Supplementary Information for

Diborane Heterolysis and P(V) Reduction by $Ph_3P{=}O$ Coordination to Magnesium

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Supplementary Methods

General considerations and starting materials.

All manipulations were carried out using standard Schlenk line and glovebox techniques under an inert atmosphere of argon. NMR experiments were conducted in J Young tap NMR tubes made up and sealed in a glovebox. NMR spectra were recorded on an Agilent ProPulse spectrometer operating at 500 MHz (^{1}H), 126 MHz (^{13}C), 160.4 MHz (^{11}B). The spectra were referenced relative to residual solvent resonances or an external $BF_3.OEt_2$ standard (^{11}B). Solvents (toluene, hexane) were dried by passage through a commercially available (Innovative Technologies) solvent purification system, under argon and stored in ampoules over molecular sieves. d_8-Toluene was purchased from Fluorochem Ltd. and Sigma-Aldrich Ltd. and dried over molten potassium before distilling under argon and storing over molecular sieves. Di-*n*-butylmagnesium (1.0 M solution in *n*-heptane) and B_2pin_2 were purchased from Sigma-Aldrich Ltd. [(BDI)Mg*n*-Bu] (BDI = HC{(Me)CNDipp}$_2$; Dipp = 2,6-*i*-$Pr_2C_6H_3$] was synthesised by a literature procedure.[1] Elemental analysis was carried out Mr Stephen Boyer of London Metropolitan Enterprises.

Synthesis of compound 11

Toluene-d_8 (0.5 mL) was added to a mixture of [(BDI)Mg*n*-Bu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol) in a NMR tube fitted with J. Young tap. After 2 h, 1 equivalent of triphenylphosphine oxide (27.8 mg, 0.1 mmol) was added. After a further 1 h at RT, NMR spectra were recorded, which showed the formation of [(BDI)Mg(Bpin)($OPPh_3$)] (**11**) and *n*-BuBpin. Colourless crystals of compound **11** suitable for X-ray diffraction analysis were obtained during the removal of toluene under reduced pressure. ^{1}H NMR (500 MHz, toluene-d_8) δ 7.19 - 6.98 (m, 21H, CH ar), 4.91 (s, 1H, NC(CH_3)C*H*), 4.14 (hept, 2H, J_{HH} = 6.8 Hz, C*H*(CH_3)$_2$), 3.48 (hept, 2H, J_{HH} = 6.8 Hz, C*H*(CH_3)$_2$), 1.74 (s, 6H, NC(C*H*$_3$)CH), 1.46 (d, 6H, J_{HH} = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.28 (s, 12H, B(OC(C*H*$_3$)$_2$)$_2$), 1.22 (d, 6H, J_{HH} = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.13 (d, 6H, J_{HH} = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.07 (d,

6H, J_{HH} = 6.8 Hz, CH(CH_3)$_2$), 1.03 (*n*-BuBpin), 0.92 (*n*-BuBpin), 0.86 (d, 6H, J_{HH} = 6.8 Hz, CH(CH_3)$_2$) ppm. ^{31}P{^{1}H} NMR (202 MHz, toluene) δ 36.35 (LMg(OBpin)(OPPh$_3$)), 35.21 (LMg(Bpin)(OPPh$_3$)), –5.26 (PPh$_3$) ppm. Due to the extreme air- and moisture-sensitivity of compound **11**, an accurate microanalysis could not be obtained.

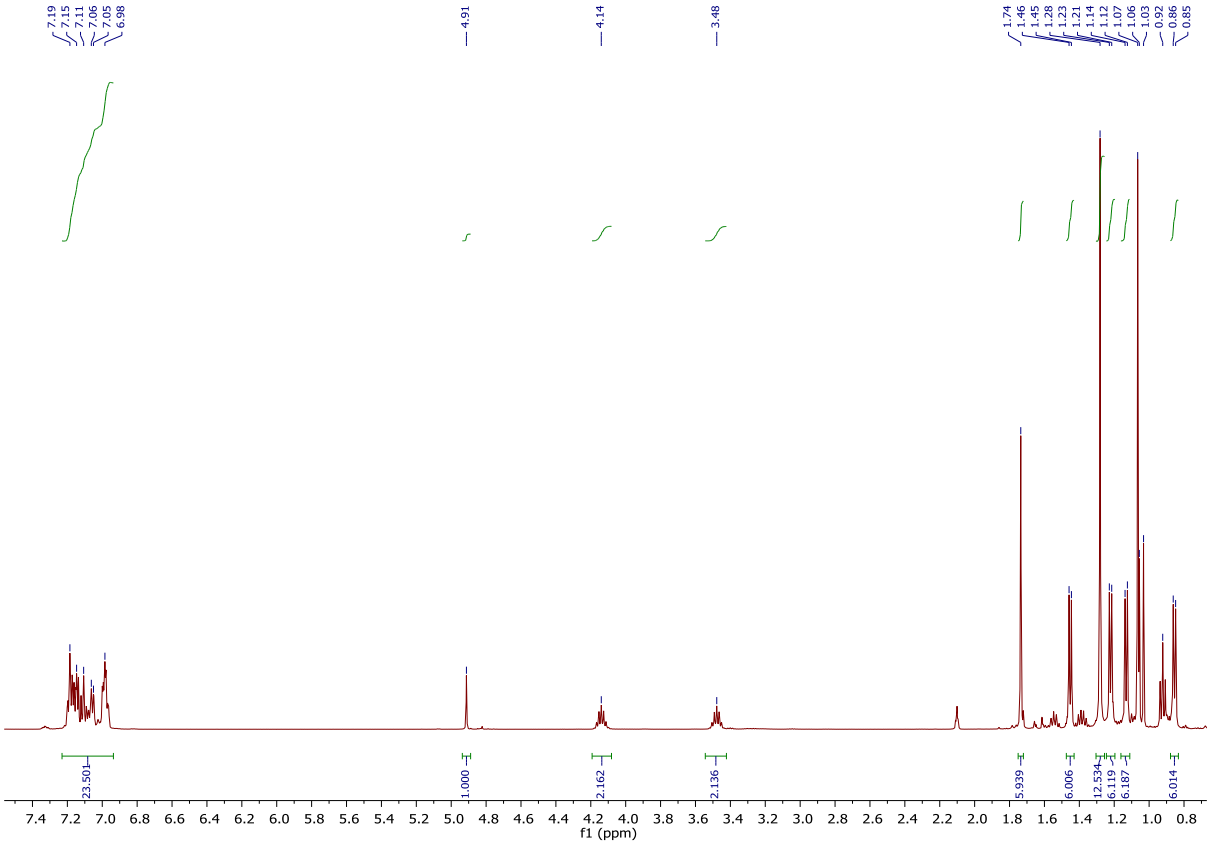


Figure S1: ^{1}H NMR spectrum of compound **11** recorded in the presence of *n*-BuBpin side-product.

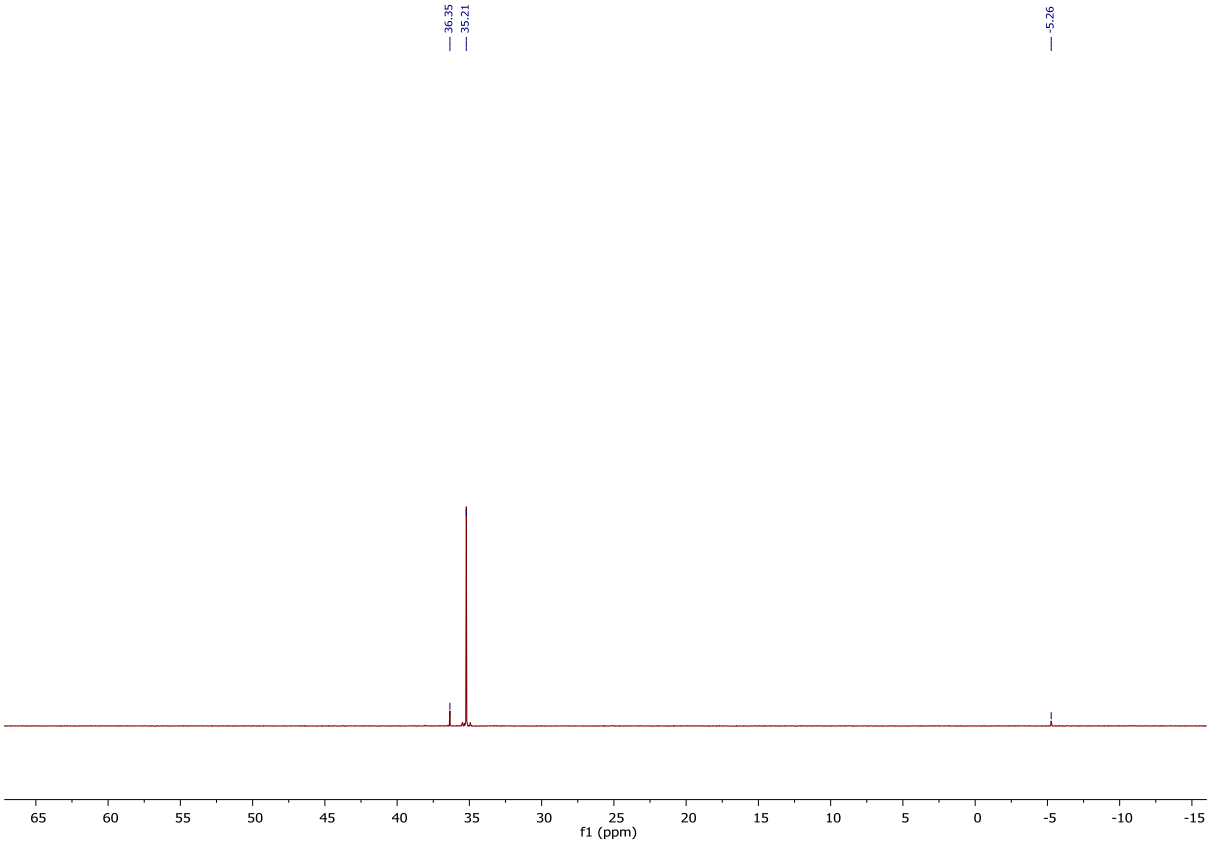


Figure S2: $^{31}P\{^{1}H\}$ NMR spectrum of compound **11**. [δ 36.35 ($LMg(OBpin)(OPPh_3)$), –5.26 (PPh_3) ppm].

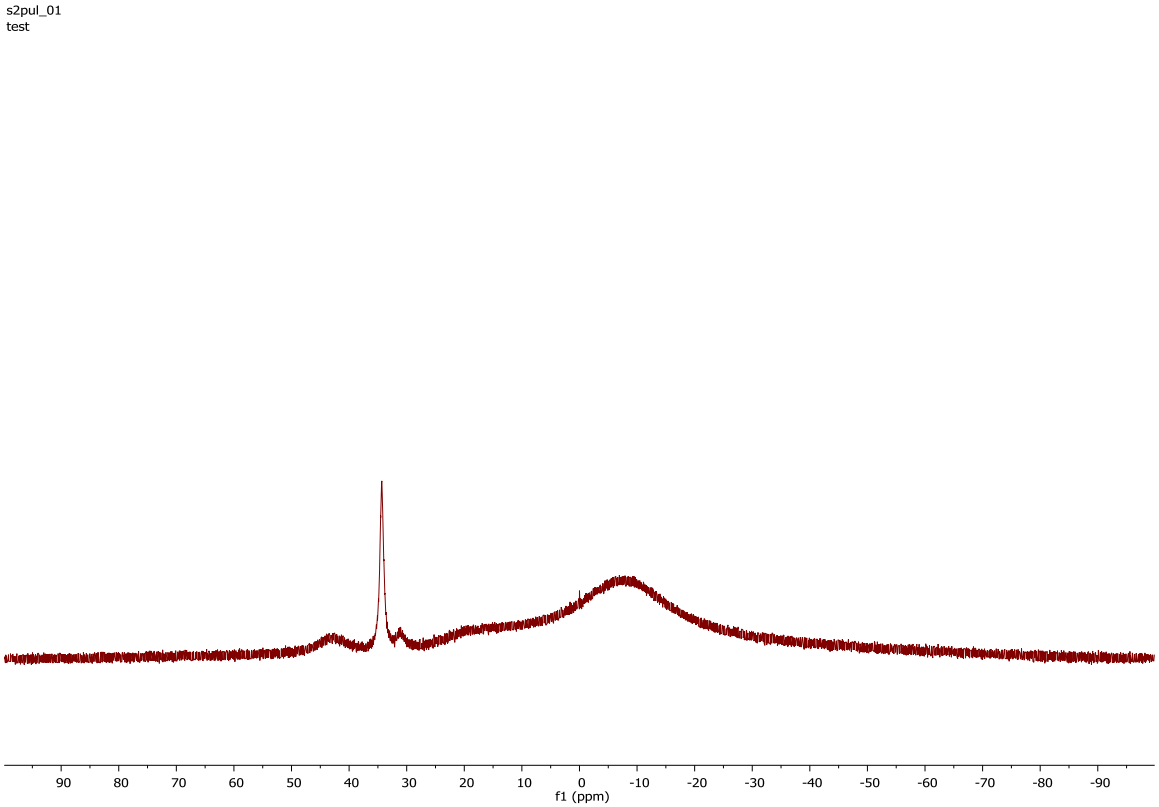


Figure S3: $^{11}B\{^{1}H\}$ NMR spectrum of compound **11** showing the formation of *n*-BuBpin.

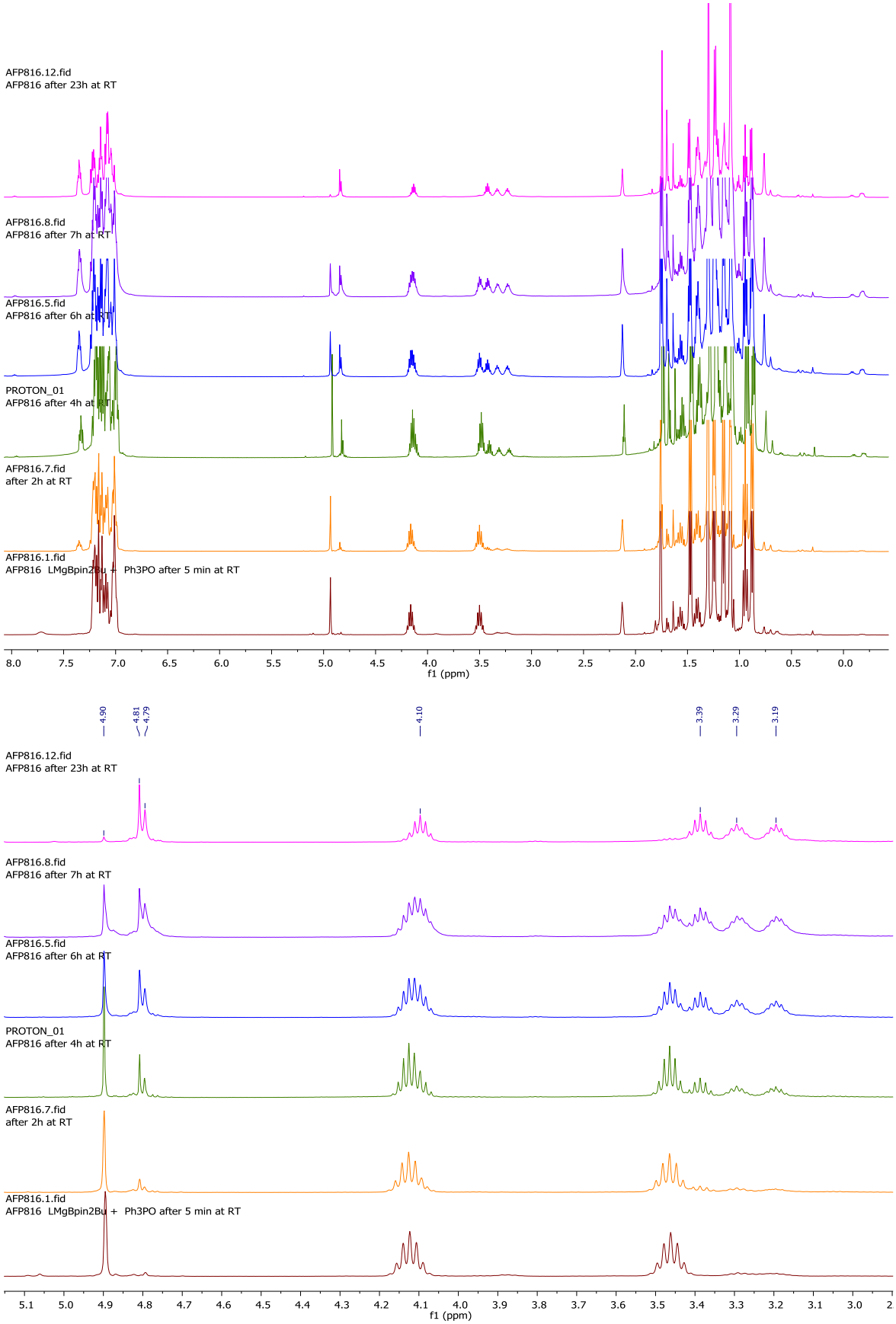


Figure S4: Stacked spectra at the various times indicated demonstrating the conversion of compound **11** to compound **12** over 23 hours.

Synthesis of compound 12

Toluene-d_8 (0.5 mL) was added to a mixture of [(BDI)MgBu] (50 mg, 0.1 mmol) and bis(pinacolato)diboron (25.4 mg, 0.1 mmol) in a NMR tube fitted with J. Young tap. After 2 h, 2 equivalents of triphenylphosphine oxide (55.7 mg, 0.2 mmol) were added. After 1 day at RT, the solvent was removed under reduced pressure and the solid was washed with hexane to yield [(BDI)Mg(OBpin)($OPPh_3$)] (**12**) (50 mg, 58%)). Colourless crystals suitable for X-ray diffraction studies were obtained from a saturated toluene solution of at RT. ^{1}H NMR (500 MHz, toluene) δ 7.22-7.18 (m, 8H, CH ar), 7.08-7.01 (m, 13H, CH ar), 4.83 (s, 1H, NC(CH_3)C*H*), 4.12 (hept, 2H, J_{HH} = 6.8 Hz, C*H*(CH_3)$_2$), 3.41 (hept, 2H, J_{HH} = 6.8 Hz, C*H*(CH_3)$_2$), 1.73 (s, 6H, NC(C*H*$_3$)CH), 1.47 (d, 6H, J_{HH} = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.28 (s, 12H, B(OC(C*H*$_3$)$_2$)$_2$), 1.22 (d, 12H, J_{HH} = 6.8 Hz, CH(C*H*$_3$)$_2$), 0.88 (d, 6H, J_{HH} = 6.8 Hz, CH(C*H*$_3$)$_2$) ppm. ^{13}C{^{1}H} NMR (126 MHz, toluene) δ 167.61 (N*C*(CH_3)CH), 146.65, 144.30, 141.96, 132.35 (CH ar), 132.26 (CH ar), 131.95 (CH ar), 128.66 (CH ar), 128.56 (CH ar), 123.93 (CH ar), 123.77 (CH ar), 122.92 (CH ar), 94.68 (NC(CH_3)*C*H), 77.92 (B(O*C*(CH_3)$_2$)$_2$), 27.69 (*C*H(CH_3)$_2$), 27.21 (*C*H(CH_3)$_2$), 25.78 (B(OC(*C*H$_3$)$_2$)$_2$), 25.32 (CH(*C*H$_3$)$_2$), 24.61 (CH(*C*H$_3$)$_2$), 24.45 (CH(*C*H$_3$)$_2$), 24.03 (CH(*C*H$_3$)$_2$), 23.75 (NC(*C*H$_3$)CH) ppm. ^{11}B{^{1}H} NMR (160 MHz, toluene) δ 20.12 ppm. ^{31}P{^{1}H} NMR (202 MHz, toluene) δ 36.35 ppm. Elemental analysis: Found C, 73.61; H, 8.06 N, 3.34 %. $C_{53}H_{68}BMgN_2O_4P$ requires: C, 73.74; H, 7.94; N, 3.25 %.

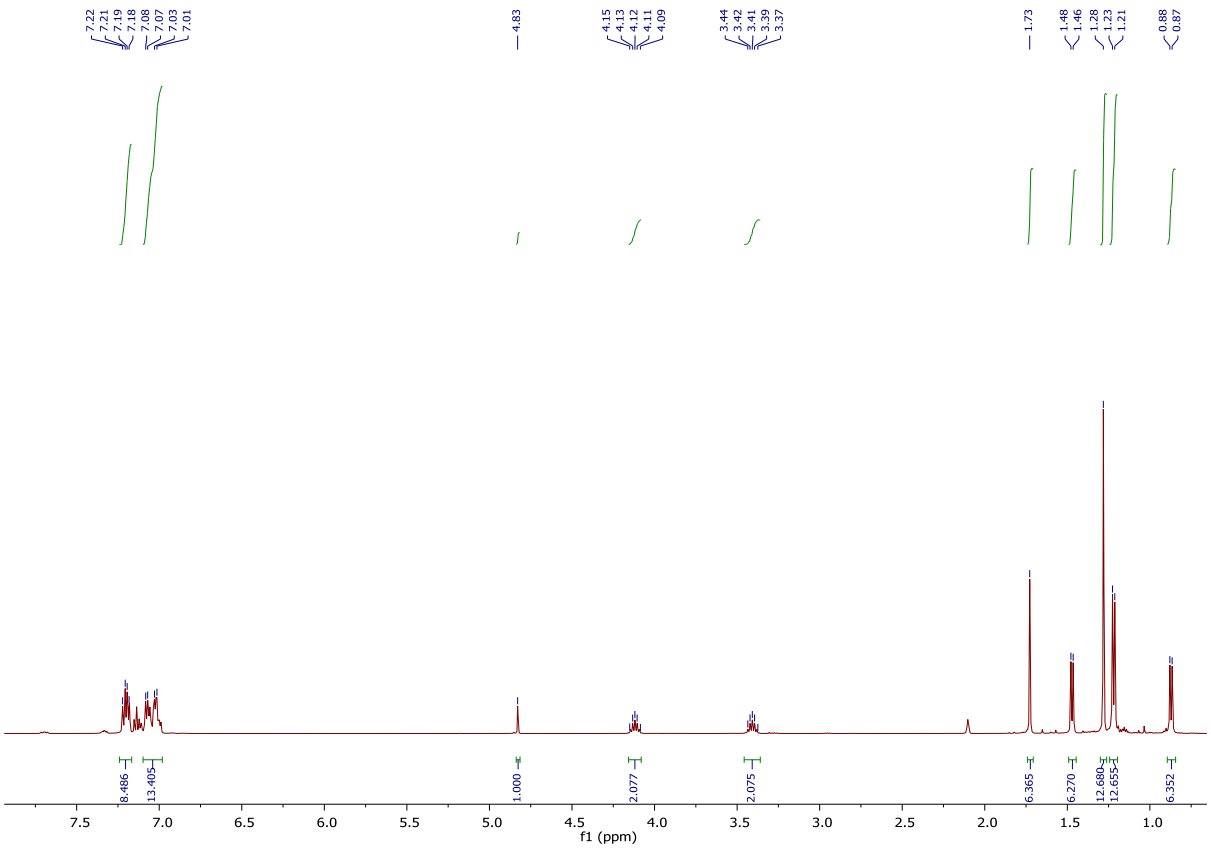


Figure S5: ^{1}H NMR spectrum of compound **12**.

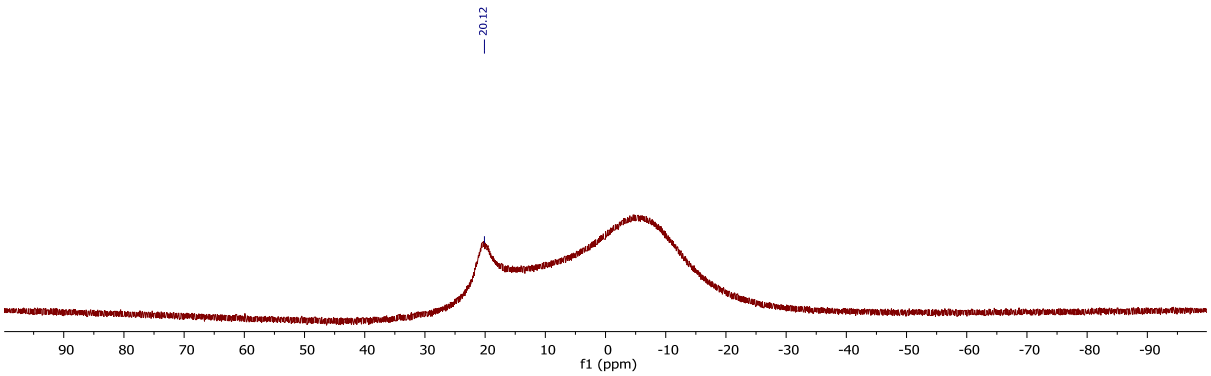


Figure S6: $^{11}B\{^{1}H\}$ of compound **12**.

