Supporting Information for

Diverse Reactivity of a Magnesium Silanide toward Ketones

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General Experimental Details

All reactions of air- and moisture-sensitive compounds were carried out using standard Schlenk line and glovebox techniques under an inert atmosphere of argon. NMR experiments involving air-sensitive compounds were conducted in J. Young tap NMR tubes made up and sealed in a glovebox under argon. NMR spectra were recorded on a Bruker AV300 Ultrashield instrument for ^{1}H (300.2 MHz), a Bruker 400 Ultrashield instrument for ^{29}Si (79.5 MHz) or an Agilent ProPulse instrument for ^{1}H (500 MHz), ^{13}C (126 MHz) and ^{29}Si (99 MHz) spectra at room temperature. The ^{1}H/^{13}C NMR spectra were referenced relative to residual solvent resonances, while ^{29}Si NMR spectra were referenced to an external standard (Me_4Si). Solvents (toluene, pentane and hexane) were dried using an MBraun solvent purification system and stored over 4 Å molecular sieves under argon. THF for use in air- and moisture-sensitive reactions was dried over sodium or potassium/benzophenone and distilled before use. C_6D_6 was purchased from Sigma-Aldrich and dried over a potassium mirror, vacuum transferred into a sealed ampoule and stored in a glovebox under argon. Di-*n*-butylmagnesium (Mg*n*-Bu_2 1.0 M solution in *n*-heptane) and carbodiimides were purchased from Sigma-Aldrich and used without further purification. The β-diketiminato magnesium alkyl complex, [(BDI)Mg*n*Bu] (BDI = CH{C(Me)NDipp}$_2$, Dipp = 2,6-*i*-$Pr_2C_6H_3$), and dimethylphenylsilyl boronic acid pinacol ester (pinBSiMe_2Ph, pin = pinacolato) were synthesised by literature procedures.[1,2] Elemental analysis was performed by Elemental Microanalysis, Okehampton, UK.

Synthesis of compound 2.

A solution of [(BDI)Mg*n*-Bu] (50 mg, 0.10 mmol) and pinBSiMe$_2$Ph (26 mg, 0.10 mmol) in C_6D_6 (0.5 mL) was added via pipette to a J. Young NMR tube. Complete conversion to compound **1** was obtained after approximately 12 hours at room temperature. Acetophenone (20 mg, 0.10 mmol) was added to the reaction mixture and complete conversion to compound **2** was obtained after 10 minutes at room temperature. Crystals suitable for single crystal X-ray diffraction analysis of **2** were obtained by slow evaporation of a hexane/toluene solution at room temperature. ^{1}H NMR (500 MHz, C_6D_6) δ 7.67 – 7.60 (m, 1H, O-Ar), 7.35 – 7.20 (m, 4H, O-Ar), 7.10 (s, 2H, Dipp-Ar), 6.94 – 6.75 (m, 4H, Dipp-Ar), 5.01 (s, 1H, C*H*{C(CH$_3$)NDipp}$_2$), 4.04 (s, 2H, OCH$_2$), 3.33 – 2.85 (m, 4H, Dipp-C*H*(CH$_3$)$_2$), 1.66 (s, 6H, CH{C(C*H*$_3$)NDipp}$_2$), 1.40 (s, 6H, Dipp-CH(C*H*$_3$)$_2$), 1.21 – 0.92 (m, 12H, Dipp-CH(C*H*$_3$)$_2$), 0.75 (s, 6H, Dipp-CH(C*H*$_3$)$_2$). ^{13}C NMR (126 MHz, C_6D_6) δ 170.2 (CH{*C*(CH$_3$)NDipp}$_2$), 160.4 (*i*, O Ar), 147.1 (*i*, Dipp Ar), 146.1 (*C*, Dipp Ar), 143.0 (*C*, Dipp Ar), 142.2 (*C*, Dipp Ar), 141.4 (*C*, Dipp Ar), 128.8 (*C*H, O Ar), 126.4 (*C*H, O Ar), 125.6 (*C*H, Dipp Ar), 123.9 (*C*H, Dipp Ar), 96.4 ({*C*H(CH$_3$)NDipp}$_2$), 91.6 (O*C*H), 32.0 (Dipp-CH(*C*H$_3$)$_2$), 28.5 (Dipp-*C*H(CH$_3$)$_2$), 24.9 (CH{C(*C*H$_3$)NDipp}$_2$), 24.5 (Dipp CH(*C*H$_3$)$_2$), 24.1 (Dipp CH(*C*H$_3$)$_2$), 23.1 (Dipp-CH(*C*H$_3$)$_2$) ppm. Elemental analysis, calculated for $C_{63}H_{68}MgN_2O_2Si$: C, 79.22; H, 8.92; N, 4.86 %. Found: C, 79.03; H, 8.78; N, 4.94 %.

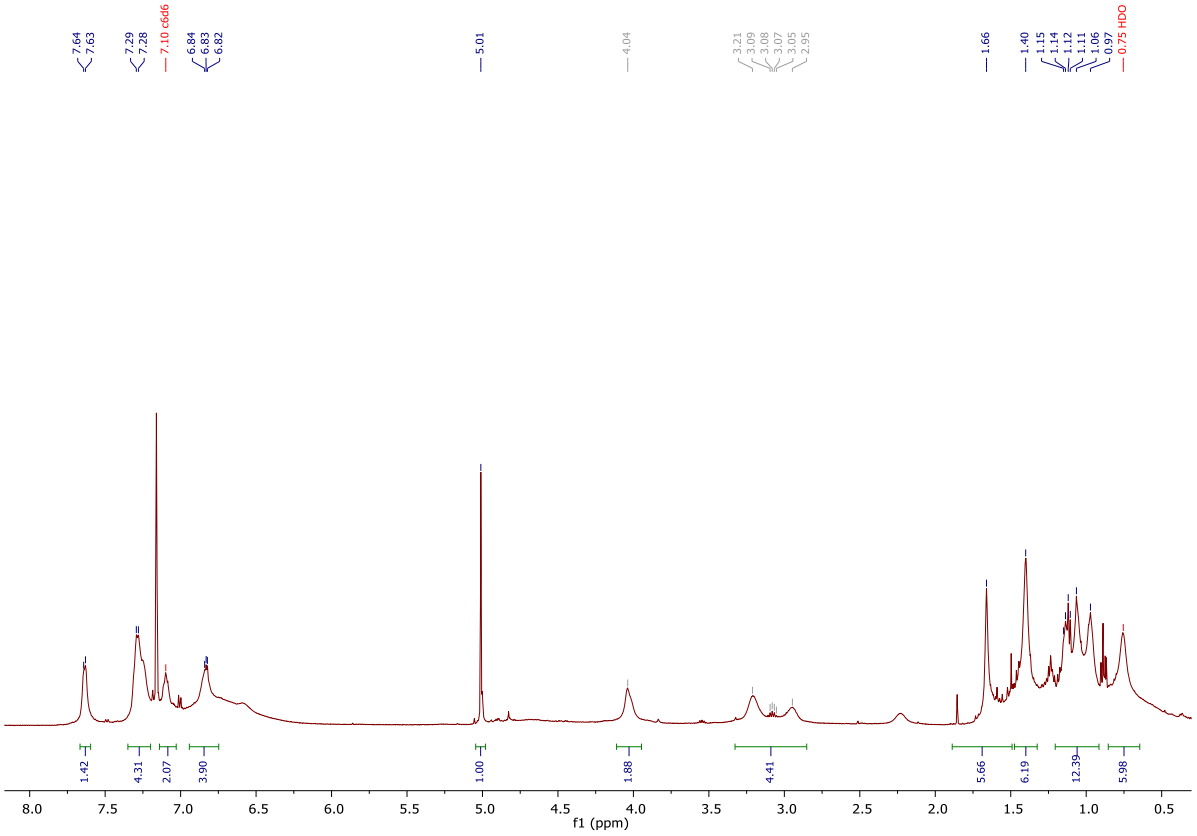


Figure S1: ^{1}H NMR spectrum (500 MHz, C_6D_6, 298 K) of compound **2**.

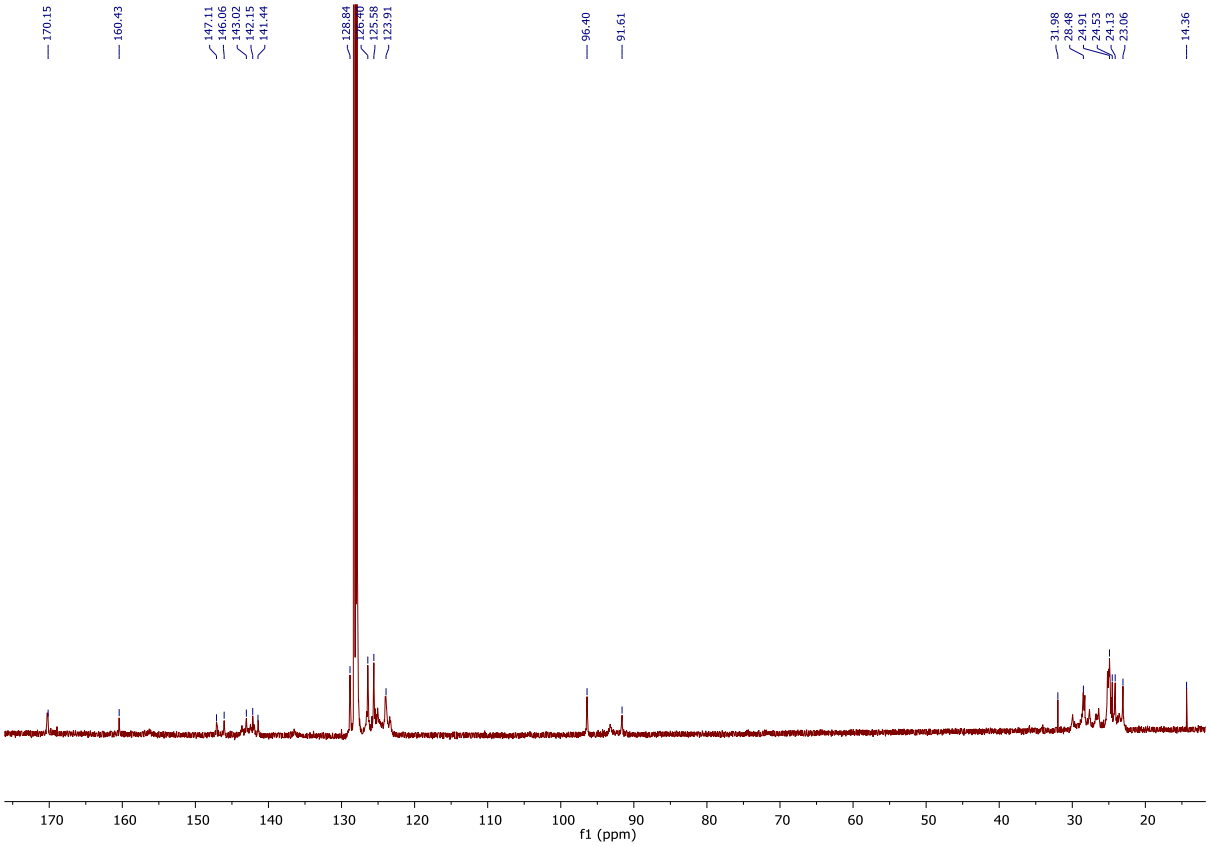


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6, 298 K) of compound **2**.

Synthesis of compound 3.

A solution of [(BDI)Mg*n*-Bu] (50 mg, 0.10 mmol) and pinBSiMe$_2$Ph (26 mg, 0.10 mmol) in C_6D_6 (0.5 mL) was added via pipette to a J. Young NMR tube. Complete conversion to compound **1** was obtained after approximately 12 hours at room temperature. Benzophenone (20 mg, 0.10 mmol) was added to the reaction mixture and complete conversion to compound **3** was obtained after immediately after reaction. Crystals suitable for single crystal X-ray diffraction analysis of **3** were obtained by cooling of hexane/toluene solution to –30 °C. ^{1}H NMR (500 MHz, C_6D_6) δ 7.31 (s, 3H, C_6H_5)Si), 7.22 (d, *J* = 7.8 Hz, 2H, C_6H_5)Si), 7.04 (dd, *J* = 16.3, 7.3 Hz, 6H, Dipp-Ar), 6.91 (d, *J* = 7.9 Hz, 3H, C=O Ar), 5.80 (dd, *J* = 9.6, 5.2 Hz, 1H, C=O Ar), 5.24 (dd, *J* = 9.7, 5.4 Hz, 1H, C=O Ar), 5.11 (s, 1H, C*H*{C(CH$_3$)NDipp}$_2$), 3.70 (d, *J* = 67.5 Hz, 2H, Dipp-C*H*(CH$_3$)$_2$), 3.34 – 2.77 (m, 2H, Dipp-C*H*(CH$_3$)$_2$), 1.72 (s, 3H Dipp-CH(C*H*$_3$)$_2$), 1.67 (s, 6H, CH{C(C*H*$_3$)NDipp}$_2$), 1.33 (d, *J* = 6.7 Hz, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.30 – 1.20 (m, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.20 – 1.09 (m, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.10 – 0.91 (m, 6H, Dipp-CH(C*H*$_3$)$_2$), 0.73 (d, *J* = 9.1 Hz, 3H, Dipp-CH(C*H*$_3$)$_2$), 0.62 (s, 6H, Si(C*H*$_3$)$_2$Ph), -0.03 (s, 3H, Dipp-CH(C*H*$_3$)$_2$) ppm. ^{13}C NMR (126 MHz, C_6D_6) δ 169.5 (CH{*C*(CH$_3$)NDipp}$_2$), 146.3 (*i*-Dipp-Ar), 140.7 (*i*-(*C*$_6$H$_5$)Si), 134.9 (O=*C*), 132.6 (*i*-Dipp-Ar),132.3 (*i*-Dipp-Ar), 125.8 (Si(*C*H$_3$)$_2$Ph), 125.4 (Si(*C*H$_3$)$_2$Ph), 124.5 (*C*(CH Dipp), 123.8 (*C*H Dipp Ar), 122.9 (*C*H O=CPh$_2$), 115.5 (*C*H O=CPh$_2$), 95.3 (s, *C*H{C(CH$_3$)NDipp}$_2$), 32.0 (Dipp *C*H(CH$_3$)$_2$), 28.9 (Dipp-*C*H(CH$_3$)$_2$), 25.0 (Dipp-CH(*C*H$_3$)$_2$), 24.7

(C(CH_3)$_3$)), 24.6 (Dipp-CH(CH_3)$_2$), 24.6 (Dipp-CH(CH_3)$_2$)', 24.5 (Dipp-CH(CH_3)$_2$)', 24.4 (Dipp-CH(CH_3)$_2$)', 24.1 (Dipp-CH(CH_3)$_2$)', 23.1 (Dipp-CH(CH_3)$_2$)', 14.4 (Dipp-CH(CH_3)$_2$)', –3.47 (Si(CH_3)$_2$Ph), –4.00 (Si(CH_3)$_2$Ph) ppm. ^{29}Si{H} NMR (99 MHz, C_6D_6, 298K) δ –115.69 ppm. Elemental analysis, calculated for $C_{50}H_{62}MgN_2OSi$: C, 79.08; H, 8.23; N, 3.69%. Found: C, 79.82; H, 7.82; N, 2.99%.

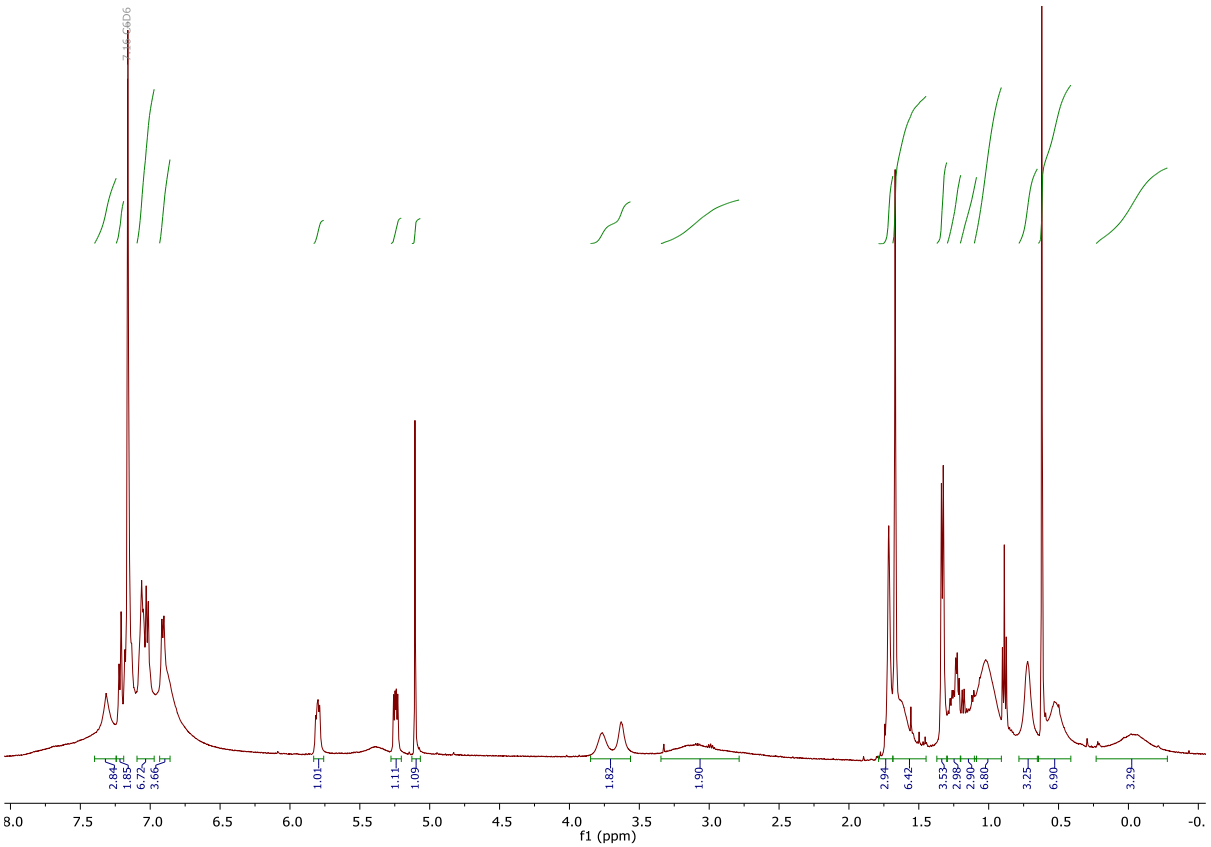


Figure S3: ^{1}H NMR spectrum (500 MHz, C_6D_6, 298 K) of compound **3**.

