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Supporting Information for

Isocyanate Deoxygenation by a Molecular Magnesium Silanide

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Figure S1: ^{1}H NMR (500 MHz, 25 °C, C_6D_6) spectrum of compound **7**.

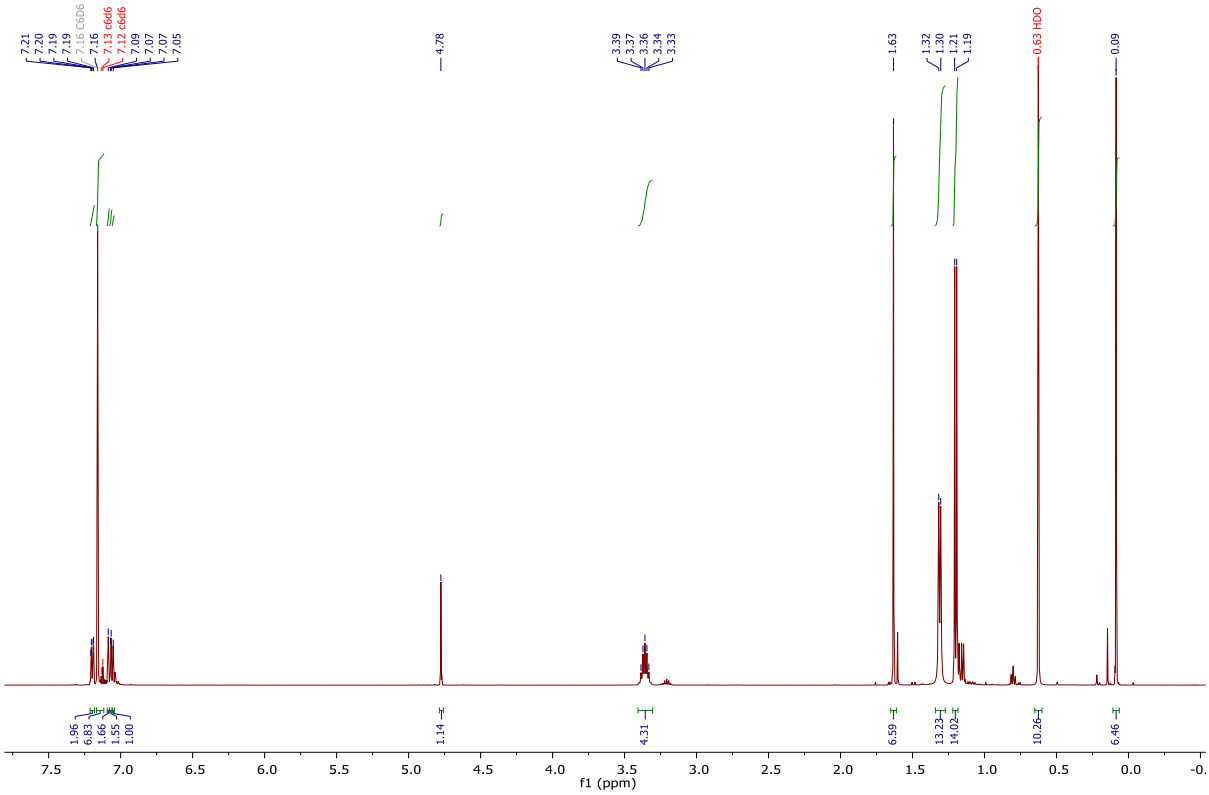


Figure S2: ^{13}C{^{1}H} NMR (126 MHz, 25 °C, C_6D_6) spectrum of compound **7**.

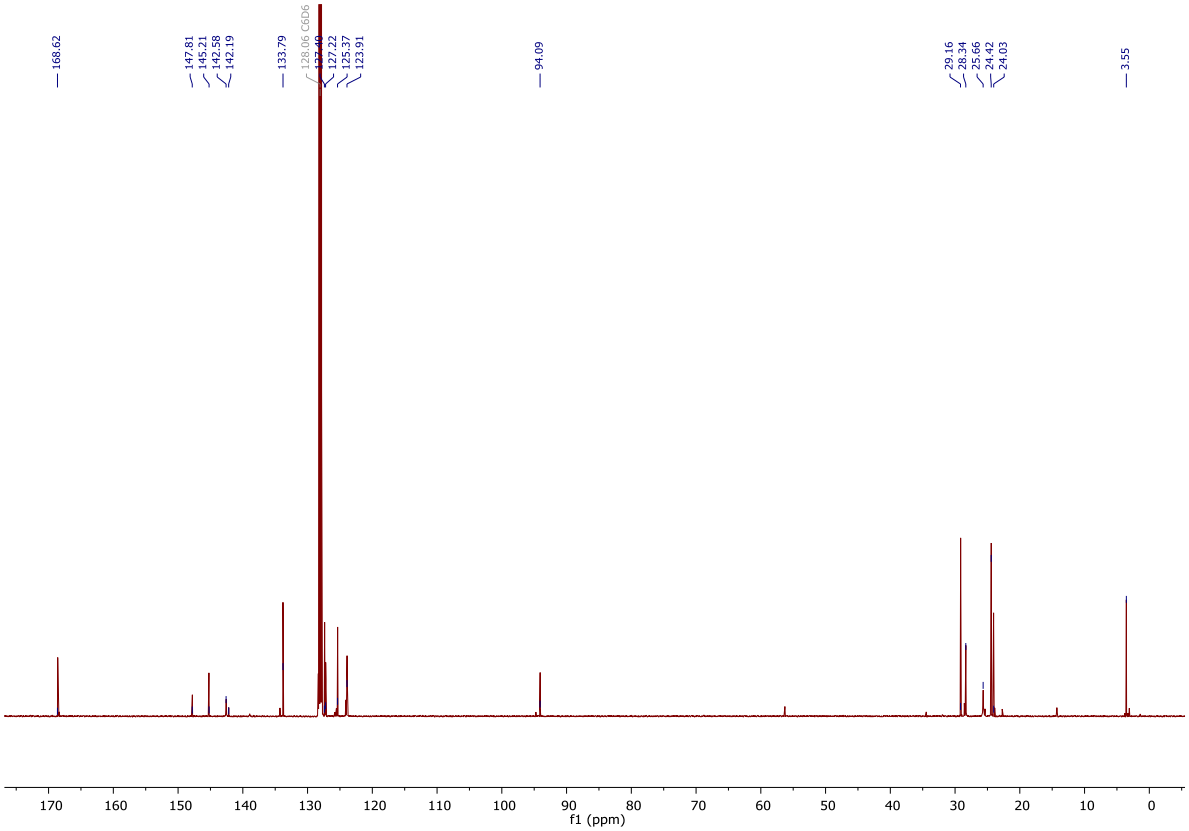


Figure S3: $^{29}Si\{^{1}H\}$ NMR (99 MHz, 25 °C, C_6D_6) NMR spectrum of compound **7**.

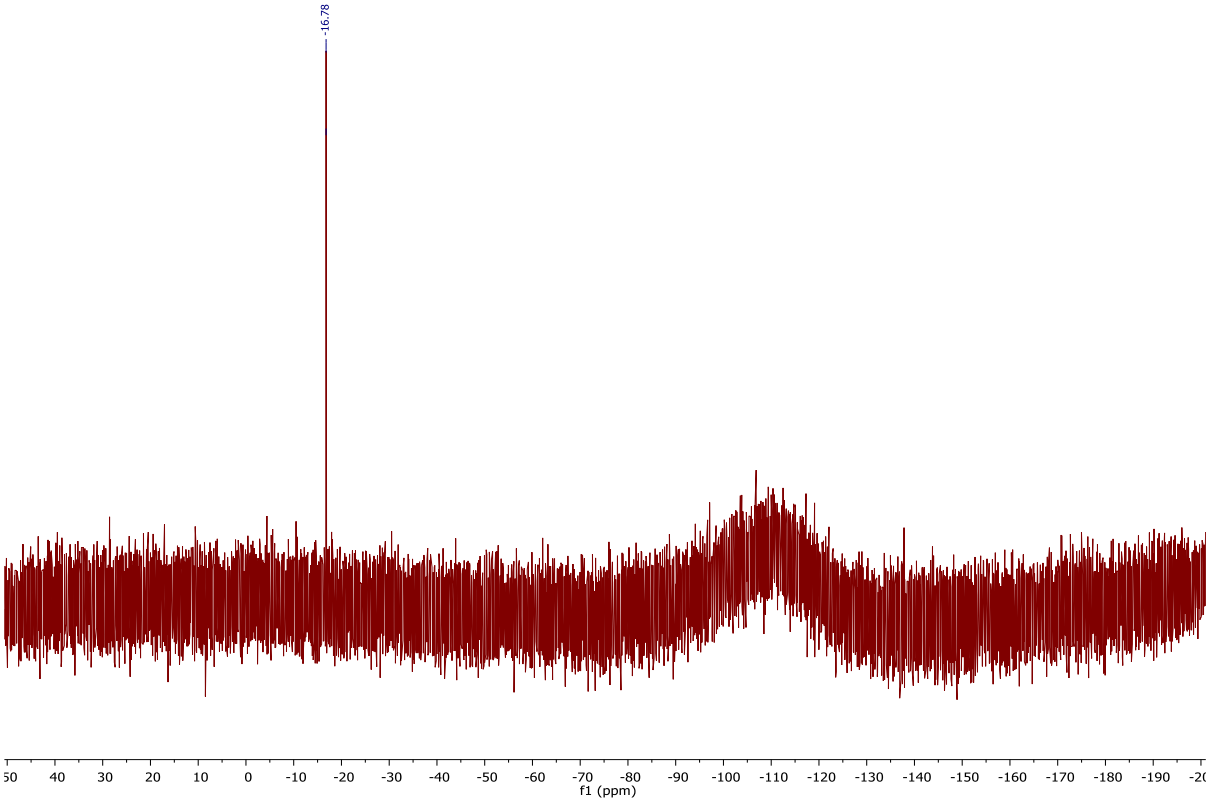


Figure S4: ^{1}H NMR (500 MHz, 25 °C, C_6D_6) spectrum of compound **8**.

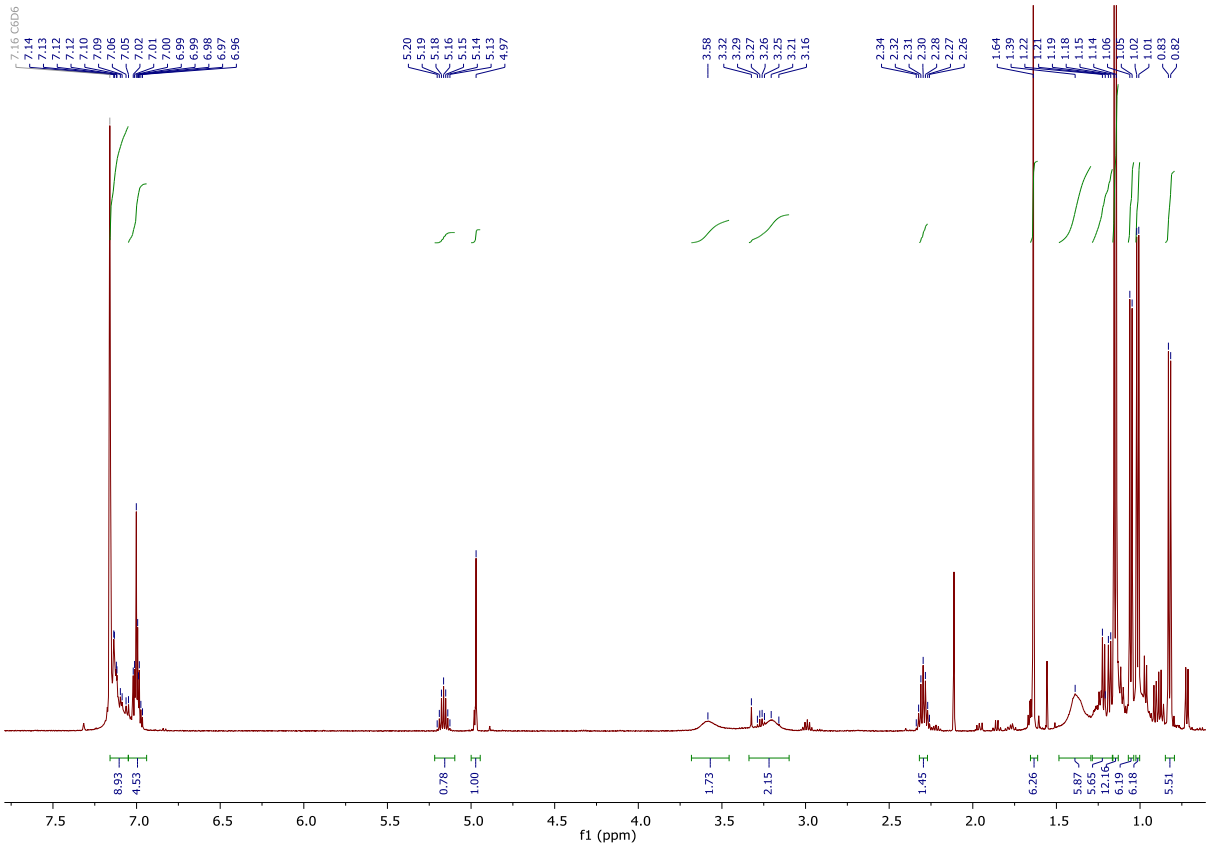


Figure S5: $^{13}C\{^{1}H\}$ NMR (126 MHz, 25 °C, C_6D_6) spectrum of compound **8**.

