Two-Coordinate Hydrido-Germylenes

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SUPPLEMENTARY INFORMATION

(23 pages)

Contents

1. Syntheses

General considerations. All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Diethyl ether was distilled over Na/K alloy (25:75), while THF, hexane and toluene were distilled over molten potassium. ^{1}H, ^{13}C{^{1}H} and ^{29}Si{^{1}H} NMR spectra were recorded on either Bruker AvanceIII or Bruker DPX300 spectrometers and were referenced to the resonances of the solvent used, or external $SiMe_4$. IR spectra were recorded for solid samples, or as Nujol mulls, using an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. Mass spectra were recorded on an Agilent Technologies 5975D inert MSD with a solid state probe. Melting points were determined in sealed glass capillaries under dinitrogen, and are uncorrected. Microanalyses were carried out at the Science Centre, London Metropolitan University. Ar†NH$_2$,[1] Ar*NH$_2$[2] and (Bu^{t}O)$_3$SiCl[3] were synthesised *via* previously reported procedures. All other reagents were used as received.

Synthesis of ^{tBuO}L*H. To a solution of Ar*NH$_2$ (10.0 g, 22.8 mmol) in THF (100 cm^3) at -80 ºC was added Bu^{n}Li (14.93 cm^3 of a 1.6 M solution, 23.9 mmol). The reaction mixture was warmed to ambient temperature and stirred for 2 h, yielding a pink/red suspension. Subsequently, (Bu^{t}O)$_3$SiCl (6.76 g, 23.94 mmol) was added at ambient temperature, and the mixture then heated at 55 ºC, with stirring, for 3 days, resulting in a colourless solution. All volatiles were removed *in vacuo*, and the residue extracted into boiling hexane, and filtered. Removal of volatiles from the filtrate *in vacuo* and washing of the residue with *ca.* 15 cm^3 of cold hexane yielded ^{tBuO}L*H as an off-white powder (13.4 g, 86 %). X-ray quality crystals were grown by slow evaporation of a diethyl ether solution of the compound. M.p.: 182-190 ºC; ^{1}H NMR (C_6D_6, 400 MHz, 298 K), δ = 1.33 (s, 27H, OC(C*H*$_3$)$_3$),

1.85 (s, 3H, *p*-CH_3), 2.20 (s, 1H, N*H*), 6.73 (s, 2H, Ph_2C*H*), 6.88 (s, 2H, *m*-Ar*H*), 7.00-7.32 (m, 20H, Ar-*H*); ^{13}C{^{1}H}NMR (C_6D_6, 75.5 MHz, 298 K), δ = 21.3 (*p*-*C*H_3), 32.0 (OC(*C*H_3)$_3$), 51.9 (Ph_2*C*H), 73.6 (O*C*(CH$_3$)$_3$), 126.4, 126.9, 128.4, 128.8, 129.6, 130.0, 130.5, 133.4, 139.5, 142.3, 143.5, 145.2 (Ar-*C*); ^{29}Si{^{1}H} NMR (C_6D_6, 80 MHz, 298 K), δ = -89.0; IR, ν/cm^{-1} (ATR): 3379 (w, NH str.), 1880 (w), 1750 (w), 1366 (m), 1183 (s), 1045 (s), 900 (m), 670 (s); MS/EI *m/z* (%): 687 (M^+, 35); acc. mass calcd for $C_{45}H_{56}NO_3Si$: 686.4029, found: 686.4019.

Synthesis of ^{tBuO}L†H. This compound was prepared following a method similar to that for ^{tBuO}L*H, using Ar†NH_2 (5.0g, 10.70 mmol), Bu^{n}Li (7.03 cm^3 of a 1.6 M solution, 11.24 mmol), and (Bu^{t}O)$_3$SiCl (3.17 g, 11.24 mmol) (4.5 g, 59 %). M.p.: 165-170 ºC; ^{1}H NMR (C_6D_6, 400 MHz, 298K), δ = 0.92 (d, $^3J_{HH}$ = 7.2 Hz, 6H, CH(CH_3)$_2$), 1.32 (s, 27H, OC(CH_3)$_3$), 2.24 (s, 1H, N*H*), 2.48 (sept, $^3J_{HH}$ = 7.2 Hz, 1H, C*H*(CH$_3$)$_2$), 6.74 (s, 2H, Ph_2C*H*), 6.92 (s, 2H, *m*-Ar*H*), 7.03-7.32 (m, 20H, Ar-*H*); ^{13}C {^{1}H}NMR (C_6D_6, 75.5 MHz, 298 K), δ = 24.1 (CH(*C*H_3)$_2$), 32.0 (OC(*C*H_3)$_3$), 33.9 (*C*H(CH$_3$)$_2$), 52.1 (Ph_2*C*H), 73.6 (O*C*(CH$_3$)$_3$), 126.4, 126.8, 127.8, 128.2, 128.4, 128.8, 130.1, 130.5, 139.8, 142.1, 144.3, 145.3 (Ar-*C*); ^{29}Si{^{1}H} NMR (C_6D_6, 80 MHz, 298 K), δ = -92.3; IR, ν/cm^{-1} (ATR): 3378 (w, NH str.), 3058 (w), 3025 (w), 1803 (w), 1752 (w), 1598 (m), 1491 (m), 1446 (m), 1363 (s), 1182 (s), 1046 (s), 902 (m), 761 (m), 673 (s); MS/EI *m/z* (%): 715 (M^+, 45); acc. mass calcd for $C_{47}H_{60}NO_3Si$: 714.4342, found: 714.4332.

