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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 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.