Supporting Information for:

Contrasting Reactivities of Silicon and Germanium Complexes Supported by an *N*-Heterocyclic Guanidine Ligand

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NMR Spectra.

Figure S1: ^{1}H NMR spectrum of IPr=N-SiBr$_3$ (**2**).

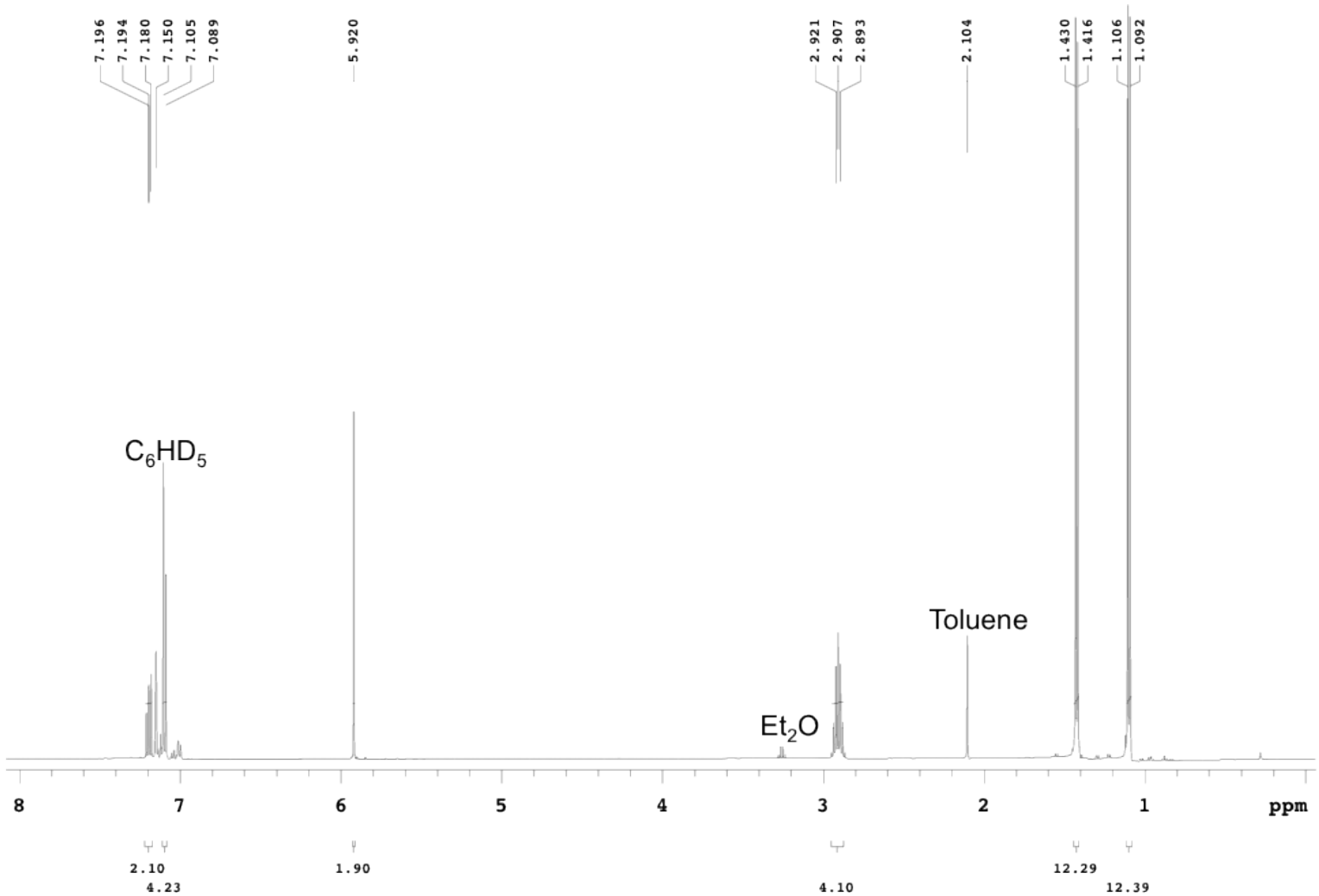


Figure S2: $^{13}C\{^{1}H\}$ NMR spectrum of IPr=N-$SiBr_3$ (**2**).

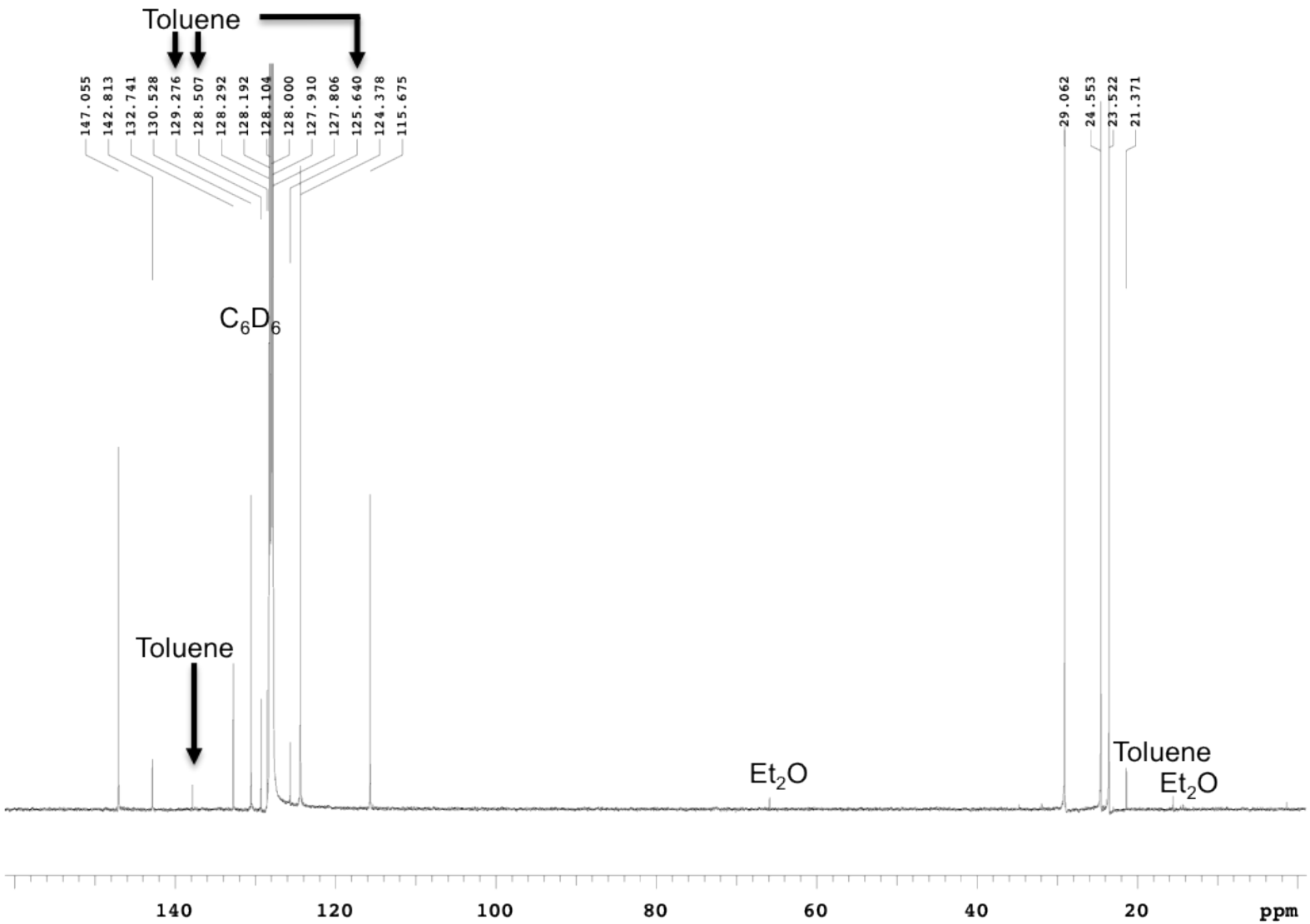


Figure S3: ^{29}Si NMR spectrum of IPr=N-$SiBr_2$ (**2**).

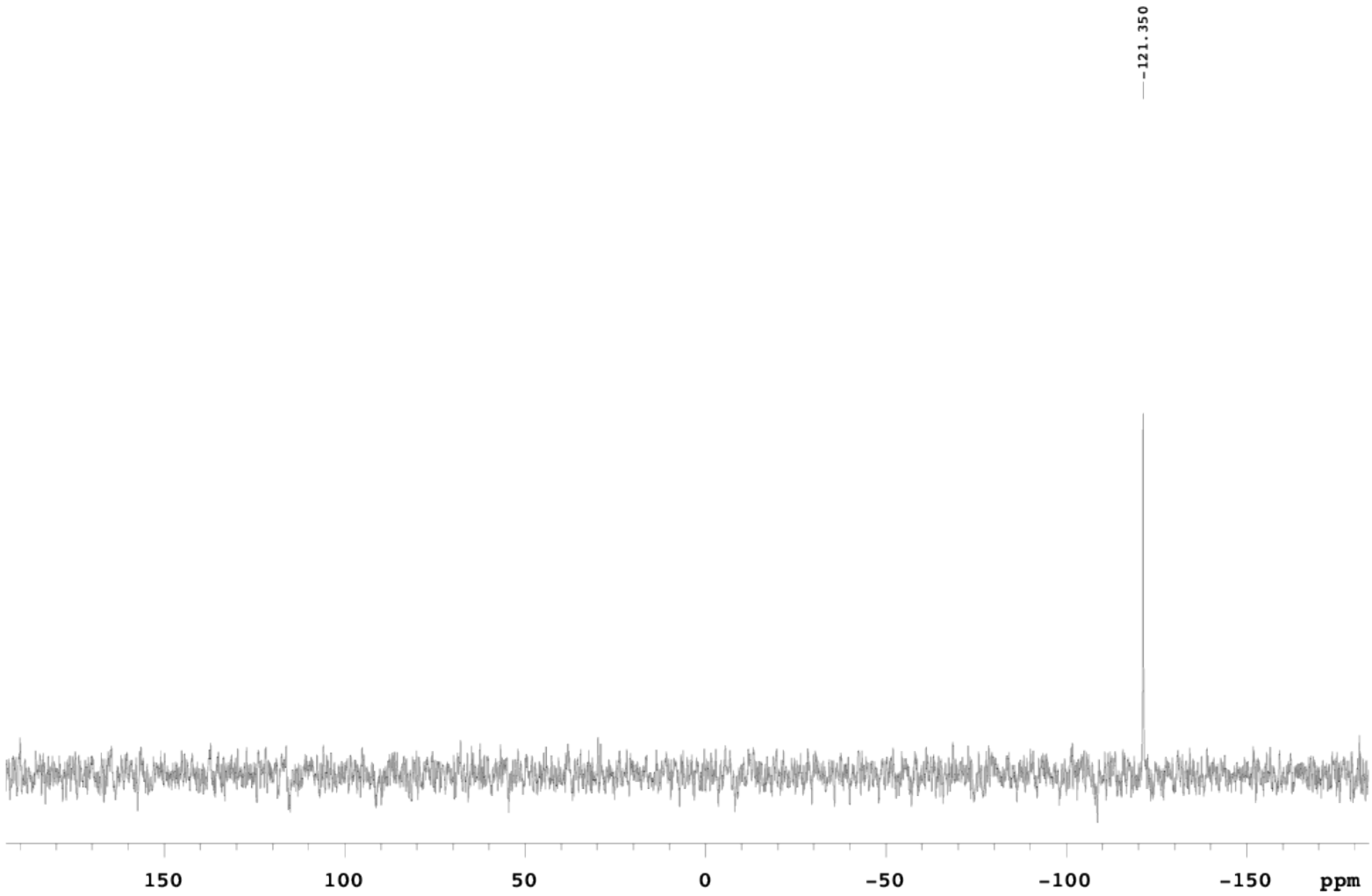


Figure S4: ^{1}H NMR spectrum of $(IPr{=}N)_2SiBr_2$ (**3**).

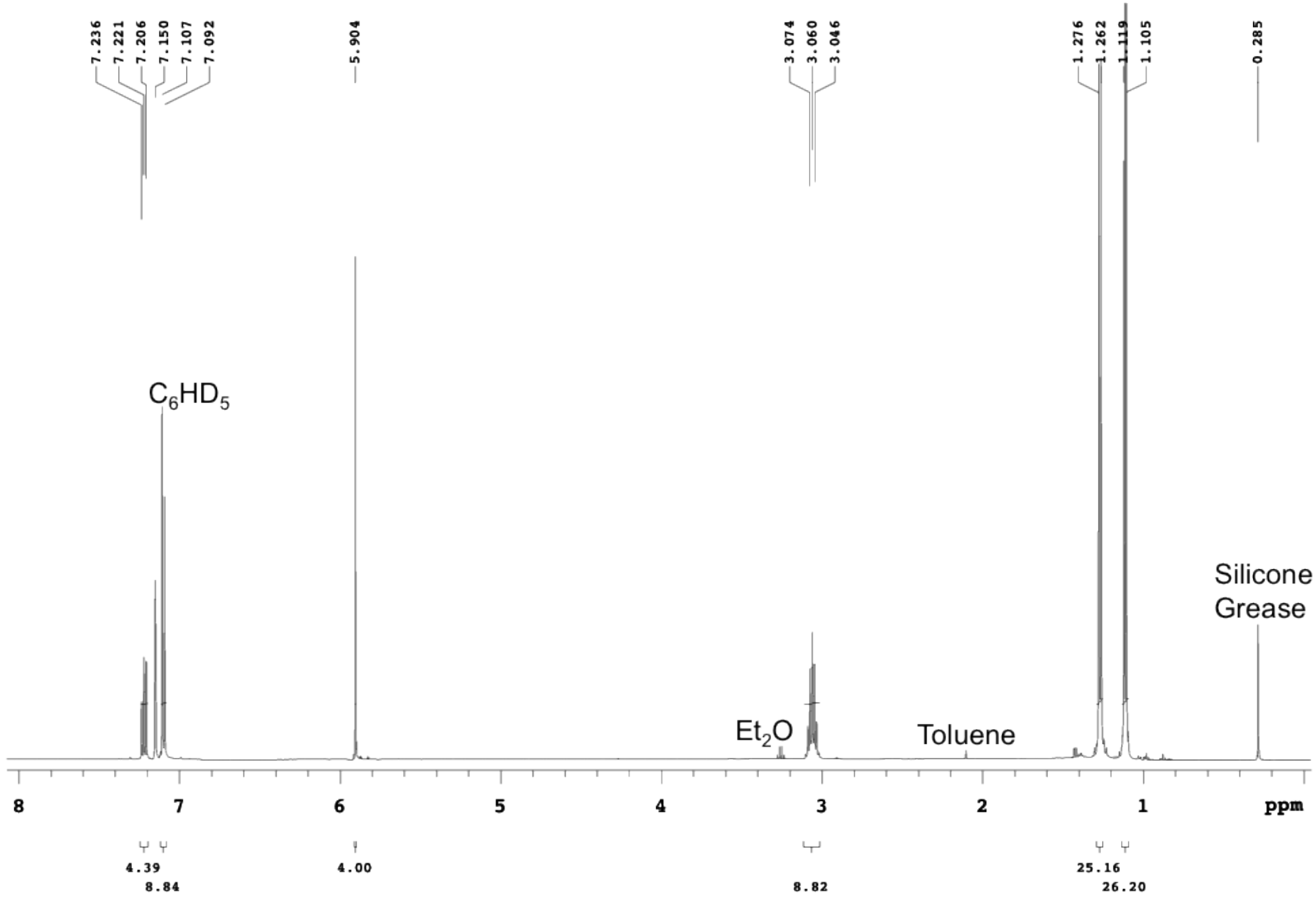


Figure S5: $^{13}C\{^{1}H\}$ NMR spectrum of $(IPr{=}N)_2SiBr_2$ (**3**).

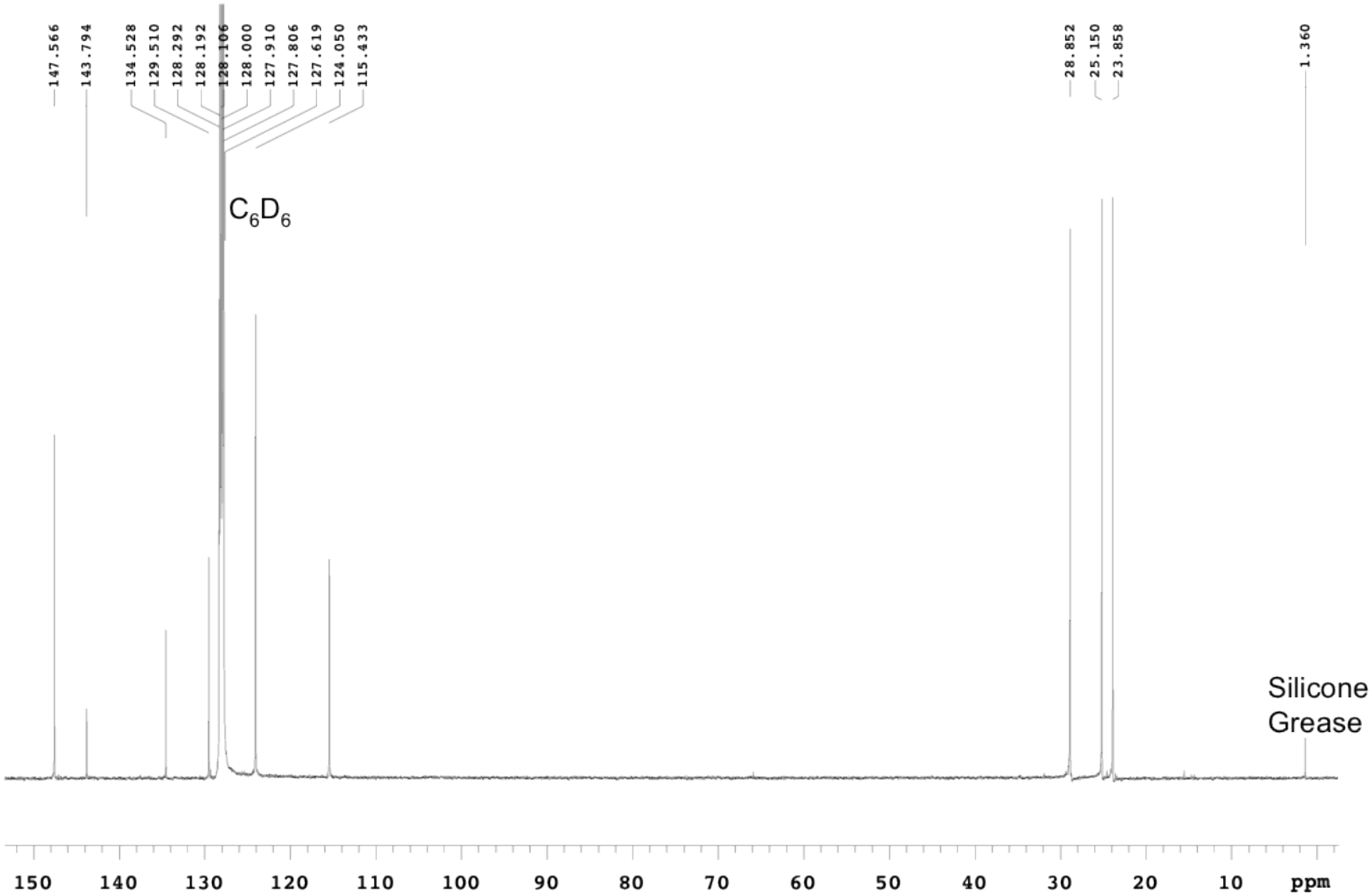


Figure S6: ^{29}Si NMR spectrum of $(IPr{=}N)_2SiBr_2$ (**3**).