Synthesis of ^{tBuO}L*K. To a mixture of ^{tBuO}L*H (5.0 g, 7.29 mmol) and KH (350 mg, 8.75 mmol) was added THF (50 cm^3) and a catalytic amount of hexamethyldisilazane (80 μL, ~5 mol%). The reaction mixture was then stirred overnight at ambient temperature under a flow of N_2. The resultant suspension was subsequently filtered, volatiles removed *in vacuo*, and the residue washed with 2 x 10 cm^3 hexane. The residue was then dried under vacuum for 1 h, affording a free-flowing off-white powder which was used without further purification (4.4 g, 76 %). ^{1}H NMR (C_6D_6, 400 MHz, 298 K), δ = 1.47 (s, 27H, OC(CH_3)$_3$), 2.20 (s, 3H, *p*-Ar-CH_3), 6.64 (br s, 2H, Ph_2C*H*), 6.77 (br s, 2H, *m*-Ar*H*), 6.85-7.41 (m, 20H, Ar-*H*); ^{13}C{^{1}H}NMR (C_6D_6, 75.5 MHz, 298 K), δ = 21.2 (*p*-Ar-*C*H_3), 32.2 (OC(*C*H_3)$_3$), 51.9 (Ph_2*C*H), 70.8 (O*C*(CH$_3$)$_3$), 118.2, 125.2, 127.6, 128.5, 128.8, 129.3, 129.8, 130.3, 130.8, 136.8, 148.8, 152.6 (Ar-*C*); ^{29}Si{^{1}H} NMR (C_6D_6, 80 MHz, 298 K), δ = -96.6; IR, *v*/cm^{-1} (ATR): 3059 (w), 1598 (m), 1372 (s), 1233 (m), 1190 (s), 1048 (s), 1013 (s), 986 (s), 810 (m), 767 (m), 705 (s), 687 (s).

N.B. Although not used in this study, the closely related compound, ^{tBuO}L*Li(THF), can be prepared by deprotonation of ^{tBuO}L*H with Bu^{n}Li in THF. Details of the crystallographic characterisation of ^{tBuO}L*Li(THF) are included below.

Synthesis of $^{tBuO}L^{\dagger}K$. This compound was prepared following a method similar to that for $^{tBuO}L^{*}K$, but using $^{tBuO}L^{\dagger}H$ (4.0 g, 5.61 mmol), KH (292 mg, 7.30 mmol), and hexamethyldisilazane (~60 µL, 5 mol%). The product was isolated as a free flowing off-white powder which was used without further purification (3.8 g, 90 %). ^{1}H NMR (C_6D_6, 400 MHz, 298K), δ = 1.11 (d, $^{3}J_{HH}$ = 7.2 Hz, 6H, CH(CH_3)$_2$), 1.47 (s, 27H, OC(CH_3)$_3$), 2.67 (sept, $^{3}J_{HH}$ = 7.2 Hz, 1H, CH(CH$_3$)$_2$), 6.65 (br s, 2H, Ph$_2$CH), 6.86 (br s, 2H, *m*-ArH), 6.90-7.42 (m, 20H, Ar-H); ^{13}C{^{1}H}NMR (C_6D_6, 75.5 MHz, 298 K), δ = 24.9 (CH(*C*H$_3$)$_2$), 32.5 (OC(*C*H$_3$)$_3$), 33.7 (*C*H(CH$_3$)$_2$), 52.4 (Ph$_2$*C*H), 71.0 (O*C*(CH$_3$)$_3$), 125.0, 125.7, 126.1, 127.3, 130.86, 131.1, 136.9, 142.1, 145.3, 147.2, 151.4, 152.9 (Ar-*C*); ^{29}Si{^{1}H} NMR (C_6D_6, 80 MHz, 298 K), δ = -95.4; IR, ν/cm^{-1} (ATR): 3055 (w), 1593 (m), 1377 (s), 1361 (s), 1234 (m), 1192 (s), 1046 (s), 1031 (s), 811 (m), 767 (m), 696 (s).

