Entering Gaussian System, Link 0=g09

Initial command:

/apps/gaussian/g09d01/g09/l1.exe "/srv/scratch/z5105842/Gau-21512.inp" -scrdir="/srv/scratch/z5105842/"

Entering Link 1 = /apps/gaussian/g09d01/g09/l1.exe PID= 21513.

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

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

Cite this work as:

Gaussian 09, Revision D.01,

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

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

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

Gaussian 09: ES64L-G09RevD.01 24-Apr-2013

17-Aug-2019

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

%nprocshared=12

Will use up to 12 processors via shared memory.

%chk=Oxy1.chk

%mem=10GB

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

#p opt=calcall b3lyp/6-311g\* scrf=(solvent=dmso,smd) empiricaldispersi

on=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=4,6=6,7=1,11=2,16=1,25=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=4,6=6,7=1,11=2,16=1,25=1,30=1,70=32205,71=2,72=21,74=-5,124=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 Sat Aug 17 17:34:55 2019, MaxMem= 1342177280 cpu: 0.9

(Enter /apps/gaussian/g09d01/g09/l101.exe)

----

Oxy1

----

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O 0. 0. 0.60729

O 0. 0. -0.60729

NAtoms= 2 NQM= 2 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

IAtWgt= 16 16

AtmWgt= 15.9949146 15.9949146

NucSpn= 0 0

AtZEff= 0.0000000 0.0000000

NQMom= 0.0000000 0.0000000

NMagM= 0.0000000 0.0000000

AtZNuc= 8.0000000 8.0000000

Leave Link 101 at Sat Aug 17 17:34:55 2019, MaxMem= 1342177280 cpu: 3.2

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

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

! Initial Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.2146 calculate D2E/DX2 analytically !

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

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

Number of steps in this run= 20 maximum allowed number of steps= 100.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:34:55 2019, MaxMem= 1342177280 cpu: 0.0

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 8 0 0.000000 0.000000 0.607290

2 8 0 0.000000 0.000000 -0.607290

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

Stoichiometry O2

Framework group D\*H[C\*(O.O)]

Deg. of freedom 1

Full point group D\*H NOp 8

Largest Abelian subgroup D2H NOp 8

Largest concise Abelian subgroup C2 NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 8 0 0.000000 0.000000 0.607290

2 8 0 0.000000 0.000000 -0.607290

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

Rotational constants (GHZ): 0.0000000 42.8364048 42.8364048

Leave Link 202 at Sat Aug 17 17:34:55 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l301.exe)

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

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

There are 10 symmetry adapted cartesian basis functions of AG symmetry.

There are 1 symmetry adapted cartesian basis functions of B1G symmetry.

There are 4 symmetry adapted cartesian basis functions of B2G symmetry.

There are 4 symmetry adapted cartesian basis functions of B3G symmetry.

There are 1 symmetry adapted cartesian basis functions of AU symmetry.

There are 10 symmetry adapted cartesian basis functions of B1U symmetry.

There are 4 symmetry adapted cartesian basis functions of B2U symmetry.

There are 4 symmetry adapted cartesian basis functions of B3U symmetry.

There are 9 symmetry adapted basis functions of AG symmetry.

There are 1 symmetry adapted basis functions of B1G symmetry.

There are 4 symmetry adapted basis functions of B2G symmetry.

There are 4 symmetry adapted basis functions of B3G symmetry.

There are 1 symmetry adapted basis functions of AU symmetry.

There are 9 symmetry adapted basis functions of B1U symmetry.

There are 4 symmetry adapted basis functions of B2U symmetry.

There are 4 symmetry adapted basis functions of B3U symmetry.

36 basis functions, 64 primitive gaussians, 38 cartesian basis functions

8 alpha electrons 8 beta electrons

nuclear repulsion energy 27.8839939319 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= 2 NActive= 2 NUniq= 1 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= -0.0004554978 Hartrees.

Nuclear repulsion after empirical dispersion term = 27.8835384341 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= 2.

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

Smoothing algorithm: Karplus/York (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

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

Spheres list:

ISph on Nord Re0 Alpha Xe Ye Ze

1 O 1 2.2940 1.000 0.000000 0.000000 0.607290

2 O 2 2.2940 1.000 0.000000 0.000000 -0.607290

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

GePol: Number of generator spheres = 2

GePol: Total number of spheres = 2

GePol: Number of exposed spheres = 2 (100.00%)

GePol: Number of points = 602

GePol: Average weight of points = 0.14

GePol: Minimum weight of points = 0.67D-02

GePol: Maximum weight of points = 0.16851

GePol: Number of points with low weight = 0

GePol: Fraction of low-weight points (<1% of avg) = 0.00%

GePol: Cavity surface area = 83.628 Ang\*\*2

GePol: Cavity volume = 70.162 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0118720665 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 27.8716663676 Hartrees.

Leave Link 301 at Sat Aug 17 17:34:55 2019, MaxMem= 1342177280 cpu: 0.9

(Enter /apps/gaussian/g09d01/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= 36 RedAO= T EigKep= 2.38D-02 NBF= 9 1 4 4 1 9 4 4

NBsUse= 36 1.00D-06 EigRej= -1.00D+00 NBFU= 9 1 4 4 1 9 4 4

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= 38 38 38 38 38 MxSgAt= 2 MxSgA2= 2.

Leave Link 302 at Sat Aug 17 17:34:56 2019, MaxMem= 1342177280 cpu: 7.3

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:34:57 2019, MaxMem= 1342177280 cpu: 1.5

(Enter /apps/gaussian/g09d01/g09/l401.exe)

ExpMin= 2.56D-01 ExpMax= 8.59D+03 ExpMxC= 1.30D+03 IAcc=1 IRadAn= 1 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 1 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 1 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= -150.327971550939

JPrj=0 DoOrth=F DoCkMO=F.

Initial guess orbital symmetries:

Occupied (SGU) (SGG) (SGG) (SGU) (SGG) (PIU) (PIU) (PIG)

Virtual (PIG) (SGU) (SGU) (PIU) (PIU) (SGG) (SGG) (PIG)

(PIG) (SGU) (PIU) (PIU) (DLTG) (DLTG) (SGG) (DLTU)

(DLTU) (PIG) (PIG) (SGU) (PIU) (PIU) (SGG) (PIG)

(PIG) (SGU) (SGG) (SGU)

Leave Link 401 at Sat Aug 17 17:34:57 2019, MaxMem= 1342177280 cpu: 9.1

(Enter /apps/gaussian/g09d01/g09/l502.exe)

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

Keep R1 ints in memory in symmetry-blocked form, NReq=3529640.

IVT= 23750 IEndB= 23750 NGot= 1342177280 MDV= 1342119376

LenX= 1342119376 LenY= 1342117491

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.

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

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

wScrn= 0.000000 ICntrl= 600 IOpCl= 0 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 666 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Cycle 1 Pass 1 IDiag 1:

Inv3: Mode=1 IEnd= 1087212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 2.89D-15 for 567.

Iteration 1 A\*A^-1 deviation from orthogonality is 1.19D-15 for 576 46.

Iteration 1 A^-1\*A deviation from unit magnitude is 3.11D-15 for 567.

Iteration 1 A^-1\*A deviation from orthogonality is 6.81D-16 for 401 305.

E= -150.306750739936

DIIS: error= 2.69D-02 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -150.306750739936 IErMin= 1 ErrMin= 2.69D-02

ErrMax= 2.69D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.88D-02 BMatP= 1.88D-02

IDIUse=3 WtCom= 7.31D-01 WtEn= 2.69D-01

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.071 Goal= None Shift= 0.000

GapD= 0.071 DampG=0.500 DampE=0.500 DampFc=0.2500 IDamp=-1.