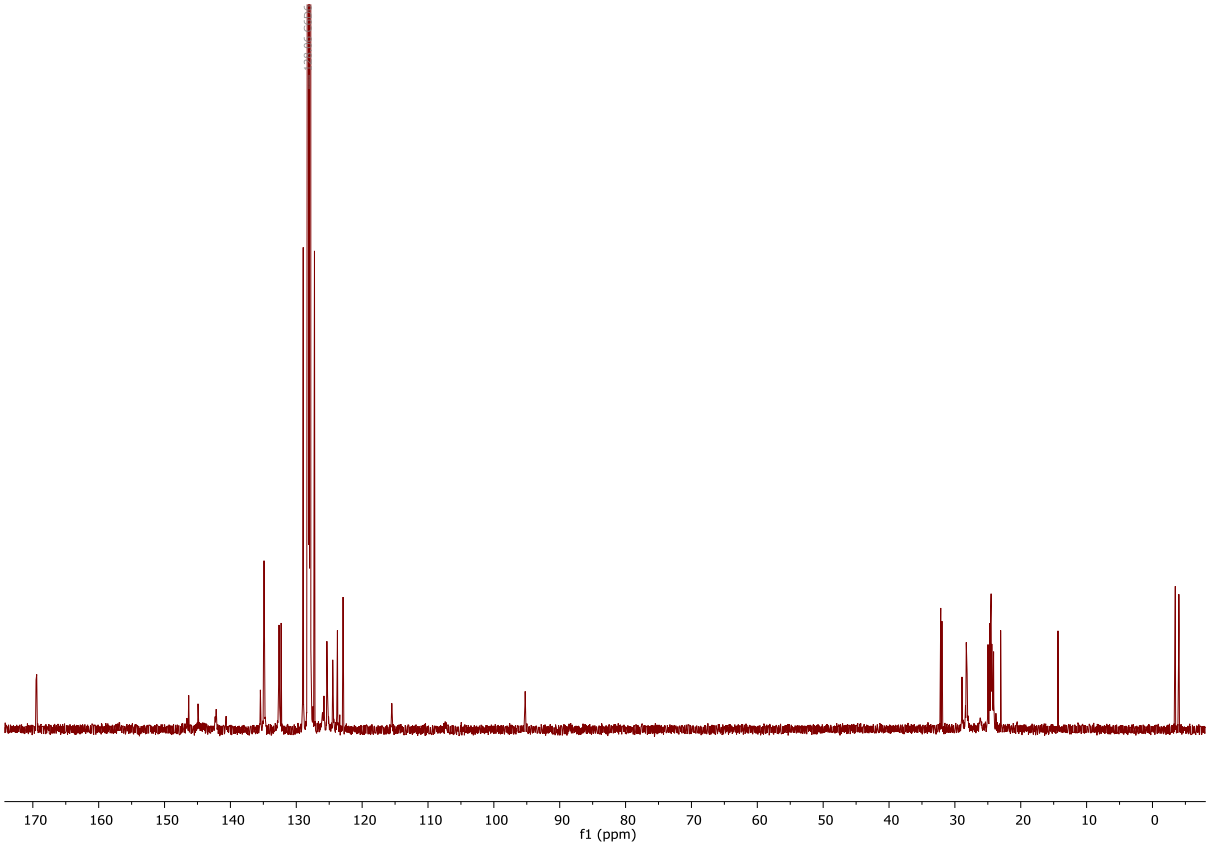


Figure S4: $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6, 298 K) of compound **3**.

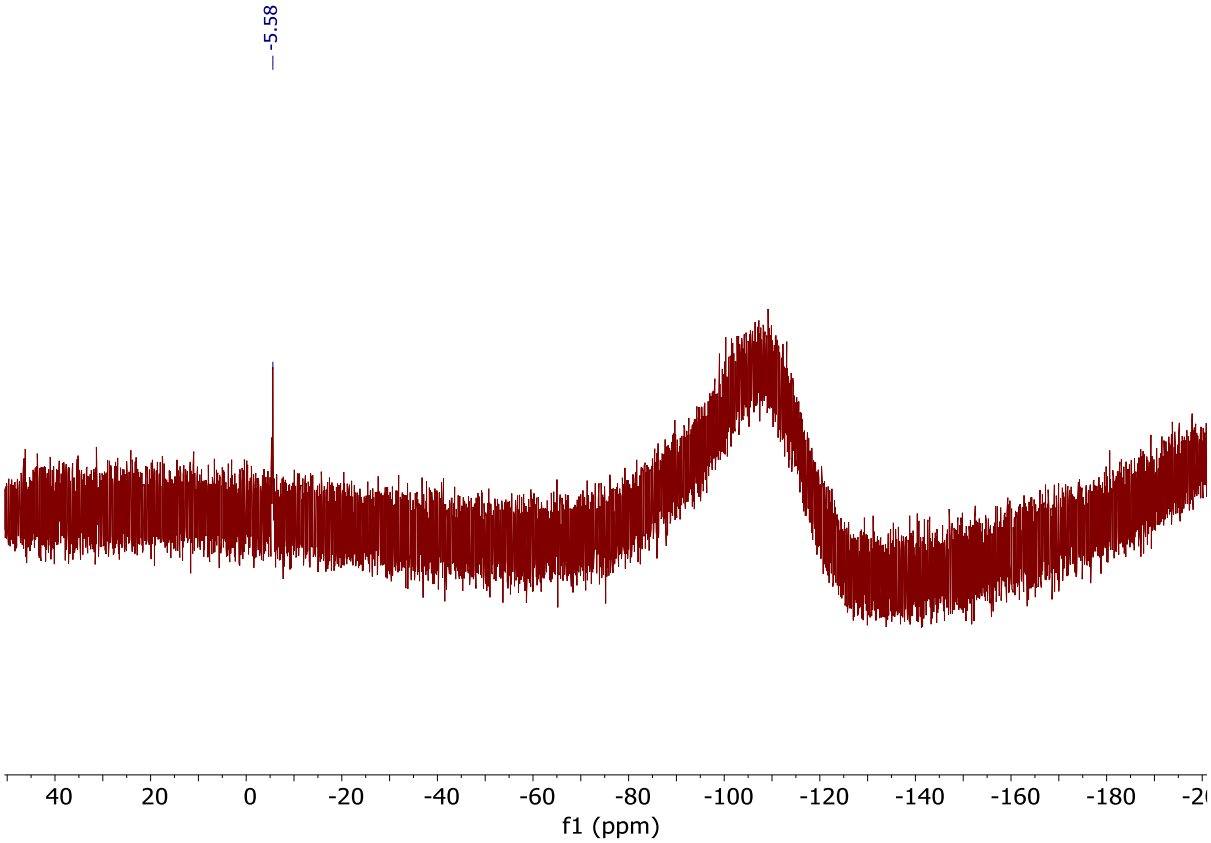


Figure S5: $^{29}Si\{^{1}H\}$ NMR spectrum (99 MHz, C_6D_6, 298 K) of compound **3**.

Synthesis of compound 4

A solution of [(BDI)Mg*n*-Bu] (50 mg, 0.10 mmol) and pinBSiMe$_2$Ph (26 mg, 0.10 mmol) in C_6D_6 (0.5 mL) was added via pipette to a J. Young NMR tube. Complete conversion to compound **1** was obtained after approximately 12 hours at room temperature. 4-fluorobenzophenone (20 mg, 0.10 mmol) was added to the reaction mixture and complete conversion to compound **4** was obtained after 48 hours at room temperature. Crystals suitable for single crystal X-ray diffraction analysis of **4** were obtained by slow evaporation of a hexane/ toluene solution at room temperature. ^{1}H NMR (500 MHz, Benzene-d_6) δ 7.61 (s, 2H, C*H*, Ar), 7.43 – 7.30 (m, 2H, C*H*, Ar), 7.24 (s, 5H, Si-Ar), 7.10 (dd, *J* = 17.9, 5.6 Hz, 6H, Dipp-Ar), 7.01 (d, *J* = 7.3 Hz, 3H, C*H*, Ar), 6.96 (d, *J* = 7.2 Hz, 2H, C*H*, Ar), 6.94 – 6.86 (m, 3H, C*H*, Ar), 6.79 (d, *J* = 4.1 Hz, 2H, C*H*, Ar), 6.11 (s, 1H, C*H*, Ar), 5.16 – 5.08 (m, 2H, C*H*, Ar), 4.82 (s, 1H, C*H*{C(CH$_3$)NDipp}$_2$), 3.32 (s, 1H, C*H*-Si), 3.00 – 2.87 (m, 4H, Dipp-C*H*(CH$_3$)$_2$), 1.55 (s, 6H, CH{C(C*H*$_3$)NDipp}$_2$), 1.22 (d, *J* = 6.9 Hz, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.18 (d, *J* = 7.0 Hz, 3H, Dipp-CH(C*H*$_3$)$_2$), 1.13 – 1.09 (m, 12H, Dipp-CH(C*H*$_3$)$_2$), 0.99 (q, *J* = 7.4, 7.0 Hz, 6H, Dipp-CH(C*H*$_3$)$_2$), 0.38 (s, 3H, Si(C*H*$_3$)$_2$Ph), 0.18 (s, 3H, Si(C*H*$_3$)$_2$Ph) ppm. ^{13}C NMR (126 MHz, Benzene-d_6) δ 167.6 (s, CH{*C*(CH$_3$)NDipp}$_2$), 146.9 (*C*, Dipp), 141.6 (*i*, Dipp), 136.4 (*i*, Dipp), 135.1 (O, *C*-Ar), 134.3 (O, C *C*-Ar), 127.4 (*C*H, Dipp Ar), 126.2 (*C*H, Ar), 124.7 (s, Si(*C*H$_3$)$_2$Ph), 124.6 (*C*H, Ar), 124.0 (*C*H, Ar), 123.4 (*C*H, Ar), 95.4 (s, *C*H{C(CH$_3$)NDipp}$_2$), 53.0 (s, CH{*C*(CH$_3$)NDipp}$_2$), 28.9 (s, Dipp *C*H(CH$_3$)$_2$), 28.4 (s, *C*H-Si), 24.4 (s, CH{C(*C*H$_3$)NDipp}$_2$), 23.8 (s, Dipp CH(*C*H$_3$)$_2$), 23.2 (s, Dipp CH(*C*H$_3$)$_2$), 23.1 (s, Dipp CH(*C*H$_3$)$_2$), 20.5 (s, Dipp CH(*C*H$_3$)$_2$), -4.2 (s, Si(*C*H$_3$)$_2$Ph) ppm. Elemental analysis, calculated for $C_{63}H_{68}MgN_2O_2Si$: C, 75.92; H, 7.05; N, 2.81 %. Found: C, 75.92; H, 7.99; N, 3.56 %.

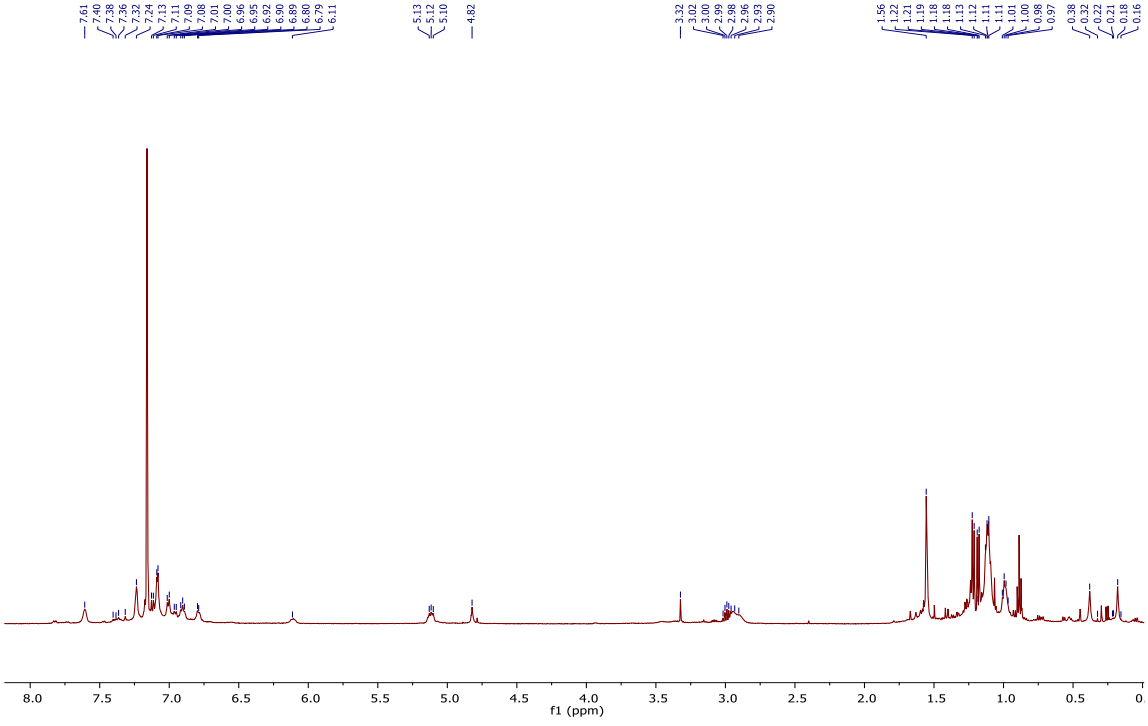


Figure S6: ^{1}H NMR spectrum (500 MHz, C_6D_6, 298 K) of compound **4**.

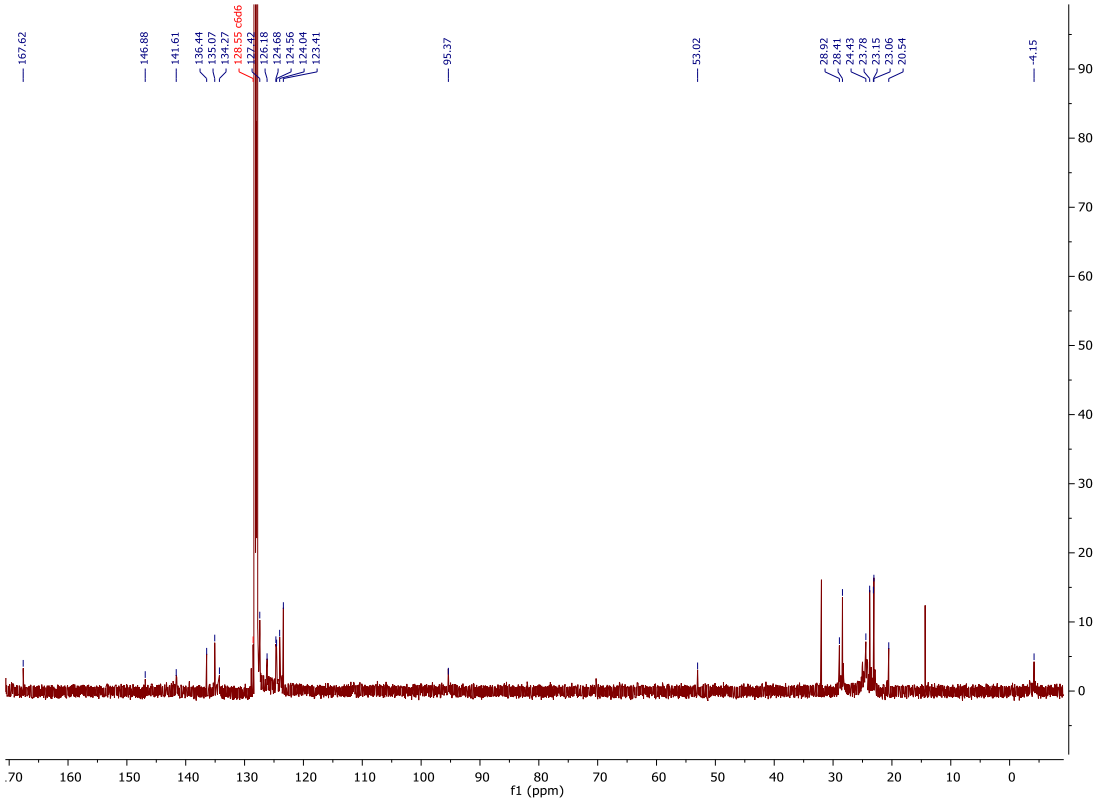


Figure S7: $^{13}C\{^{1}H\}$ NMR spectrum (126 MHz, C_6D_6, 298 K) of compound **4**.

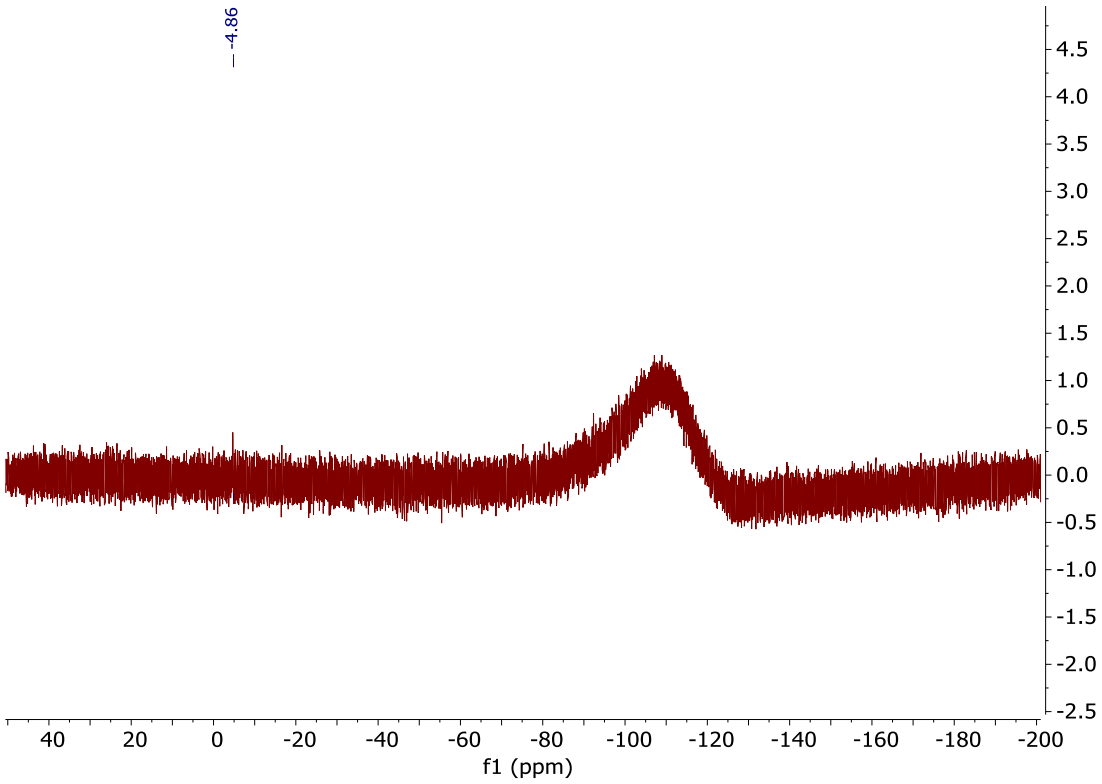


Figure S8: $^{29}Si\{^{1}H\}$ NMR spectrum (99 MHz, C_6D_6, 298 K) of compound **4**.

Synthesis of compound 5.

A solution [(BDI)Mg*n*-Bu] (50 mg, 0.10 mmol) and pinBSiMe$_2$Ph (26 mg, 0.10 mmol) in C_6D_6 (0.5 mL) was added via pipette to a J. Young NMR tube. Complete conversion to compound **1** was obtained after approximately 12 hours at room temperature. 9-fluorenone (20 mg, 0.10 mmol) was added to the reaction mixture and complete conversion to compound **5** was obtained after 48 hours at 60 °C. Crystals suitable for single crystal X-ray diffraction analysis of **5** were obtained by slow evaporation of a hexane/ toluene solution at room temperature. ^{1}H NMR (400 MHz, C_6D_6) δ 9.18 (d, *J* = 4.9 Hz, 1H, Si(C*H*$_3$)$_2$Ph), 7.59 (d, *J* = 7.8 Hz, 1H, C*H*, Ar), 7.51 (dd, *J* = 13.1, 8.1 Hz, 3H, C*H*, Ar), 7.41 – 7.32 (m, 2H, C*H*, Ar), 7.22 – 7.17 (m, 4H, Si(C*H*$_3$)$_2$Ph), 7.15 – 7.14 (m, 6H, Dipp-Ar), 7.14 – 7.11 (m, 4H, C*H*, Ar), 6.95 (q, *J* = 7.5 Hz, 3H, C*H*, Ar), 6.83 (t, *J* = 7.4 Hz, 1H, C*H*, Ar), 6.64 (t, *J* = 8.0 Hz, 1H, C*H*, Ar), 6.56 (d, *J* = 8.7 Hz, 1H, C*H*, Ar), 4.54 (s, 1H, C*H*{C(CH$_3$)NDipp}$_2$), 3.45 – 2.73 (m, 4H, Dipp-C*H*(CH$_3$)$_2$), 1.63 (s, 6H, CH{C(C*H*$_3$)NDipp}$_2$), 1.35 – 0.84 (m, 24H, Dipp-CH(C*H*$_3$)$_2$), 0.14 (s, 6H, Si(C*H*$_3$)$_2$Ph) ppm. ^{13}C NMR (101 MHz, C_6D_6) δ 168.4 (s, CH{*C*(CH$_3$)NDipp}$_2$), 147.4 (s, *i*-(*C*$_6$H$_5$)Si), 145.8 (s, *i*-Dipp-Ar), 144.6 (*i*, O, Ar), 142.5 (*C*, Ar), 141.8 (*C*,Ar), 140.0 (*C*, Ar), 139.4 (*C*, Ar), 137.5 (*C*H, Ar), 133.8 (*C*H, Ar), 132.4 (s, Si(*C*H$_3$)$_2$Ph), 130.9 (*C*H, Ar), 129.9 *C*H, Ar), 129.0 (*C*H, Ar), 128.7 (s, Si(*C*H$_3$)$_2$Ph), 127.5 (*C*H Dipp Ar), 127.0 (*C*H, Ar), 126.0 (*C*H Dipp Ar), 125.1 (*C*H, Ar), 123.8 (*C*H, Ar), 123.1 (*C*H, Ar), 121.1 (*C*H, Ar), 97.6 (*C*H{C(CH$_3$)NDipp}$_2$), 70.7 (*C*, Ar) 24.8 (s , Dipp CH(*C*H$_3$)$_2$, 24.4 (CH{C(*C*H$_3$)NDipp}$_2$), 3.5 (Si(*C*H$_3$)$_2$Ph) ppm. ^{29}Si{H} NMR (99 MHz, C_6D_6, 298K) δ – 16.09 ppm. Elemental analysis, calculated for $C_{63}H_{68}MgN_2O_2Si$: C, 80.70; H, 7.31; N, 2.99 %. Found: C, 80.40; H, 7.26; N, 3.15 %.