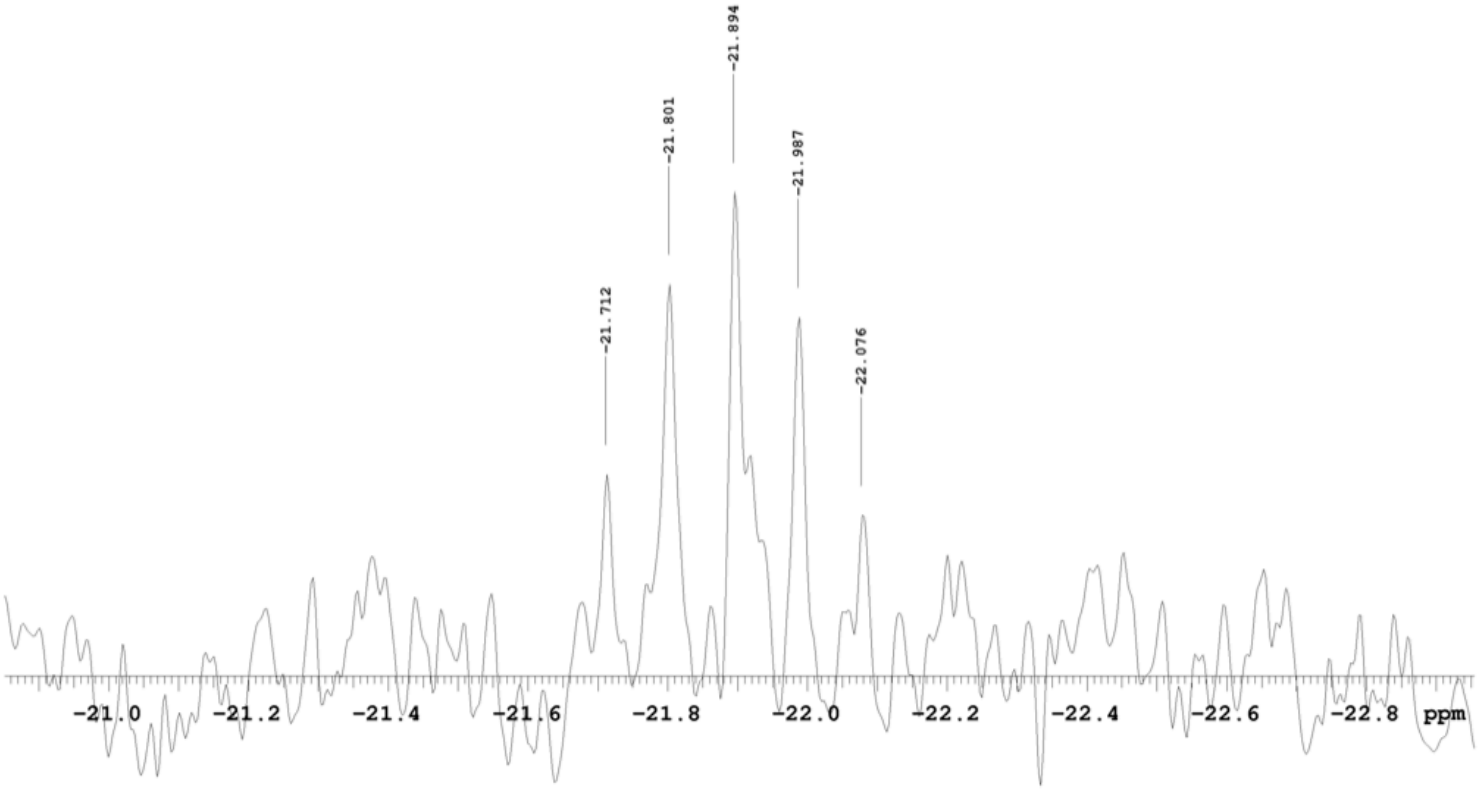


Figure S7: ^{1}H NMR spectrum of compound **5**.

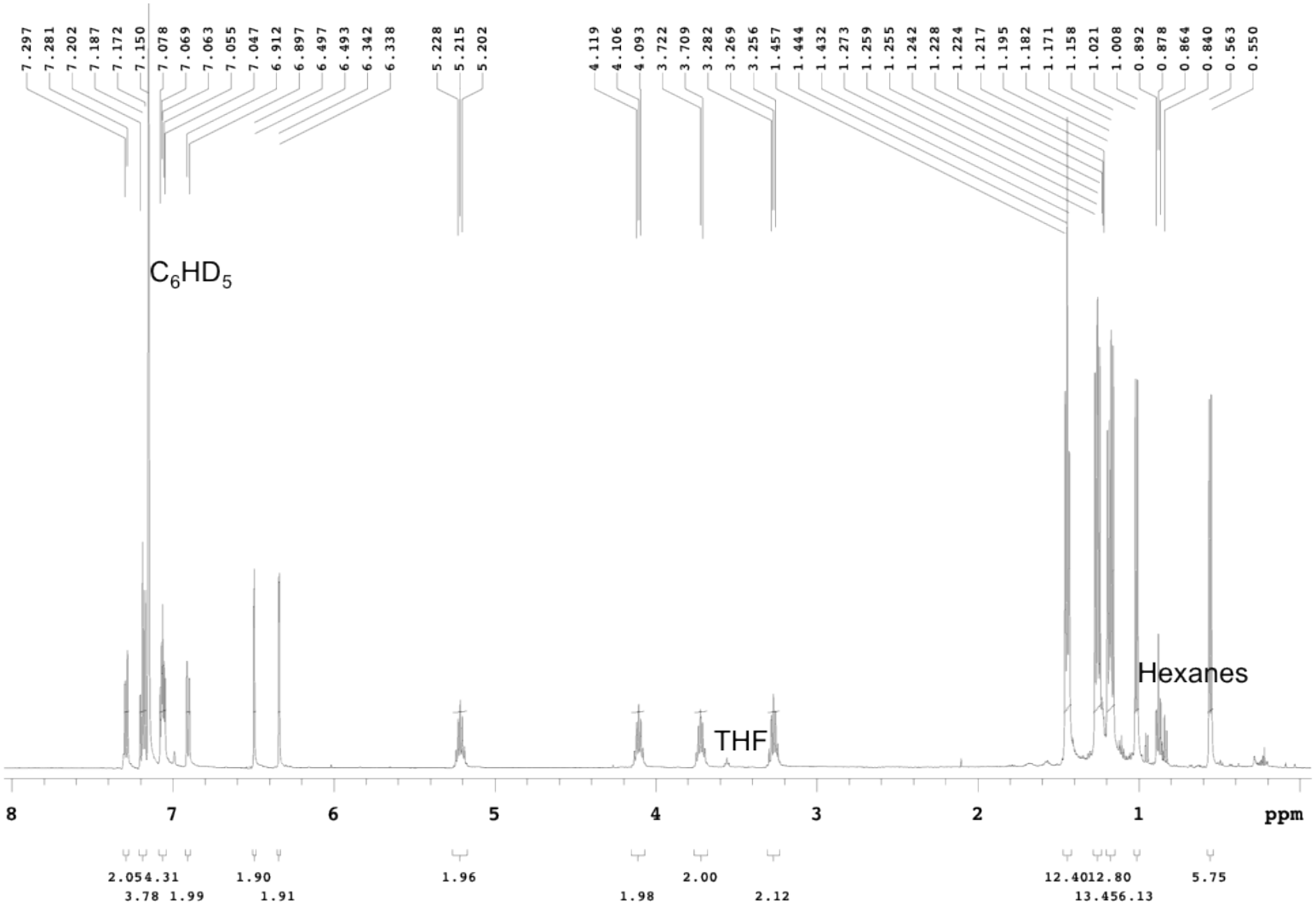


Figure S8: $^{13}C\{^{1}H\}$ NMR spectrum of compound **5**.

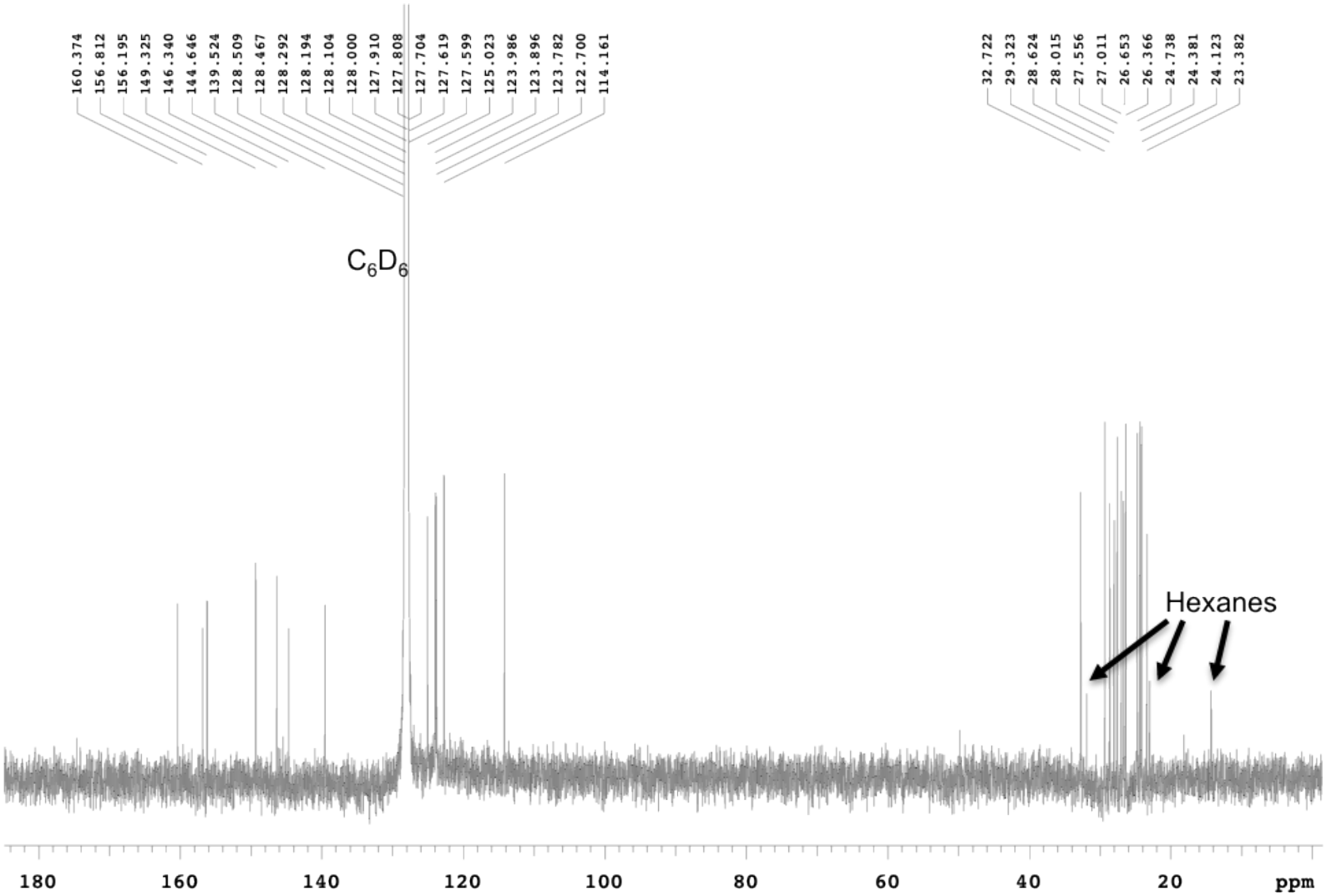


Figure S9: ^{29}Si NMR spectrum of compound **5**.

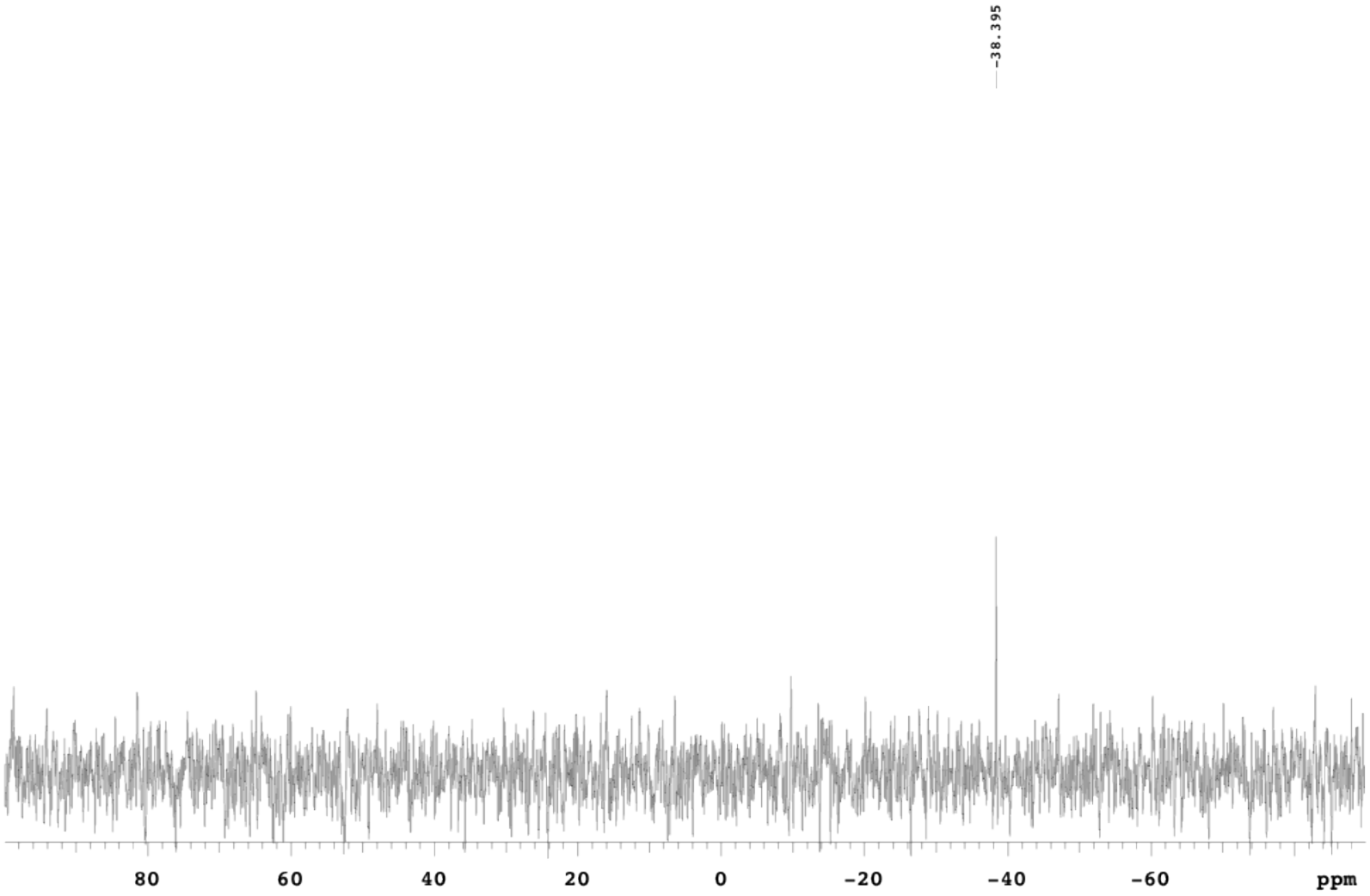


Figure S10: ^{1}H NMR spectrum of compound **10**.

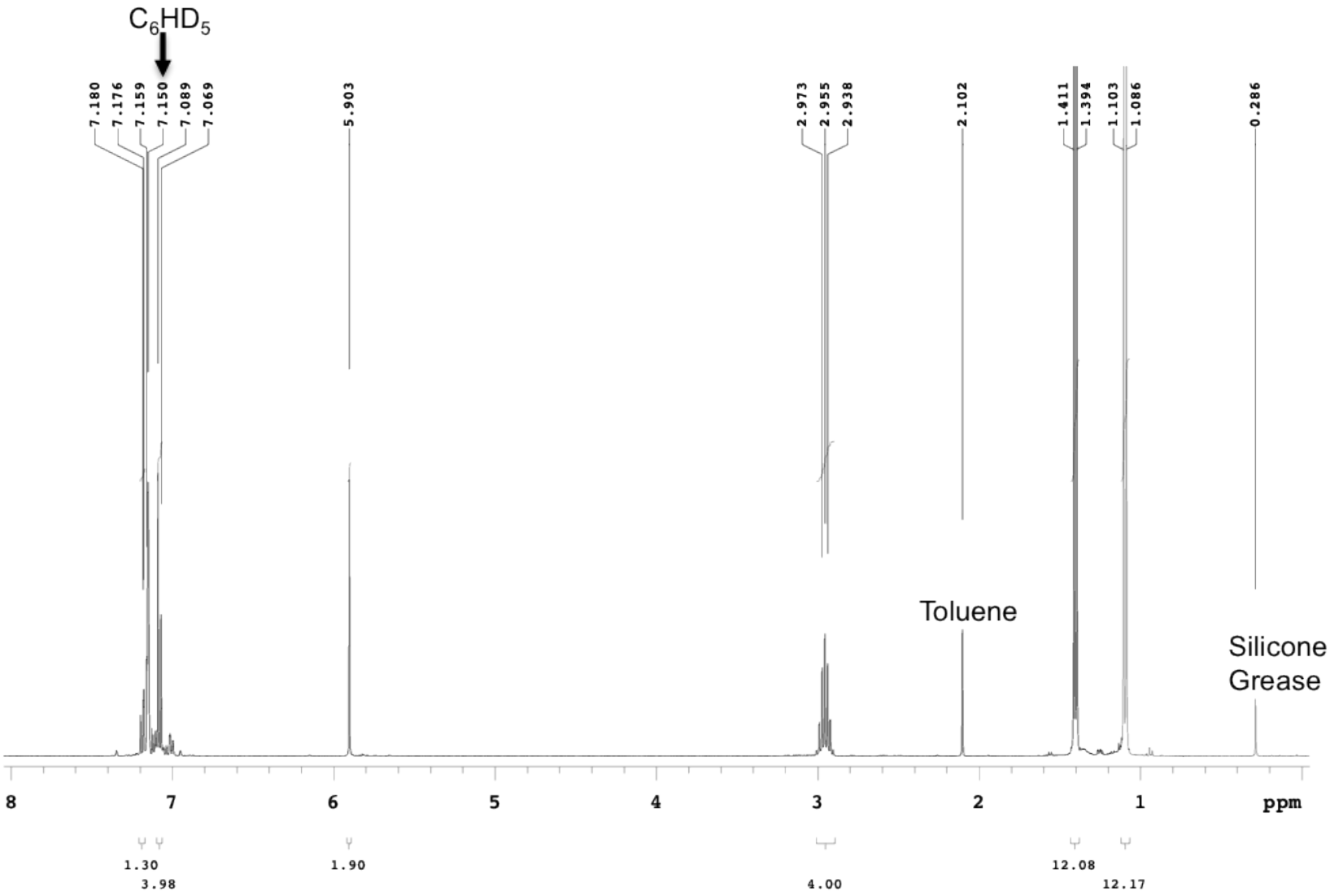


Figure S11: $^{13}C\{^{1}H\}$ NMR spectrum of compound **10**.

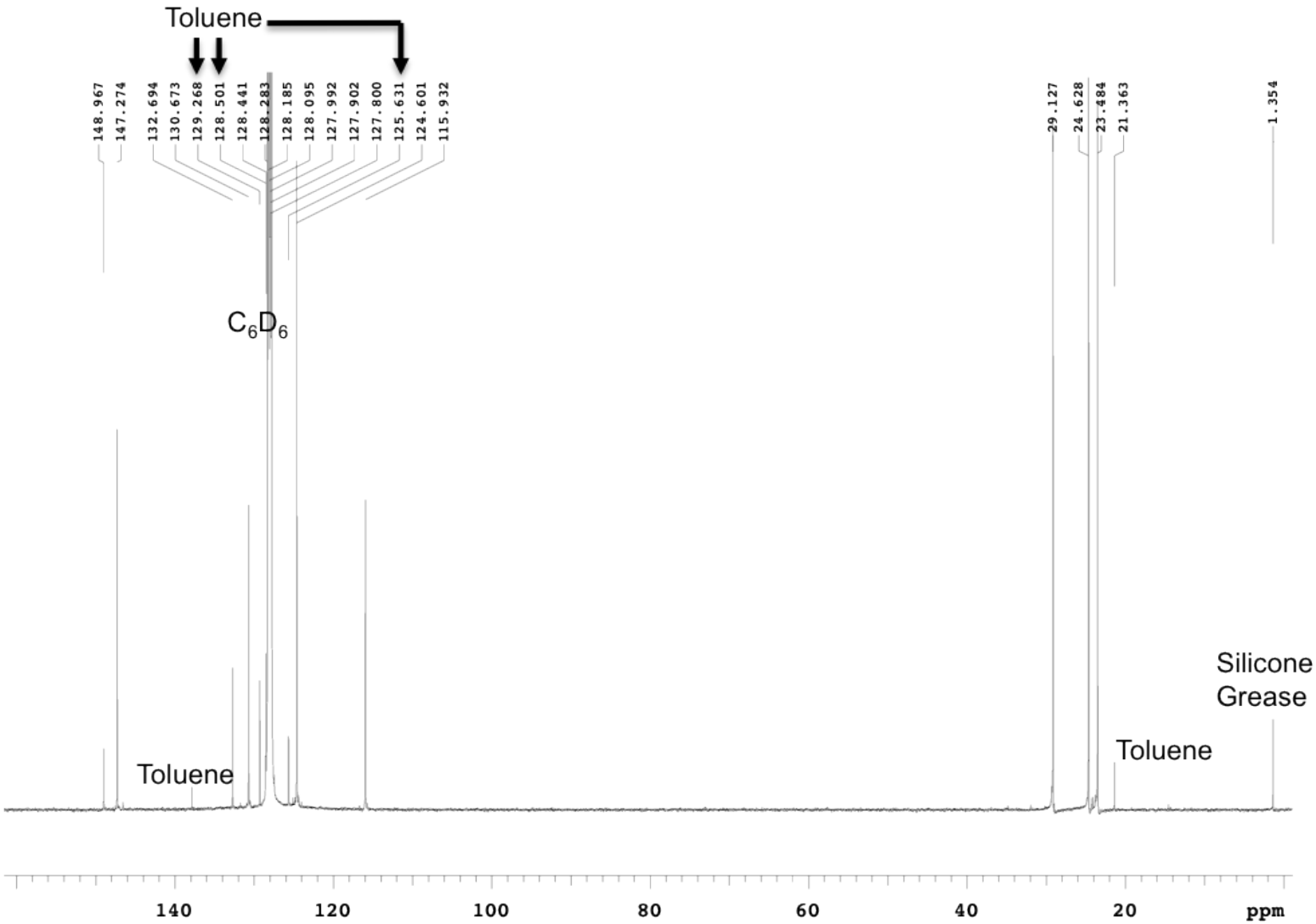


Figure S12: ^{1}H NMR spectrum of compound **11**.

