**BENZENO**

File benzene.fchk Density MP2

Angstrom

Multipoles

Limit 2

Switch 4.0

Radius H 0.35

Punch file.punch

Add TOP1 0.0 0.0 1.00

Add TOP2 0.0 0.0 -1.00

Start

Finish

G D M A

by Anthony Stone

Distributed Multipoles from Gaussian wavefunctions

version 2.3.3 (e2d289a)

Compiled with gfortran on 05 October 2021 at 19:26:39

Starting at 19:48:52 on 03 Dec 2021

Using MP2 density matrix from file benzene.fchk

Distributed Multipole Analysis

Standard DMA for products of primitives with exponent greater than 4.00000

Using 80-point Euler-MacLaurin radial quadrature

Using 590-point Lebedev quadrature

Becke smoothing parameter = 3

Positions and radii in angstrom

Multipole moments in atomic units, ea\_0^k for rank k

C x = -0.000000 y = 1.394663 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = 0.050325

|Q1| = 0.152398 Q11s = -0.152398

|Q2| = 0.711237 Q20 = -0.689378 Q22c = -0.174975

C x = -1.207814 y = 0.697332 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = 0.050323

|Q1| = 0.152398 Q11c = 0.131981 Q11s = -0.076200

|Q2| = 0.711233 Q20 = -0.689375 Q22c = 0.087482 Q22s = -0.151530

C x = -1.207814 y = -0.697332 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = 0.050323

|Q1| = 0.152398 Q11c = 0.131981 Q11s = 0.076200

|Q2| = 0.711233 Q20 = -0.689375 Q22c = 0.087482 Q22s = 0.151530

C x = -0.000000 y = -1.394663 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = 0.050325

|Q1| = 0.152398 Q11s = 0.152398

|Q2| = 0.711237 Q20 = -0.689378 Q22c = -0.174975

C x = 1.207814 y = -0.697332 z = -0.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = 0.050323

|Q1| = 0.152398 Q11c = -0.131981 Q11s = 0.076200

|Q2| = 0.711233 Q20 = -0.689375 Q22c = 0.087482 Q22s = -0.151530

C x = 1.207814 y = 0.697332 z = -0.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = 0.050323

|Q1| = 0.152398 Q11c = -0.131981 Q11s = -0.076200

|Q2| = 0.711233 Q20 = -0.689375 Q22c = 0.087482 Q22s = 0.151530

H x = -0.000000 y = 2.479089 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041400

|Q1| = 0.118058 Q11s = -0.118058

|Q2| = 0.192926 Q20 = -0.144046 Q22c = -0.128340

H x = -2.146954 y = 1.239545 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041399

|Q1| = 0.118061 Q11c = 0.102245 Q11s = -0.059028

|Q2| = 0.192911 Q20 = -0.144041 Q22c = 0.064150 Q22s = -0.111138

H x = -2.146954 y = -1.239545 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041399

|Q1| = 0.118061 Q11c = 0.102245 Q11s = 0.059028

|Q2| = 0.192911 Q20 = -0.144041 Q22c = 0.064150 Q22s = 0.111138

H x = -0.000000 y = -2.479089 z = 0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041400

|Q1| = 0.118058 Q11s = 0.118058

|Q2| = 0.192926 Q20 = -0.144046 Q22c = -0.128340

H x = 2.146954 y = -1.239545 z = -0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041399

|Q1| = 0.118061 Q11c = -0.102245 Q11s = 0.059028

|Q2| = 0.192911 Q20 = -0.144041 Q22c = 0.064150 Q22s = -0.111138

H x = 2.146954 y = 1.239545 z = -0.000000 angstrom

Maximum rank = 2 Radius = 0.350 angstrom

Q00 = 0.041399

|Q1| = 0.118061 Q11c = -0.102245 Q11s = -0.059028

|Q2| = 0.192911 Q20 = -0.144041 Q22c = 0.064150 Q22s = 0.111138

TOP1 x = 0.000000 y = 0.000000 z = 1.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = -0.275170

|Q1| = 0.289518 Q10 = 0.289518

|Q2| = 0.192943 Q20 = 0.192943 Q22c = 0.000002

TOP2 x = 0.000000 y = 0.000000 z = -1.000000 angstrom

Maximum rank = 2 Radius = 0.650 angstrom

Q00 = -0.275170

|Q1| = 0.289518 Q10 = -0.289518

|Q2| = 0.192943 Q20 = 0.192943 Q22c = 0.000002

Total multipoles referred to origin at

x = 0.000000, y = 0.000000, z = 0.000000 angstrom

Q00 = -0.000000

|Q1| = 0.000000

|Q2| = 6.145000 Q20 = -6.145000 Q22c = -0.000285

CPU time used: 1m17.217s Total: 1m17.217s

Finished at 19:50:09 on 03 Dec 2021

**GAUSSIAN**

**INPUT**

%Mem=3800MB

%NProcShared=6

%chk=/home/itamar/Aromaticity-test-set/Benzene/benzene.chk

#P MP2/6-311++G\*\* Density=MP2

14-H

0 1

6 0.000000 1.394663 0.000000

6 1.207814 0.697332 0.000000

6 1.207814 -0.697332 0.000000

6 0.000000 -1.394663 0.000000

6 -1.207814 -0.697332 0.000000

6 -1.207814 0.697332 0.000000

1 0.000000 2.479089 0.000000

1 2.146954 1.239544 0.000000

1 2.146954 -1.239544 0.000000

1 0.000000 -2.479089 0.000000

1 -2.146954 -1.239544 0.000000

1 -2.146954 1.239544 0.000000

**OUTUPT**

Entering Gaussian System, Link 0=g09

Initial command:

/apps/software//g09/l1.exe /scratch/itamar/2504.cluster.abaxnet/Gau-2498.inp -scrdir=/scratch/itamar/2504.cluster.abaxnet/

Entering Link 1 = /apps/software//g09/l1.exe PID= 2499.