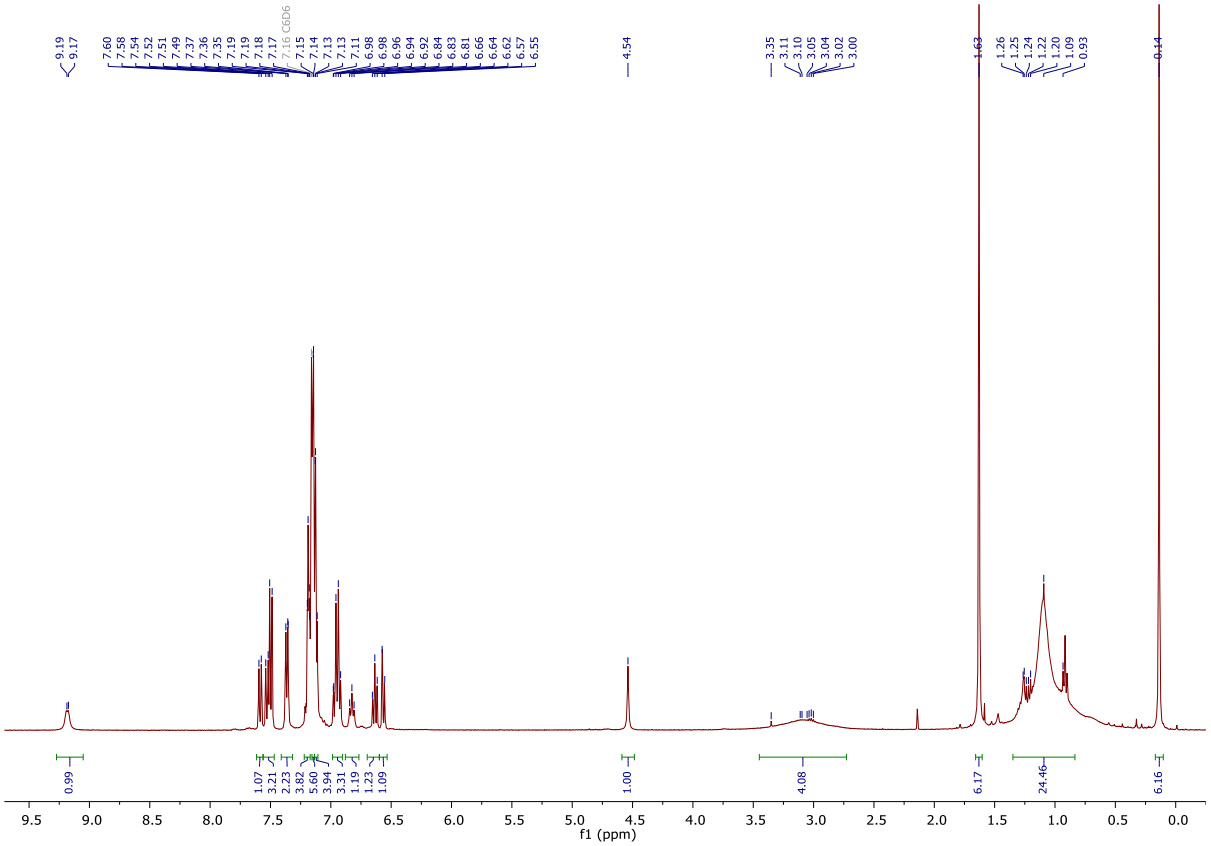


Figure S9: ^{1}H NMR spectrum (400 MHz, C_6D_6, 298 K) of compound **5**.

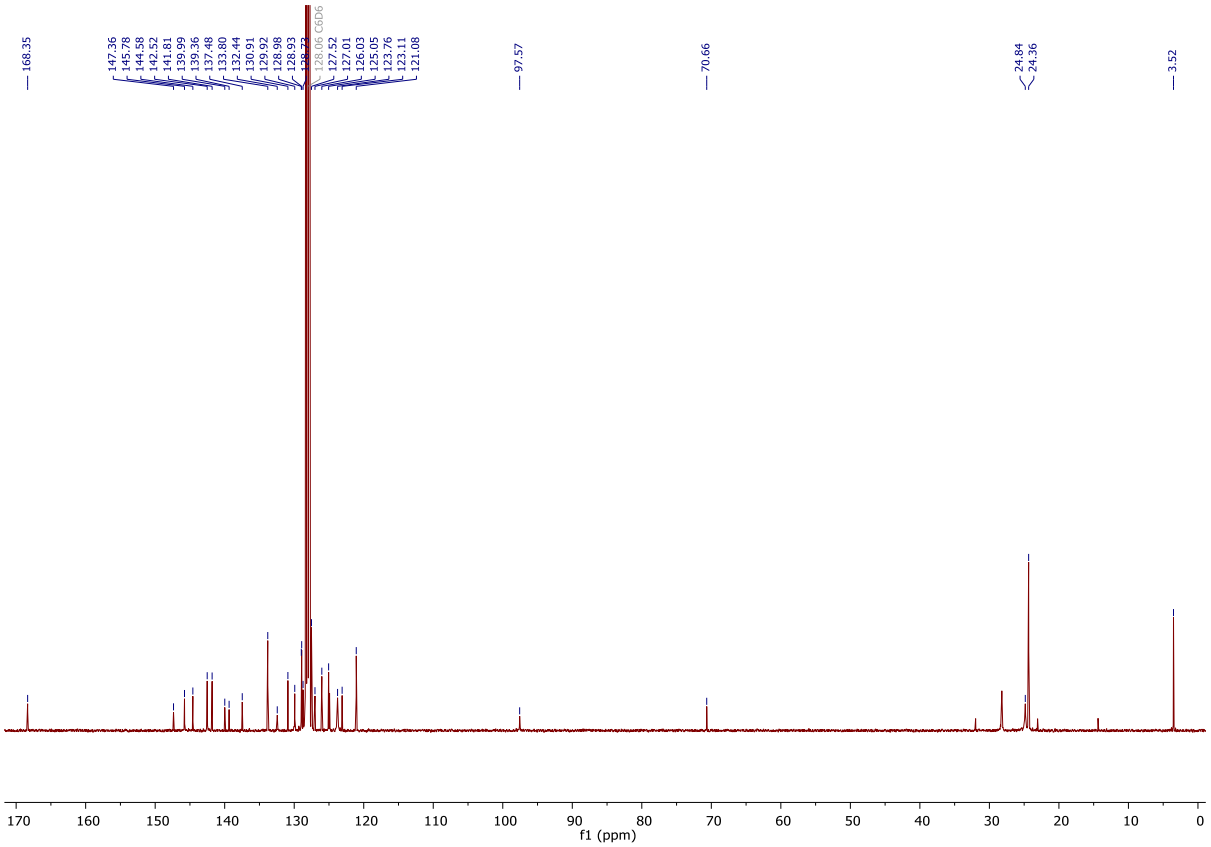


Figure S10: ^{13}C{^{1}H} NMR spectrum (101 MHz, C_6D_6, 298 K) of compound **5**.

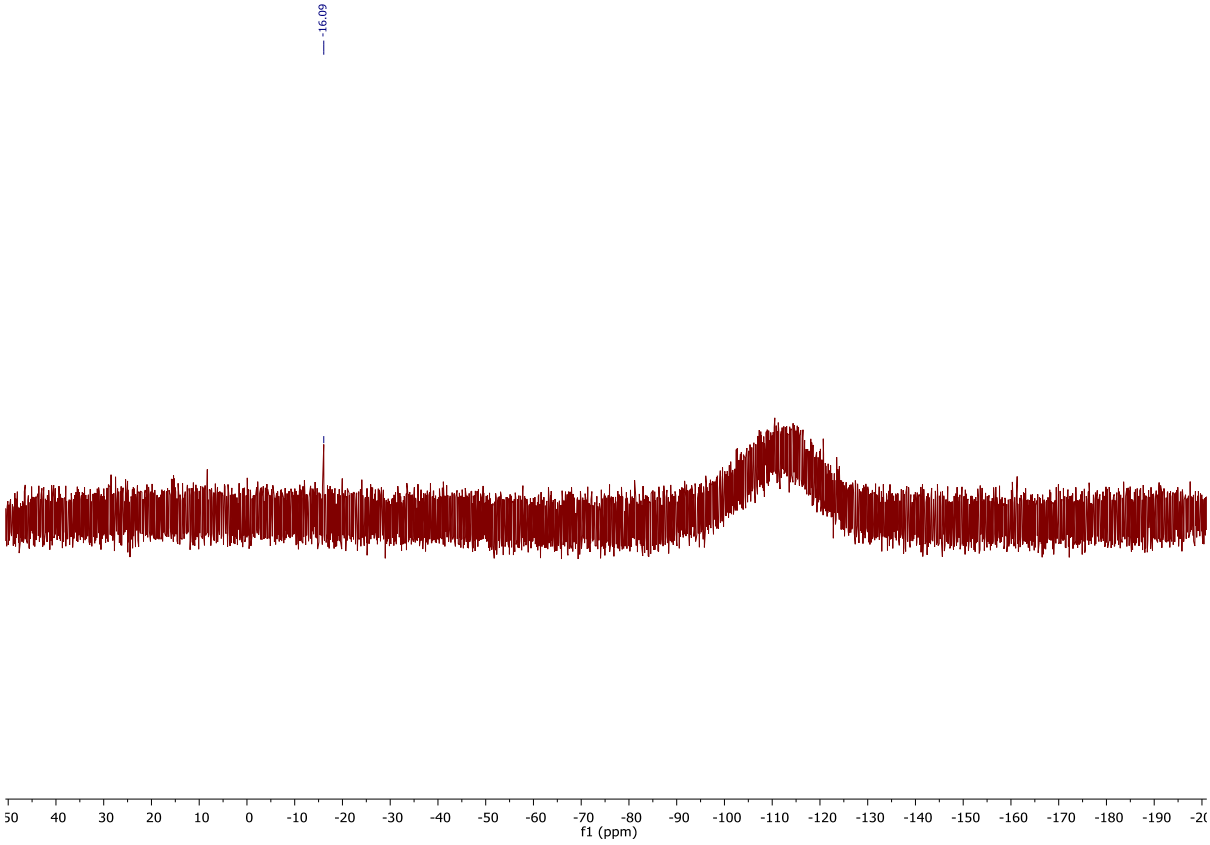


Figure S11: $^{29}Si\{^{1}H\}$ NMR spectrum (99 MHz, C_6D_6, 298 K) of compound **5**.

Single crystal X-ray analysis of compounds 2 – 5.

Data were collected for compounds **2 – 5** on a SuperNova, Dual Cu at zero, EosS2 diffractometer (Cu*K*α; λ = 1.54184 Å), with the crystals maintained at 150 K during data collection. Using Olex2,[3] the structures were solved with ShelXT[4] and refined with the ShelXL[5] using Least Squares minimisation.

The asymmetric unit in the structure of **2** comprises half of a dimer molecule, the remainder of which is generated via an inversion centre that is proximate to the core of the complex. The hydrogen atoms attached to C31 were located and refined at a distance of 0.98Å from the parent atom.

F1 was found to be disordered in the structure of **4**, such that it is present at 85% site-occupancy in the benzophenone ring based on C37, and 15% in the minor component of total ring disorder observed for the phenyl group based on C31. Distance and ADP restraints were applied to the latter moiety, to assist convergence.

Table S1: Single crystal X-ray diffraction analysis of compounds **2 – 5**.

Compound	**2**	**3**	**4**	**5**
Empirical formula	$C_{37}H_{48}MgN_2O$	$C_{50}H_{62}MgN_2OSi$	$C_{63}H_{70}F_2MgN_2O_2Si$	$C_{63}H_{68}MgN_2O_2Si$
Formula weight	561.08	759.41	977.61	937.59
Crystal system	monoclinic	triclinic	monoclinic	triclinic
Space group	$P2_1/n$	$P\bar{1}$	$P2_1/c$	$P\bar{1}$
a/Å	14.3015(2)	9.8330(3)	19.7577(7)	11.7538(2)
b/Å	13.2978(1)	10.8375(4)	13.5109(3)	12.6949(3)
c/Å	17.4919(2)	21.3220(8)	22.2296(8)	17.8590(4)
α/°	90	95.428(3)	90	90.407(2)
β/°	97.0940(10)	92.237(3)	114.878(4)	96.484(2)
γ/°	90	100.071(3)	90	94.539(2)
U/Å^3	3301.12(6)	2223.56(14)	5383.4(3)	2639.10(10)
Z	4	2	4	2
ρ_{calc}/g cm^{-3}	1.129	1.134	1.206	1.180
μ/mm^{-1}	0.681	0.878	0.909	0.852
F(000)	1216.0	820.0	2088.0	1004.0
Crystal size/mm^3	0.336 × 0.131 × 0.092	0.12 × 0.049 × 0.015	0.127 × 0.077 × 0.062	0.354 × 0.315 × 0.193
2θ range for data collection/°	7.544 to 146.18	8.33 to 146.476	7.876 to 146.1	6.986 to 146.018
Index ranges	$-17 \le h \le 17$, $-10 \le k \le 16$, $-21 \le l \le 21$	$-12 \le h \le 9$, $-12 \le k \le 13$, $-26 \le l \le 26$	$-16 \le h \le 24$, $-16 \le k \le 16$, $-27 \le l \le 17$	$-14 \le h \le 14$, $-15 \le k \le 15$, $-22 \le l \le 22$
Reflections collected	43998	27279	38292	47411
Independent reflections, R_{int}	6598, 0.0486	8885, 0.0515	10654, 0.0597	10465, 0.0334
Data/restraints/parameters	6598/2/388	8885/0/508	10654/186/691	10465/0/634
Goodness-of-fit on F^2	1.038	1.022	1.021	1.020
Final $R1$, $wR_2[I>=2\sigma(I)]$	0.0438, 0.1138	0.0443, 0.1054	0.0604, 0.1544	0.0394, 0.0992
Final $R1$, wR_2[all data]	0.0523, 0.1189	0.0590, 0.1124	0.0926, 0.1750	0.0437, 0.1023
Largest diff. peak/hole/e Å^{-3}	0.26/−0.22	0.43/−0.24	1.62/−0.52	0.28/−0.41

Computational Details / Methodology

DFT calculations were run with Gaussian 16 (C.01)[6] using the BP86 functional.[7,8] The Mg and Si centres were described with the Stuttgart RECPs and associated basis sets,[9] and 6-31G** basis sets were used for all other atoms (BS1).[10, 11] A polarization function was also added to Si (ζ_d = 0.284). Initial BP86 optimizations 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 (BS2) featuring 6-311++G** on all atoms. Corrections for the effect of benzene (ε = 2.2706) solvent were run using the polarizable continuum model and BS1.[12] Single-point dispersion corrections to the BP86 results employed Grimme's D3 parameter set with Becke-Johnson damping as implemented in Gaussian.[13]

Breakdown of Energy Contributions

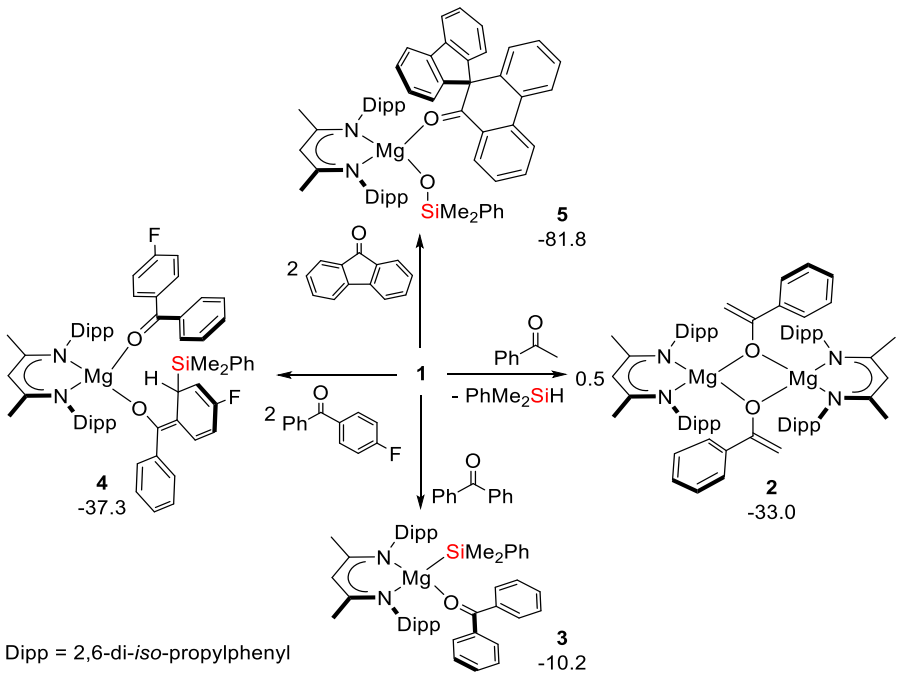
The following tables detail the evolution of the relative energies as the successive corrections to the initial SCF energy are included. Terms used are:

ΔE_{BS1}	SCF energy computed with the BP86 functional with BS1
ΔH_{BS1}	Enthalpy at 0 K with BS1
ΔG_{BS1}	Free energy at 298.15 K and 1 atm with BS1
$\Delta G_{BS1/bnz}$	Free energy corrected for benzene solvent with BS1
$\Delta G_{BS1/bnz+D3}$	Free energy corrected for benzene and dispersion effects with BS1
ΔG_{bnz}	Free energy corrected for basis set (BS2), dispersion effects and benzene solvent

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

Table S2: Relative energies (in kcal mol^{-1}) for computed structures. Data in bold are those used in the main text. All energies are quoted relative to **1** and the associated ketone at 0.0 kcal mol^{-1}.