Damping current iteration by 2.50D-01

RMSDP=2.56D-03 MaxDP=2.67D-02 OVMax= 3.45D-02

Cycle 2 Pass 1 IDiag 1:

E= -150.309295688448 Delta-E= -0.002544948512 Rises=F Damp=T

DIIS: error= 1.80D-02 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -150.309295688448 IErMin= 2 ErrMin= 1.80D-02

ErrMax= 1.80D-02 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.77D-03 BMatP= 1.88D-02

IDIUse=3 WtCom= 8.20D-01 WtEn= 1.80D-01

Coeff-Com: -0.208D+01 0.308D+01

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

Coeff: -0.170D+01 0.270D+01

Gap= 0.071 Goal= None Shift= 0.000

RMSDP=1.26D-03 MaxDP=1.20D-02 DE=-2.54D-03 OVMax= 9.76D-03

Cycle 3 Pass 1 IDiag 1:

E= -150.315215368711 Delta-E= -0.005919680263 Rises=F Damp=F

DIIS: error= 7.38D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -150.315215368711 IErMin= 3 ErrMin= 7.38D-04

ErrMax= 7.38D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.34D-05 BMatP= 8.77D-03

IDIUse=3 WtCom= 9.93D-01 WtEn= 7.38D-03

Coeff-Com: 0.229D-01-0.857D-02 0.986D+00

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

Coeff: 0.227D-01-0.851D-02 0.986D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=9.70D-05 MaxDP=1.32D-03 DE=-5.92D-03 OVMax= 8.47D-04

Cycle 4 Pass 1 IDiag 1:

E= -150.315219865819 Delta-E= -0.000004497109 Rises=F Damp=F

DIIS: error= 4.32D-04 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -150.315219865819 IErMin= 4 ErrMin= 4.32D-04

ErrMax= 4.32D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.96D-06 BMatP= 1.34D-05

IDIUse=3 WtCom= 9.96D-01 WtEn= 4.32D-03

Coeff-Com: 0.696D-01-0.940D-01 0.408D+00 0.616D+00

Coeff-En: 0.000D+00 0.000D+00 0.140D+00 0.860D+00

Coeff: 0.693D-01-0.936D-01 0.407D+00 0.617D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=3.60D-05 MaxDP=4.23D-04 DE=-4.50D-06 OVMax= 3.81D-04

Cycle 5 Pass 1 IDiag 1:

E= -150.315222364496 Delta-E= -0.000002498676 Rises=F Damp=F

DIIS: error= 1.97D-05 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -150.315222364496 IErMin= 5 ErrMin= 1.97D-05

ErrMax= 1.97D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.26D-09 BMatP= 3.96D-06

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

Coeff-Com: 0.216D-03-0.413D-03 0.871D-05 0.410D-01 0.959D+00

Coeff: 0.216D-03-0.413D-03 0.871D-05 0.410D-01 0.959D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=1.73D-06 MaxDP=2.09D-05 DE=-2.50D-06 OVMax= 1.81D-05

Cycle 6 Pass 1 IDiag 1:

E= -150.315222369562 Delta-E= -0.000000005066 Rises=F Damp=F

DIIS: error= 8.87D-07 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -150.315222369562 IErMin= 6 ErrMin= 8.87D-07

ErrMax= 8.87D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.18D-12 BMatP= 7.26D-09

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

Coeff-Com: -0.175D-03 0.233D-03-0.109D-02-0.261D-02 0.477D-02 0.999D+00

Coeff: -0.175D-03 0.233D-03-0.109D-02-0.261D-02 0.477D-02 0.999D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=4.51D-08 MaxDP=3.88D-07 DE=-5.07D-09 OVMax= 9.96D-07

Cycle 7 Pass 1 IDiag 1:

E= -150.315222369568 Delta-E= -0.000000000006 Rises=F Damp=F

DIIS: error= 1.73D-08 at cycle 7 NSaved= 7.

NSaved= 7 IEnMin= 7 EnMin= -150.315222369568 IErMin= 7 ErrMin= 1.73D-08

ErrMax= 1.73D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.24D-15 BMatP= 7.18D-12

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

Coeff-Com: 0.402D-05-0.514D-05 0.101D-04 0.524D-05-0.118D-02-0.347D-01

Coeff-Com: 0.104D+01

Coeff: 0.402D-05-0.514D-05 0.101D-04 0.524D-05-0.118D-02-0.347D-01

Coeff: 0.104D+01

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=1.33D-09 MaxDP=1.56D-08 DE=-5.85D-12 OVMax= 2.94D-08

Error on total polarization charges = 0.00004

SCF Done: E(RB3LYP) = -150.315222370 A.U. after 7 cycles

NFock= 7 Conv=0.13D-08 -V/T= 2.0020

KE= 1.500179961066D+02 PE=-4.115619873791D+02 EE= 8.335710253534D+01

SMD-CDS (non-electrostatic) energy (kcal/mol) = -7.45

(included in total energy above)

Leave Link 502 at Sat Aug 17 17:34:59 2019, MaxMem= 1342177280 cpu: 17.0

(Enter /apps/gaussian/g09d01/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 36

NBasis= 36 NAE= 8 NBE= 8 NFC= 0 NFV= 0

NROrb= 36 NOA= 8 NOB= 8 NVA= 28 NVB= 28

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.71809787D-01

Leave Link 801 at Sat Aug 17 17:34:59 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l1101.exe)

Using compressed storage, NAtomX= 2.

Will process 3 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Sat Aug 17 17:35:00 2019, MaxMem= 1342177280 cpu: 5.9

(Enter /apps/gaussian/g09d01/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Sat Aug 17 17:35:00 2019, MaxMem= 1342177280 cpu: 0.8

(Enter /apps/gaussian/g09d01/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 2.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 1342177160.

G2DrvN: will do 3 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= 0 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 = 349

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 Sat Aug 17 17:35:02 2019, MaxMem= 1342177280 cpu: 15.1

(Enter /apps/gaussian/g09d01/g09/l1002.exe)

Minotr: Closed shell wavefunction.

IDoAtm=11

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.

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= 1342177220 using IRadAn= 2.

Generate precomputed XC quadrature information.

Keep R1 ints in memory in symmetry-blocked form, NReq=2520021.

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

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

wScrn= 0.000000 ICntrl= 600 IOpCl= 0 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 666 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Solving linear equations simultaneously, MaxMat= 0.

There are 6 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 6.

6 vectors produced by pass 0 Test12= 3.73D-15 1.67D-08 XBig12= 1.46D+01 3.47D+00.

AX will form 6 AO Fock derivatives at one time.

6 vectors produced by pass 1 Test12= 3.73D-15 1.67D-08 XBig12= 9.69D+00 1.57D+00.

6 vectors produced by pass 2 Test12= 3.73D-15 1.67D-08 XBig12= 7.63D-02 9.61D-02.

6 vectors produced by pass 3 Test12= 3.73D-15 1.67D-08 XBig12= 8.43D-04 1.65D-02.

6 vectors produced by pass 4 Test12= 3.73D-15 1.67D-08 XBig12= 1.73D-05 2.95D-03.

6 vectors produced by pass 5 Test12= 3.73D-15 1.67D-08 XBig12= 4.38D-08 8.80D-05.

1 vectors produced by pass 6 Test12= 3.73D-15 1.67D-08 XBig12= 6.40D-11 3.35D-06.

1 vectors produced by pass 7 Test12= 3.73D-15 1.67D-08 XBig12= 9.67D-14 1.07D-07.

InvSVY: IOpt=1 It= 1 EMax= 4.47D-16

Solved reduced A of dimension 38 with 6 vectors.

FullF1: Do perturbations 1 to 6.

Isotropic polarizability for W= 0.000000 6.52 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 Sat Aug 17 17:35:03 2019, MaxMem= 1342177280 cpu: 9.3

(Enter /apps/gaussian/g09d01/g09/l601.exe)

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

Occupied (SGG) (SGU) (SGG) (SGU) (SGG) (PIU) (PIU) (PIG)

Virtual (PIG) (SGU) (PIU) (PIU) (SGU) (SGG) (SGG) (PIG)

(PIG) (SGU) (PIU) (PIU) (?A) (?A) (?A) (DLTU)

(DLTU) (PIG) (PIG) (SGU) (PIU) (PIU) (SGG) (PIG)

(PIG) (SGU) (SGG) (SGU)

Unable to determine electronic state: partially filled degenerate orbitals.