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

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Cite this work as:

Gaussian 09, Revision A.02,

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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, 2009.

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

Gaussian 09: EM64L-G09RevA.02 11-Jun-2009

3-Dec-2021

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

%Mem=3800MB

%NProcShared=6

Will use up to 6 processors via shared memory.

%chk=/home/itamar/Aromaticity-test-set/Benzene/benzene.chk

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

#P MP2/6-311++G\*\* Density=MP2

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

1/30=1,38=1/1;

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

3/5=4,6=6,7=1111,11=9,16=1,25=1,30=1,71=1/1,2,3;

4//1;

5/5=2,38=5/2;

8/6=4,10=2/1;

9/15=1,16=-3/6;

10/5=1,13=10/2;

6/7=2,8=2,9=2,10=2,22=2/1;

99/5=1,9=1/99;

Leave Link 1 at Fri Dec 3 19:45:16 2021, MaxMem= 498073600 cpu: 0.3

(Enter /apps/software//g09/l101.exe)

----

14-H

----

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

6 0. 1.39466 0.

6 1.20781 0.69733 0.

6 1.20781 -0.69733 0.

6 0. -1.39466 0.

6 -1.20781 -0.69733 0.

6 -1.20781 0.69733 0.

1 0. 2.47909 0.

1 2.14695 1.23954 0.

1 2.14695 -1.23954 0.

1 0. -2.47909 0.

1 -2.14695 -1.23954 0.

1 -2.14695 1.23954 0.

NAtoms= 12 NQM= 12 NQMF= 0 NMic= 0 NMicF= 0 NTot= 12.

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 12 12 12 12 1 1 1 1

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

NucSpn= 0 0 0 0 0 0 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 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000 0.0000000

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

Atom 11 12

IAtWgt= 1 1

AtmWgt= 1.0078250 1.0078250

NucSpn= 1 1

AtZEff= 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000

NMagM= 2.7928460 2.7928460

Leave Link 101 at Fri Dec 3 19:45:16 2021, MaxMem= 498073600 cpu: 0.2

(Enter /apps/software//g09/l202.exe)

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.000000 1.394663 0.000000

2 6 0 1.207814 0.697332 0.000000

3 6 0 1.207814 -0.697332 0.000000

4 6 0 0.000000 -1.394663 0.000000

5 6 0 -1.207814 -0.697332 0.000000

6 6 0 -1.207814 0.697332 0.000000

7 1 0 0.000000 2.479089 0.000000

8 1 0 2.146954 1.239544 0.000000

9 1 0 2.146954 -1.239544 0.000000

10 1 0 0.000000 -2.479089 0.000000

11 1 0 -2.146954 -1.239544 0.000000

12 1 0 -2.146954 1.239544 0.000000

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

Distance matrix (angstroms):

1 2 3 4 5

1 C 0.000000

2 C 1.394663 0.000000

3 C 2.415628 1.394664 0.000000

4 C 2.789326 2.415628 1.394663 0.000000

5 C 2.415628 2.789327 2.415628 1.394663 0.000000

6 C 1.394663 2.415628 2.789327 2.415628 1.394664

7 H 1.084426 2.152550 3.398303 3.873752 3.398303

8 H 2.152550 1.084425 2.152550 3.398302 3.873752

9 H 3.398302 2.152550 1.084425 2.152550 3.398303

10 H 3.873752 3.398303 2.152550 1.084426 2.152550

11 H 3.398302 3.873752 3.398303 2.152550 1.084425

12 H 2.152550 3.398303 3.873752 3.398302 2.152550

6 7 8 9 10

6 C 0.000000

7 H 2.152550 0.000000

8 H 3.398303 2.479089 0.000000

9 H 3.873752 4.293908 2.479088 0.000000

10 H 3.398303 4.958178 4.293908 2.479089 0.000000

11 H 2.152550 4.293908 4.958177 4.293908 2.479089

12 H 1.084425 2.479089 4.293908 4.958177 4.293908

11 12

11 H 0.000000

12 H 2.479088 0.000000

Stoichiometry C6H6

Framework group D6H[3C2'(HC.CH)]

Deg. of freedom 2

Full point group D6H NOp 24

Largest Abelian subgroup D2H NOp 8

Largest concise Abelian subgroup D2 NOp 4

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 6 0 0.000000 1.394663 0.000000

2 6 0 -1.207814 0.697332 0.000000

3 6 0 -1.207814 -0.697331 0.000000

4 6 0 0.000000 -1.394663 0.000000

5 6 0 1.207814 -0.697332 0.000000

6 6 0 1.207814 0.697331 0.000000

7 1 0 0.000000 2.479089 0.000000

8 1 0 -2.146954 1.239545 0.000000

9 1 0 -2.146954 -1.239544 0.000000

10 1 0 0.000000 -2.479089 0.000000

11 1 0 2.146954 -1.239545 0.000000

12 1 0 2.146954 1.239544 0.000000

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

Rotational constants (GHZ): 5.7037315 5.7037315 2.8518658

Leave Link 202 at Fri Dec 3 19:45:16 2021, MaxMem= 498073600 cpu: 0.1

(Enter /apps/software//g09/l301.exe)

Standard basis: 6-311++G(d,p) (5D, 7F)

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

There are 38 symmetry adapted basis functions of AG symmetry.