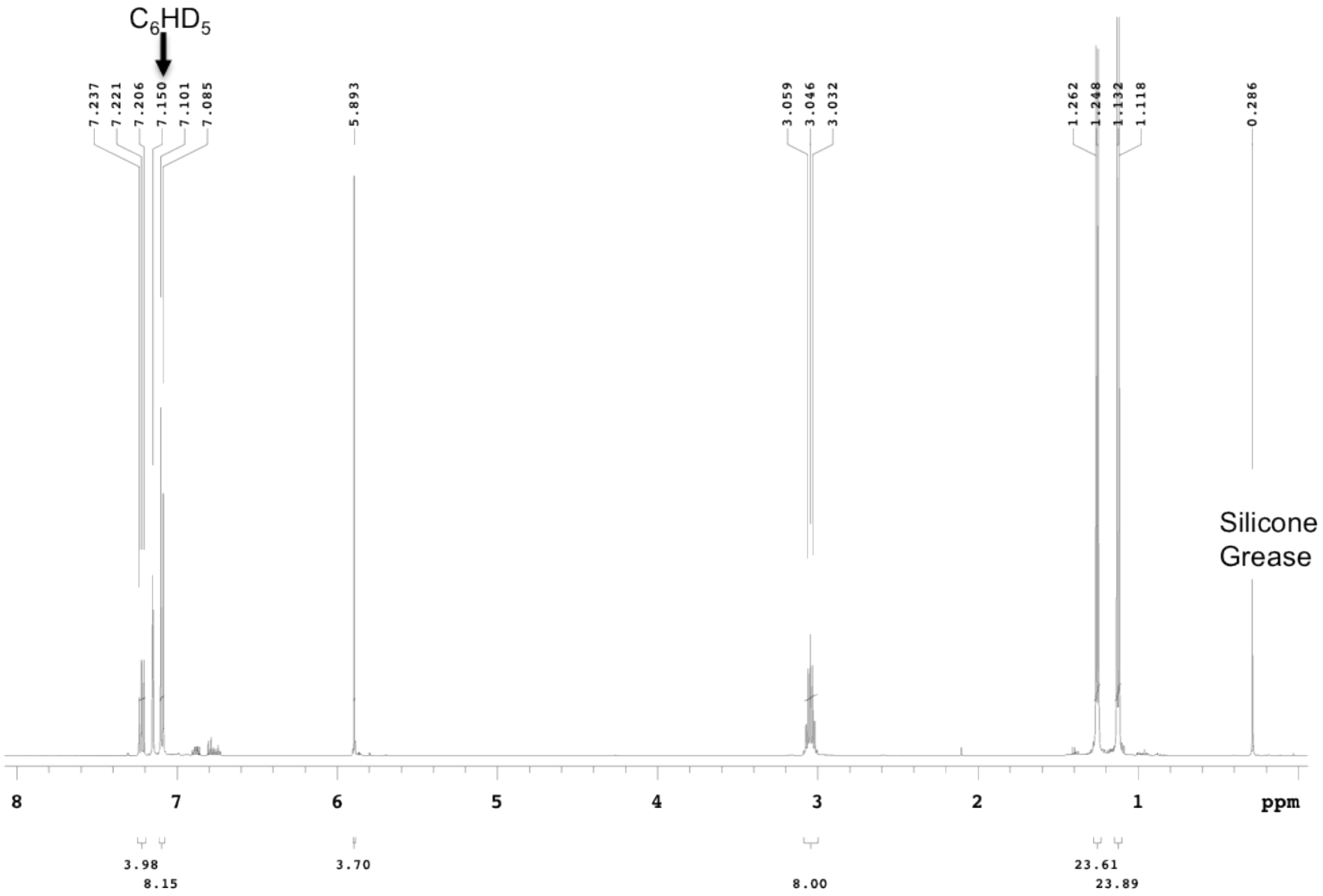


Figure S13: $^{13}C\{^{1}H\}$ NMR spectrum of compound **11**.

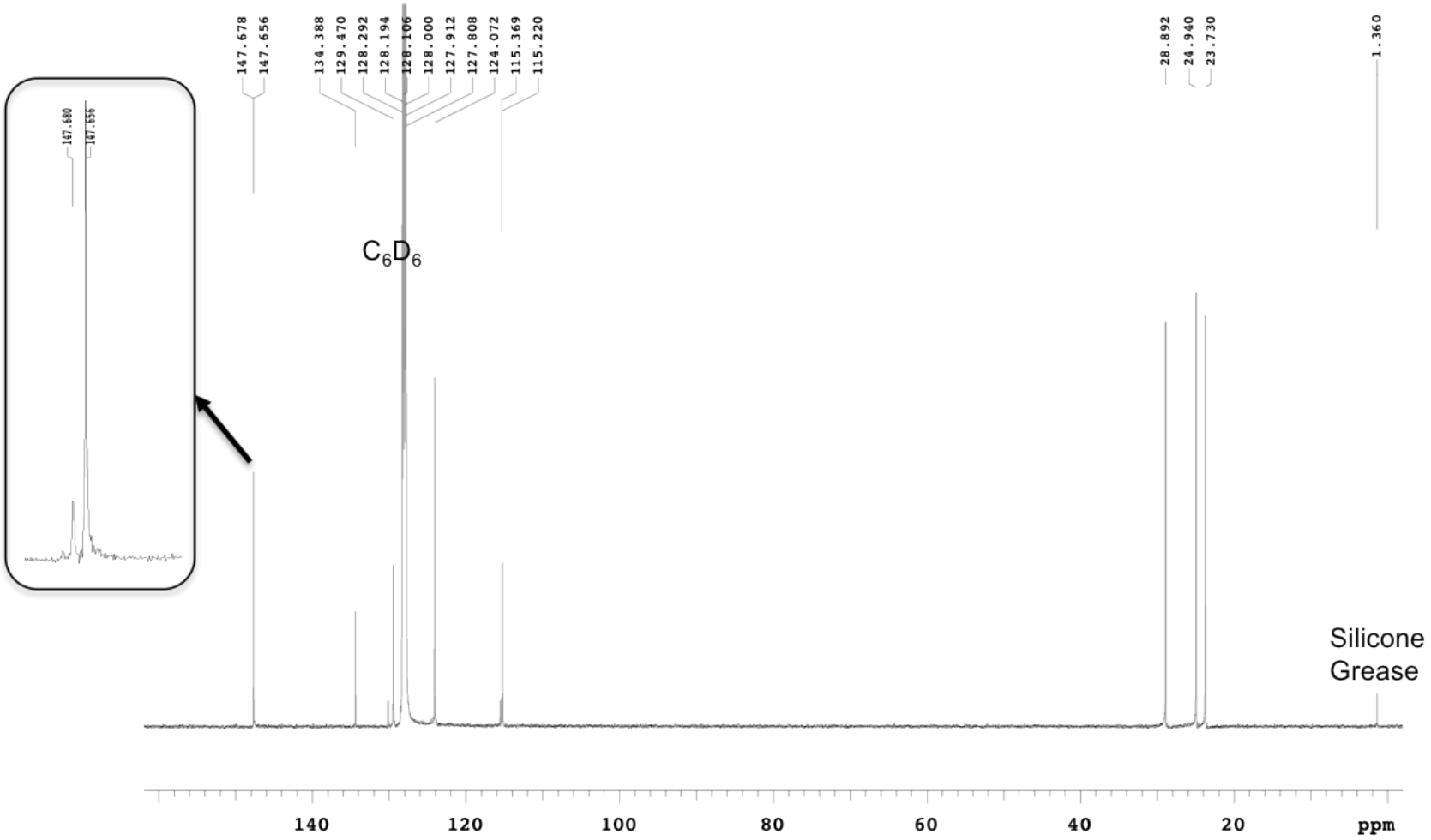


Figure S14: ^{1}H NMR spectrum of compound **12**.

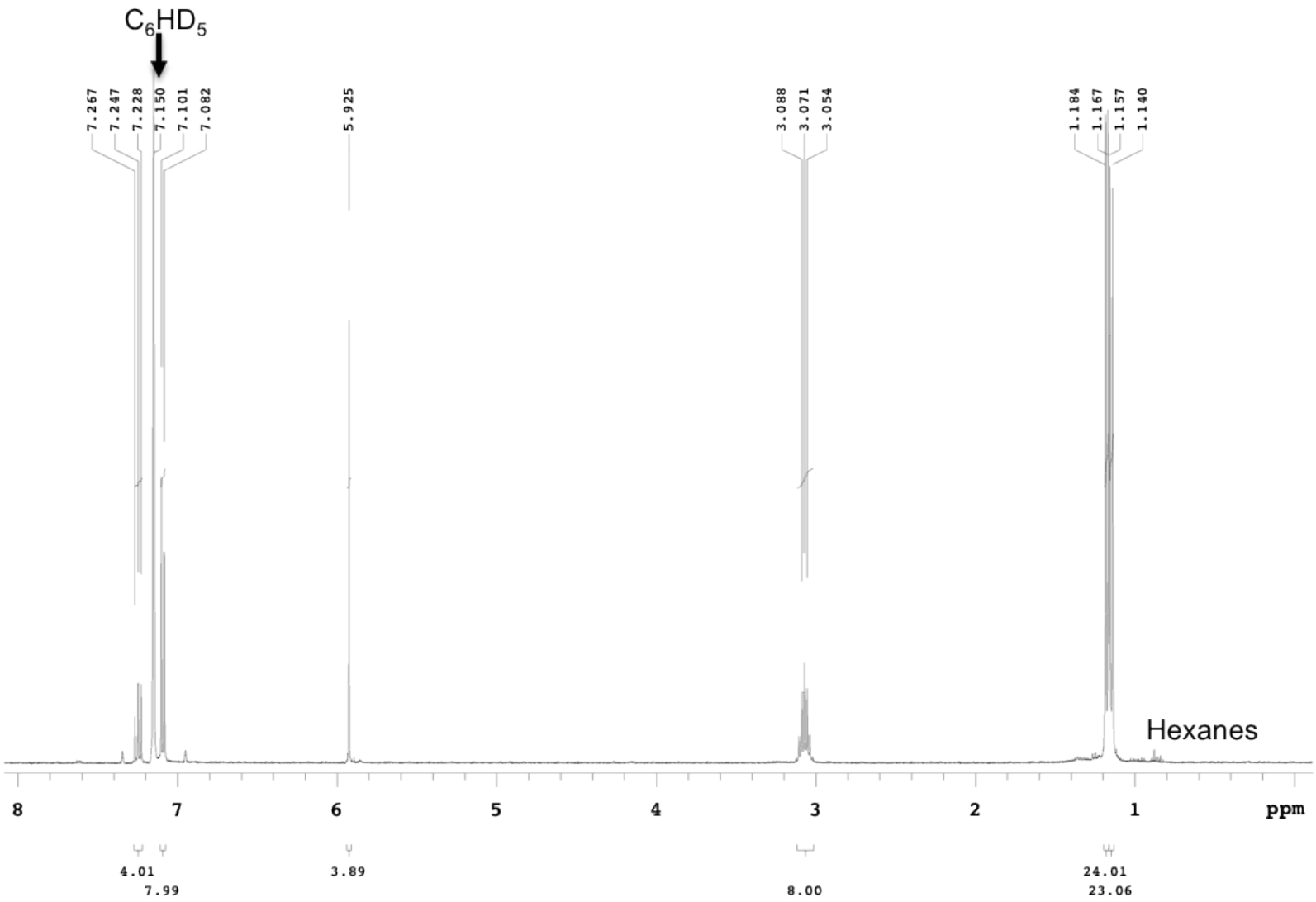
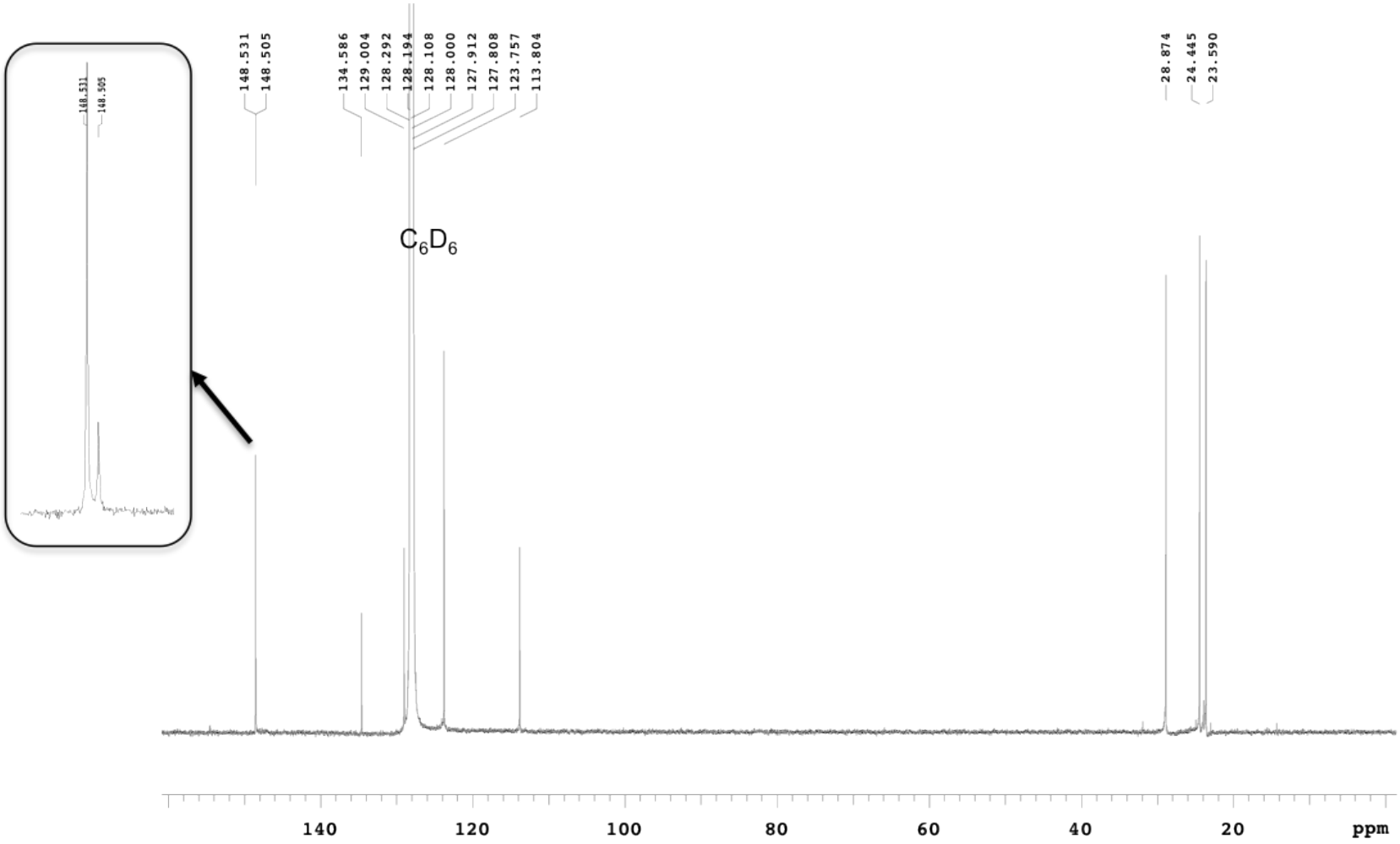


Figure S15: $^{13}C\{^{1}H\}$ NMR spectrum of compound **12**.



Crystallographic Data.

Table S1. Crystallographic Experimental Details for IPr=$NSiBr_3$• ½ C_7H_8 (compound **2**)

A. Crystal Data	
formula	$C_{30.50}H_{40}Br_3N_3Si$
formula weight	716.47
crystal dimensions (mm)	0.31 × 0.27 × 0.08
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	9.3324 (7)
b (Å)	9.5737 (7)
c (Å)	19.7142 (14)
α (deg)	91.4794 (10)
β (deg)	96.1262 (10)
γ (deg)	111.4156 (9)
V (Å^3)	1626.4 (2)
Z	2
ρ_{calcd} (g cm^{-3})	1.463
μ (mm^{-1})	3.781
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	53.54
total data collected	13645 (-11 ≤ h ≤ 11, -12 ≤ k ≤ 12, -24 ≤ l ≤ 24)
independent reflections	6903 (R_{int} = 0.0362)
number of observed reflections (*NO*)	4870 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–97*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–97*[c])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.7418–0.3879
data/restraints/parameters	6903 / 15[d] / 371
goodness-of-fit (S)[e] [all data]	1.028
final R indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0379
wR_2 [all data]	0.0837
largest difference peak and hole	1.023 and –0.874 e Å^{-3}

[a]Obtained from least-squares refinement of 4848 reflections with 4.58° < 2θ < 46.84°.

(continued)

Table S1. Crystallographic Experimental Details (continued)

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[d]A rigid-bond restraint was used on the inversion-disordered solvent toluene molecule.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0328P)^2 + 0.4796P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S2. Crystallographic Experimental Details for $(IPr{=}N)_2SiBr_2$ (compound **3**)

A. Crystal Data	
formula	$C_{60}H_{77}Br_2FN_6Si$
formula weight	1089.18
crystal dimensions (mm)	0.38 × 0.36 × 0.35
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
unit cell parameters[a]	
a (Å)	19.1921 (12)
b (Å)	12.6413 (8)
c (Å)	25.6094 (16)
β (deg)	110.5957 (7)
V (Å^3)	5816.1 (6)
Z	4
ρ_{calcd} (g cm^{-3})	1.244
μ (mm^{-1})	1.459
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	54.99
total data collected	88187 ($-24 \le h \le 24$, $-16 \le k \le 16$, $-33 \le l \le 32$)
independent reflections	13315 (R_{int} = 0.0251)
number of observed reflections (*NO*)	11139 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2013*[c])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.7656–0.5997
data/restraints/parameters	13315 / 0 / 631
goodness-of-fit (S)[d] [all data]	1.015
final R indices[e]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0326
wR_2 [all data]	0.0940
largest difference peak and hole	0.691 and –0.487 e Å^{-3}

[a]Obtained from least-squares refinement of 9827 reflections with $4.54° < 2\theta < 54.54°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table S2. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[d]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0553P)^2 + 2.0337P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[e]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S3. Crystallographic Experimental Details for Compound **5•(Et$_2$O)$_2$**.

A. Crystal Data	
formula	$C_{62}H_{92}K_2N_6O_2Si$
formula weight	1059.70
crystal dimensions (mm)	0.48 × 0.09 × 0.06
crystal system	orthorhombic
space group	*Pccn* (No. 56)
unit cell parameters[a]	
a (Å)	15.5900 (2)
b (Å)	17.6069 (3)
c (Å)	22.2395 (3)
V (Å^3)	6104.56 (15)
Z	4
ρ_{calcd} (g cm^{-3})	1.153
μ (mm^{-1})	1.904
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	Cu Kα (1.54178) (microfocus source)
temperature (°C)	–100
scan type	ω and ϕ scans (1°) (5 s exposures)
data collection 2θ limit (deg)	140.49
total data collected	38659 (-18 ≤ h ≤ 19, -21 ≤ k ≤ 21, -27 ≤ l ≤ 27)
independent reflections	5820 (R_{int} = 0.0623)
number of observed reflections (*NO*)	5207 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–97*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–97*[c])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	1.0000–0.4263
data/restraints/parameters	5820 / 2[d] / 345
goodness-of-fit (*S*)[e] [all data]	1.032
final *R* indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0475
wR_2 [all data]	0.1384
largest difference peak and hole	0.429 and –0.525 e Å^{-3}

[a]Obtained from least-squares refinement of 9894 reflections with 7.58° < 2θ < 140.18°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table S3. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[d]The O–C and C–C distances within the minor orientation of the disordered diethylether were restrained to be the same by use of the *SHELXL* **SADI** instruction.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0867P)^2 + 1.9641P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S4. Crystallographic Experimental Details for Compound **5•(tol)$_2$**.

A. Crystal Data	
formula	$C_{68}H_{88}K_2N_6Si$
formula weight	1095.73
crystal dimensions (mm)	0.37 × 0.19 × 0.13
crystal system	orthorhombic
space group	*Pccn* (No. 56)
unit cell parameters[a]	
a (Å)	15.7413 (5)
b (Å)	16.9705 (5)
c (Å)	23.1230 (7)
V (Å^3)	6177.0 (3)
Z	4
ρ_{calcd} (g cm^{-3})	1.178
μ (mm^{-1})	0.218
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	54.98
total data collected	52442 (-20 ≤ h ≤ 20, -21 ≤ k ≤ 22, -30 ≤ l ≤ 29)
independent reflections	7081 (R_{int} = 0.0409)
number of observed reflections (*NO*)	5463 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2013*[c])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	1.0000–0.9235
data/restraints/parameters	7081 / 7[d] / 338
goodness-of-fit (S)[e] [all data]	1.019
final R indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0446
wR_2 [all data]	0.1274
largest difference peak and hole	0.387 and –0.251 e Å^{-3}

[a]Obtained from least-squares refinement of 9856 reflections with 4.80° < 2θ < 50.50°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table S4. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[d]The disordered toluene molecule was constrained to be an idealized hexagon with C–C distances of 1.39 Å and distance between the methyl and ortho carbon atoms was restrained to be 2.50(1) Å. The sum of the occupancies of the three disordered toluene orientations was restrained to be 1.0000(1).