Alpha occ. eigenvalues -- -19.27479 -19.27457 -1.28378 -0.80196 -0.53638

Alpha occ. eigenvalues -- -0.52059 -0.51456 -0.25697

Alpha virt. eigenvalues -- -0.18516 0.20318 0.67520 0.69216 0.70378

Alpha virt. eigenvalues -- 0.71780 0.78541 0.79718 0.80746 1.24656

Alpha virt. eigenvalues -- 2.23778 2.26844 2.57723 2.57902 2.83051

Alpha virt. eigenvalues -- 2.83948 2.84207 3.40067 3.43174 3.75856

Alpha virt. eigenvalues -- 4.52475 4.54839 4.63696 4.81888 4.84563

Alpha virt. eigenvalues -- 5.96772 49.48856 49.67101

Condensed to atoms (all electrons):

1 2

1 O 7.970377 0.029623

2 O 0.029623 7.970377

Mulliken charges:

1

1 O 0.000000

2 O 0.000000

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 O 0.000000

2 O 0.000000

APT charges:

1

1 O 0.000000

2 O 0.000000

Sum of APT charges = 0.00000

APT charges with hydrogens summed into heavy atoms:

1

1 O 0.000000

2 O 0.000000

Electronic spatial extent (au): <R\*\*2>= 43.7074

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= -9.0078 YY= -10.8241 ZZ= -10.6132

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 1.1406 YY= -0.6758 ZZ= -0.4648

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= -5.7969 YYYY= -7.6062 ZZZZ= -28.5190 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -2.2339 XXZZ= -5.4542 YYZZ= -6.8284

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 2.787166636758D+01 E-N=-4.115619873326D+02 KE= 1.500179961066D+02

Symmetry AG KE= 6.966918434408D+01

Symmetry B1G KE= 1.030858853531D-34

Symmetry B2G KE=-5.563494811108D-33

Symmetry B3G KE= 6.042344214701D+00

Symmetry AU KE= 2.219769886934D-34

Symmetry B1U KE= 6.509062408353D+01

Symmetry B2U KE= 4.665015609570D+00

Symmetry B3U KE= 4.550827854738D+00

Exact polarizability: 3.910 0.000 2.973 0.000 0.000 12.675

Approx polarizability: 5.093 0.000 3.176 0.000 0.000 24.749

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sat Aug 17 17:35:03 2019, MaxMem= 1342177280 cpu: 3.2

(Enter /apps/gaussian/g09d01/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.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 349

Leave Link 701 at Sat Aug 17 17:35:04 2019, MaxMem= 1342177280 cpu: 10.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:35:04 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Sat Aug 17 17:35:05 2019, MaxMem= 1342177280 cpu: 6.8

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.57772181D-30 7.46297853D-34 1.46861961D-15

Polarizability= 3.91006566D+00 1.40996756D-12 2.97294627D+00

1.56217398D-11-2.83779683D-11 1.26745963D+01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 8 0.000000000 0.000000000 -0.012546088

2 8 0.000000000 0.000000000 0.012546088

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

Cartesian Forces: Max 0.012546088 RMS 0.007243487

Force constants in Cartesian coordinates:

1 2 3 4 5

1 0.647315D-02

2 0.000000D+00 0.660278D-02

3 0.000000D+00 0.000000D+00 0.757694D+00

4 -0.647315D-02 0.000000D+00 0.000000D+00 0.647315D-02

5 0.000000D+00 -0.660278D-02 0.000000D+00 0.000000D+00 0.660278D-02

6 0.000000D+00 0.000000D+00 -0.757694D+00 0.000000D+00 0.000000D+00

6

6 0.757694D+00

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Force constants in internal coordinates:

1

1 0.757694D+00

Leave Link 716 at Sat Aug 17 17:35:05 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.012546088 RMS 0.012546088

Search for a local minimum.

Step number 1 out of a maximum of 20

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .12546D-01 SwitMx=.10000D-02 MixMth= 1

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- analytic derivatives used.

The second derivative matrix:

R1

R1 0.75769

ITU= 0

Eigenvalues --- 0.75769

RFO step: Lambda=-2.07684418D-04 EMin= 7.57693729D-01

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.01170525 RMS(Int)= 0.00000000

Iteration 2 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000000

ITry= 1 IFail=0 DXMaxC= 8.28D-03 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 5.07D-19 for atom 2.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.29522 -0.01255 0.00000 -0.01655 -0.01655 2.27867

Item Value Threshold Converged?

Maximum Force 0.012546 0.000450 NO

RMS Force 0.012546 0.000300 NO

Maximum Displacement 0.008277 0.001800 NO

RMS Displacement 0.011705 0.001200 NO

Predicted change in Energy=-1.038707D-04

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:35:05 2019, MaxMem= 1342177280 cpu: 1.8

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 8 0 0.000000 0.000000 0.602910

2 8 0 0.000000 0.000000 -0.602910

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

Stoichiometry O2

Framework group D\*H[C\*(O.O)]

Deg. of freedom 1

Full point group D\*H NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup D2H NOp 8

Largest concise Abelian subgroup C2 NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 8 0 0.000000 0.000000 0.602910

2 8 0 0.000000 0.000000 -0.602910

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

Rotational constants (GHZ): 0.0000000 43.4610478 43.4610478

Leave Link 202 at Sat Aug 17 17:35:06 2019, MaxMem= 1342177280 cpu: 0.4

(Enter /apps/gaussian/g09d01/g09/l301.exe)

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

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

There are 10 symmetry adapted cartesian basis functions of AG symmetry.

There are 1 symmetry adapted cartesian basis functions of B1G symmetry.

There are 4 symmetry adapted cartesian basis functions of B2G symmetry.

There are 4 symmetry adapted cartesian basis functions of B3G symmetry.

There are 1 symmetry adapted cartesian basis functions of AU symmetry.

There are 10 symmetry adapted cartesian basis functions of B1U symmetry.

There are 4 symmetry adapted cartesian basis functions of B2U symmetry.

There are 4 symmetry adapted cartesian basis functions of B3U symmetry.

There are 9 symmetry adapted basis functions of AG symmetry.

There are 1 symmetry adapted basis functions of B1G symmetry.

There are 4 symmetry adapted basis functions of B2G symmetry.

There are 4 symmetry adapted basis functions of B3G symmetry.

There are 1 symmetry adapted basis functions of AU symmetry.

There are 9 symmetry adapted basis functions of B1U symmetry.

There are 4 symmetry adapted basis functions of B2U symmetry.

There are 4 symmetry adapted basis functions of B3U symmetry.

36 basis functions, 64 primitive gaussians, 38 cartesian basis functions

8 alpha electrons 8 beta electrons

nuclear repulsion energy 28.0865611542 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= 2 NActive= 2 NUniq= 1 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= -0.0004555178 Hartrees.

Nuclear repulsion after empirical dispersion term = 28.0861056364 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= 2.

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

Smoothing algorithm: Karplus/York (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

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

Spheres list:

ISph on Nord Re0 Alpha Xe Ye Ze

1 O 1 2.2940 1.000 0.000000 0.000000 0.602910

2 O 2 2.2940 1.000 0.000000 0.000000 -0.602910

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

GePol: Number of generator spheres = 2

GePol: Total number of spheres = 2

GePol: Number of exposed spheres = 2 (100.00%)

GePol: Number of points = 602

GePol: Average weight of points = 0.14

GePol: Minimum weight of points = 0.61D-02

GePol: Maximum weight of points = 0.16851

GePol: Number of points with low weight = 0

GePol: Fraction of low-weight points (<1% of avg) = 0.00%

GePol: Cavity surface area = 83.500 Ang\*\*2

GePol: Cavity volume = 70.025 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0118791039 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 28.0742265325 Hartrees.

Leave Link 301 at Sat Aug 17 17:35:06 2019, MaxMem= 1342177280 cpu: 0.9

(Enter /apps/gaussian/g09d01/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= 36 RedAO= T EigKep= 2.30D-02 NBF= 9 1 4 4 1 9 4 4

NBsUse= 36 1.00D-06 EigRej= -1.00D+00 NBFU= 9 1 4 4 1 9 4 4

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= 38 38 38 38 38 MxSgAt= 2 MxSgA2= 2.