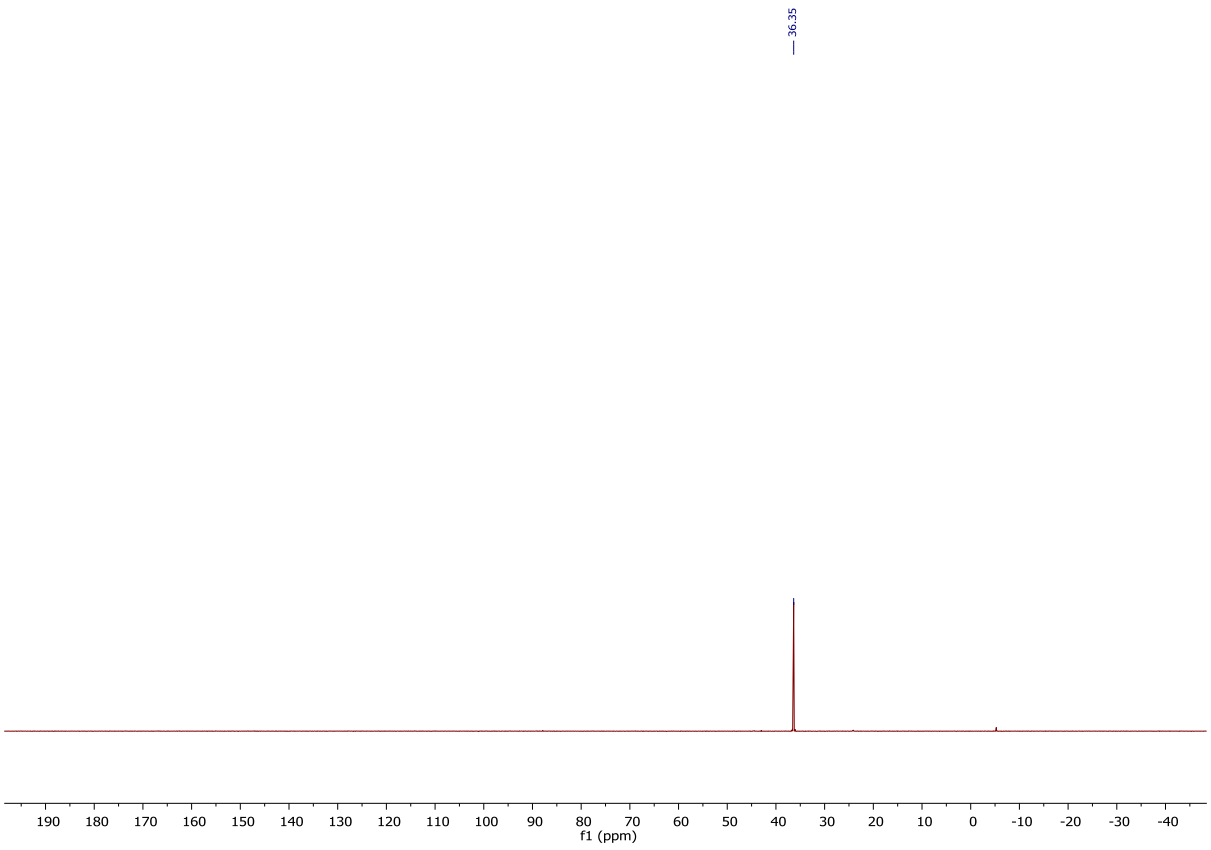


Figure S7: $^{31}P\{^{1}H\}$ NMR spectrum of compound **12**.

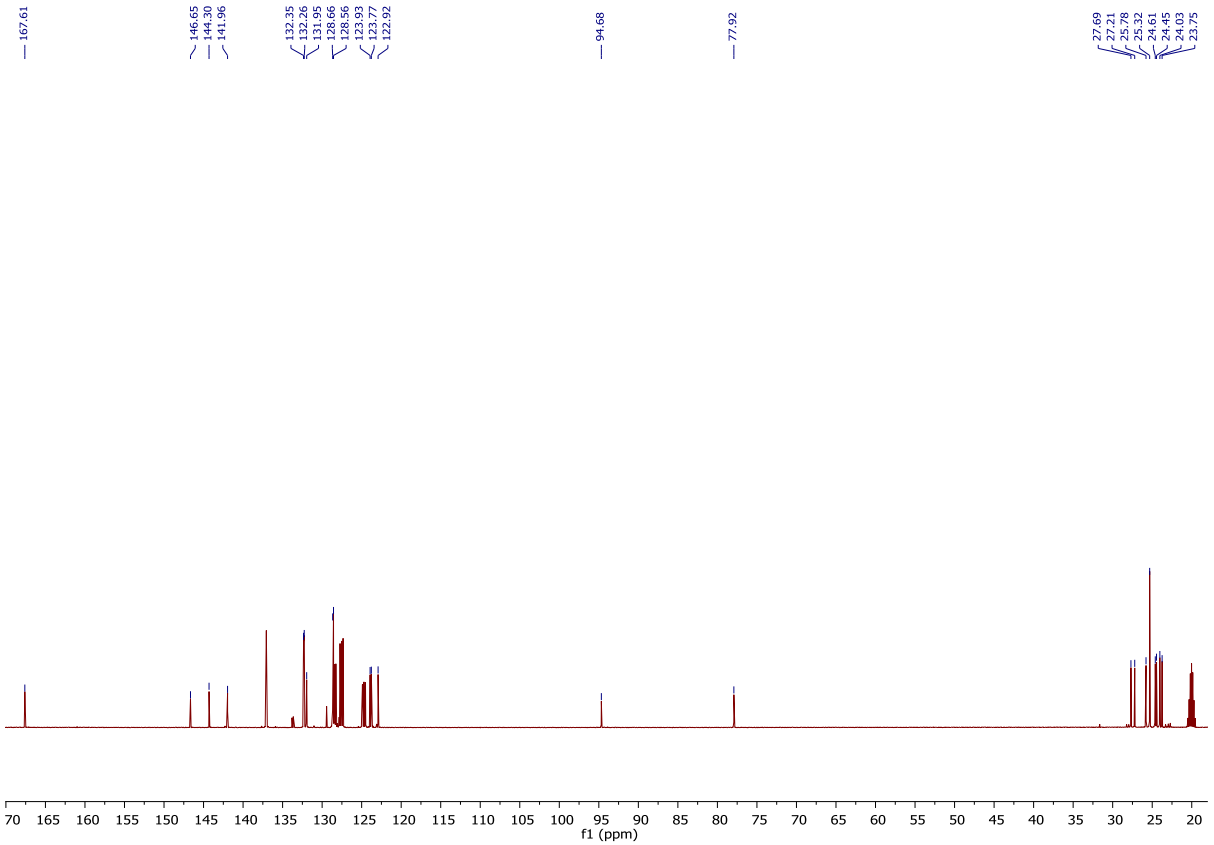


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of compound **12**.

Reaction of compound 10 and Ph_3PO

Toluene-d_8 (0.5 mL) was added to a mixture of [(BDI)MgBpin(DMAP)] (**10**) (20 mg, 0.03 mmol) and triphenylphosphine oxide (8.0 mg, 0.03 mmol) in a NMR tube fitted with a J. Young tap. The reaction was monitored by NMR over 24 h. The NMR spectra showed the formation of [(BDI)Mg(Bpin)($OPPh_3$)] (**11**), [(BDI)Mg(OBpin)($OPPh_3$)] (**12**) and unreacted compound **10**.

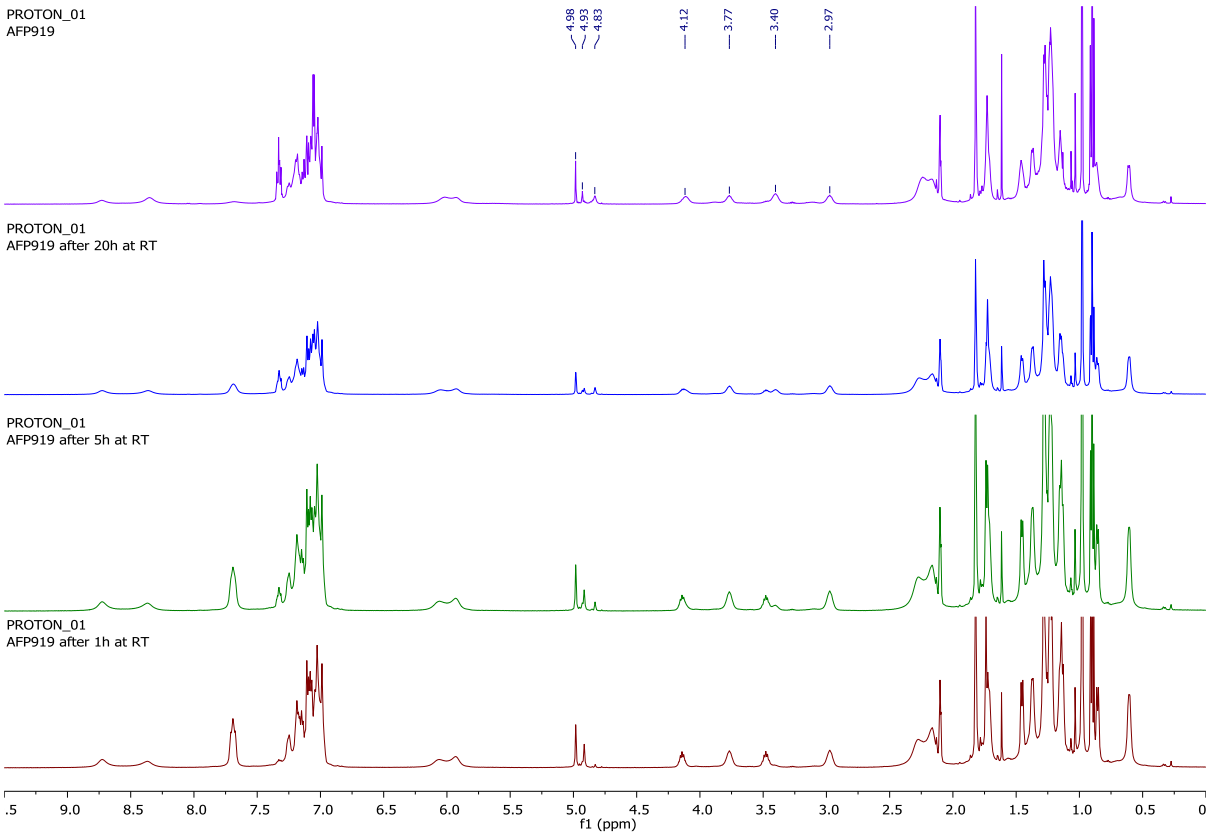


Figure S9: Stacked ^1H NMR spectra recorded at the times indicated of the reaction of compound **10** and Ph_3PO.

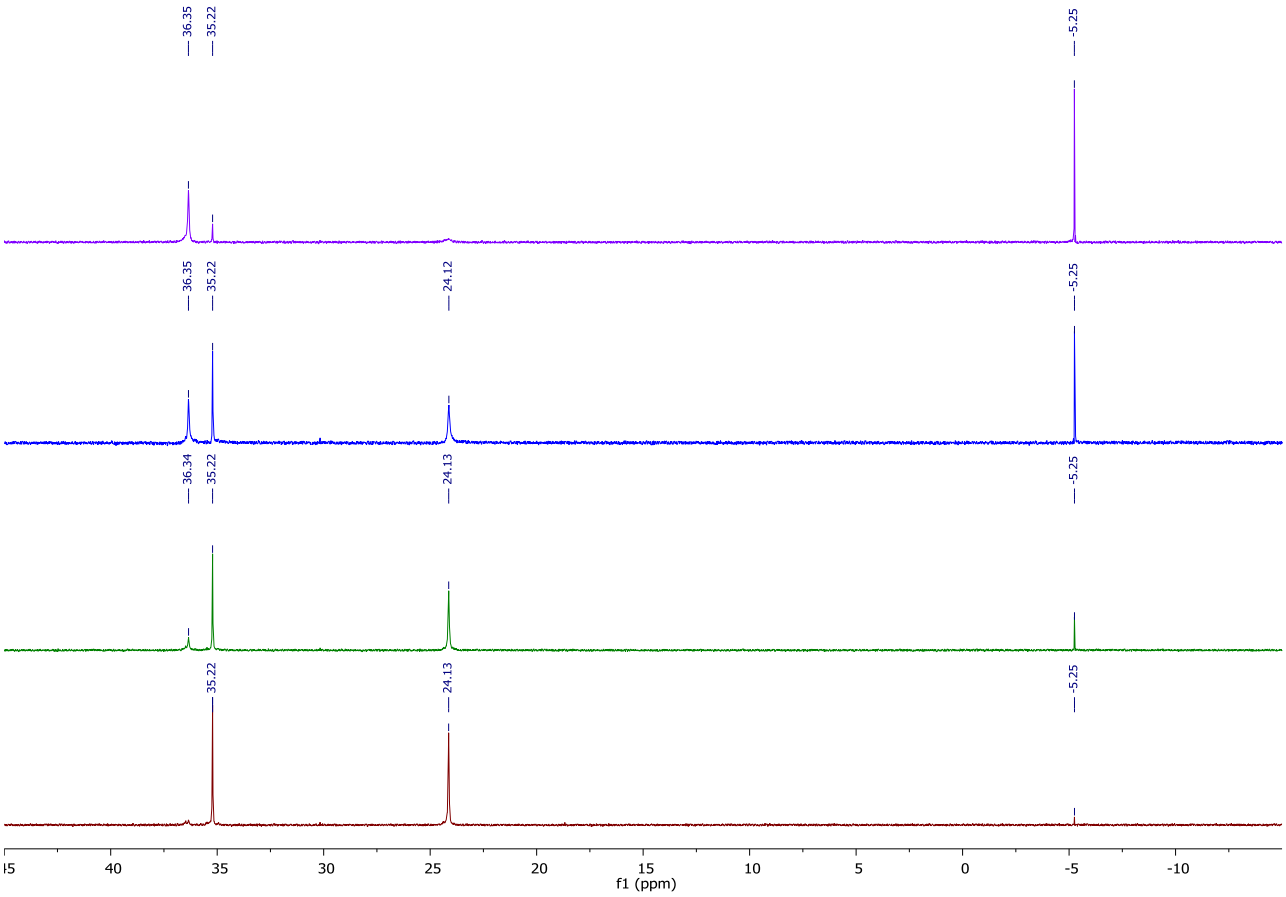


Figure S10: Stacked $^{31}P\{^{1}H\}$ NMR spectra recorded over the same time period as the data shown in Figure S9 of the reaction of compound **10** and Ph_3PO.

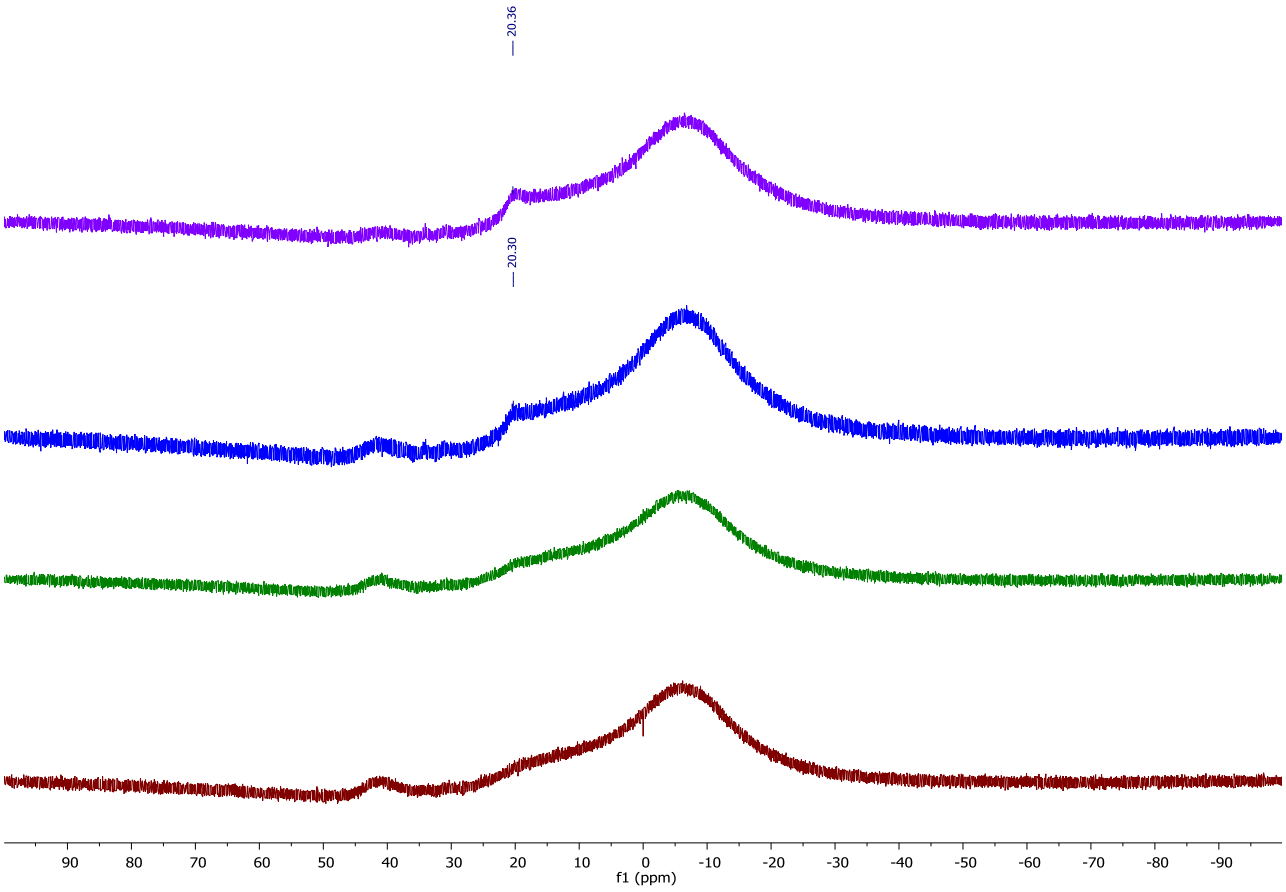


Figure S11: Stacked $^{11}B\{^{1}H\}$ NMR spectra recorded over the same time period as the data shown in Figure S9 of the reaction of compound **10** and Ph_3PO.

Single Crystal X-ray Diffraction analysis.

Single Crystal X-ray diffraction data for compounds **11** and **12** were collected using Cu*K*α (λ = 1.54184 Å) radiation on a SuperNova, Dual Cu at zero, EosS2 diffractometer. The crystals were kept at 150(2) K during data collections. The structures were solved using Olex2,[2] and refined with the ShelXL[3] refinement package using Least Squares minimisation.

The asymmetric unit in **11** comprises 2 molecules. The data were integrated for this structure in a manner that takes account of 54% sample twinning by virtue of a 180° rotation about the 1 0 0 reciprocal direction. However, raw data frames were not as clean as one might hope with some smearing of electron density in evidence. Both molecules in the asymmetric unit have similar compositions, but the highest residual electron density peak is located at 1.62 Å from Mg2, and close to B2, and has resulted in distortion of the ADPs pertaining to the latter atom. Indeed, analysis of the ADPs pinacolato ligand based on B2 suggested (since they are larger than those for the corresponding ligand containing B1) that there might be some ligand disorder involving the moiety based on B2 – possibly with a hydroxide moiety based on the highest residual electron density peak. However, efforts to model such a disorder suggested that it would be, at best, in the region of 6%. As such these were abandoned due to a lack of credibility. On balance, given the quality of the data, it appears that the residual electron density is, in fact, spurious.

The asymmetric unit of compound **12** comprises 2 molecules.

Table S1: Single Crystal X-ray Data Parameters for compounds **11** and **12**.

Compound	**11**	**12**
Empirical formula	$C_{53}H_{68}BMgN_2O_3P$	$C_{106}H_{136}B_2Mg_2N_4O_8P_2$
Formula weight	847.18	1726.36
Temperature/K	150.00(10)	149.9(5)
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a/Å	35.0861(6)	35.0559(10)
b/Å	13.1244(2)	13.3465(2)
c/Å	22.2626(4)	22.2186(7)
α/°	90	90
β/°	100.785(2)	100.589(3)
γ/°	90	90
Volume/Å^3	10070.5(3)	10218.5(5)
Z	8	4
ρ_{calc} g/cm^3	1.118	1.122
μ/mm^{-1}	0.921	0.932
F(000)	3648.0	3712.0
Crystal size/mm^3	0.296 × 0.137 × 0.095	0.096 × 0.065 × 0.035
Radiation	CuKα (λ = 1.54184 Å)	CuKα (λ = 1.54184 Å)
2Θ range for data collection/°	7.208 to 147.52	5.13 to 145.054
Index ranges	$-42 \le h \le 43$, $-16 \le k \le 16$, $-27 \le l \le 27$	$-43 \le h \le 42$, $-12 \le k \le 16$, $-26 \le l \le 27$
Reflections collected	22453	67342
Independent reflections	22453 [R_{int} = 0.0971, R_{sigma} = 0.0922]	19993 [R_{int} = 0.0589, R_{sigma} = 0.0619]
Data/restraints/parameters	22453/1/1128	19993/0/1145
Goodness-of-fit on F^2	1.079	1.014
Final R indexes [I>=2σ (I)]	R_1 = 0.0856, wR_2 = 0.1973	R_1 = 0.0535, wR_2 = 0.1226
Final R indexes [all data]	R_1 = 0.0951, wR_2 = 0.2025	R_1 = 0.0897, wR_2 = 0.1410
Largest diff. peak/hole / e Å^{-3}	0.68/-0.39	0.47/-0.30

Computational Details / Methodology

DFT calculations were run with Gaussian 09 (Revision D.01).[4] The Mg and P centers were described with the Stuttgart RECPs and associated basis sets,[5] and 6-31G** basis sets were used for all other atoms (BS1).[6] A polarisation function was also added to P (ζd =0.387). Initial BP86[7] optimisations were performed using the 'grid = ultrafine' option, with all stationary points being fully characterized via analytical frequency calculations as either minima (all positive eigenvalues) or transition states (one negative eigenvalue). IRC calculations and subsequent geometry optimizations were used to confirm the minima linked by each transition state. All energies were recomputed with a larger basis set featuring 6-311++G** basis sets on all atoms (BS2). Corrections for the effect of toluene (ε = 2.3741) solvent were run using the polarizable continuum model and BS1.[8] Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[9] The BP86-optimised geometries of **A** and **G** were used for the NBO (Natural Bonding Orbital) studies (see Table S2) to generate molecular orbital pictures.

Breakdown of Energy Contributions

The following tables detail the evolution of the relative energies as the successive corrections to the initial SCF energy are included. Terms used are:

$\mathbf{\Delta E_{BS1}}$	SCF energy computed with the BP86 functional with BS1
$\mathbf{\Delta H_{BS1}}$	Enthalpy at 0 K with BS1
$\mathbf{\Delta G_{BS1}}$	Free energy at 298.15 K and 1 atm with BS1
$\mathbf{\Delta G_{BS1/tol}}$	Free energy corrected for toluene solvent with BS1
$\mathbf{\Delta G_{BS1/tol+D3}}$	Free energy corrected for toluene and dispersion effects with BS1
$\mathbf{\Delta E_{BS2}}$	SCF energy computed with the BP86 functional with BS2
$\mathbf{\Delta G_{tol}}$	Free energy corrected for basis set (BS2), dispersion effects and toluene solvent

In each case the final data used in the main article are highlighted in bold.

Table S2 – Relative energies (kcal/mol) for computed structures. Data in bold are those used in the main text. All energies are quoted relative to **9** at 0.0 kcal/mol.

	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/tol}$	$\Delta G_{BS1/tol+D3}$	ΔE_{BS2}	ΔG_{tol}
9	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
A	+1.8	+2.4	+17.0	+18.9	-8.3	+4.3	**-5.7**
TS(A-11)	+21.7	+22.3	+37.9	+41.3	+10.4	+25.8	**+14.5**
11	-10.9	-11.8	-16.5	-13.5	-5.3	-12.0	**-6.5**
B	-8.7	-9.0	-1.8	+1.2	+3.5	-8.9	**+3.2**
TS(B-C)	+19.8	+18.4	+31.6	+36.2	+12.3	+23.0	**+15.4**
C	-82.0	-81.5	-75.7	-71.9	-70.9	-77.0	**-65.9**
12	-87.9	-88.2	-93.4	-89.3	-79.3	-83.6	**-75.0**
TS(9-D)	+15.3	+14.8	+13.5	+14.9	+18.4	+16.2	**+19.4**
D	+6.8	+6.1	+1.8	+2.7	+11.4	+6.6	**+11.2**
E	+1.0	-0.4	-21.2	-22.2	+16.5	-2.6	**+12.9**
TS(11-F)	+23.7	+21.5	+18.9	+20.6	+25.8	+25.5	**+27.7**
F	-67.9	-68.4	-80.6	-81.0	-45.5	-65.7	**-43.3**
G	-3.8	-3.4	+7.4	+9.0	-0.7	-1.6	**+1.5**
TS(G-H)	+25.6	+25.9	+42.7	+46.0	+17.3+	33.1	**24.7**
H	-67.8	-67.4	-69.5	-67.8	-61.1	-61.0	**-54.3**
TS(H-I)	-62.6	-62.6	-64.3	-62.5	-55.9	-56.9	**-50.1**
I	-69.2	-69.4	-75.3	-72.6	-61.7	-64.8	**-57.3**
J	-66.1	-66.8	-49.2	-87.9	-49.2	-64.4	**-47.5**
A'	+18.8	+19.1	+34.5	+35.2	+6.5	+20.6	**+8.4**
TS(A'-11)	+25.8	+26.6	+43.2	+46.7	+13.5	+29.2	**+16.8**

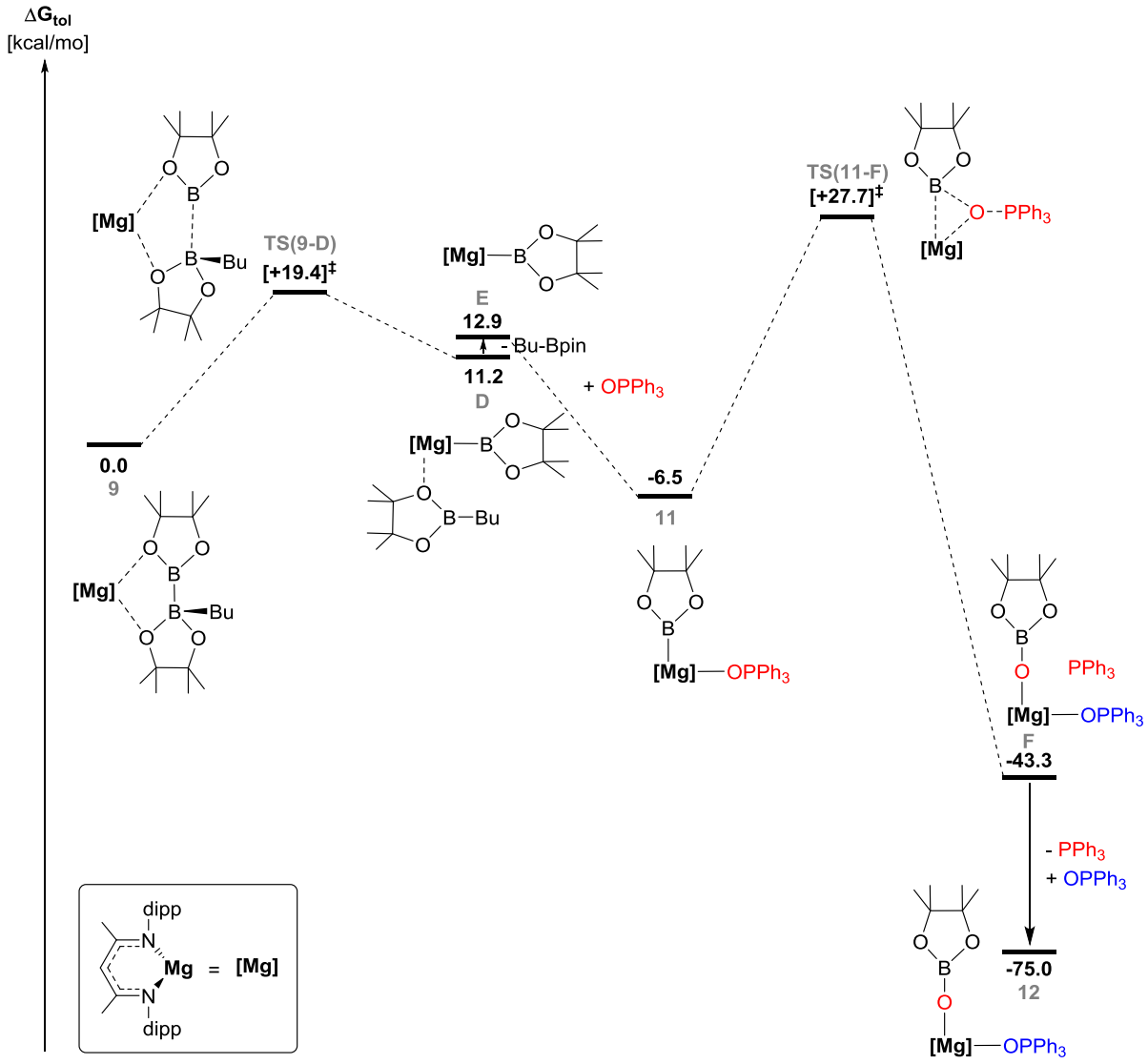


Figure S12: DFT calculated free energy (kcal mol^{-1}) profile for the reaction of **9** with $OPPh_3$ (Pathway **II**), relative to **9** + $OPPh_3$.