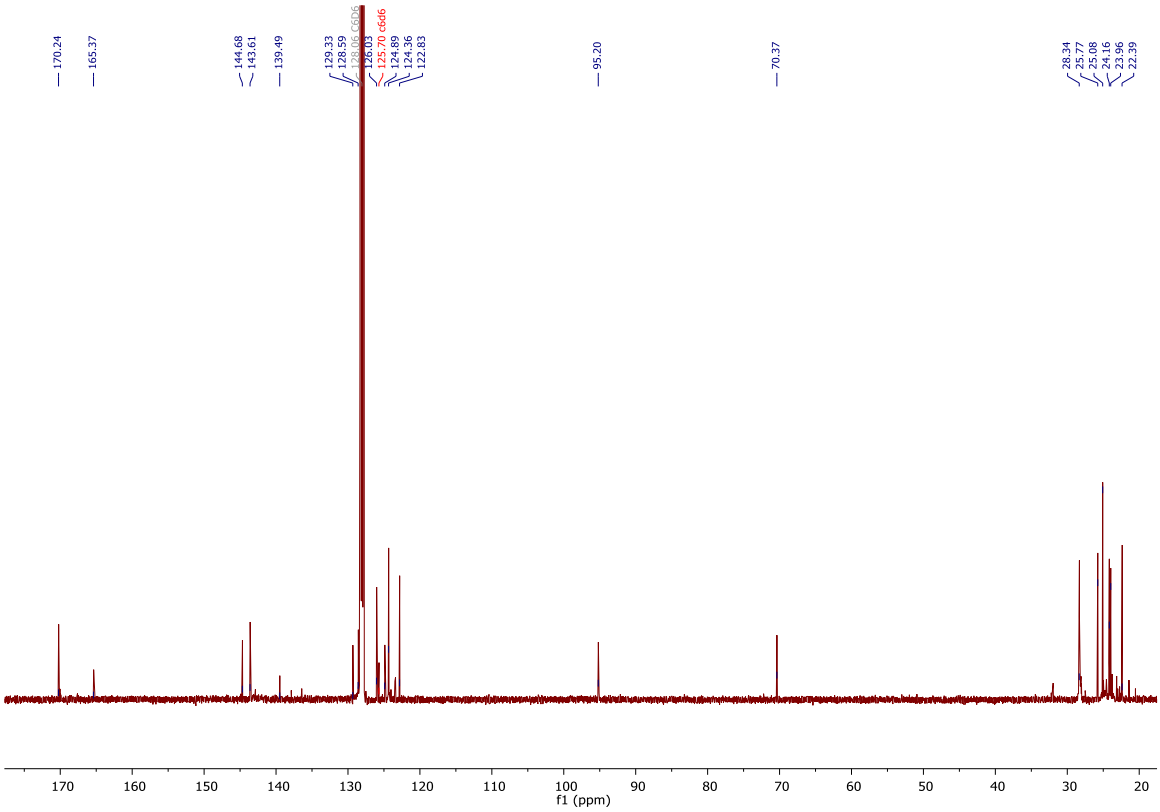


Figure S6: $^{29}Si\{^{1}H\}$ NMR (99 MHz, 25 °C, C_6D_6) NMR spectrum of compound **8**.

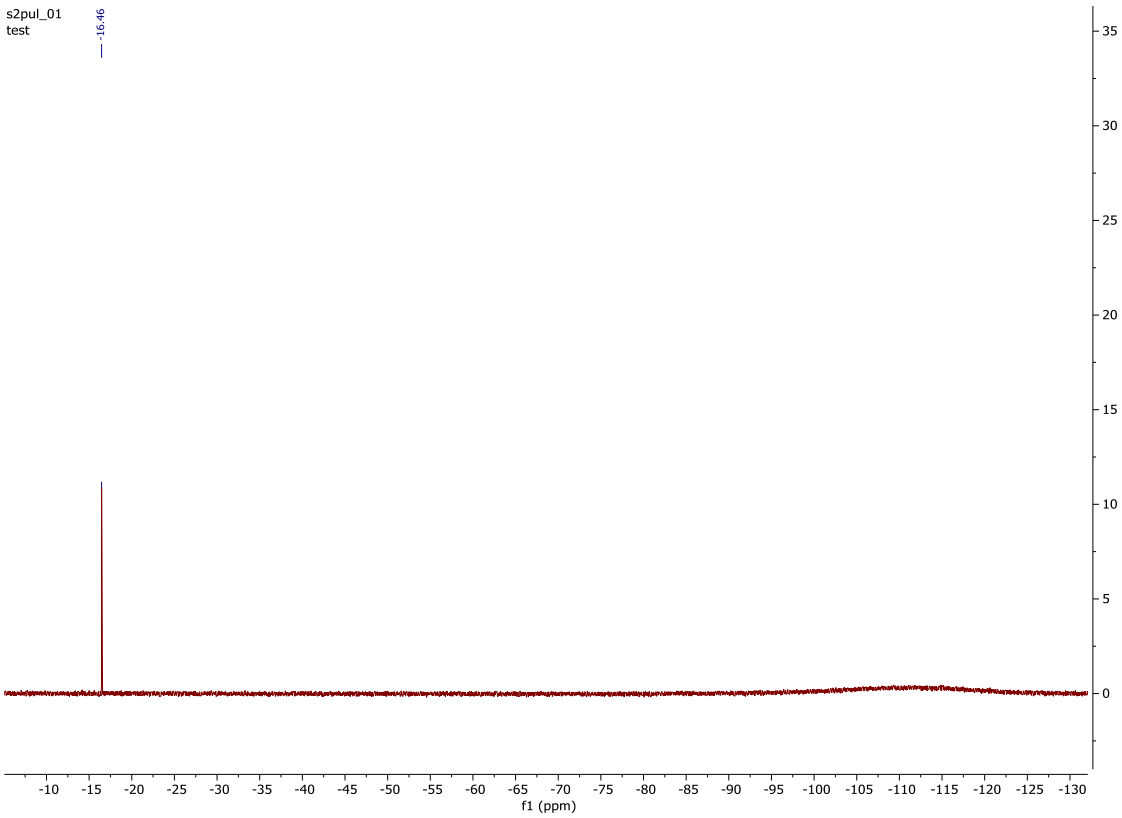


Figure S7: ^{1}H NMR (500 MHz, 25 °C, C_6D_6) spectrum of a *ca.* 3:1 mixture of compounds **10a**/**10b**.

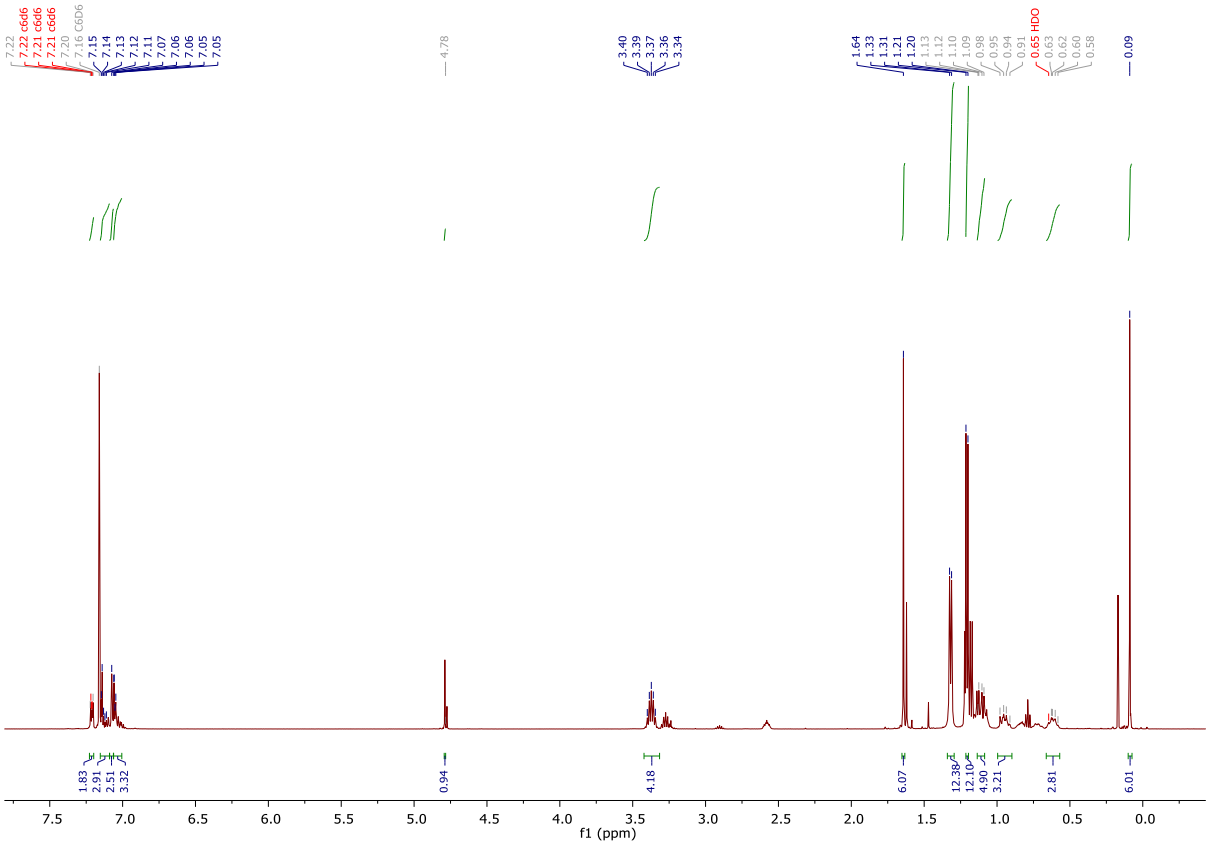


Figure S8: ^{13}C{^{1}H} NMR (126 MHz, 25 °C, C_6D_6) spectrum of a 3:1 mixture of compounds **10a**/**10b**.

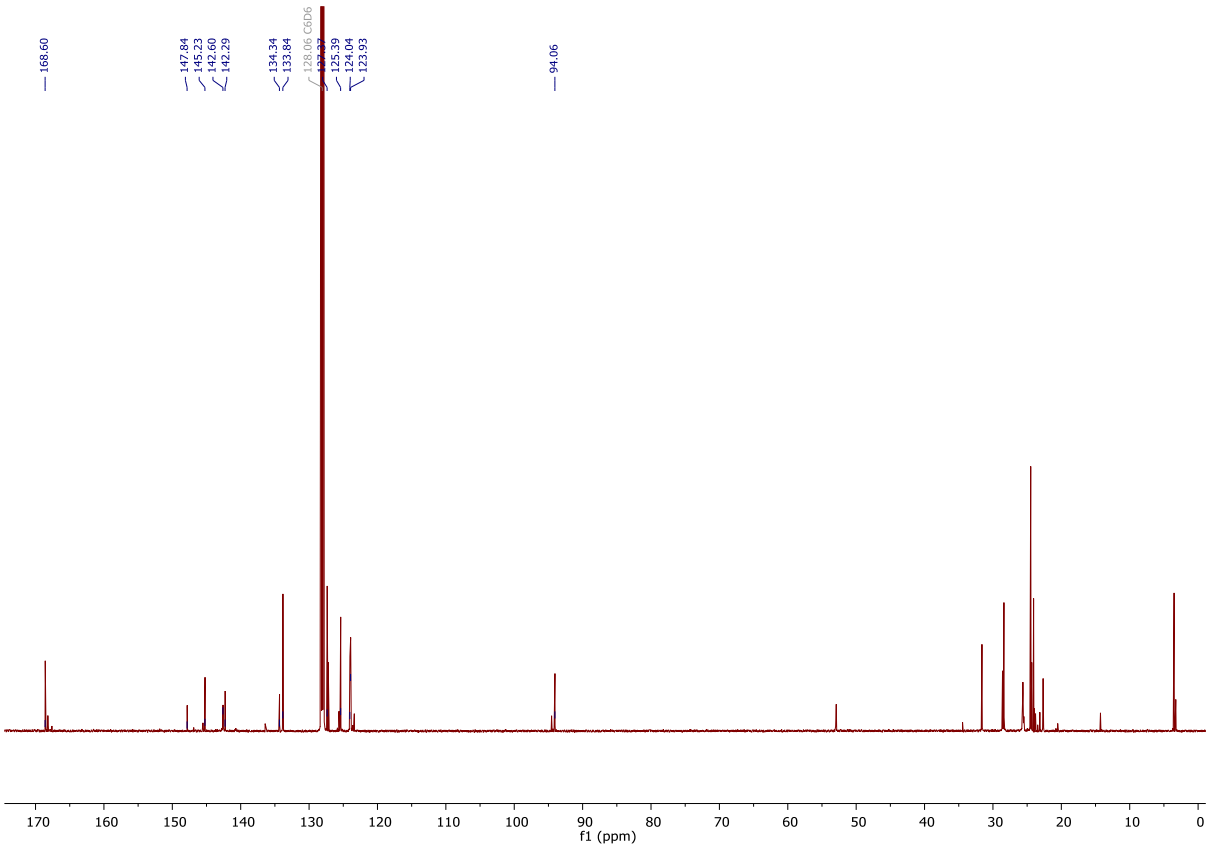


Figure S9: $^{29}Si\{^{1}H\}$ NMR (99 MHz, 25 °C, C_6D_6) NMR spectrum of a 3:1 mixture of **10a**/**10b**.

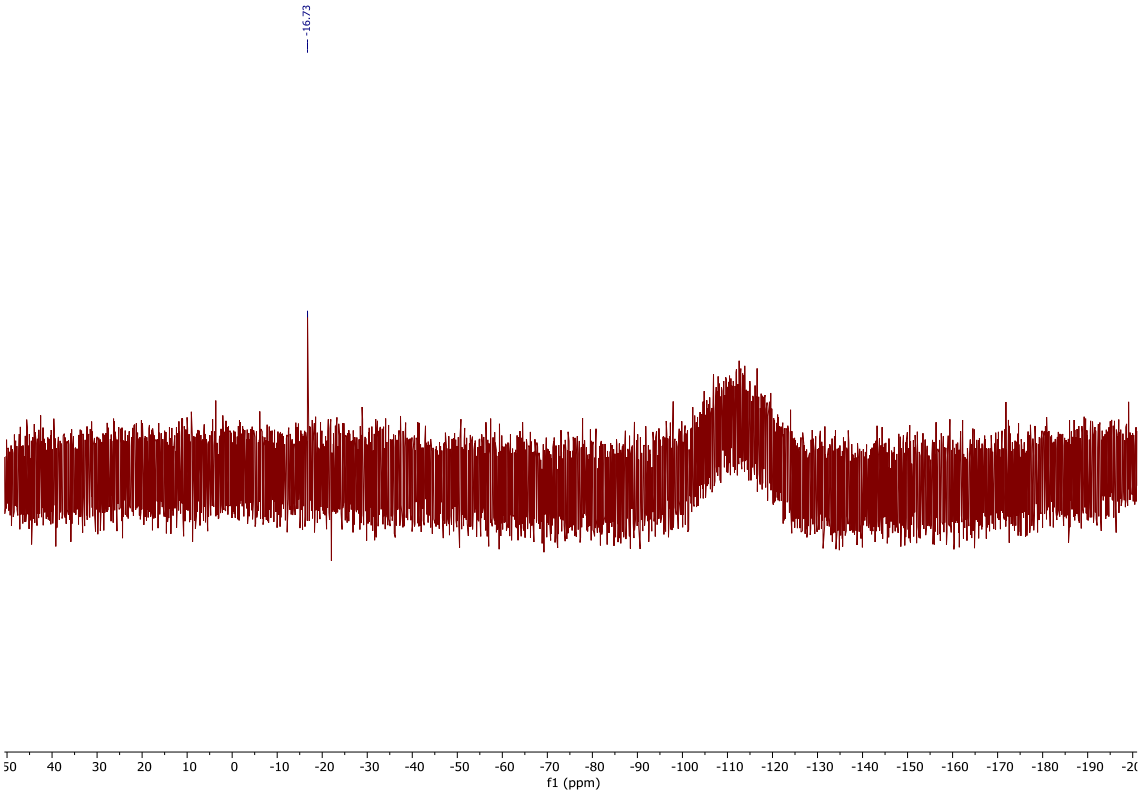


Figure S10: ^{1}H NMR (500 MHz, 25 °C, C_6D_6) spectrum resulting from the initial reaction of **6** with *i*-PrNCO illustrating the complex mixture of products produced.