	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/bnz}$	$\Delta G_{BS1/bnz+D3}$	ΔE_{BS2}	ΔG_{bnz}
1	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
2	-23.0	-23.0	-10.7	-7.3	-35.8	-20.2	**-33.0**
3	-9.4	-8.4	7.3	9.7	-13.3	-5.8	**-10.2**
4	-28.5	-27.1	2.3	6.6	-41.6	-24.3	**-37.3**
5	-76.5	-74.6	-44.1	-40.1	-84.0	-74.2	**-81.8**
4″	-28.2	-26.5	4.2	8.8	-39.2	-22.5	**-33.5**
A	-7.4	-6.8	7.7	9.5	-14.9	-4.3	**-11.7**
B	-3.7	-2.7	13.6	16.6	-11.2	-0.9	**-8.4**
TS(B-C)	11.0	11.9	30.3	32.9	2.1	13.1	**4.2**
C	-10.4	-10.0	3.9	3.7	-12.9	-10.4	**-12.8**
B′	-3.3	-2.0	14.8	17.6	-9.6	-0.3	**-7.0**
TS(B-C)′	12.2	13.0	31.1	33.8	3.3	14.6	**5.7**
C′	-8.8	-8.4	4.9	4.7	-11.8	-8.6	**-11.6**
4′	-28.2	-26.8	2.7	7.1	-41.0	-23.5	**-36.3**



Scheme S1: Synthesis of compounds **2** – **5** with DFT calculated free energies (BP86-D3(BJ)-benzene/BS2//BP86/BS1, in kcal mol^{-1}) for the reaction of **1** with the associated ketone

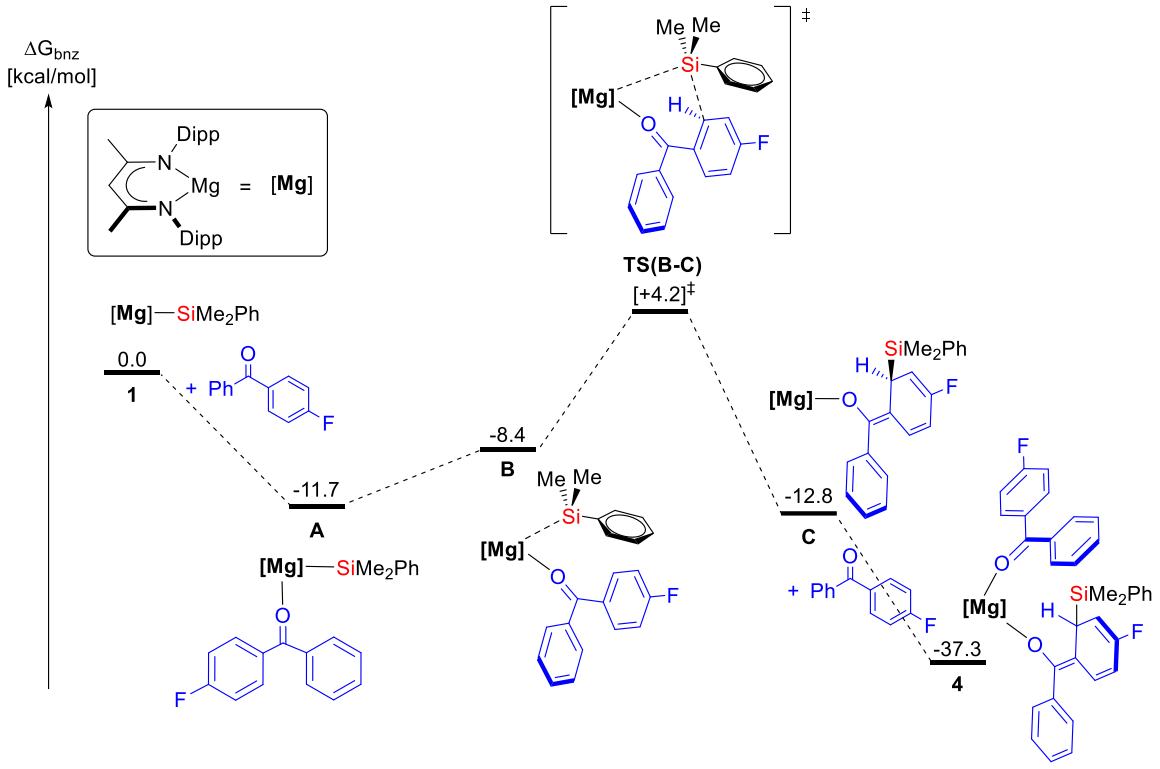


Figure S12: DFT calculated free energy profile (BP86-D3(BJ)-benzene/BS2//BP86/BS1, in kcal mol^{-1}) for the reaction of **1** with PhC(O)(C_6H_4-*p*-F) to form **4**

An alternative pathway (denoted by ′) for silylation at the *ortho* position of the non-fluorinated aryl group was also computed and is shown in Figure S13. The overall barrier is 17.4 kcal mol^{-1} to give **4′** at -36.3 kcal mol^{-1}. The equivalent silylation product for the ketone benzophenone, **4′′**, is also shown in Figure S13 at -33.5 kcal mol^{-1}.

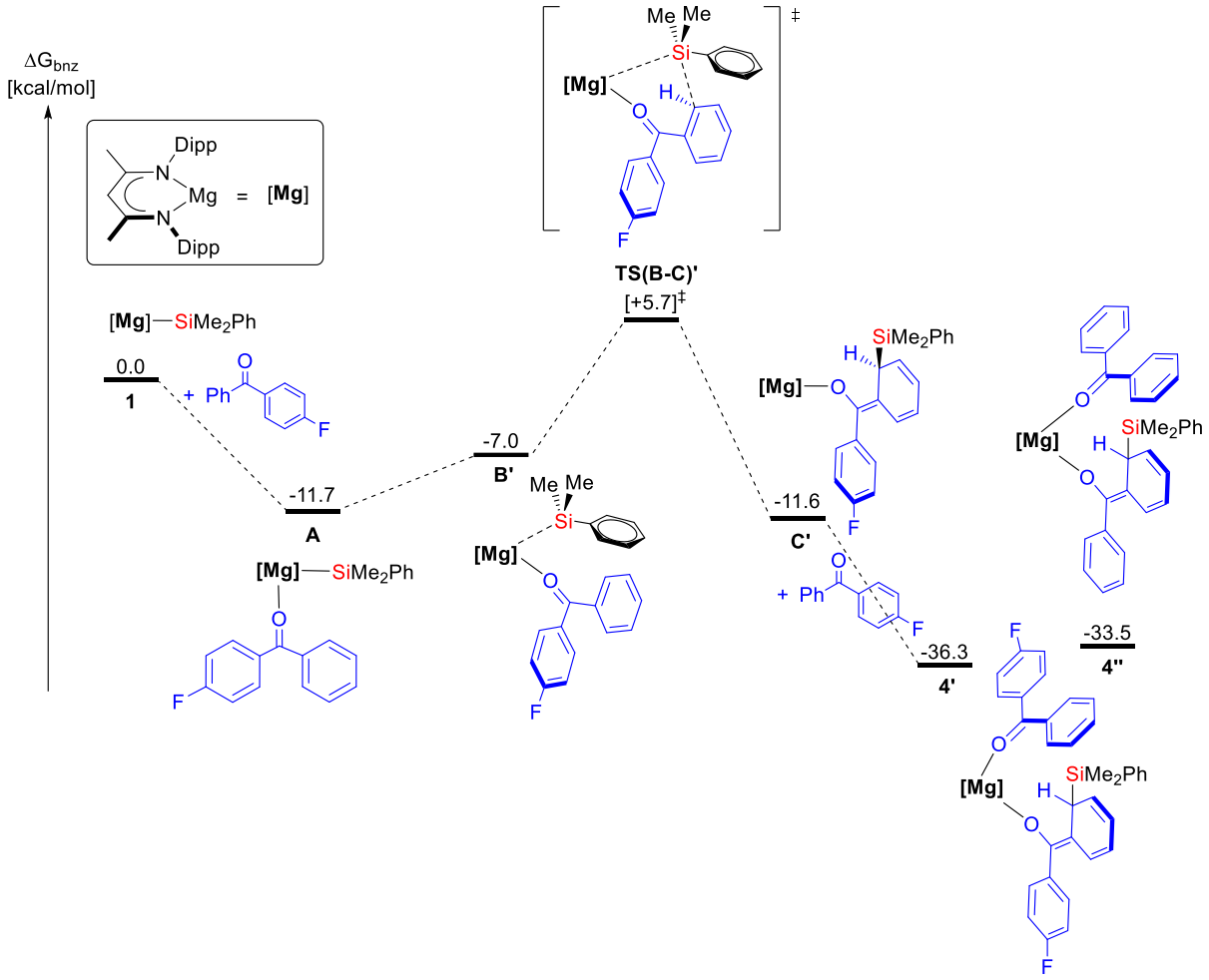


Figure S13: DFT calculated free energy profile (BP86-D3(BJ)-benzene/BS2//BP86/BS1, in kcal mol^{-1}) for the reaction of **1** with PhC(O)(C$_6$H$_4$-*p*-F) to form **4′**. Computed structure **4′′** also shown.

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Cartesian Coordinates and Computed Energies (in Hartrees)

PhC(=O)Me
SCF (BP86) Energy = -384.890526431
Enthalpy 0K = -384.756555
Enthalpy 298K = -384.747565
Free Energy 298K = -384.789429
Lowest Frequency = 66.9213 cm^{-1}
Second Frequency = 147.5339 cm^{-1}
SCF (BP86-D3BJ) Energy = -384.917634508
SCF (C6H6) Energy = -384.893162211
SCF (BS2) Energy = -384.992020751

O	-2.22489	-1.32130	0.00102
C	-1.70555	-0.20199	0.00018
C	-2.56866	1.05579	-0.00090
H	-3.62603	0.75736	-0.00055
H	-2.36407	1.67976	0.88707
H	-2.36418	1.67799	-0.89016
C	-0.20839	-0.05102	0.00006
C	0.43589	1.20516	0.00049
C	0.57525	-1.22615	-0.00044
C	1.83653	1.28319	0.00044
H	-0.15431	2.12701	0.00091
C	1.97192	-1.14819	-0.00051
H	0.05162	-2.18715	-0.00073
C	2.60573	0.10791	-0.00006
H	2.32880	2.26128	0.00080
H	2.57185	-2.06433	-0.00088
H	3.69917	0.17027	-0.00009

PhC(=O)Ph
SCF (BP86) Energy = -576.623309768
Enthalpy 0K = -576.437366
Enthalpy 298K = -576.425337
Free Energy 298K = -576.475232
Lowest Frequency = 42.1834 cm^{-1}
Second Frequency = 64.3203 cm^{-1}
SCF (BP86-D3BJ) Energy = -576.670272879
SCF (C6H6) Energy = -576.626243261
SCF (BS2) Energy = -576.769376102

C	3.83941	-0.89879	-0.11835
C	2.71931	-1.55016	-0.65916
C	1.45644	-0.94021	-0.60625
C	1.30630	0.33687	-0.02143
C	2.44557	0.99589	0.49252
C	3.69992	0.37719	0.45782
H	4.82241	-1.38047	-0.15241
H	2.82915	-2.53389	-1.12745
H	0.58975	-1.44215	-1.04698
H	2.31530	1.99815	0.91192
H	4.57412	0.88947	0.87317
C	-0.00001	1.08399	-0.00013
C	-1.30631	0.33684	0.02136
C	-1.45633	-0.94036	0.60596
C	-2.44569	0.99594	-0.49225
C	-2.71918	-1.55033	0.65899
H	-0.58955	-1.44238	1.04642
C	-3.70003	0.37723	-0.45742
H	-2.31549	1.99826	-0.91151
C	-3.83940	-0.89885	0.11854
H	-2.82893	-2.53416	1.12709
H	-4.57430	0.88960	-0.87250
H	-4.82239	-1.38055	0.15270
O	-0.00002	2.32332	-0.00022

PhC(=O)(C_6H_4-*p*-F)
SCF (BP86) Energy = -675.857861063
Enthalpy 0K = -675.679917
Enthalpy 298K = -675.667041
Free Energy 298K = -675.719054
Lowest Frequency = 39.9924 cm^{-1}
Second Frequency = 60.9980 cm^{-1}
SCF (BP86-D3BJ) Energy = -675.905169535
SCF (C6H6) Energy = -675.860736904
SCF (BS2) Energy = -676.041298969

C	0.47950	1.16134	-0.01374
O	0.57594	2.39736	-0.01474
C	-0.87852	0.51861	-0.00193
C	-1.12996	-0.76034	0.54463
C	-1.96694	1.28302	-0.48233
C	-2.43265	-1.27513	0.59466
H	-0.30637	-1.34659	0.96233
C	-3.26873	0.77668	-0.45798
H	-1.76024	2.28468	-0.87069
C	-3.48015	-0.50054	0.08205
H	-2.64736	-2.25569	1.02778
H	-4.11863	1.34884	-0.83985
C	1.72444	0.31581	-0.02341
C	1.78920	-0.95818	-0.63039
C	2.89965	0.87615	0.52536
C	3.00250	-1.66249	-0.67001
H	0.89738	-1.38325	-1.10108
C	4.10335	0.16327	0.50389
H	2.83832	1.87800	0.96109
C	4.15716	-1.10920	-0.09384
H	3.04691	-2.64269	-1.15609
H	5.00504	0.59944	0.94639
H	5.10087	-1.66437	-0.11757
F	-4.73961	-0.99681	0.11599

fluorene
SCF (BP86) Energy = -575.430864630
Enthalpy 0K = -575.266181
Enthalpy 298K = -575.255330
Free Energy 298K = -575.301574
Lowest Frequency = 94.8673 cm^{-1}
Second Frequency = 126.1437 cm^{-1}
SCF (BP86-D3BJ) Energy = -575.477105157
SCF (C6H6) Energy = -575.433882746
SCF (BS2) Energy = -575.574206025

C	3.04675	-1.40176	-0.00017
C	3.48598	-0.06565	-0.00019
C	2.55169	0.98936	-0.00011
C	1.19358	0.66990	-0.00001
C	0.74333	-0.67616	-0.00000
C	1.67214	-1.72215	-0.00008
H	3.78460	-2.21108	-0.00023
H	4.55860	0.15296	-0.00026
H	2.86851	2.03752	-0.00011
H	1.35143	-2.76933	-0.00007
C	-0.00001	1.58610	0.00013
C	-1.19376	0.66980	0.00009
C	-2.55180	0.98954	0.00010
C	-3.48609	-0.06553	0.00010
C	-3.04680	-1.40159	0.00008
C	-1.67217	-1.72210	0.00006
C	-0.74330	-0.67616	0.00006

H -2.86852 2.03771 0.00012
H -4.55875 0.15289 0.00012
H -3.78474 -2.21084 0.00008
H -1.35161 -2.76930 0.00003
O   0.00040 2.81723 -0.00001

1

SCF (BP86) Energy = -1555.60305410
Enthalpy 0K = -1554.823872
Enthalpy 298K = -1554.773580
Free Energy 298K = -1554.911662
Lowest Frequency = 6.5296 cm^{-1}
Second Frequency = 14.6959 cm^{-1}
SCF (BP86-D3BJ) Energy = -1555.83016688
SCF (C6H6) Energy = -1555.61047988
SCF (BS2) Energy = -2040.84309061

Si -0.17412 1.83588 -1.84437
Mg 0.21019 -0.19758 -0.21665
N -0.94280 -1.66299 0.67376
N   1.96018 -0.88947 0.64007
C -2.36150 -1.60791 0.41456
C   2.03531 -1.97026 1.44467
C -3.19929 -0.81621 1.25287
C -4.26042 -2.09097 -1.03284
H -4.67971 -2.58621 -1.91609
C -0.45004 -2.63178 1.47409
C   0.91994 -2.76315 1.81075
H   1.15182 -3.60543 2.46668
C -2.89540 -2.26420 -0.73217
C   3.15599 -0.14078 0.34043
C   3.51132 0.97363 1.15452
C -1.49956 3.07004 -1.18394
C -4.55715 -0.67624 0.90692
H -5.20776 -0.06232 1.53979
C -2.02776 -3.13864 -1.64092
H -1.03463 -3.22721 -1.16600
C -5.08945 -1.30109 -0.22723
H -6.14776 -1.17670 -0.47999
C   4.61600 1.76052 0.77520
H   4.89386 2.62312 1.39137
C   3.38421 -2.38436 2.01138
H   4.10717 -2.58157 1.20152
H   3.29810 -3.28604 2.63487
H   3.81800 -1.57366 2.62168
C -3.86018 3.67170 -0.82017
H -4.92216 3.42181 -0.92612
C -2.66186 -0.11288 2.50182
H -1.62099 -0.45071 2.65054
C -1.40035 -3.65806 2.07033
H -2.16336 -3.16654 2.69793
H -0.86194 -4.39478 2.68392
H -1.95034 -4.19217 1.27694
C -2.88247 2.78060 -1.28994
H -3.20605 1.83953 -1.75206
C   3.55777 -1.64567 -1.72046
H   2.76173 -2.21783 -1.21204
C   3.91472 -0.45798 -0.82324
C   2.71452 1.34327 2.40822
H   1.99519 0.52707 2.59708
C   4.75294 -2.60162 -1.93332
H   5.57448 -2.11087 -2.48400
H   4.44120 -3.48241 -2.52134
H   5.16387 -2.96042 -0.97425
C -1.14320 4.29593 -0.57183
H -0.08461 4.56563 -0.47685
C -2.63555 1.42179 2.31956
H -2.03912 1.72486 1.44217
H -2.21050 1.91176 3.21340
H -3.65255 1.82251 2.16708
C -1.82630 -2.48392 -3.02651
H -2.79006 -2.36091 -3.55156
H -1.17324 -3.10655 -3.66338
H -1.36865 -1.48351 -2.93981
C -3.47901 4.88184 -0.21592
H -4.23941 5.57908 0.15288
C   5.01050 0.36114 -1.15776
H   5.59710 0.12861 -2.05379
C   3.61208 1.46843 3.65969
H   4.19826 0.55010 3.83447
H   2.99670 1.65611 4.55674
H   4.32568 2.30597 3.56835
C -3.45720 -0.49375 3.77129
H -4.50176 -0.14010 3.71749
H -2.99883 -0.03343 4.66390
H -3.48397 -1.58597 3.92691
C   1.90167 2.64073 2.19165
H   2.56915 3.49567 1.98380
H   1.30710 2.88657 3.08902
H   1.20697 2.54964 1.33798
C -2.59856 -4.56654 -1.79493
H -2.74298 -5.05688 -0.81712
H -1.91324 -5.19289 -2.39232
H -3.57491 -4.56020 -2.31045
C -2.11510 5.19023 -0.09136
H -1.80619 6.13322 0.37458
C   2.99505 -1.16930 -3.07963
H   2.10530 -0.52892 -2.94573
H   2.70735 -2.02974 -3.70935
H   3.74520 -0.57954 -3.63536
C   1.43904 2.85941 -2.09776
H   1.86851 3.20952 -1.14416
H   1.25675 3.74075 -2.73882
H   2.20996 2.23666 -2.58311
C -0.76570 1.36651 -3.62179
H -0.05672 0.67434 -4.10901
H -0.84411 2.27065 -4.25150
H -1.75383 0.87648 -3.61185
C   5.36284 1.46437 -0.37130
H   6.21683 2.09050 -0.65031

2

SCF (BP86) Energy = -3249.06781181
Enthalpy 0K = -3247.578531
Enthalpy 298K = -3247.486235
Free Energy 298K = -3247.706584
Lowest Frequency = 5.1638 cm^{-1}
Second Frequency = 15.0562 cm^{-1}
SCF (BP86-D3BJ) Energy = -3249.59578829
SCF (C6H6) Energy = -3249.07473461
SCF (BS2) Energy = -3648.33763176

Mg 1.45899 -0.61764 0.20315
O -0.04883 0.24678 1.27322
N   3.46617 0.16014 0.23606
N   2.08672 -2.60078 0.72498
C   5.63863 0.26879 1.47536
H   5.99304 0.99996 0.73667
H   6.44589 -0.44721 1.69249
H   5.42634 0.82330 2.40784
C   4.36752 -0.45243 1.03660
C   4.22832 -1.75284 1.58119
H   5.06808 -2.05797 2.21050
C   3.25474 -2.76158 1.39325
C   3.58311 -4.09630 2.05656
H   2.94459 -4.24787 2.94452