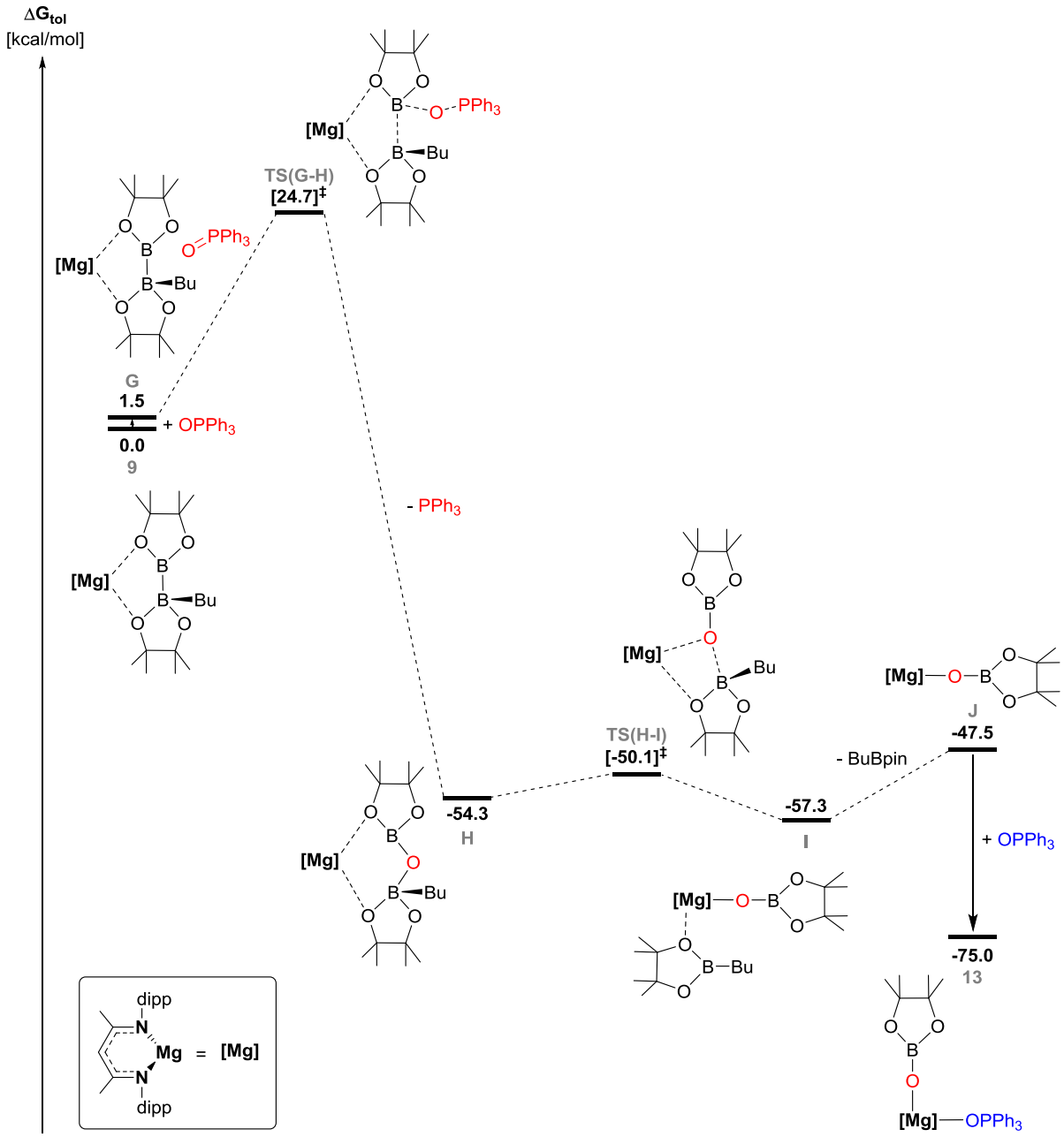
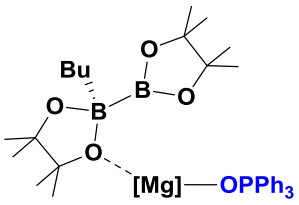
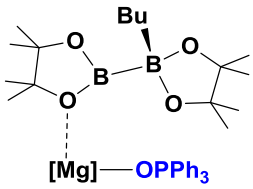
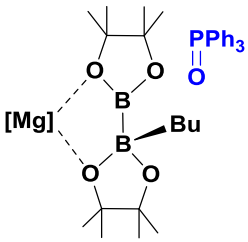
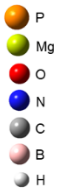


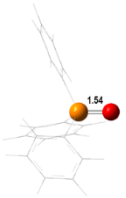
Figure S13: – DFT calculated free energy (kcal mol^{-1}) profile for the reaction of **9** with $OPPh_3$ (Pathway **III**), relative to **9** + $OPPh_3$.

Table S3: Energies (eV) of the frontier molecular orbitals computed for **A**, **A**' and **G**.

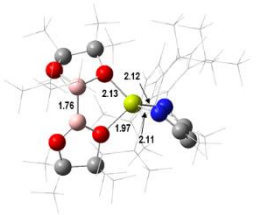
Structure	HOMO	LUMO	LUMO+11
 **A**	-3.39	-2.44	+0.19
 **A'**	-2.97	-2.42	-0.06
 **G**	-3.92`	-2.15	-1.06

DFT- computed geometries for the reaction of **9** with $OPPh_3$, relative to **9** and the free substrates. Bond lengths given in Ångstroms.

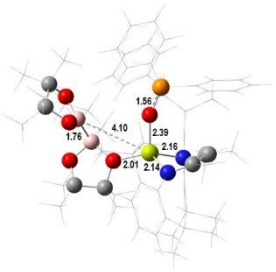




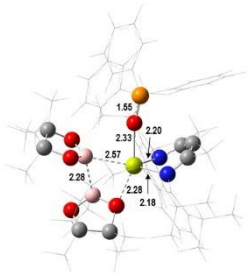
$OPPh_3$



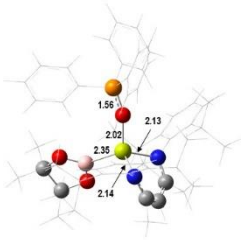
9
0.0



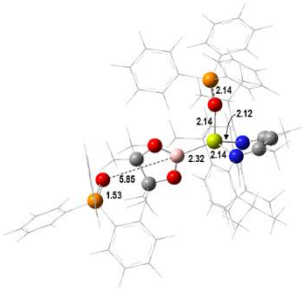
A
-5.7



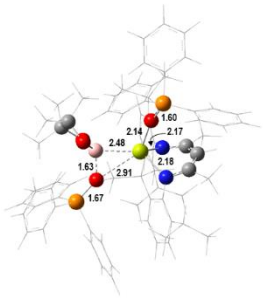
TS(A-11)
+14.5



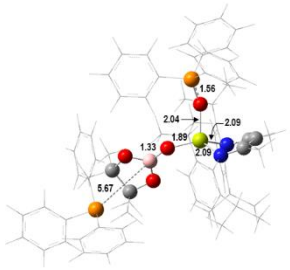
11
-6.5



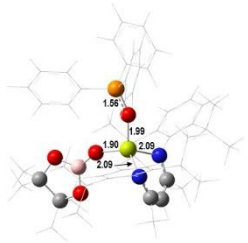
B
+3.2



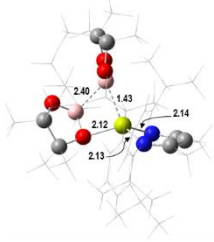
TS(B-C)
+15.4



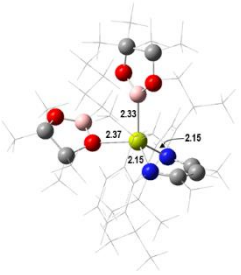
C
-65.9



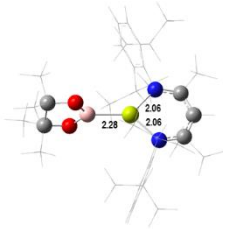
12
-75.0



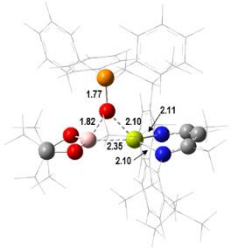
TS(9-D)
+19.4



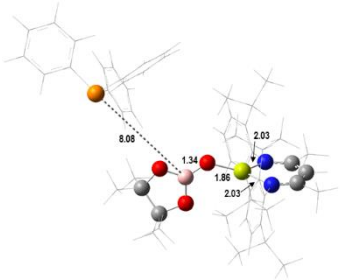
D
+11.1



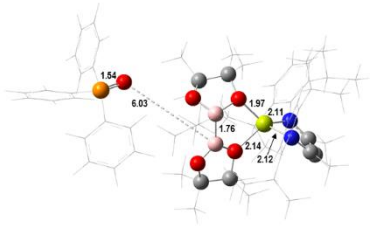
E
+12.9



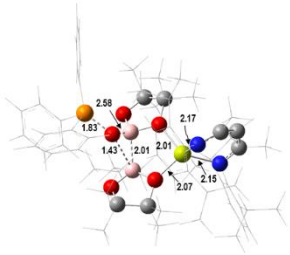
TS(11-F)
+27.7



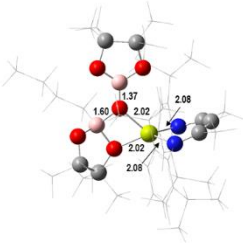
F
-43.3



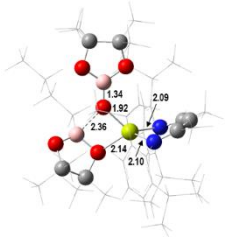
G
+1.5



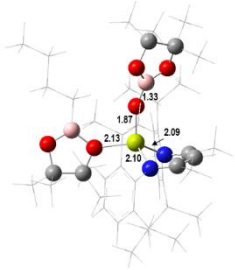
TS(G-H)
+24.7



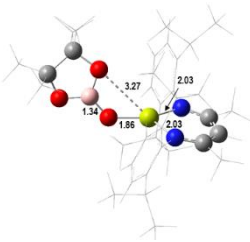
H
-54.3



TS(H-I)
-50.1



I
-57.3



J
-47.5

Cartesian Coordinates and Computed Energies (in Hartrees)

OPPh3

SCF (BP86) Energy = -776.746378277
Enthalpy 0K = -776.476359
Energy 298K = -776.458922
Free Energy 298K = -776.524191
Lowest Frequency = 14.8482 cm^{-1}
Second Frequency = 33.8839 cm^{-1}
SCF (BP86-D3BJ) Energy = -776.830662556
SCF (Toluene) Energy = -776.7518488
SCF (BS2) Energy = -1111.774142

P	0.01177	-0.02685	0.93614
C	-0.33727	1.66995	0.28447
C	0.69542	2.49879	-0.19919
C	-1.65011	2.18103	0.38068
C	0.41694	3.81889	-0.58819
H	1.71633	2.11095	-0.27195
C	-1.92427	3.49993	-0.00909
H	-2.45614	1.54495	0.76148
C	-0.89138	4.31969	-0.49521
H	1.22398	4.45631	-0.96453
H	-2.94515	3.88881	0.06663
H	-1.10699	5.34924	-0.79991
C	1.61361	-0.54824	0.16476
C	2.67604	-0.81986	1.04850
C	1.79903	-0.70021	-1.22445
C	3.91945	-1.23451	0.54442
H	2.50299	-0.70774	2.12401
C	3.04292	-1.11480	-1.72371
H	0.97425	-0.50434	-1.91768
C	4.10358	-1.38068	-0.83997
H	4.74374	-1.44581	1.23378
H	3.18447	-1.23425	-2.80312
H	5.07273	-1.70615	-1.23279
C	-1.29017	-1.10896	0.18819
C	-1.74903	-2.18257	0.97720
C	-1.81162	-0.91894	-1.10806
C	-2.70985	-3.06879	0.46632
H	-1.35248	-2.29757	1.99141
C	-2.77128	-1.80907	-1.61573
H	-1.48712	-0.06535	-1.71308
C	-3.21781	-2.88540	-0.83067
H	-3.06626	-3.90064	1.08299
H	-3.17694	-1.65725	-2.62164
H	-3.96861	-3.57674	-1.22788
O	0.05994	-0.14365	2.46606

PPh3

SCF (BP86) Energy = -701.502630498
Enthalpy 0K = -701.237091
Energy 298K = -701.220600
Free Energy 298K = -701.284016
Lowest Frequency = 23.5594 cm^{-1}
Second Frequency = 24.5927 cm^{-1}
SCF (BP86-D3BJ) Energy = -701.583032914
SCF (Toluene) Energy = -701.5053263
SCF (BS2) Energy = -1036.4965495

P	-0.00005	0.00008	-1.25095
C	-1.48732	0.77415	-0.41579
C	-2.09251	0.27954	0.75880
C	-2.04470	1.91145	-1.04201
C	-3.22314	0.91529	1.29858
H	-1.67956	-0.60836	1.24837
C	-3.16715	2.55214	-0.49585
H	-1.59593	2.29325	-1.96667
C	-3.76068	2.05326	0.67574
H	-3.68463	0.51894	2.20973
H	-3.58512	3.43503	-0.99140
H	-4.64304	2.54601	1.09771
C	0.07314	-1.67506	-0.41594
C	-0.63792	-2.72490	-1.03931
C	0.80867	-1.95358	0.75533
C	-0.63183	-4.01739	-0.49341
H	-1.19654	-2.52587	-1.96153
C	0.82316	-3.25078	1.29477
H	1.37498	-1.15327	1.24254
C	0.10156	-4.28368	0.67495
H	-1.19128	-4.81957	-0.98667
H	1.40078	-3.45360	2.20334
H	0.11574	-5.29430	1.09671
C	1.41421	0.90093	-0.41604
C	2.67860	0.81110	-1.04024
C	1.28795	1.67639	0.75577
C	3.79488	1.46286	-0.49459
H	2.78530	0.22842	-1.96288
C	2.40409	2.33778	1.29495
H	0.31197	1.76580	1.24367
C	3.65909	2.23036	0.67431
H	4.76905	1.38027	-0.98850
H	2.29116	2.93882	2.20395
H	4.52719	2.74817	1.09584

pinBBu

SCF (BP86) Energy = -569.123611712
Enthalpy 0K = -568.827988
Energy 298K = -568.812028
Free Energy 298K = -568.871243
Lowest Frequency = 17.1704 cm^{-1}
Second Frequency = 53.5444 cm^{-1}
SCF (BP86-D3BJ) Energy = -569.174139919
SCF (Toluene) Energy = -569.1253858
SCF (BS2) Energy = -569.2678874

O	-0.18305	0.73253	-0.38834
O	-0.86951	-1.32347	0.42112
C	-2.09599	-0.61210	0.04700
C	-3.15582	-0.87889	1.12040
H	-3.40478	-1.95269	1.13677
H	-4.08207	-0.31829	0.90599
H	-2.79911	-0.59817	2.12257
C	-2.54735	-1.19515	-1.30416
H	-1.79553	-1.01106	-2.08925
H	-3.50914	-0.76724	-1.63327
H	-2.67043	-2.28533	-1.19994
C	-1.60239	0.88915	-0.05321
C	-2.26940	1.72271	-1.15177
H	-1.83383	2.73533	-1.16517
H	-3.35299	1.82110	-0.96653
H	-2.12221	1.27698	-2.14680
C	-1.65437	1.63823	1.29025
H	-1.17970	1.05048	2.09310
H	-2.69058	1.86818	1.58994
H	-1.10320	2.58745	1.19199
B	0.19900	-0.53545	0.02071
C	1.69301	-1.04253	0.01354
H	1.83638	-1.74504	0.85777
H	1.83299	-1.66832	-0.89336
C	2.76817	0.06373	0.04105
H	2.59358	0.76699	-0.79542
H	2.65519	0.66794	0.96249

C 4.20766 -0.47434 -0.03506
H 4.32236 -1.07274 -0.96046
H 4.37762 -1.17954 0.80230
C 5.27348 0.63191 -0.00156
H 6.29435 0.21687 -0.05980
H 5.14848 1.33229 -0.84657
H 5.20603 1.22336 0.92902

9
SCF (BP86) Energy = -2220.57991976
Enthalpy 0K = -2219.487760
Enthalpy 298K = -2219.422702
Free Energy 298K = -2219.583101
Lowest Frequency = 18.9735 cm^{-1}
Second Frequency = 26.5885 cm^{-1}
SCF (BP86-D3BJ) Energy = -2220.90416121
SCF (Toluene) Energy = -2220.58694528
SCF (BS2) Energy = -2420.36376068

Mg -0.34476 0.01378 -0.18714
O 1.54140 -2.22807 2.66404
O 0.23112 -0.49946 1.62808
O 2.35893 -3.05123 -0.58702
O 0.47307 -1.78737 -0.98025
N 0.51453 1.72437 -1.09139
N -2.31856 0.35138 -0.85786
C 0.52128 3.21091 -3.10961
H 1.23137 3.83727 -2.55179
H -0.27347 3.84981 -3.52516
H 1.06303 2.76611 -3.96307
C -0.07685 2.11136 -2.23709
C -1.29747 1.57224 -2.73842
H -1.55178 1.93263 -3.74029
C -2.37621 0.92362 -2.08493
C -3.68846 0.97689 -2.86537
H -4.44482 0.28346 -2.47490
H -3.49885 0.74795 -3.92734
H -4.11693 1.99339 -2.83081
C -3.58012 0.07622 -0.19956
C -4.27991 1.13606 0.45445
C -5.50795 0.85688 1.08681
H -6.04588 1.67243 1.58322
C -6.05569 -0.42852 1.09327
H -7.01385 -0.62228 1.58673
C -5.36109 -1.46468 0.46179
H -5.78584 -2.47393 0.46235
C -4.12896 -1.24233 -0.18402
C -3.45154 -2.41490 -0.89197
H -2.39781 -2.12895 -1.05143
C -4.08901 -2.67981 -2.27744
H -5.16444 -2.90677 -2.16873
H -3.61217 -3.54568 -2.76980
H -3.99583 -1.81357 -2.95154
C -3.47321 -3.71728 -0.06284
H -4.49158 -4.13664 0.01548
H -3.09036 -3.56385 0.95815
H -2.84912 -4.48910 -0.54735
C -3.75936 2.57485 0.51098
H -2.77726 2.60376 0.00859
C -4.69983 3.55854 -0.22462
H -5.68564 3.61324 0.27025
H -4.87252 3.26009 -1.27138
H -4.27065 4.57572 -0.22645
C -3.56264 3.03956 1.97213
H -4.51365 3.02218 2.53234
H -3.18275 4.07550 2.00169
H -2.84709 2.39704 2.51180
C 1.66127 2.46199 -0.59421
C 1.46942 3.35241 0.50686
C 2.58182 4.02219 1.04927
H 2.43604 4.70200 1.89370
C 3.86843 3.84311 0.53151
H 4.72197 4.36877 0.97182
C 4.04690 2.99050 -0.55883
H 5.05064 2.85487 -0.97631
C 2.96910 2.29261 -1.14167
C 0.07563 3.66519 1.05162
H -0.55049 2.76348 0.91397
C -0.57072 4.80491 0.22652
H 0.04535 5.71953 0.28797
H -1.57765 5.04808 0.60918
H -0.66802 4.53353 -0.83720
C 0.06676 4.02383 2.55137
H 0.61356 3.27809 3.15151
H -0.96954 4.07474 2.92381
H 0.52274 5.01173 2.74049
C 3.28221 1.39866 -2.34317
H 2.32990 0.97938 -2.70761
C 4.20878 0.22372 -1.95175
H 4.44417 -0.39762 -2.83533
H 3.76039 -0.42235 -1.18001
H 5.16769 0.59505 -1.55095
C 3.92666 2.19470 -3.50432
H 3.32408 3.07013 -3.79544
H 4.04744 1.54914 -4.39225
H 4.93023 2.56185 -3.22754
C 0.71923 -2.53986 -2.25600
C 1.30645 -1.54898 -3.26490
H 1.45104 -2.03087 -4.24660
H 2.27400 -1.15597 -2.92583
H 0.60746 -0.70550 -3.40091
C -0.60019 -3.08965 -2.79294
H -1.26580 -2.26321 -3.08956
H -1.12198 -3.71574 -2.05601
H -0.40765 -3.70185 -3.69148
C 1.73639 -3.64723 -1.76936
C 2.84369 -3.97658 -2.77714
H 3.44517 -3.08997 -3.02619
H 2.42159 -4.39293 -3.70824
H 3.51793 -4.73147 -2.34178
C 1.05731 -4.94472 -1.29309
H 0.62269 -5.51401 -2.13197
H 0.26546 -4.73848 -0.55488
H 1.81513 -5.57543 -0.80189
C -0.37602 -0.86951 2.90607
C -1.90023 -0.81125 2.79138
H -2.24597 0.22419 2.62952
H -2.37059 -1.17054 3.72328
H -2.28208 -1.42729 1.96252
C 0.10443 0.12876 3.97487
H 1.19142 0.04849 4.12432
H -0.40125 -0.04188 4.94089
H -0.12774 1.15469 3.64460
C 0.20857 -2.32100 3.14062
C 0.25527 -2.73479 4.62236
H 0.66183 -3.75681 4.70278
H -0.75003 -2.73021 5.08018
H 0.91376 -2.06703 5.19770
C -0.55993 -3.40135 2.34292
H -0.67724 -3.10688 1.28621
H -1.56111 -3.60756 2.76108
H 0.02589 -4.33463 2.37468
B 1.63895 -1.29504 1.51821
B 1.53973 -2.08466 -0.04812

C	2.92915	-0.32134	1.71530
H	3.02134	0.42936	0.90451
H	2.79079	0.27020	2.64468
C	4.25417	-1.10467	1.82956
H	4.15187	-1.86253	2.63028
H	4.43212	-1.68159	0.89849
C	5.48588	-0.22655	2.11659
H	5.31879	0.33207	3.05884
H	5.57591	0.54480	1.32605
C	6.79762	-1.02175	2.21680
H	7.66256	-0.36830	2.42856
H	6.74423	-1.77660	3.02190
H	7.00958	-1.56239	1.27647

A

SCF (BP86) Energy = -2997.32343099
Enthalpy 0K = -2995.960224
Enthalpy 298K = -2995.875874
Free Energy 298K = -2996.080151
Lowest Frequency = 13.6199 cm^{-1}
Second Frequency = 13.9911 cm^{-1}
SCF (BP86-D3BJ) Energy = -2997.77532189
SCF (Toluene) Energy = -2997.33289136
SCF (BS2) Energy = -3532.13099936