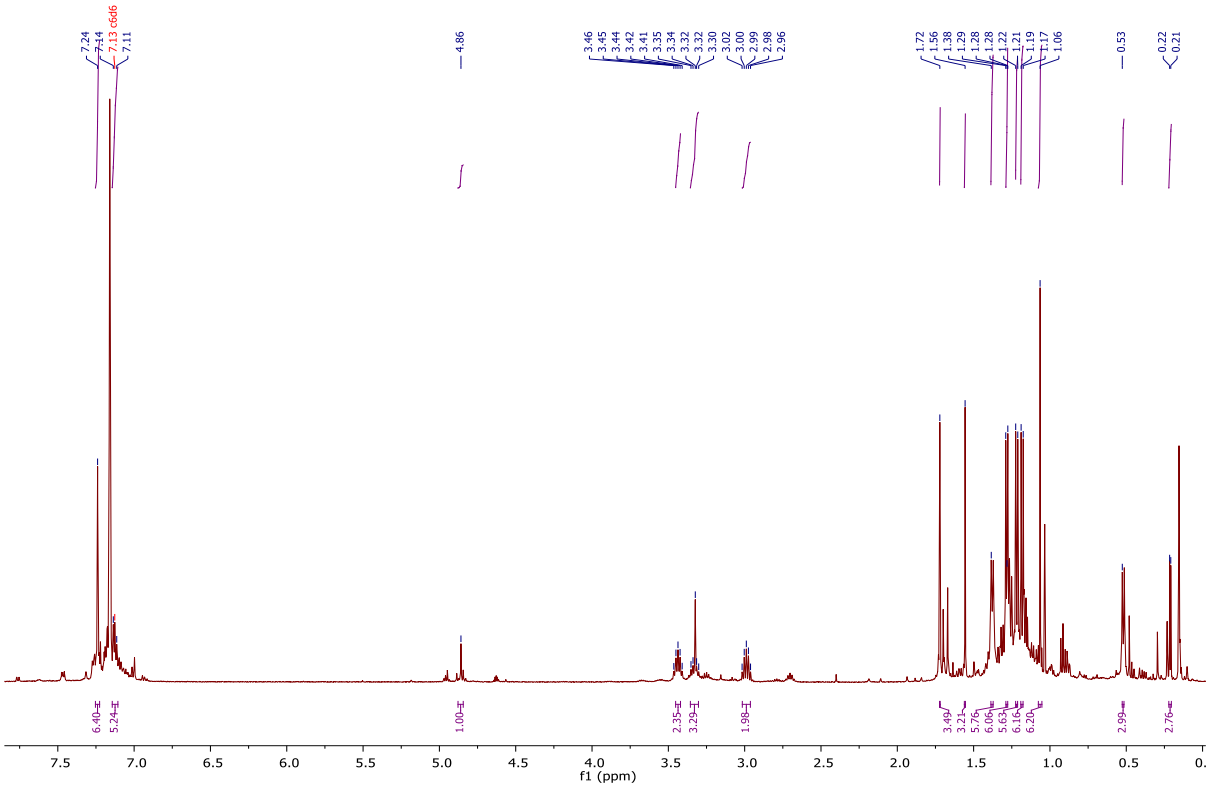


Figure S11: $^{13}C\{^{1}H\}$ NMR (126 MHz, 25 °C, C_6D_6) spectrum resulting from the initial reaction of **6** with *i*-PrNCO illustrating the complex mixture of products produced.

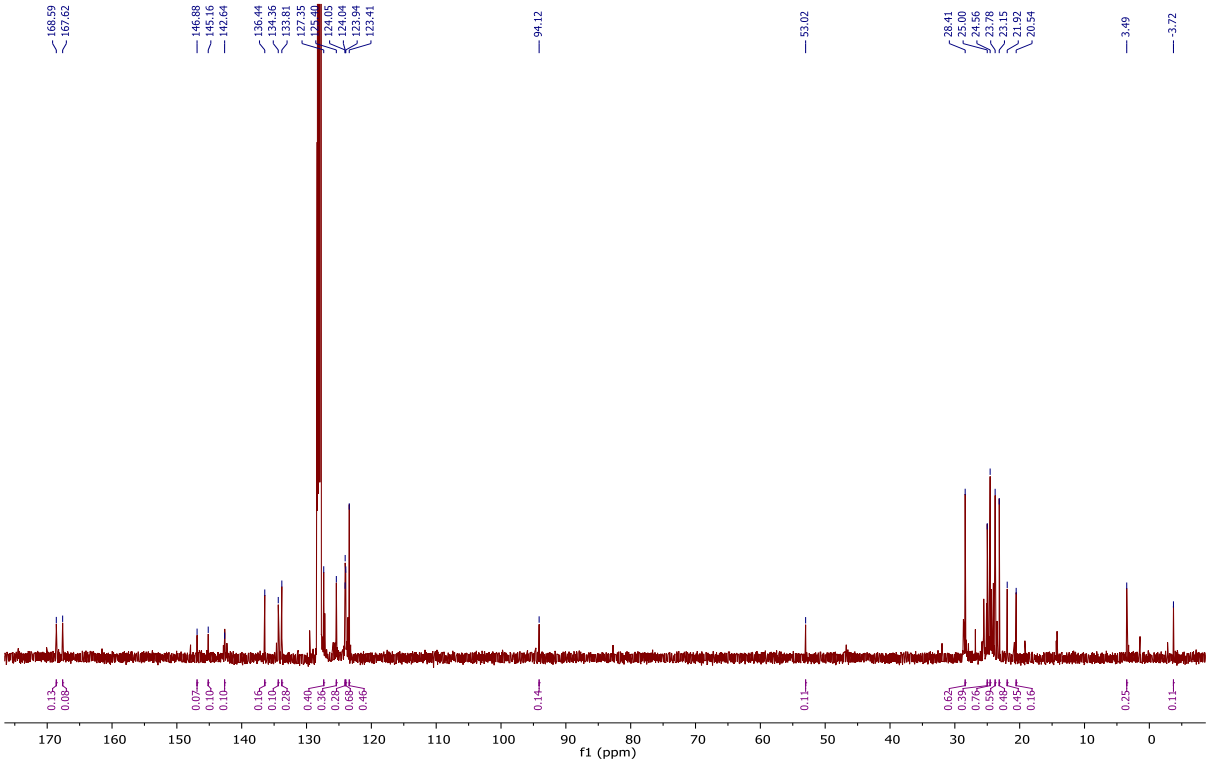


Figure S12: ^{1}H NMR (500 MHz, 25 °C, C_6D_6) spectrum of an isolated sample of compound **11**.

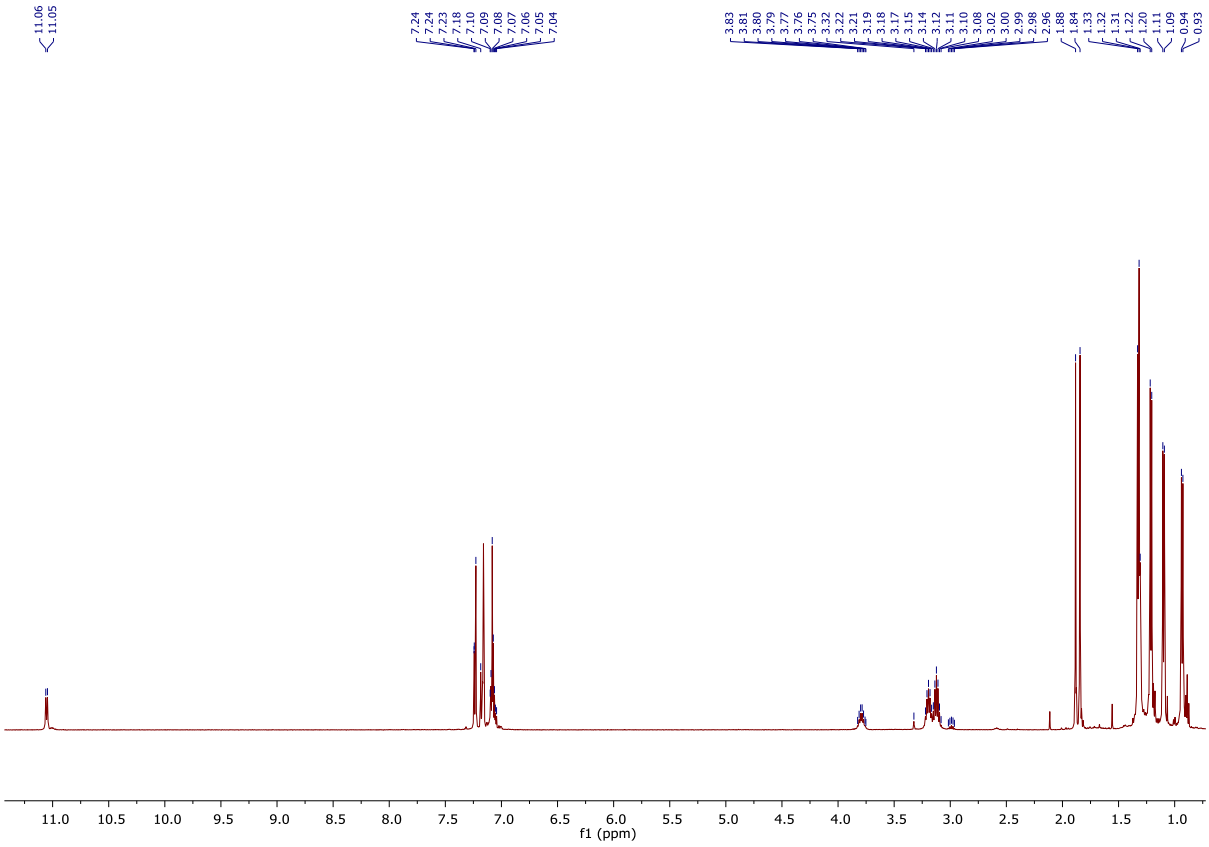
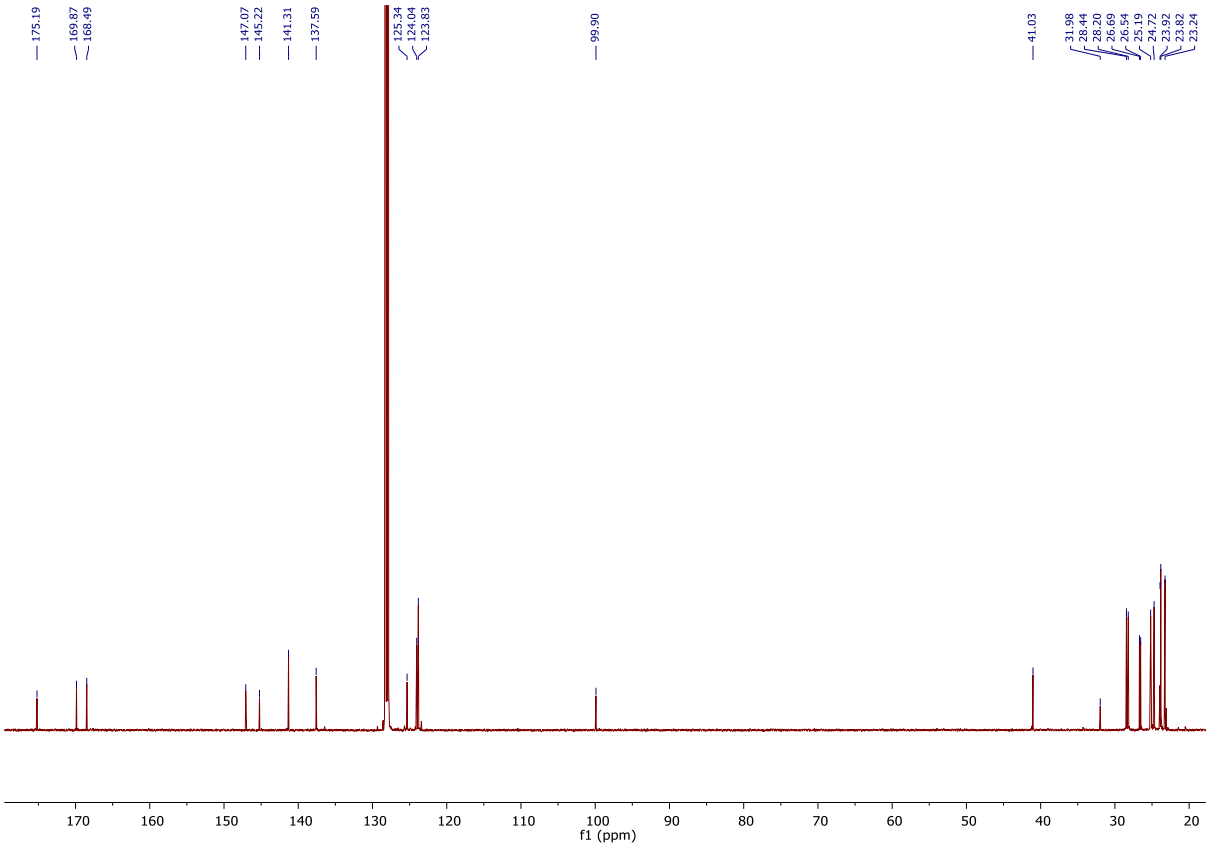


Figure S13: $^{13}C\{^{1}H\}$ NMR (126 MHz, 25 °C, C_6D_6) spectrum of an isolated sample of compound **12**.



Single crystal X-ray analysis of compounds 7, 8 and 11 – 13.

Data were collected for compounds **7**, **8**, **11** and **13** on a SuperNova, Dual Cu at zero, EosS2 diffractometer (Cu*K*α; λ = 1.54184 Å), whereas data for compound **12** were collected on a New Xcalibur, EosS2 diffractometer (MoKα; λ = 0.71073 Å). The crystals were all maintained at 150(2) K during data collection. Using Olex2,[1] the structures were solved with ShelXT[2] and refined with the ShelXL[3] using Least Squares minimisation.

The asymmetric unit in the structure of **8** contains one molecule of the magnesium complex and half of a molecule of hexane. The phenyl ring based on C45 was treated for 60:40 disorder the refinement, with the inclusion of some ADP restraints. The solvent moiety, though visible, suffers from disorder to the extent that this region of the electron density map was addressed using the solvent mask algorithm available in Olex-2. The solvent has been accounted for in the formula as presented.

Disorder was confined to 3 regions in the structure of **12**, where the asymmetric unit was seen to equate to one molecule of the magnesium complex. In particular, the methyl groups containing C14, C15, C46 and C47 were each split over 2 sites in a 70:30 ratio. Additionally, the entire ligand based on C30 was treated for 50:50 disorder. Distance and ADP restraints were employed for fractional-occupancy atoms, to assist convergence. The hydrogens attached to N3 and N7 were included at calculated positions, but their associated U_{iso} values were allowed to freely refine.