H	4.63344	-4.12526	2.38149
H	3.39398	-4.94940	1.38818
C	1.32994	-3.82255	0.51541
C	1.56409	-4.58444	-0.67055
C	0.87963	-5.80416	-0.83648
H	1.06563	-6.40203	-1.73477
C	-0.03181	-6.26783	0.11951
H	-0.55450	-7.21870	-0.03089
C	-0.26634	-5.50603	1.26822
H	-0.97850	-5.86635	2.01838
C	0.41207	-4.29251	1.49973
C	0.15416	-3.54713	2.80999
H	0.92321	-2.76297	2.90470
C	0.27402	-4.46219	4.05074
H	-0.53970	-5.20756	4.08790
H	0.20659	-3.85885	4.97242
H	1.22923	-5.01461	4.07226
C	-1.22285	-2.85124	2.79976
H	-1.30941	-2.14255	1.96156
H	-1.37863	-2.28490	3.73357
H	-2.04037	-3.58479	2.69949
C	2.57037	-4.13948	-1.73611
H	2.70581	-3.05048	-1.61923
C	2.06772	-4.39295	-3.17290
H	2.03388	-5.46977	-3.41669
H	2.74936	-3.91870	-3.90010
H	1.05870	-3.97631	-3.32238
C	3.95297	-4.80752	-1.54234
H	4.41400	-4.53391	-0.58028
H	4.64584	-4.49769	-2.34478
H	3.86557	-5.90837	-1.57878
C	3.90372	1.39561	-0.39141
C	4.59970	1.34242	-1.64034
C	4.99077	2.55184	-2.24815
H	5.52689	2.51759	-3.20249
C	4.72323	3.79175	-1.65677
H	5.03464	4.71869	-2.15045
C	4.07764	3.83063	-0.41761
H	3.89280	4.79587	0.06653
C	3.67833	2.65148	0.24298
C	3.08930	2.76975	1.64771
H	2.93118	1.75054	2.03742
C	4.05987	3.49222	2.61307
H	5.06307	3.03402	2.61194
H	3.66487	3.45263	3.64259
H	4.18159	4.55584	2.34113
C	1.72799	3.48941	1.64056
H	1.81098	4.50899	1.22937
H	1.33317	3.56806	2.66752
H	0.98556	2.94979	1.03206
C	5.01986	0.02513	-2.30229
H	4.42012	-0.78414	-1.84967
C	4.77967	0.01735	-3.82851
H	3.75721	0.33893	-4.08167
H	4.93677	-0.99767	-4.23349
H	5.48534	0.68506	-4.35356
C	6.50738	-0.29979	-2.01751
H	7.16184	0.50049	-2.40668
H	6.79645	-1.24393	-2.51234
H	6.71069	-0.40814	-0.94091
C	-0.33821	0.60487	2.56185
C	-1.61332	0.88008	2.94126
H	-2.44847	0.79743	2.24056
H	-1.85959	1.13947	3.97032
C	0.76287	0.66084	3.57240
C	1.86432	-0.21799	3.52714
H	1.94378	-0.96344	2.73157
C	2.85889	-0.19331	4.51816
H	3.69370	-0.89788	4.44902
C	2.77992	0.72140	5.57836
H	3.55560	0.74369	6.35083
C	1.69519	1.61398	5.63351
H	1.62484	2.34420	6.44692
C	0.70483	1.58642	4.64327
H	-0.12087	2.30296	4.68488
Mg	-1.45908	0.61767	-0.20301
O	0.04869	-0.24677	-1.27307
N	-3.46625	-0.16020	-0.23562
N	-2.08686	2.60076	-0.72506
C	-5.63913	-0.26872	-1.47427
H	-5.99277	-1.00063	-0.73596
H	-6.44670	0.44734	-1.69006
H	-5.42754	-0.82228	-2.40748
C	-4.36779	0.45235	-1.03594
C	-4.22863	1.75269	-1.58075
H	-5.06853	2.05776	-2.20991
C	-3.25496	2.76142	-1.39321
C	-3.58332	4.09596	-2.05690
H	-2.94486	4.24718	-2.94496
H	-4.63367	4.12489	-2.38175
H	-3.39406	4.94928	-1.38883
C	-1.33011	3.82262	-0.51581
C	-1.56446	4.58495	0.66983
C	-0.88006	5.80476	0.83542
H	-1.06622	6.40295	1.73347
C	0.03150	6.26812	-0.12061
H	0.55410	7.21909	0.02951
C	0.26622	5.50590	-1.26900
H	0.97846	5.86597	-2.01921
C	-0.41209	4.29226	-1.50014
C	-0.15384	3.54641	-2.81006
H	-0.92234	2.76165	-2.90430
C	-0.27445	4.46079	-4.05124
H	0.53866	5.20680	-4.08874
H	-0.20656	3.85708	-4.97264
H	-1.23011	5.01242	-4.07302
C	1.22370	2.85156	-2.79963
H	1.31094	2.14345	-1.96101
H	1.37977	2.28477	-3.73312
H	2.04069	3.58577	-2.69991
C	-2.57091	4.14044	1.73541
H	-2.70682	3.05150	1.61854
C	-2.06810	4.39372	3.17218
H	-2.03356	5.47054	3.41587
H	-2.75001	3.91996	3.89944
H	-1.05934	3.97645	3.32166
C	-3.95322	4.80910	1.54165
H	-4.41434	4.53575	0.57956
H	-4.64625	4.49953	2.34405
H	-3.86534	5.90991	1.57815
C	-3.90349	-1.39581	0.39180
C	-4.59912	-1.34291	1.64093
C	-4.98986	-2.55248	2.24867
H	-5.52570	-2.51845	3.20318
C	-4.72234	-3.79226	1.65702
H	-5.03351	-4.71932	2.15063
C	-4.07713	-3.83085	0.41765
H	-3.89235	-4.79599	-0.06672
C	-3.67815	-2.65156	-0.24286
C	-3.08962	-2.76955	-1.64782
H	-2.93154	-1.75026	-2.03735
C	-4.06062	-3.49170	-2.61298
H	-5.06376	-3.03336	-2.61139
H	-3.66599	-3.45194	-3.64263
H	-4.18237	-4.55536	-2.34122
C	-1.72838	-3.48935	-1.64132

H	-1.81131	-4.50899	-1.23027
H	-1.33398	-3.56786	-2.66846
H	-0.98566	-2.94990	-1.03303
C	-5.01939	-0.02580	2.30315
H	-4.42017	0.78369	1.85026
C	-4.77844	-0.01800	3.82925
H	-3.75565	-0.33899	4.08185
H	-4.93591	0.99690	4.23439
H	-5.48344	-0.68616	4.35461
C	-6.50717	0.29856	2.01910
H	-7.16115	-0.50187	2.40876
H	-6.79631	1.24269	2.51390
H	-6.71109	0.40661	0.94258
C	0.33822	-0.60430	-2.56183
C	1.61347	-0.87870	-2.94135
H	2.44858	-0.79576	-2.24064
H	1.85985	-1.13765	-3.97050
C	-0.76286	-0.66058	-3.57237
C	-1.86476	0.21769	-3.52694
H	-1.94465	0.96293	-2.73122
C	-2.85930	0.19273	-4.51797
H	-3.69445	0.89689	-4.44869
C	-2.77987	-0.72170	-5.57838
H	-3.55553	-0.74421	-6.35086
C	-1.69469	-1.61373	-5.63370
H	-1.62397	-2.34374	-6.44727
C	-0.70435	-1.58589	-4.64345
H	0.12170	-2.30201	-4.68520

3

SCF (BP86) Energy = -2132.24128814
Enthalpy 0K = -2131.274584
Enthalpy 298K = -2131.211921
Free Energy 298K = -2131.375300
Lowest Frequency = 13.7676 cm^{-1}
Second Frequency = 18.4533 cm^{-1}
SCF (BP86-D3BJ) Energy = -2132.55279427
SCF (C6H6) Energy = -2132.24780317
SCF (BS2) Energy = -2617.62170294

Si	0.51148	0.02033	2.83817
Mg	0.55919	-0.03658	0.17607
O	-1.36360	-0.48546	-0.55419
N	1.67834	-1.49788	-0.85902
N	1.15615	1.49674	-1.14955
C	2.51594	-2.50177	-2.97554
H	3.32769	-3.01426	-2.43525
H	2.89405	-2.16775	-3.95317
H	1.73097	-3.25874	-3.14943
C	1.96191	-1.33481	-2.16553
C	1.77554	-0.11985	-2.87901
H	2.01197	-0.18099	-3.94484
C	1.49477	1.19482	-2.41631
C	1.57456	2.29421	-3.46932
H	0.56076	2.51904	-3.84848
H	2.19563	1.98907	-4.32503
H	1.97205	3.23116	-3.05130
C	1.12304	2.87513	-0.72957
C	2.31676	3.47809	-0.22681
C	2.25712	4.80094	0.25247
H	3.17117	5.27071	0.63269
C	1.05949	5.52568	0.25656
H	1.03484	6.55138	0.63976
C	-0.10419	4.92691	-0.23785
H	-1.04217	5.49421	-0.24446
C	-0.09786	3.61068	-0.74074
C	-1.39333	3.02675	-1.30524
H	-1.16802	2.00495	-1.65684
C	-1.90723	3.84005	-2.51608
H	-2.20359	4.86085	-2.21578
H	-2.79131	3.35208	-2.96263
H	-1.13705	3.93749	-3.29950
C	-2.49548	2.92431	-0.22805
H	-2.16543	2.33612	0.64400
H	-3.40281	2.45040	-0.64385
H	-2.78714	3.92338	0.14168
C	3.65981	2.74275	-0.22627
H	3.45440	1.68295	-0.45774
C	4.36329	2.79702	1.14693
H	4.65416	3.82729	1.41858
H	5.28883	2.19480	1.12416
H	3.71759	2.40586	1.94893
C	4.60079	3.29066	-1.32590
H	4.15667	3.20124	-2.33080
H	5.55744	2.73878	-1.32879
H	4.82804	4.35795	-1.15318
C	2.09214	-2.71200	-0.20192
C	3.32742	-2.71699	0.51627
C	3.72325	-3.89746	1.17399
H	4.67313	-3.91292	1.71828
C	2.92567	-5.04823	1.15422
H	3.25187	-5.95540	1.67394
C	1.70259	-5.02236	0.47739
H	1.06781	-5.91591	0.47780
C	1.26317	-3.87077	-0.20528
C	-0.10452	-3.89776	-0.88982
H	-0.21879	-2.94923	-1.44352
C	-0.24258	-5.06032	-1.89900
H	0.56335	-5.05197	-2.65243
H	-1.20848	-4.99809	-2.43065
H	-0.20917	-6.04106	-1.39273
C	-1.23632	-3.96653	0.16115
H	-1.15967	-4.88949	0.76252
H	-2.22786	-3.96341	-0.32504
H	-1.19330	-3.11010	0.85367
C	4.22524	-1.47818	0.56768
H	3.57479	-0.60195	0.38797
C	4.90669	-1.28329	1.93824
H	4.17858	-1.32733	2.76483
H	5.40732	-0.30051	1.97432
H	5.68218	-2.04681	2.12781
C	5.29010	-1.49757	-0.55479
H	5.93844	-2.38735	-0.46174
H	5.93371	-0.60194	-0.49499
H	4.83085	-1.51396	-1.55611
C	-2.53017	-0.63789	-0.99558
C	-2.82201	-0.33317	-2.42600
C	-1.76677	-0.40801	-3.36616
H	-0.76454	-0.69449	-3.02963
C	-2.00208	-0.10867	-4.71272
H	-1.18276	-0.18424	-5.43467
C	-3.28160	0.29428	-5.13535
H	-3.46071	0.53363	-6.18884
C	-4.32845	0.40095	-4.20423
H	-5.31926	0.73653	-4.52654
C	-4.10521	0.08323	-2.85745
H	-4.91552	0.18776	-2.13046
C	-3.60635	-1.11916	-0.08832
C	-4.68101	-1.91424	-0.55822
H	-4.73323	-2.18953	-1.61569
C	-5.64933	-2.38837	0.33648
H	-6.46535	-3.01950	-0.02987
C	-5.56949	-2.05671	1.69990
H	-6.33512	-2.41768	2.39479
C	-4.50513	-1.26937	2.17408
H	-4.43241	-1.00184	3.23253

C	-3.51852	-0.81724	1.29124
H	-2.68539	-0.21262	1.66317
C	1.93520	1.00076	3.71235
H	2.92710	0.64576	3.38300
H	1.87923	0.88615	4.80979
H	1.87044	2.07831	3.48268
C	0.61714	-1.76035	3.58752
H	-0.23446	-2.39078	3.27592
H	0.64326	-1.74503	4.69292
H	1.53284	-2.26635	3.23549
C	-1.06852	0.80299	3.64896
C	-1.39941	2.16078	3.40965
H	-0.76987	2.75623	2.73480
C	-2.50479	2.77571	4.01996
H	-2.72478	3.83027	3.81681
C	-3.32657	2.04184	4.89243
H	-4.18911	2.51762	5.37219
C	-3.02558	0.69412	5.14821
H	-3.64905	0.11563	5.84123
C	-1.91377	0.08848	4.53334
H	-1.69068	-0.96041	4.76221

4

SCF (BP86) Energy = -2907.36423649
Enthalpy 0K = -2906.226906
Enthalpy 298K = -2906.150140
Free Energy 298K = -2906.346087
Lowest Frequency = 10.3157 cm^{-1}
Second Frequency = 10.7485 cm^{-1}
SCF (BP86-D3BJ) Energy = -2907.76267774
SCF (C6H6) Energy = -2907.37064858
SCF (BS2) Energy = -3392.96433290

Mg	1.22362	-0.53203	-0.01899
O	-0.46178	-1.07925	-0.78138
N	2.00627	-1.93777	1.34069
N	3.04236	-0.21275	-0.98445
C	3.64957	-3.74455	1.87065
H	4.39597	-3.33666	2.57552
H	4.16150	-4.50596	1.26131
H	2.86432	-4.22695	2.46976
C	3.10867	-2.62827	0.98366
C	3.88721	-2.36323	-0.17649
H	4.68221	-3.09168	-0.35611
C	3.93576	-1.22635	-1.02013
C	5.08335	-1.18962	-2.02095
H	4.69599	-1.36400	-3.04052
H	5.83349	-1.96354	-1.80165
H	5.57917	-0.20635	-2.03678
C	3.37362	1.01176	-1.67106
C	4.08013	2.03064	-0.95760
C	4.39959	3.23008	-1.62452
H	4.95578	4.00684	-1.08885
C	4.02076	3.45052	-2.95495
H	4.28486	4.38747	-3.45752
C	3.30661	2.45864	-3.63533
H	3.00379	2.62888	-4.67471
C	2.97690	1.23297	-3.02180
C	2.19944	0.19420	-3.82872
H	2.10176	-0.71463	-3.21009
C	2.92514	-0.20009	-5.13555
H	2.97431	0.64661	-5.84338
H	2.38497	-1.02332	-5.63289
H	3.96002	-0.53394	-4.94879
C	0.77487	0.70175	-4.14269
H	0.22452	0.93968	-3.21834
H	0.20566	-0.06799	-4.69075
H	0.80379	1.61517	-4.76362
C	4.51552	1.84387	0.49854
H	3.91513	1.01438	0.91285
C	4.25289	3.09697	1.36144
H	4.89302	3.94599	1.06330
H	4.47536	2.88274	2.42060
H	3.20310	3.42690	1.29241
C	6.00458	1.43537	0.59794
H	6.20434	0.48618	0.07538
H	6.30317	1.30816	1.65363
H	6.65437	2.21060	0.15373
C	1.42899	-2.20884	2.63751
C	1.99688	-1.61858	3.80528
C	1.40905	-1.88643	5.05723
H	1.84181	-1.43316	5.95631
C	0.29163	-2.71806	5.17506
H	-0.14393	-2.92491	6.15867
C	-0.26762	-3.28294	4.02210
H	-1.14399	-3.93201	4.11421
C	0.27242	-3.04166	2.74293
C	-0.36345	-3.69866	1.51481
H	-0.18791	-3.02328	0.65966
C	0.29478	-5.05926	1.18236
H	1.36719	-4.95779	0.95339
H	-0.19383	-5.51443	0.30343
H	0.19203	-5.76043	2.03015
C	-1.88894	-3.88359	1.64311
H	-2.15249	-4.66513	2.37863
H	-2.31247	-4.19120	0.67350
H	-2.39376	-2.95022	1.94216
C	3.20648	-0.68240	3.75092
H	3.58698	-0.67919	2.71490
C	2.79201	0.76437	4.10282
H	2.02977	1.14475	3.40381
H	3.66419	1.44061	4.06642
H	2.36716	0.81827	5.12055
C	4.35508	-1.14766	4.67504
H	4.06675	-1.09290	5.73962
H	5.24171	-0.50365	4.54110
H	4.65477	-2.18870	4.46806
C	-1.11132	-1.88197	-1.60818
C	-0.29853	-2.61361	-2.63109
C	0.94629	-3.18471	-2.27427
H	1.29124	-3.12989	-1.23596
C	1.73362	-3.85640	-3.22027
H	2.68515	-4.30000	-2.90849
C	1.30500	-3.96237	-4.55445
H	1.91995	-4.48628	-5.29367
C	0.08101	-3.38340	-4.93154
H	-0.25753	-3.44348	-5.97179
C	-0.70759	-2.71451	-3.98358
H	-1.64789	-2.24490	-4.29014
C	-2.50435	-2.07074	-1.48951
C	-3.18699	-3.18170	-2.10324
H	-2.65663	-3.78515	-2.84546
C	-4.43784	-3.59501	-1.69468
H	-4.92255	-4.47294	-2.12972
C	-5.06177	-2.94114	-0.56939
C	-4.52745	-1.85012	0.03848
H	-5.00979	-1.41306	0.91671
C	-3.32797	-1.17598	-0.57181
H	-2.67606	-0.73248	0.20157
C	-2.57526	1.38655	-2.28359
H	-1.88916	1.73348	-1.49457
H	-2.94046	2.26376	-2.84435
H	-1.99321	0.75573	-2.97424
C	-5.06479	1.46018	-0.41152
C	-6.36261	1.06400	-0.00344
H	-6.77899	0.11696	-0.36570

C	-7.13494	1.85880	0.85859
H	-8.13551	1.52683	1.15742
C	-6.62839	3.08029	1.33193
H	-7.23051	3.70463	2.00114
C	-5.34802	3.49853	0.93608
H	-4.95045	4.45554	1.29346
C	-4.57888	2.69589	0.07710
H	-3.58438	3.04554	-0.22435
Si	-4.01941	0.37130	-1.58350
C	-5.12559	-0.22672	-3.01112
H	-5.55923	0.63888	-3.54026
H	-4.54386	-0.82017	-3.73492
H	-5.95278	-0.85779	-2.64913
C	0.00021	2.21115	1.12961
O	0.65517	1.29358	0.54454
C	-0.09646	3.53624	0.48449
C	-1.11090	4.47431	0.81487
C	0.81561	3.85611	-0.55666
C	-1.19629	5.70050	0.14856
H	-1.85689	4.22429	1.57382
C	0.74566	5.08207	-1.21946
H	1.58912	3.13230	-0.82754
C	-0.25958	5.98972	-0.85432
H	-1.97918	6.42678	0.38180
H	1.45499	5.33813	-2.01041
C	-0.64318	1.92763	2.43632
C	-0.69754	2.89602	3.46996
C	-1.14135	0.62572	2.68891
C	-1.24931	2.56984	4.71569
H	-0.26695	3.88847	3.30692
C	-1.70284	0.31045	3.93018
H	-1.11022	-0.12247	1.89003
C	-1.75965	1.28132	4.94611
H	-1.27146	3.32076	5.51212
H	-2.08405	-0.69884	4.10890
F	-6.20365	-3.51676	-0.08998
F	-0.33529	7.17801	-1.49458
H	-2.19557	1.03084	5.91866

5

SCF (BP86) Energy = -2706.58661577
Enthalpy 0K = -2705.473492
Enthalpy 298K = -2705.401306
Free Energy 298K = -2705.585028
Lowest Frequency = 7.5912 cm^{-1}
Second Frequency = 10.1410 cm^{-1}
SCF (BP86-D3BJ) Energy = -2706.97613274
SCF (C6H6) Energy = -2706.59383262
SCF (BS2) Energy = -3192.10971605