Leave Link 302 at Sat Aug 17 17:35:07 2019, MaxMem= 1342177280 cpu: 8.2

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:35:07 2019, MaxMem= 1342177280 cpu: 1.4

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "Oxy1.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 orbital symmetries:

Occupied (SGG) (SGU) (SGG) (SGU) (SGG) (PIU) (PIU) (?A)

Virtual (SGG) (SGG) (?B) (?B) (?B) (SGG) (?B) (?A) (PIG)

(?A) (?A) (?A) (PIG) (?A) (?C) (SGU) (SGU) (?C)

(?C) (SGU) (SGU) (SGU) (PIU) (PIU) (PIU) (PIU)

(PIU) (PIU)

Leave Link 401 at Sat Aug 17 17:35:08 2019, MaxMem= 1342177280 cpu: 6.2

(Enter /apps/gaussian/g09d01/g09/l502.exe)

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

Keep R1 ints in memory in symmetry-blocked form, NReq=3529640.

IVT= 23750 IEndB= 23750 NGot= 1342177280 MDV= 1342119376

LenX= 1342119376 LenY= 1342117491

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.

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

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

wScrn= 0.000000 ICntrl= 600 IOpCl= 0 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 666 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Cycle 1 Pass 1 IDiag 1:

Inv3: Mode=1 IEnd= 1087212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 3.11D-15 for 587.

Iteration 1 A\*A^-1 deviation from orthogonality is 1.09D-15 for 586 40.

Iteration 1 A^-1\*A deviation from unit magnitude is 2.89D-15 for 587.

Iteration 1 A^-1\*A deviation from orthogonality is 5.65D-16 for 182 126.

E= -150.315256146770

DIIS: error= 1.75D-03 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -150.315256146770 IErMin= 1 ErrMin= 1.75D-03

ErrMax= 1.75D-03 0.00D+00 EMaxC= 1.00D-01 BMatC= 7.17D-05 BMatP= 7.17D-05

IDIUse=3 WtCom= 9.83D-01 WtEn= 1.75D-02

Coeff-Com: 0.100D+01

Coeff-En: 0.100D+01

Coeff: 0.100D+01

Gap= 0.193 Goal= None Shift= 0.000

GapD= 0.193 DampG=1.000 DampE=1.000 DampFc=1.0000 IDamp=-1.

RMSDP=2.00D-04 MaxDP=2.11D-03 OVMax= 2.65D-03

Cycle 2 Pass 1 IDiag 1:

E= -150.315321841799 Delta-E= -0.000065695028 Rises=F Damp=F

DIIS: error= 3.86D-04 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -150.315321841799 IErMin= 2 ErrMin= 3.86D-04

ErrMax= 3.86D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 3.06D-06 BMatP= 7.17D-05

IDIUse=3 WtCom= 9.96D-01 WtEn= 3.86D-03

Coeff-Com: 0.588D-01 0.941D+00

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

Coeff: 0.586D-01 0.941D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=5.93D-05 MaxDP=7.03D-04 DE=-6.57D-05 OVMax= 6.56D-04

Cycle 3 Pass 1 IDiag 1:

E= -150.315323037598 Delta-E= -0.000001195799 Rises=F Damp=F

DIIS: error= 2.65D-04 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -150.315323037598 IErMin= 3 ErrMin= 2.65D-04

ErrMax= 2.65D-04 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.55D-06 BMatP= 3.06D-06

IDIUse=3 WtCom= 9.97D-01 WtEn= 2.65D-03

Coeff-Com: -0.234D-01 0.409D+00 0.614D+00

Coeff-En: 0.000D+00 0.261D+00 0.739D+00

Coeff: -0.233D-01 0.409D+00 0.615D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=2.05D-05 MaxDP=2.47D-04 DE=-1.20D-06 OVMax= 2.19D-04

Cycle 4 Pass 1 IDiag 1:

E= -150.315324016489 Delta-E= -0.000000978892 Rises=F Damp=F

DIIS: error= 2.15D-06 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -150.315324016489 IErMin= 4 ErrMin= 2.15D-06

ErrMax= 2.15D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.04D-10 BMatP= 1.55D-06

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

Coeff-Com: 0.643D-04-0.908D-02-0.723D-02 0.102D+01

Coeff: 0.643D-04-0.908D-02-0.723D-02 0.102D+01

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=3.41D-07 MaxDP=3.92D-06 DE=-9.79D-07 OVMax= 6.18D-06

Cycle 5 Pass 1 IDiag 1:

E= -150.315324016611 Delta-E= -0.000000000122 Rises=F Damp=F

DIIS: error= 4.99D-07 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -150.315324016611 IErMin= 5 ErrMin= 4.99D-07

ErrMax= 4.99D-07 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.50D-12 BMatP= 1.04D-10

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

Coeff-Com: 0.427D-04-0.287D-02-0.325D-02 0.205D+00 0.801D+00

Coeff: 0.427D-04-0.287D-02-0.325D-02 0.205D+00 0.801D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=4.01D-08 MaxDP=5.33D-07 DE=-1.22D-10 OVMax= 4.39D-07

Cycle 6 Pass 1 IDiag 1:

E= -150.315324016614 Delta-E= -0.000000000003 Rises=F Damp=F

DIIS: error= 4.35D-08 at cycle 6 NSaved= 6.

NSaved= 6 IEnMin= 6 EnMin= -150.315324016614 IErMin= 6 ErrMin= 4.35D-08

ErrMax= 4.35D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 5.71D-14 BMatP= 6.50D-12

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

Coeff-Com: 0.472D-05-0.178D-05-0.164D-03-0.111D-01 0.671D-01 0.944D+00

Coeff: 0.472D-05-0.178D-05-0.164D-03-0.111D-01 0.671D-01 0.944D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=5.36D-09 MaxDP=7.05D-08 DE=-3.30D-12 OVMax= 7.68D-08

Error on total polarization charges = 0.00004

SCF Done: E(RB3LYP) = -150.315324017 A.U. after 6 cycles

NFock= 6 Conv=0.54D-08 -V/T= 2.0018

KE= 1.500467320957D+02 PE=-4.119786972130D+02 EE= 8.354241456815D+01

SMD-CDS (non-electrostatic) energy (kcal/mol) = -7.45

(included in total energy above)

Leave Link 502 at Sat Aug 17 17:35:10 2019, MaxMem= 1342177280 cpu: 16.4

(Enter /apps/gaussian/g09d01/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 36

NBasis= 36 NAE= 8 NBE= 8 NFC= 0 NFV= 0

NROrb= 36 NOA= 8 NOB= 8 NVA= 28 NVB= 28

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.71918916D-01

Leave Link 801 at Sat Aug 17 17:35:10 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l1101.exe)

Using compressed storage, NAtomX= 2.

Will process 3 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Sat Aug 17 17:35:11 2019, MaxMem= 1342177280 cpu: 5.8

(Enter /apps/gaussian/g09d01/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Sat Aug 17 17:35:11 2019, MaxMem= 1342177280 cpu: 0.9

(Enter /apps/gaussian/g09d01/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 2.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 1342177160.

G2DrvN: will do 3 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= 0 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 = 349

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 Sat Aug 17 17:35:13 2019, MaxMem= 1342177280 cpu: 23.8

(Enter /apps/gaussian/g09d01/g09/l1002.exe)

Minotr: Closed shell wavefunction.

IDoAtm=11

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.

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= 1342177220 using IRadAn= 2.

Generate precomputed XC quadrature information.

Keep R1 ints in memory in symmetry-blocked form, NReq=2520021.

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

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

wScrn= 0.000000 ICntrl= 600 IOpCl= 0 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 666 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Solving linear equations simultaneously, MaxMat= 0.

There are 6 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 6.

6 vectors produced by pass 0 Test12= 3.73D-15 1.67D-08 XBig12= 1.39D+01 3.39D+00.

AX will form 6 AO Fock derivatives at one time.