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0561P)^2 + 3.1404P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

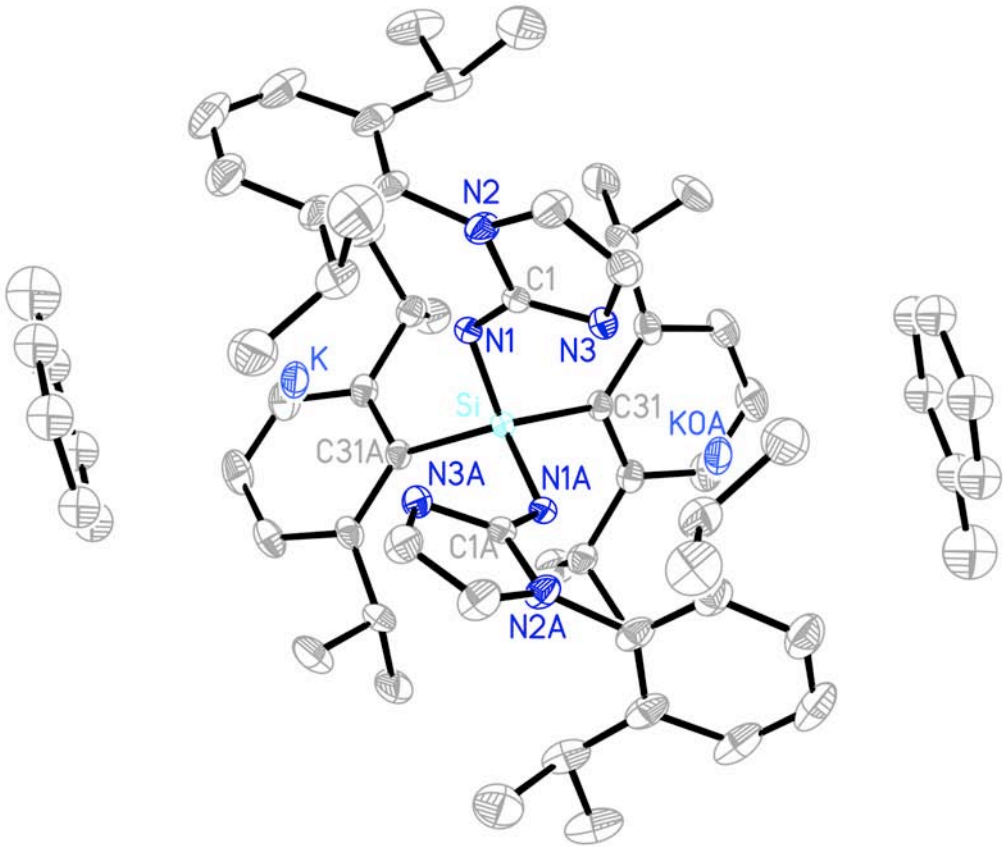


Figure S16. Molecular structure of **5•(tol)$_2$** with thermal ellipsoids at the 30% probability level. All hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): K-N(1) 2.7084(13), Si-N(1) 1.7131(13), Si-C(31) 1.9627(16), N(1)-C(1) 1.334(2); N(1)-Si-N(1A) 114.70(9), C(31)-Si-C(31A) 110.36(10), N(1)-Si-C(31A) 101.73(6) N(1)-Si-C(31) 114.38(6).

Table S5. Crystallographic Experimental Details for Compound **6**.

A. Crystal Data	
formula	$C_{56}H_{78}N_6OSi_2$
formula weight	907.42
crystal dimensions (mm)	0.30 × 0.10 × 0.09
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	12.1444 (2)
b (Å)	21.8298 (3)
c (Å)	20.3141 (3)
β (deg)	94.4491 (7)
V (Å^3)	5369.24 (14)
Z	4
ρ_{calcd} (g cm^{-3})	1.123
μ (mm^{-1})	0.921
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	Cu Kα (1.54178) (microfocus source)
temperature (°C)	–100
scan type	ω and ϕ scans (1.0°) (5 s exposures)
data collection 2θ limit (deg)	143.08
total data collected	36037 (-14 ≤ h ≤ 14, -26 ≤ k ≤ 26, -24 ≤ l ≤ 24)
independent reflections	10277 (R_{int} = 0.0639)
number of observed reflections (*NO*)	8416 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	direct methods/dual space (*SHELXD*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–97*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.9241–0.7715
data/restraints/parameters	10277 / 0 / 588
goodness-of-fit (S)[e] [all data]	1.029
final R indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0434
wR_2 [all data]	0.1238
largest difference peak and hole	0.372 and –0.398 e Å^{-3}

[a]Obtained from least-squares refinement of 9944 reflections with 5.96° < 2θ < 142.64°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.`

(continued)

Table S5. Crystallographic Experimental Details (continued)

[c]Schneider, T. R.; Sheldrick, G. M. *Acta Crystallogr.* **2002**, *D58*, 1772-1779.

[d]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0499P)^2 + 1.6377P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S6. Crystallographic Experimental Details of IPr=N-$GeCl_3$• ½ C_7H_8 (compound **10**)

A. Crystal Data	
formula	$C_{30.50}H_{40}Cl_3GeN_3$
formula weight	627.59
crystal dimensions (mm)	0.34 × 0.25 × 0.13
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	9.3618 (3)
b (Å)	9.4782 (3)
c (Å)	19.3727 (7)
α (deg)	89.2845 (4)
β (deg)	84.2790 (4)
γ (deg)	69.4191 (4)
V (Å^3)	1600.80 (9)
Z	2
ρ_{calcd} (g cm^{-3})	1.302
μ (mm^{-1})	1.230
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–100
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	55.74
total data collected	14548 (-12 ≤ h ≤ 12, -12 ≤ k ≤ 12, -25 ≤ l ≤ 25)
independent reflections	7497 (R_{int} = 0.0099)
number of observed reflections (*NO*)	6953 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2013*[c])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.9034–0.7200
data/restraints/parameters	7497 / 0 / 371
goodness-of-fit (S)[d] [all data]	1.055
final R indices[e]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0247
wR_2 [all data]	0.0676
largest difference peak and hole	0.363 and –0.259 e Å^{-3}

[a]Obtained from least-squares refinement of 9976 reflections with 4.60° < 2θ < 55.70°.

(continued)

Table S6. Crystallographic Experimental Details (continued)

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[d]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0354P)^2 + 0.4952P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[e]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S7. Crystallographic Experimental Details for $(IPr{=}N)_2GeCl_2{\bullet}C_6H_5F$ (compound **11**)

A. Crystal Data	
formula	$C_{60}H_{77}Cl_2FGeN_6$
formula weight	1044.76
crystal dimensions (mm)	0.33 × 0.25 × 0.15
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
unit cell parameters[a]	
a (Å)	19.1837 (3)
b (Å)	12.5630 (2)
c (Å)	25.6436 (4)
β (deg)	110.8290 (5)
V (Å^3)	5776.33 (16)
Z	4
ρ_{calcd} (g cm^{-3})	1.201
μ (mm^{-1})	1.915
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	Cu Kα (1.54178) (microfocus source)
temperature (°C)	–100
scan type	ω and ϕ scans (1.0°) (5 s exposures)
data collection 2θ limit (deg)	145.96
total data collected	39308 (-23 ≤ h ≤ 23, -15 ≤ k ≤ 15, -31 ≤ l ≤ 31)
independent reflections	11507 (R_{int} = 0.0173)
number of observed reflections (*NO*)	10800 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT-2013*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2013*[c])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.7984–0.6342
data/restraints/parameters	11507 / 0 / 600
goodness-of-fit (S)[d] [all data]	1.058
final R indices[e]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0373
wR_2 [all data]	0.1056
largest difference peak and hole	0.610 and –0.734 e Å^{-3}

[a]Obtained from least-squares refinement of 9824 reflections with 7.38° < 2θ < 144.36°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table S7. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[d]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0466P)^2 + 3.3122P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[e]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S8. Crystallographic Experimental Details of $[:Ge(IPr{=}N)_2]_{0.955}[(IPr{=}N)_2GeCl_2]_{0.045}$ (compound **12**)

A. Crystal Data	
formula	$C_{54}H_{72}Cl_{0.09}GeN_6$
formula weight	880.95
crystal dimensions (mm)	0.36 × 0.17 × 0.03
crystal system	orthorhombic
space group	*Pbcn* (No. 60)
unit cell parameters[a]	
a (Å)	11.8062 (3)
b (Å)	19.8956 (5)
c (Å)	21.8851 (5)
V (Å^3)	5140.6 (2)
Z	4
ρ_{calcd} (g cm^{-3})	1.138
μ (mm^{-1})	1.143
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	Cu Kα (1.54178) (microfocus source)
temperature (°C)	–100
scan type	ω and ϕ scans (1°) (5 s exposures)
data collection 2θ limit (deg)	136.82
total data collected	31779 (-14 ≤ h ≤ 14, -23 ≤ k ≤ 23, -25 ≤ l ≤ 26)
independent reflections	4722 (R_{int} = 0.0468)
number of observed reflections (*NO*)	3862 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	intrinsic phasing (*SHELXT*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–2013*[c])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.9881–0.7308
data/restraints/parameters	4722 / 0 / 280
goodness-of-fit (S)[d] [all data]	1.034
final R indices[e]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0355
wR_2 [all data]	0.0996
largest difference peak and hole	0.513 and –0.429 e Å^{-3}

[a]Obtained from least-squares refinement of 9018 reflections with 8.08° < 2θ < 136.52°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table S8. Crystallographic Experimental Details (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[d]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0505P)^2 + 2.1585P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[e]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table S9. Crystallographic Experimental Details for **[Li(N=IPr)]$_2$**.

A. Crystal Data	
formula	$C_{54}H_{72}Li_2N_6$
formula weight	819.06
crystal dimensions (mm)	0.41 × 0.21 × 0.10
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	10.9982 (2)
b (Å)	18.7313 (2)
c (Å)	12.0421 (2)
β (deg)	94.2202 (6)
V (Å^3)	2474.07 (7)
Z	2
ρ_{calcd} (g cm^{-3})	1.099
μ (mm^{-1})	0.481
B. Data Collection and Refinement Conditions	
diffractometer	Bruker D8/APEX II CCD[b]
radiation (λ [Å])	Cu Kα (1.54178) (microfocus source)
temperature (°C)	–100
scan type	ω scans (1.0°) (5 s exposures)
data collection 2θ limit (deg)	140.32
total data collected	16759 (-13 ≤ h ≤ 13, -22 ≤ k ≤ 22, -14 ≤ l ≤ 14)
independent reflections	4695 (R_{int} = 0.0219)
number of observed reflections (*NO*)	4252 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	direct methods/dual space (*SHELXD*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–97*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.9526–0.8279
data/restraints/parameters	4695 / 0 / 280
goodness-of-fit (S)[e] [all data]	1.055
final R indices[f]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0402
wR_2 [all data]	0.1103
largest difference peak and hole	0.237 and –0.229 e Å^{-3}

[a]Obtained from least-squares refinement of 9856 reflections with 9.34° < 2θ < 138.88°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table S9. Crystallographic Experimental Details (continued)

[c]Schneider, T. R.; Sheldrick, G. M. *Acta Crystallogr.* **2002**, *D58*, 1772-1779.

[d]Sheldrick, G. M. *Acta Crystallogr.* **2008**, *A64*, 112–122.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0548P)^2 + 0.5547P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

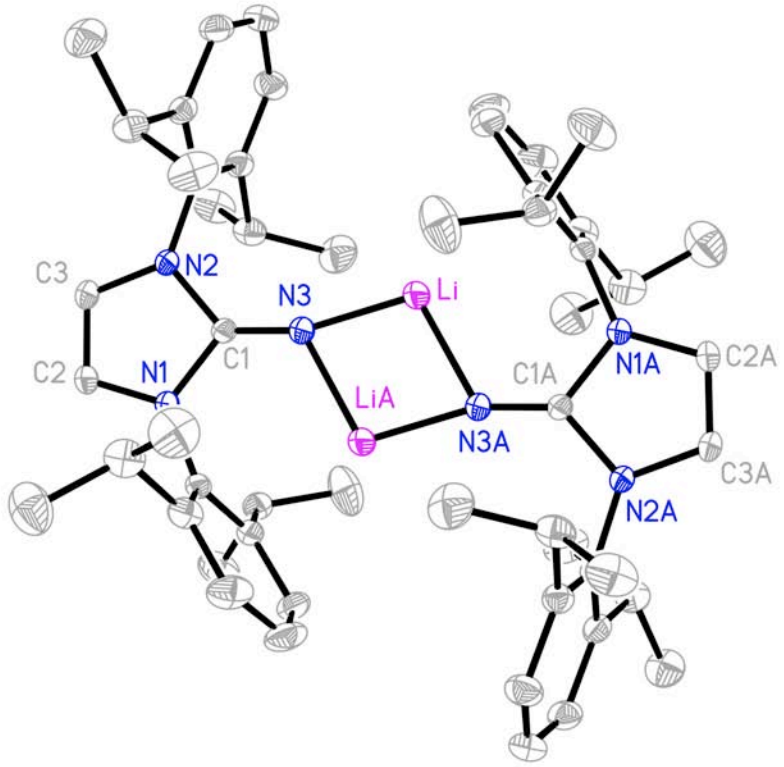


Figure S17. Molecular structure of [**Li(N=IPr)]$_2$** with thermal ellipsoids at the 30% probability level. All hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): N(3)-Li 1.853(2), N(3)-LiA 1.984(2), N(1)-C(1) 1.4365(13); C(1)-N(3)-Li 162.74(10), C(1)-N(3)-LiA 120.45(9), Li-N(3)-LiA 76.74(9).

Computational details.

All calculations were carried out using the Gaussian 09 Rev. C.01 software package.[1] Input structures were taken from the crystal structures when possible. The geometries were optimized at the B3LYP/6-31G(2d,p) level of theory in the gas phase with tight convergence criteria and an ultrafine integration grid. Potential reaction intermediates (e.g. **8**, **9** etc...; see Scheme 4 in manuscript) were subsequently generated based on related structures, and their geometries were optimized at the same level of theory. All optimized structures were then confirmed to be local energy minima on the potential energy surface by frequency analysis. The energy differences ΔE_{gas} and ΔG_{gas} (at standard conditions 1atm, 298 K) refer to the zero-point energy corrected electronic energy and the Gibbs free energy in the gas phase. In order to account for the polar solvent environment, the relative energy differences ΔE_{PCM} were calculated based on single-point energy calculations at the B3LYP/6-31G(2d,p) level of theory which employed the polarizable continuum model (IEFPCM) for diethyl ether.[2]

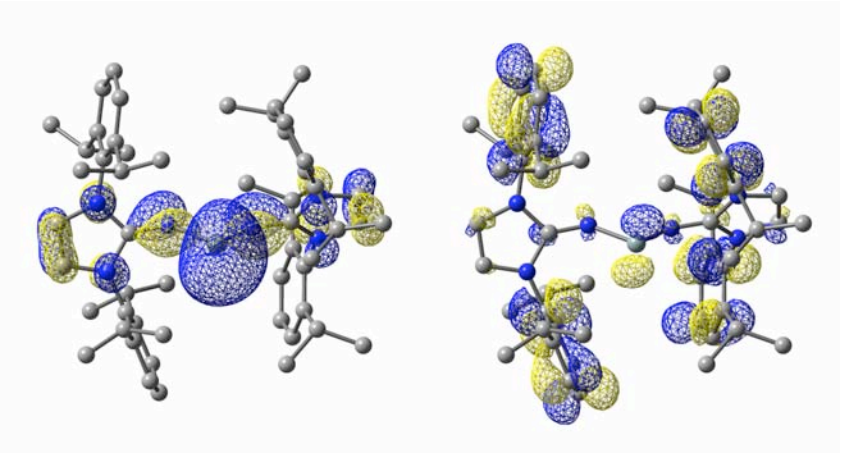


Figure S18: Calculated HOMO (left) and LUMO (right) for the putative silylene :Si(N=IPr)$_2$ (B3LYP/6-31G(2d,p) level). HOMO = -3.965 eV; LUMO = -0.0996 eV; Delta = 3.865 eV

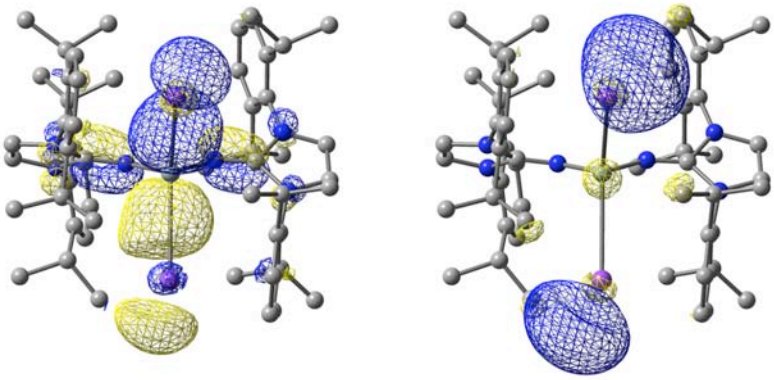


Figure S19: Calculated HOMO (left) and LUMO (right) for the dianion K_2[Si(NIPr)$_2$] (**9**) (B3LYP/6-31G(2d,p) level.

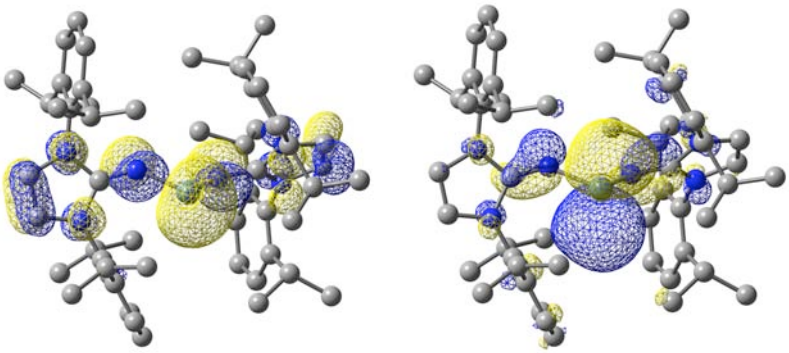


Figure S20: Calculated HOMO (left) and LUMO (right) for germylene :Ge(N=IPr)$_2$ (**12**) (B3LYP/6-31G(2d,p) level). HOMO = -4.156 eV; LUMO = -0.3385 eV; Delta = 3.817 eV

Figure S21. Detailed summary of computed reduction and isomerization pathways investigated in this study for the silicon species. Energies associated (zero-point corrected) for each process is listed in italics (kcal/mol); associated free energies and energy changes with an Et_2O solvation model are listed in parentheses and square brackets, respectively (kcal/mol).

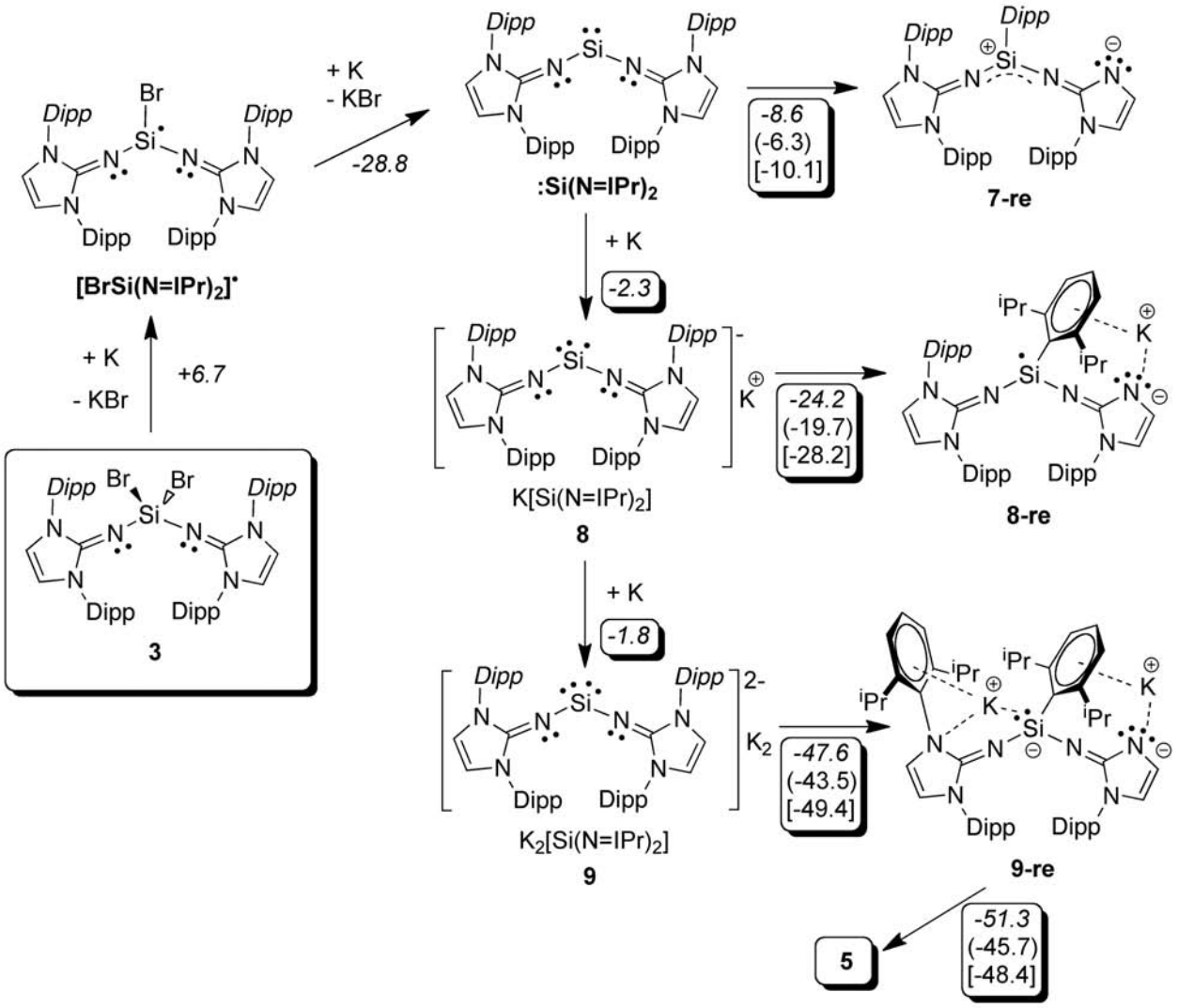


Figure S22. Detailed summary of computed reduction pathways investigated in this study for the germanium species. Associated free energies and energy changes with an Et_2O solvation model are listed in parentheses and square brackets, respectively (kcal/mol).

