0.6912853,0.0113718,0.1938188,-

1.4026096,-0.0099806,0.0030882,0.0408022,0.0396269,-0.0049116,1.967902

6,0.0016221,-0.0076115,1.1269,-0.0027309,0.0202414,-0.033369,-0.261014

2,-0.0049097,-1.9679029,-0.0016222,0.0076101,1.1269,-0.0027309,-0.0202

414,-0.0333684,-0.2610142,-3.2016572,0.6912862,-0.0113719,-0.193817,-1

.4026105,-0.0099806,-0.0030878,0.0408023,0.0396269,1.9775812,-0.000000

1,0.0000001,0.,-1.2563225,0.0213632,-0.0000001,0.0014366,-0.4105199,0.

0694701,-0.1789135,-0.0030176,-0.1101029,-0.0161068,-0.0059292,-0.0041

269,-0.0081324,0.2131161,0.0694701,0.1789135,0.0030176,0.110103,-0.016

1067,-0.0059292,0.0041269,-0.0081324,0.2131162,-0.003519,-0.0743737,0.

0031438,-0.1108611,0.0962012,0.0012913,0.0043216,0.0030805,0.205036,-0

.0035191,0.0743737,0.0031437,0.1108611,0.0962011,-0.0012913,0.0043216,

-0.0030805,0.205036,-0.0035191,-0.0743737,-0.0031438,-0.1108611,0.0962

011,-0.0012913,-0.0043216,-0.0030805,0.205036,-0.003519,0.0743737,-0.0

031437,0.1108612,0.096201,0.0012913,-0.0043216,0.0030805,0.2050361,0.0

694701,0.1789136,-0.0030176,0.1101029,-0.0161067,0.0059292,-0.0041269,

0.0081325,0.2131162,0.0694701,-0.1789136,0.0030176,-0.1101028,-0.01610

67,0.0059292,0.0041269,0.0081325,0.2131162,1.608477,0.0000002,0.,0.000

0004,1.396371,0.,0.,0.,1.3949696,3.091974,-1.1605655,-0.0010472,-0.754

6422,0.7772014,-0.0021523,0.0141654,-0.0276095,0.0182293,-0.803666,0.3

521655,-0.0000462,-0.6260873,0.4286556,-0.0001556,0.0115761,-0.0158903

,-0.0422893,-0.8036673,0.3521648,0.0000462,-0.6260888,0.4286559,0.0001

556,-0.011576,0.0158903,-0.0422894,-0.3326412,-0.6422168,0.0009725,-0.

0144967,-0.9859151,0.0010013,0.0017772,0.0123344,-0.2657857,-0.3326401

,-0.6422164,-0.0009725,-0.0144955,-0.9859152,-0.0010014,-0.0017772,-0.

0123346,-0.2657857,-0.8036672,-0.3521644,-0.0000462,0.6260882,0.428655

8,0.0001556,0.0115759,0.0158902,-0.0422894,-0.3326404,0.642216,0.00097

24,0.0144961,-0.9859154,-0.0010013,0.0017771,-0.0123343,-0.2657857,-0.

8036662,-0.3521653,0.0000461,0.626087,0.4286563,-0.0001555,-0.0115761,

-0.0158902,-0.0422893,-0.332641,0.6422165,-0.0009724,0.0144968,-0.9859

157,0.0010012,-0.0017772,0.0123343,-0.2657857,0.358033,-0.1076669,0.00

04236,-0.0777188,0.3923705,-0.0005114,0.0011106,-0.0006057,0.2655553,0

.3580327,0.1076666,-0.0004236,0.0777186,0.3923701,-0.0005114,-0.001110

4,-0.0006055,0.2655553,0.3580328,-0.1076666,-0.0004236,-0.0777186,0.39

23701,0.0005114,-0.0011106,0.0006058,0.2655553,0.3580326,0.1076667,0.0

004236,0.0777186,0.3923705,0.0005114,0.0011104,0.0006055,0.2655552\Pol

ar=1223.3080745,-0.0002415,1614.5193783,-0.0000013,0.0000023,181.33216

76\PG=C01 [X(C28H12N4Zn1)]\NImag=0\\0.69142471,0.14800269,0.69761842,0

.00482714,0.01628346,0.11324454,-0.09766278,0.04420207,0.00192486,0.64

786775,0.02307043,-0.25569199,-0.00501705,-0.05545907,0.58189134,0.000

69611,-0.00487478,-0.06631069,0.00063988,0.01069790,0.14220109,-0.0072

3877,-0.04451234,-0.00170617,-0.13557417,-0.09551413,-0.00279238,0.458

76804,-0.00294477,-0.07663017,-0.00243846,-0.07413940,-0.17760782,-0.0

0313630,-0.00000006,0.54904246,-0.00012985,-0.00269643,0.01677087,-0.0

0151702,-0.00306692,-0.06970286,-0.00000003,0.02410554,0.09445862,-0.0

5123634,-0.01961695,-0.00005398,-0.18456319,-0.02428955,-0.00032938,-0

.13557433,0.07413947,0.00151703,0.64786801,-0.07366472,-0.00695586,-0.

00035749,0.02428964,0.00803812,-0.00011735,0.09551416,-0.17760788,-0.0

0306692,0.05545905,0.58189137,-0.00187621,-0.00055839,0.01157721,0.000

32936,-0.00011736,0.01120186,0.00279239,-0.00313629,-0.06970285,-0.000

63987,0.01069789,0.14220109,-0.34702562,-0.01836728,-0.00059592,-0.051

23642,0.07366470,0.00187621,-0.00723870,0.00294478,0.00012985,-0.09766

285,-0.02307040,-0.00069611,0.69142473,0.01836727,-0.11375705,-0.00191

146,0.01961690,-0.00695587,-0.00055839,0.04451239,-0.07663018,-0.00269

643,-0.04420210,-0.25569196,-0.00487478,-0.14800270,0.69761839,0.00059

591,-0.00191146,-0.05579206,0.00005397,-0.00035749,0.01157721,0.001706

17,-0.00243846,0.01677087,-0.00192487,-0.00501705,-0.06631070,-0.00482

712,0.01628345,0.11324453,0.01258249,-0.00609211,-0.00051648,0.0610695

1,0.01667394,0.00017474,-0.08843618,-0.00404089,-0.00014668,-0.1709344

2,-0.05114656,-0.00015101,-0.02088911,-0.02071368,0.00019636,0.5551853

7,-0.00168847,-0.00506671,-0.00023762,0.01316574,-0.01124635,-0.000210

80,0.01722245,0.01702217,0.00042032,-0.04398077,-0.11706487,-0.0014127

2,-0.03601826,-0.00930911,-0.00000511,0.00114101,0.59594616,0.00005094

,-0.00028475,0.00203993,0.00076594,-0.00001468,0.00478524,-0.00019477,

0.00055810,-0.00495799,0.00096835,-0.00109588,-0.04773800,-0.00075794,

-0.00015938,0.00167850,-0.00264331,0.00417601,0.12680955,-0.00479110,0

.00180537,0.00011666,-0.01039635,-0.00760954,-0.00005681,0.01539164,0.

00231460,0.00004427,-0.01861397,-0.03650986,-0.00032622,-0.00158111,0.

00352117,-0.00000283,-0.12694607,-0.07847089,0.00056089,0.55542113,0.0

0211156,-0.00354050,-0.00019929,0.00147271,0.01131763,0.00000473,-0.00

433121,-0.00487340,-0.00013851,-0.02548226,-0.01825405,0.00047226,0.00

598140,0.00815638,0.00021854,-0.06431333,-0.20707756,-0.00152283,0.069

67122,0.66589929,-0.00007489,0.00004546,0.00022079,-0.00032956,-0.0000

6291,-0.00064201,0.00023034,-0.00008200,0.00018211,-0.00070570,0.00003

096,0.00581326,0.00009815,0.00000424,0.00258858,0.00090783,-0.00036620

,-0.05016976,-0.00584392,0.00147242,0.14834286,0.00048302,-0.00164678,

-0.00004609,0.00272455,0.00027678,-0.00010844,-0.00500927,-0.00841890,

-0.00081616,-0.00186789,0.00225153,0.00010682,-0.00059075,-0.00101754,

-0.00000303,0.01533450,0.00155059,-0.00035968,-0.18398642,0.06795614,0

.00225005,0.54157842,-0.00301882,0.00265318,0.00018692,-0.00321692,-0.

01250428,-0.00000047,-0.00022577,-0.00217507,0.00057764,0.00052000,0.0

1404773,-0.00017047,-0.00265474,-0.00502247,-0.00021688,0.01768985,-0.

11161292,0.00011845,0.08900965,-0.11356260,-0.00146980,-0.00000009,0.4

4522288,-0.00002988,0.00005605,-0.00033500,-0.00027173,0.00001575,-0.0

0023346,-0.00028787,0.00116080,0.00418195,0.00003206,0.00006088,-0.001

59927,0.00000674,0.00005823,-0.00000705,-0.00003387,-0.00016534,-0.001

09033,0.00223622,-0.00052888,-0.06749279,-0.02095774,-0.00000005,0.088

28262,-0.00047004,0.00007193,-0.00003082,0.00258512,0.00117789,-0.0000

2120,-0.00441700,-0.00129267,0.00000304,-0.00041106,-0.00432812,0.0000

8518,0.00197703,0.00230173,0.00006698,-0.00370230,0.02836476,0.0000507

8,0.01595343,-0.03444444,-0.00032178,-0.18398636,-0.08900956,0.0022362

2,0.55542107,0.00289924,-0.00316863,-0.00018943,0.00156505,0.01139349,

-0.00001825,-0.00666107,0.00107691,0.00007533,0.00191795,-0.00977219,0

.00021442,0.00186409,0.00365740,0.00016962,0.01011643,0.06518349,-0.00

047028,0.03444441,-0.18991727,-0.00031357,-0.06795609,-0.11356255,0.00

052887,-0.06967123,0.66589905,0.00005419,-0.00003155,0.00004919,0.0002

3667,0.00006212,0.00059032,-0.00017469,0.00013934,-0.00051536,0.000286

78,0.00000349,-0.00003793,-0.00003521,-0.00003591,-0.00003020,-0.00010

771,-0.00019681,0.00406345,-0.00032178,0.00031358,0.00511668,0.0022500

6,0.00146980,-0.06749280,-0.00584393,-0.00147245,0.14834287,0.00042152

,-0.00108435,-0.00003167,0.00095359,0.00010243,0.00001183,-0.00094712,

-0.00113554,-0.00003779,0.00122509,0.00021050,-0.00003877,-0.00168981,

-0.00118209,-0.00002726,-0.00891813,-0.00867512,0.00013446,-0.00756308

,-0.01950467,0.00040907,-0.06856034,-0.03732774,0.00151268,-0.22054612

,0.02933222,0.00240352,0.65906600,-0.00147964,0.00079413,0.00003246,-0

.00362582,-0.00111022,-0.00001950,0.00300492,-0.00064799,0.00003505,-0

.00656629,-0.00263810,0.00003567,0.00165760,0.00205001,0.00001970,0.00

426624,0.01861319,0.00005195,-0.06233051,-0.05646181,0.00082235,-0.012

31489,-0.00248183,0.00029645,0.01714569,-0.09103225,-0.00040283,0.1557

6610,0.76257997,0.00000977,-0.00000424,0.00019559,0.00007288,0.0000400

8,0.00023790,-0.00009223,0.00002034,-0.00060818,0.00006289,-0.00006279

,-0.00019405,0.00003650,0.00003831,-0.00026458,0.00016237,0.00039217,0

.00180161,0.00024437,-0.00008539,0.00890700,0.00136743,0.00115233,0.01

534988,0.00235082,-0.00104656,-0.06581767,-0.00921128,-0.00342406,0.12

014543,0.00231620,-0.00157160,-0.00008788,0.00674078,0.00297425,0.0000

2286,-0.00743543,-0.00047004,-0.00005142,0.01124331,0.00269875,0.00010

724,-0.00170478,-0.00201498,0.00003100,-0.01102780,-0.01952052,-0.0000

2347,-0.22054611,-0.02933220,0.00240352,-0.06856035,0.03732773,0.00151

268,-0.00756308,0.01950469,0.00040907,-0.11636333,0.01412034,0.0012362

1,0.65906601,0.00225284,-0.00234544,-0.00009932,0.00507791,0.00306882,

0.00002968,-0.00592242,0.00001918,-0.00001906,0.01126460,-0.00188333,-

0.00005075,-0.00373923,-0.00196614,0.00000168,-0.03947790,-0.02271294,

0.00025338,-0.01714570,-0.09103224,0.00040283,0.01231489,-0.00248184,-

0.00029645,0.06233052,-0.05646180,-0.00082234,-0.01412033,-0.42522337,

0.00035336,-0.15576610,0.76257997,-0.00006657,0.00007386,-0.00053915,-

0.00018500,-0.00010661,-0.00025442,0.00021434,-0.00002053,0.00024437,-

0.00024563,0.00001033,0.00535678,0.00005570,-0.00002831,0.00095167,0.0

0001650,-0.00027679,0.00186459,0.00235082,0.00104657,-0.06581768,0.001

36743,-0.00115233,0.01534988,0.00024436,0.00008540,0.00890700,0.001236

21,-0.00035333,-0.05749134,-0.00921126,0.00342400,0.12014542,-0.020889

15,0.02071370,-0.00019635,-0.17093429,0.05114651,0.00015100,-0.0884362

2,0.00404091,0.00014667,0.06106954,-0.01667400,-0.00017473,0.01258254,

0.00609214,0.00051648,-0.04500254,-0.01145062,-0.00043132,0.00446277,0

.00639585,0.00024862,0.00031282,-0.00220732,0.00009672,-0.00051643,0.0

0426966,-0.00017467,-0.00038739,0.00280795,-0.00002498,-0.00396807,-0.

00284420,0.00008962,0.55518521,0.03601824,-0.00930910,-0.00000511,0.04

398073,-0.11706489,-0.00141272,-0.01722242,0.01702216,0.00042033,-0.01

316578,-0.01124636,-0.00021080,0.00168848,-0.00506670,-0.00023762,0.01

145066,0.02494999,-0.00010809,0.00506103,-0.02990002,-0.00008438,-0.00

032348,0.02650681,-0.00002149,-0.00815069,-0.02820903,0.00007335,0.002

42683,-0.00307924,-0.00015626,0.00023024,0.00007657,0.00011499,-0.0011

4101,0.59594608,0.00075794,-0.00015938,0.00167850,-0.00096835,-0.00109

589,-0.04773799,0.00019476,0.00055810,-0.00495800,-0.00076593,-0.00001

468,0.00478524,-0.00005094,-0.00028475,0.00203993,0.00043131,-0.000108

09,0.00102884,-0.00014374,0.00022532,0.00022745,0.00005925,-0.00026086

,0.00030944,0.00006032,0.00025787,-0.00021035,-0.00000897,-0.00001514,

-0.00002955,0.00005748,0.00005170,-0.00003483,0.00264336,0.00417610,0.

12680957,-0.00158109,-0.00352119,0.00000283,-0.01861401,0.03650986,0.0

0032622,0.01539167,-0.00231460,-0.00004426,-0.01039636,0.00760957,0.00

005680,-0.00479112,-0.00180538,-0.00011666,0.00446276,-0.00506106,0.00

014375,-0.00570310,0.00862279,0.00000096,0.00012218,-0.00892363,-0.000

04777,-0.00032531,0.01028612,0.00001079,0.00127375,-0.00169458,0.00003

135,0.00251560,0.00274432,-0.00009293,-0.12694605,0.07847088,-0.000560

88,0.55542111,-0.00598137,0.00815636,0.00021854,0.02548224,-0.01825400

,0.00047225,0.00433119,-0.00487339,-0.00013851,-0.00147266,0.01131765,

0.00000473,-0.00211159,-0.00354051,-0.00019929,-0.00639590,-0.02990004

,0.00022532,-0.00862276,0.03921166,0.00007082,0.00045835,-0.03544118,-

0.00005897,0.01028610,0.03740303,-0.00006431,-0.00254504,0.00286288,0.

00021497,0.00118638,0.00114607,-0.00019053,0.06431335,-0.20707753,-0.0

0152285,-0.06967120,0.66589927,-0.00009815,0.00000424,0.00258859,0.000

70569,0.00003096,0.00581325,-0.00023034,-0.00008201,0.00018211,0.00032

955,-0.00006291,-0.00064201,0.00007489,0.00004546,0.00022079,-0.000248

61,-0.00008438,0.00022745,-0.00000097,0.00007083,-0.00026952,-0.000074

93,-0.00002604,0.00013753,-0.00001079,0.00006432,0.00014129,0.00001695

,0.00000212,0.00003822,-0.00000693,-0.00000207,0.00001145,-0.00090782,

-0.00036623,-0.05016975,0.00584394,0.00147250,0.14834285,-0.00170479,0

.00201498,-0.00003100,0.01124334,-0.00269875,-0.00010724,-0.00743545,0

.00047004,0.00005142,0.00674079,-0.00297427,-0.00002286,0.00231621,0.0

0157161,0.00008788,-0.00396808,-0.00023023,-0.00005748,0.00251560,-0.0

0118640,0.00000693,0.00007874,0.00187286,0.00003141,0.00127375,-0.0025

4505,-0.00001695,-0.00113063,0.00151470,0.00000879,-0.00156598,-0.0016

9918,0.00003231,-0.01102782,0.01952051,0.00002347,-0.22054609,0.029332

21,-0.00240352,0.65906600,0.00373924,-0.00196614,0.00000168,-0.0112646

3,-0.00188332,-0.00005075,0.00592245,0.00001918,-0.00001906,-0.0050779

3,0.00306884,0.00002968,-0.00225285,-0.00234545,-0.00009932,0.00284421

,0.00007655,0.00005170,-0.00274432,0.00114609,-0.00000207,-0.00018993,

-0.00182977,-0.00001784,-0.00169457,0.00286289,-0.00000212,0.00151470,

-0.00185779,-0.00001105,0.00169918,0.00208472,-0.00003795,0.03947792,-

0.02271292,0.00025337,0.01714568,-0.09103226,0.00040283,0.15576611,0.7

6257982,-0.00005569,-0.00002831,0.00095167,0.00024562,0.00001033,0.005

35678,-0.00021434,-0.00002053,0.00024437,0.00018500,-0.00010661,-0.000

25442,0.00006657,0.00007386,-0.00053915,-0.00008962,0.00011499,-0.0000

3483,0.00009293,-0.00019053,0.00001145,0.00000554,0.00019809,-0.000006

78,-0.00003135,-0.00021497,0.00003821,-0.00000879,0.00001105,0.0000194

9,-0.00003231,-0.00003795,-0.00001992,-0.00001649,-0.00027679,0.001864

58,-0.00235083,0.00104656,-0.06581767,0.00921132,0.00342409,0.12014544

,-0.00168981,0.00118209,0.00002726,0.00122511,-0.00021050,0.00003877,-

0.00094714,0.00113554,0.00003779,0.00095361,-0.00010244,-0.00001183,0.