The motif in **13** contains 1 molecule of a complex based on three magnesium centres and some solvent. The latter was (very) evidently hexane, but it was ultimately treated using the Olex-2 solvent mask algorithm, as it would have involved considerable disorder modelling. The latter, seen in the context of extensive disorder within the complex, would have resulted in the application of considerable additional restraints to the model – thereby risking over-paramaterisation. Allowance has been made, in the formula as presented, for the presence of six hexanes per unit cell, despite solvent address in the refinement. 2-component disorder modelling in a 58:42 ratio, was effected for the entire Dipp moiety attached to N8, and the phenyl groups bonded to Si1 and Si2. The phenyl attached to Si3 was treated for 55:45 disorder and the isopropyl carbons C131 and C132 were modelled to take account of 65:35 disorder. Distance and ADPs restraints were applied in disordered regions, to assist convergence.

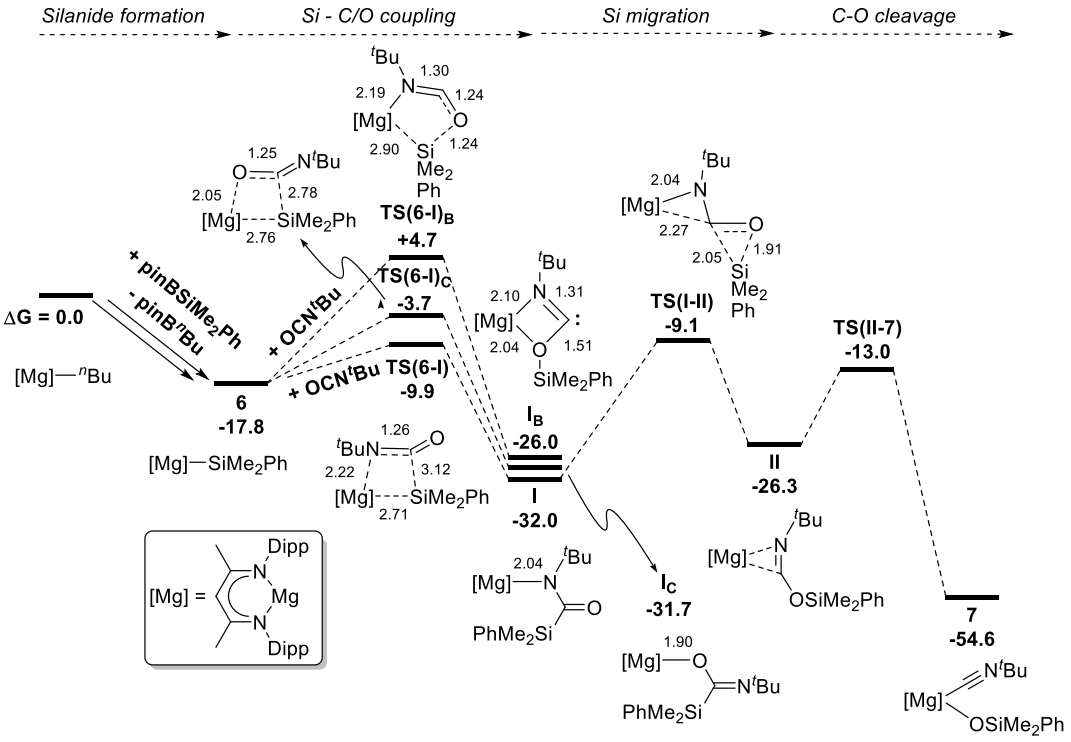
Table S1: Single crystal X-ray diffraction analysis of compounds **7**, **8** and **11 – 13**.

Compound	**7**	**8**	**11**	**12**	**13**
Empirical formula	$C_{42}H_{61}MgN_3OSi$	$C_{51.8}H_{73.2}MgN_3OSi$	$C_{66}H_{96}MgN_6O_2$	$C_{70}H_{103}MgN_7O_2$	$C_{153}H_{240}Mg_3N_{12}O_6Si_3$
Formula weight	676.33	806.33	1029.79	1098.90	2500.76
Crystal system	orthorhombic	monoclinic	orthorhombic	orthorhombic	triclinic
Space group	$P2_12_12_1$	$P2_1/n$	$P2_12_12_1$	$Pca2_1$	P-1
a/Å	11.6235(1)	13.7088(1)	15.6289(4)	15.9146(4)	16.2685(3)
b/Å	17.5314(1)	17.6095(1)	18.9135(5)	17.6992(5)	24.0536(4)
c/Å	20.1961(1)	21.7081(2)	21.0175(5)	23.9884(6)	24.3670(5)
α/°	90	90	90	90	61.681(2)
β/°	90	106.096(1)	90	90	85.617(2)
γ/°	90	90	90	90	86.756(2)
U/Å^3	4115.49(5)	5035.01(7)	6212.7(3)	6756.9(3)	8367.2(3)
Z	4	4	4	4	2
ρ_{calc}g cm^{-3}	1.092	1.064	1.101	1.080	0.993
μ/mm^{-1}	0.896	0.803	0.596	0.073	0.754
F(000)	1472.0	1756.0	2248.0	2400.0	2736.0
Crystal size/mm^3	0.21 × 0.19 × 0.16	0.25 × 0.158 × 0.144	0.164 × 0.129 × 0.079	0.583 × 0.346 × 0.262	0.294 × 0.189 × 0.183
2θ range for data collection/°	6.676 to 146.344	6.57 to 146.14	7.048 to 146.59	5.864 to 57.212	7.364 to 145.944
Index ranges	$-14 \leq h \leq 14$, $-17 \leq k \leq 21$, $-25 \leq l \leq 24$	$-16 \leq h \leq 16$, $-21 \leq k \leq 15$, $-26 \leq l \leq 26$	$-19 \leq h \leq 19$, $-22 \leq k \leq 23$, $-16 \leq l \leq 26$	$-21 \leq h \leq 21$, $-23 \leq k \leq 23$, $-32 \leq l \leq 31$	$-20 \leq h \leq 20$, $-29 \leq k \leq 19$, $-29 \leq l \leq 30$
Reflections collected	60020	66427	46377	96921	60767
Independent reflections, R_{int}	8219, 0.0363	10019, 0.0402	12319, 0.0607	15727, 0.0464	32598, 0.0309
Data/restraints/parameters	8219/0/448	10019/88/575	12319/0/702	15727/137/836	32598/493/1741
Goodness−of−fit on F^2	1.020	1.037	1.021	1.012	1.045
Final $R1$, $wR_2[I>=2\sigma(I)]$	0.0306, 0.0844	0.0449, 0.1168	0.0495, 0.1173	0.0549, 0.1164	0.0490, 0.1256
Final $R1$, wR_2[all data]	0.0315, 0.0853	0.0524, 0.1221	0.0630, 0.1251	0.0960, 0.1343	0.0682, 0.1362
Largest diff. peak/hole / e Å^{-3}	0.35/-0.36	0.34/-0.35	0.18/-0.23	0.21/-0.18	0.28/-0.22
Flack parameter	-0.008(7)	-	0.05(4)	0.31(11)	-

Computational Details

DFT optimisations were run with Gaussian 09 (Revision D.01).[4] The Mg and Si centres 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 polarization function was also added to Si ($\zeta d = 0.284$). Initial BP86[7] 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 toluene ($\varepsilon = 2.3741$) 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 were used for NBO (Natural Bond Orbital) studies, using NBO version 3 as implemented in Gaussian 09 to yield natural atomic charges and atomic contributions to notable NBOs.

Figure S14. Computed full free energy profile (BP86-D3BJ, toluene/BS2//BP86/BS1, in kcal/mol) for the reaction of silanide species **6** with OCN*t*-Bu to yield the magnesium siloxide *t*-BuNC adduct **7** relative to species **5**, including disfavoured Si-C/O coupling processes via **TS(6-I)$_B$** and **TS(6-I)$_C$**.



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
$\Delta G_{BS1/tol}$	Free energy corrected for toluene solvent with BS1
$\Delta G_{BS1/tol+D3}$	Free energy corrected for toluene and dispersion effects with BS1
ΔG_{tol}	Free energy corrected for basis set (BS2), dispersion effects and toluene solvent

In each case the final data used in the main article is 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 **5** at 0.0 kcal/mol.

	ΔE_{BS1}	ΔH_{BS1}	ΔG_{BS1}	$\Delta G_{BS1/tol}$	$\Delta G_{BS1/tol+D3}$	ΔE_{BS2}	ΔG_{tol}
5	0.0	0.0	0.0	0.0	0.0	0.0	**0.0**
6	-13.4	-12.3	-11.5	-55.7	-30.7	-13.9	**-17.8**
TS(6-I)	-6.1	32.6	14.4	-20.2	-18.8	-3.4	**-9.9**
I	-32.0	7.7	-10.2	-71.0	-67.2	-28.7	**-32.0**
$TS(6\text{-}I)_C$	-5.0	33.7	13.9	-19.6	-12.4	-1.3	**-3.7**
I_C	-37.3	2.3	-17.8	-84.8	-72.5	-33.9	**-31.7**
$TS(6\text{-}I)_B$	8.5	46.9	27.9	8.3	9.1	12.7	**4.7**
I_B	-29.4	9.6	-10.4	-68.6	-57.7	-27.2	**-26.0**
TS(I-II)	-13.2	25.5	6.7	-35.1	-26.8	-8.7	**-9.1**
II	-32.1	7.6	-12.3	-72.9	-60.9	-29.6	**-26.3**
TS(II-7)	-13.8	24.5	3.9	-40.3	-28.3	-12.2	**-13.0**
7	-55.7	-16.2	-37.9	-122.1	-111.5	-54.4	**-54.6**

Cartessian Coordinates and Calculation Energies

OCNtBu

SCF (BP86) Energy = -325.939448072
Enthalpy 0K = -325.799578
Enthalpy 298K = -325.798634
Free Energy 298K = -325.841021
Lowest Frequency = 31.2565 cm^{-1}
Second Frequency = 110.5327 cm^{-1}
SCF (BP86-D3BJ) Energy = -325.960115964
SCF (Toluene) Energy = -325.941161016
SCF (BS2) Energy = -326.031575481

C	1.74491	0.00044	-0.22105
N	0.58860	0.00100	-0.61379
O	2.91795	-0.00006	0.00273
C	-0.75105	-0.00003	0.00123
C	-0.91536	1.27190	0.86063
H	-1.92971	1.31293	1.29301
H	-0.18680	1.28228	1.68905
H	-0.76113	2.17661	0.25017
C	-1.77279	-0.00383	-1.15359
H	-1.64270	-0.89785	-1.78499
H	-2.79996	-0.00443	-0.75274
H	-1.64517	0.88794	-1.78865
C	-0.91154	-1.26899	0.86570
H	-1.92574	-1.31131	1.29831
H	-0.75469	-2.17569	0.25885
H	-0.18293	-1.27391	1.69413

CNtBu

SCF (BP86) Energy = -250.657660213
Enthalpy 0K = -250.523808
Enthalpy 298K = -250.522864
Free Energy 298K = -250.561847
Lowest Frequency = 165.0246 cm^{-1}
Second Frequency = 165.0854 cm^{-1}
SCF (BP86-D3BJ) Energy = -250.677044745
SCF (Toluene) Energy = -250.660542260
SCF (BS2) Energy = -250.723754424

C	-2.38159	0.00001	-0.00017
N	-1.19018	-0.00006	-0.00027
C	0.25778	0.00002	-0.00002
C	0.73924	1.44373	-0.26966
H	1.84158	1.47243	-0.27478
H	0.37419	1.80095	-1.24600
H	0.37376	2.12940	0.51162
C	0.73892	-0.48822	1.38526
H	0.37350	-1.50770	1.58834
H	1.84126	-0.49802	1.41298
H	0.37357	0.17866	2.18269
C	0.73948	-0.95547	-1.11529
H	1.84184	-0.97442	-1.13719
H	0.37419	-1.97956	-0.93662
H	0.37440	-0.62165	-2.09986

pinBSiMe$_2$Ph

SCF (BP86) Energy = -726.662674892
Enthalpy 0K = -726.303812
Enthalpy 298K = -726.302868
Free Energy 298K = -726.376466
Lowest Frequency = 11.0064 cm^{-1}
Second Frequency = 23.4304 cm^{-1}
SCF (BP86-D3BJ) Energy = -726.740094323
SCF (Toluene) Energy = -726.665345104
SCF (BS2) Energy = -1012.46966575

Si	1.05624	1.41511	0.24334
C	1.30054	2.76708	-1.08099
H	1.21456	2.34823	-2.09704
H	2.28635	3.25492	-0.99086
H	0.53042	3.54980	-0.97502
C	1.26942	2.19161	1.97959
H	0.53641	2.99917	2.14926
H	2.28072	2.61819	2.09302
H	1.12926	1.43290	2.76707
B	-0.78319	0.54599	0.07310
O	-1.22480	-0.45470	0.92598
O	-1.70646	0.87284	-0.90367
C	-2.64779	-0.69627	0.62370
C	-2.78368	-0.13200	-0.84612
C	-2.46113	-1.17080	-1.93417
H	-3.25386	-1.93326	-2.01665
H	-2.37285	-0.65657	-2.90472
H	-1.50412	-1.67827	-1.73074
C	-4.10950	0.56947	-1.15493
H	-4.08955	0.96214	-2.18466
H	-4.95386	-0.13711	-1.07670
H	-4.29345	1.41307	-0.47317
C	-2.92275	-2.19508	0.77503
H	-3.96844	-2.42969	0.51079
H	-2.25686	-2.79797	0.14000
H	-2.76149	-2.49786	1.82260
C	-3.45090	0.10260	1.66475
H	-4.53517	-0.07224	1.56316
H	-3.14221	-0.21272	2.67447
H	-3.25967	1.18418	1.57274
C	2.37540	0.04574	0.01663
C	2.13551	-1.27180	0.47651
C	3.62876	0.31398	-0.58206
C	3.11016	-2.27531	0.35322
H	1.16755	-1.51580	0.93063
C	4.60634	-0.68643	-0.71073
H	3.84840	1.32011	-0.95890
C	4.34911	-1.98451	-0.24092
H	2.90103	-3.28761	0.71733
H	5.56897	-0.45309	-1.17958
H	5.10960	-2.76678	-0.34087

pinBOSiMe$_2$Ph

SCF (BP86) Energy = -801.987393267
Enthalpy 0K = -801.622786
Enthalpy 298K = -801.621842
Free Energy 298K = -801.697374
Lowest Frequency = 16.4707 cm^{-1}
Second Frequency = 22.8516 cm^{-1}
SCF (BP86-D3BJ) Energy = -802.065873498
SCF (Toluene) Energy = -801.990449068
SCF (BS2) Energy = -1087.82202189