Mg	0.94572	0.06075	-0.22484
O	-1.30795	2.59791	-3.01397
O	0.08827	1.17191	-1.66353
O	-2.98650	-0.26480	-2.55906
O	-3.99223	1.39045	-1.31779
N	2.32678	0.89739	1.21606
N	2.21519	-1.60140	-0.66827
C	3.66605	0.29601	3.25617
H	3.83105	1.37525	3.37263
H	4.63966	-0.21981	3.28325
H	3.08892	-0.06822	4.12424
C	2.91138	-0.04981	1.97363
C	2.89837	-1.44474	1.68506
H	3.27038	-2.06282	2.50693
C	2.69828	-2.14805	0.47554
C	3.05401	-3.63223	0.51549
H	3.64059	-3.94088	-0.36250
H	2.12608	-4.23246	0.49688
H	3.61294	-3.89081	1.42705
C	2.53080	-2.29868	-1.89529
C	3.83878	-2.14723	-2.46211
C	4.15053	-2.82147	-3.65787
H	5.15399	-2.71201	-4.08354
C	3.21239	-3.62394	-4.31516
H	3.47400	-4.13669	-5.24687
C	1.93784	-3.76282	-3.76182
H	1.20115	-4.39949	-4.26452
C	1.57658	-3.12368	-2.55759
C	0.18366	-3.40534	-1.99547
H	0.06118	-2.80229	-1.07721
C	0.03522	-4.89751	-1.60998
H	0.09529	-5.54427	-2.50335
H	-0.94184	-5.07896	-1.12960
H	0.82798	-5.22491	-0.91618
C	-0.92297	-3.00633	-2.99543
H	-0.79505	-3.52738	-3.96042
H	-0.93405	-1.92345	-3.18878
H	-1.91835	-3.27974	-2.60788
C	4.93138	-1.29473	-1.80819
H	4.44926	-0.67680	-1.03107
C	6.00445	-2.16850	-1.11439
H	6.49621	-2.83776	-1.84307
H	5.57573	-2.79496	-0.31655
H	6.78537	-1.53349	-0.65966
C	5.61725	-0.34768	-2.81867
H	6.18211	-0.90580	-3.58579
H	6.34113	0.30360	-2.29869
H	4.88773	0.29327	-3.33965
C	2.58723	2.28999	1.53078
C	3.64985	2.96942	0.85410
C	3.86941	4.33408	1.12340
H	4.67844	4.85549	0.60322
C	3.08055	5.03771	2.03871
H	3.26460	6.10044	2.22831
C	2.06053	4.36393	2.71268
H	1.44973	4.90593	3.44286
C	1.79594	2.99763	2.48575
C	4.59718	2.24492	-0.10646
H	4.02864	1.41366	-0.56317
C	5.79330	1.62646	0.65773
H	6.35637	2.41262	1.19179
H	6.48759	1.13056	-0.04358
H	5.47037	0.87808	1.39680
C	5.13161	3.14454	-1.24164
H	4.32297	3.69159	-1.75112
H	5.65582	2.53026	-1.99219
H	5.86120	3.88450	-0.86724
C	0.70292	2.34202	3.33421
H	0.55871	1.31368	2.95579
C	-0.64518	3.08783	3.23724
H	-1.43070	2.53560	3.78152
H	-0.96700	3.21026	2.19290
H	-0.57797	4.09300	3.68968
C	1.12491	2.26795	4.82331
H	2.06013	1.70665	4.97342
H	0.33195	1.79373	5.43083
H	1.27822	3.28294	5.23025
C	-5.08592	0.55750	-1.81374
C	-6.22793	1.48312	-2.25398
H	-7.05666	0.90751	-2.70321
H	-5.88195	2.23132	-2.98219
H	-6.62633	2.02242	-1.37833
C	-5.55832	-0.33200	-0.65038
H	-5.84089	0.30784	0.20145
H	-4.75935	-1.01053	-0.31068
H	-6.43738	-0.93827	-0.93014
C	-4.39142	-0.24507	-2.98087
C	-4.43396	0.49694	-4.33052
H	-4.03599	1.51957	-4.22761
H	-5.45742	0.54688	-4.73984
H	-3.79800	-0.03932	-5.05348
C	-4.88281	-1.68364	-3.16436
H	-5.93899	-1.69940	-3.48652
H	-4.79890	-2.26528	-2.23430
H	-4.28366	-2.18405	-3.94325
C	0.86973	1.77315	-2.75990
C	1.91210	0.76436	-3.24264
H	2.69249	0.60017	-2.47777
H	2.42123	1.14381	-4.14606
H	1.46227	-0.20980	-3.48544
C	1.56010	3.04902	-2.24492
H	0.82328	3.83821	-2.03705
H	2.28694	3.43038	-2.98319
H	2.10147	2.83610	-1.30900
C	-0.24106	2.11606	-3.81882
C	0.16677	3.23677	-4.79524
H	-0.66435	3.42218	-5.49608
H	1.05514	2.95699	-5.38985
H	0.37307	4.17875	-4.26557

C	-0.67872	0.88266	-4.64098
H	-1.00302	0.06285	-3.98396
H	0.12000	0.52219	-5.31301
H	-1.54252	1.16902	-5.26321
B	-1.34202	1.91675	-1.67635
B	-2.76111	0.88430	-1.77433
C	-1.42959	3.04891	-0.49221
H	-1.74529	2.58611	0.46539
H	-0.42357	3.47545	-0.29133
C	-2.39492	4.21183	-0.81091
H	-2.09597	4.65838	-1.77857
H	-3.41218	3.80598	-0.97097
C	-2.45318	5.31437	0.26196
H	-1.43346	5.71321	0.43366
H	-2.76681	4.87178	1.22930
C	-3.40095	6.47018	-0.09971
H	-3.42700	7.24765	0.68470
H	-3.09094	6.95632	-1.04224
H	-4.43451	6.10697	-0.24578
P	-1.30507	-1.46185	2.03995
C	-2.50178	-0.29869	2.80703
C	-2.94891	-0.42843	4.14024
C	-3.07614	0.67058	1.96062
C	-3.94548	0.43160	4.62592
H	-2.52297	-1.19108	4.79965
C	-4.07661	1.52226	2.45364
H	-2.75319	0.76462	0.91952
C	-4.50773	1.40789	3.78469
H	-4.28334	0.33746	5.66312
H	-4.50651	2.27220	1.78333
H	-5.28500	2.07659	4.16903
C	-2.32814	-2.89204	1.49240
C	-2.72878	-2.97419	0.14508
C	-2.79479	-3.84133	2.42792
C	-3.56921	-4.02483	-0.26248
H	-2.39450	-2.22126	-0.57664
C	-3.63736	-4.88181	2.01201
H	-2.49610	-3.77548	3.47889
C	-4.02093	-4.97756	0.66404
H	-3.86946	-4.09690	-1.31235
H	-3.99111	-5.61855	2.74044
H	-4.67485	-5.79246	0.33698
C	-0.19524	-2.11859	3.35697
C	0.31725	-3.42969	3.24887
C	0.19624	-1.30735	4.44229
C	1.19447	-3.92579	4.22427
H	0.02491	-4.06482	2.40743
C	1.07231	-1.80968	5.41734
H	-0.18567	-0.28677	4.53102
C	1.56966	-3.11881	5.31119
H	1.58282	-4.94537	4.13567
H	1.36141	-1.17609	6.26193
H	2.24894	-3.51031	6.07548
O	-0.57577	-0.79602	0.82827

TS(A-11)

SCF (BP86) Energy = -2997.29166573
Enthalpy 0K = -2995.928514
Enthalpy 298K = -2995.844527
Free Energy 298K = -2996.046934
Lowest Frequency = -127.5229 cm^{-1}
Second Frequency = 13.2120 cm^{-1}
SCF (BP86-D3BJ) Energy = -2997.74938088
SCF (Toluene) Energy = -2997.29873156
SCF (BS2) Energy = -3532.09684168077

Mg	0.57610	-0.26050	-0.05632
O	2.99497	1.31349	-2.81231
O	2.54464	-0.32449	-1.19746
O	-0.21290	1.47338	-3.02374
O	0.13676	3.01696	-1.36459
N	1.06653	-0.02370	2.07132
N	0.13704	-2.38150	0.23086
C	0.25849	-0.41380	4.40386
H	1.26832	-0.25882	4.81345
H	-0.23303	-1.21665	4.97330
H	-0.29685	0.52405	4.57782
C	0.29474	-0.74179	2.91197
C	-0.53300	-1.83127	2.53144
H	-1.17528	-2.20064	3.33355
C	-0.55043	-2.63650	1.36980
C	-1.44025	-3.87395	1.45432
H	-0.90499	-4.79818	1.19141
H	-2.26823	-3.77808	0.73083
H	-1.87649	-3.98819	2.45723
C	0.33936	-3.52405	-0.62660
C	1.32660	-4.50230	-0.26912
C	1.51250	-5.62253	-1.10148
H	2.25919	-6.37433	-0.82153
C	0.77434	-5.79704	-2.27740
H	0.93927	-6.67383	-2.91276
C	-0.18036	-4.83780	-2.62433
H	-0.77095	-4.97423	-3.53768
C	-0.42369	-3.70762	-1.81673
C	-1.54328	-2.75495	-2.23896
H	-1.57792	-1.92881	-1.50564
C	-2.91786	-3.46586	-2.22208
H	-2.95468	-4.27716	-2.97084
H	-3.72426	-2.75141	-2.46562
H	-3.13528	-3.91668	-1.23923
C	-1.29029	-2.15598	-3.63943
H	-1.20819	-2.94757	-4.40509
H	-0.36475	-1.56125	-3.66759
H	-2.12286	-1.49588	-3.93530
C	2.19207	-4.39066	0.99360
H	2.03542	-3.38439	1.41672
C	1.79020	-5.42811	2.07029
H	1.89555	-6.45817	1.68455
H	0.75042	-5.29770	2.40744
H	2.44233	-5.33357	2.95651
C	3.69865	-4.54965	0.68454
H	3.93356	-5.55432	0.29103
H	4.29242	-4.41634	1.60566
H	4.04958	-3.81127	-0.05446
C	2.03685	0.84842	2.70258
C	3.35174	0.34070	2.94967
C	4.29063	1.15948	3.60547
H	5.29311	0.76812	3.80457
C	3.97105	2.45927	4.01345
H	4.71407	3.07840	4.52739
C	2.69333	2.95686	3.74865
H	2.44017	3.97751	4.05693
C	1.71206	2.17987	3.09872
C	3.75021	-1.08699	2.56869
H	3.12445	-1.37965	1.70624
C	3.45949	-2.07457	3.72537
H	3.98303	-1.75764	4.64543
H	3.81442	-3.08873	3.46967
H	2.38334	-2.14483	3.94793
C	5.23049	-1.20940	2.14947
H	5.50531	-0.45665	1.39271
H	5.42076	-2.20987	1.72501
H	5.91478	-1.09307	3.00899
C	0.34627	2.82772	2.86031

H	-0.31214	2.07152	2.39646
C	0.46849	4.02798	1.89121
H	-0.49442	4.56373	1.82214
H	0.75477	3.71427	0.87638
H	1.21679	4.75232	2.25819
C	-0.31023	3.30247	4.17988
H	-0.35517	2.50592	4.94151
H	-1.33940	3.65309	3.98928
H	0.25002	4.14500	4.62279
C	-0.52441	3.76822	-2.43823
C	0.23511	5.09141	-2.61061
H	-0.19922	5.69705	-3.42558
H	1.30000	4.92239	-2.82776
H	0.16654	5.67763	-1.67924
C	-1.96446	4.06353	-1.98919
H	-1.94076	4.64108	-1.05099
H	-2.53231	3.13744	-1.80708
H	-2.50668	4.66293	-2.74078
C	-0.43358	2.78046	-3.67010
C	0.77402	3.04941	-4.58564
H	1.72353	2.97683	-4.03351
H	0.69784	4.03982	-5.06603
H	0.79514	2.28904	-5.38330
C	-1.70140	2.69959	-4.52816
H	-1.87805	3.65499	-5.05327
H	-2.59593	2.46190	-3.93534
H	-1.57335	1.91584	-5.29377
C	3.39062	-0.96218	-2.22848
C	2.87067	-2.35627	-2.56379
H	2.95152	-3.02480	-1.69575
H	3.47310	-2.79193	-3.38029
H	1.81851	-2.34637	-2.88012
C	4.80657	-1.07032	-1.63651
H	5.22553	-0.08019	-1.39935
H	5.49511	-1.58771	-2.32620
H	4.75789	-1.65008	-0.70141
C	3.29760	0.04928	-3.44803
C	4.62264	0.22257	-4.21005
H	4.48585	0.96658	-5.01201
H	4.93794	-0.72656	-4.67798
H	5.43032	0.57805	-3.55316
C	2.18171	-0.28346	-4.45342
H	1.19394	-0.26376	-3.97086
H	2.34416	-1.26043	-4.93793
H	2.17454	0.48703	-5.24104
B	2.50975	1.11352	-1.49825
B	0.31618	1.67515	-1.73315
C	2.95929	2.25815	-0.46418
H	2.53089	3.21184	-0.82169
H	2.53716	2.10358	0.54337
C	4.49519	2.41988	-0.35713
H	4.93064	1.54281	0.16174
H	4.93313	2.43235	-1.37462
C	4.92964	3.69489	0.38931
H	4.48314	3.69140	1.40115
H	4.50707	4.57658	-0.13194
C	6.45539	3.84382	0.49867
H	6.74000	4.77152	1.02574
H	6.89912	2.99700	1.05253
H	6.92884	3.86859	-0.49967
P	-3.21638	0.25229	0.52275
C	-3.69981	1.80105	1.40786
C	-4.89841	1.88965	2.14932
C	-2.89969	2.94583	1.23076
C	-5.29453	3.11612	2.70277
H	-5.51697	1.00100	2.30852
C	-3.30794	4.17208	1.78168
H	-1.96698	2.87131	0.66299
C	-4.50208	4.26035	2.51471
H	-6.22163	3.17649	3.28224
H	-2.68905	5.06320	1.63620
H	-4.81348	5.21918	2.94201
C	-4.23902	0.26712	-1.01786
C	-3.58684	0.33681	-2.26315
C	-5.64986	0.25238	-0.96179
C	-4.34927	0.36345	-3.44522
H	-2.49261	0.38076	-2.30488
C	-6.40196	0.28394	-2.14434
H	-6.16472	0.21202	0.00336
C	-5.75099	0.33317	-3.38901
H	-3.83983	0.41112	-4.41261
H	-7.49560	0.26852	-2.09394
H	-6.33756	0.35303	-4.31342
C	-3.92627	-1.10426	1.56609
C	-4.63897	-2.17671	0.99070
C	-3.75492	-1.06002	2.96745
C	-5.18495	-3.18181	1.80623
H	-4.77712	-2.22400	-0.09314
C	-4.30422	-2.06414	3.77833
H	-3.20229	-0.23354	3.42387
C	-5.02180	-3.12497	3.19897
H	-5.74025	-4.00753	1.34975
H	-4.17396	-2.01633	4.86437
H	-5.45416	-3.90511	3.83417
O	-1.69907	0.19621	0.19016

A'

SCF (BP86) Energy = -2997.29640791
Enthalpy 0K = -2995.933628
Energy 298K = -2995.850452
Free Energy 298K = -2996.052370
Lowest Frequency = 8.9201 cm^{-1}
Second Frequency = 19.1772 cm^{-1}
SCF (BP86-D3BJ) Energy = -2997.75065538
SCF (Toluene) Energy = -2997.30767729
SCF (BS2) Energy = -3532.10506432

Mg	0.92781	0.18294	0.03875
O	-0.76270	3.79037	-1.64403
O	0.32881	2.11030	-0.49581
O	-3.37616	1.08062	-0.94884
O	-3.48141	3.43514	-0.68283
N	1.94916	-0.23504	1.89140
N	2.51122	-0.59386	-1.14362
C	3.14835	-2.04540	3.15175
H	3.02090	-1.40334	4.03330
H	4.21709	-2.29180	3.03884
H	2.61973	-2.99833	3.32870
C	2.61610	-1.40383	1.87414
C	2.89850	-2.16074	0.70111
H	3.27913	-3.16479	0.90720
C	2.94799	-1.78446	-0.65748
C	3.51761	-2.82699	-1.61549
H	4.23887	-2.39358	-2.32361
H	2.69655	-3.24654	-2.22459
H	3.99966	-3.65446	-1.07420
C	3.07372	-0.17675	-2.40537
C	4.41569	0.33247	-2.43434
C	4.96231	0.73873	-3.66660
H	5.98849	1.12110	-3.69312
C	4.22578	0.67181	-4.85501
H	4.66995	0.99710	-5.80171
C	2.91756	0.18283	-4.81724
H	2.34132	0.11693	-5.74700

C	2.32474	-0.25498	-3.61461
C	0.92224	-0.85967	-3.67989
H	0.61376	-1.11634	-2.65002
C	0.91817	-2.16741	-4.50844
H	1.16201	-1.96731	-5.56697
H	-0.07881	-2.63992	-4.47707
H	1.66021	-2.89314	-4.13399
C	-0.10883	0.13154	-4.25901
H	0.19548	0.49578	-5.25573
H	-0.24834	1.00828	-3.60644
H	-1.08879	-0.35877	-4.37191
C	5.28402	0.44636	-1.17403
H	4.60803	0.36821	-0.30451
C	6.32104	-0.69874	-1.06689
H	6.98093	-0.71137	-1.95288
H	5.84626	-1.68760	-0.98216
H	6.95772	-0.55633	-0.17574
C	6.02959	1.79803	-1.08483
H	6.82870	1.87493	-1.84317
H	6.51499	1.89638	-0.09799
H	5.35378	2.65619	-1.22351
C	1.83700	0.49178	3.14227
C	2.79614	1.50510	3.45836
C	2.60574	2.28632	4.61535
H	3.33427	3.06759	4.85551
C	1.51720	2.07862	5.46834
H	1.38037	2.70532	6.35572
C	0.62274	1.04219	5.18906
H	-0.20661	0.84829	5.87773
C	0.76431	0.22644	4.04831
C	4.07794	1.69988	2.64344
H	3.90914	1.25074	1.64817
C	5.25964	0.93945	3.29541
H	5.46234	1.33614	4.30615
H	6.17805	1.05965	2.69361
H	5.05551	-0.13764	3.39343
C	4.47516	3.17977	2.45348
H	3.64178	3.78809	2.06924
H	5.31518	3.25814	1.74217
H	4.81319	3.63400	3.40137
C	-0.18348	-0.96845	3.90021
H	0.00392	-1.42062	2.90999
C	-1.67437	-0.58310	3.97506
H	-2.30816	-1.47368	3.82459
H	-1.94292	0.16017	3.21069
H	-1.93086	-0.16251	4.96327
C	0.10872	-2.02962	4.99234
H	1.15399	-2.37491	4.98440
H	-0.54865	-2.90935	4.86482
H	-0.09644	-1.61540	5.99514
C	-4.62965	3.03615	-1.42293
C	-4.90646	4.09738	-2.50785
H	-5.73925	3.80350	-3.17329
H	-4.00952	4.28503	-3.11716
H	-5.18256	5.04908	-2.02191
C	-5.86196	2.96821	-0.48747
H	-5.95926	3.93289	0.03877
H	-5.74055	2.17971	0.27191
H	-6.80065	2.78416	-1.04180
C	-4.22940	1.60838	-1.98105
C	-3.43571	1.73618	-3.30217
H	-2.59764	2.44187	-3.18721
H	-4.07162	2.08321	-4.13545
H	-3.01852	0.75496	-3.58275
C	-5.41166	0.64787	-2.18697
H	-6.13618	1.05755	-2.91351
H	-5.93952	0.45572	-1.24021
H	-5.05751	-0.32278	-2.57498
C	1.24175	3.31738	-0.50592
C	2.68395	2.88620	-0.71132
H	3.03895	2.27249	0.13171
H	3.32758	3.78241	-0.75253
H	2.82453	2.31833	-1.64131
C	1.05304	3.99818	0.85737
H	0.01393	4.33578	0.99548
H	1.71998	4.87147	0.95640
H	1.29114	3.28962	1.66768
C	0.64782	4.14329	-1.69489
C	0.75877	5.66469	-1.52242
H	0.30327	6.16246	-2.39378
H	1.81443	5.98348	-1.46135
H	0.22798	6.01050	-0.62347
C	1.19169	3.73547	-3.07481
H	1.19277	2.64292	-3.21142
H	2.21871	4.10506	-3.23570
H	0.54239	4.17563	-3.84873
B	-0.99306	2.61538	-0.95492
B	-2.62871	2.25363	-0.34772
C	-2.39495	2.15411	1.29465
H	-1.93083	1.17340	1.53846
H	-1.62149	2.89946	1.58106
C	-3.62437	2.42756	2.18630
H	-4.21774	3.22401	1.70117
H	-4.28165	1.53453	2.22138
C	-3.30934	2.87564	3.62715
H	-2.69539	3.79715	3.58246
H	-2.67734	2.12228	4.13449
C	-4.56653	3.14171	4.47160
H	-4.31627	3.48828	5.49028
H	-5.20350	3.91309	4.00259
H	-5.18096	2.22830	4.57236
P	-1.30936	-2.52161	-0.05942
C	-2.01299	-2.94664	-1.70533
C	-2.50496	-1.88434	-2.49114
C	-2.21904	-4.28366	-2.11104
C	-3.15867	-2.17112	-3.70151
H	-2.42162	-0.84851	-2.13391
C	-2.86769	-4.55544	-3.32474
H	-1.88174	-5.11385	-1.48354
C	-3.33041	-3.49872	-4.12553
H	-3.54454	-1.34692	-4.30989
H	-3.01574	-5.59349	-3.63971
H	-3.83928	-3.71031	-5.07166
C	-0.18798	-3.90024	0.44148
C	0.01255	-4.19844	1.80693
C	0.54219	-4.61398	-0.53297
C	0.89885	-5.21817	2.18629
H	-0.52683	-3.63936	2.57631
C	1.42784	-5.63268	-0.14918
H	0.41632	-4.37813	-1.59364
C	1.60217	-5.94180	1.20924
H	1.03373	-5.44972	3.24780
H	1.98084	-6.18560	-0.91517
H	2.28677	-6.74291	1.50649
C	-2.78420	-2.52809	1.03772
C	-3.62231	-1.39080	1.00040
C	-3.17085	-3.67442	1.76722
C	-4.82115	-1.40428	1.73124
H	-3.38230	-0.50976	0.38416
C	-4.36818	-3.66617	2.49911
H	-2.55069	-4.57532	1.76309
C	-5.19068	-2.52800	2.48774
H	-5.46811	-0.52225	1.69895
H	-4.65844	-4.55308	3.07194

H -6.12597 -2.52346 3.05743
O -0.59301 -1.12613 -0.08955

TS(A′-11)
SCF (BP86) Energy = -2997.28511710
Enthalpy 0K = -2995.921705
Energy 298K = -2995.839369
Free Energy 298K = -2996.038387
Lowest Frequency = -45.6116 cm^{-1}
Second Frequency = 13.5158 cm^{-1}
SCF (BP86-D3BJ) Energy = -2997.74665393
SCF (Toluene) Energy = -2997.29201775
SCF (BS2) Energy = -3532.09139033

Mg 0.58659 -0.21162 0.30726
O 2.22612 2.36570 -1.94712
O 2.41819 1.59468 0.21500
O -1.26112 2.68181 -1.32895
O 0.41425 4.10199 -0.47247
N 0.37962 -1.04188 2.31511
N 1.70962 -1.89605 -0.39828
C -0.02253 -3.16273 3.61777
H -0.08663 -2.52563 4.50858
H 0.77305 -3.91029 3.77538
H -0.96750 -3.72295 3.51257
C 0.26155 -2.38213 2.33395
C 0.42370 -3.23461 1.20477
H 0.07987 -4.25796 1.37929
C 1.15467 -3.06526 0.01110
C 1.33648 -4.32739 -0.82932
H 2.39915 -4.57289 -0.98157
H 0.90656 -4.17829 -1.83399
H 0.84057 -5.18987 -0.36034
C 2.78693 -2.04361 -1.34866
C 4.09792 -2.36736 -0.85903
C 5.13328 -2.58429 -1.78906
H 6.13446 -2.83470 -1.42444
C 4.91457 -2.49061 -3.16920
H 5.73475 -2.67039 -3.87257
C 3.64179 -2.15539 -3.63550
H 3.46826 -2.07141 -4.71435
C 2.56645 -1.92528 -2.75211
C 1.20859 -1.56271 -3.35642
H 0.49481 -1.42462 -2.52431
C 0.65923 -2.67847 -4.27720
H 1.30520 -2.81986 -5.16207
H -0.34826 -2.41143 -4.64109
H 0.59332 -3.65374 -3.76457
C 1.29249 -0.23723 -4.14637
H 2.01556 -0.31894 -4.97789
H 1.60330 0.60029 -3.50298
H 0.31175 0.00861 -4.58607
C 4.40503 -2.50331 0.64056
H 3.71011 -1.82738 1.17228
C 4.16304 -3.93608 1.18135
H 4.73697 -4.67504 0.59340
H 3.10075 -4.21870 1.16208
H 4.50384 -4.00471 2.22983
C 5.85390 -2.10314 1.00389
H 6.57986 -2.87043 0.67997
H 5.95329 -2.01686 2.09983
H 6.15798 -1.14366 0.55742
C 0.20155 -0.33632 3.56680
C 1.34506 0.20710 4.22741
C 1.16976 0.89631 5.44270
H 2.04346 1.31297 5.95211
C -0.09302 1.04595 6.02529
H -0.20612 1.58036 6.97436
C -1.20611 0.50215 5.38095
H -2.19744 0.61426 5.83447
C -1.09279 -0.18485 4.15511
C 2.75930 -0.03540 3.69742
H 2.70544 -0.05523 2.59302
C 3.27852 -1.41485 4.17033
H 3.30715 -1.45833 5.27380
H 4.30200 -1.59586 3.79661
H 2.63791 -2.23619 3.81344
C 3.76452 1.06089 4.10098
H 3.40761 2.06725 3.82544
H 4.73317 0.88793 3.60184
H 3.96761 1.05633 5.18668
C -2.38003 -0.74440 3.53972
H -2.10497 -1.27738 2.61312
C -3.37243 0.37966 3.16691
H -4.27990 -0.03974 2.69767
H -2.92945 1.09963 2.46345
H -3.69135 0.93727 4.06524
C -3.09025 -1.74352 4.48617
H -2.43201 -2.56573 4.80659
H -3.97483 -2.18360 3.99037
H -3.45376 -1.23465 5.39611
C -0.25289 4.85144 -1.50879
C 0.80588 5.53302 -2.39476
H 0.33854 6.11366 -3.21016
H 1.49482 4.79627 -2.82992
H 1.39465 6.23545 -1.77960
C -1.08469 5.95545 -0.81813
H -0.41529 6.55555 -0.17904
H -1.87288 5.53341 -0.17649
H -1.55502 6.63267 -1.55305
C -1.15008 3.77084 -2.26892
C -0.49189 3.26690 -3.57204
H 0.51004 2.85462 -3.38476
H -0.40872 4.07234 -4.32265
H -1.12289 2.47564 -4.00915
C -2.57575 4.24881 -2.60001
H -2.56374 5.10416 -3.29839
H -3.12617 4.54599 -1.69425
H -3.13384 3.42754 -3.08155
C 3.72843 2.24027 -0.09074
C 4.85877 1.34014 0.39312
H 4.80649 1.22227 1.48642
H 5.83936 1.78506 0.14766
H 4.80015 0.34604 -0.07086
C 3.70358 3.56740 0.68577
H 2.83366 4.17619 0.38912
H 4.62971 4.14589 0.52732
H 3.61666 3.35024 1.76291
C 3.66560 2.42028 -1.66005
C 4.19822 3.77239 -2.15546
H 4.08386 3.83233 -3.25062
H 5.27273 3.87795 -1.92333
H 3.65551 4.61655 -1.70734
C 4.33916 1.28972 -2.45092
H 3.97959 0.29750 -2.14244
H 5.43632 1.31823 -2.33760
H 4.10518 1.41557 -3.52054
B 1.51859 1.94857 -0.81938
B -0.15666 2.73868 -0.35940
C -0.54259 2.41145 1.19934
H -1.07395 1.43768 1.30526
H 0.39824 2.31681 1.77986
C -1.39119 3.52650 1.86097
H -1.00982 4.49216 1.48520