00042153,0.00108435,0.00003168,-0.00038741,-0.00242683,0.00000897,0.00

127376,0.00254503,-0.00001695,0.00007875,-0.00187284,0.00003141,0.0025

1559,0.00118637,0.00000693,-0.00156598,0.00169917,0.00003231,-0.001130

63,-0.00151470,0.00000879,-0.00891814,0.00867510,-0.00013446,-0.007563

07,0.01950469,-0.00040907,-0.11636334,0.01412035,-0.00123621,0.6590659

9,-0.00165760,0.00205001,0.00001970,0.00656632,-0.00263809,0.00003567,

-0.00300495,-0.00064799,0.00003505,0.00362585,-0.00111023,-0.00001950,

0.00147964,0.00079414,0.00003246,-0.00280797,-0.00307922,-0.00001514,0

.00169458,0.00286285,0.00000212,0.00018993,-0.00182973,0.00001784,0.00

274431,0.00114606,0.00000207,-0.00169917,0.00208472,0.00003795,-0.0015

1470,-0.00185779,0.00001106,-0.00426626,0.01861318,0.00005195,0.062330

52,-0.05646178,0.00082234,-0.01412033,-0.42522323,-0.00035338,-0.15576

613,0.76257981,-0.00003650,0.00003831,-0.00026458,-0.00006289,-0.00006

279,-0.00019405,0.00009223,0.00002034,-0.00060818,-0.00007288,0.000040

08,0.00023790,-0.00000977,-0.00000424,0.00019559,0.00002498,-0.0001562

7,-0.00002955,-0.00003135,0.00021497,0.00003822,0.00000554,-0.00019809

,-0.00000678,0.00009293,0.00019053,0.00001145,-0.00003231,0.00003795,-

0.00001992,-0.00000879,-0.00001106,0.00001949,-0.00016237,0.00039218,0

.00180162,-0.00024436,-0.00008540,0.00890700,-0.00123621,0.00035332,-0

.05749135,0.00921130,-0.00342400,0.12014543,0.00197702,-0.00230173,-0.

00006698,-0.00041107,0.00432811,-0.00008518,-0.00441698,0.00129266,-0.

00000304,0.00258509,-0.00117789,0.00002120,-0.00047004,-0.00007193,0.0

0003082,-0.00051641,0.00815069,-0.00006032,-0.00032532,-0.01028609,0.0

0001079,0.00012217,0.00892359,-0.00004777,-0.00570309,-0.00862275,0.00

000097,0.00251560,-0.00274432,-0.00009293,0.00127376,0.00169458,0.0000

3135,-0.00370230,-0.02836473,-0.00005078,0.01595343,0.03444441,0.00032

179,-0.00756307,-0.06233052,-0.00024437,-0.22054608,-0.01714569,-0.002

35083,0.55542109,-0.00186406,0.00365737,0.00016962,-0.00191804,-0.0097

7216,0.00021441,0.00666111,0.00107691,0.00007533,-0.00156507,0.0113935

4,-0.00001825,-0.00289929,-0.00316866,-0.00018943,-0.00426967,-0.02820

908,0.00025787,-0.01028610,0.03740308,0.00006431,-0.00045835,-0.035441

23,0.00005898,0.00862279,0.03921170,-0.00007082,-0.00118639,0.00114609

,0.00019053,0.00254504,0.00286287,-0.00021497,-0.01011635,0.06518348,-

0.00047027,-0.03444445,-0.18991727,-0.00031359,-0.01950466,-0.05646181

,0.00008539,-0.02933218,-0.09103223,-0.00104657,0.06967104,0.66589888,

0.00003521,-0.00003591,-0.00003020,-0.00028678,0.00000349,-0.00003793,

0.00017469,0.00013934,-0.00051536,-0.00023667,0.00006212,0.00059032,-0

.00005419,-0.00003155,0.00004919,0.00017467,0.00007335,-0.00021035,-0.

00001079,-0.00006431,0.00014129,-0.00007493,0.00002604,0.00013753,-0.0

0000096,-0.00007082,-0.00026952,-0.00000693,0.00000207,0.00001145,0.00

001695,-0.00000212,0.00003821,0.00010771,-0.00019680,0.00406345,0.0003

2178,0.00031356,0.00511669,-0.00040908,-0.00082235,0.00890699,-0.00240

353,-0.00040283,-0.06581767,0.00584395,-0.00147244,0.14834287,-0.00059

075,0.00101754,0.00000303,-0.00186790,-0.00225153,-0.00010682,-0.00500

924,0.00841888,0.00081619,0.00272455,-0.00027677,0.00010844,0.00048302

,0.00164678,0.00004609,0.00031282,0.00032348,-0.00005925,0.00012217,-0

.00045834,0.00007493,0.00090856,0.,-0.00021073,0.00012218,0.00045835,0

.00007493,0.00007875,-0.00018993,-0.00000554,0.00007875,0.00018993,-0.

00000554,0.01533451,-0.00155056,0.00035968,-0.18398641,-0.06795618,-0.

00225007,-0.06856036,-0.01231490,-0.00136744,-0.06856036,0.01231489,-0

.00136744,-0.18398642,0.06795617,-0.00225006,0.54157848,0.00265471,-0.

00502244,-0.00021688,-0.00051996,0.01404769,-0.00017047,0.00022575,-0.

00217506,0.00057762,0.00321690,-0.01250431,-0.00000047,0.00301886,0.00

265320,0.00018692,0.00220736,0.02650685,-0.00026086,0.00892361,-0.0354

4121,-0.00002604,0.,0.03327319,0.,-0.00892362,-0.03544120,0.00002604,0

.00187286,-0.00182976,-0.00019809,-0.00187285,-0.00182974,0.00019809,-

0.01768989,-0.11161289,0.00011842,-0.08900964,-0.11356267,-0.00146982,

-0.03732776,-0.00248182,-0.00115234,0.03732773,-0.00248184,0.00115234,

0.08900969,-0.11356263,0.00146981,-0.00000002,0.44522305,-0.00000674,0

.00005822,-0.00000705,-0.00003206,0.00006088,-0.00159927,0.00028788,0.

00116078,0.00418194,0.00027173,0.00001575,-0.00023346,0.00002988,0.000

05605,-0.00033500,-0.00009672,-0.00002148,0.00030944,0.00004777,-0.000

05898,0.00013753,0.00021073,0.,-0.00112237,0.00004777,0.00005897,0.000

13753,-0.00003141,0.00001784,-0.00000678,-0.00003141,-0.00001784,-0.00

000678,0.00003387,-0.00016536,-0.00109033,-0.00223624,-0.00052889,-0.0

6749278,-0.00151269,-0.00029645,0.01534988,-0.00151268,0.00029645,0.01

534988,-0.00223622,0.00052888,-0.06749278,0.02095779,0.00000004,0.0882

8249,0.00253785,-0.00210071,0.00018660,-0.03980410,-0.00144209,0.00009

121,0.03110311,-0.00018327,-0.00007938,-0.03413053,0.00956002,0.000086

44,-0.00600548,-0.00307077,-0.00028408,0.02547674,0.00618771,0.0002724

4,-0.00051642,-0.00426968,-0.00017467,0.00031282,0.00220735,0.00009672

,0.00446275,-0.00639589,0.00024862,-0.00396806,0.00284419,0.00008962,-

0.00038739,-0.00280795,-0.00002498,0.03466457,-0.00649979,-0.00034437,

-0.00370233,0.01011641,0.00010771,-0.00891811,0.00426622,-0.00016237,-

0.01102777,-0.03947786,-0.00001650,-0.12694607,-0.06431328,-0.00090783

,0.01533450,0.01768988,0.00003387,0.55518503,0.00066798,-0.00184447,-0

.00008827,-0.00228953,0.00541734,-0.00015882,-0.00323439,0.00091167,0.

00001285,-0.00192185,-0.00776484,0.00000967,0.00215326,0.00294787,0.00

012921,0.00618770,0.02141135,-0.00015829,0.00815070,-0.02820907,-0.000

07335,0.00032348,0.02650686,0.00002148,-0.00506106,-0.02990006,0.00008

438,-0.00023023,0.00007655,-0.00011499,-0.00242683,-0.00307923,0.00015

626,0.00649973,-0.04538568,0.00027359,0.02836477,0.06518349,0.00019681

,-0.00867512,0.01861320,-0.00039217,-0.01952052,-0.02271294,0.00027679

,-0.07847078,-0.20707716,0.00036621,0.00155058,-0.11161293,0.00016534,

0.00114085,0.59594572,-0.00001788,0.00000790,-0.00004275,0.00049089,0.

00008729,-0.00009130,-0.00044494,-0.00005171,0.00025922,0.00043693,-0.

00017589,-0.00005987,0.00008804,0.00005711,0.00004901,-0.00027244,0.00

015829,-0.00001210,0.00006032,-0.00025787,-0.00021035,0.00005925,0.000

26086,0.00030944,-0.00014375,-0.00022532,0.00022745,0.00005748,-0.0000

5170,-0.00003483,-0.00000897,0.00001514,-0.00002955,-0.00034438,-0.000

27360,0.00122039,-0.00005078,0.00047028,0.00406345,-0.00013446,-0.0000

5195,0.00180161,0.00002347,-0.00025338,0.00186458,-0.00056089,0.001522

84,-0.05016976,0.00035968,-0.00011844,-0.00109033,0.00264334,-0.004176

06,0.12680956,-0.00019507,0.00039204,-0.00031186,0.05052851,0.00582648

,-0.00007286,-0.04135131,-0.00006305,0.00001938,0.04529218,-0.01139007

,-0.00003862,0.00539084,0.00271497,0.00036362,-0.03413053,-0.00192187,

-0.00043693,0.00258512,-0.00156504,0.00023667,0.00272455,0.00321690,-0

.00027173,-0.01039634,-0.00147268,-0.00032956,0.00674077,-0.00507790,-

0.00018500,0.00095359,0.00362583,0.00007288,-0.03980412,0.00228960,0.0

0049088,-0.00041102,0.00191797,-0.00028678,0.00122507,-0.00656626,-0.0

0006289,0.01124328,0.01126457,0.00024563,-0.01861393,-0.02548216,0.000

70570,-0.00186789,0.00051996,-0.00003206,-0.17093411,-0.04398073,-0.00

096835,0.64786768,-0.00590378,0.00398073,0.00016006,-0.00582652,-0.008

37111,-0.00009351,0.00847126,0.00051626,0.00010687,-0.01139004,-0.0023

7881,-0.00013477,0.00428551,0.00267974,-0.00001711,0.00956000,-0.00776

481,0.00017589,-0.00117789,0.01139351,-0.00006212,-0.00027677,-0.01250

429,-0.00001575,0.00760955,0.01131764,0.00006291,-0.00297426,0.0030688

3,0.00010661,-0.00010243,-0.00111022,-0.00004008,0.00144211,0.00541734

,-0.00008729,-0.00432812,-0.00977216,-0.00000349,0.00021050,-0.0026381

0,0.00006279,0.00269875,-0.00188332,-0.00001033,-0.03650984,-0.0182540

1,-0.00003096,0.00225153,0.01404771,-0.00006088,-0.05114646,-0.1170648

6,0.00109589,0.05545890,0.58189133,0.00011078,-0.00006679,0.00002080,-

0.00007287,0.00009351,0.00000240,0.00004025,0.00007758,0.00008769,0.00

003862,0.00013477,-0.00003514,-0.00011631,-0.00008399,-0.00005727,-0.0

0008644,-0.00000967,-0.00005987,-0.00002120,0.00001825,0.00059032,-0.0

0010844,0.00000047,-0.00023346,-0.00005680,-0.00000473,-0.00064201,0.0

0002286,-0.00002968,-0.00025442,0.00001183,0.00001950,0.00023790,0.000

09122,0.00015882,-0.00009130,-0.00008518,-0.00021442,-0.00003793,0.000

03877,-0.00003567,-0.00019405,-0.00010724,0.00005075,0.00535678,0.0003

2622,-0.00047226,0.00581323,-0.00010682,0.00017047,-0.00159927,0.00015

101,0.00141273,-0.04773799,0.00063985,-0.01069793,0.14220109,0.0053119

4,-0.00337792,-0.00009137,-0.00019503,0.00590378,0.00011078,-0.0024570

9,-0.00034044,-0.00008574,0.00539083,0.00428551,0.00011631,-0.00486266

,-0.00303839,-0.00004390,-0.00600547,0.00215324,-0.00008804,-0.0004700

3,-0.00289926,0.00005419,0.00048302,0.00301884,-0.00002988,-0.00479111

,-0.00211159,-0.00007489,0.00231621,-0.00225285,-0.00006657,0.00042152

,0.00147964,0.00000977,0.00253782,-0.00066799,-0.00001788,0.00197703,0

.00186408,0.00003521,-0.00168981,0.00165760,-0.00003650,-0.00170478,-0

.00373923,-0.00005569,-0.00158111,0.00598138,-0.00009815,-0.00059075,-

0.00265473,-0.00000674,-0.02088910,-0.03601823,0.00075794,-0.09766284,

-0.02307041,0.00069611,0.69142457,0.00337792,-0.00227247,-0.00005974,-

0.00039201,0.00398074,0.00006679,-0.00142236,-0.00032743,-0.00007199,0

.00271496,0.00267975,0.00008399,-0.00303839,-0.00195499,-0.00003145,-0

.00307077,0.00294786,-0.00005710,-0.00007193,-0.00316864,0.00003155,0.

00164678,0.00265319,-0.00005605,-0.00180538,-0.00354051,-0.00004546,0.

00157160,-0.00234544,-0.00007386,0.00108435,0.00079413,0.00000424,0.00

210070,-0.00184448,-0.00000790,0.00230173,0.00365738,0.00003591,-0.001

18209,0.00205001,-0.00003832,-0.00201498,-0.00196614,0.00002831,0.0035

2118,0.00815636,-0.00000424,-0.00101754,-0.00502245,-0.00005823,-0.020

71368,-0.00930909,0.00015938,-0.04420209,-0.25569195,0.00487480,-0.148

00272,0.69761839,-0.00009137,0.00005974,0.00001945,-0.00031186,-0.0001

6006,0.00002080,0.00031608,0.00000528,0.00001003,-0.00036362,0.0000171

1,-0.00005727,0.00004390,0.00003145,-0.00001553,0.00028408,-0.00012920

,0.00004901,-0.00003082,0.00018943,0.00004919,-0.00004609,-0.00018692,

-0.00033500,0.00011666,0.00019929,0.00022079,-0.00008788,0.00009932,-0

.00053915,-0.00003168,-0.00003246,0.00019559,0.00018660,0.00008827,-0.

00004275,-0.00006698,-0.00016962,-0.00003020,0.00002726,-0.00001971,-0

.00026458,-0.00003100,-0.00000167,0.00095167,0.00000283,-0.00021854,0.

00258858,0.00000303,0.00021688,-0.00000705,-0.00019635,0.00000511,0.00

167850,0.00192487,0.00501707,-0.06631069,0.00482710,-0.01628350,0.1132

4454,-0.00486267,0.00303839,0.00004390,0.00539081,-0.00428552,-0.00011

631,-0.00245707,0.00034044,0.00008574,-0.00019505,-0.00590378,-0.00011

078,0.00531194,0.00337792,0.00009137,0.00253784,0.00066799,0.00001788,

0.00197703,-0.00186407,-0.00003521,-0.00059076,0.00265472,0.00000674,-

0.00158110,-0.00598137,0.00009815,-0.00170478,0.00373923,0.00005570,-0

.00168981,-0.00165760,0.00003650,-0.00600545,-0.00215323,0.00008804,-0

.00047003,0.00289925,-0.00005419,0.00042152,-0.00147963,-0.00000977,0.

00231620,0.00225284,0.00006657,-0.00479110,0.00211159,0.00007489,0.000

48302,-0.00301884,0.00002988,0.01258250,-0.00168849,-0.00005094,-0.051

23635,-0.07366471,0.00187622,-0.34702549,0.01836727,-0.00059589,0.6914

2457,0.00303840,-0.00195499,-0.00003145,-0.00271495,0.00267975,0.00008

399,0.00142234,-0.00032743,-0.00007199,0.00039203,0.00398073,0.0000667

9,-0.00337792,-0.00227247,-0.00005974,-0.00210071,-0.00184448,-0.00000

790,-0.00230173,0.00365738,0.00003591,0.00101754,-0.00502245,-0.000058

23,-0.00352118,0.00815636,-0.00000424,0.00201498,-0.00196614,0.0000283

1,0.00118209,0.00205001,-0.00003831,0.00307076,0.00294785,-0.00005710,

0.00007193,-0.00316863,0.00003155,-0.00108435,0.00079413,0.00000424,-0

.00157160,-0.00234544,-0.00007386,0.00180537,-0.00354051,-0.00004546,-

0.00164678,0.00265319,-0.00005605,-0.00609211,-0.00506669,0.00028475,-

0.01961694,-0.00695587,0.00055839,-0.01836727,-0.11375705,0.00191147,0

.14800270,0.69761842,-0.00004390,0.00003145,-0.00001553,0.00036362,0.0

0001711,-0.00005727,-0.00031608,0.00000528,0.00001003,0.00031186,-0.00

016006,0.00002080,0.00009137,0.00005974,0.00001945,-0.00018660,0.00008

827,-0.00004275,0.00006698,-0.00016962,-0.00003020,-0.00000303,0.00021

688,-0.00000705,-0.00000283,-0.00021854,0.00258859,0.00003100,-0.00000

168,0.00095167,-0.00002726,-0.00001970,-0.00026458,-0.00028408,-0.0001

2920,0.00004901,0.00003082,0.00018943,0.00004919,0.00003167,-0.0000324

6,0.00019559,0.00008788,0.00009932,-0.00053915,-0.00011666,0.00019929,

0.00022079,0.00004609,-0.00018692,-0.00033500,0.00051648,0.00023762,0.

00203993,0.00005398,0.00035749,0.01157721,0.00059594,0.00191147,-0.055

79207,-0.00482720,-0.01628353,0.11324454,0.00539079,-0.00271494,-0.000

36362,0.04529225,0.01139002,0.00003862,-0.04135133,0.00006306,-0.00001

939,0.05052849,-0.00582654,0.00007287,-0.00019501,-0.00039200,0.000311

86,-0.03980408,-0.00228956,-0.00049089,-0.00041105,-0.00191799,0.00028

678,-0.00186789,-0.00051996,0.00003206,-0.01861396,0.02548222,-0.00070

570,0.01124331,-0.01126460,-0.00024562,0.00122509,0.00656629,0.0000628

9,-0.03413060,0.00192188,0.00043692,0.00258515,0.00156505,-0.00023666,

0.00095357,-0.00362580,-0.00007288,0.00674076,0.00507788,0.00018500,-0

.01039633,0.00147276,0.00032956,0.00272455,-0.00321693,0.00027173,0.06

106952,0.01316570,-0.00076594,-0.18456319,0.02428960,-0.00032936,-0.05

123639,0.01961691,-0.00005397,-0.09766281,0.04420207,-0.00192487,0.647

86793,-0.00428553,0.00267975,-0.00001711,0.01139003,-0.00237883,-0.000

13477,-0.00847124,0.00051626,0.00010686,0.00582648,-0.00837112,-0.0000

9351,0.00590379,0.00398074,0.00016006,-0.00144208,0.00541734,-0.000087

30,0.00432811,-0.00977216,-0.00000349,-0.00225153,0.01404770,-0.000060

88,0.03650986,-0.01825401,-0.00003096,-0.00269875,-0.00188333,-0.00001

033,-0.00021050,-0.00263810,0.00006279,-0.00955999,-0.00776480,0.00017

589,0.00117790,0.01139349,-0.00006212,0.00010242,-0.00111021,-0.000040

08,0.00297425,0.00306882,0.00010661,-0.00760953,0.01131765,0.00006291,

0.00027678,-0.01250428,-0.00001575,0.01667393,-0.01124637,0.00001468,-

0.02428955,0.00803812,0.00011736,0.07366470,-0.00695587,0.00035748,0.0

2307043,-0.25569197,0.00501707,-0.05545900,0.58189139,0.00011631,-0.00

008399,-0.00005727,-0.00003862,0.00013477,-0.00003514,-0.00004024,0.00

007758,0.00008769,0.00007286,0.00009351,0.00000240,-0.00011078,-0.0000

6679,0.00002080,-0.00009122,0.00015882,-0.00009130,0.00008518,-0.00021

442,-0.00003793,0.00010682,0.00017047,-0.00159927,-0.00032622,-0.00047

226,0.00581325,0.00010724,0.00005075,0.00535678,-0.00003877,-0.0000356

7,-0.00019405,0.00008645,-0.00000967,-0.00005987,0.00002120,0.00001825

,0.00059032,-0.00001183,0.00001950,0.00023790,-0.00002286,-0.00002968,

-0.00025442,0.00005681,-0.00000474,-0.00064201,0.00010844,0.00000047,-

0.00023346,-0.00017474,0.00021080,0.00478524,0.00032939,0.00011735,0.0

1120186,-0.00187621,0.00055839,0.01157721,-0.00069611,0.00487479,-0.06

631069,-0.00063993,-0.01069793,0.14220107,-0.00245705,0.00142234,0.000

31608,-0.04135134,-0.00847123,0.00004024,0.03687281,0.,0.,-0.04135130,

0.00847128,-0.00004025,-0.00245710,-0.00142237,-0.00031608,0.03110310,

-0.00323436,0.00044494,-0.00441700,0.00666107,-0.00017469,-0.00500925,

0.00022576,-0.00028788,0.01539164,0.00433119,0.00023034,-0.00743543,0.