Si	2.62840	-2.79962	0.87909
Mg	1.09463	0.16225	0.04949
O	-1.03144	0.19825	-0.04955
O	1.56520	-1.62278	0.39881
N	1.51993	1.79764	1.27830
N	1.68315	1.12654	-1.69773
C	1.25403	4.24259	1.64074
H	0.66707	4.04939	2.55400
H	0.82880	5.10799	1.11087
H	2.26892	4.51707	1.97628
C	1.29328	3.01595	0.73860
C	1.10801	3.25849	-0.64701
H	0.81635	4.28219	-0.89313
C	1.36936	2.43555	-1.77532
C	1.24952	3.10857	-3.13722
H	2.04233	2.77915	-3.82598
H	1.27907	4.20506	-3.05081
H	0.28639	2.82799	-3.60137
C	2.19939	0.45068	-2.86142
C	1.33020	-0.25362	-3.74109
C	1.88117	-0.94192	-4.84035
H	1.21248	-1.48691	-5.51636
C	3.25654	-0.93815	-5.08745
H	3.66679	-1.47211	-5.95135
C	4.10737	-0.25385	-4.21101
H	5.18583	-0.26522	-4.39713
C	3.61115	0.43492	-3.08748
C	4.58386	1.14422	-2.14060
H	4.10228	1.16047	-1.14495
C	4.83535	2.61365	-2.55715
H	5.24511	2.66318	-3.58207
H	5.56657	3.08763	-1.87808
H	3.91400	3.21544	-2.52719
C	5.93419	0.40917	-2.00645
H	5.79806	-0.65548	-1.75591
H	6.54037	0.87492	-1.21080
H	6.53009	0.46915	-2.93462
C	-0.18135	-0.30248	-3.52574
H	-0.42742	0.38398	-2.69598
C	-0.95826	0.17007	-4.77445
H	-0.64163	1.17914	-5.09000
H	-2.04128	0.19591	-4.56862
H	-0.79827	-0.50872	-5.63092
C	-0.63065	-1.72172	-3.10842
H	-0.41902	-2.45282	-3.90926
H	-1.71622	-1.74560	-2.90863
H	-0.10049	-2.05929	-2.20171
C	1.97260	1.72560	2.64490
C	3.34971	1.95279	2.95049
C	3.78001	1.84451	4.28705
H	4.83706	2.01763	4.51978
C	2.89452	1.51682	5.31938
H	3.24997	1.43946	6.35236
C	1.55108	1.28173	5.01194
H	0.85260	1.01864	5.81471
C	1.06928	1.37825	3.69180
C	-0.41269	1.10836	3.43544
H	-0.58662	1.24111	2.35294
C	-1.31959	2.11196	4.18466
H	-1.20031	2.02159	5.27872
H	-2.38399	1.92599	3.95378
H	-1.08544	3.15627	3.91412
C	-0.78790	-0.34318	3.80950
H	-0.18865	-1.07125	3.23836
H	-1.85483	-0.53873	3.60521
H	-0.61459	-0.53361	4.88335
C	4.39125	2.26783	1.87468
H	3.86545	2.35676	0.90873
C	5.40816	1.11010	1.75356
H	5.95619	0.95986	2.70048
H	6.15227	1.32267	0.96658
H	4.90592	0.16071	1.50431
C	5.13052	3.59994	2.13678
H	4.43282	4.44984	2.22606
H	5.82851	3.82164	1.31061
H	5.72257	3.55842	3.06815
C	-2.17725	-0.21194	0.24661
C	-2.43067	-1.54220	0.82275
C	-1.42597	-2.53653	0.74310
H	-0.43571	-2.28406	0.33677
C	-1.67903	-3.83166	1.20581
H	-0.90173	-4.59695	1.12447
C	-2.93378	-4.13491	1.76309
H	-3.14691	-5.15169	2.11030
C	-3.91804	-3.14570	1.89046
H	-4.88190	-3.40937	2.33461

C	-3.68913	-1.82706	1.44326
C	-4.67880	-0.74665	1.64945
C	-5.75149	-0.89044	2.56136
H	-5.83949	-1.80670	3.15212
C	-6.68804	0.13068	2.74938
H	-7.50593	-0.00477	3.46415
C	-6.56407	1.32823	2.02778
H	-7.28845	2.13717	2.16646
C	-5.49550	1.49634	1.13648
H	-5.39091	2.43426	0.58442
C	-4.54286	0.47858	0.94720
C	-3.41485	0.65650	-0.08385
C	-3.95230	0.21170	-1.47908
C	-4.45365	-1.03035	-1.87935
H	-4.46132	-1.88374	-1.19483
C	-4.96674	-1.16418	-3.18420
H	-5.36285	-2.13101	-3.51044
C	-4.98073	-0.06847	-4.06591
H	-5.38919	-0.18843	-5.07454
C	-4.47562	1.17912	-3.66349
H	-4.49255	2.03163	-4.35069
C	-3.95346	1.31771	-2.36631
C	-3.40167	2.49028	-1.67461
C	-3.06826	2.12325	-0.34771
C	-2.55755	3.06947	0.54474
H	-2.31281	2.79540	1.57529
C	-2.37823	4.39299	0.10124
H	-1.98507	5.14493	0.79261
C	-2.70371	4.75930	-1.21790
H	-2.56007	5.79449	-1.54469
C	-3.21721	3.81116	-2.11693
H	-3.47670	4.10075	-3.14074
C	4.26644	-2.72301	-0.09333
H	4.07617	-2.77484	-1.17881
H	4.93334	-3.55988	0.17837
H	4.80239	-1.78006	0.11161
C	3.01653	-2.69459	2.74224
H	3.41817	-1.69625	2.98662
H	3.76671	-3.44340	3.05233
H	2.11000	-2.84250	3.35388
C	1.86125	-4.52500	0.52292
C	1.73954	-5.52761	1.51357
H	2.08882	-5.32476	2.53299
C	1.17470	-6.78370	1.22754
H	1.09416	-7.54089	2.01624
C	0.71536	-7.06770	-0.06896
H	0.27555	-8.04519	-0.29679
C	0.82782	-6.09086	-1.07339
H	0.47431	-6.30554	-2.08848
C	1.39376	-4.84025	-0.77641
H	1.47077	-4.08935	-1.57231

4''

SCF (BP86) Energy = -2708.89455339
Enthalpy 0K = -2707.740848
Enthalpy 298K = -2707.666177
Free Energy 298K = -2707.855386
Lowest Frequency = 10.8161 cm^{-1}
Second Frequency = 12.7374 cm^{-1}
SCF (BP86-D3BJ) Energy = -2709.2920684
SCF (C6H6) Energy = -2708.90055344
SCF (BS2) Energy = -3194.41761491

Mg	-1.16222	-0.24571	-0.20176
O	0.48796	-1.21962	-0.46587
N	-2.32351	0.30027	-1.87369
N	-2.78072	-1.11313	0.80755
C	-4.21119	-0.15392	-3.44742
H	-5.00612	0.59468	-3.28299
H	-4.70328	-1.08096	-3.78200
H	-3.56619	0.22495	-4.25343
C	-3.43912	-0.40335	-2.15629
C	-4.01390	-1.37437	-1.29445
H	-4.86519	-1.90845	-1.72464
C	-3.79441	-1.63424	0.08170
C	-4.79608	-2.57274	0.74270
H	-4.32346	-3.54871	0.95057
H	-5.66837	-2.74554	0.09545
H	-5.14343	-2.17868	1.71094
C	-2.81508	-1.28654	2.23939
C	-3.38026	-0.24853	3.04477
C	-3.39982	-0.40972	4.44428
H	-3.84218	0.37545	5.06628
C	-2.86421	-1.55019	5.05581
H	-2.89402	-1.65851	6.14553
C	-2.29315	-2.54954	4.26036
H	-1.86801	-3.44055	4.73606
C	-2.25976	-2.44672	2.85479
C	-1.61119	-3.57267	2.04994
H	-1.79104	-3.37569	0.97934
C	-2.20493	-4.96052	2.38262
H	-1.96006	-5.27331	3.41340
H	-1.79084	-5.71933	1.69729
H	-3.30418	-4.97585	2.28618
C	-0.08160	-3.57925	2.26503
H	0.36447	-2.62706	1.93678
H	0.38375	-4.39011	1.67926
H	0.17053	-3.73260	3.32978
C	-3.97943	1.01561	2.42223
H	-3.54665	1.11581	1.41066
C	-3.63334	2.29410	3.21535
H	-4.14027	2.32238	4.19615
H	-3.96067	3.18728	2.65701
H	-2.54885	2.38214	3.39521
C	-5.51273	0.89188	2.25646
H	-5.78571	0.04802	1.60264
H	-5.93094	1.81219	1.81132
H	-6.00146	0.73668	3.23504
C	-2.01536	1.43917	-2.70115
C	-2.76847	2.64475	-2.56160
C	-2.42708	3.75450	-3.35904
H	-3.00076	4.68211	-3.25318
C	-1.37290	3.69800	-4.27664
H	-1.13089	4.56799	-4.89708
C	-0.63082	2.51643	-4.39728
H	0.19537	2.47332	-5.11313
C	-0.92696	1.37546	-3.62443
C	-0.11788	0.09142	-3.82229
H	-0.07155	-0.42663	-2.84708
C	-0.81067	-0.86904	-4.81870
H	-1.81228	-1.17099	-4.47452
H	-0.20891	-1.78537	-4.94528
H	-0.91868	-0.39041	-5.80873
C	1.33332	0.34432	-4.27352
H	1.38321	0.71305	-5.31433
H	1.90828	-0.59410	-4.23036
H	1.84292	1.07816	-3.62739
C	-3.90340	2.79771	-1.54503
H	-4.12483	1.80216	-1.12436
C	-3.46023	3.70520	-0.37493
H	-2.57451	3.29119	0.13317
H	-4.27293	3.80935	0.36594
H	-3.19973	4.71638	-0.73421
C	-5.20363	3.34115	-2.17997
H	-5.08230	4.38114	-2.53093
H	-6.02147	3.33982	-1.43849

H	-5.52588	2.73709	-3.04494
C	1.09257	-2.17707	-1.15412
C	0.31378	-3.43322	-1.40435
C	-1.03695	-3.37090	-1.81844
H	-1.50077	-2.39920	-2.01804
C	-1.79127	-4.53675	-2.01306
H	-2.83141	-4.45242	-2.34559
C	-1.21931	-5.79967	-1.78382
H	-1.80901	-6.71036	-1.93263
C	0.11689	-5.88069	-1.35579
H	0.57193	-6.85752	-1.15762
C	0.87146	-4.71343	-1.16580
H	1.90415	-4.78368	-0.80875
C	2.40683	-2.01530	-1.63905
C	2.97450	-2.88423	-2.64088
H	2.45026	-3.81114	-2.89183
C	4.07971	-2.52478	-3.38566
H	4.44811	-3.19538	-4.16890
C	4.66644	-1.20727	-3.24105
C	4.22518	-0.36143	-2.26491
H	4.62966	0.65282	-2.17937
C	3.25051	-0.81967	-1.21935
H	2.60412	0.00179	-0.86085
C	3.24784	-1.63579	1.85229
H	2.61730	-0.76928	2.10877
H	3.85290	-1.90228	2.73586
H	2.57704	-2.48039	1.62858
C	5.55419	0.13961	0.74222
C	6.69720	0.38308	-0.05923
H	6.89674	-0.25944	-0.92450
C	7.58393	1.43332	0.22646
H	8.46026	1.59711	-0.41083
C	7.35185	2.26939	1.33113
H	8.04426	3.08731	1.55890
C	6.22984	2.04502	2.14436
H	6.04681	2.68856	3.01282
C	5.34489	0.99358	1.85084
H	4.47880	0.83302	2.50256
Si	4.35774	-1.30007	0.34945
C	5.39352	-2.84910	-0.03338
H	6.08650	-3.05222	0.80096
H	4.74510	-3.72965	-0.16925
H	5.98553	-2.72486	-0.95391
C	0.21259	2.24817	1.31224
O	-0.51450	1.44000	0.65181
C	0.77954	1.83938	2.61989
C	1.99659	2.37508	3.11574
C	0.10731	0.85438	3.38624
C	2.50567	1.95121	4.35059
H	2.56100	3.09130	2.51258
C	0.61414	0.44533	4.62393
H	-0.83071	0.43169	3.01594
C	1.81425	0.99293	5.11194
H	3.45104	2.36464	4.71671
H	0.06522	-0.30225	5.20428
H	2.21328	0.66931	6.07885
C	0.46406	3.59567	0.75097
C	0.72937	4.72310	1.57117
C	0.37731	3.77695	-0.65304
C	0.92646	5.98523	0.99864
H	0.74226	4.61194	2.65902
C	0.59357	5.03719	-1.21905
H	0.14369	2.91897	-1.28948
C	0.87132	6.14435	-0.39723
H	1.11512	6.84970	1.64345
H	0.53214	5.15272	-2.30522
H	1.03380	7.13151	-0.84252
H	5.42336	-0.87647	-3.96153

A

SCF (BP86) Energy = -2231.47277261
Enthalpy 0K = -2230.514572
Enthalpy 298K = -2230.450759
Free Energy 298K = -2230.618446
Lowest Frequency = 9.3407 cm^{-1}
Second Frequency = 14.9938 cm^{-1}
SCF (BP86-D3BJ) Energy = -2231.78607905
SCF (C6H6) Energy = -2231.48018791
SCF (BS2) Energy = -2716.89123071

Mg	0.25634	0.08821	0.20375
O	-1.69179	-0.75917	0.27080
N	0.82642	-0.69568	-1.67495
N	-0.18878	1.98730	-0.59633
C	0.40255	-0.90809	-4.11624
H	1.39561	-0.71064	-4.55512
H	-0.35605	-0.56696	-4.83708
H	0.32445	-2.00026	-3.99584
C	0.24854	-0.18828	-2.78172
C	-0.49129	1.02596	-2.82427
H	-0.91426	1.25934	-3.80529
C	-0.59211	2.08166	-1.87539
C	-1.18343	3.38844	-2.38723
H	-2.00006	3.73738	-1.73334
H	-1.56472	3.28292	-3.41372
H	-0.42256	4.18735	-2.38273
C	-0.18467	3.17187	0.22532
C	0.96352	4.01849	0.24418
C	0.96569	5.13942	1.09759
H	1.84506	5.79355	1.11231
C	-0.12252	5.43307	1.92653
H	-0.09811	6.30906	2.58337
C	-1.23957	4.59117	1.91001
H	-2.09281	4.81402	2.56114
C	-1.29541	3.46099	1.07177
C	-2.54317	2.57792	1.10278
H	-2.41588	1.79937	0.33130
C	-3.82938	3.36577	0.76659
H	-4.04386	4.13668	1.52766
H	-4.69871	2.68609	0.72659
H	-3.75258	3.87616	-0.20854
C	-2.68804	1.86630	2.46713
H	-1.79307	1.26502	2.70166
H	-3.56748	1.19712	2.46986
H	-2.82195	2.59561	3.28554
C	2.19907	3.74838	-0.61784
H	2.00932	2.82766	-1.19634
C	3.44950	3.50480	0.25697
H	3.67444	4.38270	0.88823
H	4.33399	3.31334	-0.37453
H	3.31650	2.63537	0.92146
C	2.46472	4.89425	-1.62190
H	1.59696	5.07911	-2.27782
H	3.32892	4.65179	-2.26489
H	2.69313	5.84056	-1.10018
C	1.77341	-1.77324	-1.83446
C	3.11866	-1.48200	-2.21613
C	4.03784	-2.54302	-2.32469
H	5.07136	-2.32076	-2.61330
C	3.66609	-3.86702	-2.06757
H	4.39746	-4.67686	-2.16180
C	2.34878	-4.14301	-1.68735
H	2.05078	-5.17871	-1.48711
C	1.38845	-3.11934	-1.56384
C	-0.03783	-3.49795	-1.16328
H	-0.62182	-2.56435	-1.09688
C	-0.71336	-4.39848	-2.22361

H	-0.73652	-3.91539	-3.21523
H	-1.75394	-4.62814	-1.93266
H	-0.17874	-5.35842	-2.33441
C	-0.07148	-4.17943	0.22274
H	0.50610	-5.12069	0.22132
H	-1.10713	-4.42296	0.51577
H	0.35850	-3.52547	1.00023
C	3.61402	-0.05884	-2.48685
H	2.75305	0.62416	-2.38576
C	4.67727	0.36427	-1.44795
H	4.28909	0.30933	-0.41859
H	5.01266	1.39853	-1.64112
H	5.56569	-0.28898	-1.49945
C	4.18076	0.10078	-3.91709
H	5.08407	-0.51766	-4.06286
H	4.46629	1.15116	-4.10206
H	3.45191	-0.19282	-4.69173
C	-2.86131	-1.19395	0.43052
C	-3.97847	-0.61532	-0.36130
C	-3.68585	-0.01253	-1.61004
H	-2.65013	0.00644	-1.96985
C	-4.70215	0.55737	-2.38004
H	-4.49645	1.01188	-3.35269
C	-6.01347	0.54680	-1.88216
C	-6.33529	-0.01350	-0.63818
H	-7.36675	0.02324	-0.27845
C	-5.31317	-0.59997	0.11603
H	-5.54580	-1.02002	1.09840
C	-3.11401	-2.28770	1.40938
C	-4.14125	-3.24564	1.22911
H	-4.78276	-3.19814	0.34429
C	-4.30553	-4.28369	2.15667
H	-5.08887	-5.03229	2.00105
C	-3.46294	-4.36695	3.27841
C	-2.43634	-3.42274	3.46051
H	-1.76962	-3.48848	4.32590
C	-2.25194	-2.40063	2.52414
H	-1.44101	-1.67666	2.64091
C	3.40017	-0.51175	2.30834
C	3.77962	-1.74319	1.71869
H	3.00493	-2.43369	1.35993
C	5.12637	-2.11039	1.57259
H	5.38154	-3.07232	1.11393
C	6.14340	-1.23974	2.00044
H	7.19643	-1.51937	1.88327
C	5.79772	-0.00651	2.57506
H	6.58270	0.68133	2.91112
C	4.44507	0.34665	2.72811
H	4.20036	1.30828	3.19458
Si	1.52999	-0.07797	2.54864
C	0.95850	-1.39928	3.85677
H	-0.04047	-1.15321	4.26145
H	0.91736	-2.41966	3.43755
H	1.66329	-1.41516	4.70713
C	1.50427	1.56776	3.56185
H	1.86141	2.42959	2.97335
H	0.47150	1.80382	3.87304
H	2.11914	1.49353	4.47775
F	-6.99859	1.10071	-2.62157
H	-3.59971	-5.17431	4.00534

B

SCF (BP86) Energy = -2231.46682885
Enthalpy 0K = -2230.508051
Enthalpy 298K = -2230.444750
Free Energy 298K = -2230.609063
Lowest Frequency = 6.7246 cm^{-1}
Second Frequency = 12.4861 cm^{-1}

SCF (BP86-D3BJ) Energy = -2231.78551872
SCF (C6H6) Energy = -2231.47240465
SCF (BS2) Energy = -2716.88577102