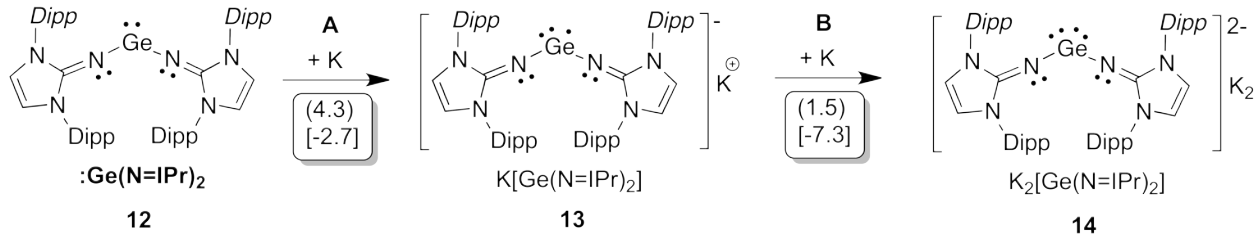


Table S10. Calculated energies in Hartrees (B3LYP/6-31G(2d,p)) for each compound in this study.

	E_{ZPC}	G	E_{SP} in PCM
$(IPr{=}N)_2SiBr_2$	-7862.04911	-7862.15886	-7863.29434
product **5**	-3918.10983	-3918.21101	-3919.33291
K	-599.891859	-599.90769	-599.895698
KBr	-3171.85305	-3171.87761	-3171.90462
8	-3318.05751	-3318.17238	-3319.27808
9	-3917.95218	-3918.06889	-3919.1771
$:Si(N{=}IPr)_2$ singlet	-2718.16194	-2718.27087	-2719.38427
$:Si(N{=}IPr)_2$ triplet	-2718.09152	-2718.20297	-2719.31342
7-re	-2718.17563	-2718.28094	-2719.40039
8-re	-3318.09605	-3318.20379	-3319.323
9-re	-3918.02807	-3918.13814	-3919.25578
12 $:Ge(N{=}IPr)_2$ singlet	-4503.88006	-4503.99014	-4505.110847
12 $:Ge(N{=}IPr)_2$ triplet	-4503.80736	-4503.91705	-4505.037155
13	-5103.77619	-5103.89097	-
14	-5703.67973	-5703.79623	-

Table S11. Computed (B3LYP/6-31G(2d,p)) Cartesian coordinates (in Å) for all the compounds investigated in this work (see also Figures S25 and S26).

$(IPr{=}N)_2SiBr_2$ **3**

charge=0, multiplicity=1

Si	0.00000000	0.00000000	0.59660000
N	0.03840000	1.38470000	-0.30030000
N	0.48510000	3.63220000	0.50730000
N	-1.08050000	3.36080000	-1.00910000
N	-0.03840000	-1.38470000	-0.30030000
N	1.08050000	-3.36080000	-1.00910000
N	-0.48510000	-3.63220000	0.50730000
C	-0.16570000	2.65100000	-0.23600000
C	0.00000000	4.89360000	0.16170000
C	-0.95950000	4.72710000	-0.76940000
C	0.16570000	-2.65100000	-0.23600000
C	0.95950000	-4.72710000	-0.76940000
C	0.00000000	-4.89360000	0.16170000
C	1.61930000	3.44440000	1.37170000
C	1.42030000	3.41740000	2.76500000
C	2.55130000	3.31560000	3.57880000
C	3.82520000	3.22380000	3.03290000
C	3.99470000	3.24410000	1.65500000
C	2.90020000	3.36570000	0.79510000
C	0.03440000	3.51320000	3.39110000
C	-0.27690000	4.95680000	3.83270000
C	-0.15090000	2.53870000	4.56640000
C	3.13360000	3.42700000	-0.70890000
C	3.99020000	4.64730000	-1.09410000
C	3.74740000	2.12040000	-1.24050000
C	-1.94420000	2.78110000	-1.99910000
C	-3.26950000	2.45690000	-1.64830000
C	-4.08560000	1.91010000	-2.64230000
C	-3.60590000	1.69050000	-3.92850000
C	-2.29920000	2.03080000	-4.25230000
C	-1.44290000	2.59000000	-3.29920000
C	-3.82840000	2.73860000	-0.25820000
C	-4.53210000	4.11080000	-0.22700000
C	-4.77680000	1.64300000	0.25240000
C	-0.02550000	2.98300000	-3.69660000
C	-0.02410000	3.99850000	-4.85400000
C	0.83130000	1.75020000	-4.03190000
C	1.94420000	-2.78110000	-1.99910000
C	3.26950000	-2.45690000	-1.64830000
C	4.08560000	-1.91010000	-2.64230000
C	3.60590000	-1.69050000	-3.92850000
C	2.29920000	-2.03080000	-4.25230000
C	1.44290000	-2.59000000	-3.29920000

C	3.82840000	-2.73860000	-0.25820000
C	4.53210000	-4.11080000	-0.22700000
C	4.77680000	-1.64300000	0.25240000
C	0.02550000	-2.98300000	-3.69660000
C	0.02410000	-3.99850000	-4.85400000
C	-0.83130000	-1.75020000	-4.03190000
C	-1.61930000	-3.44440000	1.37170000
C	-1.42030000	-3.41740000	2.76500000
C	-2.55130000	-3.31560000	3.57880000
C	-3.82520000	-3.22380000	3.03290000
C	-3.99470000	-3.24410000	1.65500000
C	-2.90020000	-3.36570000	0.79510000
C	-0.03440000	-3.51320000	3.39110000
C	0.27690000	-4.95680000	3.83270000
C	0.15090000	-2.53870000	4.56640000
C	-3.13360000	-3.42700000	-0.70890000
C	-3.99020000	-4.64730000	-1.09410000
C	-3.74740000	-2.12040000	-1.24050000
Br	-1.77570000	0.22230000	2.03770000
Br	1.77570000	-0.22230000	2.03770000
H	0.40000000	5.78570000	0.61080000
H	-1.56670000	5.44480000	-1.29290000
H	1.56670000	-5.44480000	-1.29290000
H	-0.40000000	-5.78570000	0.61080000
H	2.43040000	3.29370000	4.65580000
H	4.68890000	3.13500000	3.68460000
H	4.99350000	3.17240000	1.23690000
H	-0.69460000	3.23020000	2.62720000
H	-1.27690000	5.01350000	4.27580000
H	0.44390000	5.29960000	4.58350000
H	-0.24270000	5.65680000	2.99270000
H	0.14120000	1.52500000	4.28520000
H	-1.20270000	2.51900000	4.86800000
H	0.43360000	2.83900000	5.44320000
H	2.16450000	3.54860000	-1.19760000
H	4.09920000	4.70760000	-2.18230000
H	3.53480000	5.58000000	-0.74620000
H	4.99520000	4.58720000	-0.66360000
H	3.09870000	1.26990000	-1.01920000
H	3.88000000	2.17570000	-2.32640000
H	4.72960000	1.92860000	-0.79520000
H	-5.11090000	1.65020000	-2.40570000
H	-4.25680000	1.25870000	-4.68250000
H	-1.93610000	1.86450000	-5.26110000
H	-2.98570000	2.77560000	0.43700000
H	-4.91490000	4.32110000	0.77740000
H	-5.37890000	4.13050000	-0.92210000
H	-3.85390000	4.92290000	-0.50390000
H	-4.30180000	0.66050000	0.22380000
H	-5.04910000	1.85050000	1.29210000
H	-5.70800000	1.60120000	-0.32330000

H	0.43870000	3.47710000	-2.83990000
H	0.99950000	4.31870000	-5.07550000
H	-0.44040000	3.56920000	-5.77130000
H	-0.61220000	4.88800000	-4.60660000
H	0.86680000	1.05850000	-3.18710000
H	1.85580000	2.05360000	-4.27370000
H	0.43150000	1.21320000	-4.89870000
H	5.11090000	-1.65020000	-2.40570000
H	4.25680000	-1.25870000	-4.68250000
H	1.93610000	-1.86450000	-5.26110000
H	2.98570000	-2.77560000	0.43700000
H	4.91490000	-4.32110000	0.77740000
H	5.37890000	-4.13050000	-0.92210000
H	3.85390000	-4.92290000	-0.50390000
H	5.04910000	-1.85050000	1.29210000
H	5.70800000	-1.60120000	-0.32330000
H	4.30180000	-0.66050000	0.22380000
H	-0.43870000	-3.47710000	-2.83990000
H	0.61220000	-4.88800000	-4.60660000
H	-0.99950000	-4.31870000	-5.07550000
H	0.44040000	-3.56920000	-5.77130000
H	-0.86680000	-1.05850000	-3.18710000
H	-0.43150000	-1.21320000	-4.89870000
H	-1.85580000	-2.05360000	-4.27370000
H	-2.43040000	-3.29370000	4.65580000
H	-4.68890000	-3.13500000	3.68460000
H	-4.99350000	-3.17240000	1.23690000
H	1.27690000	-5.01350000	4.27580000
H	0.24270000	-5.65680000	2.99270000
H	-0.44390000	-5.29960000	4.58350000
H	1.20270000	-2.51900000	4.86800000
H	-0.43360000	-2.83900000	5.44320000
H	-0.14120000	-1.52500000	4.28520000
H	-2.16450000	-3.54860000	-1.19760000
H	-4.09920000	-4.70760000	-2.18230000
H	-3.53480000	-5.58000000	-0.74620000
H	-4.99520000	-4.58720000	-0.66360000
H	-3.88000000	-2.17570000	-2.32640000
H	-3.09870000	-1.26990000	-1.01920000
H	-4.72960000	-1.92860000	-0.79520000
H	0.69460000	-3.23020000	2.62720000

Compound 5

charge=0, multiplicity=1

K	1.83640000	-0.24180000	2.49580000
Si	0.00000000	1.14660000	0.00000000

N	1.43560000	0.20120000	-0.13780000
N	2.56240000	-1.82450000	-0.80850000
N	0.66420000	-1.31250000	-1.88480000
C	1.49930000	-0.89020000	-0.90080000
C	2.34860000	-2.81400000	-1.77490000
H	3.04780000	-3.61880000	-1.92340000
C	1.19870000	-2.47200000	-2.40750000
H	0.73300000	-2.98550000	-3.23640000
C	3.65590000	-1.84830000	0.11170000
C	4.83570000	-1.12370000	-0.18460000
C	5.88080000	-1.14770000	0.74450000
H	6.78640000	-0.58820000	0.54410000
C	5.78850000	-1.88480000	1.91860000
H	6.61260000	-1.88850000	2.62570000
C	4.65110000	-2.64150000	2.17060000
H	4.60850000	-3.24850000	3.06790000
C	3.57170000	-2.65200000	1.27620000
C	5.00680000	-0.38750000	-1.51080000
H	4.04660000	0.07890000	-1.74720000
C	5.34660000	-1.37550000	-2.64840000
H	5.51170000	-0.82780000	-3.58290000
H	4.54330000	-2.09290000	-2.81970000
H	6.26560000	-1.92670000	-2.41790000
C	6.07940000	0.71310000	-1.47950000
H	5.96140000	1.39100000	-0.63180000
H	6.01900000	1.30740000	-2.39670000
H	7.09020000	0.29130000	-1.44060000
C	2.38130000	-3.57380000	1.54500000
H	1.49670000	-3.13540000	1.07290000
C	2.61380000	-4.96370000	0.91370000
H	2.72540000	-4.89920000	-0.16860000
H	1.76250000	-5.61990000	1.12430000
H	3.51410000	-5.43190000	1.32810000
C	2.07060000	-3.77200000	3.03970000
H	1.94450000	-2.83170000	3.58880000
H	2.85310000	-4.34270000	3.55050000
H	1.13960000	-4.33460000	3.14440000
C	-0.41850000	2.23050000	-1.60600000
C	0.27810000	2.13790000	-2.85340000
C	-0.36450000	2.50190000	-4.04840000
H	0.16800000	2.39690000	-4.98750000
C	-1.65230000	3.02050000	-4.05990000
H	-2.13610000	3.28060000	-4.99720000
C	-2.27680000	3.27080000	-2.84530000
H	-3.24230000	3.76650000	-2.83510000
C	-1.67070000	2.91190000	-1.63390000
C	1.76160000	1.78390000	-2.98700000
H	2.09390000	1.37680000	-2.03190000
C	2.07650000	0.75070000	-4.08380000
H	1.51950000	-0.17360000	-3.92890000
H	3.14340000	0.50240000	-4.06410000

H	1.86330000	1.13650000	-5.08730000
C	2.55810000	3.07700000	-3.27160000
H	3.63460000	2.87140000	-3.27010000
H	2.35750000	3.85420000	-2.53040000
H	2.30100000	3.48770000	-4.25470000
C	-2.37320000	3.37240000	-0.36220000
H	-1.83510000	2.95450000	0.48670000
C	-2.28490000	4.90770000	-0.24700000
H	-2.73670000	5.25200000	0.68960000
H	-2.81260000	5.40140000	-1.07050000
H	-1.24470000	5.24680000	-0.26870000
C	-3.82620000	2.89360000	-0.26110000
H	-4.26960000	3.22110000	0.68460000
H	-3.86260000	1.80270000	-0.29580000
H	-4.45110000	3.29330000	-1.06770000
N	-1.43560000	0.20120000	0.13770000
N	-2.56240000	-1.82450000	0.80840000
N	-0.66420000	-1.31250000	1.88480000
C	-1.49930000	-0.89020000	0.90080000
C	-2.34860000	-2.81400000	1.77490000
H	-3.04780000	-3.61880000	1.92330000
C	-1.19870000	-2.47200000	2.40750000
H	-0.73300000	-2.98560000	3.23630000
C	-3.65590000	-1.84830000	-0.11170000
C	-4.83580000	-1.12370000	0.18460000
C	-5.88090000	-1.14760000	-0.74450000
H	-6.78650000	-0.58820000	-0.54400000
C	-5.78860000	-1.88480000	-1.91860000
H	-6.61270000	-1.88850000	-2.62560000
C	-4.65120000	-2.64140000	-2.17070000
H	-4.60860000	-3.24840000	-3.06800000
C	-3.57180000	-2.65190000	-1.27630000
C	-5.00680000	-0.38760000	1.51080000
H	-4.04660000	0.07880000	1.74720000
C	-5.34660000	-1.37550000	2.64850000
H	-5.51170000	-0.82790000	3.58290000
H	-4.54330000	-2.09300000	2.81970000
H	-6.26560000	-1.92670000	2.41790000
C	-6.07940000	0.71310000	1.47960000
H	-5.96130000	1.39100000	0.63190000
H	-6.01900000	1.30730000	2.39680000
H	-7.09020000	0.29130000	1.44070000
C	-2.38130000	-3.57370000	-1.54520000
H	-1.49670000	-3.13530000	-1.07310000
C	-2.61380000	-4.96360000	-0.91390000
H	-2.72530000	-4.89910000	0.16850000
H	-1.76240000	-5.61980000	-1.12450000
H	-3.51400000	-5.43180000	-1.32820000
C	-2.07070000	-3.77190000	-3.03990000
H	-1.94470000	-2.83160000	-3.58900000
H	-2.85320000	-4.34260000	-3.55060000

H	-1.13970000	-4.33440000	-3.14460000
C	0.41850000	2.23040000	1.60610000
C	-0.27810000	2.13780000	2.85340000
C	0.36450000	2.50170000	4.04840000
H	-0.16800000	2.39680000	4.98750000
C	1.65230000	3.02040000	4.05990000
H	2.13620000	3.28040000	4.99720000
C	2.27690000	3.27070000	2.84530000
H	3.24230000	3.76640000	2.83520000
C	1.67070000	2.91190000	1.63400000
C	-1.76160000	1.78380000	2.98700000
H	-2.09390000	1.37680000	2.03190000
C	-2.07650000	0.75060000	4.08380000
H	-1.51950000	-0.17380000	3.92890000
H	-3.14340000	0.50230000	4.06410000
H	-1.86320000	1.13640000	5.08740000
C	-2.55810000	3.07690000	3.27160000
H	-3.63460000	2.87130000	3.27020000
H	-2.35750000	3.85410000	2.53050000
H	-2.30090000	3.48750000	4.25480000
C	2.37320000	3.37240000	0.36230000
H	1.83510000	2.95450000	-0.48670000
C	2.28490000	4.90770000	0.24710000
H	2.73670000	5.25210000	-0.68940000
H	2.81260000	5.40140000	1.07070000
H	1.24470000	5.24680000	0.26880000
C	3.82620000	2.89360000	0.26120000
H	4.26960000	3.22110000	-0.68450000
H	3.86260000	1.80270000	0.29590000
H	4.45110000	3.29330000	1.06770000
K	-1.83640000	-0.24170000	-2.49580000

:Si(N=IPr)$_2$

charge=0, multiplicity=1

Si	0.00000000	0.00010000	-1.00380000
N	-1.31210000	0.28910000	0.05070000
N	-3.67500000	0.31420000	0.42630000
N	-2.79180000	2.15800000	-0.39290000
N	1.31220000	-0.28890000	0.05060000
N	2.79170000	-2.15790000	-0.39390000
N	3.67520000	-0.31430000	0.42570000
C	-2.45570000	0.85840000	0.01040000
C	-4.69660000	1.25570000	0.29740000
C	-4.15640000	2.38460000	-0.20090000
C	2.45570000	-0.85840000	0.00990000
C	4.15630000	-2.38450000	-0.20230000

C	4.69670000	-1.25580000	0.29630000
C	-3.84720000	-1.00290000	0.96260000
C	-4.06190000	-2.07690000	0.07930000
C	-4.27390000	-3.34330000	0.63120000
C	-4.26310000	-3.53650000	2.00730000
C	-4.03900000	-2.46280000	2.86090000
C	-3.82900000	-1.17500000	2.35990000
C	-4.10820000	-1.87840000	-1.43030000
C	-5.56630000	-1.81240000	-1.92500000
C	-3.31420000	-2.94780000	-2.19740000
C	-3.55330000	-0.01530000	3.30950000
C	-4.49880000	0.00450000	4.52200000
C	-2.07710000	-0.02130000	3.75230000
C	-1.87930000	3.13630000	-0.90550000
C	-1.82700000	3.35910000	-2.29540000
C	-0.97080000	4.35880000	-2.76510000
C	-0.18360000	5.09910000	-1.89160000
C	-0.24230000	4.85390000	-0.52500000
C	-1.09170000	3.87510000	-0.00200000
C	-2.67470000	2.56640000	-3.28270000
C	-3.77490000	3.44850000	-3.90280000
C	-1.81760000	1.89950000	-4.37270000
C	-1.15280000	3.65710000	1.50360000
C	-1.73560000	4.89100000	2.21790000
C	0.22010000	3.27090000	2.07980000
C	1.87900000	-3.13610000	-0.90620000
C	1.82610000	-3.35890000	-2.29600000
C	0.96980000	-4.35860000	-2.76530000
C	0.18310000	-5.09900000	-1.89150000
C	0.24230000	-4.85380000	-0.52500000
C	1.09180000	-3.87490000	-0.00230000
C	2.67320000	-2.56590000	-3.28370000
C	3.77330000	-3.44770000	-3.90420000
C	1.81540000	-1.89920000	-4.37330000
C	1.15350000	-3.65700000	1.50330000
C	1.73680000	-4.89080000	2.21730000
C	-0.21920000	-3.27120000	2.08010000
C	3.84760000	1.00270000	0.96230000
C	4.06270000	2.07680000	0.07930000
C	4.27470000	3.34300000	0.63160000
C	4.26360000	3.53600000	2.00760000
C	4.03920000	2.46200000	2.86090000
C	3.82920000	1.17440000	2.35970000
C	4.10920000	1.87870000	-1.43040000
C	5.56740000	1.81440000	-1.92500000
C	3.31410000	2.94750000	-2.19720000
C	3.55330000	0.01450000	3.30900000
C	4.49880000	-0.00560000	4.52150000
C	2.07710000	0.02060000	3.75180000
H	-5.70940000	1.02480000	0.57980000
H	-4.60390000	3.33480000	-0.43630000

H	4.60370000	-3.33460000	-0.43800000
H	5.70960000	-1.02500000	0.57840000
H	-4.45070000	-4.18830000	-0.02520000
H	-4.43030000	-4.52800000	2.41690000
H	-4.02680000	-2.62740000	3.93270000
H	-3.64100000	-0.91570000	-1.65090000
H	-5.59830000	-1.64380000	-3.00690000
H	-6.09570000	-2.74830000	-1.71400000
H	-6.11670000	-1.00030000	-1.44000000
H	-2.28520000	-3.01600000	-1.83540000
H	-3.28290000	-2.69460000	-3.26220000
H	-3.77270000	-3.93930000	-2.11400000
H	-3.72330000	0.91370000	2.75840000
H	-4.33440000	0.91430000	5.10860000
H	-5.54900000	-0.01590000	4.21400000
H	-4.32920000	-0.84510000	5.19170000
H	-1.41140000	0.02690000	2.88640000
H	-1.86880000	0.83630000	4.40200000
H	-1.84240000	-0.93280000	4.31330000
H	-0.91590000	4.55440000	-3.83080000
H	0.47780000	5.86880000	-2.27710000
H	0.37660000	5.43520000	0.15050000
H	-3.17060000	1.76590000	-2.72790000
H	-4.40000000	2.86030000	-4.58310000
H	-3.34380000	4.27620000	-4.47640000
H	-4.42440000	3.88040000	-3.13470000
H	-1.05200000	1.25790000	-3.92720000
H	-2.44930000	1.28380000	-5.02230000
H	-1.31890000	2.63980000	-5.00750000
H	-1.82870000	2.82090000	1.69460000
H	-1.81770000	4.70530000	3.29420000
H	-1.09900000	5.77180000	2.08030000
H	-2.73240000	5.13860000	1.83910000
H	0.61300000	2.37500000	1.59320000
H	0.13240000	3.06740000	3.15260000
H	0.95420000	4.07400000	1.95620000
H	0.91450000	-4.55420000	-3.83100000
H	-0.47840000	-5.86880000	-2.27680000
H	-0.37630000	-5.43520000	0.15070000
H	3.16910000	-1.76530000	-2.72900000
H	4.39800000	-2.85940000	-4.58480000
H	3.34210000	-4.27550000	-4.47780000
H	4.42320000	-3.87960000	-3.13650000
H	2.44660000	-1.28330000	-5.02300000
H	1.31670000	-2.63970000	-5.00800000
H	1.04980000	-1.25790000	-3.92730000
H	1.82930000	-2.82070000	1.69400000
H	2.73360000	-5.13810000	1.83810000
H	1.81930000	-4.70510000	3.29360000
H	1.10040000	-5.77170000	2.07980000
H	-0.61250000	-2.37520000	1.59380000