There are 28 symmetry adapted basis functions of B1G symmetry.

There are 8 symmetry adapted basis functions of B2G symmetry.

There are 13 symmetry adapted basis functions of B3G symmetry.

There are 8 symmetry adapted basis functions of AU symmetry.

There are 13 symmetry adapted basis functions of B1U symmetry.

There are 38 symmetry adapted basis functions of B2U symmetry.

There are 28 symmetry adapted basis functions of B3U symmetry.

Integral buffers will be 131072 words long.

Raffenetti 1 integral format.

Two-electron integral symmetry is turned on.

174 basis functions, 270 primitive gaussians, 180 cartesian basis functions

21 alpha electrons 21 beta electrons

nuclear repulsion energy 203.5013944183 Hartrees.

IExCor= 0 DFT=F Ex=HF Corr=None ExCW=0 ScaHFX= 1.000000

ScaDFX= 1.000000 1.000000 1.000000 1.000000 ScalE2= 1.000000 1.000000

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

NAtoms= 12 NActive= 12 NUniq= 2 SFac= 3.00D+00 NAtFMM= 80 NAOKFM=F Big=F

Leave Link 301 at Fri Dec 3 19:45:16 2021, MaxMem= 498073600 cpu: 0.3

(Enter /apps/software//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

NBasis= 174 RedAO= T NBF= 38 28 8 13 8 13 38 28

NBsUse= 173 1.00D-06 NBFU= 38 28 8 13 8 13 37 28

Leave Link 302 at Fri Dec 3 19:45:17 2021, MaxMem= 498073600 cpu: 1.6

(Enter /apps/software//g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Fri Dec 3 19:45:17 2021, MaxMem= 498073600 cpu: 0.2

(Enter /apps/software//g09/l401.exe)

Harris functional with IExCor= 205 diagonalized for initial guess.

ExpMin= 3.60D-02 ExpMax= 4.56D+03 ExpMxC= 6.82D+02 IAcc=3 IRadAn= 0 AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 0 IDoV= 1

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

Omega= 0.000000 0.000000 1.000000 0.000000 0.000000 ICntrl= 500 IOpCl= 0

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

I1Cent= 4 NGrid= 0.

Petite list used in FoFCou.

Harris En= -231.151488063891

Initial guess orbital symmetries:

Occupied (A1G) (E1U) (E1U) (E2G) (E2G) (B1U) (A1G) (E1U)

(E1U) (E2G) (E2G) (A1G) (B2U) (B1U) (E1U) (E1U)

(A2U) (E2G) (E2G) (E1G) (E1G)

Virtual (E2U) (E2U) (A1G) (B2G) (E1U) (E1U) (E2G) (E2G)

(A1G) (A2U) (B1U) (E1G) (E1G) (B2U) (A1G) (E1U)

(E1U) (E2G) (E2G) (B2G) (B2G) (E2U) (E2U) (E2G)

(E2G) (B2G) (B2G) (B2G) (B2G) (E2G) (E2G) (A1G)

(E2G) (E2G) (B2G) (B2G) (B1U) (A2G) (E1U) (E1U)

(E2G) (E2G) (B2U) (A2G) (B1U) (A1G) (A2U) (E2G)

(E2G) (E1U) (E1U) (A1G) (E1G) (E1G) (E2U) (E2U)

(B2G) (B2G) (E2G) (E2G) (B2G) (B2G) (A1G) (B2G)

(A2G) (B2G) (B2G) (E1U) (E1U) (A2U) (E2G) (E2G)

(B1G) (E1G) (E1G) (E2G) (E2G) (E2U) (E2U) (A1G)

(B1U) (B2U) (E1U) (E1U) (A1G) (E2U) (E2U) (B2G)

(E2G) (E2G) (E1U) (E1U) (A2U) (E1G) (E1G) (E2G)

(E2G) (B2U) (E1G) (E1G) (E1U) (E1U) (A2G) (B1U)

(E2G) (E2G) (E2U) (E2U) (B2G) (A1U) (A1G) (E2G)

(E2G) (E1U) (E1U) (A2U) (E1U) (E1U) (B1U) (A1G)

(E1G) (E1G) (?A) (?A) (?A) (E2G) (E2G) (E2U) (E2U)

(A2G) (E2G) (E2G) (B2U) (B2G) (E2G) (E2G) (E1U)

(E1U) (A1G) (B1U) (E2G) (E2G) (B1U) (E1U) (E1U)

(A2G) (A1G) (E1U) (E1U) (E2G) (E2G) (B1U)

The electronic state of the initial guess is 1-A1G.

Leave Link 401 at Fri Dec 3 19:45:17 2021, MaxMem= 498073600 cpu: 2.2

(Enter /apps/software//g09/l502.exe)

Closed shell SCF:

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.