00592243,0.00021434,-0.00094712,-0.00300493,-0.00009223,0.03110315,0.0

0323433,-0.00044493,-0.00441703,-0.00666106,0.00017469,-0.00094711,0.0

0300490,0.00009223,-0.00743541,-0.00592240,-0.00021434,0.01539162,-0.0

0433125,-0.00023035,-0.00500924,-0.00022572,0.00028786,-0.08843618,0.0

1722247,0.00019477,-0.13557435,0.09551419,-0.00279239,-0.00723872,0.04

451239,-0.00170617,-0.00723875,-0.04451237,0.00170618,-0.13557432,-0.0

9551422,0.00279241,0.45876820,0.00034044,-0.00032743,-0.00000528,0.000

06306,0.00051627,-0.00007758,0.,0.00136306,0.00033633,-0.00006305,0.00

051626,-0.00007758,-0.00034044,-0.00032743,-0.00000528,-0.00018327,0.0

0091168,0.00005171,0.00129267,0.00107691,-0.00013934,0.00841888,-0.002

17505,-0.00116076,-0.00231460,-0.00487340,0.00008200,0.00047004,0.0000

1918,0.00002053,0.00113553,-0.00064799,-0.00002034,0.00018327,0.000911

67,0.00005171,-0.00129266,0.00107692,-0.00013934,-0.00113553,-0.000647

99,-0.00002034,-0.00047004,0.00001918,0.00002053,0.00231460,-0.0048733

9,0.00008200,-0.00841886,-0.00217504,-0.00116081,-0.00404090,0.0170221

6,-0.00055811,0.07413949,-0.17760787,0.00313630,0.00294478,-0.07663019

,0.00243847,-0.00294478,-0.07663020,0.00243847,-0.07413950,-0.17760787

,0.00313631,0.00000001,0.54904252,-0.00008574,0.00007199,0.00001003,0.

00001939,-0.00010686,0.00008769,0.,-0.00033633,-0.00072795,-0.00001938

,-0.00010687,0.00008769,0.00008574,0.00007199,0.00001003,0.00007938,-0

.00001285,0.00025922,0.00000304,-0.00007533,-0.00051536,-0.00081621,-0

.00057762,0.00418194,0.00004427,0.00013851,0.00018211,-0.00005142,0.00

001906,0.00024437,-0.00003779,-0.00003505,-0.00060818,-0.00007939,-0.0

0001285,0.00025922,-0.00000304,-0.00007532,-0.00051536,0.00003779,-0.0

0003505,-0.00060818,0.00005142,0.00001906,0.00024437,-0.00004427,0.000

13851,0.00018211,0.00081617,-0.00057763,0.00418192,0.00014668,-0.00042

033,-0.00495800,-0.00151703,0.00306692,-0.06970284,-0.00012985,0.00269

644,0.01677087,0.00012985,0.00269645,0.01677087,0.00151704,0.00306694,

-0.06970285,0.00000001,-0.02410559,0.09445853,-0.16504540,-0.14246988,

-0.00440108,0.00999396,0.00764967,0.00024200,0.00014102,0.00357536,0.0

0010702,-0.00550305,0.00036487,0.00001087,-0.00596089,-0.02310807,-0.0

0070527,0.00048738,-0.00158506,-0.00003611,-0.00059451,0.00032835,0.00

000631,0.00011770,-0.00005651,-0.00000760,0.00002652,0.00009069,0.0000

0144,-0.00002891,-0.00005366,0.00000177,0.00011311,-0.00005534,-0.0000

0023,0.00007547,-0.00075618,-0.00000528,0.00016944,-0.00008791,-0.0000

0862,-0.00011224,0.00004303,-0.00000174,-0.00003214,-0.00008274,-0.000

00108,0.00007864,-0.00006823,0.00000427,-0.00001673,0.00001189,-0.0000

0421,0.00004052,0.00001958,-0.00000220,0.00005723,-0.00018901,0.000005

35,0.00016865,0.00010913,-0.00000359,-0.00015199,0.00009695,-0.0000014

6,0.00016831,-0.00012551,0.00000405,-0.00010312,0.00001424,-0.00000313

,0.16721968,-0.14084450,-0.24540975,-0.00656351,-0.01785820,-0.0095461

5,-0.00028099,-0.00009900,-0.00590894,-0.00039242,0.00189685,-0.000837

20,-0.00017342,0.00425138,0.00818454,0.00020751,0.00030546,0.00052252,

-0.00001737,0.00013269,0.00004899,0.00000280,-0.00026668,-0.00039792,0

.00000664,-0.00001923,0.00025944,0.00000318,-0.00004073,-0.00005105,0.

00000110,0.00002955,0.00007154,0.00000227,-0.00100127,0.00036302,0.000

04497,0.00006891,-0.00039501,0.00001119,-0.00000625,0.00003150,0.00000

153,0.00001721,-0.00007265,-0.00000126,0.00011430,-0.00014511,-0.00000

633,0.00014931,0.00022446,0.00000882,-0.00016220,0.00012132,0.00000664

,0.00024009,-0.00008013,-0.00000275,0.00004521,0.00002085,-0.00000208,

-0.00000728,-0.00000182,0.00000183,0.00025900,0.00004767,0.00000030,-0

.00022987,-0.00001080,-0.00000034,0.15443637,0.25174244,-0.00444998,-0

.00662049,-0.02687025,-0.00050827,-0.00016787,-0.00177710,-0.00014630,

-0.00029006,0.00528075,0.00012889,-0.00028194,0.00507613,0.00023923,0.

00026758,0.00097448,0.00000922,-0.00001249,0.00131812,0.00000295,-0.00

000504,-0.00032498,-0.00000316,-0.00000690,-0.00001390,-0.00000448,-0.

00000479,-0.00004501,0.00000235,-0.00000158,0.00000691,-0.00000491,0.0

0000118,-0.00017835,-0.00001193,0.00002513,-0.00180405,-0.00000097,0.0

0002671,-0.00013931,-0.00000312,-0.00000085,0.00002563,0.00000317,-0.0

0000143,0.00000736,-0.00000180,0.00001197,0.00006548,0.00000433,-0.000

01323,-0.00009124,0.00000684,-0.00000599,-0.00000695,-0.00000792,-0.00

000259,0.00000212,0.00000231,0.00000090,-0.00000173,-0.00000328,0.0000

0231,0.00000029,-0.00000602,-0.00000492,0.00001211,0.00000493,-0.00000

198,-0.00000020,0.00477815,0.00697391,0.02099842,-0.00596089,0.0231080

7,0.00070527,-0.00550305,-0.00036487,-0.00001087,0.00014102,-0.0035753

6,-0.00010702,0.00999396,-0.00764967,-0.00024200,-0.16504541,0.1424698

9,0.00440108,0.00007547,0.00075618,0.00000528,0.00016944,0.00008791,0.

00000862,-0.00001673,-0.00001189,0.00000421,0.00007864,0.00006823,-0.0

0000427,-0.00003214,0.00008274,0.00000108,-0.00011224,-0.00004303,0.00

000174,0.00048738,0.00158506,0.00003611,-0.00059452,-0.00032835,-0.000

00631,0.00011311,0.00005534,0.00000023,-0.00002891,0.00005366,-0.00000

177,0.00002652,-0.00009069,-0.00000144,0.00011770,0.00005651,0.0000076

0,-0.00019274,0.00008490,0.00000362,0.00016831,0.00012551,-0.00000405,

-0.00015199,-0.00009695,0.00000146,0.00016865,-0.00010913,0.00000359,0

.00005723,0.00018901,-0.00000535,-0.00010312,-0.00001424,0.00000313,0.

00094483,-0.00080458,-0.00002939,0.16721969,-0.00425138,0.00818454,0.0

0020751,-0.00189685,-0.00083720,-0.00017342,0.00009900,-0.00590894,-0.

00039242,0.01785820,-0.00954615,-0.00028099,0.14084450,-0.24540974,-0.

00656350,0.00100127,0.00036302,0.00004497,-0.00006891,-0.00039501,0.00

001119,-0.00014931,0.00022446,0.00000882,-0.00011430,-0.00014510,-0.00

000633,-0.00001721,-0.00007265,-0.00000126,0.00000625,0.00003150,0.000

00153,-0.00030546,0.00052252,-0.00001737,-0.00013269,0.00004899,0.0000

0280,-0.00002955,0.00007154,0.00000227,0.00004073,-0.00005105,0.000001

10,0.00001923,0.00025944,0.00000318,0.00026668,-0.00039792,0.00000664,

0.00017957,-0.00009433,-0.00000237,-0.00025900,0.00004767,0.00000030,0

.00000728,-0.00000182,0.00000183,-0.00004521,0.00002085,-0.00000208,-0

.00024009,-0.00008012,-0.00000275,0.00022987,-0.00001080,-0.00000034,0

.00080458,-0.00011359,0.00008607,-0.15443638,0.25174243,-0.00023923,0.

00026758,0.00097448,-0.00012889,-0.00028194,0.00507613,0.00014630,-0.0

0029006,0.00528075,0.00050827,-0.00016787,-0.00177710,0.00444998,-0.00

662049,-0.02687024,0.00001193,0.00002513,-0.00180405,0.00000097,0.0000

2671,-0.00013931,-0.00000433,-0.00001323,-0.00009124,0.00000180,0.0000

1197,0.00006548,-0.00000317,-0.00000143,0.00000736,0.00000312,-0.00000

085,0.00002563,-0.00000922,-0.00001249,0.00131812,-0.00000295,-0.00000

504,-0.00032498,0.00000491,0.00000118,-0.00017835,-0.00000235,-0.00000

158,0.00000691,0.00000448,-0.00000479,-0.00004501,0.00000316,-0.000006

90,-0.00001390,-0.00000347,0.00000492,-0.00001513,0.00000602,-0.000004

92,0.00001211,0.00000328,0.00000231,0.00000029,-0.00000231,0.00000090,

-0.00000173,0.00000792,-0.00000259,0.00000212,-0.00000493,-0.00000198,

-0.00000020,0.00002939,0.00008607,-0.00313922,-0.00477814,0.00697391,0

.02099842,0.00002329,-0.00008247,-0.00000266,0.00020487,0.00007057,-0.

00000251,-0.00038681,-0.00024376,-0.00000176,0.00009984,0.00018520,-0.

00000914,0.00002215,-0.00001806,-0.00000144,0.00052150,0.00017798,-0.0

0000241,-0.00106748,0.00201574,0.00016390,-0.00538325,-0.00024308,0.00

024525,-0.00907152,-0.01740944,0.00019592,-0.24575606,-0.14314395,0.00

406646,0.00853140,0.00455198,-0.00009768,-0.00003065,-0.00019842,0.000

00309,0.00004717,0.00027853,-0.00000020,-0.00000183,-0.00002242,-0.000

00115,0.00004037,0.00005056,0.00000168,-0.00010155,0.00023008,0.000003

00,-0.00001214,-0.00024105,-0.00000011,0.00018778,-0.00013885,-0.00000

732,-0.00028034,0.00018405,0.00000286,-0.00011738,-0.00001321,0.000002

31,0.00004676,-0.00001238,-0.00000325,-0.00044472,0.00006960,-0.000011

90,0.00032247,0.00010766,-0.00000229,0.00000625,-0.00001294,0.00000057

,0.00000158,-0.00000778,-0.00000042,0.25104498,-0.00004869,-0.00002029

,-0.00000099,-0.00014135,-0.00000580,0.00000047,0.00018824,0.00010441,

0.00000411,0.00008956,-0.00046395,-0.00000802,-0.00009165,0.00007783,0

.00000154,-0.00148411,0.00037126,0.00002430,0.00062834,-0.00528426,-0.

00001322,0.00387986,0.00007715,-0.00007996,0.00803292,0.01013708,-0.00

016628,-0.14379565,-0.16688735,0.00285289,-0.02358535,-0.00688393,0.00

046612,0.00006603,-0.00006179,-0.00000006,-0.00005237,0.00004246,-0.00

000047,0.00004294,-0.00005608,0.00000060,0.00004922,0.00005894,0.00000

117,-0.00007552,0.00001230,-0.00000168,-0.00000251,-0.00002635,0.00000

166,0.00014798,0.00003384,0.00000036,-0.00025489,0.00010898,-0.0000036

0,-0.00010031,-0.00005113,0.00000288,0.00004229,-0.00010573,0.00000208

,-0.00028721,0.00006811,0.00000549,0.00018044,-0.00001082,0.00000246,-

0.00001809,0.00000592,0.00000004,0.00000510,-0.00000151,-0.00000017,0.

15551207,0.16976750,0.00000503,-0.00000695,0.00002204,0.00001509,0.000

00995,-0.00010623,-0.00000475,-0.00000659,0.00013547,0.00001614,0.0000

0569,-0.00083382,-0.00000989,0.00000437,-0.00015450,-0.00001078,-0.000

02154,0.00083021,0.00024430,-0.00006922,0.00750644,0.00012682,0.000105

29,0.00399348,0.00008389,0.00032072,-0.00107837,0.00415861,0.00294800,

-0.03165592,-0.00015392,-0.00020214,0.00340093,-0.00001030,0.00000211,

0.00001877,0.00000131,-0.00000150,-0.00000109,-0.00000161,0.00000053,-

0.00000576,-0.00000012,-0.00000166,-0.00000094,0.00000293,-0.00000157,

0.00000415,0.00000038,0.00000227,0.00000398,0.00000356,-0.00000046,-0.

00002142,-0.00000314,0.00000028,0.00006857,0.00000266,0.00000093,-0.00

000836,0.,0.00000138,-0.00001160,-0.00001041,0.00000257,-0.00011556,0.

00000426,-0.00000443,-0.00011472,-0.00000039,-0.00000139,0.00005963,-0

.00000008,0.00000035,-0.00002198,-0.00438595,-0.00308453,0.02269970,-0

.00011738,0.00001320,0.00000231,-0.00028034,-0.00018405,0.00000286,0.0

0032247,-0.00010766,-0.00000229,-0.00044472,-0.00006960,-0.00001190,0.

00004676,0.00001238,-0.00000325,0.00036846,0.00049117,-0.00000696,-0.0

0907152,0.01740944,0.00019592,-0.00538325,0.00024308,0.00024525,-0.001

06748,-0.00201574,0.00016390,0.00853140,-0.00455198,-0.00009768,-0.245

75608,0.14314395,0.00406644,0.00018778,0.00013885,-0.00000732,-0.00010

155,-0.00023008,0.00000300,0.00004037,-0.00005056,0.00000168,-0.000001

83,0.00002242,-0.00000115,0.00004717,-0.00027853,-0.00000020,-0.000012

14,0.00024106,-0.00000011,-0.00003065,0.00019842,0.00000309,0.00020487

,-0.00007057,-0.00000251,0.00002329,0.00008247,-0.00000266,0.00002215,

0.00001806,-0.00000144,0.00009984,-0.00018520,-0.00000914,-0.00038682,

0.00024376,-0.00000176,-0.00000513,-0.00000875,0.00000012,0.00001048,-

0.00002610,0.00000002,-0.00006009,0.00075007,-0.00007204,0.25104500,0.

00010031,-0.00005113,-0.00000288,0.00025489,0.00010898,0.00000360,-0.0

0018044,-0.00001082,-0.00000246,0.00028722,0.00006810,-0.00000549,-0.0

0004229,-0.00010573,-0.00000208,0.00057348,0.00023460,-0.00000004,-0.0

0803292,0.01013708,0.00016628,-0.00387986,0.00007716,0.00007996,-0.000

62834,-0.00528426,0.00001322,0.02358535,-0.00688393,-0.00046612,0.1437

9565,-0.16688734,-0.00285288,-0.00014799,0.00003384,-0.00000036,0.0000

7552,0.00001230,0.00000168,-0.00004922,0.00005894,-0.00000117,-0.00004

294,-0.00005608,-0.00000060,0.00005237,0.00004247,0.00000047,0.0000025

1,-0.00002635,-0.00000166,-0.00006603,-0.00006180,0.00000006,0.0001413

5,-0.00000580,-0.00000047,0.00004869,-0.00002029,0.00000099,0.00009165

,0.00007783,-0.00000154,-0.00008956,-0.00046395,0.00000802,-0.00018823

,0.00010441,-0.00000411,0.00000584,0.00000167,0.00000019,-0.00000970,0

.00000521,0.00000088,-0.00075007,0.00099606,0.00002217,-0.15551207,0.1

6976749,0.00000267,-0.00000093,-0.00000836,-0.00000314,-0.00000028,0.0

0006857,0.00000426,0.00000443,-0.00011472,-0.00001040,-0.00000257,-0.0

0011556,0.,-0.00000138,-0.00001160,-0.00000687,0.00001983,-0.00129004,

0.00008389,-0.00032072,-0.00107837,0.00012682,-0.00010529,0.00399348,0

.00024430,0.00006922,0.00750644,-0.00015393,0.00020214,0.00340093,0.00

415859,-0.00294798,-0.03165591,0.00000356,0.00000046,-0.00002142,0.000

00293,0.00000157,0.00000415,-0.00000012,0.00000166,-0.00000094,-0.0000

0161,-0.00000053,-0.00000576,0.00000131,0.00000150,-0.00000109,0.00000

038,-0.00000227,0.00000398,-0.00001030,-0.00000211,0.00001877,0.000015

09,-0.00000995,-0.00010623,0.00000503,0.00000695,0.00002204,-0.0000098

9,-0.00000437,-0.00015450,0.00001614,-0.00000569,-0.00083382,-0.000004

75,0.00000659,0.00013547,0.00000023,0.00000002,-0.00000490,-0.00000121

,-0.00000140,0.00004675,-0.00007204,-0.00002217,-0.00419542,-0.0043859

3,0.00308452,0.02269970,0.00004676,-0.00001238,0.00000325,-0.00044472,

0.00006960,0.00001190,0.00032247,0.00010766,0.00000229,-0.00028034,0.0

0018405,-0.00000286,-0.00011738,-0.00001320,-0.00000231,0.00018778,-0.