H	-2.44249	3.45653	1.51341
C	-1.36259	3.57855	3.39793
H	-0.31059	3.67245	3.73045
H	-1.72048	2.62552	3.82379
C	-2.18774	4.74153	3.97268
H	-2.13740	4.77498	5.07535
H	-1.82796	5.71465	3.59202
H	-3.25329	4.65443	3.69110
P	-2.60866	-1.21652	-0.93963
C	-2.81722	-1.18557	-2.76769
C	-2.25224	-0.09249	-3.45500
C	-3.64039	-2.10543	-3.45139
C	-2.49711	0.05922	-4.82936
H	-1.64852	0.64051	-2.90583
C	-3.86961	-1.94946	-4.82686
H	-4.10262	-2.94088	-2.91669
C	-3.29659	-0.86861	-5.51696
H	-2.06043	0.90907	-5.36416
H	-4.49972	-2.67084	-5.35730
H	-3.47995	-0.74511	-6.58937
C	-2.80633	-2.96527	-0.39150
C	-3.37604	-3.26885	0.86342
C	-2.29072	-4.00972	-1.18868
C	-3.44917	-4.59973	1.30229
H	-3.76620	-2.46754	1.49727
C	-2.36889	-5.33909	-0.74685
H	-1.82806	-3.78480	-2.15440
C	-2.95081	-5.63636	0.49630
H	-3.89961	-4.82504	2.27428
H	-1.97286	-6.14281	-1.37573
H	-3.01406	-6.67482	0.83763
C	-4.05143	-0.24030	-0.34800
C	-3.89738	1.16132	-0.27786
C	-5.31235	-0.83070	-0.11483
C	-5.00503	1.95518	0.06054
H	-2.93433	1.63783	-0.51322
C	-6.40807	-0.02437	0.22995
H	-5.44508	-1.91343	-0.20246
C	-6.25342	1.36864	0.32398
H	-4.88438	3.04175	0.11574
H	-7.38236	-0.48613	0.42102
H	-7.10961	1.99651	0.59240
O	-1.25288	-0.57293	-0.51314

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SCF (BP86) Energy = -2428.22000193
Enthalpy 0K = -2427.155010
Enthalpy 298K = -2427.086613
Free Energy 298K = -2427.262358
Lowest Frequency = 11.1260 cm^{-1}
Second Frequency = 12.3752 cm^{-1}
SCF (BP86-D3BJ) Energy = -2428.56495539
SCF (Toluene) Energy = -2428.22597178
SCF (BS2) Energy = -2962.88917904

B	-2.75717	-0.86481	0.22020
C	-2.08628	2.92149	-3.56019
H	-3.07429	3.09979	-3.10001
H	-2.23506	2.76146	-4.63839
H	-1.49928	3.84230	-3.41360
C	-1.41323	1.71975	-2.90663
C	-1.37814	0.53270	-3.68521
H	-1.89969	0.60459	-4.64397
C	-0.62206	-0.65924	-3.52124
C	-0.54037	-1.54103	-4.76428
H	-0.21920	-2.56574	-4.52605
H	0.17382	-1.12514	-5.49650
H	-1.52372	-1.57797	-5.26162
C	0.98691	-2.05329	-2.40017
C	2.27310	-1.83972	-2.98854
C	3.23874	-2.86354	-2.91108
H	4.22251	-2.69924	-3.36676
C	2.97102	-4.07952	-2.27189
H	3.73405	-4.86448	-2.22780
C	1.70846	-4.28525	-1.70128
H	1.48799	-5.24028	-1.21258
C	0.70487	-3.29842	-1.75479
C	-0.68207	-3.60863	-1.19263
H	-1.19314	-2.64694	-0.99453
C	-1.53627	-4.36887	-2.23495
H	-1.66287	-3.78618	-3.16193
H	-2.54141	-4.58412	-1.83013
H	-1.06515	-5.33248	-2.50125
C	-0.64738	-4.38572	0.13810
H	-0.32370	-5.43363	0.00107
H	-1.65581	-4.40038	0.58292
H	0.02988	-3.91170	0.86713
C	2.65984	-0.52829	-3.67717
H	1.76984	0.12272	-3.69673
C	3.75726	0.21185	-2.88061
H	3.43084	0.42278	-1.84962
H	4.01123	1.16994	-3.36834
H	4.68270	-0.38862	-2.82292
C	3.12275	-0.74906	-5.13605
H	4.06466	-1.32475	-5.17800
H	3.30656	0.21946	-5.63345
H	2.37305	-1.30098	-5.72685
C	-0.80534	3.12086	-1.05434
C	0.42702	3.83995	-1.16558
C	0.53171	5.11305	-0.57122
H	1.46580	5.67574	-0.67484
C	-0.53341	5.67535	0.14483
H	-0.43805	6.67323	0.58756
C	-1.71918	4.94642	0.28743
H	-2.54926	5.37507	0.86092
C	-1.88140	3.67397	-0.29668
C	-3.19840	2.92961	-0.07675
H	-3.16995	1.99079	-0.65484
C	-4.42360	3.74622	-0.54759
H	-4.56885	4.65522	0.06371
H	-5.34077	3.13832	-0.46165
H	-4.32596	4.06863	-1.59814
C	-3.36252	2.53983	1.40949
H	-2.54559	1.87608	1.73916
H	-4.31452	2.00181	1.55755
H	-3.36749	3.43100	2.06281
C	1.61752	3.26274	-1.93472
H	1.46454	2.16955	-1.98416
C	1.66340	3.79294	-3.38733
H	0.75197	3.52693	-3.94638
H	2.52745	3.36928	-3.92998
H	1.76226	4.89350	-3.40062
C	2.96603	3.52733	-1.23142
H	3.23387	4.59905	-1.23803
H	3.77718	2.98906	-1.74967
H	2.95185	3.19059	-0.18112
C	-4.43745	-1.98733	1.43055
C	-5.05776	-1.33335	0.13879
C	-5.29741	-2.33806	-1.00387
H	-5.53617	-1.77998	-1.92380
H	-6.13574	-3.02238	-0.78550
H	-4.39271	-2.93617	-1.19905
C	-6.32533	-0.50328	0.37287
H	-6.15459	0.30962	1.09480

H	-7.15056	-1.13535	0.74677
H	-6.65070	-0.04996	-0.57817
C	-4.78268	-3.46695	1.63700
H	-4.46000	-4.08362	0.78481
H	-5.86978	-3.60446	1.77672
H	-4.27859	-3.84710	2.54182
C	-4.72968	-1.19960	2.72097
H	-4.11337	-1.60703	3.53982
H	-5.78954	-1.27623	3.01973
H	-4.47178	-0.13516	2.60325
C	1.06349	-1.46707	3.04632
C	-0.29108	-1.85436	3.00666
H	-1.00027	-1.37609	2.32173
C	-0.73279	-2.89833	3.83434
H	-1.78101	-3.20695	3.78015
C	0.16112	-3.54694	4.70137
H	-0.19092	-4.36100	5.34387
C	1.51268	-3.16397	4.73435
H	2.21596	-3.67894	5.39702
C	1.96930	-2.12983	3.90308
H	3.02861	-1.85201	3.90815
C	1.50374	1.45650	3.03028
C	1.77298	1.43077	4.41537
H	2.02711	0.48818	4.91139
C	1.68938	2.61490	5.16319
H	1.89557	2.59354	6.23833
C	1.32705	3.81949	4.53628
H	1.25500	4.74018	5.12488
C	1.04515	3.84190	3.16102
H	0.74513	4.76939	2.66407
C	1.13303	2.66314	2.40346
H	0.89794	2.68017	1.33469
C	3.39179	-0.37517	1.62773
C	4.43210	0.30589	2.29171
H	4.19905	1.07346	3.03648
C	5.76934	0.00309	1.98783
H	6.57641	0.53541	2.50174
C	6.06843	-0.97318	1.02396
H	7.11219	-1.20625	0.78836
C	5.03093	-1.64582	0.35596
H	5.25373	-2.39934	-0.40548
C	3.69243	-1.35112	0.65232
H	2.88997	-1.86952	0.11697
Mg	-0.73193	-0.02742	-0.63139
N	-0.90817	1.82462	-1.66097
N	0.01070	-1.00628	-2.38488
O	-2.99316	-1.87464	1.18016
O	-3.98668	-0.43733	-0.31021
O	0.79325	0.09224	0.68931
P	1.61790	-0.06219	1.99948

B

SCF (BP86) Energy = -3204.96294345
Enthalpy 0K = -3203.626884
Energy 298K = -3203.540637
Free Energy 298K = -3203.763105
Lowest Frequency = -2.8909 cm^{-1}
Second Frequency = 3.4976 cm^{-1}
SCF (BP86-D3BJ) Energy = -3205.40170247
SCF (Toluene) Energy = -3204.97429330
SCF (BS2) Energy = -4074.65841376

Mg	2.13507	-0.72108	0.04390
O	-0.02941	-2.34524	-1.80313
O	-0.28101	-0.10370	-2.24599
N	3.87316	-1.93940	0.05992
N	1.84610	-0.98400	2.14395
C	6.08878	-2.39520	1.08625
H	6.06851	-3.49339	0.97670
H	6.64886	-2.14960	2.00085
H	6.63917	-2.00951	0.21185
C	4.67109	-1.83752	1.13456
C	4.27147	-1.25589	2.37498
H	5.07377	-1.17329	3.11369
C	2.97266	-0.99064	2.88612
C	2.89338	-0.71801	4.38542
H	2.20628	0.11814	4.59742
H	3.88847	-0.48583	4.79641
H	2.50350	-1.59246	4.93240
C	0.58142	-1.06767	2.82111
C	0.17422	-2.29682	3.43284
C	-1.07749	-2.36329	4.07378
H	-1.38070	-3.30443	4.54735
C	-1.94257	-1.26350	4.11458
H	-2.90734	-1.33131	4.62895
C	-1.55430	-0.07513	3.48799
H	-2.22644	0.79028	3.51061
C	-0.30752	0.04845	2.84362
C	0.04921	1.39793	2.22353
H	1.06297	1.31051	1.79302
C	0.09585	2.51151	3.29460
H	-0.89626	2.66586	3.75503
H	0.40968	3.46946	2.84543
H	0.80597	2.26789	4.10268
C	-0.92795	1.77545	1.08813
H	-1.96581	1.84700	1.45857
H	-0.90870	1.03307	0.27276
H	-0.66296	2.75737	0.65873
C	1.00965	-3.57757	3.35752
H	1.98363	-3.32838	2.90403
C	1.27893	-4.21077	4.74177
H	0.34520	-4.55757	5.21910
H	1.76223	-3.50481	5.43854
H	1.94047	-5.08865	4.63855
C	0.31184	-4.60315	2.43515
H	-0.67206	-4.89485	2.84433
H	0.92062	-5.51970	2.33908
H	0.14896	-4.18755	1.42795
C	4.32500	-2.72216	-1.06326
C	4.01083	-4.11185	-1.13033
C	4.48348	-4.86628	-2.22205
H	4.25382	-5.93723	-2.26481
C	5.22494	-4.28092	-3.25313
H	5.58598	-4.88666	-4.09143
C	5.47756	-2.90620	-3.20992
H	6.02969	-2.43328	-4.03034
C	5.03751	-2.10893	-2.13522
C	3.14118	-4.81086	-0.08489
H	2.82713	-4.04941	0.65011
C	3.91595	-5.91306	0.67220
H	4.25207	-6.71209	-0.01269
H	3.27464	-6.38195	1.43971
H	4.81005	-5.51067	1.17896
C	1.86578	-5.38474	-0.74606
H	1.26325	-4.58159	-1.20238
H	1.24181	-5.90531	0.00039
H	2.11833	-6.11649	-1.53403
C	5.29627	-0.60428	-2.18818
H	4.96507	-0.16665	-1.23109
C	4.44304	0.03276	-3.30991
H	4.61633	1.12142	-3.36223
H	3.36712	-0.13798	-3.13547
H	4.69821	-0.39719	-4.29506
C	6.79106	-0.26329	-2.37568

H	7.41406	-0.71506	-1.58430
H	6.94426	0.82910	-2.34680
H	7.17467	-0.62687	-3.34576
C	-1.08644	-0.80119	-3.26312
C	-0.26104	-0.77554	-4.56377
H	-0.81518	-1.21655	-5.41062
H	0.68884	-1.32082	-4.44145
H	-0.02269	0.27092	-4.81641
C	-2.40371	-0.04360	-3.46138
H	-2.19896	0.95195	-3.89255
H	-2.96218	0.10145	-2.52436
H	-3.05343	-0.58100	-4.17604
C	-1.22975	-2.24124	-2.64650
C	-1.20774	-3.38909	-3.66211
H	-0.27582	-3.39780	-4.24717
H	-2.06174	-3.31632	-4.35910
H	-1.28472	-4.35351	-3.13296
C	-2.44307	-2.38480	-1.71135
H	-3.39436	-2.39773	-2.27030
H	-2.48091	-1.56044	-0.98240
H	-2.35529	-3.33178	-1.15430
B	0.43105	-1.05710	-1.49192
P	-6.39838	0.52663	-0.47099
C	-7.71666	0.23549	-1.73888
C	-7.28084	-0.12016	-3.03135
C	-9.09542	0.36452	-1.47528
C	-8.21889	-0.36545	-4.04562
H	-6.20571	-0.18134	-3.22848
C	-10.03045	0.11515	-2.49302
H	-9.43928	0.67919	-0.48407
C	-9.59329	-0.25324	-3.77616
H	-7.87673	-0.63955	-5.04919
H	-11.10092	0.21853	-2.28585
H	-10.32441	-0.44321	-4.56914
C	-6.29188	-1.02382	0.53085
C	-5.06502	-1.27986	1.17787
C	-7.35713	-1.93807	0.66026
C	-4.91024	-2.43517	1.95882
H	-4.23242	-0.58061	1.05186
C	-7.19846	-3.09130	1.44616
H	-8.30084	-1.76207	0.13306
C	-5.97793	-3.33858	2.09587
H	-3.95229	-2.62435	2.45413
H	-8.02620	-3.80227	1.54135
H	-5.85561	-4.24231	2.70246
C	-7.07450	1.81722	0.67144
C	-6.67175	3.14799	0.44011
C	-7.94585	1.52342	1.73969
C	-7.15493	4.17910	1.25997
H	-5.96641	3.35414	-0.37152
C	-8.42961	2.55958	2.55503
H	-8.22877	0.48583	1.94822
C	-8.03761	3.88667	2.31353
H	-6.83787	5.21186	1.08021
H	-9.10416	2.32846	3.38632
H	-8.41225	4.69234	2.95386
O	-5.05914	0.93835	-1.09933
P	3.32830	2.69102	-0.15605
C	4.99326	3.13769	-0.83175
C	5.14552	3.52099	-2.18151
C	6.12893	3.07983	0.00456
C	6.41569	3.84565	-2.68381
H	4.27164	3.57489	-2.83727
C	7.39657	3.39775	-0.50422
H	6.02172	2.79780	1.05646
C	7.54145	3.78535	-1.84690
H	6.52325	4.14546	-3.73120
H	8.27137	3.35032	0.15222
H	8.53088	4.04138	-2.23971
C	2.10560	3.58464	-1.19511
C	1.01440	2.85035	-1.69936
C	2.23992	4.95819	-1.50480
C	0.04790	3.49715	-2.48696
H	0.91582	1.77743	-1.50426
C	1.26609	5.59492	-2.28783
H	3.11193	5.52412	-1.16003
C	0.16645	4.86536	-2.77401
H	-0.79500	2.91300	-2.86760
H	1.37125	6.65856	-2.52569
H	-0.59171	5.36555	-3.38585
C	3.33498	3.38331	1.55522
C	3.79531	2.53705	2.58714
C	2.97140	4.71373	1.84622
C	3.91038	3.03464	3.89532
H	4.04414	1.49144	2.36747
C	3.08241	5.19915	3.15838
H	2.58504	5.36738	1.05884
C	3.55923	4.36385	4.18172
H	4.26769	2.37593	4.69327
H	2.79061	6.23068	3.38099
H	3.64702	4.74622	5.20399
O	3.05999	1.15906	-0.11978

TS(B-C)

SCF (BP86) Energy = -3204.91745163
Enthalpy 0K = -3203.583095
Energy 298K = -3203.497501
Free Energy 298K = -3203.709877
Lowest Frequency = -219.2312 cm^{-1}
Second Frequency = 9.3553 cm^{-1}
SCF (BP86-D3BJ) Energy = -3205.39778279
SCF (Toluene) Energy = -3204.92639750
SCF (BS2) Energy = -4074.60758034

Mg	0.53503	0.39440	0.34295
O	-1.24771	-2.15904	1.78049
O	-0.63008	-2.75239	-0.38865
N	0.91887	1.76381	1.97804
N	0.57473	2.06253	-1.06485
C	2.54445	3.43422	2.85925
H	1.80821	3.93294	3.51079
H	3.24511	4.19285	2.47982
H	3.09730	2.73213	3.50652
C	1.85359	2.69648	1.71627
C	2.26581	3.06577	0.40759
H	3.12091	3.74626	0.37550
C	1.62675	2.88254	-0.84569
C	2.20046	3.72522	-1.98254
H	2.01758	3.25902	-2.96249
H	3.28541	3.85195	-1.84119
H	1.75238	4.73285	-2.00963
C	-0.22019	2.35004	-2.22715
C	-0.99172	3.55772	-2.28527
C	-1.74141	3.84086	-3.44206
H	-2.32218	4.76957	-3.48092
C	-1.77009	2.96762	-4.53486
H	-2.34978	3.21347	-5.43162
C	-1.04266	1.77613	-4.46240
H	-1.05414	1.08606	-5.31402
C	-0.26470	1.44975	-3.33300
C	0.54651	0.15717	-3.37873
H	1.06836	0.05229	-2.41030
C	1.62637	0.21717	-4.48422
H	1.16893	0.31714	-5.48471

H	2.23191	-0.70647	-4.48424
H	2.30274	1.07711	-4.34027
C	-0.36904	-1.07028	-3.56889
H	-0.95866	-0.99122	-4.49946
H	-1.06320	-1.17402	-2.72101
H	0.22791	-1.99522	-3.63512
C	-1.09787	4.53975	-1.11409
H	-0.37808	4.23444	-0.33680
C	-0.77557	5.99898	-1.51157
H	-1.52602	6.40391	-2.21380
H	0.21156	6.09480	-1.99404
H	-0.78040	6.64769	-0.61818
C	-2.51405	4.47110	-0.50069
H	-3.27776	4.77905	-1.23565
H	-2.59497	5.14428	0.37128
H	-2.76357	3.44795	-0.17771
C	0.46618	1.64760	3.34157
C	-0.66677	2.39912	3.77775
C	-1.07690	2.30153	5.12212
H	-1.93523	2.89344	5.45986
C	-0.41213	1.47496	6.03384
H	-0.74353	1.41752	7.07644
C	0.67512	0.71532	5.59161
H	1.18960	0.05042	6.29503
C	1.12955	0.78238	4.26012
C	-1.43857	3.33071	2.84196
H	-1.09130	3.12647	1.81398
C	-1.14413	4.81549	3.16125
H	-1.43288	5.06031	4.19933
H	-1.71208	5.48252	2.48860
H	-0.07384	5.05368	3.04505
C	-2.95924	3.06567	2.89425
H	-3.19007	2.01086	2.67222
H	-3.48666	3.69172	2.15546
H	-3.38253	3.30022	3.88719
C	2.28712	-0.12244	3.84087
H	2.54643	0.11856	2.79491
C	1.81659	-1.59252	3.88188
H	2.62359	-2.27325	3.55924
H	0.93960	-1.73591	3.22893
H	1.52471	-1.88397	4.90696
C	3.55255	0.06807	4.70624
H	3.90412	1.11443	4.70325
H	4.37256	-0.56725	4.32840
H	3.37140	-0.21510	5.75851
C	-0.41626	-3.92109	0.44694
C	1.08428	-4.01155	0.79427
H	1.30796	-4.89544	1.41667
H	1.40191	-3.10382	1.33125
H	1.67345	-4.09055	-0.13305
C	-0.82018	-5.18075	-0.33411
H	-0.18100	-5.28522	-1.22785
H	-1.86905	-5.14670	-0.66466
H	-0.68184	-6.08636	0.28340
C	-1.29971	-3.61286	1.71422
C	-0.76452	-4.18698	3.03554
H	0.24790	-3.82694	3.26508
H	-0.74685	-5.29153	3.00624
H	-1.42677	-3.88210	3.86324
C	-2.75923	-4.08255	1.55238
H	-2.83323	-5.18371	1.60770
H	-3.19480	-3.75989	0.59421
H	-3.37152	-3.65825	2.36332
B	-0.92425	-1.60693	0.48257
P	-3.76534	-0.84230	-0.35098
C	-4.62305	-1.30517	1.21239
C	-4.05551	-0.88609	2.43538
C	-5.83828	-2.02197	1.21386
C	-4.71406	-1.16354	3.64328
H	-3.08092	-0.39097	2.43738
C	-6.48091	-2.31121	2.42734
H	-6.27544	-2.36657	0.27155
C	-5.92515	-1.87627	3.64243
H	-4.26563	-0.83640	4.58681
H	-7.41876	-2.87684	2.42227
H	-6.43032	-2.10149	4.58768
C	-4.55199	0.73223	-0.85738
C	-4.33082	1.21966	-2.16923
C	-5.38528	1.46623	0.02034
C	-4.96254	2.39275	-2.59905
H	-3.66424	0.68316	-2.85163
C	-6.00475	2.64578	-0.41734
H	-5.56348	1.10214	1.03602
C	-5.80736	3.10658	-1.72990
H	-4.78104	2.75494	-3.61537
H	-6.65594	3.19852	0.26822
H	-6.30282	4.02118	-2.07207
C	-4.28075	-2.02923	-1.66988
C	-3.36434	-3.01587	-2.09261
C	-5.55216	-1.94347	-2.28434
C	-3.73386	-3.92396	-3.09883
H	-2.36276	-3.04653	-1.64088
C	-5.90949	-2.85476	-3.28926
H	-6.25504	-1.15823	-1.98824
C	-5.00292	-3.84968	-3.69462
H	-3.01829	-4.68638	-3.42468
H	-6.89644	-2.78448	-3.75902
H	-5.28312	-4.55674	-4.48277
O	-2.12020	-0.68386	-0.14137
P	3.91296	-0.64926	-0.59740
C	5.07801	-1.33312	0.66255
C	4.58347	-2.34428	1.51438
C	6.43743	-0.96330	0.74072
C	5.43419	-2.96448	2.44034
H	3.53289	-2.64146	1.44750
C	7.28342	-1.58513	1.67330
H	6.83719	-0.18922	0.07943
C	6.78486	-2.58418	2.52418
H	5.04044	-3.74674	3.09737
H	8.33545	-1.28686	1.73196
H	7.44734	-3.06867	3.24892
C	3.83532	-1.97508	-1.87631
C	2.59641	-2.58561	-2.14869
C	5.00767	-2.43456	-2.51515
C	2.53638	-3.64599	-3.07066
H	1.69054	-2.25150	-1.62973
C	4.93580	-3.48503	-3.44077
H	5.97635	-1.97780	-2.28546
C	3.69825	-4.09138	-3.71954
H	1.57274	-4.12312	-3.27601
H	5.84601	-3.83561	-3.93822
H	3.64350	-4.91629	-4.43772
C	4.78498	0.79056	-1.34586
C	5.25549	1.81954	-0.49711
C	4.97225	0.90288	-2.74001
C	5.93320	2.92231	-1.03700
H	5.09294	1.75492	0.58251
C	5.64108	2.01536	-3.27497
H	4.60091	0.11988	-3.40677
C	6.12939	3.02137	-2.42599
H	6.30532	3.70827	-0.37182
H	5.78278	2.09209	-4.35775
H	6.65839	3.88390	-2.84443
O	2.49735	-0.37250	-0.00362

C

SCF (BP86) Energy = -3205.07974721
Enthalpy 0K = -3203.742409
Energy 298K = -3203.655586
Free Energy 298K = -3203.880885
Lowest Frequency = 3.1023 cm^{-1}
Second Frequency = 6.7670 cm^{-1}
SCF (BP86-D3BJ) Energy = -3205.52051569
SCF (Toluene) Energy = -3205.08979613
SCF (BS2) Energy = -4074.76690958