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

Keep R1 ints in memory in canonical form, NReq=135774799.

IEnd= 119810 IEndB= 119810 NGot= 498073600 MDV= 365312788

LenX= 365312788 LenY= 365279947

Symmetry not used in FoFDir.

MinBra= 0 MaxBra= 2 Meth= 1.

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.

Cycle 1 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-04

Density has only Abelian symmetry.

E= -230.452981724818

DIIS: error= 6.92D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -230.452981724818 IErMin= 1 ErrMin= 6.92D-02

ErrMax= 6.92D-02 EMaxC= 1.00D-01 BMatC= 5.17D-01 BMatP= 5.17D-01

IDIUse=3 WtCom= 3.08D-01 WtEn= 6.92D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.327 Goal= None Shift= 0.000

GapD= 0.327 DampG=1.000 DampE=0.500 DampFc=0.5000 IDamp=-1.

Damping current iteration by 5.00D-01

RMSDP=3.66D-03 MaxDP=7.10D-02 OVMax= 1.60D-01

Cycle 2 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.612392670408 Delta-E= -0.159410945589 Rises=F Damp=T

DIIS: error= 3.42D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -230.612392670408 IErMin= 2 ErrMin= 3.42D-02

ErrMax= 3.42D-02 EMaxC= 1.00D-01 BMatC= 1.11D-01 BMatP= 5.17D-01

IDIUse=3 WtCom= 6.58D-01 WtEn= 3.42D-01

Coeff-Com: -0.686D+00 0.169D+01

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

Coeff: -0.451D+00 0.145D+01

Gap= 0.387 Goal= None Shift= 0.000

RMSDP=2.36D-03 MaxDP=6.00D-02 DE=-1.59D-01 OVMax= 4.87D-02

Cycle 3 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.755018446574 Delta-E= -0.142625776167 Rises=F Damp=F

DIIS: error= 3.33D-03 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -230.755018446574 IErMin= 3 ErrMin= 3.33D-03

ErrMax= 3.33D-03 EMaxC= 1.00D-01 BMatC= 1.07D-03 BMatP= 1.11D-01

IDIUse=3 WtCom= 9.67D-01 WtEn= 3.33D-02

Coeff-Com: -0.810D-01 0.124D+00 0.957D+00

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

Coeff: -0.783D-01 0.120D+00 0.958D+00

Gap= 0.379 Goal= None Shift= 0.000

RMSDP=4.11D-04 MaxDP=9.71D-03 DE=-1.43D-01 OVMax= 8.70D-03

Cycle 4 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.756033214449 Delta-E= -0.001014767874 Rises=F Damp=F

DIIS: error= 6.24D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -230.756033214449 IErMin= 4 ErrMin= 6.24D-04

ErrMax= 6.24D-04 EMaxC= 1.00D-01 BMatC= 2.48D-05 BMatP= 1.07D-03

IDIUse=3 WtCom= 9.94D-01 WtEn= 6.24D-03

Coeff-Com: 0.784D-02-0.190D-01-0.117D-01 0.102D+01

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

Coeff: 0.779D-02-0.189D-01-0.116D-01 0.102D+01

Gap= 0.379 Goal= None Shift= 0.000

RMSDP=8.73D-05 MaxDP=1.86D-03 DE=-1.01D-03 OVMax= 1.81D-03

Cycle 5 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.756075972548 Delta-E= -0.000042758100 Rises=F Damp=F

DIIS: error= 1.80D-04 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -230.756075972548 IErMin= 5 ErrMin= 1.80D-04

ErrMax= 1.80D-04 EMaxC= 1.00D-01 BMatC= 1.69D-06 BMatP= 2.48D-05

IDIUse=3 WtCom= 9.98D-01 WtEn= 1.80D-03

Coeff-Com: 0.273D-02-0.341D-02-0.423D-01-0.191D+00 0.123D+01

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

Coeff: 0.272D-02-0.341D-02-0.422D-01-0.191D+00 0.123D+01

Gap= 0.379 Goal= None Shift= 0.000

RMSDP=3.59D-05 MaxDP=7.79D-04 DE=-4.28D-05 OVMax= 6.72D-04

Cycle 6 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.756079547693 Delta-E= -0.000003575144 Rises=F Damp=F

DIIS: error= 1.24D-05 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -230.756079547693 IErMin= 6 ErrMin= 1.24D-05

ErrMax= 1.24D-05 EMaxC= 1.00D-01 BMatC= 8.39D-09 BMatP= 1.69D-06

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

Coeff-Com: -0.389D-03 0.518D-03 0.683D-02 0.227D-01-0.204D+00 0.117D+01

Coeff: -0.389D-03 0.518D-03 0.683D-02 0.227D-01-0.204D+00 0.117D+01

Gap= 0.379 Goal= None Shift= 0.000

RMSDP=3.57D-06 MaxDP=5.55D-05 DE=-3.58D-06 OVMax= 4.97D-05

Cycle 7 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.756079566767 Delta-E= -0.000000019075 Rises=F Damp=F

DIIS: error= 1.32D-06 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -230.756079566767 IErMin= 7 ErrMin= 1.32D-06

ErrMax= 1.32D-06 EMaxC= 1.00D-01 BMatC= 1.53D-10 BMatP= 8.39D-09

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

Coeff-Com: 0.522D-04-0.689D-04-0.114D-02-0.324D-02 0.337D-01-0.288D+00

Coeff-Com: 0.126D+01

Coeff: 0.522D-04-0.689D-04-0.114D-02-0.324D-02 0.337D-01-0.288D+00

Coeff: 0.126D+01

Gap= 0.379 Goal= None Shift= 0.000

RMSDP=4.87D-07 MaxDP=7.82D-06 DE=-1.91D-08 OVMax= 5.99D-06

Cycle 8 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.756079567121 Delta-E= -0.000000000354 Rises=F Damp=F

DIIS: error= 1.21D-07 at cycle 8 NSaved= 8.