6 vectors produced by pass 1 Test12= 3.73D-15 1.67D-08 XBig12= 9.11D+00 1.52D+00.

6 vectors produced by pass 2 Test12= 3.73D-15 1.67D-08 XBig12= 7.11D-02 9.35D-02.

6 vectors produced by pass 3 Test12= 3.73D-15 1.67D-08 XBig12= 7.74D-04 1.57D-02.

6 vectors produced by pass 4 Test12= 3.73D-15 1.67D-08 XBig12= 1.53D-05 2.77D-03.

6 vectors produced by pass 5 Test12= 3.73D-15 1.67D-08 XBig12= 3.80D-08 8.17D-05.

1 vectors produced by pass 6 Test12= 3.73D-15 1.67D-08 XBig12= 5.66D-11 3.16D-06.

1 vectors produced by pass 7 Test12= 3.73D-15 1.67D-08 XBig12= 8.62D-14 1.01D-07.

InvSVY: IOpt=1 It= 1 EMax= 1.41D-16

Solved reduced A of dimension 38 with 6 vectors.

FullF1: Do perturbations 1 to 6.

Isotropic polarizability for W= 0.000000 6.46 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 Sat Aug 17 17:35:15 2019, MaxMem= 1342177280 cpu: 22.0

(Enter /apps/gaussian/g09d01/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.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 349

Leave Link 701 at Sat Aug 17 17:35:17 2019, MaxMem= 1342177280 cpu: 12.5

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:35:17 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Sat Aug 17 17:35:18 2019, MaxMem= 1342177280 cpu: 9.6

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-5.91645679D-31 2.20278237D-33-5.78242966D-15

Polarizability= 3.90884370D+00 1.28283469D-12 2.97767295D+00

1.98736801D-11-2.51487651D-11 1.24889133D+01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 8 0.000000000 0.000000000 0.000401632

2 8 0.000000000 0.000000000 -0.000401632

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

Cartesian Forces: Max 0.000401632 RMS 0.000231883

Force constants in Cartesian coordinates:

1 2 3 4 5

1 0.115120D-02

2 0.000000D+00 0.127463D-02

3 0.000000D+00 0.000000D+00 0.807140D+00

4 -0.115120D-02 0.000000D+00 0.000000D+00 0.115120D-02

5 0.000000D+00 -0.127463D-02 0.000000D+00 0.000000D+00 0.127463D-02

6 0.000000D+00 0.000000D+00 -0.807140D+00 0.000000D+00 0.000000D+00

6

6 0.807140D+00

Red2BG is reusing G-inverse.

Force constants in internal coordinates:

1

1 0.807140D+00

Leave Link 716 at Sat Aug 17 17:35:18 2019, MaxMem= 1342177280 cpu: 0.6

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000401632 RMS 0.000401632

Search for a local minimum.

Step number 2 out of a maximum of 20

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .40163D-03 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Second derivative matrix not updated -- analytic derivatives used.

DE= -1.02D-04 DEPred=-1.04D-04 R= 9.79D-01

TightC=F SS= 1.41D+00 RLast= 1.66D-02 DXNew= 5.0454D-01 4.9661D-02

Trust test= 9.79D-01 RLast= 1.66D-02 DXMaxT set to 3.00D-01

The second derivative matrix:

R1

R1 0.80714

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues --- 0.80714

RFO step: Lambda= 0.00000000D+00 EMin= 8.07140476D-01

Quintic linear search produced a step of -0.03009.

Iteration 1 RMS(Cart)= 0.00035219 RMS(Int)= 0.00000000

Iteration 2 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000000

ITry= 1 IFail=0 DXMaxC= 2.49D-04 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 1.52D-20 for atom 1.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.27867 0.00040 0.00050 0.00000 0.00050 2.27917

Item Value Threshold Converged?

Maximum Force 0.000402 0.000450 YES

RMS Force 0.000402 0.000300 NO

Maximum Displacement 0.000249 0.001800 YES

RMS Displacement 0.000352 0.001200 YES

Predicted change in Energy=-9.992583D-08

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Leave Link 103 at Sat Aug 17 17:35:19 2019, MaxMem= 1342177280 cpu: 1.6

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 8 0 0.000000 0.000000 0.603042

2 8 0 0.000000 0.000000 -0.603042

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

Stoichiometry O2

Framework group D\*H[C\*(O.O)]

Deg. of freedom 1

Full point group D\*H NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup D2H NOp 8

Largest concise Abelian subgroup C2 NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 8 0 0.000000 0.000000 0.603042

2 8 0 0.000000 0.000000 -0.603042

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

Rotational constants (GHZ): 0.0000000 43.4420545 43.4420545

Leave Link 202 at Sat Aug 17 17:35:19 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l301.exe)

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

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

There are 10 symmetry adapted cartesian basis functions of AG symmetry.

There are 1 symmetry adapted cartesian basis functions of B1G symmetry.

There are 4 symmetry adapted cartesian basis functions of B2G symmetry.

There are 4 symmetry adapted cartesian basis functions of B3G symmetry.

There are 1 symmetry adapted cartesian basis functions of AU symmetry.

There are 10 symmetry adapted cartesian basis functions of B1U symmetry.

There are 4 symmetry adapted cartesian basis functions of B2U symmetry.

There are 4 symmetry adapted cartesian basis functions of B3U symmetry.

There are 9 symmetry adapted basis functions of AG symmetry.

There are 1 symmetry adapted basis functions of B1G symmetry.

There are 4 symmetry adapted basis functions of B2G symmetry.

There are 4 symmetry adapted basis functions of B3G symmetry.

There are 1 symmetry adapted basis functions of AU symmetry.

There are 9 symmetry adapted basis functions of B1U symmetry.

There are 4 symmetry adapted basis functions of B2U symmetry.

There are 4 symmetry adapted basis functions of B3U symmetry.

36 basis functions, 64 primitive gaussians, 38 cartesian basis functions

8 alpha electrons 8 beta electrons

nuclear repulsion energy 28.0804233313 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= 2 NActive= 2 NUniq= 1 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= -0.0004555172 Hartrees.

Nuclear repulsion after empirical dispersion term = 28.0799678141 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= 2.

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

Smoothing algorithm: Karplus/York (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

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

Spheres list:

ISph on Nord Re0 Alpha Xe Ye Ze

1 O 1 2.2940 1.000 0.000000 0.000000 0.603042

2 O 2 2.2940 1.000 0.000000 0.000000 -0.603042

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

GePol: Number of generator spheres = 2

GePol: Total number of spheres = 2

GePol: Number of exposed spheres = 2 (100.00%)

GePol: Number of points = 602

GePol: Average weight of points = 0.14

GePol: Minimum weight of points = 0.61D-02

GePol: Maximum weight of points = 0.16851

GePol: Number of points with low weight = 0

GePol: Fraction of low-weight points (<1% of avg) = 0.00%

GePol: Cavity surface area = 83.503 Ang\*\*2

GePol: Cavity volume = 70.029 Ang\*\*3

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

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

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

PCM non-electrostatic energy = -0.0118789031 Hartrees.

Nuclear repulsion after PCM non-electrostatic terms = 28.0680889110 Hartrees.

Leave Link 301 at Sat Aug 17 17:35:19 2019, MaxMem= 1342177280 cpu: 0.9

(Enter /apps/gaussian/g09d01/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= 36 RedAO= T EigKep= 2.30D-02 NBF= 9 1 4 4 1 9 4 4

NBsUse= 36 1.00D-06 EigRej= -1.00D+00 NBFU= 9 1 4 4 1 9 4 4

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= 38 38 38 38 38 MxSgAt= 2 MxSgA2= 2.

Leave Link 302 at Sat Aug 17 17:35:20 2019, MaxMem= 1342177280 cpu: 8.4

(Enter /apps/gaussian/g09d01/g09/l303.exe)

DipDrv: MaxL=1.