O	1.88600	0.85023	-0.12578
O	1.95465	-1.45654	0.18644
B	1.15775	-0.33070	0.03142
C	3.28160	0.51784	0.16859
C	3.32292	-1.04159	-0.11759
C	4.18388	1.36768	-0.73074
H	4.06288	2.43422	-0.47861
H	5.24511	1.10283	-0.58386
H	3.93357	1.23897	-1.79436
C	3.52032	0.86434	1.64898
H	3.26871	1.92452	1.81482
H	2.88157	0.25347	2.30805
H	4.57258	0.70934	1.94059
C	4.28022	-1.83834	0.77402
H	5.32355	-1.51317	0.61994
H	4.02962	-1.72665	1.83947
H	4.21708	-2.90940	0.52086
C	3.57049	-1.37468	-1.60008
H	3.37087	-2.44611	-1.76272
H	2.89545	-0.79941	-2.25517
Si	-1.33663	0.88948	-0.08252

```
C  -1.10195  2.07234  1.37716
H  -1.85403  2.87970  1.35367
H  -1.20876  1.53757  2.33516
H  -0.10007  2.53033  1.33916
C  -1.10199  1.78693 -1.73295
H  -1.84884  2.59062 -1.85283
H  -0.09674  2.23647 -1.78360
H  -1.21794  1.08815 -2.57762
C  -3.01669  0.02002 -0.00229
C  -3.11026 -1.38508  0.12155
C  -4.21880  0.76347 -0.06565
H  -2.19071 -1.97773  0.17228
H  -4.18449  1.85646 -0.16198
C  -4.35968 -2.02410  0.17991
C  -5.46960  0.12949 -0.00776
H  -4.41096 -3.11436  0.27601
H  -6.38828  0.72432 -0.05853
C  -5.54123 -1.26825  0.11536
H  -6.51616 -1.76583  0.16083
H   4.61123 -1.16552 -1.89938
O  -0.20397 -0.39721  0.03370
```

6

SCF (BP86) Energy = -1555.60305410
Enthalpy 0K = -1554.774524
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 (Toluene) Energy = -1555.61062849
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
```

TS(6-I)

SCF (BP86) Energy = -1881.53092732
Enthalpy 0K = -1880.561311
Enthalpy 298K = -1880.560366
Free Energy 298K = -1880.711374
Lowest Frequency = -110.0912 cm^{-1}
Second Frequency = 19.0069 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.81625069
SCF (Toluene) Energy = -1881.53654216
SCF (BS2) Energy = -2366.85792565

```
Si -0.62166 -0.96682 -2.35812
Mg  0.25289 -0.36401  0.13970
O  -1.16044 -3.71207 -0.65276
N   2.20120  0.30318  0.56418
N  -0.67835  1.12604  1.28163
N  -0.06810 -2.36280  1.05429
C   3.32499  0.23349 -0.33839
C  -0.03160  1.48449  2.41230
C   3.91316 -1.02654 -0.65982
C   4.87763  1.31683 -1.88441
H   5.25352  2.22740 -2.36457
C   2.38686  0.80275  1.80365
```

C	1.33777	1.21006	2.67277
H	1.67527	1.50789	3.66934
C	3.81965	1.42230	-0.96036
C	-1.98324	1.69469	1.03106
C	-3.17077	1.03708	1.46280
C	-2.52533	-1.10997	-2.58344
C	4.97190	-1.07264	-1.58776
H	5.43033	-2.03933	-1.82344
C	3.24273	2.81476	-0.68961
H	2.45325	2.71978	0.07526
C	0.12820	-3.20204	2.34013
C	5.45687	0.08502	-2.20349
H	6.28007	0.02803	-2.92334
C	-4.41749	1.64289	1.20978
H	-5.33050	1.13881	1.54581
C	-0.78368	2.22123	3.51458
H	-1.34852	3.07708	3.11269
H	-0.09912	2.58231	4.29605
H	-1.52581	1.55193	3.98408
C	-4.53066	-2.38603	-3.22403
H	-4.97654	-3.32040	-3.58447
C	3.48339	-2.32724	0.01914
H	2.55223	-2.11901	0.57601
C	3.79357	0.99641	2.35777
H	3.80340	0.79635	3.44143
H	4.13024	2.03839	2.21919
H	4.52598	0.34330	1.86071
C	-3.13978	-2.29964	-3.04361
H	-2.52151	-3.17522	-3.27046
C	-0.83247	3.63111	-0.24639
H	-0.05311	2.85836	-0.38339
C	-0.62253	-2.92897	0.06554
C	-2.07408	2.92078	0.30059
C	-3.15360	-0.32104	2.16275
H	-2.09454	-0.60136	2.30867
C	-1.24727	-3.51793	2.95194
H	-1.78470	-2.59539	3.21963
H	-1.11581	-4.11765	3.86931
H	-1.87227	-4.10010	2.25412
C	-0.27374	4.67577	0.74946
H	-1.03949	5.43553	0.98816
H	0.59570	5.19922	0.31326
H	0.05478	4.21193	1.69287
C	-3.37314	-0.00966	-2.30380
H	-2.94409	0.92936	-1.93198
C	3.18370	-3.45136	-0.99573
H	2.40309	-3.14965	-1.71226
H	2.83777	-4.36293	-0.47779
H	4.08174	-3.73159	-1.57327
C	2.59538	3.40446	-1.96330
H	3.33828	3.51598	-2.77269
H	2.17855	4.40590	-1.75610
H	1.78281	2.76336	-2.34149
C	-5.34740	-1.27768	-2.94915
H	-6.43182	-1.34142	-3.09301
C	-3.34548	3.48677	0.08254
H	-3.42212	4.43202	-0.46387
C	-3.83388	-0.27975	3.55068
H	-3.39028	0.48604	4.20942
H	-3.74559	-1.25772	4.05680
H	-4.91114	-0.05477	3.46201
C	0.96378	-2.33506	3.28987
H	1.95754	-2.12478	2.86304
H	1.10349	-2.86428	4.24788
H	0.47037	-1.37033	3.48985
C	4.54908	-2.78939	1.04193
H	5.51051	-2.99763	0.54015
H	4.23202	-3.71597	1.55377
H	4.73523	-2.02218	1.81238
C	-3.81809	-1.39933	1.27540
H	-4.87991	-1.15937	1.09334
H	-3.78120	-2.38812	1.76493
H	-3.33096	-1.47609	0.28978
C	4.31399	3.79263	-0.15079
H	4.82986	3.39575	0.73924
H	3.85226	4.75728	0.12312
H	5.08639	4.00042	-0.91217
C	-4.76269	-0.08631	-2.48755
H	-5.38817	0.78509	-2.26423
C	-1.08632	4.30114	-1.61431
H	-1.55837	3.60813	-2.33072
H	-0.13422	4.64638	-2.04999
H	-1.73878	5.18762	-1.52407
C	-0.11798	0.64406	-3.30992
H	-0.56305	1.54862	-2.86328
H	-0.45013	0.58705	-4.36222
H	0.97924	0.76529	-3.30281
C	0.16929	-2.38086	-3.39696
H	1.25475	-2.20944	-3.50038
H	-0.26281	-2.39319	-4.41393
H	0.02037	-3.37707	-2.95092
C	0.86865	-4.50596	1.99388
H	0.28975	-5.12609	1.28876
H	1.02588	-5.09818	2.91168
H	1.85363	-4.29529	1.54920
C	-4.51337	2.86576	0.54089
H	-5.49093	3.32669	0.36380

I

SCF (BP86) Energy = -1881.57211495
Enthalpy 0K = -1880.600928
Enthalpy 298K = -1880.599984
Free Energy 298K = -1880.750574
Lowest Frequency = 14.0265 cm^{-1}
Second Frequency = 18.7836 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.85371296
SCF (Toluene) Energy = -1881.57830980
SCF (BS2) Energy = -2366.89823341

Si	-1.31115	-2.07003	-1.69298
Mg	0.33272	-0.27683	0.57334
O	-1.87134	-3.80998	0.27337
N	2.37419	0.12113	0.51144
N	-0.28629	1.63237	1.07598
N	-0.55604	-2.03475	1.09035
C	3.39406	-0.34238	-0.39953
C	0.52451	2.17126	2.01783
C	3.71726	-1.73258	-0.47634
C	5.02475	0.10383	-2.16721
H	5.52843	0.81490	-2.83154
C	2.73536	0.89857	1.55780
C	1.83520	1.70271	2.31132
H	2.29538	2.18081	3.18028
C	4.05372	0.58447	-1.26650
C	-1.46922	2.38450	0.70966
C	-2.73550	2.09061	1.29721
C	-3.13167	-1.72764	-2.13145
C	4.69533	-2.15519	-1.39753
H	4.95074	-3.21767	-1.45005
C	3.72804	2.07980	-1.31071
H	2.99653	2.30393	-0.51591
C	-0.51135	-2.59570	2.48947
C	5.35344	-1.25181	-2.23807
H	6.11282	-1.60370	-2.94418
C	-3.83432	2.91882	0.99270
H	-4.80167	2.70659	1.46071
C	0.05405	3.37043	2.82952
H	0.03373	4.28112	2.20711
H	0.72184	3.55524	3.68356
H	-0.97450	3.22695	3.19697
C	-5.50346	-2.32227	-1.92385
H	-6.28230	-2.95620	-1.48546
C	3.09275	-2.76552	0.46121
H	2.09204	-2.39830	0.75746
C	4.19005	0.97865	2.00533
H	4.23954	0.94299	3.10629
H	4.64621	1.93436	1.69541
H	4.79780	0.16250	1.58967
C	-4.15871	-2.53388	-1.58048
H	-3.88564	-3.32430	-0.87211
C	-0.08185	3.71951	-1.04062
H	0.64738	2.92793	-0.79263

C	-1.24125	-2.72539	0.13436
C	-1.36232	3.43815	-0.24932
C	-2.96771	0.90649	2.23575
H	-2.03484	0.31564	2.26918
C	-1.92605	-2.68989	3.10578
H	-2.38744	-1.69301	3.18396
H	-1.86803	-3.11739	4.12311
H	-2.56534	-3.33356	2.48421
C	0.55268	5.08118	-0.67570
H	-0.14407	5.91318	-0.88046
H	1.46605	5.25675	-1.27117
H	0.83302	5.13282	0.38933
C	-3.50482	-0.70395	-3.03424
H	-2.74039	-0.05630	-3.48022
C	2.88951	-4.14542	-0.19889
H	2.36264	-4.06295	-1.16412
H	2.28894	-4.79591	0.45773
H	3.84760	-4.66437	-0.37769
C	3.07864	2.44591	-2.66467
H	3.76493	2.23599	-3.50368
H	2.82912	3.52087	-2.69827
H	2.15398	1.87073	-2.83662
C	-5.85245	-1.30237	-2.82465
H	-6.90216	-1.13838	-3.09210
C	-2.49311	4.23544	-0.51381
H	-2.40693	5.05780	-1.23279
C	-3.29241	1.35423	3.67971
H	-2.48544	1.96735	4.11544
H	-3.43775	0.47581	4.33268
H	-4.22077	1.95148	3.71152
C	0.34388	-1.62784	3.33204
H	1.37594	-1.55447	2.94133
H	0.41472	-1.97355	4.37789
H	-0.09727	-0.61276	3.35694
C	3.93676	-2.90987	1.75075
H	4.95849	-3.25116	1.50670
H	3.48582	-3.64970	2.43513
H	4.02117	-1.95388	2.29341
C	-4.08720	-0.01179	1.69289
H	-5.05421	0.51838	1.64573
H	-4.22380	-0.88759	2.34879
H	-3.85685	-0.38077	0.68043
C	4.97433	2.96402	-1.07137
H	5.49365	2.70414	-0.13434
H	4.68644	4.02844	-1.01981
H	5.70583	2.86022	-1.89192
C	-4.84969	-0.49117	-3.37900
H	-5.11383	0.30938	-4.07890
C	-0.36101	3.65410	-2.56121
H	-0.78897	2.67949	-2.85029
H	0.56748	3.80524	-3.13612
H	-1.07487	4.43505	-2.87511
C	-0.30783	-0.44454	-2.00571
H	-0.71243	0.45525	-1.49905
H	-0.36817	-0.20038	-3.08173
H	0.78165	-0.54659	-1.82192
C	-0.59054	-3.41993	-2.81990
H	0.50018	-3.51765	-2.68595
H	-0.79345	-3.20736	-3.88279
H	-1.05693	-4.38358	-2.55967
C	0.13692	-3.99986	2.51536
H	-0.44890	-4.69714	1.89918
H	0.17456	-4.37995	3.55224
H	1.16874	-3.96367	2.13157
C	-3.71914	4.00007	0.11503
H	-4.58308	4.63931	-0.09501

TS(6-I)$_B$

SCF (BP86) Energy = -1881.50759392
Enthalpy 0K = -1880.538411
Enthalpy 298K = -1880.537467
Free Energy 298K = -1880.689926
Lowest Frequency = -113.2504 cm^{-1}
Second Frequency = 11.6242 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.79389472
SCF (Toluene) Energy = -1881.51260940
SCF (BS2) Energy = -2366.83234827

Si	0.66835	-1.16170	2.30745
Mg	-0.27704	-0.51478	-0.36127
O	0.76744	-3.00224	1.01574
N	-2.19483	0.33529	-0.54521
N	0.67817	1.07664	-1.32600
N	0.01368	-2.54886	-1.12101
C	-3.25563	0.26670	0.42825
C	0.00870	1.51600	-2.41802
C	-3.82095	-0.99697	0.77976
C	-4.66240	1.32963	2.12198
H	-4.99807	2.23448	2.64103
C	-2.41245	0.91380	-1.74418
C	-1.38013	1.32164	-2.63383
H	-1.74077	1.66716	-3.60705
C	-3.69654	1.44998	1.10288
C	2.00014	1.60276	-1.07426
C	3.16477	0.87343	-1.45098
C	2.54479	-1.17303	2.63688
C	-4.78262	-1.05623	1.80702
H	-5.22142	-2.02535	2.06784
C	-3.18439	2.85566	0.77132
H	-2.42321	2.76988	-0.02292
C	-0.23241	-3.17743	-2.46612
C	-5.20181	0.09234	2.48541
H	-5.94953	0.02502	3.28258
C	4.43302	1.42963	-1.19129
H	5.32747	0.86943	-1.48561
C	0.76554	2.22336	-3.53617
H	0.07853	2.71024	-4.24397
H	1.37264	1.48806	-4.09516
H	1.46832	2.97383	-3.14425
C	4.57834	-2.37142	3.32585
H	5.05837	-3.29735	3.66233
C	-3.49486	-2.27858	0.01298
H	-2.60560	-2.08191	-0.61249
C	-3.82887	1.15865	-2.25258
H	-3.93991	0.70340	-3.25206
H	-4.02865	2.23686	-2.37050
H	-4.58923	0.73374	-1.58228
C	3.19959	-2.35439	3.06583
H	2.62234	-3.27626	3.19749
C	0.92417	3.66730	0.08087
H	0.06834	2.96992	0.13824
C	0.50062	-3.27606	-0.16236
C	2.13410	2.85994	-0.40292
C	3.10123	-0.49420	-2.12878
H	2.03432	-0.75442	-2.25373
C	-1.18210	-4.38509	-2.31795
H	-0.73605	-5.14098	-1.64997
H	-1.37032	-4.85130	-3.30091
H	-2.15033	-4.07563	-1.89284
C	0.53981	4.79492	-0.90722
H	1.38645	5.48864	-1.05701
H	-0.30970	5.38058	-0.51315
H	0.24520	4.40041	-1.89214
C	3.33630	-0.01148	2.46720
H	2.87446	0.92128	2.12374
C	-3.15606	-3.46730	0.93647
H	-2.30892	-3.23436	1.60144
H	-2.87863	-4.35151	0.33770
H	-4.01534	-3.75689	1.56621
C	-2.51517	3.52599	1.99251
H	-3.23001	3.64855	2.82510
H	-2.14858	4.53226	1.72336
H	-1.66271	2.93650	2.36554
C	5.34219	-1.20435	3.15583
H	6.41886	-1.21613	3.35829
C	3.42673	3.37494	-0.18190
H	3.53567	4.34433	0.31540
C	3.74854	-0.47167	-3.53318
H	3.29511	0.29534	-4.18383
H	3.63667	-1.45173	-4.03000
H	4.82969	-0.25598	-3.47135
C	1.10167	-3.65034	-3.08070

H	1.79411	-2.80535	-3.22154
H	0.92788	-4.12130	-4.06414
H	1.58500	-4.38837	-2.41877
C	-4.66087	-2.64078	-0.93888
H	-5.58468	-2.84194	-0.36811
H	-4.42522	-3.54617	-1.52625
H	-4.87695	-1.82174	-1.64549
C	3.75536	-1.58428	-1.24960
H	4.82896	-1.37814	-1.09595
H	3.67105	-2.57428	-1.72987
H	3.28412	-1.64400	-0.25543
C	-4.32404	3.76258	0.24615
H	-4.85246	3.31224	-0.60943
H	-3.92388	4.74111	-0.07243
H	-5.07436	3.95168	1.03413
C	4.71710	-0.02420	2.72245
H	5.30337	0.88982	2.57857
C	1.14709	4.26950	1.48677
H	1.46947	3.50704	2.21520
H	0.21310	4.72241	1.85859
H	1.91037	5.06710	1.47551
C	0.05925	0.66298	2.60097
H	0.48550	1.39227	1.89345
H	0.35465	0.96530	3.62381
H	-1.04049	0.71047	2.53025
C	-0.23420	-2.18183	3.64441
H	-1.32758	-2.09433	3.52510
H	0.02669	-1.80629	4.64948
H	0.02990	-3.24925	3.58968
C	-0.87841	-2.11201	-3.36735
H	-1.84116	-1.76879	-2.95217
H	-1.06957	-2.52734	-4.37116
H	-0.22386	-1.23161	-3.48339
C	4.57342	2.67639	-0.57650
H	5.56801	3.09809	-0.39646

I_B

SCF (BP86) Energy = -1881.56811601
Enthalpy 0K = -1880.597996
Enthalpy 298K = -1880.597052
Free Energy 298K = -1880.750917
Lowest Frequency = 11.1979 cm^{-1}
Second Frequency = 15.0555 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.83834162
SCF (Toluene) Energy = -1881.57412195
SCF (BS2) Energy = -2366.89580893

Si	-1.67392	-1.77417	-2.20154
Mg	0.33028	-0.22864	0.50314
O	-0.86772	-1.36013	-0.70185
N	2.40490	-0.05211	0.49089
N	-0.06172	1.74423	1.01003
N	-0.59005	-1.87282	1.43908
C	3.40509	-0.64717	-0.36168
C	0.77148	2.17183	1.98423
C	3.59573	-2.06088	-0.38235
C	5.15188	-0.41570	-2.05798
H	5.75135	0.22164	-2.71794
C	2.81771	0.63691	1.57896
C	2.00236	1.53892	2.31736
H	2.48555	1.94359	3.21034
C	4.19084	0.18312	-1.22094
C	-1.16150	2.60337	0.63308
C	-2.44870	2.43848	1.22443
C	-3.56081	-1.68877	-2.02795
C	4.57634	-2.60558	-1.23549
H	4.73365	-3.68974	-1.23675
C	4.00434	1.69962	-1.31583
H	3.27134	2.00702	-0.55079
C	-0.72280	-2.59323	2.74401
C	5.35696	-1.79876	-2.06805
H	6.11520	-2.24357	-2.72110
C	-3.47776	3.33535	0.87447
H	-4.46310	3.21742	1.33897
C	0.42612	3.41669	2.78926
H	1.09805	3.53006	3.65239
H	-0.61717	3.39039	3.14226
H	0.51603	4.32078	2.16286
C	-5.65637	-2.48665	-1.03116
H	-6.17409	-3.12111	-0.30314
C	2.81136	-3.01510	0.51804
H	2.00118	-2.44124	1.00260
C	4.25154	0.50206	2.07569
H	4.29455	0.66879	3.16339
H	4.90606	1.25451	1.60276
H	4.67167	-0.48794	1.84205
C	-4.25474	-2.50295	-1.09911
H	-3.67268	-3.12716	-0.41152
C	0.35864	3.77990	-1.11362
H	1.02080	2.94686	-0.81851
C	-1.23371	-2.32584	0.39484
C	-0.95909	3.61648	-0.35217
C	-2.77396	1.31621	2.21106
H	-1.86531	0.69906	2.33225
C	-0.51466	-4.11232	2.56572
H	-1.24441	-4.51650	1.84690
H	-0.63334	-4.63284	3.53222
H	0.49720	-4.32510	2.18341
C	1.07669	5.10381	-0.76464
H	0.45364	5.97687	-1.02797
H	2.02623	5.19047	-1.32199
H	1.31141	5.17298	0.31059
C	-4.32420	-0.85889	-2.88253
H	-3.82170	-0.21224	-3.61116
C	2.15405	-4.15480	-0.28945
H	1.47704	-3.75689	-1.06221
H	1.55904	-4.80710	0.37115
H	2.90669	-4.78984	-0.78852
C	3.43065	2.08303	-2.69902
H	4.11759	1.78354	-3.51000
H	3.28373	3.17500	-2.77112
H	2.46107	1.59179	-2.88377
C	-6.39591	-1.65717	-1.89127
H	-7.49017	-1.64477	-1.83774
C	-2.02132	4.48872	-0.66049
H	-1.86166	5.27893	-1.40283
C	-3.16672	1.85497	3.60635
H	-2.37246	2.47955	4.04923
H	-3.36501	1.01950	4.30073
H	-4.08357	2.46835	3.55509
C	-2.12431	-2.33828	3.33886
H	-2.28596	-1.26217	3.51503
H	-2.23668	-2.86387	4.30361
H	-2.90242	-2.69766	2.64620
C	3.70869	-3.58816	1.64040
H	4.54336	-4.17641	1.21941
H	3.12821	-4.25436	2.30290
H	4.14500	-2.78775	2.26189
C	-3.89274	0.40824	1.65126
H	-4.82284	0.97843	1.48279
H	-4.12456	-0.40486	2.35911
H	-3.60116	-0.05136	0.69350
C	5.31470	2.47878	-1.05736
H	5.77409	2.21016	-0.09145
H	5.12094	3.56554	-1.05117
H	6.06445	2.28208	-1.84383
C	-5.72744	-0.84125	-2.81715
H	-6.29739	-0.18801	-3.48705
C	0.12470	3.68706	-2.63953
H	-0.34784	2.72975	-2.91704
H	1.07848	3.76785	-3.18707
H	-0.53248	4.49809	-2.99837
C	-1.05472	-0.43703	-3.39277
H	-1.38453	0.56770	-3.07952
H	-1.42488	-0.61352	-4.41700
H	0.04772	-0.44341	-3.43459
C	-1.11751	-3.49197	-2.75855
H	-0.02652	-3.52333	-2.91782
H	-1.61304	-3.76241	-3.70697
H	-1.38139	-4.24168	-1.99699
C	0.35183	-2.02073	3.68925
H	1.36550	-2.20861	3.29564