00013885,0.00000732,-0.00010155,0.00023008,-0.00000300,-0.00001214,-0.

00024105,0.00000011,0.00004717,0.00027853,0.00000020,-0.00000183,-0.00

002242,0.00000115,0.00004037,0.00005056,-0.00000168,0.00036846,-0.0004

9117,0.00000696,-0.00907152,-0.01740944,-0.00019592,-0.24575606,-0.143

14396,-0.00406648,0.00853140,0.00455199,0.00009768,-0.00106748,0.00201

574,-0.00016390,-0.00538325,-0.00024308,-0.00024525,0.00052149,0.00017

798,0.00000241,0.00009984,0.00018520,0.00000914,0.00002215,-0.00001806

,0.00000144,0.00002329,-0.00008247,0.00000266,0.00020487,0.00007057,0.

00000251,-0.00038681,-0.00024376,0.00000176,0.00001048,0.00002610,-0.0

0000002,-0.00000513,0.00000875,-0.00000012,-0.00000017,-0.00000096,0.0

0000011,-0.00000487,0.00000152,-0.00000003,0.25104498,0.00004229,-0.00

010573,-0.00000208,-0.00028722,0.00006810,-0.00000549,0.00018044,-0.00

001082,-0.00000246,-0.00025489,0.00010898,0.00000360,-0.00010031,-0.00

005113,-0.00000288,0.00014799,0.00003384,-0.00000036,-0.00007552,0.000

01230,0.00000168,-0.00000251,-0.00002635,-0.00000166,-0.00005237,0.000

04247,0.00000047,0.00004294,-0.00005608,-0.00000060,0.00004922,0.00005

894,-0.00000117,-0.00057348,0.00023460,-0.00000004,0.00803292,0.010137

08,0.00016628,-0.14379565,-0.16688736,-0.00285291,-0.02358535,-0.00688

393,-0.00046612,0.00062834,-0.00528426,0.00001322,0.00387986,0.0000771

6,0.00007996,-0.00148411,0.00037127,-0.00002430,0.00008956,-0.00046395

,0.00000802,-0.00009165,0.00007784,-0.00000154,-0.00004869,-0.00002029

,0.00000099,-0.00014135,-0.00000579,-0.00000047,0.00018823,0.00010441,

-0.00000411,0.00000970,0.00000521,0.00000088,-0.00000584,0.00000167,0.

00000019,-0.00000096,-0.00000197,0.00000008,-0.00000152,0.00000226,0.0

0000002,0.15551208,0.16976750,0.,-0.00000138,-0.00001160,0.00001040,-0

.00000257,-0.00011556,-0.00000426,0.00000443,-0.00011472,0.00000314,-0

.00000028,0.00006857,-0.00000266,-0.00000093,-0.00000836,-0.00000356,0

.00000046,-0.00002142,-0.00000293,0.00000157,0.00000415,-0.00000038,-0

.00000227,0.00000398,-0.00000131,0.00000150,-0.00000109,0.00000161,-0.

00000053,-0.00000576,0.00000012,0.00000166,-0.00000094,0.00000687,0.00

001983,-0.00129004,-0.00008389,-0.00032072,-0.00107837,-0.00415863,-0.

00294801,-0.03165591,0.00015392,0.00020214,0.00340093,-0.00024430,0.00

006922,0.00750644,-0.00012682,-0.00010529,0.00399349,0.00001078,0.0000

2154,0.00083021,-0.00001614,-0.00000569,-0.00083382,0.00000989,-0.0000

0437,-0.00015450,-0.00000503,0.00000695,0.00002204,-0.00001509,-0.0000

0995,-0.00010623,0.00000475,0.00000659,0.00013547,0.00000121,-0.000001

40,0.00004675,-0.00000023,0.00000002,-0.00000490,-0.00000011,-0.000000

08,0.00000074,0.00000003,0.00000002,0.00000226,0.00438597,0.00308455,0

.02269970,0.00002215,0.00001806,0.00000144,0.00009984,-0.00018520,0.00

000914,-0.00038681,0.00024376,0.00000176,0.00020487,-0.00007057,0.0000

0251,0.00002329,0.00008247,0.00000266,-0.00003065,0.00019842,-0.000003

09,0.00004717,-0.00027853,0.00000020,-0.00001214,0.00024105,0.00000011

,-0.00010155,-0.00023008,-0.00000300,0.00004037,-0.00005056,-0.0000016

8,-0.00000183,0.00002242,0.00000115,0.00052150,-0.00017798,0.00000241,

-0.00106748,-0.00201574,-0.00016390,0.00853140,-0.00455198,0.00009768,

-0.24575608,0.14314395,-0.00406646,-0.00907152,0.01740944,-0.00019592,

-0.00538325,0.00024308,-0.00024525,0.00036846,0.00049117,0.00000696,-0

.00044472,-0.00006960,0.00001190,0.00004676,0.00001238,0.00000325,-0.0

0011738,0.00001320,-0.00000231,-0.00028034,-0.00018405,-0.00000286,0.0

0032247,-0.00010766,0.00000229,0.00000158,0.00000778,0.00000042,0.0000

0625,0.00001294,-0.00000057,-0.00000487,-0.00000152,-0.00000003,-0.000

00017,0.00000096,0.00000011,-0.00006009,0.00075007,0.00007204,0.251045

00,0.00009165,0.00007784,0.00000154,-0.00008956,-0.00046395,-0.0000080

2,-0.00018824,0.00010441,0.00000411,0.00014135,-0.00000580,0.00000047,

0.00004869,-0.00002029,-0.00000099,-0.00006603,-0.00006180,-0.00000006

,0.00005237,0.00004246,-0.00000047,0.00000251,-0.00002635,0.00000166,0

.00007552,0.00001230,-0.00000168,-0.00004922,0.00005894,0.00000117,-0.

00004294,-0.00005608,0.00000060,0.00148411,0.00037127,0.00002430,-0.00

062834,-0.00528426,-0.00001322,0.02358535,-0.00688393,0.00046612,0.143

79565,-0.16688734,0.00285289,-0.00803292,0.01013708,-0.00016628,-0.003

87986,0.00007716,-0.00007996,0.00057348,0.00023460,0.00000004,0.000287

21,0.00006810,0.00000549,-0.00004229,-0.00010573,0.00000208,0.00010031

,-0.00005113,0.00000288,0.00025489,0.00010898,-0.00000360,-0.00018044,

-0.00001082,0.00000246,-0.00000510,-0.00000151,-0.00000017,0.00001809,

0.00000592,0.00000004,0.00000152,0.00000226,-0.00000002,0.00000096,-0.

00000197,-0.00000008,-0.00075007,0.00099606,-0.00002217,-0.15551207,0.

16976748,0.00000989,0.00000437,-0.00015450,-0.00001614,0.00000569,-0.0

0083382,0.00000475,-0.00000659,0.00013547,-0.00001509,0.00000995,-0.00

010623,-0.00000503,-0.00000695,0.00002204,0.00001030,0.00000211,0.0000

1877,-0.00000131,-0.00000150,-0.00000109,-0.00000038,0.00000227,0.0000

0398,-0.00000293,-0.00000157,0.00000415,0.00000012,-0.00000166,-0.0000

0094,0.00000161,0.00000053,-0.00000576,0.00001078,-0.00002154,0.000830

22,-0.00024430,-0.00006922,0.00750644,0.00015393,-0.00020214,0.0034009

3,-0.00415861,0.00294800,-0.03165591,-0.00008389,0.00032072,-0.0010783

7,-0.00012682,0.00010529,0.00399349,0.00000687,-0.00001983,-0.00129004

,0.00001040,0.00000257,-0.00011556,0.,0.00000138,-0.00001160,-0.000002

66,0.00000093,-0.00000836,0.00000314,0.00000028,0.00006857,-0.00000426

,-0.00000443,-0.00011472,0.00000008,0.00000035,-0.00002198,0.00000039,

-0.00000139,0.00005963,0.00000003,-0.00000002,0.00000226,-0.00000011,0

.00000008,0.00000074,0.00007204,0.00002217,-0.00419542,0.00438595,-0.0

0308453,0.02269970,0.00016865,-0.00010913,-0.00000359,0.00005723,0.000

18901,0.00000535,-0.00010312,-0.00001424,-0.00000313,0.00016831,0.0001

2551,0.00000405,-0.00015199,-0.00009695,-0.00000146,-0.00019274,0.0000

8490,-0.00000362,0.00002652,-0.00009069,0.00000144,0.00011770,0.000056

51,-0.00000760,-0.00059451,-0.00032835,0.00000631,0.00011311,0.0000553

4,-0.00000023,-0.00002891,0.00005366,0.00000177,0.00004052,-0.00001958

,-0.00000220,0.00007864,0.00006823,0.00000427,-0.00003214,0.00008274,-

0.00000108,-0.00011224,-0.00004303,-0.00000174,0.00016944,0.00008791,-

0.00000862,-0.00001673,-0.00001188,-0.00000421,0.00007547,0.00075618,-

0.00000528,0.00999396,-0.00764967,0.00024200,-0.16504541,0.14246989,-0

.00440108,-0.00596089,0.02310807,-0.00070527,-0.00550305,-0.00036487,0

.00001087,0.00014102,-0.00357536,0.00010702,0.00000677,0.00000228,0.00

000007,-0.00000594,0.00000090,0.00000019,-0.00000513,-0.00000584,0.000

00023,0.00000625,0.00001809,-0.00000039,0.00000158,0.00000510,0.000000

08,0.00001048,-0.00000970,0.00000121,0.16721968,-0.00004521,0.00002085

,0.00000208,-0.00024009,-0.00008013,0.00000275,0.00022987,-0.00001080,

0.00000034,-0.00025900,0.00004767,-0.00000030,0.00000728,-0.00000182,-

0.00000183,0.00017957,-0.00009433,0.00000237,0.00001923,0.00025944,-0.

00000318,0.00026668,-0.00039792,-0.00000664,-0.00013269,0.00004899,-0.

00000280,-0.00002955,0.00007154,-0.00000227,0.00004073,-0.00005105,-0.

00000110,0.00016220,0.00012132,-0.00000664,-0.00011430,-0.00014510,0.0

0000633,-0.00001721,-0.00007265,0.00000126,0.00000625,0.00003150,-0.00

000153,-0.00006891,-0.00039501,-0.00001119,-0.00014931,0.00022445,-0.0

0000882,0.00100127,0.00036302,-0.00004497,0.01785820,-0.00954615,0.000

28099,0.14084450,-0.24540974,0.00656352,-0.00425138,0.00818454,-0.0002

0751,-0.00189685,-0.00083720,0.00017342,0.00009900,-0.00590894,0.00039

242,-0.00000228,-0.00000422,-0.00000016,0.00000090,-0.00000114,-0.0000

0008,0.00000875,0.00000167,-0.00000002,0.00001294,0.00000592,0.0000013

9,-0.00000778,-0.00000151,-0.00000035,-0.00002610,0.00000521,0.0000014

0,-0.15443638,0.25174243,0.00000231,-0.00000090,-0.00000173,-0.0000079

2,0.00000259,0.00000212,0.00000493,0.00000198,-0.00000020,-0.00000602,

0.00000492,0.00001211,-0.00000328,-0.00000231,0.00000029,0.00000347,-0

.00000492,-0.00001513,-0.00000448,0.00000479,-0.00004501,-0.00000316,0

.00000690,-0.00001390,0.00000295,0.00000504,-0.00032498,-0.00000491,-0

.00000118,-0.00017835,0.00000235,0.00000158,0.00000691,0.00000684,0.00

000599,-0.00000695,-0.00000180,-0.00001197,0.00006548,0.00000317,0.000

00143,0.00000736,-0.00000312,0.00000085,0.00002563,-0.00000097,-0.0000

2671,-0.00013931,0.00000433,0.00001323,-0.00009124,-0.00001193,-0.0000

2513,-0.00180404,-0.00050827,0.00016787,-0.00177710,-0.00444999,0.0066

2051,-0.02687024,0.00023923,-0.00026758,0.00097448,0.00012889,0.000281

94,0.00507613,-0.00014630,0.00029006,0.00528076,0.00000007,0.00000016,

-0.00000224,-0.00000019,0.00000008,0.00000281,0.00000012,-0.00000019,-

0.00000490,0.00000057,-0.00000004,0.00005963,0.00000042,0.00000017,-0.

00002198,-0.00000002,-0.00000088,0.00004675,0.00477815,-0.00697392,0.0

2099841,-0.00015199,0.00009695,0.00000146,0.00016831,-0.00012551,-0.00

000405,-0.00010312,0.00001424,0.00000313,0.00005723,-0.00018901,-0.000

00535,0.00016865,0.00010913,0.00000359,0.00004052,0.00001958,0.0000022

0,0.00007864,-0.00006823,-0.00000427,-0.00001673,0.00001189,0.00000421

,0.00016944,-0.00008791,0.00000862,-0.00011224,0.00004303,0.00000174,-

0.00003214,-0.00008274,0.00000108,-0.00019274,-0.00008490,0.00000362,0

.00002652,0.00009069,-0.00000144,-0.00002891,-0.00005366,-0.00000177,0

.00011311,-0.00005534,0.00000023,-0.00059451,0.00032835,-0.00000631,0.

00011770,-0.00005651,0.00000760,0.00048738,-0.00158506,0.00003611,-0.0

0550305,0.00036487,-0.00001087,-0.00596089,-0.02310807,0.00070528,-0.1

6504540,-0.14246989,0.00440111,0.00999396,0.00764967,-0.00024200,0.000

14102,0.00357536,-0.00010702,-0.00000594,-0.00000090,-0.00000019,0.000

00677,-0.00000228,-0.00000007,0.00001048,0.00000970,-0.00000121,0.0000

0158,-0.00000510,-0.00000008,0.00000625,-0.00001809,0.00000039,-0.0000

0513,0.00000584,-0.00000023,0.00094483,0.00080458,-0.00002940,0.167219

67,-0.00000728,-0.00000182,-0.00000183,0.00025900,0.00004767,-0.000000

30,-0.00022987,-0.00001080,0.00000034,0.00024009,-0.00008013,0.0000027

5,0.00004521,0.00002085,0.00000208,-0.00016220,0.00012132,-0.00000664,

0.00011430,-0.00014511,0.00000633,0.00014931,0.00022446,-0.00000882,0.

00006891,-0.00039501,-0.00001119,-0.00000625,0.00003150,-0.00000153,0.

00001721,-0.00007265,0.00000126,-0.00017957,-0.00009433,0.00000237,-0.

00001923,0.00025944,-0.00000318,-0.00004073,-0.00005105,-0.00000110,0.

00002955,0.00007154,-0.00000227,0.00013269,0.00004899,-0.00000280,-0.0

0026668,-0.00039792,-0.00000664,0.00030546,0.00052252,0.00001737,0.001

89685,-0.00083719,0.00017342,0.00425138,0.00818454,-0.00020751,-0.1408

4450,-0.24540975,0.00656354,-0.01785820,-0.00954615,0.00028099,-0.0000

9900,-0.00590894,0.00039242,-0.00000090,-0.00000114,-0.00000008,0.0000

0228,-0.00000422,-0.00000016,0.00002610,0.00000521,0.00000140,0.000007

78,-0.00000151,-0.00000035,-0.00001294,0.00000592,0.00000139,-0.000008

75,0.00000167,-0.00000002,-0.00080458,-0.00011359,-0.00008607,0.154436

37,0.25174244,0.00000328,-0.00000231,0.00000029,0.00000602,0.00000492,

0.00001211,-0.00000493,0.00000198,-0.00000020,0.00000792,0.00000259,0.

00000212,-0.00000231,-0.00000090,-0.00000173,-0.00000684,0.00000599,-0

.00000695,0.00000180,-0.00001197,0.00006548,-0.00000433,0.00001323,-0.

00009124,0.00000097,-0.00002671,-0.00013931,0.00000312,0.00000085,0.00

002563,-0.00000317,0.00000143,0.00000736,-0.00000347,-0.00000492,-0.00

001513,0.00000448,0.00000479,-0.00004501,-0.00000235,0.00000158,0.0000

0691,0.00000491,-0.00000118,-0.00017835,-0.00000295,0.00000504,-0.0003

2498,0.00000316,0.00000690,-0.00001390,-0.00000922,0.00001249,0.001318

12,-0.00012889,0.00028194,0.00507613,-0.00023923,-0.00026758,0.0009744

8,0.00445001,0.00662053,-0.02687024,0.00050827,0.00016787,-0.00177710,

0.00014630,0.00029006,0.00528076,0.00000019,0.00000008,0.00000281,-0.0

0000007,0.00000016,-0.00000224,0.00000002,-0.00000088,0.00004675,-0.00

000042,0.00000017,-0.00002198,-0.00000057,-0.00000004,0.00005963,-0.00

000012,-0.00000019,-0.00000490,0.00002939,-0.00008607,-0.00313922,-0.0

0477817,-0.00697395,0.02099841,-0.00096931,-0.00097794,-0.00002133,-0.

00408386,-0.00533173,-0.00026619,-0.00329586,0.,0.,-0.00408385,0.00533

173,0.00026619,-0.00096931,0.00097794,0.00002133,0.00336046,0.00246841

,0.00006698,-0.00990098,0.00861989,0.00023691,-0.05220176,0.00000002,0

.01427106,-0.00990098,-0.00861988,0.00023691,0.00683952,-0.00356198,-0

.00005916,0.00683952,0.00356198,-0.00005916,0.00336047,-0.00246841,-0.

00006698,-0.00990098,-0.00861989,-0.00023691,0.00683952,-0.00356198,0.

00005916,0.00683952,0.00356198,0.00005916,-0.00990099,0.00861989,-0.00

023691,-0.05220178,0.,-0.01427106,0.00336046,0.00246841,-0.00006698,-0

.00408384,0.00533173,-0.00026619,-0.00096931,0.00097794,-0.00002133,-0

.00096931,-0.00097794,0.00002133,-0.00408385,-0.00533173,0.00026619,-0

.00329587,-0.00000003,0.,0.00003970,-0.00012688,0.00001400,0.00003970,

0.00012688,-0.00001400,0.00076117,-0.00023838,0.00001303,0.00076117,0.

00023838,0.00001303,0.00076117,-0.00023838,-0.00001303,0.00076117,0.00

023838,-0.00001303,0.00003970,0.00012688,0.00001400,0.00003970,-0.0001

2688,-0.00001400,0.12878920,-0.00553671,0.00816841,0.00017191,-0.00737

750,-0.01162446,-0.00034374,-0.00000002,-0.05319840,-0.01405398,0.0073

7751,-0.01162446,-0.00034374,0.00553671,0.00816841,0.00017191,0.003864

77,-0.00034913,-0.00001838,0.00457822,0.00098479,-0.00029010,0.0000000

4,-0.00788091,0.,-0.00457822,0.00098480,0.00029010,-0.00099862,-0.0007

2228,0.00004515,0.00099862,-0.00072228,-0.00004515,-0.00386478,-0.0003

4914,-0.00001838,-0.00457822,0.00098480,-0.00029010,-0.00099862,-0.000

72228,-0.00004515,0.00099862,-0.00072228,0.00004515,0.00457822,0.00098

480,0.00029010,0.,-0.00788093,0.,0.00386478,-0.00034914,0.00001838,0.0

0737750,-0.01162446,0.00034374,0.00553671,0.00816840,-0.00017191,-0.00

553671,0.00816841,-0.00017191,-0.00737751,-0.01162446,0.00034374,-0.00

000002,-0.05319841,0.01405397,-0.00020055,0.00083445,0.00000115,0.0002

0055,0.00083445,0.00000115,-0.00009372,0.00005153,-0.00001565,0.000093

72,0.00005153,0.00001565,-0.00009372,0.00005153,0.00001565,0.00009372,

0.00005153,-0.00001565,0.00020055,0.00083445,-0.00000115,-0.00020055,0

.00083445,-0.00000115,0.,0.13157109,-0.00004762,0.00035642,0.00039666,

-0.00044826,-0.00038958,-0.00050789,0.00000002,-0.01557552,-0.00367187

,0.00044826,-0.00038958,-0.00050789,0.00004762,0.00035642,0.00039666,0

.00010473,-0.00008669,-0.00032052,0.00028957,-0.00047720,-0.00027427,0

.01576671,0.00000003,-0.00467585,0.00028957,0.00047720,-0.00027427,-0.