Leave Link 303 at Sat Aug 17 17:35:20 2019, MaxMem= 1342177280 cpu: 2.0

(Enter /apps/gaussian/g09d01/g09/l401.exe)

Initial guess from the checkpoint file: "Oxy1.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 orbital symmetries:

Occupied (SGG) (SGU) (SGG) (SGU) (SGG) (PIU) (PIU) (?A)

Virtual (SGG) (SGG) (?B) (?B) (?B) (SGG) (?B) (?A) (PIG)

(?A) (?A) (?A) (PIG) (?A) (?C) (SGU) (SGU) (?C)

(?C) (SGU) (SGU) (SGU) (PIU) (PIU) (PIU) (PIU)

(PIU) (PIU)

Leave Link 401 at Sat Aug 17 17:35:21 2019, MaxMem= 1342177280 cpu: 7.1

(Enter /apps/gaussian/g09d01/g09/l502.exe)

Closed shell SCF:

Using DIIS extrapolation, IDIIS= 1040.

Integral symmetry usage will be decided dynamically.

Keep R1 ints in memory in symmetry-blocked form, NReq=3529640.

IVT= 23750 IEndB= 23750 NGot= 1342177280 MDV= 1342119376

LenX= 1342119376 LenY= 1342117491

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.

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

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

wScrn= 0.000000 ICntrl= 600 IOpCl= 0 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 666 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Cycle 1 Pass 1 IDiag 1:

Inv3: Mode=1 IEnd= 1087212.

Iteration 1 A\*A^-1 deviation from unit magnitude is 3.77D-15 for 595.

Iteration 1 A\*A^-1 deviation from orthogonality is 2.15D-15 for 586 40.

Iteration 1 A^-1\*A deviation from unit magnitude is 3.77D-15 for 595.

Iteration 1 A^-1\*A deviation from orthogonality is 7.39D-16 for 600 599.

E= -150.315324054432

DIIS: error= 5.31D-05 at cycle 1 NSaved= 1.

NSaved= 1 IEnMin= 1 EnMin= -150.315324054432 IErMin= 1 ErrMin= 5.31D-05

ErrMax= 5.31D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.60D-08 BMatP= 6.60D-08

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

Coeff-Com: 0.100D+01

Coeff: 0.100D+01

Gap= 0.193 Goal= None Shift= 0.000

RMSDP=6.04D-06 MaxDP=6.38D-05 OVMax= 8.00D-05

Cycle 2 Pass 1 IDiag 1:

E= -150.315324114600 Delta-E= -0.000000060168 Rises=F Damp=F

DIIS: error= 1.17D-05 at cycle 2 NSaved= 2.

NSaved= 2 IEnMin= 2 EnMin= -150.315324114600 IErMin= 2 ErrMin= 1.17D-05

ErrMax= 1.17D-05 0.00D+00 EMaxC= 1.00D-01 BMatC= 2.82D-09 BMatP= 6.60D-08

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

Coeff-Com: 0.592D-01 0.941D+00

Coeff: 0.592D-01 0.941D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=1.80D-06 MaxDP=2.13D-05 DE=-6.02D-08 OVMax= 1.99D-05

Cycle 3 Pass 1 IDiag 1:

E= -150.315324115703 Delta-E= -0.000000001103 Rises=F Damp=F

DIIS: error= 8.04D-06 at cycle 3 NSaved= 3.

NSaved= 3 IEnMin= 3 EnMin= -150.315324115703 IErMin= 3 ErrMin= 8.04D-06

ErrMax= 8.04D-06 0.00D+00 EMaxC= 1.00D-01 BMatC= 1.43D-09 BMatP= 2.82D-09

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

Coeff-Com: -0.233D-01 0.409D+00 0.615D+00

Coeff: -0.233D-01 0.409D+00 0.615D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=6.22D-07 MaxDP=7.48D-06 DE=-1.10D-09 OVMax= 6.62D-06

Cycle 4 Pass 1 IDiag 1:

E= -150.315324116602 Delta-E= -0.000000000899 Rises=F Damp=F

DIIS: error= 6.51D-08 at cycle 4 NSaved= 4.

NSaved= 4 IEnMin= 4 EnMin= -150.315324116602 IErMin= 4 ErrMin= 6.51D-08

ErrMax= 6.51D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 8.97D-14 BMatP= 1.43D-09

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

Coeff-Com: 0.598D-04-0.889D-02-0.758D-02 0.102D+01

Coeff: 0.598D-04-0.889D-02-0.758D-02 0.102D+01

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=1.02D-08 MaxDP=1.14D-07 DE=-8.99D-10 OVMax= 1.88D-07

Cycle 5 Pass 1 IDiag 1:

E= -150.315324116602 Delta-E= 0.000000000000 Rises=F Damp=F

DIIS: error= 1.60D-08 at cycle 5 NSaved= 5.

NSaved= 5 IEnMin= 5 EnMin= -150.315324116602 IErMin= 5 ErrMin= 1.60D-08

ErrMax= 1.60D-08 0.00D+00 EMaxC= 1.00D-01 BMatC= 6.66D-15 BMatP= 8.97D-14

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

Coeff-Com: 0.448D-04-0.300D-02-0.351D-02 0.218D+00 0.789D+00

Coeff: 0.448D-04-0.300D-02-0.351D-02 0.218D+00 0.789D+00

Gap= 0.072 Goal= None Shift= 0.000

RMSDP=1.27D-09 MaxDP=1.68D-08 DE=-3.41D-13 OVMax= 1.41D-08

Error on total polarization charges = 0.00004

SCF Done: E(RB3LYP) = -150.315324117 A.U. after 5 cycles

NFock= 5 Conv=0.13D-08 -V/T= 2.0018

KE= 1.500458507985D+02 PE=-4.119660687621D+02 EE= 8.353680493595D+01

SMD-CDS (non-electrostatic) energy (kcal/mol) = -7.45

(included in total energy above)

Leave Link 502 at Sat Aug 17 17:35:25 2019, MaxMem= 1342177280 cpu: 30.8

(Enter /apps/gaussian/g09d01/g09/l801.exe)

DoSCS=F DFT=T ScalE2(SS,OS)= 1.000000 1.000000

Range of M.O.s used for correlation: 1 36

NBasis= 36 NAE= 8 NBE= 8 NFC= 0 NFV= 0

NROrb= 36 NOA= 8 NOB= 8 NVA= 28 NVB= 28

\*\*\*\* Warning!!: The smallest alpha delta epsilon is 0.71915653D-01

Leave Link 801 at Sat Aug 17 17:35:25 2019, MaxMem= 1342177280 cpu: 0.3

(Enter /apps/gaussian/g09d01/g09/l1101.exe)

Using compressed storage, NAtomX= 2.

Will process 3 centers per pass.

R6Disp: Adding Grimme-D3(BJ) dispersion energy 1st derivatives to the gradient.

Leave Link 1101 at Sat Aug 17 17:35:26 2019, MaxMem= 1342177280 cpu: 6.3

(Enter /apps/gaussian/g09d01/g09/l1102.exe)

Symmetrizing basis deriv contribution to polar:

IMax=3 JMax=2 DiffMx= 0.00D+00

Leave Link 1102 at Sat Aug 17 17:35:26 2019, MaxMem= 1342177280 cpu: 0.8

(Enter /apps/gaussian/g09d01/g09/l1110.exe)

Forming Gx(P) for the SCF density, NAtomX= 2.

Integral derivatives from FoFJK, PRISM(SPDF).

Do as many integral derivatives as possible in FoFJK.

G2DrvN: MDV= 1342177160.

G2DrvN: will do 3 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= 0 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 = 349

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 Sat Aug 17 17:35:30 2019, MaxMem= 1342177280 cpu: 33.3

(Enter /apps/gaussian/g09d01/g09/l1002.exe)

Minotr: Closed shell wavefunction.

IDoAtm=11

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.

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= 1342177220 using IRadAn= 2.

Generate precomputed XC quadrature information.

Keep R1 ints in memory in symmetry-blocked form, NReq=2520021.

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

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

wScrn= 0.000000 ICntrl= 600 IOpCl= 0 I1Cent= 0 NGrid= 0

NMat0= 1 NMatS0= 666 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Solving linear equations simultaneously, MaxMat= 0.