```
H   0.28146 -2.48638  4.68758
H   0.22990 -0.92954  3.80891
C  -3.27091  4.36787 -0.04467
H  -4.08137  5.06158 -0.29218
```

INT(6-I)$_C$

SCF (BP86) Energy = -1881.55060295
Enthalpy 0K = -1880.579370
Enthalpy 298K = -1880.578426
Free Energy 298K = -1880.736853
Lowest Frequency = 11.6938 cm^{-1}
Second Frequency = 19.8721 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.81909328
SCF (Toluene) Energy = -1881.55621556
SCF (BS2) Energy = -2366.87740812

```
Si  0.35523  0.27443 -2.47768
Mg -0.48087 -0.06392  0.01573
O   1.22744  0.65766  1.20865
N  -2.03247  0.99843  0.93345
N  -0.86520 -1.81937  1.09813
N   3.36463  1.63356  1.70059
C  -2.56639  2.17889  0.30237
C  -1.55322 -1.77996  2.25666
C  -1.94178  3.44559  0.49347
C  -4.14546  3.20782 -1.24852
H  -5.00019  3.11945 -1.92903
C  -2.55804  0.59217  2.10736
C  -2.25597 -0.64263  2.73443
H  -2.73362 -0.78491  3.70719
C  -3.68456  2.05976 -0.57587
C  -0.33312 -3.07189  0.62451
C   0.93956 -3.54484  1.05879
C   2.28755  0.20723 -2.62435
C  -2.44468  4.56418 -0.19944
H  -1.96762  5.54035 -0.05352
C  -4.38147  0.72008 -0.82434
H  -3.93473 -0.02106 -0.13928
C   4.70475  2.13864  1.37371
C  -3.53702  4.45533 -1.06684
H  -3.91170  5.33643 -1.59848
C   1.43834 -4.74618  0.51572
H   2.41597 -5.11477  0.84742
C  -1.60915 -3.00870  3.15729
H  -1.63077 -3.94193  2.57421
H  -2.48802 -2.97678  3.81873
H  -0.70978 -3.04933  3.79735
C   4.46134  1.21420 -3.21459
H   5.02947  2.07835 -3.57945
C  -0.74011  3.62477  1.42258
H  -0.52744  2.64299  1.87983
C  -3.58247  1.46926  2.81396
H  -3.81220  1.08504  3.81863
H  -4.52269  1.50885  2.23652
H  -3.22844  2.50962  2.89963
C   3.06399  1.30346 -3.07299
H   2.56590  2.24333 -3.33939
C  -2.44693 -3.31931 -0.83400
H  -2.44495 -2.21496 -0.75979
C   2.32157  1.14276  1.37254
C  -1.07383 -3.80152 -0.35725
C   1.79190 -2.78933  2.08057
H   1.21286 -1.91075  2.41432
C   5.25350  2.81163  2.64917
H   4.60908  3.64998  2.96010
H   6.26504  3.20328  2.45392
H   5.31324  2.09007  3.48015
C  -3.57861 -3.83530  0.08741
H  -3.59481 -4.93982  0.10109
H  -4.56190 -3.48638 -0.27497
H  -3.45827 -3.48259  1.12362
C   2.98795 -0.98560 -2.31401
H   2.42741 -1.86379 -1.96633
C   0.51454  4.05983  0.63165
H   0.74967  3.34384 -0.17405
H   1.39068  4.13301  1.30073
H   0.36906  5.04899  0.16263
C  -4.13439  0.22849 -2.26877
H  -4.54606  0.93826 -3.00808
H  -4.61674 -0.75067 -2.43757
H  -3.05577  0.11996 -2.47424
C   5.12690  0.01565 -2.90842
H   6.21319 -0.06147 -3.02912
C  -0.53063 -4.99810 -0.86206
H  -1.09155 -5.56637 -1.61061
C   2.11999 -3.65129  3.32195
H   1.21066 -4.05393  3.79801
H   2.66567 -3.05504  4.07447
H   2.75952 -4.51113  3.05480
C   4.58141  3.15812  0.22284
H   4.18825  2.67615 -0.68724
H   5.57766  3.57204 -0.00705
H   3.91709  3.99107  0.50512
C  -1.02708  4.62634  2.56449
H  -1.22559  5.63948  2.17242
H  -0.16059  4.69661  3.24568
H  -1.90352  4.32487  3.16263
C   3.10183 -2.27458  1.44144
H   3.74446 -3.11475  1.12344
H   3.67767 -1.67233  2.16686
H   2.90699 -1.65554  0.55034
C  -5.89611  0.78234 -0.52411
H  -6.09509  1.12401  0.50602
H  -6.35427 -0.21479 -0.64567
H  -6.41925  1.47224 -1.20957
C   4.38178 -1.08825 -2.45620
H   4.88713 -2.03257 -2.22234
C  -2.75558 -3.68917 -2.29879
H  -1.94597 -3.37946 -2.97914
H  -3.68418 -3.18890 -2.62344
H  -2.91634 -4.77469 -2.42579
C  -0.22093 -1.03995 -3.77672
H   0.13158 -2.04930 -3.50351
H   0.17044 -0.80338 -4.78219
H  -1.32254 -1.07732 -3.84059
C  -0.14887  1.97514 -3.24434
H  -1.24851  2.06300 -3.27814
H   0.23077  2.09164 -4.27611
H   0.21765  2.82792 -2.64669
C   5.58905  0.94366  0.96074
H   5.64280  0.19753  1.77019
H   6.61120  1.30188  0.75191
H   5.19937  0.45903  0.05086
C   0.71432 -5.47496 -0.43252
H   1.11835 -6.40768 -0.84030
```

TS(6-I)$_C$

SCF (BP86) Energy = -1881.52919238
Enthalpy 0K = -1880.559574
Enthalpy 298K = -1880.558629
Free Energy 298K = -1880.712158
Lowest Frequency = -159.4034 cm^{-1}
Second Frequency = 15.7396 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.80533665
SCF (Toluene) Energy = -1881.53481650
SCF (BS2) Energy = -2366.85464499