Mg	0.77724	-0.38425	0.01657
O	-0.81354	0.56345	-0.87628
N	0.58020	-2.31601	-0.90016
N	2.69737	-0.07235	-0.80115
C	1.33449	-4.13024	-2.46128
H	2.29582	-4.66257	-2.36724
H	1.11898	-4.04942	-3.54029
H	0.54872	-4.73941	-1.99445
C	1.45365	-2.74207	-1.83315
C	2.57029	-2.00249	-2.30052
H	3.11942	-2.49396	-3.10927
C	3.18239	-0.82598	-1.81136
C	4.51413	-0.46394	-2.45955
H	4.62139	0.62542	-2.57938
H	4.61315	-0.94775	-3.44320
H	5.36098	-0.79647	-1.83397
C	3.59333	0.89041	-0.21062
C	4.59735	0.44282	0.70311
C	5.43409	1.39777	1.31077
H	6.19917	1.06276	2.02013
C	5.31239	2.76349	1.02711
H	5.97785	3.48926	1.50652
C	4.33288	3.19072	0.12507
H	4.24219	4.25842	-0.10488
C	3.45960	2.27819	-0.50072
C	2.42339	2.80522	-1.49515
H	1.76753	1.95995	-1.77097
C	3.09147	3.32129	-2.79120
H	3.77084	4.16579	-2.57821
H	2.32725	3.67580	-3.50547
H	3.68291	2.53469	-3.28938
C	1.53824	3.90731	-0.87567
H	1.01967	3.53960	0.02480
H	0.77334	4.24124	-1.59660
H	2.13260	4.79145	-0.58490
C	4.77300	-1.03710	1.06203
H	4.19181	-1.63364	0.33892
C	4.20188	-1.33957	2.46632
H	4.72900	-0.75745	3.24311
H	4.31344	-2.41093	2.71190
H	3.13074	-1.08254	2.52494
C	6.24374	-1.50273	0.97123
H	6.68771	-1.27522	-0.01311
H	6.30965	-2.59313	1.13088
H	6.87559	-1.02168	1.73848
C	-0.56298	-3.12511	-0.57188
C	-0.62285	-3.74257	0.71886
C	-1.79245	-4.43538	1.08643
H	-1.84689	-4.90996	2.07039
C	-2.88342	-4.54554	0.21417
H	-3.78206	-5.09214	0.51978
C	-2.80372	-3.96986	-1.05676
H	-3.64876	-4.07205	-1.74715
C	-1.66118	-3.26089	-1.47981
C	-1.65326	-2.70190	-2.90856
H	-0.68334	-2.20389	-3.07670
C	-1.80926	-3.82899	-3.95957
H	-1.06583	-4.63079	-3.82895
H	-1.69981	-3.42099	-4.97997
H	-2.80982	-4.29212	-3.89632
C	-2.76020	-1.64887	-3.13493
H	-3.76450	-2.08787	-3.00032
H	-2.70736	-1.25117	-4.16404
H	-2.66849	-0.80822	-2.43346

C	0.58654	-3.72065	1.66014
H	1.00895	-2.69528	1.63747
C	0.24483	-4.04696	3.12639
H	-0.57982	-3.42595	3.51186
H	1.12614	-3.86753	3.76435
H	-0.03540	-5.10843	3.25168
C	1.69484	-4.68450	1.17059
H	1.31683	-5.72180	1.13764
H	2.55694	-4.65918	1.86024
H	2.05809	-4.41876	0.16694
C	-1.87892	1.24041	-0.93446
C	-1.86480	2.51161	-1.72049
C	-1.20577	2.51308	-2.97108
H	-0.73643	1.58976	-3.32345
C	-1.17736	3.67446	-3.75388
H	-0.68624	3.65969	-4.73222
C	-1.77501	4.85642	-3.28166
H	-1.74526	5.76642	-3.88990
C	-2.40144	4.87135	-2.02410
H	-2.84396	5.79732	-1.64274
C	-2.45904	3.70407	-1.24846
H	-2.91537	3.72307	-0.25373
C	-3.12508	0.73963	-0.31638
C	-4.39143	1.32142	-0.58508
H	-4.46562	2.18326	-1.25237
C	-5.55833	0.78680	-0.03239
H	-6.54062	1.22095	-0.23546
C	-5.45587	-0.34512	0.78748
C	-4.22579	-0.95985	1.06222
H	-4.18938	-1.85463	1.68784
C	-3.06925	-0.41579	0.50536
H	-2.10243	-0.88656	0.69901
C	0.30593	-0.50245	4.02112
H	-0.56860	-1.17190	3.95895
H	0.23089	0.06671	4.96522
H	1.20139	-1.14453	4.08389
C	-1.14411	1.82464	2.71217
C	-1.13815	3.17719	2.29154
H	-0.23134	3.59665	1.83950
C	-2.25097	4.01862	2.46831
H	-2.19835	5.06662	2.14917
C	-3.41952	3.52419	3.07123
H	-4.28744	4.17668	3.21813
C	-3.45493	2.18664	3.50053
H	-4.35499	1.79104	3.98551
C	-2.33512	1.35851	3.32189
H	-2.38770	0.32336	3.67968
Si	0.42361	0.70050	2.51016
C	1.87081	1.89450	2.97665
H	1.67392	2.37713	3.95097
H	2.82393	1.34526	3.04810
H	2.02172	2.68533	2.22367
F	-6.58324	-0.87157	1.31609

TS(B-C)

SCF (BP86) Energy = -2231.44335686
Enthalpy 0K = -2230.484775
Enthalpy 298K = -2230.422564
Free Energy 298K = -2230.582452
Lowest Frequency = -175.5360 cm^{-1}
Second Frequency = 13.5463 cm^{-1}
SCF (BP86-D3BJ) Energy = -2231.76676459
SCF (C6H6) Energy = -2231.44952066
SCF (BS2) Energy = -2716.86350727

Mg	0.77373	-0.01635	0.33318
O	-0.75381	-0.55558	1.40203
N	1.75504	1.72019	0.99041
N	2.42319	-1.26773	0.55067
C	3.41935	2.76551	2.53963
H	4.51156	2.65254	2.62181
H	3.01901	2.83076	3.56654
H	3.19381	3.71442	2.03289
C	2.80959	1.56655	1.81998
C	3.43976	0.32932	2.10780
H	4.23171	0.39907	2.85858
C	3.33901	-0.93975	1.48867
C	4.40056	-1.95060	1.90316
H	4.01202	-2.97987	1.89204
H	4.78406	-1.71758	2.90819
H	5.25652	-1.92342	1.20611
C	2.61217	-2.50197	-0.17209
C	3.54731	-2.54783	-1.25089
C	3.65729	-3.73624	-1.99851
H	4.36299	-3.77586	-2.83612
C	2.88954	-4.86573	-1.69288
H	2.99330	-5.78118	-2.28497
C	1.99375	-4.81660	-0.61926
H	1.40362	-5.70543	-0.37004
C	1.83132	-3.64966	0.15406
C	0.85900	-3.66954	1.33681
H	0.73635	-2.63383	1.69682
C	1.41829	-4.51105	2.50901
H	1.56853	-5.56276	2.20608
H	0.71429	-4.50122	3.35946
H	2.38688	-4.12486	2.86820
C	-0.54217	-4.18287	0.94196
H	-0.96363	-3.59748	0.10782
H	-1.23478	-4.09493	1.79537
H	-0.52166	-5.24306	0.63306
C	4.42891	-1.35191	-1.63147
H	4.29985	-0.57424	-0.85968
C	4.00548	-0.73367	-2.98420
H	4.07262	-1.47443	-3.80036
H	4.66166	0.11564	-3.24524
H	2.96709	-0.36308	-2.95662
C	5.92871	-1.72722	-1.67462
H	6.26288	-2.19992	-0.73560
H	6.54570	-0.82737	-1.84282
H	6.14695	-2.43401	-2.49438
C	1.26185	3.04896	0.71295
C	1.60847	3.65874	-0.53380
C	1.05887	4.91719	-0.84549
H	1.31700	5.39512	-1.79510
C	0.18995	5.57331	0.03630
H	-0.23065	6.54898	-0.22892
C	-0.13064	4.97509	1.25771
H	-0.80405	5.49226	1.95020
C	0.39328	3.71911	1.62674
C	0.02016	3.15142	3.00076
H	0.54411	2.18762	3.12384
C	0.46868	4.09588	4.14319
H	1.53737	4.35660	4.07778
H	0.28805	3.62349	5.12465
H	-0.10260	5.04066	4.12278
C	-1.49573	2.87983	3.13009
H	-2.07736	3.81239	3.02284
H	-1.72404	2.45899	4.12519
H	-1.85704	2.17114	2.36976
C	2.59812	2.99053	-1.49431
H	2.40283	1.90002	-1.46038
C	2.45595	3.45332	-2.95803
H	1.41478	3.39919	-3.31446
H	3.07517	2.81738	-3.61348
H	2.80931	4.49126	-3.09255
C	4.06231	3.19967	-1.03559

H	4.30134	4.27692	-0.98871
H	4.75959	2.72859	-1.75085
H	4.25233	2.76212	-0.04411
C	-2.05340	-0.45057	1.34465
C	-2.81555	-1.40743	2.20046
C	-2.33606	-1.66285	3.50728
H	-1.44475	-1.13016	3.85182
C	-2.99127	-2.57274	4.34653
H	-2.61504	-2.74490	5.36074
C	-4.12674	-3.26477	3.88964
H	-4.63701	-3.97935	4.54401
C	-4.59335	-3.04458	2.58374
H	-5.45933	-3.60109	2.20950
C	-3.94569	-2.12558	1.74388
H	-4.28758	-1.99707	0.71231
C	-2.64350	0.51782	0.48579
C	-4.05694	0.72071	0.36324
H	-4.73173	0.12277	0.98007
C	-4.58886	1.67278	-0.48271
H	-5.66568	1.82932	-0.57738
C	-3.69383	2.50216	-1.22166
C	-2.32599	2.40979	-1.11877
H	-1.69061	3.16273	-1.59059
C	-1.73779	1.34641	-0.33159
H	-0.81152	1.66330	0.16052
C	-0.44121	1.08805	-3.59794
H	-0.91936	2.07635	-3.50930
H	-0.72824	0.65928	-4.57468
H	0.65139	1.23395	-3.60556
C	-2.70769	-0.74813	-2.58273
C	-3.18527	-1.96608	-2.04134
H	-2.54286	-2.55373	-1.37435
C	-4.46611	-2.45432	-2.34558
H	-4.80375	-3.40581	-1.91885
C	-5.30791	-1.73006	-3.20677
H	-6.30625	-2.10990	-3.45025
C	-4.85562	-0.52307	-3.76170
H	-5.50173	0.04539	-4.44015
C	-3.57247	-0.04113	-3.45133
H	-3.24003	0.90167	-3.89938
Si	-0.93870	-0.12498	-2.19979
C	0.12416	-1.71784	-2.53434
H	-0.08200	-2.03977	-3.57239
H	1.20891	-1.55405	-2.43896
H	-0.13959	-2.55226	-1.86548
F	-4.24211	3.48953	-1.97784

C

SCF (BP86) Energy = -2231.47753691
Enthalpy 0K = -2230.519648
Enthalpy 298K = -2230.456233
Free Energy 298K = -2230.624550
Lowest Frequency = 8.2068 cm^{-1}
Second Frequency = 9.9955 cm^{-1}
SCF (BP86-D3BJ) Energy = -2231.77826819
SCF (C6H6) Energy = -2231.48818206
SCF (BS2) Energy = -2716.90095009

Mg	-1.32850	-0.30853	-0.12879
O	0.21905	-0.38605	0.87921
N	-1.87489	-1.48365	-1.69951
N	-2.95087	0.91666	-0.11887
C	-3.57625	-2.38643	-3.26652
H	-3.15616	-2.03442	-4.22522
H	-4.67107	-2.41884	-3.36470
H	-3.19401	-3.40844	-3.11795
C	-3.15408	-1.46209	-2.13560
C	-4.15446	-0.58777	-1.63717
H	-5.14579	-0.74852	-2.06741
C	-4.06574	0.54637	-0.78996
C	-5.31667	1.40656	-0.69871
H	-5.47819	1.78072	0.32399
H	-6.20427	0.84500	-1.02546
H	-5.22112	2.29514	-1.34758
C	-2.93774	2.19597	0.55635
C	-2.63416	3.37581	-0.18547
C	-2.59139	4.60828	0.49380
H	-2.35415	5.51903	-0.06744
C	-2.84520	4.69275	1.86738
H	-2.81469	5.66192	2.37616
C	-3.12914	3.52708	2.58637
H	-3.31970	3.59168	3.66311
C	-3.17252	2.26569	1.95962
C	-3.47835	1.02806	2.80527
H	-3.32070	0.13865	2.16751
C	-4.95266	1.00473	3.27305
H	-5.17881	1.87948	3.90814
H	-5.15450	0.09656	3.86743
H	-5.65670	1.01679	2.42401
C	-2.52770	0.91295	4.01639
H	-1.47209	0.92116	3.70164
H	-2.70756	-0.03041	4.55770
H	-2.67816	1.74314	4.72875
C	-2.31437	3.34229	-1.68228
H	-2.51867	2.32167	-2.05040
C	-0.81592	3.63697	-1.92592
H	-0.54808	4.64522	-1.56439
H	-0.57471	3.58861	-3.00214
H	-0.16811	2.91507	-1.39921
C	-3.19181	4.31694	-2.49967
H	-4.26764	4.13561	-2.33622
H	-2.98770	4.20594	-3.57876
H	-2.98925	5.36874	-2.23230
C	-0.91246	-2.30197	-2.40669
C	-0.22448	-1.75395	-3.52861
C	0.72381	-2.55238	-4.19616
H	1.25878	-2.13709	-5.05759
C	0.99904	-3.85943	-3.77972
H	1.73670	-4.46629	-4.31488
C	0.33525	-4.37796	-2.66314
H	0.56308	-5.39502	-2.32563
C	-0.61685	-3.61964	-1.95353
C	-1.28014	-4.23616	-0.72044
H	-1.92934	-3.46093	-0.27168
C	-2.18183	-5.43940	-1.08239
H	-2.98164	-5.16059	-1.78900
H	-2.65974	-5.85074	-0.17610
H	-1.59298	-6.24972	-1.54697
C	-0.22629	-4.65359	0.33102
H	0.40873	-5.47377	-0.04694
H	-0.71720	-5.01097	1.25240
H	0.43749	-3.81559	0.60005
C	-0.44770	-0.31598	-4.00303
H	-1.27209	0.11224	-3.40536
C	0.81452	0.54124	-3.75017
H	1.10702	0.53230	-2.68590
H	0.64587	1.58984	-4.05054
H	1.67558	0.16070	-4.32645
C	-0.86434	-0.24034	-5.48906
H	-0.06647	-0.61631	-6.15299
H	-1.07115	0.80446	-5.77937
H	-1.77155	-0.83490	-5.69080
C	0.94141	-1.01393	1.81770
C	0.18096	-1.58569	2.96601
C	-1.05933	-2.23678	2.75410
H	-1.42456	-2.37539	1.72874

C	-1.79994	-2.77151	3.81678
H	-2.74285	-3.29162	3.61430
C	-1.33117	-2.65024	5.13654
H	-1.90795	-3.06492	5.96962
C	-0.11838	-1.98059	5.37304
H	0.24716	-1.85510	6.39814
C	0.62261	-1.45220	4.30660
H	1.54842	-0.90397	4.50680
C	2.32862	-1.11245	1.67779
C	3.14760	-1.99443	2.48026
H	2.69926	-2.49389	3.34394
C	4.43232	-2.32524	2.12287
H	5.02468	-3.03644	2.70484
C	4.97243	-1.82951	0.87549
C	4.30854	-0.95629	0.07938
H	4.73077	-0.64914	-0.88115
C	3.02343	-0.33625	0.56222
H	2.31864	-0.18036	-0.27562
C	1.89134	2.36362	1.82946
H	1.13747	2.50096	1.03819
H	2.14659	3.35321	2.24571
H	1.42259	1.76402	2.62667
C	4.20628	2.46362	-0.25698
C	5.54294	2.24467	-0.67314
H	6.16226	1.51224	-0.14245
C	6.09924	2.94707	-1.75413
H	7.13624	2.75719	-2.05304
C	5.32962	3.89557	-2.44762
H	5.76238	4.44781	-3.28906
C	4.00404	4.13520	-2.05193
H	3.39862	4.87838	-2.58316
C	3.45376	3.42600	-0.97125
H	2.41948	3.63549	-0.67388
Si	3.45243	1.47813	1.19712
C	4.72722	1.37814	2.60625
H	5.00818	2.39145	2.93983
H	4.31168	0.83137	3.46834
H	5.64238	0.85311	2.28927
F	6.18018	-2.34512	0.49626

B′

SCF (BP86) Energy = -2231.46615583
Enthalpy 0K = -2230.506972
Enthalpy 298K = -2230.443968
Free Energy 298K = -2230.607089
Lowest Frequency = 9.5308 cm^{-1}
Second Frequency = 12.0422 cm^{-1}
SCF (BP86-D3BJ) Energy = -2231.78456828
SCF (C6H6) Energy = -2231.47196903
SCF (BS2) Energy = -2716.88491445

Mg	0.83320	-0.04761	-0.00718
O	-1.12715	-0.15008	-0.63726
N	1.68743	-1.67534	-1.10511
N	2.06874	1.38420	-0.94839
C	3.06610	-2.61613	-2.97758
H	4.14410	-2.44761	-3.13515
H	2.60155	-2.67457	-3.97688
H	2.92973	-3.58445	-2.47676
C	2.46999	-1.45707	-2.18001
C	2.85204	-0.17859	-2.66142
H	3.44622	-0.21043	-3.57990
C	2.75530	1.10590	-2.07668
C	3.56391	2.19367	-2.77912
H	3.12870	3.19338	-2.63464
H	3.63506	1.98077	-3.85757
H	4.59440	2.22925	-2.38366
C	2.32352	2.64725	-0.30689
C	3.54361	2.84547	0.40874
C	3.75239	4.07589	1.06146
H	4.68253	4.23348	1.61882
C	2.79819	5.09746	1.01675
H	2.98163	6.04839	1.52808
C	1.60143	4.89126	0.31999
H	0.85522	5.69122	0.29273
C	1.33602	3.67656	-0.34215
C	0.02561	3.49091	-1.11199
H	-0.25865	2.42422	-1.02763
C	0.20155	3.79419	-2.61912
H	0.55258	4.83087	-2.76864
H	-0.76128	3.68424	-3.14907
H	0.92782	3.11450	-3.09121
C	-1.14142	4.32757	-0.55015
H	-1.24257	4.21209	0.54212
H	-2.08874	4.01351	-1.01959
H	-1.01529	5.40424	-0.76338
C	4.61317	1.75321	0.52568
H	4.38130	0.96552	-0.21061
C	4.57971	1.09190	1.92296
H	4.78727	1.83128	2.71692
H	5.34090	0.29447	1.99592
H	3.59257	0.64557	2.13077
C	6.03513	2.27420	0.21735
H	6.08373	2.78634	-0.75879
H	6.75403	1.43656	0.20047
H	6.38530	2.98864	0.98300
C	1.35570	-3.02220	-0.71869
C	1.94262	-3.55728	0.47306
C	1.52668	-4.82391	0.92494
H	1.96704	-5.23857	1.83632
C	0.56908	-5.57173	0.22753
H	0.25920	-6.55483	0.59798
C	0.03101	-5.06042	-0.95626
H	-0.70063	-5.65483	-1.51540
C	0.40775	-3.79764	-1.45739
C	-0.19654	-3.34597	-2.79270
H	0.21842	-2.35308	-3.03634
C	0.16926	-4.32203	-3.93852
H	1.25454	-4.49158	-4.01633
H	-0.18851	-3.93005	-4.90713
H	-0.30867	-5.30570	-3.78501
C	-1.73260	-3.20463	-2.72672
H	-2.21504	-4.17474	-2.51332
H	-2.12781	-2.84330	-3.69288
H	-2.04047	-2.50244	-1.94019
C	3.05836	-2.80619	1.20777
H	2.77481	-1.73457	1.23793
C	3.27715	-3.26976	2.66068
H	2.34338	-3.26912	3.24514
H	3.99001	-2.59449	3.16352
H	3.71152	-4.28489	2.70247
C	4.39816	-2.90315	0.43774
H	4.71072	-3.95802	0.33965
H	5.19314	-2.36286	0.98159
H	4.32674	-2.47057	-0.57107
C	-2.38379	-0.22925	-0.52801
C	-3.21931	0.80526	-1.20056
C	-2.78747	1.30421	-2.45234
H	-1.86110	0.91630	-2.88513
C	-3.54066	2.25966	-3.14234
H	-3.23543	2.63456	-4.12277
C	-4.71767	2.74041	-2.55095
C	-5.15712	2.29403	-1.29752
H	-6.06600	2.71703	-0.86159
C	-4.40896	1.31703	-0.62961
H	-4.71630	0.98578	0.36628