There are 6 degrees of freedom in the 1st order CPHF. IDoFFX=4 NUNeed= 6.

6 vectors produced by pass 0 Test12= 3.73D-15 1.67D-08 XBig12= 1.40D+01 3.39D+00.

AX will form 6 AO Fock derivatives at one time.

6 vectors produced by pass 1 Test12= 3.73D-15 1.67D-08 XBig12= 9.13D+00 1.52D+00.

6 vectors produced by pass 2 Test12= 3.73D-15 1.67D-08 XBig12= 7.13D-02 9.36D-02.

6 vectors produced by pass 3 Test12= 3.73D-15 1.67D-08 XBig12= 7.76D-04 1.57D-02.

6 vectors produced by pass 4 Test12= 3.73D-15 1.67D-08 XBig12= 1.53D-05 2.77D-03.

6 vectors produced by pass 5 Test12= 3.73D-15 1.67D-08 XBig12= 3.81D-08 8.19D-05.

1 vectors produced by pass 6 Test12= 3.73D-15 1.67D-08 XBig12= 5.68D-11 3.17D-06.

1 vectors produced by pass 7 Test12= 3.73D-15 1.67D-08 XBig12= 8.65D-14 1.01D-07.

InvSVY: IOpt=1 It= 1 EMax= 1.33D-15

Solved reduced A of dimension 38 with 6 vectors.

FullF1: Do perturbations 1 to 6.

Isotropic polarizability for W= 0.000000 6.46 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 Sat Aug 17 17:35:31 2019, MaxMem= 1342177280 cpu: 14.9

(Enter /apps/gaussian/g09d01/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.

D2PCM: PCM CHGder 2nd derivatives, FixD1E=F FixD2E=F DoIter=F DoCFld=F I1PDM=0

GePol: Maximum number of non-zero 2nd derivatives = 349

Leave Link 701 at Sat Aug 17 17:35:33 2019, MaxMem= 1342177280 cpu: 17.0

(Enter /apps/gaussian/g09d01/g09/l702.exe)

L702 exits ... SP integral derivatives will be done elsewhere.

Leave Link 702 at Sat Aug 17 17:35:33 2019, MaxMem= 1342177280 cpu: 0.2

(Enter /apps/gaussian/g09d01/g09/l703.exe)

Compute integral second derivatives, UseDBF=F ICtDFT= 0.

Integral derivatives from FoFJK, PRISM(SPDF).

Calling FoFJK, ICntrl= 100127 FMM=F ISym2X=1 I1Cent= 0 IOpClX= 0 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= 0 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 Sat Aug 17 17:35:34 2019, MaxMem= 1342177280 cpu: 7.8

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Dipole =-1.38050658D-30 1.20370622D-33-1.69874152D-15

Polarizability= 3.90888313D+00 1.28736359D-12 2.97753116D+00

1.98349064D-11-2.50004836D-11 1.24944842D+01

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 8 0.000000000 0.000000000 0.000000007

2 8 0.000000000 0.000000000 -0.000000007

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

Cartesian Forces: Max 0.000000007 RMS 0.000000004

Force constants in Cartesian coordinates:

1 2 3 4 5

1 0.131835D-02

2 0.000000D+00 0.144196D-02

3 0.000000D+00 0.000000D+00 0.805611D+00

4 -0.131835D-02 0.000000D+00 0.000000D+00 0.131835D-02

5 0.000000D+00 -0.144196D-02 0.000000D+00 0.000000D+00 0.144196D-02

6 0.000000D+00 0.000000D+00 -0.805611D+00 0.000000D+00 0.000000D+00

6

6 0.805611D+00

Red2BG is reusing G-inverse.

Force constants in internal coordinates:

1

1 0.805611D+00

Leave Link 716 at Sat Aug 17 17:35:34 2019, MaxMem= 1342177280 cpu: 0.7

(Enter /apps/gaussian/g09d01/g09/l103.exe)

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

Red2BG is reusing G-inverse.

Internal Forces: Max 0.000000007 RMS 0.000000007

Search for a local minimum.

Step number 3 out of a maximum of 20

All quantities printed in internal units (Hartrees-Bohrs-Radians)

RMS Force = .70253D-08 SwitMx=.10000D-02 MixMth= 2

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Second derivative matrix not updated -- analytic derivatives used.

DE= -1.00D-07 DEPred=-9.99D-08 R= 1.00D+00

Trust test= 1.00D+00 RLast= 4.98D-04 DXMaxT set to 3.00D-01

The second derivative matrix:

R1

R1 0.80561

ITU= 0 1

Eigenvalues --- 0.80561

En-DIIS/RFO-DIIS IScMMF= 0 using points: 3 2

RFO step: Lambda=-5.55111512D-17.

NNeg= 0 NP= 2 Switch= 2.50D-03 Rises=F DC= 1.00D-07 SmlDif= 1.00D-05

RMS Error= 0.7827124816D-08 NUsed= 2 EDIIS=F

DidBck=F Rises=F RFO-DIIS coefs: 1.00002 -0.00002

Iteration 1 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000000

ITry= 1 IFail=0 DXMaxC= 4.36D-09 DCOld= 1.00D+10 DXMaxT= 3.00D-01 DXLimC= 3.00D+00 Rises=F

ClnCor: largest displacement from symmetrization is 2.67D-25 for atom 1.

Variable Old X -DE/DX Delta X Delta X Delta X New X

(Linear) (Quad) (Total)

R1 2.27917 0.00000 0.00000 0.00000 0.00000 2.27917

Item Value Threshold Converged?

Maximum Force 0.000000 0.000450 YES

RMS Force 0.000000 0.000300 YES

Maximum Displacement 0.000000 0.001800 YES

RMS Displacement 0.000000 0.001200 YES

Predicted change in Energy=-3.063192D-17

Optimization completed.

-- Stationary point found.

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

! Optimized Parameters !

! (Angstroms and Degrees) !

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

! Name Definition Value Derivative Info. !

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

! R1 R(1,2) 1.2061 -DE/DX = 0.0 !

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

Lowest energy point so far. Saving SCF results.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Largest change from initial coordinates is atom 1 0.004 Angstoms.

Leave Link 103 at Sat Aug 17 17:35:34 2019, MaxMem= 1342177280 cpu: 1.3

(Enter /apps/gaussian/g09d01/g09/l202.exe)

Input orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 8 0 0.000000 0.000000 0.603042

2 8 0 0.000000 0.000000 -0.603042

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

Stoichiometry O2

Framework group D\*H[C\*(O.O)]

Deg. of freedom 1

Full point group D\*H NOp 8

RotChk: IX=0 Diff= 0.00D+00

Largest Abelian subgroup D2H NOp 8

Largest concise Abelian subgroup C2 NOp 2

Standard orientation:

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

Center Atomic Atomic Coordinates (Angstroms)

Number Number Type X Y Z

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

1 8 0 0.000000 0.000000 0.603042

2 8 0 0.000000 0.000000 -0.603042

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

Rotational constants (GHZ): 0.0000000 43.4420545 43.4420545

Leave Link 202 at Sat Aug 17 17:35:35 2019, MaxMem= 1342177280 cpu: 1.0

(Enter /apps/gaussian/g09d01/g09/l601.exe)

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

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

Population analysis using the SCF density.

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

Orbital symmetries:

Occupied (SGG) (SGU) (SGG) (SGU) (SGG) (PIU) (PIU) (PIG)

Virtual (PIG) (SGU) (PIU) (PIU) (SGU) (SGG) (SGG) (PIG)

(PIG) (SGU) (PIU) (PIU) (?A) (?A) (DLTU) (DLTU)

(?A) (PIG) (PIG) (SGU) (PIU) (PIU) (SGG) (PIG)

(PIG) (SGU) (SGG) (SGU)

Unable to determine electronic state: partially filled degenerate orbitals.