```
Si -0.80319 -1.14395 -1.82189
Mg  0.39596 -0.05011  0.40417
O  -0.56545 -1.36494  1.64621
N   2.44699 -0.07945  0.73528
N   0.12111  1.87696  1.11847
N  -2.01373 -2.84932  0.39332
C   3.34904 -0.89656 -0.03602
C   0.94423  2.28123  2.11120
C   3.35740 -2.31159  0.15065
C   4.95707 -1.13918 -1.85468
H   5.58648 -0.68838 -2.63051
C   2.90971  0.64038  1.77725
C   2.16148  1.63901  2.45413
H   2.67189  2.07189  3.31875
```

C	4.17527	-0.29974	-1.03694
C	-0.98942	2.71429	0.73835
C	-2.24922	2.60655	1.39577
C	-2.65461	-0.76745	-2.15083
C	4.16467	-3.10158	-0.69124
H	4.18006	-4.18776	-0.54783
C	4.26409	1.21585	-1.24503
H	3.60805	1.70060	-0.50171
C	-2.91165	-3.83693	1.05453
C	4.95273	-2.52934	-1.69600
H	5.56837	-3.16198	-2.34412
C	-3.30920	3.42935	0.96479
H	-4.27958	3.35282	1.46823
C	0.57453	3.49225	2.95822
H	0.13370	4.29570	2.34833
H	1.45056	3.88665	3.49406
H	-0.18451	3.20981	3.70914
C	-4.89670	-1.46409	-2.89011
H	-5.56370	-2.24980	-3.26387
C	2.57576	-2.98644	1.28077
H	1.89688	-2.23447	1.71819
C	4.33352	0.44374	2.28110
H	4.36773	0.55689	3.37649
H	5.00431	1.21012	1.85453
H	4.73717	-0.54136	2.00538
C	-3.54749	-1.75772	-2.62502
H	-3.18091	-2.77546	-2.80175
C	0.51382	3.73682	-1.09498
H	1.02742	2.76213	-0.99212
C	-1.22597	-2.00104	0.79256
C	-0.82338	3.61624	-0.35837
C	-2.50312	1.61081	2.52911
H	-1.55114	1.09575	2.74564
C	-2.49722	-4.04088	2.52514
H	-1.46540	-4.42363	2.59604
H	-3.16851	-4.77300	3.00683
H	-2.55714	-3.09627	3.09015
C	1.43069	4.80154	-0.44579
H	0.94300	5.79269	-0.45474
H	2.37997	4.88613	-1.00401
H	1.67663	4.55089	0.59803
C	-3.17526	0.53366	-1.94902
H	-2.52128	1.33405	-1.57905
C	1.70978	-4.16535	0.78766
H	1.00904	-3.85314	-0.00352
H	1.12062	-4.57891	1.62508
H	2.32751	-4.98794	0.38581
C	3.77431	1.64230	-2.64732
H	4.38604	1.18187	-3.44324
H	3.84892	2.73815	-2.76422
H	2.72621	1.35068	-2.82042
C	-5.38802	-0.16503	-2.68311
H	-6.43874	0.06700	-2.88961
C	-1.91530	4.41719	-0.74499
H	-1.79744	5.11636	-1.57892
C	-2.98128	2.30194	3.82690
H	-2.28163	3.08570	4.16245
H	-3.08318	1.56342	4.64119
H	-3.96759	2.77897	3.68794
C	-2.78959	-5.15553	0.26612
H	-3.06988	-5.00300	-0.78871
H	-3.45890	-5.91865	0.69851
H	-1.75659	-5.53943	0.30010
C	3.52942	-3.45817	2.40491
H	4.23934	-4.21623	2.02878
H	2.95773	-3.91126	3.23405
H	4.11971	-2.62318	2.81748
C	-3.52855	0.53708	2.09710
H	-4.52222	0.98607	1.92178
H	-3.63966	-0.22744	2.88655
H	-3.22676	0.03564	1.16331
C	5.70514	1.73257	-1.01720
H	6.10297	1.42809	-0.03499
H	5.73433	2.83485	-1.07349
H	6.39519	1.34289	-1.78636
C	-4.52116	0.83513	-2.21186
H	-4.89071	1.85283	-2.04471
C	0.35509	4.03442	-2.60087
H	-0.35673	3.34559	-3.08571
H	1.32899	3.93361	-3.10932
H	0.00216	5.06532	-2.78178
C	0.16538	0.00830	-3.05237
H	0.02993	1.08044	-2.83480
H	-0.18834	-0.17385	-4.08344
H	1.24440	-0.22060	-3.01793
C	-0.40728	-2.90400	-2.47063
H	0.68209	-3.07870	-2.44796
H	-0.73974	-3.01207	-3.51886
H	-0.89650	-3.68516	-1.86810
C	-4.34829	-3.28502	0.95656
H	-4.45069	-2.35436	1.53796
H	-5.06332	-4.02585	1.35443
H	-4.60785	-3.06453	-0.09109
C	-3.15002	4.33524	-0.08847
H	-3.98493	4.97042	-0.40315

I_C

SCF (BP86) Energy = -1881.58070678
Enthalpy 0K = -1880.609534
Enthalpy 298K = -1880.608590
Free Energy 298K = -1880.762678
Lowest Frequency = 8.6852 cm^{-1}
Second Frequency = 9.6845 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.84867457
SCF (Toluene) Energy = -1881.58827041
SCF (BS2) Energy = -2366.90655124

Si	-1.70041	-2.41531	0.10513
Mg	0.64570	0.30874	-0.13579
O	-0.47152	-0.16760	1.32073
N	2.59494	-0.13807	-0.64184
N	0.53775	2.10507	-1.10533
N	-2.29732	-1.21102	2.44722
C	3.24613	-1.30377	-0.08198
C	1.58878	2.59432	-1.79855
C	3.75354	-1.24812	1.24878
C	3.92638	-3.63971	-0.23355
H	4.00618	-4.56992	-0.80631
C	3.33717	0.74548	-1.34771
C	2.83725	1.93702	-1.93093
H	3.57609	2.49285	-2.51367
C	3.33404	-2.51276	-0.83824
C	-0.60588	2.96122	-0.88056
C	-0.57323	3.89384	0.19870
C	-3.51783	-2.62885	-0.43103
C	4.32165	-2.40929	1.80749
H	4.70457	-2.37422	2.83348
C	2.84205	-2.62513	-2.28617
H	2.21841	-1.73715	-2.49528
C	-2.37331	-0.31298	3.62608
C	4.41275	-3.59912	1.07790
H	4.86263	-4.49052	1.52743
C	-1.71991	4.66979	0.45181
H	-1.71040	5.38112	1.28473
C	1.48915	3.96933	-2.44171
H	0.50818	4.12193	-2.91773
H	2.28234	4.11346	-3.19007
H	1.59340	4.76082	-1.67825
C	-5.15779	-3.39171	-2.09577
H	-5.37243	-3.83381	-3.07528
C	3.69745	0.02830	2.09069
H	3.32217	0.84114	1.44276
C	4.83835	0.53568	-1.49003
H	5.35278	0.97806	-0.61708
H	5.22409	1.03797	-2.39007
H	5.11655	-0.52695	-1.51670
C	-3.82764	-3.19727	-1.69036
H	-3.02229	-3.49893	-2.37216
C	-1.84271	1.85323	-2.86509
H	-0.93186	1.22674	-2.82870
C	-1.45497	-1.07814	1.46797
C	-1.77197	2.82673	-1.68648
C	0.65339	4.04193	1.10399

H	1.50338	3.54465	0.60476
C	-1.02825	-0.21729	4.38114
H	-0.65814	-1.22594	4.63478
H	-1.15368	0.34643	5.32357
H	-0.26854	0.28656	3.76684
C	-1.83178	2.59788	-4.22139
H	-2.70981	3.26135	-4.31274
H	-1.86383	1.87922	-5.05914
H	-0.92873	3.21888	-4.34363
C	-4.59293	-2.26349	0.41263
H	-4.35684	-1.83141	1.39221
C	2.71075	-0.12921	3.26925
H	1.69594	-0.37417	2.91395
H	2.65254	0.80343	3.85742
H	3.03290	-0.93642	3.95040
C	1.97997	-3.88772	-2.51846
H	2.58977	-4.80693	-2.47315
H	1.51884	-3.85506	-3.52094
H	1.17680	-3.98618	-1.77079
C	-6.21092	-3.01818	-1.24478
H	-7.25006	-3.16744	-1.55869
C	-2.88747	3.63781	-1.39693
H	-3.78709	3.54713	-2.01555
C	1.05555	5.51551	1.33243
H	1.20022	6.05387	0.37998
H	1.99925	5.56915	1.90243
H	0.29316	6.06424	1.91237
C	-3.43034	-0.93508	4.56670
H	-4.40286	-1.02207	4.05282
H	-3.56835	-0.31831	5.47266
H	-3.12223	-1.94814	4.87677
C	5.09483	0.45420	2.59540
H	5.51485	-0.28626	3.29838
H	5.03236	1.41787	3.13008
H	5.81238	0.56821	1.76506
C	0.42756	3.32304	2.45467
H	-0.41192	3.78088	3.00669
H	1.32835	3.39219	3.09032
H	0.18192	2.25634	2.31303
C	4.01395	-2.61768	-3.29821
H	4.60554	-1.69038	-3.24568
H	3.63172	-2.71437	-4.32967
H	4.69676	-3.46519	-3.11066
C	-5.92463	-2.45465	0.00918
H	-6.74265	-2.16329	0.67778
C	-3.07491	0.92439	-2.78169
H	-3.13352	0.39366	-1.81719
H	-3.04516	0.16956	-3.58647
H	-4.01492	1.49079	-2.90081
C	-0.72225	-1.79426	-1.43191
H	-1.05611	-0.78432	-1.74032
H	-0.87984	-2.43537	-2.31546
H	0.37329	-1.81416	-1.26816
C	-0.97184	-4.08469	0.65807
H	0.10958	-4.00143	0.86108
H	-1.12568	-4.86574	-0.10607
H	-1.47019	-4.41065	1.58559
C	-2.84924	1.08974	3.18080
H	-2.12396	1.54968	2.49219
H	-2.97755	1.75430	4.05459
H	-3.82022	1.01716	2.66140
C	-2.87021	4.55080	-0.33753
H	-3.75050	5.16659	-0.12552

TS(I-II)

SCF (BP86) Energy = -1881.54219056
Enthalpy 0K = -1880.572568
Enthalpy 298K = -1880.571623
Free Energy 298K = -1880.723617
Lowest Frequency = -188.8966 cm^{-1}
Second Frequency = 9.4932 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.81663935
SCF (Toluene) Energy = -1881.54803147
SCF (BS2) Energy = -2366.86631791

Si	-0.57506	-2.16993	-2.07155
Mg	0.30410	-0.25123	0.59039
O	-0.76785	-3.43682	-0.65908
N	2.23156	0.50482	0.66132
N	-0.67962	1.46928	1.19628
N	-0.20500	-2.12469	1.26065
C	3.38029	0.28665	-0.18597
C	-0.00025	2.12461	2.16190
C	4.03998	-0.97761	-0.21436
C	4.97939	1.13041	-1.83233
H	5.33822	1.94412	-2.47275
C	2.40803	1.25602	1.77452
C	1.35708	1.86488	2.50948
H	1.69190	2.39036	3.40764
C	3.84926	1.34855	-1.02158
C	-1.99592	1.95824	0.84344
C	-3.15309	1.45511	1.50910
C	-2.41011	-1.81840	-2.44072
C	5.17120	-1.13742	-1.04022
H	5.69060	-2.10177	-1.04690
C	3.14683	2.70580	-1.11742
H	2.32243	2.71859	-0.38444
C	-0.36467	-3.19009	2.30761
C	5.65012	-0.09654	-1.84053
H	6.53336	-0.24270	-2.47117
C	-4.40737	2.02022	1.20450
H	-5.29615	1.65381	1.72967
C	-0.65024	3.26609	2.93353
H	-0.49265	4.21986	2.39892
H	-0.19113	3.36929	3.92869
H	-1.73613	3.13716	3.04266
C	-4.78974	-2.36367	-2.16748
H	-5.57033	-2.96604	-1.68929
C	3.59492	-2.16488	0.64041
H	2.61710	-1.91379	1.08971
C	3.81346	1.53753	2.29044
H	3.78856	1.76629	3.36692
H	4.25641	2.40756	1.77616
H	4.48754	0.68530	2.11454
C	-3.44102	-2.57992	-1.84168
H	-3.17340	-3.35159	-1.11192
C	-0.95112	3.45167	-1.00311
H	-0.07012	2.84098	-0.73573
C	-0.41031	-2.31159	-0.02988
C	-2.13318	2.94927	-0.17224
C	-3.09350	0.32725	2.54217
H	-2.07093	-0.09061	2.52457
C	-1.75079	-3.86548	2.21113
H	-2.55484	-3.11444	2.24878
H	-1.88866	-4.56048	3.05872
H	-1.84724	-4.43055	1.27226
C	-0.61200	4.92879	-0.69874
H	-1.46428	5.58882	-0.93909
H	0.25075	5.26365	-1.30135
H	-0.36158	5.08170	0.36414
C	-2.78513	-0.83120	-3.38234
H	-2.01493	-0.22369	-3.87218
C	3.41012	-3.44059	-0.21114
H	2.67995	-3.28150	-1.02172
H	3.04690	-4.27397	0.41174
H	4.35924	-3.76420	-0.67236
C	2.53114	2.89223	-2.52360
H	3.31345	2.88998	-3.30298
H	1.99737	3.85674	-2.58965
H	1.82017	2.08379	-2.76086
C	-5.13852	-1.37833	-3.10576
H	-6.19027	-1.20741	-3.36037
C	-3.41227	3.47493	-0.44037
H	-3.51851	4.24798	-1.20957
C	-3.37624	0.82886	3.97792
H	-2.65074	1.59270	4.30166
H	-3.32659	-0.00825	4.69655
H	-4.38546	1.27196	4.04993
C	-0.21276	-2.49054	3.67204
H	0.76209	-1.97704	3.74127
H	-0.27560	-3.22411	4.49438
H	-1.00695	-1.73919	3.82143

C	4.58469	-2.42994	1.79943
H	5.58871	-2.67958	1.41298
H	4.24267	-3.27840	2.41834
H	4.68818	-1.55140	2.45819
C	-4.07373	-0.81060	2.17891
H	-5.12236	-0.46627	2.20157
H	-3.98957	-1.63539	2.90755
H	-3.87438	-1.21138	1.17147
C	4.08704	3.88976	-0.79404
H	4.55372	3.79169	0.20039
H	3.52674	4.84075	-0.81192
H	4.90215	3.97274	-1.53432
C	-4.13213	-0.61229	-3.71515
H	-4.39591	0.15826	-4.44806
C	-1.22056	3.26555	-2.51463
H	-1.48524	2.22138	-2.75059
H	-0.33013	3.53930	-3.10516
H	-2.05399	3.90344	-2.85727
C	0.39579	-0.54947	-2.49790
H	-0.06013	0.34354	-2.02381
H	0.41823	-0.35404	-3.58655
H	1.45009	-0.62322	-2.17238
C	0.19172	-3.42450	-3.29305
H	1.24588	-3.63606	-3.04173
H	0.17003	-3.01983	-4.31989
H	-0.35921	-4.37795	-3.27227
C	0.73796	-4.25917	2.14816
H	0.67927	-4.73212	1.15550
H	0.61855	-5.04363	2.91667
H	1.73799	-3.81236	2.27280
C	-4.54392	3.03458	0.25198
H	-5.52781	3.46511	0.03807

II

SCF (BP86) Energy = -1881.57235687
Enthalpy 0K = -1880.601142
Enthalpy 298K = -1880.600198
Free Energy 298K = -1880.753969
Lowest Frequency = 4.9890 cm^{-1}