00034448,-0.00000664,0.00041921,-0.00034448,0.00000664,0.00041921,-0.0

0010473,-0.00008669,-0.00032052,-0.00028957,-0.00047720,-0.00027427,0.

00034448,0.00000664,0.00041921,0.00034448,-0.00000664,0.00041921,-0.00

028957,0.00047720,-0.00027427,-0.01576672,-0.00000002,-0.00467572,-0.0

0010473,0.00008669,-0.00032052,-0.00044826,0.00038958,-0.00050789,-0.0

0004762,-0.00035642,0.00039666,0.00004762,-0.00035642,0.00039666,0.000

44826,0.00038958,-0.00050789,-0.00000002,0.01557552,-0.00367178,-0.000

00799,0.00006804,0.00040327,0.00000799,0.00006804,0.00040327,-0.000073

38,0.00001711,0.00030101,-0.00007338,-0.00001711,0.00030101,0.00007338

,-0.00001711,0.00030101,0.00007338,0.00001711,0.00030101,-0.00000799,-

0.00006804,0.00040327,0.00000799,-0.00006804,0.00040327,0.,0.,0.015200

57,-0.00600544,0.00307075,0.00028408,-0.03413059,-0.00955999,-0.000086

45,0.03110313,0.00018327,0.00007939,-0.03980409,0.00144213,-0.00009122

,0.00253781,0.00210069,-0.00018660,0.03466455,0.00649976,0.00034438,-0

.00370231,-0.01011638,-0.00010771,0.01533450,-0.01768989,-0.00003387,-

0.12694605,0.06431329,0.00090784,-0.01102780,0.03947789,0.00001650,-0.

00891812,-0.00426624,0.00016237,0.02547679,-0.00618771,-0.00027244,-0.

00051645,0.00426966,0.00017467,-0.00038738,0.00280793,0.00002498,-0.00

396805,-0.00284418,-0.00008963,0.00446275,0.00639583,-0.00024862,0.000

31281,-0.00220732,-0.00009672,-0.04500254,-0.01145061,0.00043132,0.061

06953,-0.01667397,0.00017473,0.01258252,0.00609213,-0.00051648,-0.0208

8912,0.02071369,0.00019636,-0.17093434,0.05114654,-0.00015099,-0.08843

622,0.00404091,-0.00014667,-0.00019274,-0.00017957,0.00000347,0.000040

52,0.00016220,-0.00000684,0.00036846,-0.00057348,-0.00000687,0.0005214

9,0.00148411,-0.00001078,-0.00003065,0.00006603,0.00001030,0.00018778,

-0.00014798,-0.00000356,0.00048738,-0.00030546,0.00000922,0.00007547,-

0.00100127,0.00001193,0.00336046,-0.00386478,0.00010473,0.55518531,-0.

00215323,0.00294785,0.00012920,0.00192189,-0.00776480,0.00000967,0.003

23434,0.00091167,0.00001285,0.00228961,0.00541736,-0.00015882,-0.00066

800,-0.00184449,-0.00008827,-0.00649980,-0.04538569,0.00027360,-0.0283

6474,0.06518348,0.00019680,-0.00155056,-0.11161287,0.00016535,0.078470

82,-0.20707743,0.00036621,0.01952051,-0.02271294,0.00027679,0.00867511

,0.01861318,-0.00039217,-0.00618771,0.02141132,-0.00015828,-0.00815070

,-0.02820903,-0.00007336,0.00242684,-0.00307924,0.00015627,0.00023025,

0.00007658,-0.00011499,0.00506103,-0.02990005,0.00008438,-0.00032349,0

.02650682,0.00002149,0.01145065,0.02495001,0.00010809,-0.01316578,-0.0

1124635,0.00021080,0.00168848,-0.00506670,0.00023762,0.03601824,-0.009

30910,0.00000511,0.04398078,-0.11706490,0.00141272,-0.01722242,0.01702

217,-0.00042032,-0.00008490,-0.00009433,0.00000492,-0.00001958,0.00012

132,-0.00000599,-0.00049117,0.00023460,-0.00001983,-0.00017798,0.00037

126,0.00002154,-0.00019842,-0.00006180,-0.00000211,0.00013885,0.000033

84,-0.00000046,0.00158506,0.00052252,0.00001249,-0.00075618,0.00036302

,-0.00002513,-0.00246842,-0.00034913,0.00008669,-0.00114099,0.59594595

,-0.00008804,0.00005710,0.00004901,-0.00043692,-0.00017589,-0.00005987

,0.00044493,-0.00005171,0.00025922,-0.00049088,0.00008729,-0.00009130,

0.00001788,0.00000790,-0.00004275,0.00034438,-0.00027360,0.00122039,0.

00005078,0.00047027,0.00406345,-0.00035968,-0.00011844,-0.00109033,0.0

0056089,0.00152283,-0.05016976,-0.00002347,-0.00025337,0.00186458,0.00

013446,-0.00005195,0.00180161,0.00027244,0.00015829,-0.00001210,-0.000

06032,-0.00025787,-0.00021035,0.00000897,0.00001514,-0.00002955,-0.000

05748,-0.00005170,-0.00003483,0.00014374,-0.00022532,0.00022745,-0.000

05925,0.00026086,0.00030944,-0.00043131,0.00010809,0.00102884,0.000765

93,0.00001469,0.00478524,0.00005094,0.00028475,0.00203993,-0.00075794,

0.00015938,0.00167849,0.00096836,0.00109588,-0.04773798,-0.00019476,-0

.00055811,-0.00495800,-0.00000362,-0.00000237,-0.00001513,0.00000220,0

.00000664,-0.00000695,-0.00000696,0.00000004,-0.00129004,-0.00000241,-

0.00002430,0.00083021,-0.00000309,0.00000006,0.00001877,0.00000732,0.0

0000036,-0.00002142,-0.00003611,0.00001737,0.00131812,0.00000528,-0.00

004497,-0.00180405,0.00006698,0.00001838,-0.00032052,-0.00264337,-0.00

417606,0.12680956,0.00331298,-0.00242533,-0.00015274,0.01116019,0.0067

3737,0.00004323,-0.01202863,-0.00034084,-0.00002046,0.01373256,-0.0016

8742,0.00009382,-0.00111143,-0.00048236,0.00008701,-0.01001237,0.01312

151,-0.00020519,0.00776058,-0.02046143,0.00001667,0.00165191,0.0280352

3,-0.00004164,0.01035802,-0.04289995,-0.00010715,-0.00196926,0.0041857

2,-0.00013866,-0.00281163,-0.00309863,0.00016238,-0.00680699,-0.004134

06,0.00014805,0.00350144,0.00678710,-0.00003765,-0.00098372,0.00034746

,-0.00006561,0.00097667,0.00055611,0.00006275,-0.00224792,0.00705486,0

.00006667,-0.00004107,-0.00725642,0.00005609,0.01204829,-0.00307902,-0

.00017779,-0.02031257,0.00329100,0.00005125,-0.00185156,-0.00211805,0.

00022497,-0.00204305,-0.00095167,-0.00015429,-0.06239549,-0.02558931,0

.00027891,0.01469632,0.00387160,-0.00004476,0.00010800,0.00010496,-0.0

0000291,-0.00002032,-0.00009611,0.00000485,-0.00025414,0.00077866,-0.0

0000116,0.00011496,0.00002633,0.00000386,0.00007434,0.00000096,-0.0000

0211,-0.00010829,0.00003601,0.00000077,0.00002431,0.00018916,-0.000001

84,-0.00160632,-0.00005678,-0.00000575,-0.00126073,0.00105158,-0.00005

761,-0.17269841,-0.08652222,0.00173729,0.71886640,0.00378978,-0.002789

70,-0.00015861,0.01041795,0.00730419,0.00005343,-0.01185062,-0.0004523

8,-0.00002185,0.01351541,-0.00122888,0.00010927,-0.00157616,-0.0006989

5,0.00008319,-0.00925120,0.01444673,-0.00023634,0.00532044,-0.02424865

,0.00008307,0.00629141,0.02380827,-0.00005219,-0.02896328,-0.07646368,

0.00033815,0.00007495,-0.00285506,-0.00013955,-0.00233622,-0.00231292,

0.00016489,-0.00593599,-0.00449690,0.00013933,0.00345949,0.00708339,-0

.00002861,-0.00087775,0.00029724,-0.00006507,0.00100148,0.00061858,0.0

0006083,-0.00231751,0.00707238,0.00006273,-0.00002002,-0.00722113,0.00

005313,0.01195473,-0.00377363,-0.00015570,-0.01805285,0.00541594,-0.00

004221,-0.00222931,-0.00240775,0.00022585,0.00407231,-0.00339588,-0.00

008538,-0.03306723,0.01311919,-0.00030331,0.02058692,-0.00053034,0.000

06489,0.00012109,0.00010198,-0.00000284,-0.00003045,-0.00009769,0.0000

0439,-0.00021737,-0.00191590,0.00000160,0.00020432,0.00011175,0.000000

34,0.00007959,0.00000215,-0.00000209,-0.00010513,0.00003124,0.00000145

,-0.00004991,0.00009918,0.00000350,0.00079166,-0.00007016,-0.00002008,

-0.00080478,0.00049802,-0.00004719,-0.09326930,-0.16207578,0.00189041,

0.61315008,0.74383405,-0.00008390,0.00005845,0.00002425,-0.00028216,-0

.00015466,0.00000387,0.00029336,0.00000727,-0.00000988,-0.00034629,0.0

0003140,0.00010981,0.00003477,0.00001695,-0.00000464,0.00024705,-0.000

24374,-0.00053545,-0.00011269,0.00041759,0.00030395,-0.00002448,-0.000

45722,0.00615322,0.00023577,0.00090831,0.00112856,-0.00007898,-0.00005

436,-0.00297497,0.00005894,0.00004522,0.00087152,0.00017137,0.00008438

,0.00001613,-0.00006782,-0.00014757,-0.00003586,0.00001859,-0.00000473

,-0.00001332,-0.00002475,-0.00001417,0.00002843,0.00005896,-0.00014401

,-0.00009945,0.00000017,0.00015271,0.00002990,-0.00028029,0.00005007,-

0.00026366,0.00043123,-0.00012734,-0.00059452,0.00008305,0.00008298,0.

00083540,-0.00014019,0.00002212,-0.00121456,0.00080839,0.00003106,0.00

239510,-0.00039454,0.00004645,0.00384474,-0.00000287,-0.00000229,-0.00

000763,0.00000058,0.00000171,-0.00000343,0.00000264,0.00000878,0.00034

075,0.00000259,-0.00000095,0.00025240,-0.00000171,-0.00000009,-0.00000

098,0.00000154,-0.00000109,0.00000321,0.00000085,-0.00000617,-0.000085

14,0.00001433,-0.00000022,0.00025994,0.00002105,-0.00002694,-0.0000440

9,0.00121459,0.00134411,-0.04714002,-0.00774415,-0.00822377,0.06241343

,-0.00204305,-0.00095167,0.00015429,-0.06239549,-0.02558933,-0.0002789

1,0.01469633,0.00387160,0.00004476,-0.02031257,0.00329102,-0.00005125,

-0.00185157,-0.00211806,-0.00022497,0.01204828,-0.00307902,0.00017779,

-0.00224793,0.00705485,-0.00006667,-0.00004107,-0.00725642,-0.00005610

,0.00350143,0.00678712,0.00003765,-0.00098371,0.00034745,0.00006561,0.

00097668,0.00055613,-0.00006275,-0.17269837,-0.08652224,-0.00173729,0.

01035802,-0.04289992,0.00010714,-0.00196926,0.00418570,0.00013866,-0.0

0281162,-0.00309862,-0.00016238,0.00776058,-0.02046144,-0.00001667,0.0

0165192,0.02803523,0.00004164,-0.01001238,0.01312152,0.00020519,0.0137

3257,-0.00168740,-0.00009381,-0.00111143,-0.00048237,-0.00008701,0.003

31298,-0.00242534,0.00015274,0.01116020,0.00673737,-0.00004323,-0.0120

2862,-0.00034084,0.00002046,-0.00160633,-0.00005678,0.00000575,0.00002

431,0.00018916,0.00000184,0.00007434,0.00000095,0.00000211,-0.00010829

,0.00003602,-0.00000076,-0.00025414,0.00077866,0.00000116,0.00011495,0

.00002633,-0.00000386,-0.00002032,-0.00009610,-0.00000485,0.00010800,0

.00010496,0.00000291,-0.00126074,0.00105159,0.00005761,-0.00680698,-0.

00413407,-0.00014805,0.00318358,0.00295777,-0.00008045,0.71886622,0.00

407232,-0.00339588,0.00008538,-0.03306725,0.01311917,0.00030331,0.0205

8694,-0.00053034,-0.00006489,-0.01805286,0.00541596,0.00004221,-0.0022

2932,-0.00240775,-0.00022585,0.01195473,-0.00377362,0.00015570,-0.0023

1753,0.00707237,-0.00006273,-0.00002002,-0.00722114,-0.00005314,0.0034

5948,0.00708341,0.00002862,-0.00087775,0.00029723,0.00006507,0.0010014

9,0.00061860,-0.00006083,-0.09326930,-0.16207582,-0.00189042,-0.028963

28,-0.07646369,-0.00033816,0.00007495,-0.00285507,0.00013955,-0.002336

22,-0.00231291,-0.00016489,0.00532044,-0.02424868,-0.00008307,0.006291

42,0.02380829,0.00005219,-0.00925123,0.01444675,0.00023634,0.01351543,

-0.00122887,-0.00010927,-0.00157617,-0.00069897,-0.00008319,0.00378978

,-0.00278971,0.00015861,0.01041796,0.00730420,-0.00005343,-0.01185063,

-0.00045238,0.00002185,0.00079166,-0.00007016,0.00002008,-0.00004990,0

.00009918,-0.00000350,0.00007959,0.00000214,0.00000209,-0.00010513,0.0

0003125,-0.00000144,-0.00021737,-0.00191590,-0.00000160,0.00020432,0.0

0011175,-0.00000034,-0.00003045,-0.00009769,-0.00000439,0.00012109,0.0

0010198,0.00000284,-0.00080479,0.00049803,0.00004719,-0.00593599,-0.00

449691,-0.00013933,0.00295777,0.00268490,-0.00007424,0.61315010,0.7438

3429,0.00014019,-0.00002212,-0.00121456,-0.00080839,-0.00003106,0.0023

9510,0.00039454,-0.00004645,0.00384474,-0.00043123,0.00012734,-0.00059

452,-0.00008305,-0.00008298,0.00083540,0.00028029,-0.00005007,-0.00026

366,-0.00005897,0.00014401,-0.00009944,-0.00000017,-0.00015271,0.00002

990,0.00006782,0.00014757,-0.00003586,-0.00001859,0.00000473,-0.000013

32,0.00002475,0.00001417,0.00002843,-0.00121460,-0.00134411,-0.0471400

2,-0.00023577,-0.00090832,0.00112856,0.00007898,0.00005436,-0.00297497

,-0.00005894,-0.00004523,0.00087152,0.00011270,-0.00041760,0.00030395,

0.00002448,0.00045723,0.00615323,-0.00024706,0.00024375,-0.00053545,0.

00034629,-0.00003140,0.00010981,-0.00003477,-0.00001695,-0.00000464,0.

00008390,-0.00005846,0.00002425,0.00028216,0.00015466,0.00000387,-0.00

029336,-0.00000727,-0.00000988,-0.00001433,0.00000022,0.00025994,-0.00

000085,0.00000617,-0.00008514,0.00000171,0.00000009,-0.00000098,-0.000

00154,0.00000109,0.00000321,-0.00000264,-0.00000878,0.00034075,-0.0000

0259,0.00000095,0.00025240,-0.00000058,-0.00000171,-0.00000343,0.00000

287,0.00000229,-0.00000763,-0.00002105,0.00002694,-0.00004409,-0.00017

137,-0.00008438,0.00001613,0.00008045,0.00007424,-0.00001389,0.0077442

2,0.00822385,0.06241344,-0.00222844,0.00158735,0.00009564,-0.00670339,

-0.00416397,-0.00002668,0.00719895,0.00019171,0.00002115,-0.00804935,0

.00094466,-0.00006058,0.00088998,0.00037989,-0.00004988,0.00598366,-0.

00787458,0.00012718,-0.00407948,0.01232197,-0.00001697,-0.00058159,-0.

01570143,0.00004832,-0.00305848,0.02313802,0.00007692,-0.00071594,0.00

112690,0.00009190,0.00155280,0.00097237,-0.00009398,0.00379514,0.00324

710,-0.00008762,-0.00224904,-0.00515098,0.00001722,0.00068943,-0.00051

998,0.00004326,-0.00038509,-0.00013286,-0.00003743,0.00140383,-0.00540

400,-0.00002464,-0.00009102,0.00521296,-0.00001505,-0.00453009,0.00332

268,0.00009821,0.00753862,-0.00322375,0.00000764,0.00118151,0.00105391

,-0.00010443,-0.00027922,0.00098388,0.00006419,0.01477923,-0.00142138,

0.00009673,-0.00957252,0.00010593,-0.00001144,-0.00008211,-0.00007234,

0.00000093,0.00002875,0.00004715,-0.00000355,0.00071123,0.00038946,-0.

00000958,-0.00006542,-0.00006059,-0.00000189,-0.00006163,-0.00001452,0

.00000051,0.00004971,-0.00000594,-0.00000084,-0.00002374,-0.00003796,-

0.00000415,-0.00057440,-0.00022791,0.00001700,0.00077679,-0.00017243,-

0.00006594,-0.01766723,-0.03163446,0.00010734,-0.50410697,-0.48953673,

0.00597605,-0.00218975,-0.00206840,-0.00005016,0.73122093,-0.00241187,

0.00165663,0.00010276,-0.00779827,-0.00438105,-0.00002930,0.00812938,0

.00017723,0.00002377,-0.00932380,0.00087308,-0.00006191,0.00099274,0.0

0049106,-0.00005564,0.00698822,-0.00707226,0.00014547,-0.00416321,0.01

117340,-0.00003121,-0.00123251,-0.01550007,0.00006153,-0.00069422,0.02

293643,0.00006341,0.00014188,0.00017415,0.00006973,0.00102398,0.001127

30,-0.00007543,0.00465876,0.00280028,-0.00009313,-0.00218416,-0.004691

06,0.00002094,0.00066941,-0.00041991,0.00004317,-0.00049478,-0.0001883

1,-0.00003689,0.00148902,-0.00484881,-0.00003307,-0.00007655,0.0048193

6,-0.00001761,-0.00587649,0.00289315,0.00009130,0.00942423,-0.00305491

,0.00001820,0.00074577,0.00153486,-0.00012891,0.00090239,0.00019141,0.