Alpha occ. eigenvalues -- -19.27383 -19.27359 -1.29058 -0.79931 -0.53744

Alpha occ. eigenvalues -- -0.52362 -0.51731 -0.25417

Alpha virt. eigenvalues -- -0.18226 0.21419 0.67450 0.69158 0.70611

Alpha virt. eigenvalues -- 0.71607 0.78370 0.79771 0.80795 1.24922

Alpha virt. eigenvalues -- 2.23459 2.26536 2.57231 2.57418 2.84376

Alpha virt. eigenvalues -- 2.84635 2.85021 3.41515 3.44628 3.76556

Alpha virt. eigenvalues -- 4.52466 4.54832 4.64952 4.82501 4.85191

Alpha virt. eigenvalues -- 5.98273 49.48860 49.68437

Condensed to atoms (all electrons):

1 2

1 O 7.976263 0.023737

2 O 0.023737 7.976263

Mulliken charges:

1

1 O 0.000000

2 O 0.000000

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

1

1 O 0.000000

2 O 0.000000

APT charges:

1

1 O 0.000000

2 O 0.000000

Sum of APT charges = 0.00000

APT charges with hydrogens summed into heavy atoms:

1

1 O 0.000000

2 O 0.000000

Electronic spatial extent (au): <R\*\*2>= 43.4026

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= -8.9918 YY= -10.8100 ZZ= -10.6284

XY= 0.0000 XZ= 0.0000 YZ= 0.0000

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

XX= 1.1516 YY= -0.6666 ZZ= -0.4850

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= -5.7765 YYYY= -7.5899 ZZZZ= -28.2480 XXXY= 0.0000

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

ZZZY= 0.0000 XXYY= -2.2277 XXZZ= -5.4050 YYZZ= -6.7745

XXYZ= 0.0000 YYXZ= 0.0000 ZZXY= 0.0000

N-N= 2.806808891102D+01 E-N=-4.119660686947D+02 KE= 1.500458507985D+02

Symmetry AG KE= 6.969500365645D+01

Symmetry B1G KE= 1.074031685389D-34

Symmetry B2G KE=-3.649616606237D-33

Symmetry B3G KE= 6.048882263504D+00

Symmetry AU KE= 2.316171835560D-34

Symmetry B1U KE= 6.508084191109D+01

Symmetry B2U KE= 4.667259738061D+00

Symmetry B3U KE= 4.553863229445D+00

Exact polarizability: 3.909 0.000 2.978 0.000 0.000 12.494

Approx polarizability: 5.093 0.000 3.183 0.000 0.000 24.026

No NMR shielding tensors so no spin-rotation constants.

Leave Link 601 at Sat Aug 17 17:35:36 2019, MaxMem= 1342177280 cpu: 7.4

(Enter /apps/gaussian/g09d01/g09/l716.exe)

Rotating derivatives to standard orientation.

Dipole =-1.38050658D-30 1.20370622D-33-1.69874152D-15

Polarizability= 3.90888313D+00 1.28736359D-12 2.97753116D+00

1.98349064D-11-2.50004836D-11 1.24944842D+01

Full mass-weighted force constant matrix:

Low frequencies --- -0.0009 0.0008 0.0013 65.9999 69.0246 1631.5151

Diagonal vibrational polarizability:

0.0000000 0.0000000 0.0000000

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

SGG

Frequencies -- 1631.5151

Red. masses -- 15.9949

Frc consts -- 25.0850

IR Inten -- 0.0000

Atom AN X Y Z

1 8 0.00 0.00 0.71

2 8 0.00 0.00 -0.71

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

- Thermochemistry -

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

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Atom 1 has atomic number 8 and mass 15.99491

Atom 2 has atomic number 8 and mass 15.99491

Molecular mass: 31.98983 amu.

Principal axes and moments of inertia in atomic units:

1 2 3

Eigenvalues -- 0.00000 41.54364 41.54364

X 0.00000 1.00000 0.00000

Y 0.00000 0.00000 1.00000

Z 1.00000 0.00000 0.00000

This molecule is a prolate symmetric top.

Rotational symmetry number 2.

Rotational temperature (Kelvin) 2.08489

Rotational constant (GHZ): 43.442055

Zero-point vibrational energy 9758.6 (Joules/Mol)

2.33237 (Kcal/Mol)

Vibrational temperatures: 2347.38

(Kelvin)

Zero-point correction= 0.003717 (Hartree/Particle)

Thermal correction to Energy= 0.006080

Thermal correction to Enthalpy= 0.007024

Thermal correction to Gibbs Free Energy= -0.015212

Sum of electronic and zero-point Energies= -150.311607

Sum of electronic and thermal Energies= -150.309244

Sum of electronic and thermal Enthalpies= -150.308300

Sum of electronic and thermal Free Energies= -150.330536

E (Thermal) CV S

KCal/Mol Cal/Mol-Kelvin Cal/Mol-Kelvin

Total 3.815 5.015 46.799

Electronic 0.000 0.000 0.000

Translational 0.889 2.981 36.321

Rotational 0.592 1.987 10.472

Vibrational 2.334 0.047 0.007

Q Log10(Q) Ln(Q)

Total Bot 0.992717D+07 6.996825 16.110786

Total V=0 0.508699D+09 8.706461 20.047367

Vib (Bot) 0.195223D-01 -1.709470 -3.936200

Vib (V=0) 0.100038D+01 0.000165 0.000381

Electronic 0.100000D+01 0.000000 0.000000

Translational 0.711169D+07 6.851973 15.777251

Rotational 0.715027D+02 1.854322 4.269735

\*\*\*\*\* Axes restored to original set \*\*\*\*\*

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

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

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

1 8 0.000000000 0.000000000 0.000000007

2 8 0.000000000 0.000000000 -0.000000007

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

Cartesian Forces: Max 0.000000007 RMS 0.000000004

Force constants in Cartesian coordinates:

1 2 3 4 5

1 0.131835D-02

2 0.000000D+00 0.144196D-02

3 0.000000D+00 0.000000D+00 0.805611D+00

4 -0.131835D-02 0.000000D+00 0.000000D+00 0.131835D-02

5 0.000000D+00 -0.144196D-02 0.000000D+00 0.000000D+00 0.144196D-02

6 0.000000D+00 0.000000D+00 -0.805611D+00 0.000000D+00 0.000000D+00

6

6 0.805611D+00

Red2BG is reusing G-inverse.

Force constants in internal coordinates:

1

1 0.805611D+00

Leave Link 716 at Sat Aug 17 17:35:36 2019, MaxMem= 1342177280 cpu: 2.7

(Enter /apps/gaussian/g09d01/g09/l9999.exe)

1\1\GINC-K152\Freq\RB3LYP\6-311G(d)\O2\Z5105842\17-Aug-2019\0\\#p opt=

calcall b3lyp/6-311g\* scrf=(solvent=dmso,smd) empiricaldispersion=gd3b

j\\Oxy1\\0,1\O,0.,0.,0.6030418586\O,0.,0.,-0.6030418586\\Version=ES64L

-G09RevD.01\HF=-150.3153241\RMSD=1.269e-09\RMSF=4.056e-09\ZeroPoint=0.

0037169\Thermal=0.0060802\Dipole=0.,0.,0.\DipoleDeriv=0.,0.,0.,0.,0.,0

.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.,0.\Polar=3.9088831,0.,2.9775312,0.,

0.,12.4944842\PG=D\*H [C\*(O1.O1)]\NImag=0\\0.00131835,0.,0.00144196,0.,

0.,0.80561131,-0.00131835,0.,0.,0.00131835,0.,-0.00144196,0.,0.,0.0014

4196,0.,0.,-0.80561131,0.,0.,0.80561131\\0.,0.,0.,0.,0.,0.\\\@

WHERE THERE IS MUCH DESIRE TO LEARN, THERE OF NECESSITY WILL BE

MUCH ARGUING, MUCH WRITING, MANY OPINIONS; FOR OPINION IN GOOD MEN

IS BUT KNOWLEDGE IN THE MAKING. -- JOHN MILTON.

Job cpu time: 0 days 0 hours 6 minutes 8.2 seconds.

File lengths (MBytes): RWF= 93 Int= 0 D2E= 0 Chk= 3 Scr= 2

Normal termination of Gaussian 09 at Sat Aug 17 17:35:36 2019.