Second Frequency = 11.1469 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.84088695
SCF (Toluene) Energy = -1881.57795193
SCF (BS2) Energy = -2366.89961069

Si	-1.40681	-3.67462	0.46605
Mg	0.58374	0.48315	0.34263
O	-0.83612	-2.47883	1.57906
N	2.43140	0.85037	-0.54741
N	-0.28784	2.25617	-0.31425
N	0.18726	-0.48129	2.14653
C	3.37605	-0.22351	-0.72256
C	0.43690	3.22141	-0.91719
C	4.15664	-0.66603	0.38815
C	4.37398	-1.95871	-2.11589
H	4.45664	-2.47090	-3.08092
C	2.73565	2.06117	-1.06396
C	1.83363	3.15000	-1.15145
H	2.26375	4.05542	-1.58762
C	3.48353	-0.87500	-1.98729
C	-1.71915	2.42078	-0.24578
C	-2.31521	2.89132	0.96329
C	-2.99484	-3.04523	-0.35708
C	5.03964	-1.74701	0.19888
H	5.64897	-2.09504	1.03797
C	2.63579	-0.46127	-3.19465
H	2.18610	0.52202	-2.97604
C	0.11279	-0.70963	3.62896
C	5.15274	-2.39260	-1.03869
H	5.84378	-3.23365	-1.15953
C	-3.71647	3.02718	1.00916
H	-4.18994	3.39439	1.92463
C	-0.25069	4.46809	-1.46219
H	-0.65286	4.26337	-2.47083
H	0.46419	5.30010	-1.55373
H	-1.09929	4.78547	-0.83857
C	-4.95728	-1.57121	-0.35559
H	-5.51099	-0.74099	0.09507
C	4.05526	0.02262	1.75355
H	2.98383	0.25111	1.91981
C	4.11507	2.31394	-1.66384
H	4.36176	3.38614	-1.62322
H	4.13707	2.01014	-2.72552
H	4.90126	1.74195	-1.14922
C	-3.74101	-1.98637	0.21022
H	-3.36031	-1.47523	1.10086
C	-1.92761	1.50305	-2.65383
H	-0.83480	1.65336	-2.60958
C	-0.24993	-1.29149	1.19676
C	-2.52825	2.06822	-1.36434
C	-1.46106	3.25101	2.18424
H	-0.62195	2.52852	2.20793
C	-1.36067	-0.80281	4.08623
H	-1.92251	0.08941	3.76329
H	-1.41578	-0.86132	5.18827
H	-1.84737	-1.69399	3.66351
C	-2.44447	2.22275	-3.91934
H	-3.52214	2.04399	-4.08007
H	-1.91535	1.85069	-4.81393
H	-2.29412	3.31452	-3.86236
C	-3.50971	-3.67239	-1.51615
H	-2.95484	-4.49293	-1.98795
C	4.52209	-0.86538	2.92403
H	4.05363	-1.86341	2.89967
H	4.26257	-0.38909	3.88482
H	5.61821	-1.00451	2.92028
C	1.47126	-1.45342	-3.41341
H	1.84985	-2.47474	-3.59516
H	0.85919	-1.15688	-4.28359
H	0.81047	-1.48967	-2.53087
C	-5.45411	-2.21219	-1.50248
H	-6.40432	-1.89194	-1.94388
C	-3.92546	2.21196	-1.25899
H	-4.55584	1.93787	-2.11199
C	-0.84037	4.66543	2.08378
H	-0.14758	4.75467	1.23385
H	-0.27314	4.89945	3.00218
H	-1.62908	5.43057	1.97038
C	0.78115	0.50879	4.29703
H	1.83359	0.60210	3.97810
H	0.76252	0.41061	5.39651
H	0.25851	1.44172	4.02604
C	4.82154	1.36650	1.79512
H	5.89254	1.21138	1.57330
H	4.74760	1.81868	2.80015
H	4.42041	2.09251	1.07229
C	-2.22350	3.12759	3.51918
H	-2.97137	3.93195	3.63873
H	-1.52034	3.21620	4.36488
H	-2.74759	2.16190	3.61074
C	3.46749	-0.31522	-4.48855
H	4.32982	0.35869	-4.34860
H	2.84164	0.09320	-5.30097
H	3.85986	-1.28677	-4.83669
C	-4.72717	-3.26436	-2.08417
H	-5.10764	-3.76496	-2.98144
C	-2.18310	-0.01842	-2.75203
H	-1.77395	-0.55356	-1.87846
H	-1.71762	-0.43472	-3.66289
H	-3.26368	-0.23967	-2.78918
C	-0.07778	-4.14163	-0.79310
H	0.22286	-3.27437	-1.39943
H	-0.44381	-4.93085	-1.47237
H	0.81707	-4.52717	-0.27675
C	-1.79962	-5.14189	1.59632
H	-0.89026	-5.51011	2.10023
H	-2.22929	-5.97287	1.01111
H	-2.53312	-4.85725	2.36818
C	0.87663	-1.99160	4.03215
H	0.40034	-2.88560	3.60509
H	0.89337	-2.09135	5.13258
H	1.91986	-1.94795	3.67892
C	-4.52018	2.69673	-0.08965

H -5.60775 2.81310 -0.02988

TS(II-7)

SCF (BP86) Energy = -1881.54311777
Enthalpy 0K = -1880.574156
Enthalpy 298K = -1880.573211
Free Energy 298K = -1880.728156
Lowest Frequency = -201.3783 cm^{-1}
Second Frequency = 8.1076 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.81168018
SCF (Toluene) Energy = -1881.55178663
SCF (BS2) Energy = -2366.87198534

Si 0.92489 0.96684 2.95401
Mg -0.06825 0.28882 -0.79519
O -0.10662 1.29516 1.63122
N 1.33023 -0.76081 -1.88398
N -1.71139 -0.55107 -1.72274
N 0.09498 3.35143 0.14035
C 2.70608 -0.79414 -1.44962
C -1.58019 -1.20126 -2.89840
C 3.56225 0.31422 -1.71794
C 4.49601 -1.87357 -0.19445
H 4.86559 -2.72146 0.39340
C 0.98916 -1.37469 -3.03872
C -0.33816 -1.50223 -3.51436
H -0.42541 -1.99631 -4.48529
C 3.17975 -1.90857 -0.69488
C -3.01889 -0.43729 -1.12551
C -3.68890 0.82298 -1.15271
C 0.30734 -0.66440 3.72743
C 4.87156 0.29372 -1.19782
H 5.53715 1.14042 -1.40034
C 2.30406 -3.13238 -0.41064
H 1.36486 -3.01168 -0.97788
C 0.00874 4.50663 1.05246
C 5.33967 -0.78261 -0.43596
H 6.35986 -0.77504 -0.03786
C -4.94146 0.92839 -0.51794
H -5.47035 1.88603 -0.53304
C -2.81302 -1.70058 -3.64109
H -3.07768 -2.71937 -3.30688
H -2.61617 -1.75084 -4.72315
H -3.69059 -1.06218 -3.46083
C -1.55184 -2.05017 4.54298
H -2.63007 -2.22465 4.63003
C 3.12423 1.49815 -2.58487
H 2.06305 1.34297 -2.85023
C 2.07082 -2.01212 -3.89729
H 1.69521 -2.23160 -4.90753
H 2.41085 -2.96163 -3.44739
H 2.95922 -1.36584 -3.97416
C -1.07862 -0.92239 3.85194
H -1.79710 -0.22723 3.40183
C -2.89050 -2.90959 -0.35574
H -2.01834 -2.89018 -1.03145
C 0.09410 2.10268 0.25015
C -3.59798 -1.55479 -0.45547
C -3.08614 2.02910 -1.88038
H -1.98698 1.97403 -1.76114
C -1.06077 4.31252 2.14927
H -2.05371 4.17476 1.68864
H -1.10815 5.20606 2.79699
H -0.85149 3.43041 2.76733
C -3.79537 -4.08480 -0.79060
H -4.64199 -4.22437 -0.09571
H -3.22124 -5.02762 -0.79965
H -4.21806 -3.93099 -1.79801
C 1.20141 -1.58737 4.31966
H 2.28288 -1.42146 4.24453
C 3.22934 2.84398 -1.83478
H 2.59039 2.85325 -0.93794
H 2.90140 3.67096 -2.48856
H 4.26955 3.05428 -1.52870
C 1.93483 -3.22756 1.08610
H 2.83789 -3.34265 1.71120
H 1.28309 -4.09819 1.27544
H 1.40418 -2.32871 1.44068
C -0.64470 -2.95280 5.12215
H -1.01180 -3.83266 5.66190
C -4.84968 -1.38902 0.16904
H -5.30117 -2.23924 0.69248
C -3.38641 1.99209 -3.39775
H -2.97192 1.09180 -3.87771
H -2.94741 2.87295 -3.89863
H -4.47594 2.00605 -3.57934
C -0.37779 5.72456 0.17943
H 0.36058 5.87302 -0.62574
H -0.42392 6.64260 0.79099
H -1.36488 5.56867 -0.28640
C 3.93036 1.55498 -3.90465
H 5.00361 1.72617 -3.70846
H 3.56972 2.38225 -4.54065
H 3.84319 0.62006 -4.48365
C -3.52393 3.38382 -1.29191
H -4.58824 3.59997 -1.49439
H -2.93490 4.19522 -1.75107
H -3.36605 3.42146 -0.20164
C 2.97103 -4.44592 -0.88014
H 3.25859 -4.40563 -1.94461
H 2.28086 -5.29678 -0.74474
H 3.88415 -4.66642 -0.29981
C 0.73541 -2.72074 5.00689
H 1.44921 -3.42138 5.45465
C -2.35754 -3.14764 1.07486
H -1.67219 -2.34752 1.39855
H -1.81540 -4.10767 1.13707
H -3.18627 -3.18147 1.80377
C 2.73189 0.81271 2.39083
H 2.87781 -0.00670 1.66736
H 3.40047 0.63263 3.25073
H 3.06356 1.74645 1.90625
C 0.82916 2.21253 4.39787
H 1.20782 3.21935 4.16391
H 1.43707 1.80559 5.22631
H -0.20496 2.30805 4.76911
C 1.41117 4.75838 1.65217
H 1.75114 3.90423 2.25677
H 1.39697 5.65605 2.29493
H 2.14694 4.92265 0.84706
C -5.52321 -0.16379 0.13779
H -6.49711 -0.05654 0.62717

7

SCF (BP86) Energy = -1881.60990385
Enthalpy 0K = -1880.639042
Enthalpy 298K = -1880.638098
Free Energy 298K = -1880.794745
Lowest Frequency = 9.9863 cm^{-1}
Second Frequency = 12.9444 cm^{-1}
SCF (BP86-D3BJ) Energy = -1881.88066750
SCF (Toluene) Energy = -1881.61559096
SCF (BS2) Energy = -2366.93921558

Si -0.68710 1.24962 2.67985
Mg 0.44746 -0.29249 -0.14225
O -0.08342 0.14490 1.60914
N 2.44369 -0.42793 -0.72855
N -0.10498 -2.09390 -1.03744
N -1.21389 2.48020 -1.40895
C 3.39315 0.49050 -0.15090
C 0.75867 -2.84097 -1.75427
C 3.62759 1.75397 -0.76947
C 4.91618 1.10255 1.65244
H 5.41446 0.85733 2.59712
C 2.90477 -1.43355 -1.50039
C 2.10506 -2.48323 -2.01719
H 2.64669 -3.19588 -2.64461
C 4.04832 0.15754 1.07221
C -1.41141 -2.63147 -0.75022

C	-2.52350	-2.25930	-1.56243
C	-2.52530	1.62561	2.25571
C	4.51942	2.65546	-0.15566
H	4.71608	3.62220	-0.63283
C	3.82195	-1.18067	1.78034
H	3.25420	-1.83164	1.09300
C	-1.95261	3.70730	-1.66630
C	5.15935	2.34157	1.04852
H	5.84471	3.05835	1.51338
C	-3.79955	-2.76008	-1.23643
H	-4.65594	-2.49216	-1.86530
C	0.32778	-4.20208	-2.28614
H	0.40669	-4.96191	-1.48766
H	0.97403	-4.52313	-3.11707
H	-0.72107	-4.20411	-2.61912
C	-4.65841	0.87740	1.27876
H	-5.22859	0.11126	0.74123
C	2.96408	2.13918	-2.09395
H	2.16309	1.40213	-2.28449
C	4.39237	-1.52857	-1.81553
H	4.56706	-2.15195	-2.70545
H	4.93165	-1.99290	-0.97021
H	4.84564	-0.53781	-1.97097
C	-3.29530	0.66923	1.55162
H	-2.81685	-0.26042	1.22122
C	-0.44223	-3.89136	1.29366
H	0.49580	-3.56224	0.81337
C	-0.61297	1.49958	-1.14982
C	-1.59955	-3.48191	0.37970
C	-2.35925	-1.35380	-2.78540
H	-1.36346	-0.88100	-2.70739
C	-3.45832	3.40461	-1.50852
H	-3.79017	2.66098	-2.24948
H	-4.02199	4.33767	-1.67308
H	-3.68494	3.02854	-0.49862
C	-0.35741	-5.42289	1.48270
H	-1.23175	-5.81510	2.03155
H	0.54097	-5.68599	2.06785
H	-0.30548	-5.95640	0.51776
C	-3.18223	2.80959	2.66789
H	-2.62449	3.57492	3.22296
C	2.31932	3.54074	-2.03647
H	1.61568	3.62366	-1.19168
H	1.77151	3.74767	-2.97332
H	3.07628	4.33614	-1.92116
C	2.96281	-0.99431	3.05245
H	3.46121	-0.31410	3.76657
H	2.81041	-1.96301	3.56120
H	1.97349	-0.57593	2.80071
C	-5.28752	2.06188	1.70037
H	-6.35084	2.22694	1.49300
C	-2.89920	-3.93951	0.67126
H	-3.05232	-4.58470	1.54360
C	-2.39289	-2.15548	-4.10798
H	-1.58682	-2.90521	-4.15441
H	-2.27589	-1.48162	-4.97553
H	-3.35492	-2.68680	-4.21969
C	-1.62259	4.16387	-3.10449
H	-0.54574	4.36573	-3.21828
H	-2.17789	5.09069	-3.32167
H	-1.92057	3.39850	-3.83894
C	3.95880	2.06691	-3.27670
H	4.80127	2.76497	-3.12471
H	3.46024	2.33932	-4.22413
H	4.37887	1.05527	-3.39700
C	-3.41887	-0.23193	-2.82312
H	-4.42902	-0.62998	-3.02519
H	-3.18731	0.48528	-3.63111
H	-3.45972	0.31364	-1.86631
C	5.14832	-1.90007	2.11460
H	5.78686	-2.02463	1.22291
H	4.94451	-2.90150	2.53205
H	5.73544	-1.34532	2.86763
C	-4.54412	3.03132	2.39519
H	-5.02730	3.95672	2.73013
C	-0.53899	-3.17258	2.65942
H	-0.50136	-2.07743	2.53042
H	0.29784	-3.47459	3.31435
H	-1.48057	-3.43435	3.17509
C	-0.65582	0.57464	4.46246
H	-1.22878	-0.36488	4.53390
H	-1.09896	1.29614	5.17119
H	0.37867	0.36815	4.78655
C	0.28866	2.89179	2.65889
H	1.33868	2.70350	2.94143
H	-0.11935	3.63359	3.36828
H	0.29266	3.34682	1.65375
C	-1.49554	4.75307	-0.62487
H	-1.72402	4.40697	0.39531
H	-2.03681	5.69581	-0.80746
H	-0.41453	4.94918	-0.70683
C	-3.99448	-3.59225	-0.12786
H	-4.99499	-3.96764	0.11229

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