00009592,0.01649381,-0.00437979,0.00017027,-0.01049859,0.00066252,-0.0

0002333,-0.00008928,-0.00007764,0.00000103,0.00003166,0.00004919,-0.00

000338,-0.00007828,-0.00045722,0.00000328,-0.00005334,-0.00007121,-0.0

0000309,-0.00006190,-0.00001201,0.00000065,0.00005293,-0.00000926,-0.0

0000118,-0.00001449,-0.00005277,-0.00000368,0.00052415,0.00061008,-0.0

0000062,0.00093048,-0.00023021,-0.00006981,-0.02518984,-0.02624349,0.0

0007448,-0.49077157,-0.53006508,0.00634414,-0.00235399,-0.00220096,-0.

00005451,0.70444964,0.76953625,0.00003859,-0.00002669,-0.00000654,0.00

011966,0.00006839,-0.00000279,-0.00012424,-0.00000267,0.00000217,0.000

14372,-0.00001442,-0.00001245,-0.00001679,-0.00000780,0.00000250,-0.00

010931,0.00011100,-0.00004580,0.00005038,-0.00017732,-0.00012356,0.000

01969,0.00022395,-0.00023121,0.00004911,-0.00031477,0.00193666,0.00002

469,-0.00001551,0.00026285,-0.00002135,-0.00000737,-0.00018604,-0.0000

6941,-0.00004711,-0.00000073,0.00003386,0.00007828,0.00001169,-0.00001

086,0.00000787,-0.00000382,0.00000655,0.00000198,0.00000660,-0.0000248

9,0.00008114,0.00001652,0.00000106,-0.00007930,-0.00000790,0.00008108,

-0.00005308,-0.00009126,-0.00013391,0.00004018,-0.00002507,-0.00000941

,-0.00003010,-0.00017537,-0.00001335,0.00001509,0.00018037,-0.00021635

,0.00007914,0.00147249,0.00013976,0.00000250,0.00005363,0.00000145,0.0

0000122,0.00000156,-0.00000050,-0.00000057,-0.00000165,-0.00000863,-0.

00000924,-0.00011669,0.00000116,0.00000051,0.00003227,0.00000103,0.000

00023,-0.00000137,-0.00000060,0.00000017,-0.00000118,-0.00000009,0.000

00275,0.00006384,-0.00001666,-0.00001639,-0.00013130,-0.00001716,0.000

00188,-0.00000724,0.00027836,0.00037059,0.00238582,0.00612313,0.006467

35,-0.02650431,0.00003746,0.00003508,0.00000340,-0.00900615,-0.0096125

4,0.03747094,-0.00027922,0.00098388,-0.00006419,0.01477923,-0.00142136

,-0.00009673,-0.00957253,0.00010593,0.00001144,0.00753862,-0.00322376,

-0.00000764,0.00118151,0.00105391,0.00010443,-0.00453008,0.00332268,-0

.00009821,0.00140384,-0.00540399,0.00002464,-0.00009102,0.00521296,0.0

0001505,-0.00224903,-0.00515098,-0.00001722,0.00068943,-0.00051997,-0.

00004326,-0.00038510,-0.00013286,0.00003743,-0.01766721,-0.03163445,-0

.00010735,-0.00305847,0.02313801,-0.00007692,-0.00071594,0.00112691,-0

.00009190,0.00155279,0.00097236,0.00009398,-0.00407947,0.01232198,0.00

001697,-0.00058159,-0.01570144,-0.00004832,0.00598366,-0.00787458,-0.0

0012718,-0.00804935,0.00094465,0.00006058,0.00088998,0.00037990,0.0000

4988,-0.00222844,0.00158736,-0.00009564,-0.00670340,-0.00416397,0.0000

2668,0.00719895,0.00019171,-0.00002115,-0.00057440,-0.00022791,-0.0000

1700,-0.00002374,-0.00003796,0.00000415,-0.00006163,-0.00001451,-0.000

00051,0.00004971,-0.00000594,0.00000084,0.00071123,0.00038946,0.000009

58,-0.00006542,-0.00006059,0.00000189,0.00002875,0.00004715,0.00000355

,-0.00008211,-0.00007234,-0.00000093,0.00077679,-0.00017244,0.00006594

,0.00379514,0.00324711,0.00008762,-0.00218975,-0.00206840,0.00005016,-

0.50410683,-0.48953674,-0.00597610,0.00132781,0.00139726,-0.00002183,0

.73122071,0.00090239,0.00019141,-0.00009592,0.01649382,-0.00437977,-0.

00017026,-0.01049861,0.00066252,0.00002333,0.00942424,-0.00305493,-0.0

0001820,0.00074578,0.00153486,0.00012891,-0.00587649,0.00289315,-0.000

09130,0.00148903,-0.00484881,0.00003307,-0.00007655,0.00481937,0.00001

761,-0.00218416,-0.00469108,-0.00002094,0.00066941,-0.00041990,-0.0000

4317,-0.00049479,-0.00018832,0.00003689,-0.02518984,-0.02624350,-0.000

07448,-0.00069422,0.02293644,-0.00006340,0.00014187,0.00017416,-0.0000

6973,0.00102398,0.00112729,0.00007544,-0.00416320,0.01117342,0.0000312

1,-0.00123251,-0.01550008,-0.00006154,0.00698824,-0.00707227,-0.000145

47,-0.00932381,0.00087307,0.00006191,0.00099275,0.00049107,0.00005564,

-0.00241187,0.00165663,-0.00010276,-0.00779827,-0.00438105,0.00002930,

0.00812938,0.00017723,-0.00002377,0.00052415,0.00061008,0.00000062,-0.

00001449,-0.00005277,0.00000368,-0.00006190,-0.00001201,-0.00000065,0.

00005293,-0.00000926,0.00000118,-0.00007828,-0.00045722,-0.00000328,-0

.00005334,-0.00007121,0.00000309,0.00003166,0.00004919,0.00000338,-0.0

0008928,-0.00007764,-0.00000103,0.00093049,-0.00023021,0.00006981,0.00

465876,0.00280029,0.00009313,-0.00235399,-0.00220096,0.00005451,-0.490

77159,-0.53006527,-0.00634420,0.00139726,0.00149851,-0.00002326,0.7044

4964,0.76953650,0.00001335,-0.00001509,0.00018037,0.00021635,-0.000079

14,0.00147249,-0.00013976,-0.00000250,0.00005363,0.00013391,-0.0000401

8,-0.00002507,0.00000941,0.00003010,-0.00017538,-0.00008108,0.00005308

,-0.00009126,0.00002489,-0.00008114,0.00001652,-0.00000105,0.00007930,

-0.00000790,-0.00003386,-0.00007828,0.00001169,0.00001086,-0.00000787,

-0.00000382,-0.00000655,-0.00000198,0.00000660,-0.00027836,-0.00037059

,0.00238582,-0.00004911,0.00031478,0.00193666,-0.00002469,0.00001551,0

.00026285,0.00002135,0.00000737,-0.00018604,-0.00005038,0.00017732,-0.

00012356,-0.00001969,-0.00022395,-0.00023121,0.00010931,-0.00011100,-0

.00004580,-0.00014372,0.00001442,-0.00001245,0.00001679,0.00000780,0.0

0000250,-0.00003859,0.00002669,-0.00000654,-0.00011966,-0.00006839,-0.

00000279,0.00012424,0.00000267,0.00000217,0.00001666,0.00001639,-0.000

13130,0.00000009,-0.00000275,0.00006384,-0.00000103,-0.00000023,-0.000

00137,0.00000060,-0.00000017,-0.00000118,0.00000863,0.00000924,-0.0001

1669,-0.00000116,-0.00000051,0.00003227,0.00000050,0.00000057,-0.00000

165,-0.00000145,-0.00000122,0.00000156,0.00001716,-0.00000188,-0.00000

724,0.00006941,0.00004711,-0.00000073,-0.00003746,-0.00003508,0.000003

40,-0.00612318,-0.00646741,-0.02650432,0.00002183,0.00002326,-0.000000

37,0.00900622,0.00961262,0.03747096,-0.00185155,0.00211804,0.00022497,

-0.02031257,-0.00329100,0.00005125,0.01469632,-0.00387161,-0.00004476,

-0.06239547,0.02558934,0.00027889,-0.00204307,0.00095166,-0.00015429,-

0.17269843,0.08652223,0.00173726,0.01035803,0.04289995,-0.00010716,0.0

0165193,-0.02803523,-0.00004164,0.00776059,0.02046142,0.00001667,-0.00

281163,0.00309863,0.00016238,-0.00196927,-0.00418572,-0.00013866,0.012

04829,0.00307901,-0.00017779,-0.00224794,-0.00705484,0.00006667,0.0009

7669,-0.00055613,0.00006275,-0.00098371,-0.00034744,-0.00006561,0.0035

0142,-0.00678713,-0.00003765,-0.00004107,0.00725642,0.00005610,-0.0068

0697,0.00413408,0.00014805,0.01116017,-0.00673737,0.00004323,0.0033129

9,0.00242534,-0.00015275,-0.00111144,0.00048237,0.00008701,0.01373257,

0.00168739,0.00009381,-0.01202861,0.00034085,-0.00002046,0.00002431,-0

.00018916,-0.00000184,-0.00160632,0.00005678,-0.00000575,0.00011495,-0

.00002633,0.00000386,-0.00025414,-0.00077867,-0.00000116,-0.00010829,-

0.00003602,0.00000077,0.00007434,-0.00000095,-0.00000211,0.00010800,-0

.00010496,-0.00000291,-0.00002032,0.00009611,0.00000485,-0.00126074,-0

.00105158,-0.00005762,-0.01001238,-0.01312149,-0.00020519,0.00820295,0

.00868166,-0.00018851,-0.00572148,-0.00551491,-0.00012554,-0.00487237,

-0.00503418,0.00007920,0.00267890,0.00291392,0.00004242,0.71886624,0.0

0222930,-0.00240773,-0.00022585,0.01805285,0.00541593,0.00004221,-0.02

058692,-0.00053033,-0.00006489,0.03306722,0.01311916,0.00030331,-0.004

07230,-0.00339587,0.00008538,0.09326935,-0.16207581,-0.00189038,0.0289

6327,-0.07646370,-0.00033814,-0.00629142,0.02380828,0.00005219,-0.0053

2045,-0.02424865,-0.00008306,0.00233623,-0.00231292,-0.00016489,-0.000

07494,-0.00285506,0.00013955,-0.01195473,-0.00377361,0.00015570,0.0023

1753,0.00707236,-0.00006273,-0.00100150,0.00061860,-0.00006083,0.00087

775,0.00029722,0.00006507,-0.00345947,0.00708341,0.00002862,0.00002002

,-0.00722113,-0.00005314,0.00593597,-0.00449691,-0.00013933,-0.0104179

3,0.00730420,-0.00005343,-0.00378979,-0.00278971,0.00015861,0.00157618

,-0.00069897,-0.00008319,-0.01351542,-0.00122885,-0.00010927,0.0118506

1,-0.00045239,0.00002185,0.00004990,0.00009918,-0.00000350,-0.00079165

,-0.00007016,0.00002008,-0.00020432,0.00011175,-0.00000034,0.00021737,

-0.00191591,-0.00000160,0.00010513,0.00003125,-0.00000144,-0.00007959,

0.00000215,0.00000209,-0.00012109,0.00010198,0.00000284,0.00003045,-0.

00009769,-0.00000439,0.00080479,0.00049802,0.00004719,0.00925123,0.014

44672,0.00023634,-0.00868167,-0.00942527,0.00019707,0.00551490,0.00555

367,0.00012574,0.00511076,0.00527054,-0.00008132,-0.00272797,-0.002972

83,-0.00004472,-0.61315009,0.74383429,0.00008305,-0.00008298,0.0008354

0,0.00043122,0.00012733,-0.00059452,-0.00039453,-0.00004645,0.00384474

,0.00080838,-0.00003106,0.00239510,-0.00014019,-0.00002212,-0.00121456

,0.00121456,-0.00134407,-0.04714002,0.00023576,-0.00090830,0.00112857,

-0.00002448,0.00045722,0.00615322,-0.00011269,-0.00041759,0.00030395,0

.00005894,-0.00004522,0.00087152,-0.00007898,0.00005436,-0.00297497,-0

.00028029,-0.00005007,-0.00026366,0.00005896,0.00014400,-0.00009944,-0

.00002475,0.00001417,0.00002843,0.00001859,0.00000473,-0.00001332,-0.0

0006782,0.00014757,-0.00003586,0.00000017,-0.00015271,0.00002990,0.000

17137,-0.00008438,0.00001613,-0.00028216,0.00015466,0.00000387,-0.0000

8390,-0.00005845,0.00002425,0.00003477,-0.00001695,-0.00000464,-0.0003

4629,-0.00003140,0.00010981,0.00029336,-0.00000727,-0.00000988,0.00000

085,0.00000617,-0.00008514,0.00001433,0.00000022,0.00025994,0.00000259

,0.00000095,0.00025240,0.00000264,-0.00000878,0.00034075,0.00000154,0.

00000109,0.00000321,-0.00000171,0.00000009,-0.00000098,-0.00000287,0.0

0000229,-0.00000763,0.00000058,-0.00000171,-0.00000343,0.00002105,0.00

002694,-0.00004409,0.00024705,0.00024374,-0.00053545,-0.00018851,-0.00

019707,-0.00024597,0.00012554,0.00012574,0.00017496,0.00011356,0.00011

495,0.00005260,-0.00005927,-0.00007030,0.00000514,-0.00774392,0.008223

54,0.06241344,0.00118150,-0.00105390,-0.00010443,0.00753862,0.00322374

,0.00000764,-0.00957252,-0.00010592,-0.00001144,0.01477922,0.00142136,

0.00009673,-0.00027921,-0.00098387,0.00006419,-0.01766720,0.03163446,0

.00010734,-0.00305848,-0.02313802,0.00007692,-0.00058160,0.01570143,0.

00004832,-0.00407948,-0.01232196,-0.00001697,0.00155280,-0.00097237,-0

.00009398,-0.00071594,-0.00112690,0.00009190,-0.00453009,-0.00332267,0

.00009821,0.00140384,0.00540399,-0.00002463,-0.00038510,0.00013287,-0.

00003743,0.00068943,0.00051996,0.00004327,-0.00224903,0.00515099,0.000

01722,-0.00009102,-0.00521296,-0.00001505,0.00379513,-0.00324712,-0.00

008762,-0.00670338,0.00416397,-0.00002668,-0.00222844,-0.00158736,0.00

009564,0.00088999,-0.00037990,-0.00004988,-0.00804935,-0.00094465,-0.0

0006058,0.00719894,-0.00019172,0.00002115,-0.00002374,0.00003796,-0.00

000415,-0.00057440,0.00022791,0.00001700,-0.00006542,0.00006059,-0.000

00189,0.00071123,-0.00038946,-0.00000958,0.00004971,0.00000594,-0.0000

0084,-0.00006163,0.00001451,0.00000051,-0.00008211,0.00007234,0.000000

93,0.00002875,-0.00004715,-0.00000355,0.00077679,0.00017243,-0.0000659

4,0.00598367,0.00787456,0.00012718,-0.00487236,-0.00511074,0.00011356,

0.00267890,0.00272797,0.00005927,0.00300975,0.00311495,-0.00004945,-0.

00152851,-0.00161201,-0.00002447,-0.50410681,0.48953671,0.00597587,0.7

3122068,-0.00074577,0.00153485,0.00012891,-0.00942424,-0.00305491,-0.0

0001820,0.01049860,0.00066252,0.00002334,-0.01649381,-0.00437977,-0.00

017027,-0.00090240,0.00019140,-0.00009592,0.02518983,-0.02624351,-0.00

007447,0.00069423,0.02293645,-0.00006341,0.00123252,-0.01550008,-0.000

06153,0.00416321,0.01117340,0.00003121,-0.00102398,0.00112730,0.000075

43,-0.00014188,0.00017416,-0.00006973,0.00587649,0.00289314,-0.0000913

0,-0.00148903,-0.00484880,0.00003306,0.00049479,-0.00018832,0.00003689

,-0.00066941,-0.00041990,-0.00004318,0.00218416,-0.00469108,-0.0000209

4,0.00007655,0.00481937,0.00001761,-0.00465875,0.00280029,0.00009313,0

.00779826,-0.00438105,0.00002930,0.00241188,0.00165663,-0.00010276,-0.

00099275,0.00049107,0.00005564,0.00932381,0.00087306,0.00006191,-0.008

12938,0.00017724,-0.00002377,0.00001449,-0.00005277,0.00000368,-0.0005

2415,0.00061008,0.00000062,0.00005334,-0.00007121,0.00000309,0.0000782

8,-0.00045722,-0.00000328,-0.00005293,-0.00000926,0.00000118,0.0000619

0,-0.00001201,-0.00000065,0.00008927,-0.00007764,-0.00000103,-0.000031

66,0.00004919,0.00000338,-0.00093049,-0.00023021,0.00006981,-0.0069882

4,-0.00707225,-0.00014547,0.00503418,0.00527055,-0.00011495,-0.0029139

2,-0.00297283,-0.00007030,-0.00311496,-0.00326355,0.00005035,0.0016120

1,0.00172861,0.00002717,0.49077156,-0.53006525,-0.00634396,-0.70444961

,0.76953649,-0.00000941,0.00003010,-0.00017538,-0.00013391,-0.00004018

,-0.00002507,0.00013976,-0.00000250,0.00005363,-0.00021635,-0.00007914

,0.00147249,-0.00001335,-0.00001509,0.00018037,0.00027836,-0.00037058,

0.00238582,0.00004911,0.00031477,0.00193666,0.00001969,-0.00022394,-0.

00023121,0.00005038,0.00017732,-0.00012356,-0.00002135,0.00000737,-0.0

0018604,0.00002469,0.00001551,0.00026285,0.00008108,0.00005308,-0.0000

9126,-0.00002489,-0.00008113,0.00001652,0.00000655,-0.00000198,0.00000

660,-0.00001086,-0.00000787,-0.00000382,0.00003386,-0.00007828,0.00001

169,0.00000106,0.00007930,-0.00000790,-0.00006941,0.00004711,-0.000000

73,0.00011966,-0.00006839,-0.00000279,0.00003859,0.00002669,-0.0000065

4,-0.00001679,0.00000780,0.00000250,0.00014372,0.00001442,-0.00001245,

-0.00012424,0.00000267,0.00000217,-0.00000009,-0.00000275,0.00006384,-

0.00001666,0.00001639,-0.00013130,0.00000116,-0.00000051,0.00003227,-0

.00000863,0.00000924,-0.00011669,-0.00000060,-0.00000017,-0.00000118,0

.00000103,-0.00000023,-0.00000137,0.00000145,-0.00000122,0.00000156,-0

.00000050,0.00000057,-0.00000165,-0.00001716,-0.00000188,-0.00000724,-

0.00010931,-0.00011100,-0.00004580,0.00007920,0.00008132,0.00005260,-0

.00004242,-0.00004471,0.00000514,-0.00004945,-0.00005035,0.00000873,0.

00002447,0.00002717,-0.00000121,0.00612295,-0.00646717,-0.02650431,-0.