NSaved= 8 IEnMin= 8 EnMin= -230.756079567121 IErMin= 8 ErrMin= 1.21D-07

ErrMax= 1.21D-07 EMaxC= 1.00D-01 BMatC= 1.46D-12 BMatP= 1.53D-10

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

Coeff-Com: -0.908D-05 0.114D-04 0.219D-03 0.609D-03-0.631D-02 0.577D-01

Coeff-Com: -0.297D+00 0.125D+01

Coeff: -0.908D-05 0.114D-04 0.219D-03 0.609D-03-0.631D-02 0.577D-01

Coeff: -0.297D+00 0.125D+01

Gap= 0.379 Goal= None Shift= 0.000

RMSDP=3.74D-08 MaxDP=7.52D-07 DE=-3.54D-10 OVMax= 6.21D-07

Cycle 9 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.756079567126 Delta-E= -0.000000000005 Rises=F Damp=F

DIIS: error= 2.46D-08 at cycle 9 NSaved= 9.

NSaved= 9 IEnMin= 9 EnMin= -230.756079567126 IErMin= 9 ErrMin= 2.46D-08

ErrMax= 2.46D-08 EMaxC= 1.00D-01 BMatC= 3.89D-14 BMatP= 1.46D-12

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

Coeff-Com: 0.137D-05-0.150D-05-0.408D-04-0.107D-03 0.112D-02-0.108D-01

Coeff-Com: 0.602D-01-0.354D+00 0.130D+01

Coeff: 0.137D-05-0.150D-05-0.408D-04-0.107D-03 0.112D-02-0.108D-01

Coeff: 0.602D-01-0.354D+00 0.130D+01

Gap= 0.379 Goal= None Shift= 0.000

RMSDP=1.26D-08 MaxDP=2.02D-07 DE=-4.77D-12 OVMax= 1.81D-07

Cycle 10 Pass 1 IDiag 1:

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

E= -230.756079567127 Delta-E= -0.000000000001 Rises=F Damp=F

DIIS: error= 3.91D-09 at cycle 10 NSaved= 10.

NSaved=10 IEnMin=10 EnMin= -230.756079567127 IErMin=10 ErrMin= 3.91D-09

ErrMax= 3.91D-09 EMaxC= 1.00D-01 BMatC= 1.11D-15 BMatP= 3.89D-14

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

Coeff-Com: -0.165D-06 0.193D-06 0.388D-05 0.108D-04-0.100D-03 0.958D-03

Coeff-Com: -0.580D-02 0.472D-01-0.294D+00 0.125D+01

Coeff: -0.165D-06 0.193D-06 0.388D-05 0.108D-04-0.100D-03 0.958D-03

Coeff: -0.580D-02 0.472D-01-0.294D+00 0.125D+01

Gap= 0.379 Goal= None Shift= 0.000

RMSDP=1.26D-09 MaxDP=3.31D-08 DE=-1.25D-12 OVMax= 3.10D-08

Density matrix breaks symmetry, PCut= 1.00D-07

Density has only Abelian symmetry.

SCF Done: E(RHF) = -230.756079567 A.U. after 10 cycles

Convg = 0.1264D-08 -V/T = 2.0013

KE= 2.304576554469D+02 PE=-9.438004226684D+02 EE= 2.790852932362D+02

Leave Link 502 at Fri Dec 3 19:45:22 2021, MaxMem= 498073600 cpu: 31.6

(Enter /apps/software//g09/l801.exe)

ExpMin= 3.60D-02 ExpMax= 4.56D+03 ExpMxC= 6.82D+02 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

HarFok: IExCor= 205 AccDes= 0.00D+00 IRadAn= 5 IDoV=-2

ScaDFX= 1.000000 1.000000 1.000000 1.000000

Largest valence mixing into a core orbital is 1.52D-04

Largest core mixing into a valence orbital is 3.99D-05

Range of M.O.s used for correlation: 7 173

NBasis= 174 NAE= 21 NBE= 21 NFC= 6 NFV= 0

NROrb= 167 NOA= 15 NOB= 15 NVA= 152 NVB= 152

\*\*\*\* Warning!!: The largest alpha MO coefficient is 0.98864499D+02

Leave Link 801 at Fri Dec 3 19:45:23 2021, MaxMem= 498073600 cpu: 1.2

(Enter /apps/software//g09/l906.exe)

Frozen-core derivative calculation, NFC= 6 NFV= 0.

FulOut=F Deriv=T AODrv=F NAtomX= 12

MMem= 574 MDisk= 15 MDiskD= 15

W3Min= 653940 MinDsk= 1009670 NBas6D= 180

NBas2D= 16542 NTT= 16290 LW2= 2040000

MDV= 497685314 MDiskM= 38247 NBas2p= 4804

Fully in-core method, ICMem= 280915704.