C	-3.00685	-1.37516	0.17981
C	-4.36566	-1.73218	-0.01301
H	-4.99391	-1.14479	-0.68738
C	-4.89851	-2.86230	0.61931
H	-5.94628	-3.13276	0.45390
C	-2.73509	-3.31712	1.63840
H	-2.09577	-3.93777	2.27304
C	-2.19680	-2.19514	1.00342
H	-1.14403	-1.93319	1.14176
C	0.90967	-0.76890	3.93964
H	0.51561	-1.78650	3.77259
H	0.61929	-0.45318	4.95840
H	2.01054	-0.83653	3.91265
C	-1.60590	0.68381	3.01222
C	-2.34761	1.76501	2.47751
H	-1.85219	2.47388	1.80216
C	-3.69801	1.97678	2.80527
H	-4.23065	2.84186	2.39231
C	-4.35980	1.08912	3.67057
H	-5.41126	1.25064	3.93348
C	-3.65333	-0.00121	4.20506
H	-4.15592	-0.69805	4.88610
C	-2.30029	-0.19379	3.88029
H	-1.76975	-1.04307	4.32634
Si	0.28183	0.49409	2.61688
C	0.98819	2.19422	3.20989
H	0.71557	2.37361	4.26549
H	2.08635	2.22834	3.12370
H	0.59472	3.02867	2.60637
C	-4.08749	-3.65396	1.44925
H	-4.50504	-4.54039	1.93833
F	-5.44971	3.66722	-3.20992

TS(B-C)'

SCF (BP86) Energy = -2231.44155777
Enthalpy 0K = -2230.483057
Enthalpy 298K = -2230.420828
Free Energy 298K = -2230.581127
Lowest Frequency = -180.3813 cm^{-1}
Second Frequency = 14.1351 cm^{-1}
SCF (BP86-D3BJ) Energy = -2231.76460051
SCF (C6H6) Energy = -2231.44765131
SCF (BS2) Energy = -2716.86115891

Mg	0.73011	0.18117	-0.32083
O	-1.02823	0.04700	-1.12798
N	2.21172	-1.03890	-1.17480
N	1.70032	1.97867	-0.72951
C	3.91353	-1.37617	-2.97813
H	4.83743	-0.83265	-3.22949
H	3.42086	-1.64279	-3.92954
H	4.17600	-2.31275	-2.46606
C	2.98768	-0.50001	-2.14015
C	3.02602	0.87778	-2.47275
H	3.66247	1.10965	-3.33117
C	2.52284	2.01773	-1.80078
C	3.02657	3.35538	-2.32810
H	2.27748	4.15203	-2.20802
H	3.30129	3.27168	-3.39074
H	3.92809	3.67592	-1.77686
C	1.49294	3.20290	0.00496
C	2.48392	3.63952	0.93646
C	2.22650	4.79140	1.70479
H	2.97578	5.12635	2.43115
C	1.03934	5.51777	1.55804
H	0.86089	6.41300	2.16307
C	0.08603	5.09378	0.62582
H	-0.83660	5.67103	0.49979
C	0.28346	3.94019	-0.15929
C	-0.78144	3.54639	-1.18670
H	-0.54332	2.53396	-1.55514
C	-0.76941	4.50421	-2.40218
H	-0.99393	5.54050	-2.09227
H	-1.53187	4.19925	-3.14021
H	0.20885	4.51168	-2.91119
C	-2.19854	3.48694	-0.57778
H	-2.23277	2.81320	0.29451
H	-2.91715	3.10694	-1.32285
H	-2.54980	4.48123	-0.24951
C	3.81255	2.90008	1.13733
H	3.88639	2.11592	0.36484
C	3.87824	2.19854	2.51389
H	3.76780	2.92482	3.33831
H	4.84904	1.68766	2.64301
H	3.08160	1.44422	2.62649
C	5.02982	3.83979	0.97140
H	5.00333	4.38375	0.01214
H	5.96985	3.26231	1.01127
H	5.07269	4.59450	1.77624
C	2.33530	-2.44647	-0.87647
C	3.07076	-2.83440	0.28740
C	3.12795	-4.20001	0.62601
H	3.68996	-4.51009	1.51198
C	2.48290	-5.17213	-0.14979
H	2.53653	-6.22842	0.13427
C	1.77555	-4.78321	-1.29037
H	1.27617	-5.54446	-1.90000
C	1.68884	-3.43165	-1.68251
C	0.92155	-3.09510	-2.96596
H	0.99582	-2.00597	-3.13009
C	1.53090	-3.81288	-4.19543
H	2.61268	-3.62852	-4.29673
H	1.03481	-3.47445	-5.12191
H	1.38834	-4.90574	-4.12681
C	-0.57860	-3.45132	-2.85985
H	-0.71926	-4.53485	-2.69967
H	-1.10105	-3.18348	-3.79519
H	-1.07308	-2.92419	-2.03013
C	3.82776	-1.79969	1.12664
H	3.20496	-0.88316	1.15616
C	4.08604	-2.24460	2.57993
H	3.17091	-2.60843	3.07427
H	4.47816	-1.39670	3.16711
H	4.84361	-3.04695	2.63131
C	5.17327	-1.40864	0.46756
H	5.81858	-2.29753	0.35226
H	5.71151	-0.67847	1.09754
H	5.03190	-0.95548	-0.52507
C	-2.15342	-0.57482	-0.89311
C	-3.34896	-0.02370	-1.59350
C	-3.20032	0.40144	-2.93603
H	-2.22622	0.28311	-3.41900
C	-4.27063	0.95778	-3.64554
H	-4.16757	1.27208	-4.68787
C	-5.50134	1.11157	-2.99389
C	-5.68000	0.73546	-1.65803
H	-6.64626	0.90233	-1.17411
C	-4.60117	0.17025	-0.96310
H	-4.71944	-0.07830	0.09561
C	-2.17221	-1.68035	0.00302
C	-3.34675	-2.43881	0.32265
H	-4.28829	-2.18600	-0.17087
C	-3.30649	-3.50384	1.20101
H	-4.21667	-4.07024	1.41926
C	-0.89333	-3.23703	1.48036
H	0.07082	-3.61905	1.82913

C	-0.90295	-2.04954	0.65033
H	-0.00516	-1.96870	0.02663
C	0.60049	-1.21690	3.73983
H	0.51820	-2.31463	3.70261
H	0.31219	-0.88849	4.75441
H	1.65846	-0.94608	3.58937
C	-2.30907	-0.41733	3.07285
C	-3.28415	0.50177	2.61570
H	-3.01042	1.26003	1.87208
C	-4.60185	0.47850	3.10028
H	-5.33138	1.21049	2.73501
C	-4.97969	-0.47297	4.06287
H	-6.00538	-0.49122	4.44742
C	-4.02993	-1.39095	4.53695
H	-4.31307	-2.13125	5.29386
C	-2.71375	-1.36144	4.04595
H	-1.98834	-2.08495	4.43323
Si	-0.50260	-0.32917	2.44734
C	-0.09609	1.55754	2.67965
H	-0.27450	1.80362	3.74338
H	0.94689	1.81800	2.44127
H	-0.74311	2.20887	2.07120
C	-2.06162	-3.90396	1.78476
H	-2.02733	-4.79798	2.41780
F	-6.54400	1.65345	-3.67315

C′

SCF (BP86) Energy = -2231.47490414
Enthalpy 0K = -2230.517163
Enthalpy 298K = -2230.453771
Free Energy 298K = -2230.622944
Lowest Frequency = 4.1124 cm^{-1}
Second Frequency = 9.2093 cm^{-1}
SCF (BP86-D3BJ) Energy = -2231.77554362
SCF (C6H6) Energy = -2231.48550318
SCF (BS2) Energy = -2716.89804836

Mg	1.41858	0.08366	-0.21160
O	-0.40356	0.02198	-0.43075
N	2.82766	-1.36807	-0.44277
N	2.67836	1.61584	0.22977
C	5.15930	-2.09561	-0.89335
H	6.09689	-1.65574	-1.26351
H	4.79132	-2.83486	-1.62192
H	5.38705	-2.65509	0.03114
C	4.12175	-1.01856	-0.61838
C	4.61186	0.30954	-0.52184
H	5.67675	0.41244	-0.74303
C	3.99448	1.50000	-0.06002
C	4.91283	2.69322	0.15035
H	4.46940	3.61717	-0.25355
H	5.89299	2.52658	-0.31946
H	5.07474	2.87118	1.22792
C	2.20684	2.83067	0.85785
C	2.27382	2.95487	2.27705
C	1.77263	4.12597	2.87686
H	1.81674	4.22801	3.96706
C	1.22100	5.15885	2.11044
H	0.84166	6.06440	2.59534
C	1.15109	5.02058	0.72032
H	0.71200	5.82521	0.12015
C	1.62932	3.86623	0.06894
C	1.50592	3.77136	-1.45305
H	1.87973	2.77652	-1.75778
C	2.37390	4.83199	-2.16962
H	2.04818	5.85440	-1.90908
H	2.28902	4.72320	-3.26486
H	3.44062	4.74378	-1.90214
C	0.03287	3.88389	-1.90442
H	-0.59220	3.11067	-1.43021
H	-0.04839	3.75715	-2.99689
H	-0.38977	4.87109	-1.64769
C	2.83986	1.84734	3.16986
H	3.26665	1.06893	2.51329
C	1.71794	1.19159	4.00806
H	1.24211	1.92718	4.67971
H	2.11942	0.37459	4.63282
H	0.92361	0.77220	3.36654
C	3.97293	2.35186	4.09182
H	4.78855	2.82361	3.51803
H	4.40302	1.51423	4.66801
H	3.60418	3.09749	4.81762
C	2.48680	-2.77317	-0.39356
C	2.59684	-3.47543	0.84255
C	2.24094	-4.83699	0.88057
H	2.32045	-5.38313	1.82728
C	1.78580	-5.50345	-0.26256
H	1.51938	-6.56440	-0.21452
C	1.65957	-4.79831	-1.46380
H	1.28790	-5.31560	-2.35500
C	1.99325	-3.43243	-1.55562
C	1.80744	-2.71463	-2.89387
H	2.02328	-1.64215	-2.72686
C	2.80201	-3.22100	-3.96466
H	3.85106	-3.08594	-3.65157
H	2.65915	-2.67594	-4.91409
H	2.64920	-4.29536	-4.16887
C	0.35414	-2.84098	-3.40464
H	0.10464	-3.88963	-3.64300
H	0.21497	-2.25094	-4.32655
H	-0.37436	-2.48510	-2.65749
C	3.03913	-2.78724	2.13633
H	3.37044	-1.76560	1.87990
C	1.84832	-2.66296	3.11566
H	1.00462	-2.11571	2.65985
H	2.14733	-2.13019	4.03520
H	1.47110	-3.65824	3.40865
C	4.22546	-3.50441	2.81833
H	3.94884	-4.51927	3.15340
H	4.55622	-2.94169	3.70857
H	5.08896	-3.60375	2.13896
C	-1.55717	-0.20835	-1.07974
C	-1.70669	0.46999	-2.39884
C	-0.60933	0.56108	-3.28962
H	0.33899	0.08507	-3.01737
C	-0.71046	1.20969	-4.52719
H	0.13383	1.25849	-5.22106
C	-1.92962	1.80256	-4.87756
C	-3.03351	1.76572	-4.01789
H	-3.96267	2.26355	-4.30951
C	-2.91249	1.10750	-2.78642
H	-3.76138	1.10288	-2.09604
C	-2.52998	-1.03534	-0.51716
C	-3.66667	-1.55307	-1.24965
H	-3.86842	-1.16492	-2.25233
C	-4.41895	-2.60307	-0.78212
H	-5.24191	-2.99400	-1.38916
C	-3.04705	-2.81391	1.22709
H	-2.73293	-3.35734	2.12597
C	-2.37869	-1.50238	0.92612
H	-1.30756	-1.52148	1.20890
C	-2.83972	-0.76031	3.93619
H	-3.36670	-1.70488	4.14968
H	-3.19170	-0.00679	4.66094
H	-1.76351	-0.92775	4.11716
C	-5.01543	0.04856	1.86775

C	-5.52442	1.16604	1.16399
H	-4.83282	1.92058	0.77141
C	-6.90302	1.33869	0.95989
H	-7.26936	2.21463	0.41262
C	-7.81050	0.39143	1.46046
H	-8.88697	0.52384	1.30531
C	-7.33049	-0.72462	2.16492
H	-8.03281	-1.46707	2.56041
C	-5.95092	-0.89014	2.36520
H	-5.59701	-1.77014	2.91329
Si	-3.14286	-0.16204	2.14820
C	-2.29236	1.52108	1.89308
H	-2.80161	2.30808	2.47530
H	-1.24046	1.48084	2.22000
H	-2.29516	1.81261	0.83065
C	-4.05775	-3.28663	0.44752
H	-4.57245	-4.21804	0.71018
F	-2.03759	2.44010	-6.07402

4′

SCF (BP86) Energy = -2907.36365593
Enthalpy 0K = -2906.226430
Enthalpy 298K = -2906.149690
Free Energy 298K = -2906.345533
Lowest Frequency = 10.4427 cm^{-1}
Second Frequency = 11.7701 cm^{-1}
SCF (BP86-D3BJ) Energy = -2907.76196768
SCF (C6H6) Energy = -2907.36974043
SCF (BS2) Energy = -3392.96320765

Mg	-1.17195	0.15218	0.24592
O	0.26139	1.36625	-0.18580
N	-2.15134	0.66134	2.04091
N	-2.93881	-0.17815	-0.81020
C	-4.11616	1.66016	3.21893
H	-4.69223	0.83980	3.68303
H	-4.83438	2.45346	2.95832
H	-3.41737	2.03830	3.97861
C	-3.40523	1.15369	1.96844
C	-4.18866	1.19752	0.78243
H	-5.14077	1.72248	0.89588
C	-4.04124	0.51611	-0.45112
C	-5.22567	0.60446	-1.40482
H	-4.97300	1.26023	-2.25689
H	-6.11406	1.01828	-0.90556
H	-5.48102	-0.37905	-1.82966
C	-3.03205	-1.06650	-1.94277
C	-3.41731	-2.42577	-1.71891
C	-3.50584	-3.29720	-2.82260
H	-3.81706	-4.33457	-2.66013
C	-3.20236	-2.86666	-4.12061
H	-3.28366	-3.55846	-4.96617
C	-2.79865	-1.54308	-4.32477
H	-2.55374	-1.20386	-5.33764
C	-2.71129	-0.62459	-3.25893
C	-2.26523	0.80599	-3.55797
H	-2.33275	1.38551	-2.62096
C	-3.16501	1.49615	-4.60859
H	-3.07922	1.01082	-5.59716
H	-2.86742	2.55170	-4.72817
H	-4.22984	1.47219	-4.32119
C	-0.79130	0.83168	-4.01913
H	-0.12890	0.38677	-3.25946
H	-0.46172	1.86980	-4.19471
H	-0.65672	0.26568	-4.95836
C	-3.75376	-2.94848	-0.31940
H	-3.30382	-2.24613	0.40511
C	-3.16457	-4.34983	-0.05041
H	-3.64467	-5.12673	-0.67127
H	-3.32766	-4.63441	1.00293
H	-2.08059	-4.38185	-0.24963
C	-5.28045	-2.95919	-0.06835
H	-5.71494	-1.94987	-0.14703
H	-5.50541	-3.34488	0.94187
H	-5.79353	-3.60840	-0.80034
C	-1.55769	0.51843	3.35067
C	-1.88818	-0.60798	4.16097
C	-1.29056	-0.73092	5.43077
H	-1.54105	-1.59596	6.05531
C	-0.39155	0.22656	5.90945
H	0.05242	0.12079	6.90529
C	-0.06082	1.32129	5.10117
H	0.64618	2.06892	5.47422
C	-0.61893	1.48927	3.81803
C	-0.23592	2.71094	2.97844
H	-0.31792	2.41340	1.91871
C	-1.20139	3.89786	3.21087
H	-2.23858	3.65068	2.93495
H	-0.89100	4.76647	2.60452
H	-1.19552	4.20437	4.27249
C	1.21617	3.17667	3.20814
H	1.35176	3.63900	4.20281
H	1.49250	3.93196	2.45498
H	1.93359	2.34406	3.11958
C	-2.84789	-1.70565	3.69536
H	-3.28861	-1.38662	2.73508
C	-2.08481	-3.02638	3.44556
H	-1.30512	-2.90061	2.67704
H	-2.77639	-3.81974	3.11140
H	-1.58993	-3.37868	4.36761
C	-4.00593	-1.93951	4.69236
H	-3.63902	-2.34170	5.65314
H	-4.72447	-2.67074	4.28275
H	-4.55471	-1.00853	4.91280
C	0.63769	2.56468	-0.60508
C	-0.40617	3.41996	-1.25223
C	-1.71448	3.47591	-0.71436
H	-1.94981	2.92700	0.20350
C	-2.72061	4.24978	-1.30819
H	-3.72529	4.29893	-0.87968
C	-2.41995	4.97116	-2.46938
C	-1.14580	4.92992	-3.04848
H	-0.95034	5.49020	-3.96725
C	-0.15172	4.15147	-2.43850
H	0.84037	4.09398	-2.89697
C	1.95433	3.02546	-0.39857
C	2.32028	4.41676	-0.50193
H	1.60814	5.11919	-0.94518
C	3.47640	4.91569	0.06301
H	3.69070	5.98772	0.00272
C	4.33513	4.06156	0.85958
C	4.08978	2.72174	0.93868
H	4.70760	2.07577	1.57204
C	3.03510	2.07266	0.09095
H	2.57798	1.20125	0.59276
C	2.76127	0.30295	-2.51647
H	2.24967	-0.48560	-1.94193
H	3.26773	-0.16093	-3.37990
H	1.98812	0.98836	-2.89862
C	5.35843	0.12034	-0.80523
C	6.56626	0.63490	-0.27246
H	6.71887	1.71952	-0.22859
C	7.57862	-0.21366	0.20307
H	8.50293	0.21238	0.60921
C	7.40969	-1.60712	0.15200
H	8.19957	-2.27203	0.51827

C	6.22459	-2.14175	-0.37774
H	6.09006	-3.22837	-0.42952
C	5.21412	-1.28644	-0.84794
H	4.30010	-1.72610	-1.26434
Si	3.98738	1.28503	-1.45057
C	4.79103	2.65479	-2.49665
H	5.39163	2.20897	-3.30771
H	4.02227	3.30238	-2.94821
H	5.45004	3.29428	-1.88815
C	0.74250	-2.42800	0.20728
O	-0.15262	-1.54267	0.02878
C	1.09271	-3.31893	-0.91682
C	2.32037	-4.03207	-0.97376
C	0.20011	-3.41091	-2.01851
C	2.63490	-4.82981	-2.07807
H	3.04559	-3.93194	-0.16195
C	0.49999	-4.21354	-3.11995
H	-0.73972	-2.85292	-1.98935
C	1.71440	-4.91534	-3.13267
H	3.58116	-5.37329	-2.14200
H	-0.19141	-4.29859	-3.96206
C	1.40203	-2.54013	1.53123
C	1.76655	-3.79414	2.08315
C	1.59510	-1.36921	2.30545
C	2.32195	-3.86757	3.36714
H	1.57205	-4.71165	1.51990
C	2.16071	-1.44816	3.58182
H	1.32455	-0.39710	1.88029
C	2.52746	-2.69654	4.11577
H	2.58466	-4.84319	3.78893
H	2.30207	-0.53455	4.16612
F	2.01303	-5.69244	-4.19836
H	2.96610	-2.75635	5.11711
F	-3.39021	5.72126	-3.05525
H	5.14742	4.51290	1.44080