00900588,0.00961227,0.03747094,-0.00111144,0.00048237,-0.00008701,0.01

373259,0.00168740,-0.00009381,-0.01202863,0.00034084,0.00002046,0.0111

6019,-0.00673740,-0.00004323,0.00331300,0.00242535,0.00015275,-0.00680

697,0.00413408,-0.00014805,0.00350142,-0.00678712,0.00003765,-0.000041

07,0.00725643,-0.00005610,-0.00224793,-0.00705486,-0.00006667,0.000976

68,-0.00055613,-0.00006275,-0.00098371,-0.00034744,0.00006561,-0.01001

240,-0.01312150,0.00020518,0.00776060,0.02046143,-0.00001667,-0.002811

64,0.00309865,-0.00016238,-0.00196928,-0.00418573,0.00013866,0.0103580

4,0.04289998,0.00010715,0.00165192,-0.02803525,0.00004164,-0.17269839,

0.08652219,-0.00173728,-0.06239549,0.02558932,-0.00027890,-0.00204306,

0.00095167,0.00015429,-0.00185156,0.00211804,-0.00022497,-0.02031259,-

0.00329100,-0.00005125,0.01469633,-0.00387161,0.00004476,-0.00002032,0

.00009611,-0.00000485,0.00010800,-0.00010496,0.00000291,-0.00010829,-0

.00003601,-0.00000077,0.00007434,-0.00000096,0.00000211,0.00011495,-0.

00002633,-0.00000386,-0.00025414,-0.00077866,0.00000116,-0.00160632,0.

00005678,0.00000575,0.00002431,-0.00018916,0.00000184,-0.00126073,-0.0

0105158,0.00005761,0.01204830,0.00307902,0.00017779,-0.00572148,-0.005

51491,0.00012554,0.00820296,0.00868168,0.00018852,0.00267890,0.0029139

3,-0.00004242,-0.00487238,-0.00503419,-0.00007921,0.00318359,-0.002957

77,-0.00008045,-0.00218975,0.00235399,0.00003746,0.71886613,0.00157619

,-0.00069897,0.00008319,-0.01351545,-0.00122886,0.00010927,0.01185063,

-0.00045238,-0.00002186,-0.01041794,0.00730422,0.00005343,-0.00378980,

-0.00278972,-0.00015861,0.00593597,-0.00449692,0.00013933,-0.00345948,

0.00708341,-0.00002862,0.00002002,-0.00722114,0.00005314,0.00231752,0.

00707238,0.00006273,-0.00100149,0.00061860,0.00006083,0.00087775,0.000

29723,-0.00006507,0.00925124,0.01444673,-0.00023633,-0.00532047,-0.024

24866,0.00008306,0.00233623,-0.00231293,0.00016489,-0.00007493,-0.0028

5505,-0.00013955,0.02896326,-0.07646373,0.00033815,-0.00629142,0.02380

830,-0.00005219,0.09326931,-0.16207576,0.00189041,0.03306724,0.0131191

7,-0.00030331,-0.00407230,-0.00339588,-0.00008538,0.00222931,-0.002407

74,0.00022585,0.01805287,0.00541595,-0.00004221,-0.02058694,-0.0005303

4,0.00006489,0.00003045,-0.00009769,0.00000439,-0.00012109,0.00010198,

-0.00000284,0.00010513,0.00003124,0.00000145,-0.00007959,0.00000215,-0

.00000209,-0.00020432,0.00011175,0.00000034,0.00021737,-0.00191590,0.0

0000160,-0.00079166,-0.00007015,-0.00002008,0.00004990,0.00009918,0.00

000350,0.00080479,0.00049802,-0.00004719,-0.01195474,-0.00377362,-0.00

015570,0.00551490,0.00555367,-0.00012574,-0.00868168,-0.00942530,-0.00

019708,-0.00272797,-0.00297283,0.00004472,0.00511076,0.00527056,0.0000

8133,-0.00295777,0.00268490,0.00007424,0.00206840,-0.00220096,-0.00003

508,-0.61315000,0.74383419,-0.00003477,0.00001695,-0.00000464,0.000346

29,0.00003140,0.00010981,-0.00029336,0.00000727,-0.00000988,0.00028216

,-0.00015466,0.00000387,0.00008390,0.00005846,0.00002425,-0.00017137,0

.00008438,0.00001613,0.00006782,-0.00014757,-0.00003586,-0.00000017,0.

00015271,0.00002990,-0.00005896,-0.00014401,-0.00009945,0.00002475,-0.

00001417,0.00002843,-0.00001859,-0.00000473,-0.00001332,-0.00024705,-0

.00024375,-0.00053545,0.00011270,0.00041759,0.00030395,-0.00005894,0.0

0004523,0.00087151,0.00007898,-0.00005436,-0.00297497,-0.00023577,0.00

090831,0.00112856,0.00002448,-0.00045722,0.00615322,-0.00121458,0.0013

4410,-0.04714001,-0.00080838,0.00003106,0.00239510,0.00014019,0.000022

12,-0.00121456,-0.00008305,0.00008298,0.00083540,-0.00043123,-0.000127

33,-0.00059452,0.00039454,0.00004645,0.00384474,-0.00000058,0.00000171

,-0.00000343,0.00000287,-0.00000229,-0.00000763,-0.00000154,-0.0000010

9,0.00000321,0.00000171,-0.00000009,-0.00000098,-0.00000259,-0.0000009

5,0.00025240,-0.00000264,0.00000878,0.00034075,-0.00001433,-0.00000022

,0.00025994,-0.00000085,-0.00000617,-0.00008514,-0.00002105,-0.0000269

4,-0.00004409,0.00028029,0.00005007,-0.00026366,-0.00012554,-0.0001257

4,0.00017496,0.00018851,0.00019707,-0.00024597,0.00005927,0.00007030,0

.00000514,-0.00011356,-0.00011495,0.00005260,0.00008045,-0.00007424,-0

.00001389,-0.00005016,0.00005451,0.00000340,0.00774408,-0.00822371,0.0

6241343,0.00088999,-0.00037990,0.00004988,-0.00804937,-0.00094465,0.00

006058,0.00719895,-0.00019171,-0.00002115,-0.00670339,0.00416399,0.000

02668,-0.00222845,-0.00158737,-0.00009564,0.00379513,-0.00324712,0.000

08762,-0.00224903,0.00515099,-0.00001722,-0.00009102,-0.00521296,0.000

01505,0.00140384,0.00540400,0.00002464,-0.00038510,0.00013287,0.000037

43,0.00068943,0.00051997,-0.00004326,0.00598367,0.00787457,-0.00012718

,-0.00407949,-0.01232196,0.00001697,0.00155281,-0.00097237,0.00009398,

-0.00071593,-0.00112689,-0.00009190,-0.00305849,-0.02313804,-0.0000769

2,-0.00058159,0.01570145,-0.00004832,-0.01766723,0.03163450,-0.0001073

4,0.01477924,0.00142137,-0.00009673,-0.00027922,-0.00098388,-0.0000641

9,0.00118151,-0.00105390,0.00010443,0.00753863,0.00322375,-0.00000764,

-0.00957253,-0.00010592,0.00001144,0.00002875,-0.00004715,0.00000355,-

0.00008211,0.00007234,-0.00000093,0.00004971,0.00000593,0.00000084,-0.

00006163,0.00001452,-0.00000051,-0.00006542,0.00006059,0.00000189,0.00

071123,-0.00038946,0.00000958,-0.00057440,0.00022791,-0.00001700,-0.00

002374,0.00003796,0.00000415,0.00077679,0.00017243,0.00006594,-0.00453

009,-0.00332268,-0.00009821,0.00267890,0.00272798,-0.00005927,-0.00487

238,-0.00511076,-0.00011356,-0.00152851,-0.00161202,0.00002447,0.00300

975,0.00311496,0.00004945,-0.00218975,0.00206840,0.00005016,0.00132781

,-0.00139727,-0.00002183,-0.50410675,0.48953665,-0.00597600,0.73122064

,-0.00099276,0.00049107,-0.00005564,0.00932383,0.00087307,-0.00006190,

-0.00812939,0.00017723,0.00002377,0.00779827,-0.00438107,-0.00002930,0

.00241189,0.00165664,0.00010276,-0.00465875,0.00280029,-0.00009313,0.0

0218416,-0.00469108,0.00002094,0.00007655,0.00481937,-0.00001761,-0.00

148903,-0.00484881,-0.00003307,0.00049479,-0.00018833,-0.00003689,-0.0

0066941,-0.00041990,0.00004318,-0.00698825,-0.00707226,0.00014547,0.00

416322,0.01117341,-0.00003121,-0.00102399,0.00112731,-0.00007543,-0.00

014189,0.00017415,0.00006973,0.00069423,0.02293647,0.00006341,0.001232

51,-0.01550009,0.00006153,0.02518985,-0.02624354,0.00007447,-0.0164938

2,-0.00437977,0.00017027,-0.00090240,0.00019141,0.00009592,-0.00074577

,0.00153485,-0.00012891,-0.00942425,-0.00305492,0.00001820,0.01049861,

0.00066252,-0.00002334,-0.00003166,0.00004919,-0.00000338,0.00008927,-

0.00007764,0.00000103,-0.00005293,-0.00000926,-0.00000118,0.00006190,-

0.00001201,0.00000065,0.00005334,-0.00007121,-0.00000309,0.00007828,-0

.00045722,0.00000328,-0.00052415,0.00061008,-0.00000062,0.00001449,-0.

00005277,-0.00000368,-0.00093048,-0.00023021,-0.00006981,0.00587650,0.

00289315,0.00009130,-0.00291392,-0.00297283,0.00007030,0.00503419,0.00

527056,0.00011495,0.00161201,0.00172861,-0.00002717,-0.00311497,-0.003

26356,-0.00005036,0.00235399,-0.00220096,-0.00005451,-0.00139727,0.001

49852,0.00002326,0.49077150,-0.53006520,0.00634409,-0.70444958,0.76953

646,0.00001679,-0.00000780,0.00000250,-0.00014372,-0.00001442,-0.00001

245,0.00012424,-0.00000267,0.00000217,-0.00011966,0.00006839,-0.000002

79,-0.00003859,-0.00002669,-0.00000654,0.00006941,-0.00004711,-0.00000

073,-0.00003386,0.00007828,0.00001169,-0.00000106,-0.00007930,-0.00000

790,0.00002489,0.00008114,0.00001652,-0.00000655,0.00000198,0.00000660

,0.00001086,0.00000787,-0.00000382,0.00010931,0.00011100,-0.00004580,-

0.00005038,-0.00017732,-0.00012356,0.00002135,-0.00000737,-0.00018604,

-0.00002469,-0.00001551,0.00026285,-0.00004911,-0.00031477,0.00193666,

-0.00001969,0.00022394,-0.00023121,-0.00027836,0.00037059,0.00238582,0

.00021635,0.00007914,0.00147249,0.00001335,0.00001509,0.00018037,0.000

00941,-0.00003010,-0.00017538,0.00013391,0.00004018,-0.00002507,-0.000

13976,0.00000250,0.00005363,0.00000050,-0.00000057,-0.00000165,-0.0000

0145,0.00000122,0.00000156,0.00000060,0.00000017,-0.00000118,-0.000001

03,0.00000023,-0.00000137,-0.00000116,0.00000051,0.00003227,0.00000863

,-0.00000924,-0.00011669,0.00001666,-0.00001639,-0.00013130,0.00000009

,0.00000275,0.00006384,0.00001716,0.00000188,-0.00000724,-0.00008108,-

0.00005308,-0.00009126,0.00004242,0.00004472,0.00000514,-0.00007920,-0

.00008132,0.00005260,-0.00002447,-0.00002717,-0.00000121,0.00004945,0.

00005035,0.00000873,-0.00003746,0.00003508,0.00000340,0.00002183,-0.00

002326,-0.00000037,-0.00612308,0.00646731,-0.02650432,0.00900608,-0.00

961248,0.03747094,-0.00007533,0.00003705,-0.00000267,0.00050650,0.0000

4292,-0.00000305,-0.00045991,0.00000901,0.00000268,0.00046353,-0.00022

767,-0.00000148,0.00014955,0.00009670,0.00000597,-0.00024916,0.0002364

1,-0.00000506,0.00012133,-0.00038344,0.00000093,0.00001318,0.00036221,

0.00000205,-0.00009524,-0.00039230,0.00000050,0.00000377,0.00001353,-0

.00000211,-0.00004709,-0.00005712,0.00000264,-0.00038642,-0.00023875,0

.00000707,0.00008172,0.00041688,-0.00000224,0.00000133,-0.00001518,-0.

00000250,0.00006894,0.00012027,0.00000282,-0.00081571,0.00107043,-0.00

000867,0.00015922,-0.00041602,0.00000566,0.00368705,0.00237137,-0.0000

3200,0.00016281,-0.00070219,0.00001364,0.00007019,-0.00004142,0.000002

80,-0.00007612,0.00004690,-0.00000212,0.00002501,-0.00025176,0.0000016

8,0.00039137,0.00013281,-0.00000269,-0.00000377,0.00000131,-0.00000031

,0.00000682,-0.00000499,-0.00000005,-0.00000114,0.00000140,-0.00000009

,0.00000523,-0.00000232,-0.00000005,0.00000358,-0.00001045,-0.00000005

,0.00001503,0.00001889,-0.00000034,0.00002961,-0.00003188,0.00000093,-

0.00000130,0.00000247,-0.00000058,-0.00001124,0.00000668,-0.00001212,-

0.00004285,0.00031238,0.00000447,-0.00005680,-0.00006964,0.00000144,0.

00022279,0.00023768,0.00000615,0.00007124,0.00006814,-0.00000114,-0.00

015960,-0.00017038,-0.00000285,0.00017646,-0.00017123,-0.00000339,-0.0

0008038,0.00008306,0.00000122,0.00465959,-0.00364760,0.00004400,-0.210

95244,0.19487598,-0.00265598,0.20241404,0.00006628,-0.00003494,0.00000

320,-0.00055525,-0.00005742,0.00000268,0.00049517,-0.00000352,-0.00000

287,-0.00052090,0.00022702,0.00000123,-0.00014655,-0.00009064,-0.00000

599,0.00029873,-0.00022670,0.00000545,-0.00012605,0.00038333,-0.000000

98,-0.00001059,-0.00037523,-0.00000187,0.00009538,0.00039805,-0.000000

46,-0.00000510,-0.00001727,0.00000198,0.00005356,0.00005958,-0.0000028

7,0.00045693,0.00021846,-0.00000824,-0.00022337,-0.00030433,0.00000154

,0.00001021,-0.00002608,0.00000150,-0.00010429,0.00002869,-0.00000310,

-0.00064182,-0.00024887,-0.00001019,0.00006427,0.00070620,-0.00000600,

0.00269980,0.00395826,0.00003497,0.00056768,-0.00072272,0.00000857,0.0

0006275,0.00003436,-0.00000209,0.00003088,-0.00003777,0.00000292,0.000

06824,0.00011081,-0.00000063,-0.00007732,0.00008479,-0.00000387,0.0000

0369,-0.00000153,0.00000028,-0.00000689,0.00000558,0.00000002,0.000001

20,-0.00000130,0.00000013,-0.00000515,0.00000236,0.00000006,0.00000082

,0.00000094,0.00000023,-0.00002289,0.00002232,0.00000026,0.00002260,0.

00001723,0.00000062,-0.00000913,0.00000233,0.00000013,0.00005246,0.000

03577,0.00001231,0.00003624,-0.00028223,-0.00000257,0.00007233,0.00007

007,-0.00000238,-0.00022963,-0.00022894,-0.00000534,-0.00007213,-0.000

07000,0.00000137,0.00016330,0.00017661,0.00000267,-0.00019248,0.000186

97,0.00000378,0.00008773,-0.00009227,-0.00000136,-0.00305300,0.0043179

9,-0.00005051,0.19433195,-0.22002607,0.00286219,-0.19373424,0.21180476

,-0.00000005,-0.00000026,0.00000153,-0.00000636,-0.00000048,-0.0000056

8,0.00000590,0.00000014,-0.00000135,-0.00000592,0.00000196,-0.00000263

,-0.00000065,-0.00000033,-0.00000259,0.00000415,-0.00000022,0.00000282

,-0.00000079,0.00000092,0.00000059,-0.00000032,-0.00000097,-0.00000159

,0.00000073,-0.00000005,0.00000185,-0.00000090,0.00000063,-0.00000237,

0.00000014,-0.00000050,0.00000050,0.00000381,0.00000302,0.00004216,-0.

00000075,-0.00000558,-0.00005592,0.00000027,-0.00000145,0.00001463,-0.

00000257,0.00000002,0.00011346,0.00000767,-0.00000567,-0.00004265,0.00

000321,0.00000494,-0.00029104,-0.00004255,0.00003634,0.00519079,0.0000

1222,-0.00000216,-0.00008154,-0.00000132,-0.00000261,-0.00004858,0.000

00237,0.00000002,0.00003935,0.00001114,0.00000191,0.00000683,-0.000008

18,-0.00000517,-0.00017185,-0.00000001,-0.00000011,0.00000133,-0.00000

001,-0.00000002,0.00000050,0.00000009,0.00000003,0.00000043,0.00000002

,-0.00000002,0.00000054,0.00000031,-0.00000001,-0.00002401,-0.00000017

,0.00000003,0.00004111,-0.00000016,0.00000193,0.00006823,0.00000021,-0

.00000019,-0.00000997,-0.00000218,0.00000260,0.00000751,-0.00000828,0.

00000250,0.00002979,0.00000307,0.00000254,-0.00001637,-0.00000291,-0.0

0000354,0.00001492,-0.00000101,-0.00000115,0.00000188,0.00000156,0.000

00184,-0.00000882,-0.00000122,0.00000111,0.00000012,0.00000089,-0.0000

0102,-0.00000044,0.00005551,-0.00007034,0.00054236,-0.00266168,0.00287

616,-0.01628453,0.00263490,-0.00283676,0.01092681,0.00014955,-0.000096

70,-0.00000597,0.00046353,0.00022766,0.00000148,-0.00045991,-0.0000090

1,-0.00000268,0.00050650,-0.00004292,0.00000305,-0.00007533,-0.0000370

5,0.00000267,-0.00038642,0.00023875,-0.00000707,0.00008172,-0.00041688

,0.00000224,0.00015922,0.00041602,-0.00000566,-0.00081571,-0.00107043,

0.00000867,0.00006894,-0.00012027,-0.00000282,0.00000133,0.00001518,0.

00000250,-0.00024916,-0.00023641,0.00000506,0.00012133,0.00038344,-0.0

0000093,-0.00004709,0.00005712,-0.00000264,0.00000377,-0.00001353,0.00

000211,-0.00009524,0.00039230,-0.00000050,0.00001318,-0.00036221,-0.00

000205,-0.00004285,-0.00031238,-0.00000447,0.00002501,0.00025176,-0.00

000168,-0.00007612,-0.00004690,0.00000212,0.00007019,0.00004142,-0.000

00280,0.00016281,0.00070219,-0.00001364,0.00039137,-0.00013281,0.00000

269,0.00000682,0.00000499,0.00000005,-0.00000377,-0.00000131,0.0000003

1,0.00001503,-0.00001889,0.00000034,0.00000358,0.00001045,0.00000005,0

.00000523,0.00000232,0.00000005,-0.00000114,-0.00000140,0.00000009,-0.