IMap= 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20

IMap= 21

JobTyp=1 Pass 1 fully in-core, NPsUse= 6.

Compute canonical integrals, IntTyp= 4.

Symmetry not used in FoFDir.

MinBra= 0 MaxBra= 2 Meth= 1.

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.

Spin components of T(2) and E(2):

alpha-alpha T2 = 0.4231958300D-01 E2= -0.1077297806D+00

alpha-beta T2 = 0.2225623976D+00 E2= -0.6124852812D+00

beta-beta T2 = 0.4231958300D-01 E2= -0.1077297806D+00

The integrals were generated 1 times.

ANorm= 0.1143329158D+01

E2 = -0.8279448424D+00 EUMP2 = -0.23158402440958D+03

Leave Link 906 at Fri Dec 3 19:46:08 2021, MaxMem= 498073600 cpu: 272.6

(Enter /apps/software//g09/l1002.exe)

Minotr: Closed shell wavefunction.

Computing MP2/KS-MP2 derivatives.

Using Z-Vector for PSCF gradient.

Skipping F1 and S1 gradient terms here.

Frozen-core window.

Direct CPHF calculation.

Differentiating once with respect to electric field.

with respect to dipole field.

Electric field/nuclear overlap derivatives assumed to be zero.

Using symmetry in CPHF.

Requested convergence is 1.0D-10 RMS, and 1.0D-09 maximum.

NewPWx=F KeepS1=T KeepF1=T KeepIn=T MapXYZ=F SortEE=F KeepMc=T.

MDV= 498073500 using IRadAn= 0.

Keep R1 ints in memory in canonical form, NReq=133514357.

Symmetry not used in FoFDir.

MinBra= 0 MaxBra= 2 Meth= 1.

IRaf= 0 NMat= 1 IRICut= 1 DoRegI=T DoRafI=F ISym2E= 0 JSym2E=0.

Solving linear equations separately, MaxMat= 0.

There are 1 degrees of freedom in the 1st order CPHF. IDoFFX=0.

LinEq1: Iter= 0 NonCon= 1 RMS=3.40D-03 Max=7.25D-02

AX will form 1 AO Fock derivatives at one time.

LinEq1: Iter= 1 NonCon= 1 RMS=8.38D-04 Max=1.51D-02

LinEq1: Iter= 2 NonCon= 1 RMS=2.34D-04 Max=5.39D-03

LinEq1: Iter= 3 NonCon= 1 RMS=4.87D-05 Max=8.47D-04

LinEq1: Iter= 4 NonCon= 1 RMS=6.98D-06 Max=1.00D-04

LinEq1: Iter= 5 NonCon= 1 RMS=6.43D-07 Max=8.70D-06

LinEq1: Iter= 6 NonCon= 1 RMS=5.66D-08 Max=1.07D-06

LinEq1: Iter= 7 NonCon= 1 RMS=4.29D-09 Max=4.37D-08

LinEq1: Iter= 8 NonCon= 1 RMS=3.49D-10 Max=5.32D-09

LinEq1: Iter= 9 NonCon= 0 RMS=3.01D-11 Max=3.96D-10

Linear equations converged to 1.000D-10 1.000D-09 after 9 iterations.

End of Minotr Frequency-dependent properties file 721 does not exist.

End of Minotr Frequency-dependent properties file 722 does not exist.

Leave Link 1002 at Fri Dec 3 19:46:16 2021, MaxMem= 498073600 cpu: 47.6

(Enter /apps/software//g09/l601.exe)

Copying SCF densities to generalized density rwf, IOpCl= 0 IROHF=0.

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

Population analysis using the MP2 density.

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

Orbital symmetries:

Occupied (A1G) (E1U) (E1U) (E2G) (E2G) (B1U) (A1G) (E1U)

(E1U) (E2G) (E2G) (A1G) (B1U) (B2U) (E1U) (E1U)

(A2U) (E2G) (E2G) (E1G) (E1G)

Virtual (A1G) (E1U) (E1U) (E2G) (E2G) (B2G) (E2U) (E2U)

(A2U) (E1G) (E1G) (A1G) (B2U) (E2G) (E2G) (E1U)

(E1U) (A1G) (B2G) (E2G) (E2G) (E2U) (E2U) (B2G)

(B2G) (B2G) (B2G) (B2G) (E2G) (E2G) (A2G) (A1G)

(B2G) (B2G) (B2G) (B2G) (E2G) (E2G) (E2G) (E2G)

(E1U) (E1U) (B2U) (A1G) (A2U) (B2G) (B2G) (B2G)

(E2G) (E2G) (A2G) (E1G) (E1G) (A1G) (E2U) (E2U)

(B2G) (B2G) (B2G) (B2G) (E2G) (E2G) (A1G) (E1U)

(E1U) (E2G) (E2G) (B1U) (E1U) (E1U) (A2G) (A2U)

(E2G) (E2G) (B1G) (E1G) (E1G) (E2U) (E2U) (B1U)

(A1G) (B2U) (E1U) (E1U) (A1G) (B2G) (E2U) (E2U)

(E2G) (E2G) (E1U) (E1U) (A2U) (E1G) (E1G) (E2G)

(E2G) (B2U) (E1G) (E1G) (A2G) (E1U) (E1U) (B1U)

(E2G) (E2G) (E2U) (E2U) (B2G) (A1U) (E2G) (E2G)

(A1G) (E1U) (E1U) (?A) (?A) (?A) (A1G) (?A) (?A)

(?A) (E2G) (E2G) (A2U) (E1G) (E1G) (A2G) (E2U)

(E2U) (E2G) (E2G) (B2G) (B2U) (E2G) (E2G) (E1U)

(E1U) (A1G) (B1U) (E2G) (E2G) (B1U) (E1U) (E1U)

(A2G) (A1G) (E1U) (E1U) (E2G) (E2G) (B1U)

The electronic state is 1-A1G.