Mg	-1.91703	0.69641	0.36113
O	0.58129	2.52341	-1.88532
O	1.27199	0.39465	-2.53658
N	-3.39285	2.17413	0.37470
N	-1.58585	0.80426	2.42670
C	-5.57083	2.82881	1.37525
H	-5.40921	3.91920	1.32316
H	-6.17918	2.61001	2.26516
H	-6.14379	2.56007	0.47179
C	-4.23796	2.09269	1.41861
C	-3.96373	1.36498	2.61466
H	-4.80049	1.31948	3.31692
C	-2.73074	0.89091	3.13798
C	-2.73935	0.48467	4.60734
H	-2.17550	-0.45115	4.75849
H	-3.76914	0.35472	4.97451
H	-2.25262	1.24826	5.23667
C	-0.34228	0.66815	3.14019
C	0.21206	1.79080	3.83200
C	1.44778	1.64582	4.49066
H	1.87108	2.50771	5.01922
C	2.15200	0.43715	4.47445
H	3.11006	0.34551	4.99758
C	1.61470	-0.65126	3.78083
H	2.16195	-1.60034	3.75803
C	0.37533	-0.56318	3.11695
C	-0.15470	-1.80272	2.40145
H	-1.17436	-1.56939	2.04572
C	-0.26332	-3.01349	3.35475
H	0.73074	-3.33531	3.71237
H	-0.72427	-3.87217	2.83722
H	-0.87749	-2.77994	4.24099
C	0.71569	-2.14778	1.17259
H	1.75631	-2.36401	1.47055
H	0.73276	-1.31426	0.45073
H	0.32426	-3.04274	0.65706
C	-0.44493	3.17341	3.83438
H	-1.41964	3.09288	3.32411
C	-0.69798	3.71721	5.25926
H	0.24869	3.88369	5.80310
H	-1.31018	3.02922	5.86691
H	-1.22601	4.68572	5.21213
C	0.42264	4.17221	3.03506
H	1.41522	4.29715	3.50309
H	-0.05878	5.16554	2.99938
H	0.58033	3.82576	2.00112
C	-3.70427	3.09972	-0.68830
C	-3.21765	4.43825	-0.62487
C	-3.57058	5.33985	-1.64809
H	-3.21054	6.37340	-1.59090
C	-4.35499	4.94448	-2.73615
H	-4.62081	5.66266	-3.51937
C	-4.77275	3.61276	-2.82338
H	-5.35753	3.28660	-3.69116
C	-4.45885	2.67505	-1.82021
C	-2.28900	4.92386	0.48830
H	-2.06906	4.05887	1.13827
C	-2.94702	6.01830	1.35865
H	-3.19424	6.91294	0.75953
H	-2.26326	6.33714	2.16537
H	-3.88022	5.66263	1.82835
C	-0.95086	5.42059	-0.10807
H	-0.44972	4.61869	-0.67588
H	-0.27171	5.75927	0.69268
H	-1.10943	6.27536	-0.78954
C	-4.88901	1.22223	-2.01510
H	-4.65027	0.66772	-1.09160
C	-4.06880	0.58881	-3.16363
H	-4.36696	-0.46153	-3.32350
H	-2.98851	0.61197	-2.94220
H	-4.22970	1.13288	-4.11139
C	-6.40382	1.07452	-2.27738
H	-7.00309	1.53011	-1.47009
H	-6.68050	0.00840	-2.34611
H	-6.70429	1.55686	-3.22460
C	1.83673	1.33150	-3.49696
C	0.93013	1.30695	-4.74378
H	1.32553	1.94232	-5.55457
H	-0.08852	1.64920	-4.49708
H	0.86256	0.27220	-5.11897
C	3.25236	0.87909	-3.86814
H	3.21292	-0.09916	-4.37687
H	3.89399	0.77596	-2.98010
H	3.72725	1.59808	-4.55828
C	1.75945	2.70618	-2.71552
C	1.55105	3.93974	-3.60229
H	0.61343	3.87229	-4.17446
H	2.39023	4.06506	-4.30892
H	1.49952	4.84467	-2.97417
C	2.95837	2.92624	-1.77391
H	3.88291	3.15527	-2.33118
H	3.14335	2.03959	-1.14524
H	2.73613	3.77656	-1.10844
B	0.39614	1.13641	-1.69542
P	5.71769	-0.03942	-0.11374
C	6.96566	0.22158	-1.48713
C	7.42488	1.54495	-1.68134
C	7.42297	-0.78819	-2.35919
C	8.33548	1.84577	-2.70466
H	7.06410	2.34452	-1.02348
C	8.32499	-0.48286	-3.39290
H	7.07105	-1.81647	-2.22939
C	8.78652	0.83126	-3.56639
H	8.68570	2.87538	-2.83602
H	8.66901	-1.27822	-4.06339
H	9.48979	1.06633	-4.37242
C	6.84032	-0.15206	1.38278
C	6.22547	-0.00809	2.64686
C	8.23791	-0.33703	1.32224
C	6.98853	-0.06987	3.82287
H	5.14323	0.15776	2.70758
C	9.00117	-0.38874	2.50069
H	8.72942	-0.43428	0.34871
C	8.37898	-0.25873	3.75269
H	6.49832	0.04115	4.79622
H	10.08579	-0.53117	2.43872
H	8.97585	-0.29713	4.67025
C	5.23645	-1.83322	-0.35434
C	4.00100	-2.08352	-0.99214
C	6.01654	-2.92612	0.08173
C	3.56687	-3.40272	-1.20499
H	3.36821	-1.24788	-1.31458

C	5.57740	-4.24299	-0.12859
H	6.96609	-2.74294	0.59565
C	4.35312	-4.48353	-0.77446
H	2.60305	-3.58161	-1.69311
H	6.19128	-5.08239	0.21664
H	4.00870	-5.51140	-0.93256
O	-0.48568	0.57977	-0.86608
P	-3.33298	-2.46821	-0.35972
C	-5.01708	-2.68745	-1.09530
C	-5.19238	-2.90257	-2.47853
C	-6.14984	-2.61320	-0.25574
C	-6.48369	-3.04562	-3.01167
H	-4.32231	-2.96485	-3.13824
C	-7.43713	-2.74781	-0.79464
H	-6.02663	-2.46013	0.82083
C	-7.60600	-2.96845	-2.17217
H	-6.60965	-3.21551	-4.08576
H	-8.30941	-2.68787	-0.13593
H	-8.61181	-3.08153	-2.58966
C	-2.13570	-3.16532	-1.56311
C	-1.05161	-2.35000	-1.94620
C	-2.29522	-4.45180	-2.13081
C	-0.12557	-2.82828	-2.88960
H	-0.91821	-1.33849	-1.53183
C	-1.35663	-4.92266	-3.06046
H	-3.15952	-5.07394	-1.87453
C	-0.27189	-4.11092	-3.44023
H	0.69787	-2.16774	-3.18061
H	-1.48059	-5.91842	-3.49870
H	0.45087	-4.47955	-4.17617
C	-3.38799	-3.46594	1.19128
C	-3.79874	-2.79682	2.36502
C	-3.12080	-4.84902	1.22712
C	-3.96437	-3.51945	3.55709
H	-3.96820	-1.71409	2.34136
C	-3.28139	-5.56172	2.42577
H	-2.77207	-5.36967	0.33059
C	-3.71210	-4.90072	3.58772
H	-4.28288	-2.99831	4.46553
H	-3.06500	-6.63461	2.45137
H	-3.83911	-5.46043	4.52008
O	-3.02945	-0.98274	-0.00176

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SCF (BP86) Energy = -2503.58652475
Enthalpy 0K = -2502.515935
Enthalpy 298K = -2502.446716
Free Energy 298K = -2502.625057
Lowest Frequency = 8.4027 cm^{-1}
Second Frequency = 13.0097 cm^{-1}
SCF (BP86-D3BJ) Energy = -2503.93245599
SCF (Toluene) Energy = -2503.59346698
SCF (BS2) Energy = -3038.28081376

B	-3.24900	-0.34401	0.55714
C	-0.95883	-1.49745	-4.66561
H	-1.75961	-1.13598	-5.32833
H	-1.19470	-2.52284	-4.33961
H	-0.03157	-1.55638	-5.26296
C	-0.77751	-0.56281	-3.47717
C	-1.25500	0.76292	-3.65156
H	-1.81385	0.92547	-4.57658
C	-1.01432	1.93866	-2.89471
C	-1.52204	3.23938	-3.50435
H	-1.80482	3.10625	-4.55898
H	-0.77252	4.04333	-3.43305
H	-2.41195	3.59003	-2.95153
C	-0.00717	3.22004	-1.12860
C	1.28995	3.74504	-1.42504
C	1.66582	4.98362	-0.86751
H	2.64749	5.40359	-1.11381
C	0.81039	5.68973	-0.01162
H	1.11644	6.65669	0.40300
C	-0.43832	5.14538	0.30864
H	-1.10330	5.68685	0.99116
C	-0.87129	3.91925	-0.23409
C	-2.24510	3.37909	0.16636
H	-2.42381	2.45088	-0.40290
C	-2.27603	3.00847	1.66712
H	-1.49779	2.26810	1.90976
H	-3.24647	2.55894	1.93859
H	-2.11907	3.89909	2.30207
C	-3.37969	4.37451	-0.16676
H	-3.29220	5.30291	0.42560
H	-4.36242	3.92738	0.06218
H	-3.37682	4.66099	-1.23230
C	2.26661	3.00542	-2.34433
H	1.90592	1.96459	-2.42612
C	3.70072	2.96826	-1.77241
H	4.15402	3.97443	-1.72702
H	4.35111	2.34930	-2.41364
H	3.72466	2.54217	-0.75552
C	2.28194	3.61061	-3.76800
H	1.28913	3.56282	-4.24330
H	2.99163	3.06501	-4.41506
H	2.59453	4.67010	-3.74187
C	0.50160	-2.27504	-2.37561
C	1.79627	-2.39645	-2.96814
C	2.46261	-3.63558	-2.90211
H	3.45553	-3.73026	-3.35701
C	1.88415	-4.74566	-2.27349
H	2.41356	-5.70440	-2.24270
C	0.61559	-4.61850	-1.69561
H	0.15415	-5.48700	-1.21208
C	-0.09447	-3.40138	-1.73218
C	-1.49438	-3.34136	-1.11874
H	-1.83591	-2.29251	-1.14301
C	-2.50133	-4.17729	-1.94276
H	-2.55147	-3.83778	-2.99102
H	-3.51471	-4.09099	-1.51335
H	-2.22470	-5.24711	-1.94869
C	-1.49564	-3.79342	0.35706
H	-1.20307	-4.85363	0.46231
H	-2.50325	-3.68273	0.79230
H	-0.80611	-3.18704	0.96579
C	2.50171	-1.21294	-3.63435
H	1.77596	-0.38572	-3.70977
C	3.67579	-0.71811	-2.75984
H	3.32487	-0.40264	-1.76366
H	4.18264	0.13945	-3.23669
H	4.42705	-1.51484	-2.61550
C	2.99318	-1.54160	-5.06203
H	3.78999	-2.30645	-5.05459
H	3.41004	-0.63888	-5.54178
H	2.17733	-1.92094	-5.70066
C	0.80804	-1.33577	3.09898
C	-0.59119	-1.16338	3.05751
H	-1.06679	-0.55280	2.27508
C	-1.39414	-1.84024	3.98964
H	-2.47884	-1.70698	3.93105
C	-0.81037	-2.67427	4.95677
H	-1.44138	-3.19848	5.68269
C	0.58394	-2.85256	4.98758
H	1.03857	-3.51739	5.72950

C	1.39833	-2.18935	4.05694
H	2.48204	-2.34834	4.06639
C	3.38825	-1.32724	1.65978
C	3.33311	-2.38263	0.72353
H	2.41175	-2.58529	0.16798
C	4.47427	-3.16332	0.48977
H	4.42335	-3.97475	-0.24254
C	5.66747	-2.89718	1.18266
H	6.55650	-3.50883	0.99628
C	5.72469	-1.84224	2.10764
H	6.65687	-1.62591	2.63962
C	4.58789	-1.05339	2.34711
H	4.63826	-0.22096	3.05617
C	2.28196	1.20046	2.80270
C	2.59279	1.21836	4.17936
H	2.54892	0.29586	4.76793
C	2.92995	2.42982	4.80119
H	3.16972	2.44324	5.86942
C	2.94008	3.62337	4.05900
H	3.19324	4.56871	4.55037
C	2.60987	3.60810	2.69457
H	2.58805	4.53425	2.11256
C	2.28267	2.39846	2.06177
H	2.00553	2.38925	1.00337
C	-5.50554	-0.39690	0.03525
C	-5.28367	-0.90734	1.52129
C	-6.21474	-0.28105	2.56740
H	-6.10239	0.81304	2.60356
H	-5.97250	-0.67880	3.56748
H	-7.27127	-0.52058	2.35443
C	-5.33160	-2.44364	1.63298
H	-6.35451	-2.83752	1.50577
H	-4.96799	-2.74431	2.62963
H	-4.68098	-2.91203	0.87612
C	-5.98374	1.06718	-0.02643
H	-7.02757	1.17889	0.31383
H	-5.91793	1.41938	-1.06886
H	-5.34251	1.71561	0.59357
C	-6.42329	-1.27702	-0.82293
H	-6.03422	-2.30273	-0.90994
H	-6.49449	-0.85587	-1.83970
H	-7.44263	-1.32055	-0.40066
Mg	-0.40468	0.15345	-0.64154
N	-0.16237	-1.00281	-2.36174
N	-0.39487	1.95718	-1.69475
O	1.16034	-0.05850	0.57210
O	-1.93794	-0.14819	0.43971
O	-4.16658	-0.43942	-0.51695
O	-3.92290	-0.48999	1.79998
P	1.84694	-0.36368	1.93994

TS(9-D)

SCF (BP86) Energy = -2220.55559966
Enthalpy 0K = -2219.464203
Enthalpy 298K = -2219.398983
Free Energy 298K = -2219.561574
Lowest Frequency = -135.2496 cm^{-1}
Second Frequency = 16.4369 cm^{-1}
SCF (BP86-D3BJ) Energy = -2220.87424985
SCF (Toluene) Energy = -2220.56037645
SCF (BS2) Energy = -2420.33788036

Mg	-0.32142	0.19964	-0.27727
O	1.10101	-2.09990	2.39477
O	-0.20968	-0.24940	1.79385
O	2.44987	-1.96098	-0.81597
O	0.34966	-2.86043	-1.02158
N	0.40108	2.04054	-1.09514
N	-2.26708	0.45999	-1.09207
C	0.32569	3.81422	-2.86964
H	1.14792	4.28793	-2.31723
H	-0.48264	4.55107	-3.00746
H	0.69269	3.54904	-3.87644
C	-0.21582	2.57123	-2.16726
C	-1.42115	2.07954	-2.73280
H	-1.72253	2.59590	-3.64947
C	-2.41213	1.22666	-2.19949
C	-3.75034	1.28793	-2.93397
H	-4.37103	0.39762	-2.76376
H	-3.57905	1.40715	-4.01601
H	-4.33162	2.16544	-2.60066
C	-3.47500	-0.06272	-0.50421
C	-4.32669	0.80629	0.24519
C	-5.46640	0.26454	0.87191
H	-6.11634	0.92369	1.45875
C	-5.78759	-1.09107	0.75595
H	-6.67999	-1.49293	1.24764
C	-4.96278	-1.93010	-0.00364
H	-5.22608	-2.98720	-0.10229
C	-3.80272	-1.44740	-0.64264
C	-2.94506	-2.39413	-1.48870
H	-1.88308	-2.13119	-1.32924
C	-3.22192	-2.23590	-3.00368
H	-4.28815	-2.41616	-3.23100
H	-2.62766	-2.97025	-3.57611
H	-2.95376	-1.23431	-3.37070
C	-3.10303	-3.87806	-1.10248
H	-4.08632	-4.28184	-1.40493
H	-2.98422	-4.04187	-0.01899
H	-2.33368	-4.47535	-1.61873
C	-4.05439	2.30795	0.40050
H	-3.21965	2.57716	-0.26812
C	-5.27742	3.16417	-0.00505
H	-6.11824	3.03080	0.69826
H	-5.64672	2.90555	-1.01142
H	-5.01337	4.23605	-0.00115
C	-3.62280	2.66805	1.84035
H	-4.39440	2.37453	2.57439
H	-3.46496	3.75696	1.93746
H	-2.68108	2.16620	2.11727
C	1.57933	2.69550	-0.57684
C	1.45759	3.47895	0.61051
C	2.61085	4.06784	1.16171
H	2.52093	4.67359	2.06948
C	3.86740	3.90189	0.56853
H	4.75471	4.36534	1.01246
C	3.97589	3.14663	-0.60329
H	4.95695	3.02744	-1.07662
C	2.85429	2.53595	-1.20105
C	0.09395	3.75460	1.24569
H	-0.59870	2.96647	0.89804
C	-0.46972	5.10674	0.74645
H	0.19523	5.93783	1.04196
H	-1.46802	5.30009	1.17807
H	-0.56275	5.12584	-0.35182
C	0.11883	3.71768	2.78684
H	0.56163	2.77918	3.15844
H	-0.90728	3.79976	3.18573
H	0.69651	4.55720	3.21214
C	3.06698	1.75701	-2.50329
H	2.08998	1.35280	-2.82136
C	4.03051	0.56450	-2.31088
H	4.16378	0.02919	-3.26852
H	3.65126	-0.15505	-1.56995

H	5.02868	0.91067	-1.98817
C	3.60356	2.67210	-3.63188
H	2.96905	3.55753	-3.79589
H	3.66456	2.11233	-4.58186
H	4.62069	3.03263	-3.39677
C	1.23944	-3.76249	-1.77344
C	1.03885	-3.43631	-3.26414
H	1.61899	-4.11466	-3.91295
H	1.33350	-2.39800	-3.48653
H	-0.02837	-3.54818	-3.51634
C	0.82715	-5.20968	-1.48806
H	-0.18063	-5.40135	-1.89234
H	0.80782	-5.42004	-0.40859
H	1.52311	-5.91761	-1.97177
C	2.65928	-3.35889	-1.22779
C	3.78699	-3.39818	-2.26416
H	3.57714	-2.74660	-3.12525
H	3.94351	-4.42769	-2.63168
H	4.72783	-3.05792	-1.80155
C	3.07303	-4.13633	0.03461
H	3.25872	-5.20095	-0.18814
H	2.30505	-4.05720	0.82023
H	4.00353	-3.70367	0.43593
C	-0.86999	-0.89772	2.95694
C	-2.38583	-0.89613	2.79095
H	-2.78399	0.12866	2.83219
H	-2.84509	-1.46243	3.62018
H	-2.70854	-1.35212	1.84429
C	-0.47077	-0.07349	4.19375
H	0.61982	-0.08205	4.35102
H	-0.95841	-0.45773	5.10532
H	-0.79012	0.97093	4.04958
C	-0.22450	-2.34043	2.94223
C	-0.04214	-2.95270	4.33884
H	0.42695	-3.94562	4.24442
H	-1.01587	-3.08370	4.84206
H	0.60553	-2.33173	4.97529
C	-0.95800	-3.33682	2.03150
H	-1.05989	-2.95395	1.00573
H	-1.95494	-3.58890	2.43022
H	-0.36728	-4.26609	1.97770
B	1.11696	-0.89995	1.67268
B	1.08933	-1.75114	-0.57522
C	2.44500	-0.01238	1.69895
H	2.55932	0.62351	0.80403
H	2.27248	0.70454	2.53394
C	3.76113	-0.77000	1.96501
H	3.62270	-1.46528	2.81516
H	3.98931	-1.39839	1.08572
C	4.95397	0.15885	2.25356
H	4.72648	0.78100	3.14204
H	5.07291	0.86983	1.41350
C	6.27056	-0.60000	2.48289
H	7.10897	0.08682	2.69321
H	6.18747	-1.29647	3.33678
H	6.54495	-1.19940	1.59621

D

SCF (BP86) Energy = -2220.56913551
Enthalpy 0K = -2219.478107
Enthalpy 298K = -2219.411349
Free Energy 298K = -2219.580199
Lowest Frequency = 14.3165 cm^{-1}
Second Frequency = 17.9582 cm^{-1}
SCF (BP86-D3BJ) Energy = -2220.87954776
SCF (Toluene) Energy = -2220.57479419
SCF (BS2) Energy = -2420.35330441

Mg	0.32233	0.05980	-0.40496
O	-1.54899	0.56611	3.62572
O	-0.21797	-0.19885	1.88484
O	-1.76725	2.66086	-0.04460
O	-0.17843	3.10699	-1.64336
N	-0.36795	-1.63443	-1.53458
N	2.35332	-0.25679	-1.04354
C	-0.34979	-2.82155	-3.73955
H	-1.03052	-3.55462	-3.28318
H	0.44476	-3.35743	-4.28160
H	-0.92913	-2.25113	-4.48686
C	0.25270	-1.87364	-2.70552
C	1.48795	-1.29235	-3.09386
H	1.78374	-1.52003	-4.12176
C	2.48870	-0.64521	-2.33186
C	3.81868	-0.44950	-3.05125
H	4.29780	0.49978	-2.76776
H	3.67413	-0.46791	-4.14211
H	4.52946	-1.25402	-2.79456
C	3.55762	0.08915	-0.33532
C	4.37852	-0.94937	0.20865
C	5.50345	-0.59631	0.97953
H	6.12838	-1.39066	1.40437
C	5.84316	0.74198	1.20867
H	6.72314	0.99555	1.80956
C	5.05479	1.75125	0.64520
H	5.33344	2.80023	0.79898
C	3.91568	1.45582	-0.13062
C	3.13869	2.61096	-0.76673
H	2.25197	2.19550	-1.27428
C	3.99052	3.34293	-1.83128
H	4.87982	3.81780	-1.37902
H	3.39389	4.13387	-2.31765
H	4.34455	2.65655	-2.61857
C	2.63120	3.62507	0.27997
H	3.46009	4.08119	0.85022
H	1.94110	3.15145	0.99861
H	2.07690	4.43488	-0.22248
C	4.08310	-2.43737	-0.01432
H	3.20605	-2.51256	-0.67899
C	5.26464	-3.16671	-0.69644
H	6.15421	-3.19216	-0.04237
H	5.56399	-2.67916	-1.63907
H	4.99178	-4.21158	-0.92616
C	3.72923	-3.15478	1.30770
H	4.56350	-3.10349	2.02974
H	3.50892	-4.22175	1.12610
H	2.84516	-2.70352	1.78730
C	-1.57772	-2.34939	-1.22792
C	-1.51389	-3.42907	-0.29228
C	-2.70289	-4.09129	0.06577
H	-2.66269	-4.91956	0.77995
C	-3.93813	-3.71601	-0.47827
H	-4.85269	-4.24420	-0.18847
C	-3.99035	-2.66556	-1.39950
H	-4.95565	-2.37588	-1.82984
C	-2.83081	-1.96640	-1.79379
C	-0.16980	-3.90044	0.26706
H	0.47778	-3.00702	0.35243
C	0.52857	-4.87259	-0.71463
H	-0.09759	-5.76638	-0.88565
H	1.49717	-5.20994	-0.30431
H	0.72195	-4.39895	-1.68957
C	-0.27364	-4.55480	1.65886
H	-0.83585	-3.92631	2.36914
H	0.73531	-4.72587	2.07244

H -0.77018 -5.54046 1.61308
C -2.97837 -0.83620 -2.81742
H -1.96867 -0.46608 -3.06582
C -3.77781 0.35525 -2.24269
H -3.94372 1.11479 -3.02794
H -3.24391 0.83697 -1.40837
H -4.76917 0.03270 -1.87849
C -3.64836 -1.32987 -4.12266
H -3.14349 -2.21584 -4.54149
H -3.63440 -0.53211 -4.88579
H -4.70503 -1.60218 -3.95262
C -1.16109 4.19277 -1.76496
C -1.98416 3.89902 -3.03245
H -2.71669 4.69764 -3.24209
H -2.52087 2.94178 -2.94286
H -1.29880 3.82354 -3.89247
C -0.40857 5.51741 -1.94068
H 0.18433 5.48446 -2.86972
H 0.27942 5.71556 -1.10512
H -1.11332 6.36423 -2.01879
C -1.98709 4.06566 -0.42654
C -3.49620 4.29605 -0.56735
H -3.94911 3.60062 -1.28953
H -3.70993 5.32928 -0.89370
H -3.98762 4.14125 0.40760
C -1.43451 4.92599 0.72409
H -1.61223 6.00207 0.55463
H -0.35232 4.76561 0.85667
H -1.93932 4.63728 1.66052
C 0.64939 -0.11222 3.10983
C 2.03852 0.38260 2.73542
H 2.57753 -0.35472 2.12122
H 2.63426 0.54349 3.65047
H 2.00631 1.33159 2.18160
C 0.70773 -1.53081 3.69303
H -0.28753 -1.87316 4.02021
H 1.39527 -1.57770 4.55364
H 1.07390 -2.22814 2.92417
C -0.17281 0.88009 4.00654
C -0.02201 0.65371 5.51401
H -0.65144 1.37620 6.05835
H 1.02371 0.80811 5.83065
H -0.33501 -0.35890 5.80884
C 0.06085 2.35883 3.65422
H -0.04922 2.53080 2.57070
H 1.05923 2.70124 3.97305
H -0.69546 2.96950 4.17320
B -1.53971 0.06512 2.34276
B -0.63196 2.16298 -0.71059
C -2.86120 -0.16500 1.53490
H -2.95811 0.71527 0.86573
H -2.77929 -1.04130 0.86709
C -4.12365 -0.27883 2.42161
H -4.04483 -1.17512 3.06793
H -4.16773 0.58405 3.11268
C -5.43178 -0.35692 1.61609
H -5.37440 -1.21412 0.91835
H -5.51923 0.54644 0.98135
C -6.68031 -0.48860 2.50198
H -7.60438 -0.53879 1.90043
H -6.63608 -1.40218 3.12180
H -6.77606 0.37084 3.18965

E
SCF (BP86) Energy = -1651.45464809
Enthalpy 0K = -1650.660452
Energy 298K = -1650.611955
Free Energy 298K = -1650.745687
Lowest Frequency = 12.0457 cm^{-1}
Second Frequency = 14.6873 cm^{-1}
SCF (BP86-D3BJ) Energy = -1651.66661971
SCF (Toluene) Energy = -1651.46147315
SCF (BS2) Energy = -1851.09994995

Mg 0.00022 -0.20716 -0.00034
O 0.07130 2.85693 1.14925
O -0.07424 2.85648 -1.15121
N -1.50049 -1.61801 0.01359
N 1.50215 -1.61678 -0.01289
C -2.47650 -3.89532 0.02029
H -3.10506 -3.72554 0.91133
H -2.15520 -4.94693 0.01097
H -3.12594 -3.71571 -0.85364
C -1.28561 -2.94966 0.01130
C 0.00158 -3.54358 0.00115
H 0.00204 -4.63614 0.00166
C 1.28828 -2.94860 -0.00935
C 2.47992 -3.89334 -0.01699
H 3.10873 -3.72396 -0.90792
H 2.15944 -4.94520 -0.00677
H 3.12883 -3.71235 0.85704
C -2.84904 -1.10895 0.02548
C -3.48200 -0.81666 1.26838
C -2.78645 -1.07402 2.60688
H -1.86045 -1.63768 2.39612
C -2.38221 0.25927 3.28013
H -1.73919 0.87314 2.62548
H -1.83606 0.07183 4.22166
H -3.27472 0.86278 3.52348
C -3.64265 -1.93136 3.56504
H -3.08123 -2.15192 4.48970
H -3.93208 -2.89178 3.10521
H -4.57059 -1.41026 3.85944
C -4.76525 -0.23688 1.25184
H -5.25912 -0.00675 2.20273
C -5.41743 0.05630 0.04817
H -6.41595 0.50617 0.05698
C -4.77971 -0.22163 -1.16674
H -5.28482 0.02034 -2.10877
C -3.49661 -0.80066 -1.20591
C -2.81784 -1.04194 -2.55588
H -1.88431 -1.59935 -2.36208
C -3.68076 -1.90072 -3.50682
H -4.61892 -1.38689 -3.78097
H -3.95233 -2.86787 -3.05020
H -3.13271 -2.10780 -4.44256
C -2.43504 0.29920 -3.22617
H -1.89894 0.12160 -4.17539
H -1.79078 0.91713 -2.57662
H -3.33694 0.89396 -3.45638
C 2.85034 -1.10676 -0.02489
C 3.49730 -0.79656 1.20631
C 2.81839 -1.03688 2.55640
H 1.88532 -1.59519 2.36301
C 2.43442 0.30468 3.22517
H 1.89843 0.12772 4.17457
H 1.78966 0.92133 2.57490
H 3.33581 0.90046 3.45475
C 3.68174 -1.89405 3.50840
H 4.61949 -1.37926 3.78219
H 3.95411 -2.86147 3.05282
H 3.13367 -2.10057 4.44426
C 4.77999 -0.21659 1.16687
H 5.28460 0.02684 2.10879