H	-0.95320000	-4.07440000	1.95670000
H	-0.13110000	-3.06780000	3.15290000
H	4.45180000	4.18810000	-0.02470000
H	4.43090000	4.52740000	2.41750000
H	4.02680000	2.62640000	3.93280000
H	5.59970000	1.64610000	-3.00690000
H	6.11870000	1.00280000	-1.44010000
H	6.09580000	2.75080000	-1.71380000
H	3.28330000	2.69470000	-3.26200000
H	3.77140000	3.93950000	-2.11320000
H	2.28490000	3.01430000	-1.83530000
H	3.72320000	-0.91430000	2.75770000
H	4.33430000	-0.91550000	5.10790000
H	5.54900000	0.01470000	4.21350000
H	4.32930000	0.84380000	5.19130000
H	1.86870000	-0.83700000	4.40130000
H	1.41140000	-0.02740000	2.88590000
H	1.84250000	0.93210000	4.31300000
H	3.64320000	0.91560000	-1.65120000

Compound 7-re

charge=0, multiplicity=1

Si	-0.11930000	-0.01280000	-1.02310000
N	-1.34220000	0.19210000	0.05100000
N	-2.73640000	-0.68710000	1.78660000
N	-1.65710000	1.17540000	2.22040000
N	1.33190000	-0.60330000	-0.57480000
N	2.10250000	-1.45800000	-2.70340000
N	3.60620000	-1.24440000	-1.07040000
C	-1.83480000	0.21420000	1.23730000
C	-3.08560000	-0.28180000	3.07600000
C	-2.42520000	0.86180000	3.34100000
C	2.27380000	-1.07070000	-1.43710000
C	3.32950000	-1.86940000	-3.16140000
C	4.27450000	-1.74820000	-2.18540000
C	-3.40210000	-1.75510000	1.09120000
C	-4.71400000	-1.53510000	0.62940000
C	-5.38270000	-2.60990000	0.03590000
C	-4.77020000	-3.84860000	-0.09970000
C	-3.46670000	-4.03440000	0.34660000
C	-2.75300000	-2.99550000	0.95050000
C	-5.41530000	-0.18520000	0.73670000
C	-6.73910000	-0.28590000	1.51590000
C	-5.63290000	0.44010000	-0.65370000
C	-1.34200000	-3.22830000	1.47500000
C	-1.38610000	-3.79400000	2.90860000
C	-0.50460000	-4.13060000	0.55580000
C	-0.87540000	2.36980000	2.07580000

C	-1.42690000	3.45810000	1.37180000
C	-0.64490000	4.60900000	1.24670000
C	0.62510000	4.67930000	1.80880000
C	1.13220000	3.60220000	2.52470000
C	0.39360000	2.42440000	2.67770000
C	-2.84850000	3.44180000	0.82150000
C	-3.75230000	4.38030000	1.64520000
C	-2.91720000	3.78240000	-0.67600000
C	0.95340000	1.27810000	3.50960000
C	1.06890000	1.68480000	4.99150000
C	2.29520000	0.76970000	2.96370000
C	-0.64070000	0.53080000	-2.74230000
C	-0.11580000	1.71740000	-3.30090000
C	-0.60020000	2.16340000	-4.53580000
C	-1.56020000	1.44030000	-5.22840000
C	-2.03340000	0.24150000	-4.70690000
C	-1.58520000	-0.23220000	-3.47240000
C	1.02530000	2.49070000	-2.64870000
C	2.31330000	2.30840000	-3.47570000
C	0.71660000	3.98120000	-2.43510000
C	-2.03970000	-1.60400000	-2.98650000
C	-1.12520000	-2.70170000	-3.56980000
C	-3.51460000	-1.91400000	-3.28480000
C	4.27460000	-0.96710000	0.16620000
C	4.94510000	0.26060000	0.32230000
C	5.70450000	0.45750000	1.48020000
C	5.79230000	-0.52610000	2.45580000
C	5.10830000	-1.72570000	2.29330000
C	4.33910000	-1.97180000	1.15290000
C	4.89240000	1.35040000	-0.73930000
C	6.24120000	1.47650000	-1.47220000
C	4.45400000	2.70490000	-0.15540000
C	3.63740000	-3.31200000	0.97010000
C	4.58900000	-4.35050000	0.34340000
C	3.03810000	-3.85510000	2.27740000
H	-3.77070000	-0.85790000	3.67330000
H	-2.41260000	1.48460000	4.21850000
H	3.46020000	-2.23730000	-4.16910000
H	5.33020000	-1.96120000	-2.15200000
H	-6.39460000	-2.47040000	-0.32960000
H	-5.30720000	-4.67180000	-0.56030000
H	-2.99730000	-5.00380000	0.22810000
H	-4.76830000	0.49380000	1.29670000
H	-7.18880000	0.70600000	1.62910000
H	-7.46700000	-0.92060000	1.00030000
H	-6.58360000	-0.70390000	2.51550000
H	-4.68230000	0.57100000	-1.17820000
H	-6.11020000	1.42160000	-0.55930000
H	-6.28000000	-0.18560000	-1.27740000
H	-0.83370000	-2.26170000	1.51490000
H	-0.37140000	-3.93740000	3.29410000

H	-1.91470000	-3.12090000	3.59080000
H	-1.89690000	-4.76320000	2.93090000
H	-0.49810000	-3.76140000	-0.47320000
H	0.52930000	-4.15210000	0.90760000
H	-0.86650000	-5.16440000	0.54820000
H	-1.04070000	5.46550000	0.71120000
H	1.21620000	5.58290000	1.69850000
H	2.11620000	3.67360000	2.97540000
H	-3.24360000	2.43010000	0.93520000
H	-4.78510000	4.33120000	1.28420000
H	-3.42010000	5.42100000	1.56740000
H	-3.74920000	4.10900000	2.70560000
H	-2.32160000	3.08480000	-1.27000000
H	-3.95320000	3.72300000	-1.02580000
H	-0.17860000	4.12230000	-1.82470000
H	0.24760000	0.44550000	3.45480000
H	1.42230000	0.83910000	5.59050000
H	1.77990000	2.50710000	5.12510000
H	0.10630000	2.01120000	5.39930000
H	2.19560000	0.41900000	1.93330000
H	2.65780000	-0.06510000	3.57140000
H	3.06560000	1.54660000	2.99030000
H	-0.20970000	3.08030000	-4.96530000
H	-1.92700000	1.79910000	-6.18550000
H	-2.75550000	-0.33500000	-5.27430000
H	1.21410000	2.05240000	-1.65850000
H	3.15790000	2.80910000	-2.99130000
H	2.19750000	2.74400000	-4.47440000
H	2.55310000	1.24870000	-3.59520000
H	1.55320000	4.47020000	-1.92480000
H	0.56300000	4.50200000	-3.38620000
H	-2.56240000	4.79820000	-0.88030000
H	-1.93070000	-1.62350000	-1.89370000
H	-0.07220000	-2.50520000	-3.34590000
H	-1.40190000	-3.68240000	-3.16530000
H	-1.23590000	-2.74630000	-4.65960000
H	-4.17580000	-1.11340000	-2.94140000
H	-3.68860000	-2.06080000	-4.35620000
H	-3.81050000	-2.83770000	-2.77940000
H	6.24050000	1.39180000	1.61270000
H	6.39210000	-0.35920000	3.34540000
H	5.18310000	-2.48650000	3.06220000
H	6.18330000	2.24110000	-2.25460000
H	6.52220000	0.53120000	-1.94520000
H	7.04450000	1.76100000	-0.78330000
H	4.36890000	3.45080000	-0.95310000
H	5.17750000	3.09070000	0.57120000
H	3.48350000	2.62720000	0.34310000
H	2.81180000	-3.15400000	0.27090000
H	4.07510000	-5.30830000	0.20640000
H	4.94740000	-4.01870000	-0.63410000

H	5.45870000	-4.52250000	0.98800000
H	2.45350000	-4.75820000	2.07360000
H	2.38060000	-3.12020000	2.75200000
H	3.80980000	-4.13610000	3.00180000
H	4.14580000	1.05500000	-1.47880000

Compound 8

charge=0, multiplicity=2

Si	0.04920000	0.34410000	0.89870000
N	-1.31390000	0.20190000	-0.11500000
N	-2.84930000	2.06600000	-0.35870000
N	-3.62710000	0.03190000	-0.69600000
N	1.33500000	-0.26890000	-0.02410000
N	3.66140000	-0.50520000	-0.54730000
N	2.79130000	-2.01540000	0.80260000
C	-2.46110000	0.71800000	-0.33970000
C	-4.19000000	2.17630000	-0.73380000
C	-4.66430000	0.93310000	-0.93870000
C	2.46530000	-0.85580000	0.08700000
C	4.65560000	-1.44010000	-0.25140000
C	4.12420000	-2.36330000	0.57110000
C	-2.05330000	3.16030000	0.10870000
C	-2.30640000	3.68460000	1.39110000
C	-1.52850000	4.76780000	1.81690000
C	-0.53730000	5.30330000	1.00100000
C	-0.31080000	4.77130000	-0.26500000
C	-1.06370000	3.69450000	-0.74070000
C	-3.38930000	3.12660000	2.30920000
C	-4.48660000	4.17310000	2.57930000
C	-2.80690000	2.58560000	3.62690000
C	-0.86110000	3.15340000	-2.15100000
C	-1.79660000	3.87930000	-3.13940000
C	0.59490000	3.22240000	-2.63080000
C	-3.75370000	-1.38790000	-0.84540000
C	-3.92460000	-2.18370000	0.30480000
C	-4.12390000	-3.55390000	0.12360000
C	-4.15830000	-4.11380000	-1.14950000
C	-3.97810000	-3.31140000	-2.26790000
C	-3.76480000	-1.93470000	-2.14130000
C	-3.95180000	-1.57040000	1.69990000
C	-5.39210000	-1.18400000	2.09210000
C	-3.32100000	-2.47080000	2.77290000
C	-3.56750000	-1.08460000	-3.39060000
C	-4.85170000	-1.02810000	-4.23880000
C	-2.37320000	-1.57150000	-4.22960000
C	3.83330000	0.55670000	-1.49680000
C	4.31940000	1.80120000	-1.05170000
C	4.55620000	2.79060000	-2.01040000

C	4.30730000	2.55960000	-3.35800000
C	3.81470000	1.32910000	-3.77300000
C	3.57380000	0.30140000	-2.85660000
C	4.61790000	2.06830000	0.41780000
C	6.10970000	1.84040000	0.73100000
C	4.18390000	3.47260000	0.86740000
C	3.02860000	-1.03380000	-3.34500000
C	3.85690000	-1.61800000	-4.50250000
C	1.54190000	-0.90500000	-3.72620000
C	1.87740000	-2.83530000	1.54380000
C	1.84400000	-2.72600000	2.94760000
C	1.00120000	-3.59150000	3.65050000
C	0.20930000	-4.52010000	2.98600000
C	0.24960000	-4.60290000	1.59960000
C	1.08630000	-3.77130000	0.85000000
C	2.70890000	-1.72710000	3.70510000
C	3.92310000	-2.42090000	4.35180000
C	1.90760000	-0.94170000	4.75660000
C	1.13440000	-3.92330000	-0.66400000
C	1.71120000	-5.29430000	-1.06430000
C	-0.24260000	-3.68410000	-1.30500000
H	-4.67150000	3.13560000	-0.81400000
H	-5.63930000	0.59350000	-1.24280000
H	5.64520000	-1.35150000	-0.66500000
H	4.55790000	-3.24080000	1.01830000
H	-1.70130000	5.19980000	2.79780000
H	0.05720000	6.14070000	1.35310000
H	0.46020000	5.20370000	-0.89170000
H	-3.86320000	2.28430000	1.80080000
H	-5.28300000	3.74010000	3.19330000
H	-4.08920000	5.04200000	3.11420000
H	-4.93400000	4.53300000	1.64740000
H	-2.07190000	1.79620000	3.43580000
H	-3.60210000	2.15900000	4.24800000
H	-2.32240000	3.37330000	4.21500000
H	-1.13890000	2.09650000	-2.13950000
H	-1.67310000	3.47440000	-4.14960000
H	-2.84780000	3.76730000	-2.85780000
H	-1.56990000	4.95070000	-3.17560000
H	1.27280000	2.72910000	-1.92980000
H	0.68840000	2.71500000	-3.59570000
H	0.93650000	4.25280000	-2.77710000
H	-4.26200000	-4.19200000	0.98880000
H	-4.32420000	-5.18010000	-1.26780000
H	-4.00030000	-3.75790000	-3.25660000
H	-3.35620000	-0.65500000	1.66810000
H	-5.40870000	-0.72170000	3.08510000
H	-6.03830000	-2.06840000	2.12150000
H	-5.82670000	-0.47420000	1.38200000
H	-2.31770000	-2.79570000	2.48480000
H	-3.24180000	-1.92030000	3.71590000

H	-3.92650000	-3.36180000	2.97280000
H	-3.34060000	-0.06470000	-3.07110000
H	-4.70580000	-0.38460000	-5.11280000
H	-5.13510000	-2.02250000	-4.60010000
H	-5.69510000	-0.63210000	-3.66450000
H	-1.45650000	-1.58370000	-3.63480000
H	-2.21720000	-0.90720000	-5.08620000
H	-2.53660000	-2.58110000	-4.62150000
H	4.93980000	3.75510000	-1.69750000
H	4.49700000	3.34200000	-4.08610000
H	3.61800000	1.15980000	-4.82630000
H	4.04260000	1.34680000	1.00630000
H	6.30890000	2.02070000	1.79270000
H	6.73930000	2.52180000	0.14820000
H	6.41800000	0.81680000	0.49930000
H	4.27710000	3.56500000	1.95520000
H	4.80550000	4.25990000	0.42660000
H	3.14310000	3.67700000	0.59610000
H	3.09300000	-1.74490000	-2.51770000
H	4.91360000	-1.70900000	-4.23230000
H	3.48620000	-2.61460000	-4.76380000
H	3.79470000	-1.00100000	-5.40490000
H	0.95400000	-0.56020000	-2.87130000
H	1.40710000	-0.19460000	-4.54970000
H	1.14660000	-1.87300000	-4.05310000
H	0.96310000	-3.53510000	4.73280000
H	-0.43950000	-5.18220000	3.55100000
H	-0.37110000	-5.33100000	1.08810000
H	4.54720000	-1.68950000	4.87620000
H	4.54580000	-2.92210000	3.60460000
H	3.60320000	-3.17440000	5.07980000
H	2.52500000	-0.14460000	5.18510000
H	1.57970000	-1.57710000	5.58650000
H	1.01690000	-0.48710000	4.31100000
H	1.80950000	-3.16070000	-1.05730000
H	1.78560000	-5.37300000	-2.15410000
H	2.71070000	-5.44550000	-0.64410000
H	1.07530000	-6.11470000	-0.71470000
H	-0.16700000	-3.75850000	-2.39530000
H	-0.62660000	-2.69210000	-1.05400000
H	-0.97890000	-4.42480000	-0.97710000
H	3.09060000	-1.00250000	2.97990000
K	1.07330000	2.84440000	3.48270000

Compound 8-re

charge=0, multiplicity=2

Si	-0.10400000	-0.99670000	-0.26060000
N	1.56840000	-0.65000000	-0.36950000

N	3.82600000	-0.95110000	0.44940000
N	2.68470000	-2.78500000	-0.13550000
N	-1.03570000	0.43390000	-0.02670000
N	-2.19090000	2.28030000	0.92510000
N	-2.44870000	0.34530000	1.97210000
C	2.59030000	-1.43150000	-0.02760000
C	4.66570000	-2.05040000	0.65070000
C	3.94560000	-3.14670000	0.29430000
C	-1.80390000	0.92870000	0.85910000
C	-3.00770000	2.49850000	2.03470000
C	-3.16750000	1.32450000	2.67010000
C	4.29010000	0.38760000	0.65430000
C	4.86390000	1.09050000	-0.42570000
C	5.45240000	2.33180000	-0.17300000
C	5.48320000	2.86330000	1.11130000
C	4.89970000	2.16680000	2.16080000
C	4.28520000	0.92670000	1.95410000
C	4.89790000	0.49750000	-1.82950000
C	6.20720000	-0.28050000	-2.07170000
C	4.68200000	1.54500000	-2.93340000
C	3.66200000	0.18740000	3.12960000
C	4.74370000	-0.39680000	4.05760000
C	2.68660000	1.07970000	3.91650000
C	-1.93940000	3.25670000	-0.09440000
C	-2.97500000	3.59360000	-0.99120000
C	-2.71110000	4.55640000	-1.96980000
C	-1.46680000	5.16720000	-2.06070000
C	-0.46660000	4.83300000	-1.15730000
C	-0.68060000	3.88140000	-0.15550000
C	-4.36720000	2.97630000	-0.92240000
C	-5.43060000	4.03680000	-0.57920000
C	-4.73100000	2.23000000	-2.21760000
C	0.42290000	3.59730000	0.85120000
C	0.66130000	4.82510000	1.75190000
C	1.72070000	3.14140000	0.16800000
C	-2.72180000	-1.05210000	2.17120000
C	-3.86000000	-1.61140000	1.55390000
C	-4.18850000	-2.93590000	1.85580000
C	-3.41950000	-3.68230000	2.73880000
C	-2.29530000	-3.11650000	3.32820000
C	-1.92040000	-1.79800000	3.05670000
C	-4.75240000	-0.82010000	0.60590000
C	-6.13130000	-0.55020000	1.23700000
C	-4.89500000	-1.50270000	-0.76560000
C	-0.70380000	-1.19510000	3.74430000
C	-1.05680000	-0.74150000	5.17430000
C	0.49930000	-2.15210000	3.75090000
H	5.66620000	-1.92460000	1.03050000
H	4.25190000	-4.18320000	0.33390000
H	-3.36790000	3.48360000	2.27750000
H	-3.71330000	1.07880000	3.56480000

H	5.90450000	2.88640000	-0.98770000
H	5.95690000	3.82350000	1.29090000
H	4.92260000	2.58980000	3.15980000
H	4.06890000	-0.21450000	-1.88760000
H	6.22190000	-0.70830000	-3.08190000
H	7.07410000	0.38310000	-1.97940000
H	6.32260000	-1.09640000	-1.35390000
H	3.78650000	2.14350000	-2.74810000
H	4.56680000	1.05050000	-3.90430000
H	5.53480000	2.22590000	-3.02380000
H	3.08810000	-0.64830000	2.72280000
H	4.28400000	-0.94480000	4.88740000
H	5.39540000	-1.08940000	3.51740000
H	5.37080000	0.39420000	4.48440000
H	1.90160000	1.47460000	3.26510000
H	2.20850000	0.50500000	4.71670000
H	3.19370000	1.92780000	4.38870000
H	-3.49420000	4.83130000	-2.66910000
H	-1.28080000	5.91150000	-2.82900000
H	0.49770000	5.32600000	-1.22070000
H	-4.37510000	2.24420000	-0.11310000
H	-6.41730000	3.57160000	-0.48080000
H	-5.50000000	4.80350000	-1.35800000
H	-5.19910000	4.54290000	0.36330000
H	-5.72400000	1.77560000	-2.12880000
H	-4.75230000	2.90260000	-3.08130000
H	-4.00940000	1.43640000	-2.42790000
H	0.08930000	2.77960000	1.49400000
H	-0.25640000	5.13120000	2.26490000
H	1.41640000	4.59710000	2.51140000
H	1.02030000	5.68310000	1.17270000
H	1.57340000	2.19160000	-0.35120000
H	2.08590000	3.88840000	-0.54570000
H	2.50560000	2.99390000	0.91360000
H	-5.06440000	-3.38400000	1.39820000
H	-3.69640000	-4.70650000	2.96940000
H	-1.69950000	-3.70880000	4.01320000
H	-6.75190000	0.04880000	0.56160000
H	-6.03560000	-0.00560000	2.18110000
H	-6.66620000	-1.48400000	1.44120000
H	-5.49930000	-0.88100000	-1.43470000
H	-5.39040000	-2.47630000	-0.68720000
H	-0.41300000	-0.30720000	3.17610000
H	-0.18710000	-0.28530000	5.65920000
H	-1.86580000	-0.00450000	5.17400000
H	-1.37750000	-1.59080000	5.78800000
H	1.37180000	-1.65050000	4.17910000
H	0.75320000	-2.47280000	2.73650000
H	0.31390000	-3.04340000	4.35990000
H	-4.27960000	0.14720000	0.42990000
C	-0.67090000	-1.77230000	-1.96780000