Alpha occ. eigenvalues -- -11.23911 -11.23854 -11.23854 -11.23731 -11.23731

Alpha occ. eigenvalues -- -11.23670 -1.15218 -1.01639 -1.01639 -0.82524

Alpha occ. eigenvalues -- -0.82524 -0.71064 -0.64444 -0.62081 -0.58948

Alpha occ. eigenvalues -- -0.58948 -0.50201 -0.49607 -0.49607 -0.33709

Alpha occ. eigenvalues -- -0.33709

Alpha virt. eigenvalues -- 0.04211 0.04896 0.04896 0.06625 0.06625

Alpha virt. eigenvalues -- 0.09787 0.10916 0.10916 0.12935 0.15260

Alpha virt. eigenvalues -- 0.15260 0.15802 0.16283 0.18107 0.18107

Alpha virt. eigenvalues -- 0.18340 0.18341 0.19249 0.20920 0.21225

Alpha virt. eigenvalues -- 0.21225 0.21620 0.21620 0.22818 0.22818

Alpha virt. eigenvalues -- 0.24704 0.25034 0.25150 0.28896 0.28896

Alpha virt. eigenvalues -- 0.30307 0.33421 0.36848 0.40810 0.40829

Alpha virt. eigenvalues -- 0.41029 0.42968 0.42968 0.49812 0.49812

Alpha virt. eigenvalues -- 0.50860 0.50861 0.60407 0.60915 0.71539

Alpha virt. eigenvalues -- 0.71752 0.72273 0.72275 0.75025 0.75025

Alpha virt. eigenvalues -- 0.75089 0.75768 0.75768 0.79661 0.81957

Alpha virt. eigenvalues -- 0.81957 0.87294 0.88591 0.93974 0.93980

Alpha virt. eigenvalues -- 0.95071 0.95071 0.97527 1.01594 1.01594

Alpha virt. eigenvalues -- 1.05928 1.05928 1.10216 1.12082 1.12082

Alpha virt. eigenvalues -- 1.12974 1.16947 1.21739 1.21739 1.24907

Alpha virt. eigenvalues -- 1.32318 1.32318 1.39100 1.39100 1.49923

Alpha virt. eigenvalues -- 1.55610 1.71115 1.78517 1.78518 1.79536

Alpha virt. eigenvalues -- 1.82533 1.84417 1.84417 1.90698 1.90698

Alpha virt. eigenvalues -- 1.93224 1.93224 1.98963 2.05400 2.05400

Alpha virt. eigenvalues -- 2.10284 2.10284 2.12822 2.23618 2.23618

Alpha virt. eigenvalues -- 2.23880 2.24761 2.24764 2.29511 2.34552

Alpha virt. eigenvalues -- 2.34552 2.37710 2.37710 2.63703 2.66180

Alpha virt. eigenvalues -- 2.74088 2.74088 2.74217 2.81378 2.81380

Alpha virt. eigenvalues -- 2.95872 2.95873 2.96864 2.98864 3.02180

Alpha virt. eigenvalues -- 3.02183 3.02590 3.04641 3.04641 3.05762

Alpha virt. eigenvalues -- 3.19115 3.19115 3.26173 3.29281 3.29281

Alpha virt. eigenvalues -- 3.32488 3.32488 3.48092 3.54701 3.77420

Alpha virt. eigenvalues -- 3.77420 3.90428 3.90428 3.91835 4.07405

Alpha virt. eigenvalues -- 4.40501 4.40501 4.49228 4.57282 4.57283

Alpha virt. eigenvalues -- 5.27705 24.74675 25.13433 25.13433 25.25640

Alpha virt. eigenvalues -- 25.25640 25.36108

Condensed to atoms (all electrons):