C	5.41788	0.06037	-0.04814
H	6.41606	0.51099	-0.05721
C	4.76629	-0.23471	-1.25169
H	5.26030	-0.00528	-2.20269
C	3.48349	-0.81543	-1.26797
C	2.78847	-1.07472	-2.60634
H	1.86315	-1.63941	-2.39532
C	3.64596	-1.93157	-3.56378
H	3.08498	-2.15355	-4.48837
H	3.93667	-2.89127	-3.10325
H	4.57322	-1.40940	-3.85845
C	2.38253	0.25755	-3.28061
H	1.73856	0.87099	-2.62649
H	1.83681	0.06868	-4.22210
H	3.27426	0.86209	-3.52421
B	-0.00097	2.06807	-0.00087
C	0.26139	4.26020	0.74192
C	-0.26622	4.25960	-0.74433
C	-0.52143	5.15156	1.71172
H	-0.10486	5.04895	2.72740
H	-0.44598	6.21380	1.41952
H	-1.58518	4.87368	1.75176
C	1.76932	4.54706	0.85856
H	2.09565	4.33127	1.88888
H	2.35024	3.90426	0.17764
H	2.00397	5.60203	0.63531
C	0.51539	5.15172	-1.71441
H	0.43852	6.21395	-1.42254
H	1.57951	4.87526	-1.75438
H	0.09894	5.04824	-2.73006
C	-1.77455	4.54440	-0.86109
H	-2.10054	4.32782	-1.89135
H	-2.35463	3.90105	-0.17998
H	-2.01062	5.59914	-0.63821

TS(11-F)

SCF (BP86) Energy = -2428.16496127
Enthalpy 0K = -2427.101889
Energy 298K = -2427.035036
Free Energy 298K = -2427.205962
Lowest Frequency = -543.8482 cm^{-1}
Second Frequency = 14.1791 cm^{-1}
SCF (BP86-D3BJ) Energy = -2428.51462255
SCF (Toluene) Energy = -2428.17292045
SCF (BS2) Energy = -2962.82939725

Mg	-1.01004	0.01301	0.09097
O	0.48596	-1.46153	2.66338
O	0.73732	0.83528	2.87157
N	-1.95514	1.65049	-0.84713
N	-2.08040	-1.42424	-1.01222
C	-3.16943	2.66582	-2.76560
H	-3.98242	3.07980	-2.14420
H	-3.59075	2.36769	-3.73660
H	-2.45480	3.48852	-2.92515
C	-2.52162	1.48314	-2.05823
C	-2.61176	0.23658	-2.73814
H	-2.99477	0.30950	-3.75941
C	-2.52106	-1.09042	-2.24662
C	-3.02004	-2.17780	-3.19172
H	-2.35726	-3.05774	-3.16983
H	-3.08771	-1.80032	-4.22333
H	-4.02021	-2.53579	-2.89459
C	-2.07994	2.94608	-0.21338
C	-3.09721	3.14643	0.76625
C	-4.06231	2.04028	1.19323
H	-3.80418	1.12953	0.62391
C	-3.89947	1.72162	2.69688
H	-2.86680	1.40500	2.92246
H	-4.58456	0.91275	3.00230
H	-4.12396	2.60424	3.32130
C	-5.52737	2.39847	0.85550
H	-6.20583	1.57486	1.13962
H	-5.65868	2.59049	-0.22308
H	-5.85632	3.30238	1.39808
C	-3.22283	4.41026	1.37557
H	-4.01045	4.56337	2.12213
C	-2.37063	5.46851	1.04758
H	-2.48833	6.44626	1.52688
C	-1.35697	5.25634	0.10836
H	-0.67192	6.07568	-0.13753
C	-1.18515	4.01190	-0.52928
C	-0.00377	3.85296	-1.48767
H	-0.05478	2.84442	-1.93314
C	-0.01062	4.88528	-2.63854
H	0.11416	5.91490	-2.25906
H	-0.94724	4.86069	-3.22120
H	0.82330	4.68252	-3.33242
C	1.32080	3.95832	-0.69904
H	2.18684	3.81065	-1.36558
H	1.36645	3.20210	0.09996
H	1.42055	4.95118	-0.22552
C	-2.43183	-2.74158	-0.52735
C	-3.75704	-2.97411	-0.04333
C	-4.80925	-1.86657	0.05996
H	-4.37283	-0.94090	-0.35248
C	-5.16127	-1.60561	1.54265
H	-5.88348	-0.77503	1.63379
H	-4.26194	-1.35015	2.12704
H	-5.61796	-2.49760	2.00656
C	-6.09216	-2.17963	-0.74335
H	-6.59811	-3.08366	-0.36089
H	-5.88042	-2.34512	-1.81306
H	-6.80760	-1.34198	-0.66802
C	-4.10548	-4.26193	0.40549
H	-5.12275	-4.43957	0.77314
C	-3.18373	-5.31384	0.39709
H	-3.47535	-6.31116	0.74343
C	-1.88144	-5.07009	-0.04659
H	-1.15050	-5.88629	-0.04328
C	-1.47884	-3.79942	-0.50558
C	-0.03393	-3.62895	-0.97173
H	0.11605	-2.56174	-1.21638
C	0.25259	-4.45294	-2.24854
H	1.29578	-4.30192	-2.57573
H	-0.41358	-4.16973	-3.08205
H	0.11181	-5.53280	-2.06407
C	0.95952	-3.99623	0.15280
H	0.81475	-3.34977	1.03381
H	1.99722	-3.87915	-0.19950
H	0.83395	-5.04758	0.46783
B	0.31402	-0.21897	2.02038
C	1.20957	-1.23993	3.91790
C	0.90726	0.27862	4.21479
C	0.67580	-2.22739	4.96142
H	0.90953	-3.25908	4.64995
H	1.14418	-2.05506	5.94680
H	-0.41597	-2.14753	5.07114
C	2.70059	-1.51505	3.64927
H	2.80425	-2.52191	3.21270
H	3.11184	-0.78319	2.93476
H	3.30123	-1.47429	4.57496
C	2.03275	1.03907	4.92574
H	2.22285	0.61329	5.92691

H	2.97152	1.01339	4.35200
H	1.74063	2.09445	5.05877
C	-0.42120	0.49268	4.96567
H	-0.67231	1.56572	4.94686
H	-1.24096	-0.05894	4.47790
H	-0.35538	0.16996	6.01910
O	1.06307	-0.13890	0.36797
P	2.58152	-0.08254	-0.54749
C	3.81706	0.99779	0.30063
C	5.16744	1.02268	-0.12163
C	3.40887	1.81011	1.37894
C	6.08847	1.87065	0.51138
H	5.49956	0.37049	-0.93558
C	4.34045	2.65435	2.00779
H	2.37894	1.74810	1.75018
C	5.67459	2.69215	1.57399
H	7.13101	1.88576	0.17627
H	4.01670	3.27955	2.84630
H	6.39523	3.35225	2.06837
C	3.54473	-1.60760	-0.91417
C	3.49550	-2.24960	-2.17573
C	4.29826	-2.20795	0.12695
C	4.19083	-3.44863	-2.38818
H	2.92876	-1.80067	-2.99678
C	4.99046	-3.40490	-0.09550
H	4.34625	-1.73010	1.11007
C	4.94048	-4.03311	-1.35262
H	4.15531	-3.92269	-3.37501
H	5.57268	-3.84973	0.71850
H	5.48226	-4.96868	-1.52398
C	2.26450	0.64942	-2.21342
C	3.10503	1.62503	-2.79387
C	1.13031	0.20581	-2.93210
C	2.82147	2.13327	-4.07074
H	3.98146	1.98673	-2.24797
C	0.85504	0.71342	-4.21133
H	0.45322	-0.53703	-2.49538
C	1.69979	1.67761	-4.78459
H	3.48375	2.88662	-4.51065
H	-0.03373	0.36271	-4.74454
H	1.48233	2.07739	-5.78037

F

SCF (BP86) Energy = -2428.31094711
Enthalpy 0K = -2427.245123
Energy 298K = -2427.177011
Free Energy 298K = -2427.364509
Lowest Frequency = 2.6620 cm^{-1}
Second Frequency = 3.1129 cm^{-1}
SCF (BP86-D3BJ) Energy = -2428.61240846
SCF (Toluene) Energy = -2428.32231814
SCF (BS2) Energy = -2962.97465215

Mg	-3.01232	-0.22607	-0.36227
O	-1.99937	1.07562	2.51883
O	0.19472	1.43239	1.82391
N	-4.40099	0.66091	-1.54115
N	-3.77914	-2.09695	-0.48005
C	-6.29235	0.68099	-3.13745
H	-6.88335	1.43141	-2.58497
H	-6.98332	-0.01693	-3.63166
H	-5.73361	1.23608	-3.91032
C	-5.33946	-0.04750	-2.20460
C	-5.50056	-1.45222	-2.09214
H	-6.30160	-1.86930	-2.70672
C	-4.80734	-2.40271	-1.29988
C	-5.26933	-3.84698	-1.39779
H	-4.42779	-4.50844	-1.66541
H	-6.06636	-3.96397	-2.14606
H	-5.64623	-4.20439	-0.42409
C	-4.32447	2.09330	-1.70384
C	-5.05251	2.94211	-0.82182
C	-5.97267	2.38252	0.26557
H	-6.03284	1.28929	0.12080
C	-5.38749	2.63837	1.67481
H	-4.38148	2.20064	1.79633
H	-6.04364	2.20586	2.45087
H	-5.30359	3.72161	1.87375
C	-7.40884	2.94401	0.16471
H	-8.06155	2.46977	0.91823
H	-7.85059	2.76322	-0.83019
H	-7.43258	4.03300	0.34557
C	-4.88722	4.33565	-0.94222
H	-5.44083	4.99878	-0.26786
C	-4.02730	4.88749	-1.89905
H	-3.91230	5.97388	-1.97561
C	-3.30919	4.04120	-2.75247
H	-2.62771	4.47420	-3.49311
C	-3.43837	2.64114	-2.67551
C	-2.60108	1.75038	-3.59604
H	-2.97441	0.71622	-3.48624
C	-2.74633	2.13375	-5.08520
H	-2.34117	3.14032	-5.28934
H	-3.80158	2.12719	-5.40810
H	-2.19051	1.42177	-5.71972
C	-1.11384	1.76177	-3.16632
H	-0.51813	1.09176	-3.81148
H	-0.98357	1.43961	-2.11824
H	-0.69015	2.77780	-3.25592
C	-3.15946	-3.12472	0.32221
C	-3.67794	-3.41562	1.61692
C	-4.92296	-2.71446	2.16571
H	-5.37524	-2.13971	1.33845
C	-4.54568	-1.70924	3.27994
H	-5.44339	-1.18030	3.64653
H	-3.82037	-0.95319	2.93204
H	-4.09004	-2.23253	4.13954
C	-5.98748	-3.71214	2.67399
H	-5.62541	-4.28594	3.54502
H	-6.27367	-4.43849	1.89410
H	-6.89848	-3.17452	2.98970
C	-2.99337	-4.34828	2.41968
H	-3.37955	-4.57765	3.41921
C	-1.82775	-4.98020	1.96989
H	-1.30897	-5.70057	2.61114
C	-1.32604	-4.68073	0.69784
H	-0.40905	-5.16966	0.35069
C	-1.97260	-3.75727	-0.14638
C	-1.37322	-3.43498	-1.51706
H	-2.10656	-2.81159	-2.06032
C	-1.13349	-4.70301	-2.36639
H	-0.77386	-4.42759	-3.37304
H	-2.05635	-5.29667	-2.48374
H	-0.36990	-5.35877	-1.91272
C	-0.06934	-2.61336	-1.37270
H	-0.23316	-1.67104	-0.82111
H	0.34343	-2.36409	-2.36636
H	0.69839	-3.18929	-0.82646
B	-1.06907	0.94222	1.45461
C	-1.24225	1.44939	3.70927
C	0.03658	2.14489	3.08453
C	-2.11063	2.35840	4.58469
H	-2.98490	1.79678	4.95403
H	-1.54438	2.71767	5.46153

H	-2.47826	3.23026	4.02297
C	-0.90254	0.14957	4.46183
H	-1.83634	-0.38976	4.68957
H	-0.26860	-0.50908	3.84562
H	-0.37930	0.35032	5.41207
C	1.32280	1.98776	3.90251
H	1.22091	2.46389	4.89322
H	1.58380	0.92859	4.04648
H	2.16040	2.47433	3.37600
C	-0.19812	3.62824	2.74133
H	0.63994	3.98831	2.12286
H	-1.12897	3.75853	2.16487
H	-0.25468	4.25641	3.64652
O	-1.38088	0.41828	0.26255
P	6.88733	-0.32279	0.81128
C	5.63549	0.91569	0.17752
C	5.93256	1.96414	-0.71899
C	4.31531	0.78765	0.66448
C	4.92556	2.85582	-1.12447
H	6.95395	2.08468	-1.09468
C	3.30425	1.67127	0.25285
H	4.07767	-0.01232	1.37579
C	3.61416	2.70918	-0.64314
H	5.16887	3.66766	-1.81923
H	2.28505	1.55704	0.64030
H	2.83166	3.40653	-0.96137
C	8.50561	0.52521	0.39432
C	9.21703	0.34381	-0.81046
C	9.04893	1.37596	1.38295
C	10.43788	1.00584	-1.02345
H	8.81463	-0.32105	-1.58155
C	10.26248	2.04541	1.16494
H	8.51562	1.51035	2.33151
C	10.96173	1.85962	-0.03946
H	10.98026	0.85377	-1.96321
H	10.66783	2.70458	1.94028
H	11.91418	2.37365	-0.20733
C	6.81584	-1.65296	-0.50662
C	6.16108	-1.51196	-1.74810
C	7.43167	-2.88698	-0.19861
C	6.13310	-2.57792	-2.66313
H	5.66865	-0.56601	-1.99542
C	7.41331	-3.94673	-1.11777
H	7.92596	-3.01654	0.77156
C	6.76096	-3.79491	-2.35296
H	5.61854	-2.45485	-3.62257
H	7.89944	-4.89536	-0.86519
H	6.73688	-4.62449	-3.06769

G

SCF (BP86) Energy = -2997.33241049
Enthalpy 0K = -2995.969546
Energy 298K = -2995.885630
Free Energy 298K = -2996.095517
Lowest Frequency = 4.1733 cm^{-1}
Second Frequency = 9.5333 cm^{-1}
SCF (BP86-D3BJ) Energy = -2997.75644120
SCF (Toluene) Energy = -2997.34230932
SCF (BS2) Energy = -3532.14042606

Mg	2.61926	-0.25072	0.20705
O	-1.22350	0.43200	-0.98487
O	1.13535	-0.02492	-1.07422
O	-0.57642	1.26625	2.29143
O	1.26214	-0.04586	1.84363
N	4.12547	1.23730	0.26654
N	3.90854	-1.90586	0.44964
C	6.27733	1.95812	1.33112
H	6.25906	2.79474	0.61884
H	7.27198	1.48618	1.30713
H	6.13781	2.37490	2.34435
C	5.18972	0.93066	1.03171
C	5.42476	-0.34971	1.61176
H	6.28094	-0.36678	2.29376
C	4.97266	-1.64369	1.24632
C	5.84987	-2.77394	1.78222
H	5.37851	-3.76084	1.68677
H	6.08985	-2.58671	2.84229
H	6.81045	-2.80698	1.23992
C	3.81984	-3.23789	-0.11594
C	4.61360	-3.57399	-1.25520
C	4.51881	-4.87188	-1.79581
H	5.13191	-5.12927	-2.66688
C	3.66761	-5.83535	-1.24869
H	3.61199	-6.83919	-1.68267
C	2.88594	-5.49831	-0.13958
H	2.21784	-6.24941	0.29426
C	2.93988	-4.21569	0.44068
C	2.09249	-3.93784	1.68155
H	2.01859	-2.84143	1.78215
C	2.77111	-4.48958	2.95893
H	2.92561	-5.57969	2.87108
H	2.13895	-4.31173	3.84676
H	3.75309	-4.02577	3.14381
C	0.66066	-4.50614	1.57889
H	0.65367	-5.60944	1.62230
H	0.15884	-4.19885	0.64850
H	0.04784	-4.15224	2.42677
C	5.57113	-2.58862	-1.93098
H	5.48781	-1.61882	-1.41116
C	7.04277	-3.05594	-1.83374
H	7.19906	-3.99809	-2.38843
H	7.35208	-3.23236	-0.79078
H	7.71880	-2.29796	-2.26665
C	5.19388	-2.37023	-3.41404
H	5.25110	-3.31178	-3.98744
H	5.88659	-1.65377	-3.88876
H	4.16890	-1.97800	-3.52091
C	4.07502	2.51944	-0.41056
C	4.33762	2.55662	-1.81481
C	4.21917	3.77860	-2.50248
H	4.41672	3.80714	-3.57795
C	3.85954	4.95823	-1.84304
H	3.76662	5.89774	-2.39755
C	3.62886	4.92159	-0.46709
H	3.35898	5.84483	0.05739
C	3.73117	3.72528	0.27239
C	4.83179	1.32308	-2.57077
H	4.39670	0.43106	-2.08200
C	6.37126	1.21013	-2.44879
H	6.85663	2.10339	-2.88057
H	6.74657	0.32460	-2.99140
H	6.69222	1.12583	-1.39787
C	4.41418	1.30138	-4.05504
H	3.33395	1.48437	-4.17703
H	4.65116	0.32201	-4.50208
H	4.95588	2.06143	-4.64546
C	3.47397	3.80821	1.77818
H	3.65086	2.80719	2.20503
C	2.01277	4.21122	2.08410
H	1.85150	4.29300	3.17479
H	1.28792	3.48775	1.67793
H	1.77537	5.19571	1.64526
C	4.43714	4.79970	2.47560

H	5.49405	4.58020	2.25427
H	4.29992	4.76295	3.57089
H	4.24125	5.83793	2.15570
C	1.17771	0.02569	3.34134
C	2.26155	0.99874	3.81413
H	2.29524	1.03996	4.91598
H	2.08463	2.01380	3.43434
H	3.24704	0.65225	3.45724
C	1.43618	-1.35516	3.93866
H	2.47508	-1.66672	3.74510
H	0.75702	-2.11781	3.53321
H	1.29761	-1.31607	5.03344
C	-0.29726	0.55291	3.54111
C	-0.46506	1.53852	4.70271
H	0.16467	2.43150	4.57532
H	-0.21346	1.06097	5.66554
H	-1.51587	1.86617	4.75192
C	-1.34718	-0.56825	3.64441
H	-1.27269	-1.11285	4.60083
H	-1.25256	-1.28865	2.81587
H	-2.34965	-0.11715	3.57665
C	0.44643	-0.83859	-2.07857
C	1.11947	-2.20858	-2.17450
H	2.14528	-2.11752	-2.57187
H	0.55919	-2.86510	-2.86248
H	1.17649	-2.71669	-1.19927
C	0.54537	-0.11739	-3.43496
H	0.00137	0.83824	-3.41336
H	0.13413	-0.73934	-4.24827
H	1.60472	0.08789	-3.66181
C	-1.03333	-0.87590	-1.52483
C	-2.09052	-1.11114	-2.61746
H	-3.08580	-1.19207	-2.14977
H	-1.89592	-2.05167	-3.16458
H	-2.10390	-0.27813	-3.33690
C	-1.22653	-1.93099	-0.41275
H	-0.47167	-1.81370	0.38429
H	-1.16625	-2.96262	-0.80243
H	-2.23100	-1.79889	0.02032
B	0.04855	0.99166	-0.45850
B	0.21908	0.77726	1.27609
C	0.25522	2.51704	-0.99390
H	1.22808	2.94099	-0.67146
H	0.29826	2.50279	-2.10295
C	-0.87486	3.47670	-0.56830
H	-1.84763	3.04286	-0.87137
H	-0.91069	3.54781	0.53921
C	-0.75203	4.89700	-1.15069
H	-0.74010	4.83177	-2.25664
H	0.23126	5.32199	-0.86712
C	-1.87589	5.84606	-0.70454
H	-1.76519	6.85330	-1.14412
H	-2.86621	5.45787	-1.00319
H	-1.88854	5.96157	0.39464
P	-6.04596	-0.74244	-0.39267
C	-7.56532	-1.58089	0.25971
C	-7.37003	-2.79953	0.94049
C	-8.86997	-1.07456	0.09128
C	-8.46988	-3.49459	1.46606
H	-6.35364	-3.19668	1.03025
C	-9.96751	-1.77218	0.62149
H	-9.03157	-0.14805	-0.47030
C	-9.76794	-2.97937	1.31160
H	-8.31457	-4.44277	1.99177
H	-10.98019	-1.37745	0.48638
H	-10.62596	-3.52394	1.72002
C	-5.62018	0.58323	0.82191
C	-4.27967	1.02455	0.86187
C	-6.57317	1.14002	1.70062
C	-3.90500	2.02368	1.77565
H	-3.52334	0.59584	0.19299
C	-6.19244	2.14570	2.60336
H	-7.60651	0.77736	1.69351
C	-4.85937	2.58649	2.64046
H	-2.85918	2.34256	1.81265
H	-6.93558	2.57576	3.28366
H	-4.56283	3.36829	3.34855
C	-6.58866	0.12808	-1.93267
C	-6.41035	-0.55332	-3.15369
C	-7.15913	1.41674	-1.92484
C	-6.81662	0.04491	-4.35584
H	-5.93559	-1.53979	-3.14757
C	-7.56750	2.00958	-3.13076
H	-7.26388	1.96439	-0.98204
C	-7.39939	1.32359	-4.34476
H	-6.67230	-0.48445	-5.30363
H	-8.00582	3.01320	-3.12276
H	-7.71297	1.79054	-5.28451
O	-4.90692	-1.74476	-0.64092

TS(G-H)

SCF (BP86) Energy = -2997.28547065
Enthalpy 0K = -2995.922906
Energy 298K = -2995.840994
Free Energy 298K = -2996.039171
Lowest Frequency = -342.3941 cm^{-1}
Second Frequency = 8.4959 cm^{-1}
SCF (BP86-D3BJ) Energy = -2997.73978307
SCF (Toluene) Energy = -2997.29272996
SCF (BS2) Energy = -3532.08520790

Mg	1.61771	-0.15600	0.40253
O	-0.76583	1.68329	-2.52542
O	1.01822	0.75641	-1.28965
O	-1.88890	2.05773	1.23465
O	-0.09725	0.52656	1.32845
N	3.59599	0.45732	0.97741
N	1.97313	-2.25414	0.82061
C	5.27466	0.27173	2.84532
H	5.68418	1.21607	2.46475
H	6.07503	-0.48647	2.83610
H	4.98637	0.40894	3.90253
C	4.06072	-0.21568	2.05336
C	3.51709	-1.42937	2.55019
H	3.98180	-1.76117	3.48432
C	2.72755	-2.43342	1.92720
C	2.80826	-3.79094	2.62297
H	2.48277	-4.61281	1.97076
H	2.16053	-3.79151	3.51741
H	3.83517	-3.99225	2.96586
C	1.38719	-3.41860	0.17855
C	2.03570	-3.98581	-0.96697
C	1.40187	-5.03091	-1.66722
H	1.89084	-5.45440	-2.54891
C	0.17084	-5.55189	-1.25612
H	-0.30466	-6.36298	-1.81794
C	-0.41799	-5.05102	-0.09415
H	-1.35351	-5.49129	0.26830
C	0.17250	-4.00676	0.64888
C	-0.49720	-3.63436	1.97290
H	0.09670	-2.82659	2.43415
C	-0.52068	-4.83814	2.94881
H	-1.19370	-5.63144	2.57905
H	-0.89871	-4.52053	3.93654