00000130,-0.00000247,0.00000058,0.00002962,0.00003188,-0.00000093,-0.0

0001124,-0.00000668,0.00001212,0.00368705,-0.00237137,0.00003200,0.004

65960,0.00364760,-0.00004400,0.00017646,0.00017123,0.00000339,-0.21095

253,-0.19487598,0.00265601,-0.00008038,-0.00008305,-0.00000122,0.00022

279,-0.00023768,-0.00000615,-0.00015960,0.00017038,0.00000285,-0.00005

680,0.00006963,-0.00000144,0.00007123,-0.00006814,0.00000114,-0.000009

21,0.00000781,-0.00000002,0.20241412,0.00014655,-0.00009064,-0.0000059

9,0.00052090,0.00022702,0.00000123,-0.00049516,-0.00000352,-0.00000287

,0.00055525,-0.00005742,0.00000268,-0.00006628,-0.00003494,0.00000320,

-0.00045692,0.00021846,-0.00000824,0.00022337,-0.00030433,0.00000154,-

0.00006427,0.00070620,-0.00000600,0.00064182,-0.00024887,-0.00001019,0

.00010429,0.00002869,-0.00000310,-0.00001021,-0.00002608,0.00000150,-0

.00029873,-0.00022670,0.00000545,0.00012605,0.00038333,-0.00000098,-0.

00005356,0.00005958,-0.00000287,0.00000510,-0.00001727,0.00000198,-0.0

0009538,0.00039805,-0.00000046,0.00001059,-0.00037523,-0.00000187,-0.0

0003624,-0.00028223,-0.00000257,-0.00006824,0.00011081,-0.00000062,-0.

00003088,-0.00003776,0.00000292,-0.00006275,0.00003436,-0.00000209,-0.

00056768,-0.00072272,0.00000857,0.00007732,0.00008479,-0.00000387,0.00

000689,0.00000558,0.00000002,-0.00000369,-0.00000153,0.00000028,0.0000

2289,0.00002232,0.00000026,-0.00000082,0.00000094,0.00000023,0.0000051

5,0.00000236,0.00000006,-0.00000120,-0.00000130,0.00000013,0.00000913,

0.00000233,0.00000013,-0.00002260,0.00001723,0.00000062,-0.00005246,0.

00003577,0.00001231,-0.00269980,0.00395826,0.00003497,0.00305300,0.004

31800,-0.00005051,0.00019248,0.00018697,0.00000378,-0.19433195,-0.2200

2599,0.00286220,-0.00008774,-0.00009227,-0.00000136,0.00022963,-0.0002

2894,-0.00000534,-0.00016330,0.00017661,0.00000267,-0.00007232,0.00007

007,-0.00000238,0.00007212,-0.00007000,0.00000137,-0.00000781,0.000008

97,-0.00000003,0.19373424,0.21180467,0.00000065,-0.00000033,-0.0000025

9,0.00000592,0.00000196,-0.00000263,-0.00000590,0.00000014,-0.00000135

,0.00000636,-0.00000048,-0.00000568,0.00000005,-0.00000026,0.00000153,

-0.00000381,0.00000302,0.00004216,0.00000075,-0.00000558,-0.00005592,-

0.00000321,0.00000494,-0.00029104,-0.00000767,-0.00000567,-0.00004265,

0.00000257,0.00000002,0.00011346,-0.00000027,-0.00000145,0.00001463,-0

.00000415,-0.00000022,0.00000282,0.00000079,0.00000092,0.00000059,-0.0

0000014,-0.00000050,0.00000050,0.00000090,0.00000063,-0.00000237,-0.00

000073,-0.00000005,0.00000185,0.00000032,-0.00000097,-0.00000159,0.000

00828,0.00000250,0.00002979,-0.00001114,0.00000191,0.00000683,-0.00000

237,0.00000002,0.00003935,0.00000132,-0.00000261,-0.00004858,-0.000012

22,-0.00000216,-0.00008154,0.00000818,-0.00000517,-0.00017185,0.000000

01,-0.00000002,0.00000050,0.00000001,-0.00000011,0.00000133,0.00000017

,0.00000003,0.00004111,-0.00000031,-0.00000001,-0.00002401,-0.00000002

,-0.00000002,0.00000054,-0.00000009,0.00000003,0.00000043,-0.00000021,

-0.00000019,-0.00000997,0.00000016,0.00000193,0.00006823,0.00000218,0.

00000260,0.00000751,0.00004255,0.00003634,0.00519079,-0.00005551,-0.00

007034,0.00054237,0.00000123,0.00000111,0.00000012,0.00266171,0.002876

17,-0.01628453,-0.00000089,-0.00000102,-0.00000044,0.00000291,-0.00000

354,0.00001492,-0.00000156,0.00000184,-0.00000882,-0.00000307,0.000002

54,-0.00001637,0.00000101,-0.00000115,0.00000188,0.00000002,-0.0000000

3,0.00000008,-0.00263492,-0.00283677,0.01092681,-0.00007612,0.00004690

,0.00000212,0.00002501,-0.00025176,-0.00000168,0.00039137,0.00013281,0

.00000269,0.00016281,-0.00070219,-0.00001364,0.00007019,-0.00004142,-0

.00000280,0.00368705,0.00237137,0.00003200,-0.00081571,0.00107043,0.00

000867,0.00015922,-0.00041602,-0.00000566,0.00008172,0.00041687,0.0000

0224,0.00000133,-0.00001518,0.00000250,0.00006894,0.00012027,-0.000002

82,-0.00004285,0.00031238,-0.00000447,-0.00009524,-0.00039230,-0.00000

050,0.00000377,0.00001353,0.00000211,-0.00004709,-0.00005712,-0.000002

64,0.00012133,-0.00038344,-0.00000093,0.00001318,0.00036221,-0.0000020

5,-0.00024916,0.00023641,0.00000506,0.00046353,-0.00022767,0.00000148,

0.00014955,0.00009670,-0.00000597,-0.00007533,0.00003705,0.00000267,0.

00050650,0.00004292,0.00000305,-0.00045991,0.00000900,-0.00000268,-0.0

0000130,0.00000247,0.00000058,0.00002962,-0.00003188,-0.00000093,0.000

00358,-0.00001045,0.00000005,0.00001503,0.00001889,0.00000034,-0.00000

114,0.00000140,0.00000009,0.00000523,-0.00000232,0.00000005,0.00000682

,-0.00000499,0.00000005,-0.00000377,0.00000131,0.00000031,-0.00001124,

0.00000668,0.00001212,-0.00038642,-0.00023875,-0.00000707,0.00022279,0

.00023768,-0.00000615,-0.00005680,-0.00006963,-0.00000144,-0.00015959,

-0.00017038,0.00000285,0.00007123,0.00006814,0.00000114,0.00465960,-0.

00364760,-0.00004400,-0.21095245,0.19487598,0.00265592,0.00017646,-0.0

0017123,0.00000339,-0.00008038,0.00008305,-0.00000122,0.00000061,-0.00

000066,-0.00000008,0.00001317,0.00001256,0.00000006,0.20241404,0.00003

088,-0.00003777,-0.00000292,0.00006824,0.00011081,0.00000062,-0.000077

33,0.00008479,0.00000387,0.00056768,-0.00072273,-0.00000857,0.00006275

,0.00003436,0.00000209,0.00269980,0.00395826,-0.00003497,-0.00064182,-

0.00024887,0.00001019,0.00006427,0.00070620,0.00000600,-0.00022337,-0.

00030433,-0.00000154,0.00001021,-0.00002608,-0.00000150,-0.00010429,0.

00002869,0.00000310,0.00003624,-0.00028223,0.00000257,0.00009538,0.000

39805,0.00000046,-0.00000510,-0.00001727,-0.00000198,0.00005355,0.0000

5958,0.00000287,-0.00012605,0.00038333,0.00000098,-0.00001059,-0.00037

523,0.00000187,0.00029874,-0.00022670,-0.00000545,-0.00052090,0.000227

02,-0.00000123,-0.00014655,-0.00009064,0.00000599,0.00006628,-0.000034

94,-0.00000320,-0.00055526,-0.00005742,-0.00000268,0.00049517,-0.00000

352,0.00000287,-0.00000913,0.00000233,-0.00000013,0.00002260,0.0000172

3,-0.00000062,0.00000082,0.00000094,-0.00000023,-0.00002289,0.00002232

,-0.00000026,0.00000120,-0.00000130,-0.00000013,-0.00000515,0.00000236

,-0.00000006,-0.00000689,0.00000558,-0.00000002,0.00000369,-0.00000153

,-0.00000028,0.00005246,0.00003577,-0.00001231,0.00045693,0.00021846,0

.00000824,-0.00022963,-0.00022895,0.00000534,0.00007233,0.00007007,0.0

0000238,0.00016330,0.00017662,-0.00000267,-0.00007213,-0.00007000,-0.0

0000137,-0.00305300,0.00431800,0.00005051,0.19433195,-0.22002607,-0.00

286212,-0.00019249,0.00018698,-0.00000378,0.00008774,-0.00009227,0.000

00136,-0.00000066,0.00000108,0.00000009,-0.00001256,-0.00001468,-0.000

00008,-0.19373424,0.21180475,-0.00000237,-0.00000002,0.00003935,-0.000

01114,-0.00000191,0.00000683,0.00000818,0.00000517,-0.00017185,-0.0000

1222,0.00000216,-0.00008154,0.00000132,0.00000261,-0.00004858,0.000042

55,-0.00003634,0.00519079,-0.00000767,0.00000567,-0.00004265,-0.000003

21,-0.00000494,-0.00029104,0.00000075,0.00000558,-0.00005592,-0.000000

27,0.00000145,0.00001463,0.00000257,-0.00000002,0.00011346,0.00000828,

-0.00000250,0.00002979,-0.00000073,0.00000005,0.00000185,0.00000090,-0

.00000063,-0.00000237,-0.00000014,0.00000050,0.00000050,0.00000079,-0.

00000092,0.00000059,0.00000032,0.00000097,-0.00000159,-0.00000415,0.00

000022,0.00000282,0.00000592,-0.00000196,-0.00000263,0.00000065,0.0000

0033,-0.00000259,0.00000005,0.00000026,0.00000153,0.00000636,0.0000004

8,-0.00000568,-0.00000590,-0.00000014,-0.00000135,-0.00000021,0.000000

19,-0.00000997,0.00000016,-0.00000193,0.00006823,-0.00000031,0.0000000

1,-0.00002401,0.00000017,-0.00000003,0.00004111,-0.00000009,-0.0000000

3,0.00000043,-0.00000002,0.00000002,0.00000054,0.00000001,0.00000002,0

.00000050,0.00000001,0.00000011,0.00000133,0.00000218,-0.00000260,0.00

000751,-0.00000381,-0.00000302,0.00004216,0.00000291,0.00000354,0.0000

1492,-0.00000307,-0.00000254,-0.00001637,-0.00000156,-0.00000184,-0.00

000882,0.00000101,0.00000115,0.00000188,-0.00005550,0.00007033,0.00054

237,0.00266162,-0.00287608,-0.01628453,0.00000123,-0.00000111,0.000000

12,-0.00000089,0.00000102,-0.00000044,0.00000008,-0.00000009,0.0000000

7,0.00000006,0.00000008,0.00000174,-0.00263483,0.00283669,0.01092681,0

.00007019,0.00004142,0.00000280,0.00016281,0.00070219,0.00001364,0.000

39137,-0.00013281,-0.00000269,0.00002501,0.00025176,0.00000168,-0.0000

7612,-0.00004690,-0.00000212,-0.00004285,-0.00031238,0.00000447,-0.000

09524,0.00039230,0.00000050,0.00001318,-0.00036221,0.00000205,0.000121

33,0.00038343,0.00000093,-0.00004709,0.00005712,0.00000264,0.00000377,

-0.00001353,-0.00000211,0.00368705,-0.00237137,-0.00003200,-0.00081571

,-0.00107043,-0.00000867,0.00006894,-0.00012027,0.00000282,0.00000133,

0.00001518,-0.00000250,0.00008172,-0.00041688,-0.00000224,0.00015922,0

.00041602,0.00000566,-0.00038642,0.00023875,0.00000707,0.00050650,-0.0

0004292,-0.00000305,-0.00007533,-0.00003705,-0.00000267,0.00014955,-0.

00009670,0.00000597,0.00046353,0.00022767,-0.00000148,-0.00045991,-0.0

0000901,0.00000268,0.00002961,0.00003188,0.00000093,-0.00000130,-0.000

00247,-0.00000058,0.00000523,0.00000232,-0.00000005,-0.00000114,-0.000

00140,-0.00000009,0.00001503,-0.00001889,-0.00000034,0.00000358,0.0000

1045,-0.00000005,-0.00000377,-0.00000131,-0.00000031,0.00000682,0.0000

0499,-0.00000005,-0.00001124,-0.00000668,-0.00001212,-0.00024916,-0.00

023641,-0.00000506,0.00017646,0.00017123,-0.00000339,0.00465959,0.0036

4760,0.00004400,-0.00008038,-0.00008305,0.00000122,-0.21095246,-0.1948

7598,-0.00265602,-0.00005680,0.00006963,0.00000144,0.00007123,-0.00006

814,-0.00000114,0.00022279,-0.00023768,0.00000615,-0.00015959,0.000170

37,-0.00000285,0.00001317,-0.00001256,-0.00000006,0.00000061,0.0000006

6,0.00000008,-0.00000921,0.00000781,0.00000002,0.20241405,-0.00006275,

0.00003436,0.00000209,-0.00056768,-0.00072272,-0.00000857,0.00007733,0

.00008479,0.00000387,-0.00006824,0.00011081,0.00000062,-0.00003088,-0.

00003777,-0.00000292,-0.00003624,-0.00028223,0.00000257,-0.00009538,0.

00039805,0.00000046,0.00001059,-0.00037523,0.00000187,0.00012606,0.000

38333,0.00000098,-0.00005356,0.00005958,0.00000287,0.00000510,-0.00001

727,-0.00000198,-0.00269980,0.00395826,-0.00003497,0.00064182,-0.00024

887,0.00001019,0.00010429,0.00002869,0.00000310,-0.00001021,-0.0000260

8,-0.00000150,0.00022337,-0.00030433,-0.00000154,-0.00006427,0.0007062

0,0.00000600,-0.00045693,0.00021846,0.00000824,0.00055526,-0.00005742,

-0.00000268,-0.00006628,-0.00003494,-0.00000320,0.00014655,-0.00009064

,0.00000599,0.00052090,0.00022702,-0.00000123,-0.00049517,-0.00000352,

0.00000287,-0.00002260,0.00001723,-0.00000062,0.00000913,0.00000233,-0

.00000013,0.00000515,0.00000236,-0.00000006,-0.00000120,-0.00000130,-0

.00000013,0.00002289,0.00002232,-0.00000026,-0.00000082,0.00000094,-0.

00000023,-0.00000369,-0.00000153,-0.00000028,0.00000689,0.00000558,-0.

00000002,-0.00005246,0.00003577,-0.00001231,-0.00029874,-0.00022670,-0

.00000545,0.00019249,0.00018698,-0.00000378,0.00305300,0.00431799,0.00

005051,-0.00008774,-0.00009227,0.00000136,-0.19433194,-0.22002605,-0.0

0286223,-0.00007232,0.00007007,0.00000238,0.00007212,-0.00007000,-0.00

000137,0.00022963,-0.00022894,0.00000534,-0.00016330,0.00017662,-0.000

00267,0.00001256,-0.00001468,-0.00000008,0.00000066,0.00000108,0.00000

009,-0.00000781,0.00000897,0.00000003,0.19373424,0.21180473,-0.0000013

2,0.00000261,-0.00004858,0.00001222,0.00000216,-0.00008154,-0.00000818

,0.00000517,-0.00017185,0.00001114,-0.00000191,0.00000683,0.00000237,-

0.00000002,0.00003935,-0.00000828,-0.00000250,0.00002979,0.00000073,0.

00000005,0.00000185,-0.00000032,0.00000097,-0.00000159,-0.00000079,-0.

00000092,0.00000059,0.00000014,0.00000050,0.00000050,-0.00000090,-0.00

000063,-0.00000237,-0.00004255,-0.00003634,0.00519079,0.00000767,0.000

00567,-0.00004265,-0.00000257,-0.00000002,0.00011346,0.00000027,0.0000

0145,0.00001463,-0.00000075,0.00000558,-0.00005592,0.00000321,-0.00000

494,-0.00029104,0.00000381,-0.00000302,0.00004216,-0.00000636,0.000000

48,-0.00000568,-0.00000005,0.00000026,0.00000153,-0.00000065,0.0000003

3,-0.00000259,-0.00000592,-0.00000196,-0.00000263,0.00000590,-0.000000

14,-0.00000135,-0.00000016,-0.00000193,0.00006823,0.00000021,0.0000001

9,-0.00000997,0.00000002,0.00000002,0.00000054,0.00000009,-0.00000003,

0.00000043,-0.00000017,-0.00000003,0.00004111,0.00000031,0.00000001,-0

.00002401,-0.00000001,0.00000011,0.00000133,-0.00000001,0.00000002,0.0

0000050,-0.00000218,-0.00000260,0.00000751,0.00000415,0.00000022,0.000

00282,-0.00000123,-0.00000111,0.00000012,0.00005551,0.00007034,0.00054

237,0.00000089,0.00000102,-0.00000044,-0.00266172,-0.00287619,-0.01628

454,0.00000307,-0.00000254,-0.00001637,-0.00000101,0.00000115,0.000001

88,-0.00000291,0.00000354,0.00001492,0.00000156,-0.00000184,-0.0000088

2,-0.00000006,0.00000008,0.00000174,-0.00000008,-0.00000009,0.00000007

,-0.00000002,0.00000003,0.00000008,0.00263493,0.00283680,0.01092682\\-

0.00000001,0.00000001,0.,0.00000005,-0.00000007,0.,0.00000005,0.000000

55,-0.00000167,-0.00000005,-0.00000003,0.,0.00000002,0.00000001,0.,0.0

0000017,0.00000006,0.,-0.00000013,-0.00000004,-0.00000001,-0.00000049,

-0.00000006,-0.00000130,-0.00000008,0.00000002,-0.00000001,0.00000003,

-0.00000004,0.,0.00000003,0.00000003,0.,-0.00000017,0.00000006,0.,0.00

000013,-0.00000003,0.,-0.00000003,0.,0.,-0.00000003,-0.00000001,0.,0.0

0000010,-0.00000004,0.,0.00000040,-0.00000002,-0.00000130,-0.00000020,

-0.00000001,0.,0.00000012,0.00000005,0.,-0.00000003,0.,0.,0.00000004,-

0.00000001,0.,-0.00000005,0.00000002,0.,0.00000003,-0.00000046,-0.0000

0166,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.00000001,0.,0.,0.,0.,0.,0.,0.,0.,

0.,0.,0.,0.,0.,-0.00000002,0.00000003,0.00000596,0.00000015,-0.0000000

4,0.,-0.00000014,-0.00000015,0.,0.00000015,0.00000014,0.,0.00000002,0.

00000002,0.00000001,-0.00000002,-0.00000002,0.00000001,-0.00000016,0.0

0000017,0.,0.00000003,-0.00000003,0.00000001,0.00000015,-0.00000015,0.

,-0.00000003,0.00000003,0.00000001,-0.00000003,0.00000003,0.,0.0000000

3,0.00000003,0.,0.00000003,-0.00000003,0.,-0.00000003,-0.00000003,0.\\

\@

THE REAL VOYAGE OF DISCOVERY CONSISTS NOT IN SEEKING NEW LANDSCAPES

BUT IN HAVING NEW EYES.

-- MARCEL PROUST

Job cpu time: 4 days 4 hours 18 minutes 3.3 seconds.

File lengths (MBytes): RWF= 3973 Int= 0 D2E= 0 Chk= 54 Scr= 1

Normal termination of Gaussian 09 at Tue Jul 30 03:39:15 2019.