C	-0.57980000	-1.04150000	-3.19030000
C	-0.92530000	-3.17140000	-2.04590000
C	-0.61820000	-1.71920000	-4.41800000
C	-0.95790000	-3.81400000	-3.29460000
C	-0.77960000	-3.10210000	-4.47590000
H	-0.53050000	-1.15820000	-5.34360000
H	-1.13530000	-4.88420000	-3.34160000
H	-0.80350000	-3.61250000	-5.43470000
C	-0.41110000	0.47900000	-3.22450000
H	-0.65240000	0.85710000	-2.22960000
C	-1.17880000	-4.03370000	-0.80740000
H	-1.23290000	-3.35360000	0.05040000
C	-2.52290000	-4.77790000	-0.90380000
H	-2.74230000	-5.27530000	0.04610000
H	-3.34670000	-4.09410000	-1.12430000
H	-2.50820000	-5.54900000	-1.68280000
C	-0.03100000	-5.02220000	-0.53160000
H	-0.26250000	-5.63310000	0.34850000
H	0.11320000	-5.70990000	-1.37540000
H	0.90530000	-4.49060000	-0.33540000
C	-1.37760000	1.15380000	-4.21450000
H	-1.10880000	0.96180000	-5.25990000
H	-2.40570000	0.80990000	-4.06740000
H	-1.36080000	2.23840000	-4.06700000
C	1.04280000	0.88400000	-3.52930000
H	1.13530000	1.97480000	-3.57350000
H	1.70830000	0.53410000	-2.73410000
H	1.37740000	0.48740000	-4.49800000
K	2.06980000	-2.54240000	-2.70250000
H	-3.91820000	-1.65350000	-1.23360000

Compound 9

charge=0, multiplicity=1

Si	0.08380000	-1.03220000	-0.04450000
N	1.32120000	0.15660000	0.30520000
N	3.69990000	-0.45540000	0.05780000
N	3.15670000	1.30030000	1.30530000
N	-1.29870000	-0.01240000	-0.40710000
N	-3.34370000	0.82060000	-1.30700000
N	-3.53490000	-0.99340000	-0.03920000
C	2.55920000	0.29330000	0.50440000
C	4.87890000	0.14590000	0.52120000
C	4.54450000	1.20270000	1.28240000
C	-2.55290000	-0.07470000	-0.54150000
C	-4.69460000	0.49710000	-1.21940000
C	-4.81630000	-0.59610000	-0.44690000
C	3.74020000	-1.42440000	-0.98980000
C	3.68480000	-2.79800000	-0.66220000

C	3.84140000	-3.73220000	-1.69010000
C	4.02700000	-3.32640000	-3.01150000
C	4.09480000	-1.96860000	-3.31520000
C	3.96830000	-0.99520000	-2.31770000
C	3.52850000	-3.25880000	0.78060000
C	4.90770000	-3.51460000	1.41980000
C	2.62470000	-4.49120000	0.92730000
C	4.04670000	0.48070000	-2.69080000
C	5.29460000	0.80830000	-3.52880000
C	2.75940000	0.93480000	-3.40300000
C	2.44370000	2.34700000	1.96870000
C	2.15470000	2.21730000	3.34120000
C	1.51540000	3.28120000	3.98370000
C	1.16050000	4.43040000	3.28720000
C	1.44580000	4.53530000	1.93180000
C	2.09460000	3.50370000	1.24720000
C	2.54590000	0.97530000	4.13100000
C	3.78020000	1.24190000	5.01340000
C	1.38340000	0.42710000	4.97500000
C	2.41020000	3.66330000	-0.23330000
C	3.32450000	4.87500000	-0.49010000
C	1.12530000	3.73690000	-1.07500000
C	-2.85550000	1.98740000	-1.97520000
C	-2.37400000	1.87150000	-3.29380000
C	-1.96520000	3.03560000	-3.94900000
C	-2.02760000	4.27300000	-3.31800000
C	-2.50160000	4.36650000	-2.01600000
C	-2.92550000	3.23090000	-1.31860000
C	-2.34720000	0.52650000	-4.00810000
C	-3.65410000	0.29560000	-4.79210000
C	-1.13090000	0.35580000	-4.93060000
C	-3.41270000	3.35550000	0.11980000
C	-4.39880000	4.51890000	0.31900000
C	-2.21880000	3.46310000	1.08700000
C	-3.38100000	-1.95240000	1.00760000
C	-3.15910000	-3.30840000	0.67500000
C	-3.15870000	-4.25230000	1.70560000
C	-3.35750000	-3.87290000	3.03340000
C	-3.58880000	-2.53400000	3.34210000
C	-3.61180000	-1.55360000	2.34430000
C	-2.98930000	-3.75000000	-0.77220000
C	-4.33000000	-4.24560000	-1.34850000
C	-1.89280000	-4.80960000	-0.95260000
C	-3.88050000	-0.10280000	2.72550000
C	-5.29350000	0.07140000	3.31150000
C	-2.80690000	0.44060000	3.68450000
H	5.84590000	-0.25300000	0.26490000
H	5.16490000	1.89790000	1.82210000
H	-5.44330000	1.07480000	-1.73460000
H	-5.69110000	-1.15190000	-0.15430000
H	3.81590000	-4.79180000	-1.46090000

H	4.14660000	-4.06630000	-3.79670000
H	4.25860000	-1.66240000	-4.34310000
H	3.05520000	-2.43900000	1.32930000
H	4.79370000	-3.82160000	2.46520000
H	5.44380000	-4.31060000	0.89080000
H	5.52980000	-2.61570000	1.39890000
H	1.64950000	-4.32150000	0.45880000
H	2.46200000	-4.70750000	1.99010000
H	3.06690000	-5.39100000	0.48640000
H	4.12530000	1.05450000	-1.76520000
H	5.36030000	1.88850000	-3.69480000
H	6.21040000	0.48670000	-3.02330000
H	5.26840000	0.32900000	-4.51310000
H	1.88350000	0.77370000	-2.76650000
H	2.80910000	2.00240000	-3.64220000
H	2.61420000	0.39180000	-4.34510000
H	1.29340000	3.20990000	5.04330000
H	0.66280000	5.24590000	3.80290000
H	1.16680000	5.43610000	1.39450000
H	2.81720000	0.20010000	3.40910000
H	4.06800000	0.33620000	5.55870000
H	3.57620000	2.02750000	5.74930000
H	4.63770000	1.56150000	4.41380000
H	0.49050000	0.27250000	4.36060000
H	1.66160000	-0.53190000	5.42750000
H	1.11030000	1.10360000	5.79210000
H	2.95510000	2.77250000	-0.55260000
H	3.58550000	4.93600000	-1.55220000
H	2.83570000	5.81660000	-0.21760000
H	4.25380000	4.80450000	0.08440000
H	0.50920000	2.84730000	-0.92290000
H	1.37070000	3.80890000	-2.14030000
H	0.52690000	4.61730000	-0.81770000
H	-1.59810000	2.97700000	-4.96750000
H	-1.70660000	5.16660000	-3.84440000
H	-2.54280000	5.33640000	-1.53210000
H	-2.28000000	-0.24750000	-3.23830000
H	-3.63860000	-0.68200000	-5.28720000
H	-3.78720000	1.06300000	-5.56300000
H	-4.52610000	0.32500000	-4.13300000
H	-1.08670000	-0.67480000	-5.30380000
H	-1.17960000	1.00780000	-5.80980000
H	-0.19720000	0.57190000	-4.40260000
H	-3.95250000	2.43780000	0.36700000
H	-5.24030000	4.45750000	-0.37830000
H	-4.80010000	4.49870000	1.33780000
H	-3.92020000	5.49410000	0.18120000
H	-1.54530000	2.60940000	0.97570000
H	-1.64130000	4.37410000	0.89770000
H	-2.56810000	3.50090000	2.12520000
H	-3.00310000	-5.30010000	1.47240000

H	-3.36070000	-4.62180000	3.81920000
H	-3.76130000	-2.24840000	4.37480000
H	-4.21060000	-4.53820000	-2.39730000
H	-5.09670000	-3.46720000	-1.30140000
H	-4.69780000	-5.11700000	-0.79500000
H	-1.74450000	-5.01180000	-2.02000000
H	-2.14940000	-5.76410000	-0.48050000
H	-0.94150000	-4.46160000	-0.53650000
H	-3.82720000	0.49620000	1.81500000
H	-5.48460000	1.12620000	3.53520000
H	-6.05930000	-0.26940000	2.60820000
H	-5.41720000	-0.49320000	4.24210000
H	-3.00470000	1.49130000	3.92020000
H	-1.81340000	0.38660000	3.22770000
H	-2.78590000	-0.11150000	4.63120000
H	-2.68650000	-2.86790000	-1.34340000
K	0.81430000	-2.58070000	-2.93270000
K	-0.29670000	-2.70900000	2.82960000

Compound 9-re

charge=0, multiplicity=1

Si	-0.05010000	-0.95000000	0.83460000
N	-1.42930000	-1.17860000	-0.26180000
N	-3.66210000	-1.89120000	-0.76780000
N	-2.29950000	-3.42440000	0.15390000
N	0.78320000	0.47310000	-0.01670000
N	1.41220000	2.45560000	1.30660000
N	2.88330000	1.67540000	-0.16990000
C	-2.34030000	-2.11620000	-0.26020000
C	-4.40340000	-3.07240000	-0.62330000
C	-3.54810000	-3.97380000	-0.08130000
C	1.57290000	1.39510000	0.33030000
C	2.54380000	3.27390000	1.33850000
C	3.42990000	2.80110000	0.44670000
C	-4.21320000	-0.61110000	-1.01490000
C	-4.92750000	0.05610000	0.01020000
C	-5.38060000	1.35850000	-0.23380000
C	-5.14720000	1.98730000	-1.45570000
C	-4.47860000	1.30430000	-2.46820000
C	-4.01340000	-0.00260000	-2.27380000
C	-5.17630000	-0.60320000	1.36410000
C	-6.61360000	-0.39020000	1.86850000
C	-4.14780000	-0.13640000	2.41200000
C	-3.33460000	-0.74610000	-3.41550000
C	-4.30020000	-0.94040000	-4.59900000
C	-2.03510000	-0.05500000	-3.85920000

C	0.16060000	2.90520000	1.83200000
C	-0.30690000	2.38870000	3.06120000
C	-1.54970000	2.82800000	3.52990000
C	-2.29930000	3.76600000	2.82670000
C	-1.79850000	4.31270000	1.65070000
C	-0.55950000	3.90640000	1.13590000
C	0.56010000	1.46840000	3.90950000
C	1.46920000	2.31250000	4.82760000
C	-0.23720000	0.44230000	4.72310000
C	-0.00750000	4.61110000	-0.10280000
C	0.39450000	6.05840000	0.24690000
C	-0.97290000	4.60470000	-1.30220000
C	3.54280000	1.08190000	-1.29830000
C	4.61750000	0.19690000	-1.07910000
C	5.35900000	-0.22840000	-2.18670000
C	5.04290000	0.19230000	-3.47100000
C	3.96590000	1.04600000	-3.67160000
C	3.20080000	1.50870000	-2.59840000
C	5.01240000	-0.27480000	0.31470000
C	6.21680000	0.52030000	0.85690000
C	2.07670000	2.50380000	-2.85310000
C	2.64380000	3.92350000	-3.04990000
C	1.18310000	2.10320000	-4.03820000
H	-5.41740000	-3.15310000	-0.98040000
H	-3.76080000	-5.01210000	0.14560000
H	2.61390000	4.11170000	2.01190000
H	4.41400000	3.15410000	0.19070000
H	-5.92630000	1.88850000	0.53980000
H	-5.50750000	2.99780000	-1.62510000
H	-4.32930000	1.78630000	-3.42960000
H	-5.03720000	-1.67880000	1.23160000
H	-6.78140000	-0.98570000	2.77170000
H	-6.81370000	0.65470000	2.13090000
H	-7.35120000	-0.69610000	1.11990000
H	-3.12490000	-0.39420000	2.11640000
H	-4.34050000	-0.62240000	3.37510000
H	-4.20810000	0.94760000	2.57330000
H	-3.06600000	-1.73400000	-3.03680000
H	-3.82280000	-1.53760000	-5.38310000
H	-5.21210000	-1.45860000	-4.28650000
H	-4.59510000	0.01630000	-5.04530000
H	-1.32500000	-0.01440000	-3.02850000
H	-1.56510000	-0.61490000	-4.67500000
H	-2.21730000	0.96330000	-4.22380000
H	-1.93660000	2.43230000	4.46100000
H	-3.26210000	4.09000000	3.21010000
H	-2.36650000	5.08030000	1.13450000
H	1.19640000	0.90840000	3.22100000
H	2.12010000	1.65910000	5.41820000
H	0.87660000	2.91590000	5.52490000
H	2.10790000	2.99070000	4.25410000

H	0.45670000	-0.21470000	5.25810000
H	-0.87740000	0.90970000	5.47990000
H	-0.84340000	-0.17690000	4.05540000
H	0.89990000	4.09200000	-0.41330000
H	1.11560000	6.07990000	1.06860000
H	0.85220000	6.54820000	-0.61890000
H	-0.47540000	6.65140000	0.54980000
H	-1.15820000	3.59270000	-1.67900000
H	-1.93860000	5.06200000	-1.06340000
H	-0.54060000	5.17130000	-2.13320000
H	6.19690000	-0.90040000	-2.03860000
H	5.63200000	-0.14930000	-4.31640000
H	3.72280000	1.36900000	-4.67800000
H	6.48750000	0.16820000	1.85830000
H	6.00130000	1.58990000	0.92640000
H	7.09160000	0.39460000	0.20900000
H	1.44120000	2.51300000	-1.96590000
H	1.83590000	4.64360000	-3.22410000
H	3.20860000	4.25250000	-2.17250000
H	3.31520000	3.95990000	-3.91490000
H	0.32500000	2.78110000	-4.10660000
H	0.80520000	1.08480000	-3.91960000
H	1.71350000	2.16100000	-4.99460000
H	4.16090000	-0.08710000	0.97510000
C	1.28160000	-2.44240000	0.45070000
C	1.93860000	-3.03790000	1.57020000
C	1.44930000	-3.08620000	-0.81060000
C	2.66540000	-4.23330000	1.43300000
C	2.16200000	-4.29340000	-0.91310000
C	2.76620000	-4.87420000	0.20020000
H	3.16410000	-4.66550000	2.29670000
H	2.26270000	-4.77800000	-1.88100000
H	3.33150000	-5.79740000	0.10230000
C	1.84960000	-2.43990000	2.97940000
H	1.33980000	-1.47670000	2.87220000
C	0.88200000	-2.50030000	-2.10270000
H	0.36130000	-1.58100000	-1.83540000
C	2.00680000	-2.14870000	-3.09080000
H	1.59340000	-1.65300000	-3.97680000
H	2.73590000	-1.47630000	-2.63620000
H	2.54060000	-3.04210000	-3.43740000
C	-0.14390000	-3.43700000	-2.76810000
H	-0.55530000	-2.96840000	-3.66960000
H	0.31430000	-4.38440000	-3.08100000
H	-0.97650000	-3.65520000	-2.09360000
C	3.22230000	-2.19400000	3.62420000
H	3.78280000	-3.12020000	3.79740000
H	3.84120000	-1.54400000	2.99920000
H	3.09950000	-1.70440000	4.59750000
C	0.95520000	-3.29450000	3.89510000
H	0.93410000	-2.89120000	4.91410000

H	-0.07980000	-3.28480000	3.52900000
H	1.30770000	-4.33240000	3.96220000
K	-0.35620000	-4.90530000	0.98410000
K	-1.97860000	1.40750000	-0.10350000
C	5.31090000	-1.78290000	0.35470000
H	5.47520000	-2.10460000	1.38750000
H	4.48170000	-2.36440000	-0.05340000
H	6.21760000	-2.03380000	-0.20640000

:Ge(IPr=N)$_2$ 12 (singlet)

Charge=0 multiplicity=1

Ge	0.00000000	0.00000000	-0.96509500
N	-0.97606900	1.00448900	0.22137100
N	-2.73899100	2.57007300	0.62145300
N	-0.94673200	3.36216100	-0.38551900
N	0.97606900	-1.00448900	0.22137100
N	0.94673200	-3.36216100	-0.38551900
N	2.73899100	-2.57007300	0.62145300
C	-1.48842800	2.17298400	0.13189100
C	-2.92930500	3.93797900	0.42573400
C	-1.83202000	4.42400900	-0.18674700
C	1.48842800	-2.17298400	0.13189100
C	1.83202000	-4.42400900	-0.18674700
C	2.92930500	-3.93797900	0.42573400
C	-3.70404200	1.68058600	1.19282800
C	-4.61436800	1.02659300	0.34323300
C	-5.56006300	0.17793800	0.92655500
C	-5.59610400	-0.01671900	2.30136500
C	-4.68570900	0.63943300	3.12254900
C	-3.72444800	1.50194700	2.58960100
C	-4.60814000	1.22844500	-1.16653000
C	-5.89136800	1.93692800	-1.63871000
C	-4.39100300	-0.09408500	-1.92195700
C	-2.71289800	2.19028500	3.49757900
C	-3.34095200	2.74621800	4.78595000
C	-1.53968500	1.24088900	3.81141700
C	0.32649300	3.47395500	-1.02929200
C	0.37889700	3.52093000	-2.43707300
C	1.63063000	3.66723900	-3.04042100
C	2.78928300	3.75197600	-2.27807700
C	2.71595900	3.69205800	-0.89168200
C	1.48843500	3.55606900	-0.23738100
C	-0.87318100	3.43907800	-3.30235900
C	-1.18655100	4.80076500	-3.95091200
C	-0.77653200	2.33012500	-4.36466700
C	1.44199100	3.52911300	1.28441100
C	1.82762700	4.90166100	1.86797900
C	2.31503600	2.40502000	1.86765200

C	-0.32649300	-3.47395500	-1.02929200
C	-0.37889700	-3.52093000	-2.43707300
C	-1.63063000	-3.66723900	-3.04042100
C	-2.78928300	-3.75197600	-2.27807700
C	-2.71595900	-3.69205800	-0.89168200
C	-1.48843500	-3.55606900	-0.23738100
C	0.87318100	-3.43907800	-3.30235900
C	1.18655100	-4.80076500	-3.95091200
C	0.77653200	-2.33012500	-4.36466700
C	-1.44199100	-3.52911300	1.28441100
C	-1.82762700	-4.90166100	1.86797900
C	-2.31503600	-2.40502000	1.86765200
C	3.70404200	-1.68058600	1.19282800
C	4.61436800	-1.02659300	0.34323300
C	5.56006300	-0.17793800	0.92655500
C	5.59610400	0.01671900	2.30136500
C	4.68570900	-0.63943300	3.12254900
C	3.72444800	-1.50194700	2.58960100
C	4.60814000	-1.22844500	-1.16653000
C	5.89136800	-1.93692800	-1.63871000
C	4.39100300	0.09408500	-1.92195700
C	2.71289800	-2.19028500	3.49757900
C	3.34095200	-2.74621800	4.78595000
C	1.53968500	-1.24088900	3.81141700
H	-3.83056200	4.43015300	0.74894400
H	-1.58333200	5.42556400	-0.49285900
H	1.58333200	-5.42556400	-0.49285900
H	3.83056200	-4.43015300	0.74894400
H	-6.27748900	-0.33471100	0.29386600
H	-6.33761800	-0.67974900	2.73647800
H	-4.72329300	0.47844400	4.19425900
H	-3.76687700	1.88078000	-1.41220100
H	-5.85397600	2.11761100	-2.71833800
H	-6.78160500	1.33264600	-1.43309700
H	-6.02138300	2.90123100	-1.13740900
H	-3.45921000	-0.57589300	-1.61571600
H	-4.34096400	0.09056900	-3.00047000
H	-5.21086800	-0.79913700	-1.74578000
H	-2.30321400	3.04251600	2.94770100
H	-2.59901200	3.33124300	5.33922800
H	-4.19496200	3.39651500	4.57124700
H	-3.68480000	1.94990000	5.45436900
H	-1.06218300	0.89711100	2.89011600
H	-0.79027900	1.75011500	4.42785300
H	-1.88958700	0.36238100	4.36549800
H	1.69817200	3.71160300	-4.12234500
H	3.75264100	3.86243400	-2.76612100
H	3.62556700	3.75754600	-0.30406900
H	-1.71204800	3.18632900	-2.64898000
H	-2.10689500	4.74208800	-4.54177600
H	-0.37847600	5.11597300	-4.62004400

H	-1.31753700	5.58374000	-3.19742900
H	-0.57543100	1.36117700	-3.89916200
H	-1.71874800	2.25859300	-4.91880000
H	0.01656100	2.53041200	-5.09289700
H	0.41218000	3.32442800	1.58383000
H	1.75066600	4.88694700	2.96044400
H	2.85798600	5.17027700	1.61020600
H	1.17298800	5.69475100	1.49229000
H	2.02330200	1.43042500	1.46819700
H	2.20528500	2.37477600	2.95704900
H	3.37762100	2.55831200	1.65081200
H	-1.69817200	-3.71160300	-4.12234500
H	-3.75264100	-3.86243400	-2.76612100
H	-3.62556700	-3.75754600	-0.30406900
H	1.71204800	-3.18632900	-2.64898000
H	2.10689500	-4.74208800	-4.54177600
H	0.37847600	-5.11597300	-4.62004400
H	1.31753700	-5.58374000	-3.19742900
H	1.71874800	-2.25859300	-4.91880000
H	-0.01656100	-2.53041200	-5.09289700
H	0.57543100	-1.36117700	-3.89916200
H	-0.41218000	-3.32442800	1.58383000
H	-1.17298800	-5.69475100	1.49229000
H	-1.75066600	-4.88694700	2.96044400
H	-2.85798600	-5.17027700	1.61020600
H	-2.02330200	-1.43042500	1.46819700
H	-3.37762100	-2.55831200	1.65081200
H	-2.20528500	-2.37477600	2.95704900
H	6.27748900	0.33471100	0.29386600
H	6.33761800	0.67974900	2.73647800
H	4.72329300	-0.47844400	4.19425900
H	5.85397600	-2.11761100	-2.71833800
H	6.02138300	-2.90123100	-1.13740900
H	6.78160500	-1.33264600	-1.43309700
H	4.34096400	-0.09056900	-3.00047000
H	5.21086800	0.79913700	-1.74578000
H	3.45921000	0.57589300	-1.61571600
H	2.30321400	-3.04251600	2.94770100
H	2.59901200	-3.33124300	5.33922800
H	4.19496200	-3.39651500	4.57124700
H	3.68480000	-1.94990000	5.45436900
H	0.79027900	-1.75011500	4.42785300
H	1.06218300	-0.89711100	2.89011600
H	1.88958700	-0.36238100	4.36549800
H	3.76687700	-1.88078000	-1.41220100