H	0.47433	-5.28897	3.08921
C	-1.93565	-3.11997	1.77347
H	-2.55356	-3.86766	1.24710
H	-1.94929	-2.18566	1.19044
H	-2.42054	-2.92059	2.74356
C	3.44360	-3.56403	-1.39461
H	3.54939	-2.48725	-1.17363
C	4.51521	-4.30875	-0.56031
H	4.41695	-5.40123	-0.68970
H	4.43219	-4.08387	0.51380
H	5.52954	-4.01872	-0.88797
C	3.72498	-3.78830	-2.89521
H	3.82455	-4.86214	-3.13338
H	4.67668	-3.31074	-3.17875
H	2.93073	-3.37174	-3.53528
C	4.49257	1.42385	0.36731
C	5.57300	0.96082	-0.44930
C	6.44429	1.90016	-1.03717
H	7.27423	1.53904	-1.65446
C	6.27993	3.27237	-0.84591
H	6.96677	3.98703	-1.31140
C	5.22446	3.72127	-0.04718
H	5.09687	4.79588	0.10839
C	4.32518	2.82987	0.57126
C	5.86662	-0.51973	-0.70809
H	5.04312	-1.11444	-0.27680
C	7.18498	-0.96623	-0.03043
H	8.04966	-0.43543	-0.46696
H	7.34852	-2.04860	-0.17573
H	7.18568	-0.76321	1.05154
C	5.94866	-0.83004	-2.21966
H	5.02613	-0.54579	-2.75142
H	6.12453	-1.90747	-2.38061
H	6.78470	-0.29083	-2.69787
C	3.24685	3.40889	1.48928
H	2.36704	2.74167	1.41535
C	2.80238	4.83119	1.08921
H	1.91088	5.12349	1.66869
H	2.54861	4.90238	0.02029
H	3.58456	5.57789	1.31398
C	3.70251	3.43111	2.96886
H	3.90155	2.42361	3.36201
H	2.92639	3.89515	3.60298
H	4.62590	4.02758	3.07630
C	-0.44099	0.87707	2.72354
C	0.84493	1.05806	3.53389
H	0.60511	1.35636	4.56949
H	1.50482	1.82411	3.10457
H	1.40641	0.10742	3.58491
C	-1.25350	-0.27265	3.33329
H	-0.65829	-1.19718	3.30206
H	-2.19252	-0.44331	2.78745
H	-1.49530	-0.06499	4.38959
C	-1.30975	2.19251	2.54655
C	-0.48826	3.49333	2.63891
H	0.41539	3.45999	2.01716
H	-0.18580	3.70223	3.67981
H	-1.11084	4.33059	2.28477
C	-2.46282	2.31328	3.56082
H	-2.07898	2.39141	4.59340
H	-3.15294	1.45997	3.50770
H	-3.03416	3.23101	3.34292
C	1.29112	0.53673	-2.72044
C	1.91125	-0.84506	-2.90386
H	2.92307	-0.87045	-2.46612
H	2.01615	-1.07634	-3.97797
H	1.30476	-1.63986	-2.44145
C	2.28336	1.61376	-3.19522
H	1.83596	2.61802	-3.16286
H	2.61525	1.41555	-4.22900
H	3.17095	1.61033	-2.54082
C	-0.14704	0.68817	-3.35198
C	-0.13372	1.20956	-4.79883
H	-1.17104	1.29466	-5.16267
H	0.40423	0.51765	-5.47111
H	0.33075	2.20480	-4.86705
C	-0.96253	-0.61536	-3.28448
H	-0.98524	-1.00951	-2.25891
H	-0.56975	-1.38862	-3.96737
H	-2.00249	-0.39916	-3.57575
B	-0.17415	1.73624	-1.20555
B	-1.19690	1.10360	0.40093
C	0.20725	3.28204	-0.83274
H	0.58384	3.38409	0.19628
H	1.06318	3.55213	-1.48924
C	-0.93289	4.28923	-1.06973
H	-1.30627	4.16122	-2.10420
H	-1.77857	4.04340	-0.40099
C	-0.53055	5.76122	-0.86220
H	0.33565	6.00017	-1.51143
H	-0.17404	5.90232	0.17735
C	-1.67214	6.75033	-1.14837
H	-1.36104	7.79737	-0.98615
H	-2.01973	6.66369	-2.19368
H	-2.54217	6.55348	-0.49680
P	-3.82263	-0.13900	-0.05918
C	-4.65132	1.38235	-0.70764
C	-5.98725	1.70913	-0.38212
C	-3.94791	2.18607	-1.63220
C	-6.59969	2.83655	-0.95241
H	-6.55221	1.08469	0.31548
C	-4.57224	3.30622	-2.20079
H	-2.91801	1.93653	-1.91103
C	-5.89378	3.64015	-1.86147
H	-7.63364	3.08120	-0.68574
H	-4.01318	3.92436	-2.91075
H	-6.37262	4.51922	-2.30606
C	-4.10664	-1.39779	-1.39492
C	-3.22046	-2.48280	-1.55534
C	-5.23974	-1.30905	-2.23175
C	-3.47072	-3.46864	-2.52366
H	-2.32650	-2.55293	-0.93181
C	-5.48406	-2.29277	-3.20262
H	-5.92833	-0.46493	-2.12783
C	-4.60267	-3.37674	-3.34849
H	-2.76803	-4.30111	-2.63385
H	-6.36590	-2.20967	-3.84688
H	-4.79494	-4.14311	-4.10701
C	-4.94275	-0.73856	1.30546
C	-5.30274	-2.10453	1.42654
C	-5.27737	0.14321	2.36689
C	-5.99312	-2.56184	2.55809
H	-5.05891	-2.80378	0.62092
C	-5.97703	-0.31959	3.48896
H	-4.99987	1.19991	2.29634
C	-6.33593	-1.67581	3.59422
H	-6.27691	-3.61815	2.62425
H	-6.24359	0.38305	4.28623
H	-6.87737	-2.03734	4.47436
O	-2.04589	0.19997	-0.30872

H

SCF (BP86) Energy = -2295.93172227

Enthalpy 0K = -2294.834434

Energy 298K = -2294.769155
Free Energy 298K = -2294.934065
Lowest Frequency = 11.0147 cm^{-1}
Second Frequency = 16.2041 cm^{-1}
SCF (BP86-D3BJ) Energy = -2296.24915893
SCF (Toluene) Energy = -2295.93884723
SCF (BS2) Energy = -2495.73851316

Mg	-0.54090	0.23947	-0.07344
O	1.08937	-1.49104	2.73513
O	-0.08897	0.36521	1.89209
O	3.27014	-1.97071	-0.14657
O	2.14993	-0.95415	-1.91355
N	-0.69779	1.99897	-1.18094
N	-2.01011	-0.78939	-1.12206
C	-1.19363	3.15317	-3.34373
H	-1.12593	4.09382	-2.77841
H	-2.09782	3.17323	-3.97175
H	-0.32390	3.10863	-4.02267
C	-1.20490	1.93457	-2.42802
C	-1.78182	0.76982	-3.00056
H	-2.03880	0.87553	-4.05809
C	-2.20494	-0.44721	-2.41840
C	-2.91610	-1.41234	-3.35936
H	-3.74890	-1.93484	-2.86529
H	-2.20493	-2.18806	-3.69546
H	-3.29604	-0.89477	-4.25277
C	-2.76331	-1.89776	-0.58434
C	-4.03507	-1.62525	0.01570
C	-4.75869	-2.69306	0.57979
H	-5.73265	-2.49627	1.03908
C	-4.25908	-4.00139	0.56689
H	-4.83788	-4.81738	1.01248
C	-3.01614	-4.25554	-0.01896
H	-2.62577	-5.27937	-0.02949
C	-2.24843	-3.22633	-0.60242
C	-0.90814	-3.59339	-1.24585
H	-0.47282	-2.67108	-1.67106
C	-1.09777	-4.61088	-2.39660
H	-1.45305	-5.58394	-2.01388
H	-0.13981	-4.79034	-2.91513
H	-1.83169	-4.26315	-3.14257
C	0.09012	-4.15604	-0.20718
H	-0.32601	-5.04228	0.30367
H	0.35306	-3.41140	0.55924
H	1.02508	-4.47493	-0.70056
C	-4.63341	-0.21334	0.02132
H	-3.78606	0.49757	-0.00199
C	-5.48446	0.05320	-1.24460
H	-6.30798	-0.67920	-1.31977
H	-4.88567	-0.00805	-2.16583
H	-5.93088	1.06250	-1.20233
C	-5.48047	0.09247	1.27515
H	-6.43294	-0.46671	1.27320
H	-5.74128	1.16471	1.29858
H	-4.94787	-0.15149	2.20851
C	-0.22543	3.26079	-0.66042
C	-1.04907	3.96281	0.27321
C	-0.56464	5.15379	0.84479
H	-1.18850	5.69815	1.56024
C	0.69969	5.65829	0.51663
H	1.06097	6.58425	0.97629
C	1.49278	4.97136	-0.40582
H	2.47945	5.36931	-0.66837
C	1.05657	3.77567	-1.01249
C	-2.45974	3.47231	0.60671
H	-2.44485	2.36637	0.55358
C	-3.48157	3.95753	-0.44972
H	-3.51170	5.06117	-0.47896
H	-4.49613	3.59563	-0.20519
H	-3.22865	3.59639	-1.45874
C	-2.93942	3.86729	2.01741
H	-2.20079	3.60437	2.79323
H	-3.88602	3.35108	2.25303
H	-3.13894	4.95074	2.09526
C	1.98183	3.09948	-2.02810
H	1.46694	2.20758	-2.42443
C	3.29104	2.61881	-1.36621
H	3.95066	2.14748	-2.11603
H	3.08949	1.88405	-0.57114
H	3.84599	3.45954	-0.91436
C	2.31515	4.03763	-3.21340
H	1.40912	4.44294	-3.69242
H	2.89757	3.49684	-3.97989
H	2.92459	4.89691	-2.88238
C	3.22921	-1.73217	-2.52607
C	3.87019	-0.88559	-3.63092
H	4.72383	-1.41706	-4.08560
H	4.22405	0.08296	-3.24823
H	3.13017	-0.69046	-4.42453
C	2.58977	-2.98789	-3.14125
H	1.81591	-2.67889	-3.86273
H	2.10894	-3.61028	-2.37018
H	3.33366	-3.60357	-3.67399
C	4.18144	-2.04607	-1.28814
C	5.26551	-0.97734	-1.06529
H	4.83032	0.03414	-1.02853
H	6.03200	-1.00232	-1.85801
H	5.75993	-1.16720	-0.09924
C	4.81560	-3.44122	-1.30033
H	5.48195	-3.56318	-2.17155
H	4.05433	-4.23504	-1.32429
H	5.41905	-3.57800	-0.38827
C	-0.70215	0.03289	3.17387
C	-2.22369	0.13077	3.03787
H	-2.52456	1.17174	2.83332
H	-2.71558	-0.18006	3.97571
H	-2.60406	-0.51447	2.22978
C	-0.21249	1.06204	4.21023
H	0.87418	0.99490	4.36830
H	-0.71474	0.92028	5.18177
H	-0.44048	2.07713	3.84511
C	-0.16096	-1.44009	3.44032
C	0.11534	-1.73436	4.92688
H	0.50079	-2.76258	5.02534
H	-0.80440	-1.65701	5.53373
H	0.87238	-1.05177	5.34092
C	-1.09573	-2.53466	2.89137
H	-1.35998	-2.36849	1.83553
H	-2.03216	-2.61427	3.47026
H	-0.57228	-3.50238	2.95346
B	1.26911	-0.38106	1.83332
B	2.17900	-1.21738	-0.54400
C	2.59587	0.51631	2.11537
H	2.97201	0.98973	1.18609
H	2.30694	1.37343	2.75731
C	3.76045	-0.23152	2.79912
H	3.38540	-0.71023	3.72387
H	4.09408	-1.06411	2.15132
C	4.96384	0.66608	3.13818
H	4.62455	1.50581	3.77733
H	5.34564	1.13478	2.20908
C	6.10725	-0.08314	3.84126
H	6.95746	0.58297	4.07090

H 5.76513 -0.52908 4.79241
H 6.48920 -0.90846 3.21350
O 1.18338 -0.75756 0.27853

TS(H-I)
SCF (BP86) Energy = -2295.92347492
Enthalpy 0K = -2294.826719
Energy 298K = -2294.761692
Free Energy 298K = -2294.925822
Lowest Frequency = -45.8396 cm^{-1}
Second Frequency = 6.2262 cm^{-1}
SCF (BP86-D3BJ) Energy = -2296.24107548
SCF (Toluene) Energy = -2295.93027322
SCF (BS2) Energy = -2495.73202606

Mg -0.41050 0.17930 -0.09953
O 0.67742 -0.54463 3.60495
O -0.34491 0.75097 1.96512
O 2.93958 -2.47518 0.36814
O 2.29705 -1.38719 -1.58696
N -0.32010 1.79834 -1.42286
N -1.95744 -0.79479 -1.13674
C -0.40283 2.63818 -3.77839
H -0.23479 3.63710 -3.35105
H -1.23664 2.68817 -4.49625
H 0.50180 2.35955 -4.34696
C -0.68286 1.59342 -2.70377
C -1.33617 0.42404 -3.17304
H -1.45470 0.38617 -4.25955
C -1.95976 -0.64043 -2.48246
C -2.64881 -1.67236 -3.36909
H -3.54045 -2.10473 -2.89187
H -1.94962 -2.50464 -3.56688
H -2.93435 -1.24026 -4.34014
C -2.87186 -1.74450 -0.55120
C -4.17813 -1.28898 -0.17542
C -5.04994 -2.18829 0.46797
H -6.04929 -1.84972 0.75945
C -4.66478 -3.50584 0.74711
H -5.35612 -4.18726 1.25442
C -3.39605 -3.94566 0.35990
H -3.10209 -4.98247 0.55903
C -2.48564 -3.09426 -0.30069
C -1.15588 -3.68487 -0.78033
H -0.59454 -2.88268 -1.29155
C -1.40248 -4.82738 -1.79662
H -1.87845 -5.69688 -1.30955
H -0.44632 -5.17207 -2.22763
H -2.05929 -4.51328 -2.62450
C -0.28107 -4.20179 0.38389
H -0.83154 -4.92646 1.00970
H 0.07073 -3.37779 1.02156
H 0.61440 -4.71648 -0.00526
C -4.64728 0.13832 -0.48432
H -3.74651 0.78080 -0.48074
C -5.27682 0.24734 -1.89521
H -6.13366 -0.44299 -1.99242
H -4.55452 0.01320 -2.69081
H -5.64633 1.27320 -2.07119
C -5.64729 0.69829 0.55031
H -6.63715 0.21571 0.46418
H -5.80357 1.77681 0.37529
H -5.29921 0.56563 1.58732
C 0.25925 3.05755 -1.02644
C -0.56504 3.99180 -0.32460
C 0.01489 5.17883 0.15923
H -0.60669 5.90041 0.69823
C 1.37389 5.45744 -0.03584
H 1.80885 6.38331 0.35527
C 2.16544 4.54973 -0.74415
H 3.22439 4.77664 -0.91204
C 1.63644 3.34779 -1.25898
C -2.06550 3.73933 -0.15293
H -2.19881 2.64893 -0.01157
C -2.84934 4.12472 -1.43121
H -2.70926 5.19581 -1.66123
H -3.93039 3.94523 -1.29224
H -2.52159 3.54109 -2.30461
C -2.68698 4.45704 1.06146
H -2.11433 4.28214 1.98748
H -3.71968 4.10273 1.22305
H -2.74451 5.54903 0.90566
C 2.55985 2.44085 -2.07998
H 1.97624 1.57128 -2.42637
C 3.73671 1.89008 -1.24600
H 4.41739 1.30622 -1.88953
H 3.38144 1.22523 -0.44436
H 4.32418 2.70454 -0.78664
C 3.11408 3.18550 -3.31984
H 2.31394 3.63976 -3.92641
H 3.68192 2.49026 -3.96266
H 3.80221 3.99650 -3.02235
C 3.24663 -2.41081 -1.99310
C 4.18040 -1.82726 -3.06062
H 4.94735 -2.56308 -3.35927
H 4.68800 -0.91886 -2.70358
H 3.59752 -1.56209 -3.95854
C 2.43793 -3.57302 -2.59903
H 1.82826 -3.18740 -3.43269
H 1.75676 -4.01105 -1.85189
H 3.09147 -4.37228 -2.98804
C 3.95498 -2.79147 -0.62170
C 5.18435 -1.91520 -0.31646
H 4.94114 -0.84386 -0.40407
H 6.02935 -2.13992 -0.98944
H 5.50807 -2.10664 0.71971
C 4.32856 -4.27253 -0.47836
H 5.06420 -4.57242 -1.24494
H 3.44585 -4.92399 -0.56399
H 4.78044 -4.44461 0.51256
C -1.30311 0.63139 3.09732
C -2.72069 0.51821 2.55384
H -3.00439 1.44778 2.03297
H -3.43059 0.37374 3.38638
H -2.84068 -0.32903 1.86093
C -1.14609 1.91191 3.93450
H -0.13539 1.99103 4.36606
H -1.87957 1.94192 4.75695
H -1.31225 2.78798 3.28876
C -0.76014 -0.65031 3.83492
C -0.99193 -0.65248 5.35119
H -0.56475 -1.57118 5.78485
H -2.07063 -0.63660 5.58453
H -0.51036 0.20784 5.83932
C -1.25787 -1.96498 3.22192
H -1.13427 -1.97720 2.12913
H -2.32021 -2.14789 3.45421
H -0.66348 -2.79620 3.63351
B 0.91836 0.26044 2.50802
B 2.04759 -1.55013 -0.20267
C 2.29217 1.01236 2.34612
H 2.43262 1.38626 1.31814
H 2.19114 1.93016 2.96882
C 3.52753 0.22289 2.82555

H	3.33408	-0.16517	3.84407
H	3.66078	-0.66797	2.18441
C	4.82105	1.05682	2.84009
H	4.66420	1.96150	3.46096
H	5.03019	1.42753	1.81744
C	6.03869	0.28078	3.36567
H	6.95120	0.90197	3.36690
H	5.87099	-0.07049	4.39958
H	6.24177	-0.61033	2.74549
O	1.07287	-0.90376	0.45925

I

SCF (BP86) Energy = -2295.93401651
Enthalpy 0K = -2294.837658
Energy 298K = -2294.770999
Free Energy 298K = -2294.943304
Lowest Frequency = 8.2984 cm^{-1}
Second Frequency = 13.6700 cm^{-1}
SCF (BP86-D3BJ) Energy = -2296.24478231
SCF (Toluene) Energy = -2295.93942306
SCF (BS2) Energy = -2495.74466500

Mg	-0.21176	0.14614	-0.11824
O	0.01190	-1.75203	3.81917
O	-0.41203	-0.56337	1.88189
O	3.90129	-0.27977	-0.92628
O	3.19547	1.91157	-1.29012
N	-1.34721	1.81748	-0.63801
N	-1.03804	-1.05873	-1.61993
C	-1.37639	3.44400	-2.52858
H	-2.06921	4.06860	-1.94588
H	-1.69099	3.43920	-3.58311
H	-0.38392	3.92773	-2.47392
C	-1.27182	2.03042	-1.97155
C	-1.03640	1.00903	-2.92801
H	-0.92477	1.37027	-3.95409
C	-1.00620	-0.40517	-2.80117
C	-0.86205	-1.17218	-4.11110
H	-1.22795	-2.20557	-4.03233
H	0.20934	-1.22160	-4.37896
H	-1.38316	-0.66256	-4.93659
C	-1.25111	-2.48101	-1.59577
C	-2.58693	-2.99300	-1.66284
C	-2.78192	-4.38631	-1.58606
H	-3.80011	-4.78607	-1.64590
C	-1.70627	-5.26963	-1.43441
H	-1.88187	-6.34924	-1.37653
C	-0.40587	-4.75894	-1.35986
H	0.43966	-5.44746	-1.24945
C	-0.14952	-3.37530	-1.44089
C	1.29823	-2.88607	-1.40572
H	1.29652	-1.78330	-1.37722
C	2.07273	-3.31069	-2.67539
H	2.17494	-4.40953	-2.73477
H	3.08455	-2.87125	-2.65899
H	1.56509	-2.97472	-3.59504
C	2.05563	-3.36099	-0.14688
H	2.20985	-4.45521	-0.14607
H	1.50890	-3.10194	0.77627
H	3.04205	-2.87041	-0.10490
C	-3.80094	-2.07336	-1.83931
H	-3.47892	-1.05569	-1.55363
C	-4.27402	-2.02122	-3.31240
H	-4.57292	-3.02657	-3.65956
H	-3.48775	-1.65220	-3.98793
H	-5.14850	-1.35441	-3.41500
C	-4.99538	-2.47008	-0.94227
H	-5.45693	-3.41789	-1.27129
H	-5.78093	-1.69611	-0.99292
H	-4.70175	-2.59213	0.11279
C	-1.77904	2.88657	0.22339
C	-3.17632	3.07338	0.46680
C	-3.57956	4.08911	1.35596
H	-4.64866	4.24394	1.53939
C	-2.64603	4.90307	2.00898
H	-2.98166	5.68539	2.69820
C	-1.28148	4.70894	1.76869
H	-0.54760	5.34886	2.27201
C	-0.82189	3.71697	0.87951
C	-4.24185	2.22030	-0.22881
H	-3.72476	1.34544	-0.66344
C	-4.91729	2.98502	-1.39265
H	-5.41966	3.89616	-1.02141
H	-5.68007	2.35366	-1.88186
H	-4.18980	3.29099	-2.16079
C	-5.32369	1.70571	0.74729
H	-4.88191	1.20002	1.62169
H	-5.99057	0.98940	0.23638
H	-5.95826	2.52716	1.12384
C	0.68033	3.57790	0.63424
H	0.84437	2.77040	-0.09865
C	1.43405	3.17419	1.92059
H	2.49946	3.00225	1.69342
H	1.02534	2.24400	2.34984
H	1.36815	3.96017	2.69466
C	1.29308	4.86603	0.03952
H	0.75144	5.19431	-0.86368
H	2.34323	4.68068	-0.24088
H	1.26955	5.70109	0.76301
C	4.44988	1.75654	-2.00355
C	5.26959	3.04331	-1.85105
H	6.26227	2.94055	-2.32333
H	5.41044	3.30859	-0.79223
H	4.74540	3.87917	-2.34423
C	4.10668	1.52285	-3.48809
H	3.48451	2.35941	-3.84626
H	3.53148	0.59075	-3.61465
H	5.00991	1.46656	-4.11960
C	5.07863	0.47619	-1.31359
C	5.85213	0.81704	-0.02507
H	5.24499	1.45224	0.64076
H	6.80203	1.33737	-0.23629
H	6.08254	-0.11763	0.51210
C	5.94680	-0.39425	-2.23022
H	6.82465	0.16656	-2.59616
H	5.37762	-0.76003	-3.09830
H	6.31442	-1.27117	-1.67126
C	-1.73393	-0.74138	2.58281
C	-2.80493	-1.02579	1.53869
H	-2.95223	-0.15065	0.88464
H	-3.76673	-1.22919	2.03922
H	-2.54877	-1.89152	0.90984
C	-2.00456	0.57510	3.32246
H	-1.22918	0.77848	4.07905
H	-2.98313	0.54312	3.82916
H	-2.02101	1.41196	2.60570
C	-1.41273	-1.94688	3.53904
C	-2.17066	-1.91997	4.86977
H	-1.86492	-2.78294	5.48289
H	-3.25884	-1.99097	4.70182
H	-1.95998	-1.00389	5.44097
C	-1.55181	-3.32321	2.86686
H	-1.03499	-3.35987	1.89389
H	-2.60920	-3.59101	2.70762

H	-1.09883	-4.08363	3.52286
B	0.58333	-1.03886	2.79527
B	2.82654	0.63638	-0.79445
C	2.11984	-0.76181	2.69236
H	2.42093	-0.75009	1.62861
H	2.28455	0.28561	3.02499
C	3.00211	-1.71368	3.52887
H	2.66188	-1.71808	4.58221
H	2.86801	-2.75196	3.16780
C	4.49645	-1.35295	3.47394
H	4.63335	-0.31823	3.84552
H	4.82331	-1.33991	2.41661
C	5.38263	-2.31257	4.28264
H	6.44733	-2.02763	4.22748
H	5.09409	-2.32146	5.34909
H	5.29467	-3.34834	3.90875
O	1.64700	0.33085	-0.26198

J

SCF (BP86) Energy = -1726.80531598
Enthalpy 0K = -1726.005559
Energy 298K = -1725.956469
Free Energy 298K = -1726.090799
Lowest Frequency = 12.5754 cm^{-1}
Second Frequency = 13.1118 cm^{-1}
SCF (BP86-D3BJ) Energy = -1727.02112890
SCF (Toluene) Energy = -1726.81471062
SCF (BS2) Energy = -1926.47609891

Mg	0.03421	-0.46528	-0.31445
N	-1.40217	-1.75343	0.30641
N	1.61324	-1.60360	0.24810
C	-2.24905	-3.93093	1.12304
H	-2.85554	-3.51093	1.94378
H	-1.87290	-4.91642	1.43313
H	-2.93471	-4.06327	0.26878
C	-1.11168	-2.99125	0.75918
C	1.46318	-2.86431	0.70779
C	2.70098	-3.68720	1.02386
H	3.37722	-3.72579	0.15296
H	2.43694	-4.71373	1.31609
H	3.27834	-3.22642	1.84382
C	2.93249	-1.03653	0.10220
C	3.56816	-1.06268	-1.17215
C	4.80953	-0.41337	-1.31669
H	5.30571	-0.42272	-2.29354
C	5.41681	0.24565	-0.24137
H	6.38229	0.74492	-0.37520
C	4.77898	0.26778	1.00479
H	5.25139	0.79229	1.84296
C	3.53599	-0.36340	1.20341
C	2.85197	-0.27349	2.56969
H	1.97356	-0.94210	2.54871
C	3.76706	-0.74521	3.72164
H	4.64363	-0.08483	3.84246
H	4.14366	-1.76872	3.55317
H	3.21557	-0.73820	4.67791
C	2.33900	1.16177	2.83679
H	3.18082	1.87620	2.87380
H	1.81318	1.21230	3.80686
H	1.64517	1.50932	2.05165
C	2.92554	-1.74540	-2.38169
H	2.04431	-2.30368	-2.01668
C	3.87072	-2.76927	-3.04880
H	4.75861	-2.27955	-3.48565
H	3.34950	-3.29552	-3.86730
H	4.22731	-3.52565	-2.32868
C	2.42988	-0.70015	-3.41032
H	1.70068	0.00136	-2.96844
H	1.94954	-1.20102	-4.26969
H	3.27394	-0.10343	-3.79934
C	-2.77652	-1.32589	0.19400
C	-3.45143	-1.45981	-1.05333
C	-4.75849	-0.94838	-1.16771
H	-5.28573	-1.04164	-2.12364
C	-5.39201	-0.31891	-0.08967
H	-6.40889	0.07240	-0.20004
C	-4.71405	-0.18585	1.12785
H	-5.20708	0.31662	1.96773
C	-3.40535	-0.67830	1.29590
C	-2.68659	-0.47094	2.63106
H	-1.73290	-1.02581	2.58621
C	-3.49205	-1.02847	3.82599
H	-2.91376	-0.92687	4.76086
H	-3.73788	-2.09586	3.69196
H	-4.44240	-0.48390	3.96524
C	-2.35015	1.02303	2.85263
H	-3.27268	1.62816	2.90606
H	-1.72974	1.43752	2.03911
H	-1.80388	1.16086	3.80263
C	-2.78156	-2.10281	-2.26978
H	-1.83686	-2.56065	-1.92475
C	-3.63771	-3.23074	-2.88716
H	-3.89376	-4.00425	-2.14279
H	-3.09084	-3.71873	-3.71259
H	-4.58359	-2.84276	-3.30401
C	-2.42683	-1.03413	-3.33222
H	-3.33973	-0.53903	-3.70814
H	-1.91883	-1.50042	-4.19523
H	-1.76662	-0.24921	-2.92329
O	-0.10493	1.02887	-1.41659
B	-0.17073	2.31760	-1.05339
O	-0.35201	3.40326	-1.91932
O	-0.06602	2.74703	0.29910
C	-0.62607	4.57189	-1.10010
C	0.06731	4.20015	0.27550
C	1.57338	4.52173	0.28567
H	1.76036	5.60821	0.32890
H	2.03632	4.05637	1.17111
H	2.06864	4.11679	-0.61221
C	-0.60823	4.78279	1.52085
H	-0.07266	4.45249	2.42665
H	-0.58728	5.88636	1.49944
H	-1.65488	4.45365	1.60464
C	-2.15758	4.69560	-0.98161
H	-2.45845	5.60947	-0.44137
H	-2.59020	4.73234	-1.99458
H	-2.58503	3.82287	-0.46074
C	-0.04964	5.80690	-1.80204
H	-0.17827	6.71173	-1.18274
H	1.02037	5.68110	-2.02581
H	-0.57797	5.96997	-2.75604
C	0.20733	-3.48749	0.92147
H	0.26544	-4.51530	1.28695

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