1 2 3 4 5 6

1 C 5.766259 0.143636 -0.308966 0.461689 -0.308966 0.143636

2 C 0.143636 5.737465 0.157525 -0.308966 0.476273 -0.315972

3 C -0.308966 0.157525 5.737465 0.143636 -0.315972 0.476273

4 C 0.461689 -0.308966 0.143636 5.766259 0.143636 -0.308966

5 C -0.308966 0.476273 -0.315972 0.143636 5.737465 0.157525

6 C 0.143636 -0.315972 0.476273 -0.308966 0.157525 5.737465

7 H 0.439037 -0.084281 -0.015316 0.041641 -0.015316 -0.084281

8 H -0.083295 0.436963 -0.083328 -0.015632 0.041744 -0.015688

9 H -0.015632 -0.083328 0.436963 -0.083295 -0.015688 0.041744

10 H 0.041641 -0.015316 -0.084281 0.439037 -0.084281 -0.015316

11 H -0.015632 0.041744 -0.015688 -0.083295 0.436963 -0.083328

12 H -0.083295 -0.015688 0.041744 -0.015632 -0.083328 0.436963

7 8 9 10 11 12

1 C 0.439037 -0.083295 -0.015632 0.041641 -0.015632 -0.083295

2 C -0.084281 0.436963 -0.083328 -0.015316 0.041744 -0.015688

3 C -0.015316 -0.083328 0.436963 -0.084281 -0.015688 0.041744

4 C 0.041641 -0.015632 -0.083295 0.439037 -0.083295 -0.015632

5 C -0.015316 0.041744 -0.015688 -0.084281 0.436963 -0.083328

6 C -0.084281 -0.015688 0.041744 -0.015316 -0.083328 0.436963

7 H 0.566805 -0.009513 -0.001984 0.002123 -0.001984 -0.009513

8 H -0.009513 0.566226 -0.009435 -0.001984 0.002111 -0.001984

9 H -0.001984 -0.009435 0.566226 -0.009513 -0.001984 0.002111

10 H 0.002123 -0.001984 -0.009513 0.566805 -0.009513 -0.001984

11 H -0.001984 0.002111 -0.001984 -0.009513 0.566226 -0.009435

12 H -0.009513 -0.001984 0.002111 -0.001984 -0.009435 0.566226

Mulliken atomic charges:

1

1 C -0.180109

2 C -0.170053

3 C -0.170053

4 C -0.180109

5 C -0.170053

6 C -0.170053

7 H 0.172583

8 H 0.173816

9 H 0.173816

10 H 0.172583

11 H 0.173816

12 H 0.173816

Sum of Mulliken atomic charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 C -0.007526

2 C 0.003763

3 C 0.003763

4 C -0.007526

5 C 0.003763

6 C 0.003763

Sum of Mulliken charges with hydrogens summed into heavy atoms = 0.00000

Electronic spatial extent (au): <R\*\*2>= 460.4875

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 0.0000 Y= 0.0000 Z= 0.0000 Tot= 0.0000

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -32.5507 YY= -32.5503 ZZ= -40.8158

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 2.7549 YY= 2.7553 ZZ= -5.5102

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

Octapole moment (field-independent basis, Debye-Ang\*\*2):

XXX= 0.0000 YYY= 0.0000 ZZZ= 0.0000 XYY= 0.0000

XXY= 0.0000 XXZ= 0.0000 XZZ= 0.0000 YZZ= 0.0000

YYZ= 0.0000 XYZ= 0.0000

Hexadecapole moment (field-independent basis, Debye-Ang\*\*3):

XXXX= -279.6360 YYYY= -279.6278 ZZZZ= -51.3381 XXXY= 0.0000

XXXZ= 0.0000 YYYX= 0.0000 YYYZ= 0.0000 ZZZX= 0.0000

ZZZY= 0.0000 XXYY= -93.2104 XXZZ= -66.2038 YYZZ= -66.2034

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 2.035013944183D+02 E-N=-9.446532204707D+02 KE= 2.314769309438D+02

Symmetry AG KE= 7.451944781309D+01

Symmetry B1G KE= 3.780570046607D+01

Symmetry B2G KE= 2.121162061608D+00

Symmetry B3G KE= 2.183680501206D+00

Symmetry AU KE= 1.469222092705D-01

Symmetry B1U KE= 1.943473550160D+00

Symmetry B2U KE= 7.228795242943D+01

Symmetry B3U KE= 4.046859191296D+01

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Fri Dec 3 19:46:17 2021, MaxMem= 498073600 cpu: 2.1

(Enter /apps/software//g09/l9999.exe)

1\1\GINC-DLT01\SP\RMP2-FC\6-311++G(d,p)\C6H6\ITAMAR\03-Dec-2021\0\\#P

MP2/6-311++G\*\* Density=MP2\\14-H\\0,1\C,0,0.,1.394663,0.\C,0,1.207814,

0.697332,0.\C,0,1.207814,-0.697332,0.\C,0,0.,-1.394663,0.\C,0,-1.20781

4,-0.697332,0.\C,0,-1.207814,0.697332,0.\H,0,0.,2.479089,0.\H,0,2.1469

54,1.239544,0.\H,0,2.146954,-1.239544,0.\H,0,0.,-2.479089,0.\H,0,-2.14

6954,-1.239544,0.\H,0,-2.146954,1.239544,0.\\Version=EM64L-G09RevA.02\

State=1-A1G\HF=-230.7560796\MP2=-231.5840244\RMSD=1.264e-09\Dipole=0.,

0.,0.\Quadrupole=2.048201,2.048466,-4.096667,0.,0.,0.\PG=D06H [3C2'(H1

C1.C1H1)]\\@

SOME PHYSICISTS WOULD PREFER TO COME BACK TO THE IDEA OF AN OBJECTIVE

REAL WORLD WHOSE SMALLEST PARTS EXIST OBJECTIVELY IN THE SAME SENSE AS

STONES OR TREES EXIST INDEPENDENTLY OF WHETHER WE OBSERVE THEM.

THIS, HOWEVER, IS IMPOSSIBLE. -- WERNER HEISENBERG

Job cpu time: 0 days 0 hours 6 minutes 1.1 seconds.

File lengths (MBytes): RWF= 14 Int= 0 D2E= 0 Chk= 4 Scr= 1

Normal termination of Gaussian 09 at Fri Dec 3 19:46:17 2021.