:Ge(IPr=N)$_2$ 12 (singlet)

Charge=0 multiplicity=3

Ge	-0.00034600	-0.84728800	0.00068500

N	-1.44998100	0.28686300	0.01003500
N	-3.65131700	1.12972500	-0.12295900
N	-3.43230000	-1.01126800	-0.63325700
N	1.45017000	0.28576200	-0.00932800
N	3.43130600	-1.01465000	0.63296500
N	3.65259400	1.12605900	0.12242900
C	-2.69590200	0.11230900	-0.22847100
C	-4.91160800	0.64082000	-0.46385400
C	-4.78192400	-0.66305000	-0.77631700
C	2.69603000	0.10978700	0.22851400
C	4.78141800	-0.66802800	0.77529000
C	4.91248700	0.63566900	0.46267800
C	-3.35789400	2.45408800	0.33706100
C	-3.56342700	2.76043400	1.69655000
C	-3.27945100	4.05985700	2.12368700
C	-2.79841700	5.01676600	1.23716500
C	-2.58984700	4.68820000	-0.09596200
C	-2.86395700	3.40373500	-0.57507400
C	-4.01546400	1.70342100	2.69696100
C	-5.08636100	2.21436800	3.67443500
C	-2.79748100	1.13323700	3.45194200
C	-2.59324300	3.06644300	-2.03464400
C	-3.31095700	4.02998100	-2.99599100
C	-1.07800500	3.01692900	-2.31016700
C	-2.88965700	-2.30102300	-0.92983700
C	-2.67926300	-3.21225600	0.12695000
C	-2.16884700	-4.47263200	-0.19339300
C	-1.89044900	-4.82126300	-1.51007300
C	-2.10907200	-3.90981400	-2.53579600
C	-2.60342400	-2.63019900	-2.26852000
C	-3.04432900	-2.86081400	1.56465000
C	-4.49214900	-3.29251900	1.87347700
C	-2.07011500	-3.44281100	2.59994200
C	-2.79807200	-1.64077100	-3.41026600
C	-3.81560700	-2.15714300	-4.44333800
C	-1.45531100	-1.28444400	-4.07408700
C	2.88726600	-2.30374200	0.92987300
C	2.67521400	-3.21475400	-0.12678200
C	2.16341700	-4.47449400	0.19386100
C	1.88527800	-4.82274100	1.51069900
C	2.10550400	-3.91151700	2.53627500
C	2.60123700	-2.63250100	2.26869800
C	3.03988100	-2.86372400	-1.56469000
C	4.48731400	-3.29632400	-1.87410600
C	2.06490300	-3.44533600	-2.59947900
C	2.79741000	-1.64320000	3.41028500
C	3.81530900	-2.16028900	4.44264100
C	1.45534900	-1.28595200	4.07503000
C	3.36047600	2.45075800	-0.33746100
C	3.56529900	2.75676000	-1.69714000
C	3.28250100	4.05647900	-2.12415100

C	2.80332500	5.01403300	-1.23731200
C	2.59551700	4.68584500	0.09602400
C	2.86849000	3.40108900	0.57501500
C	4.01545100	1.69915000	-2.69777600
C	5.08560300	2.20904800	-3.67661000
C	2.79624300	1.12959100	-3.45125700
C	2.59865200	3.06426600	2.03485700
C	3.31815200	4.02719100	2.99548000
C	1.08359200	3.01635200	2.31163600
H	-5.77933500	1.27797900	-0.45375800
H	-5.51260300	-1.38668900	-1.09397500
H	5.51140900	-1.39251400	1.09259700
H	5.78096900	1.27179100	0.45206800
H	-3.42727000	4.32446200	3.16496400
H	-2.58252300	6.02100300	1.58892000
H	-2.20317500	5.43831100	-0.77781300
H	-4.46442500	0.88034400	2.13435100
H	-5.45077000	1.38874700	4.29457500
H	-4.69453100	2.97826300	4.35404000
H	-5.94215700	2.64436600	3.14449900
H	-2.06026600	0.72445900	2.75507200
H	-3.10913400	0.33829700	4.13901600
H	-2.30604500	1.91472200	4.04240600
H	-2.99205900	2.06628300	-2.22342100
H	-3.15477000	3.71388800	-4.03285800
H	-4.38907300	4.05614500	-2.80741100
H	-2.93190200	5.05353000	-2.90669300
H	-0.58938300	2.28669200	-1.66054600
H	-0.89145900	2.73563500	-3.35273600
H	-0.61067000	3.99302000	-2.13878700
H	-1.98998900	-5.19257200	0.59670900
H	-1.49955600	-5.80837900	-1.73698500
H	-1.88050500	-4.18973000	-3.55896500
H	-2.99533100	-1.77305400	1.65994800
H	-4.76199100	-3.02349600	2.90050200
H	-4.60681800	-4.37714700	1.76745300
H	-5.20745800	-2.81097900	1.20043300
H	-1.03667900	-3.17762600	2.36028200
H	-2.30556300	-3.04321100	3.59187600
H	-2.14206700	-4.53396900	2.66833100
H	-3.20440000	-0.71862100	-2.98822100
H	-3.97466300	-1.40943300	-5.22752500
H	-3.46816100	-3.07577300	-4.92803600
H	-4.78318500	-2.37236700	-3.97869600
H	-0.74770400	-0.90129800	-3.33238300
H	-1.60271000	-0.51900000	-4.84373000
H	-1.00160500	-2.15750200	-4.55585200
H	1.98320100	-5.19421000	-0.59613200
H	1.49328700	-5.80936700	1.73784600
H	1.87707400	-4.19109500	3.55956700
H	2.99146500	-1.77593800	-1.66012400

H	4.75684900	-3.02759600	-2.90128900
H	4.60137600	-4.38100800	-1.76799700
H	5.20322400	-2.81512800	-1.20146100
H	2.29999600	-3.04582200	-3.59153000
H	2.13644300	-4.53652000	-2.66791400
H	1.03167800	-3.17978600	-2.35929500
H	3.20408400	-0.72133900	2.98794100
H	4.78245400	-2.37604600	3.97734200
H	3.97534100	-1.41275700	5.22680100
H	3.46762700	-3.07876600	4.92746100
H	0.74744000	-0.90250200	3.33376800
H	1.00146400	-2.15866100	4.55725900
H	1.60376200	-0.52047800	4.84444800
H	3.42980700	4.32084100	-3.16555900
H	2.58832700	6.01849300	-1.58897800
H	2.21033600	5.43648100	0.77814100
H	5.44884100	1.38294100	-4.29678900
H	5.94223100	2.63876000	-3.14778800
H	4.69349100	2.97287400	-4.35612800
H	3.10661300	0.33431400	-4.13852200
H	2.30465200	1.91127700	-4.04132700
H	2.05953300	0.72143700	-2.75348800
H	2.99659500	2.06371600	2.22343300
H	3.16255600	3.71135700	4.03251500
H	4.39612700	4.05227600	2.80595900
H	2.94002700	5.05110400	2.90641600
H	0.89759700	2.73551800	3.35442600
H	0.59374100	2.28643800	1.66258500
H	0.61710300	3.99286600	2.14035300
H	4.46447400	0.87592100	-2.13543100

Compound 13

Charge=0 multiplicity=2

Ge	0.00482800	0.28294300	-0.97220000
N	1.35055700	0.16942500	0.27418500
N	2.80090600	2.11172200	0.53784700
N	3.65448300	0.11162800	0.91294200
N	-1.42383600	-0.23077900	0.07637200
N	-3.71059600	-0.77525100	0.50153700
N	-2.69675500	-1.99488200	-1.03418200
C	2.46228700	0.74118500	0.51536000
C	4.12436100	2.27778400	0.95817000
C	4.64332700	1.05684800	1.18387000
C	-2.47575600	-0.91617700	-0.15410100
C	-4.60727800	-1.75366100	0.07027800
C	-3.98920300	-2.49998000	-0.86382400
C	1.97574000	3.18855900	0.09237700
C	2.25951500	3.79268800	-1.15105300

C	1.49420600	4.90046800	-1.53175600
C	0.47546200	5.38506800	-0.71514600
C	0.20345300	4.76374800	0.50023300
C	0.94522000	3.65929700	0.93168000
C	3.35761100	3.28320000	-2.07936000
C	4.43528000	4.35468000	-2.32617700
C	2.77962900	2.76157600	-3.40802700
C	0.67750200	3.04439800	2.29927600
C	1.27316000	3.93592600	3.40670400
C	-0.81330000	2.76463900	2.54562100
C	3.86127200	-1.30324000	0.95726500
C	4.13652900	-1.99186400	-0.24002600
C	4.39513500	-3.36265500	-0.16074700
C	4.38603800	-4.02679000	1.06050900
C	4.10904300	-3.32843500	2.22908200
C	3.83613600	-1.95751300	2.20281000
C	4.21312700	-1.28220700	-1.58606200
C	5.67622600	-1.16404400	-2.05465200
C	3.33868900	-1.95333700	-2.65754500
C	3.54343300	-1.21854400	3.50231900
C	4.79132200	-1.15638400	4.40285800
C	2.34911000	-1.83129300	4.25320000
C	-3.98625500	0.15869200	1.55216700
C	-4.60750600	1.38189800	1.23470300
C	-4.91990900	2.25118000	2.28360100
C	-4.61191600	1.92707000	3.59941200
C	-3.98887200	0.72011400	3.89007200
C	-3.67062200	-0.19094900	2.87868900
C	-4.96245600	1.75200600	-0.19940100
C	-6.43999100	1.43829800	-0.50530500
C	-4.64623100	3.21980500	-0.52956000
C	-2.98554100	-1.50438400	3.22977400
C	-3.70188000	-2.25590200	4.36521900
C	-1.49913400	-1.27133900	3.55973300
C	-1.70494700	-2.63784700	-1.84332700
C	-1.63915800	-2.33330600	-3.21782300
C	-0.72371400	-3.03880400	-4.00271900
C	0.10845800	-4.00145200	-3.44380100
C	0.04165000	-4.27317400	-2.08308300
C	-0.86559300	-3.60519100	-1.25594400
C	-2.54582500	-1.28933000	-3.85592400
C	-3.72055200	-1.95139400	-4.60084000
C	-1.77662200	-0.33721500	-4.78724300
C	-0.93139800	-3.95465500	0.22442500
C	-1.44069900	-5.39344200	0.43096300
C	0.41996700	-3.73011500	0.92409000
H	4.55805000	3.25707400	1.06717300
H	5.62277300	0.76202500	1.51938900
H	-5.60045400	-1.82188100	0.47959600
H	-4.33606000	-3.34874700	-1.42761400
H	1.69818700	5.39328000	-2.47737200

H	-0.10147900	6.25126900	-1.02510800
H	-0.58833800	5.15227500	1.13121900
H	3.84753200	2.43940500	-1.58925800
H	5.24088000	3.94719800	-2.94570200
H	4.02644600	5.22723100	-2.84659400
H	4.87410400	4.70361700	-1.38620100
H	2.06608600	1.94926800	-3.23423100
H	3.58181500	2.37365100	-4.04528600
H	2.26997600	3.55382700	-3.96853700
H	1.18821100	2.08063700	2.33542900
H	1.12121600	3.47585500	4.38876100
H	2.34829800	4.08627700	3.26555400
H	0.79633900	4.92243600	3.42092600
H	-1.21793400	2.08431100	1.79155100
H	-0.94316000	2.29005300	3.52331500
H	-1.41321000	3.68117100	2.55191500
H	4.61834500	-3.91523800	-1.06743200
H	4.59740800	-5.09090000	1.10131500
H	4.10360300	-3.85443700	3.17819500
H	3.82871900	-0.26892300	-1.45249200
H	5.73321200	-0.61979100	-3.00359800
H	6.12462100	-2.15180200	-2.20796300
H	6.28801800	-0.63090900	-1.32015700
H	2.29581600	-2.01329000	-2.33710400
H	3.37625400	-1.37501800	-3.58705100
H	3.68235500	-2.96704600	-2.89063000
H	3.27068700	-0.19174900	3.24697700
H	4.57810200	-0.58976400	5.31553000
H	5.11840300	-2.15854400	4.70063600
H	5.63027700	-0.67258400	3.89269200
H	1.45881400	-1.84779500	3.61996100
H	2.12204700	-1.24221700	5.14819200
H	2.55514000	-2.85683900	4.57811600
H	-5.40839600	3.19500700	2.06792300
H	-4.85896300	2.61741800	4.40003900
H	-3.74923600	0.47731700	4.91985800
H	-4.34967100	1.13014900	-0.85904100
H	-6.68073900	1.69522100	-1.54257800
H	-7.10476100	2.01382700	0.14832700
H	-6.66296500	0.37742000	-0.36053600
H	-4.76502400	3.40034000	-1.60381200
H	-5.31602400	3.91523900	-0.01184300
H	-3.61949900	3.47983100	-0.25075500
H	-3.02712300	-2.14739000	2.34690000
H	-4.76063300	-2.41389500	4.13667000
H	-3.23722400	-3.23572100	4.51725100
H	-3.64189500	-1.71777000	5.31698200
H	-0.98255300	-0.81539700	2.71086000
H	-1.38928500	-0.61490900	4.43067100
H	-1.01051800	-2.22282200	3.79695600
H	-0.66027000	-2.83105100	-5.06524100

H	0.81363700	-4.53818300	-4.07074900
H	0.69873200	-5.02202100	-1.65352600
H	-4.37401600	-1.19058800	-5.04117800
H	-4.32537300	-2.56744200	-3.92890400
H	-3.35866900	-2.59461600	-5.41056400
H	-2.42691400	0.48450500	-5.10774100
H	-1.42400500	-0.84097000	-5.69373800
H	-0.90455500	0.08585500	-4.27816400
H	-1.65261400	-3.28386200	0.69524200
H	-1.52422000	-5.61856700	1.49957900
H	-2.42588500	-5.53781900	-0.02394400
H	-0.75824700	-6.12744100	-0.01113100
H	0.32571000	-3.93888200	1.99529800
H	0.76041600	-2.69812400	0.80428600
H	1.19842800	-4.39157700	0.53009000
H	-2.96740300	-0.68427500	-3.04764000
K	-1.22001900	3.15176700	-2.72402900

Compound 14

Charge=0 multiplicity=1

Ge	0.11358800	-1.15664300	-0.05295000
N	1.34510000	0.23597200	0.33331400
N	3.73558500	-0.35981400	0.02361800
N	3.19835400	1.45583700	1.19906300
N	-1.35110500	-0.01278500	-0.45478200
N	-3.46612400	0.75416600	-1.24274600
N	-3.54479300	-1.05246900	0.05887300
C	2.58424800	0.39232000	0.47115700
C	4.91667200	0.29297400	0.41321200
C	4.58568600	1.38089100	1.13051000
C	-2.60402900	-0.11614800	-0.51169300
C	-4.80159200	0.40093400	-1.07271600
C	-4.85621100	-0.68355000	-0.28048000
C	3.76079600	-1.35360400	-0.99806900
C	3.69545300	-2.71759000	-0.63361400
C	3.84025300	-3.68319400	-1.63386700
C	4.03028400	-3.31747900	-2.96593600
C	4.10092500	-1.96898400	-3.30986400
C	3.97565400	-0.96589900	-2.34122300
C	3.54514700	-3.13046500	0.82423100
C	4.92802900	-3.36948000	1.46119900
C	2.63337900	-4.35017600	1.01796200
C	4.02843600	0.49905000	-2.76012200
C	5.22934000	0.81498100	-3.66754600
C	2.70218700	0.92106500	-3.42023200
C	2.48095800	2.50519900	1.84826300
C	2.24158400	2.41757600	3.23395200
C	1.59216800	3.48303200	3.86323000

C	1.17220300	4.59299600	3.13970700
C	1.40040200	4.65432600	1.77078900
C	2.06012300	3.62046600	1.09980600
C	2.68870200	1.20978500	4.04662800
C	3.95275200	1.52289200	4.86929300
C	1.57164200	0.67054800	4.95651400
C	2.29853900	3.72440700	-0.39969500
C	3.08432500	4.99517100	-0.76936200
C	0.97419200	3.63073000	-1.17749900
C	-3.03324200	1.89850700	-1.97986900
C	-2.57186800	1.72948700	-3.29969600
C	-2.21297700	2.86863000	-4.02436800
C	-2.30496400	4.13522300	-3.45871400
C	-2.75414200	4.28275400	-2.15255400
C	-3.12338900	3.17283300	-1.38649800
C	-2.51284900	0.34772300	-3.93786800
C	-3.83280800	0.02086000	-4.66329700
C	-1.31966300	0.17214500	-4.88981300
C	-3.56165200	3.34465000	0.06302000
C	-4.43811600	4.58609000	0.29357100
C	-2.33255200	3.35224200	0.99327900
C	-3.31032100	-1.96136000	1.13192700
C	-3.00743600	-3.31088100	0.83893700
C	-2.92832800	-4.22053400	1.89665500
C	-3.12517400	-3.81198000	3.21620300
C	-3.42471900	-2.47910000	3.48951800
C	-3.52563600	-1.53309100	2.46194800
C	-2.83794300	-3.77863300	-0.60017200
C	-4.17199800	-4.31576800	-1.15406400
C	-1.71640500	-4.81288100	-0.77141100
C	-3.84468900	-0.08319600	2.80785600
C	-5.22684100	0.05142000	3.47164900
C	-2.74147000	0.54204700	3.68086700
H	5.88422600	-0.10052800	0.14962500
H	5.21254100	2.11287300	1.61167200
H	-5.59241300	0.94822100	-1.55808900
H	-5.70249400	-1.25491200	0.06253300
H	3.80738300	-4.73521500	-1.37299000
H	4.15001800	-4.08080400	-3.72875800
H	4.26667000	-1.69387800	-4.34632000
H	3.08068300	-2.28874900	1.34587900
H	4.82187600	-3.63895100	2.51787200
H	5.45699300	-4.18613700	0.95685500
H	5.55298600	-2.47402900	1.40279800
H	1.65340500	-4.17968600	0.56117400
H	2.48453200	-4.53509700	2.08871900
H	3.06130500	-5.26603100	0.59597300
H	4.14604500	1.09914500	-1.85567900
H	5.27906400	1.89169500	-3.85930700
H	6.17186800	0.50982900	-3.20256900
H	5.15717000	0.31579200	-4.63979800

H	1.85988800	0.76999400	-2.73703800
H	2.72668600	1.98188200	-3.69096900
H	2.52014900	0.35200900	-4.34129400
H	1.41126800	3.44390200	4.93254100
H	0.66627300	5.41057700	3.64408100
H	1.06573900	5.52210100	1.21148700
H	2.94395700	0.41744600	3.33762900
H	4.27601400	0.64163500	5.43469900
H	3.76638800	2.33221200	5.58401400
H	4.78022000	1.83140300	4.22390500
H	0.64670300	0.50961300	4.39207300
H	1.87547000	-0.28027600	5.41065600
H	1.33709800	1.35831100	5.77614700
H	2.90946600	2.86840000	-0.69434800
H	3.29960900	5.00844000	-1.84340700
H	2.51982600	5.90505400	-0.53876700
H	4.03649800	5.04888400	-0.23151600
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H	1.16172700	3.66754000	-2.25647700
H	0.30875000	4.46587000	-0.93378100
H	-1.86326100	2.76801400	-5.04581600
H	-2.02524000	5.00960400	-4.03841600
H	-2.81677900	5.27550100	-1.72086100
H	-2.38782800	-0.37525000	-3.12749100
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H	-4.02176200	0.73702500	-5.47100400
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H	-1.41983100	0.77124000	-5.80163800
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H	-4.82359100	4.58427400	1.31859000
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H	-2.64610900	3.41002400	2.04205600
H	-2.71115900	-5.26305500	1.69203000
H	-3.07176900	-4.53520400	4.02421600
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H	-4.05501200	-4.62781900	-2.19767500
H	-4.95504800	-3.55339800	-1.11640500
H	-4.51504900	-5.18369600	-0.57937600
H	-1.57344600	-5.02936400	-1.83666300
H	-1.94450300	-5.76573300	-0.28127900
H	-0.77232400	-4.42988800	-0.37157100
H	-3.87260300	0.48318200	1.87579200
H	-5.45415400	1.10485300	3.66574400
H	-6.01481300	-0.35170900	2.82850600
H	-5.27073500	-0.47908900	4.42918400
H	-2.98122400	1.58522900	3.91061100

H	-1.78010200	0.53778700	3.15598300
H	-2.62632100	0.01388100	4.63504100
H	-2.56176900	-2.90019000	-1.19007000
K	0.86361200	-2.42281300	-3.02038300
K	-0.21139600	-2.29781800	3.02310000

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