Synthesis of $^{tBuO}L^{\dagger}GeOBu^{t}$, 2. A solution of $^{tBuO}L^{\dagger}K$ (1.5 g, 2.00 mmol) in THF (50 cm^3) was added to a stirred solution of $GeCl_2$.dioxane (486 mg, 2.10 mmol) in THF (15 cm^3) at -80 ºC. The reaction mixture was stirred for 30 min before being warmed to ambient temperature and stirred for a further 2 h. Subsequently, all volatiles were removed *in vacuo* and the residue extracted into toluene (40 cm^3). The extract was filtered onto a suspension of KOBu^t (268 mg, 2.40 mmol) in toluene (15 cm^3) at -80 ºC, and the mixture warmed to ambient temperature, then stirred for 3 h. Volatiles were subsequently removed *in vacuo*, the residue extracted into hot hexane (50 cm^3), and the extract filtered, yielding a pale yellow solution. Removal of volatiles from the filtrate and washing the residue with *ca.* 3 cm^3 of hexane yielded **2** as an analytically pure off-white powder (900 mg, 53 %). M.p.: 217-221 ºC (decomp.); ^{1}H NMR (C_6D_6, 400 MHz, 298 K), δ = 1.00 (d, $^{3}J_{HH}$ = 6.8 Hz, 6H, CH(CH_3)$_2$), 1.16 (s, 9H, GeOC(CH_3)$_3$), 1.55 (s, 27H, SiOC(CH_3)$_3$), 2.57 (sept, $^{3}J_{HH}$ = 6.8 Hz, 1H, CH(CH$_3$)$_2$), 6.62 (s, 2H, Ph$_2$CH), 6.93 (m, 2H, *m*-ArH), 7.07-7.56 (m, 20H, Ar-H); ^{13}C{^{1}H}NMR (C_6D_6, 75.5 MHz, 298 K), δ = 24.3 (CH(*C*H$_3$)$_2$), 32.8 (SiOC(*C*H$_3$)$_3$), 34.0 (*C*H(CH$_3$)$_2$), 34.6 (GeOC(*C*H$_3$)$_3$), 52.2 (Ph$_2$*C*H), 73.1 (GeO*C*(CH$_3$)$_3$), 74.4 (SiO*C*(CH$_3$)$_3$), 126.4, 126.9, 127.0, 128.2, 129.0, 131.0, 131.1, 142.9, 144.1, 144.5, 145.5, 145.6 (Ar-*C*); ^{29}Si{^{1}H} NMR (C_6D_6, 80 MHz, 298 K), δ = -96.4; IR, ν/cm^{-1} (ATR): 3062 (w), 3029 (w), 1598 (w), 1359 (s), 1238 (m), 1182 (s), 1074 (s), 1041 (s), 932 (m), 905 (s), 838 (s), 748 (s); MS/EI *m/z* (%): 859.7 (M$^+$, 1), 785.7 (M$^+$-OBu^t, 5), 167.2 (Ph$_2$C$^+$, 100); anal. calc. for $C_{51}H_{67}GeNO_4Si$: C, 71.33 %; H, 7.86 %; N, 1.63 %; found: C, 71.12 %; H, 7.90 %; N, 1.71 %.

Synthesis of $^{tBuO}L^{*}GeOBu^{t}$, 3. This compound was prepared following a method similar to that used for **2**, but using $^{tBuO}L^{*}K$ (1.0 g, 1.38 mmol), $GeCl_2$.dioxane (336 mg, 1.45 mmol), and KOBu^t (186 mg, 1.66 mmol). The product was isolated as a colourless micro-crystalline powder.

Recrystallision from hexane at -25 ºC yielded X-ray quality colourless crystals of **3**. (940 mg, 82 %). M.p.: 225-230 ºC (decomp.); ^{1}H NMR (C_6D_6, 400 MHz, 298 K), δ = 1.14 (s, 9H, GeOC(C*H*$_3$)$_3$), 1.56 (s, 27H, SiOC(C*H*$_3$)$_3$), 1.94 (s, 3H, *p*-C*H*$_3$), 6.55 (s, 2H, Ph$_2$C*H*), 6.92 (m, 2H, *m*-Ar*H*), 7.06-7.56 (m, 20H, Ar-*H*); ^{13}C{^{1}H}NMR (C_6D_6, 75.5 MHz, 298 K), ∂ = 21.3 (*p*-*C*H$_3$), 32.8 (SiOC(*C*H$_3$)$_3$), 34.6 (GeOC(*C*H$_3$)$_3$), 52.0 (Ph$_2$*C*H), 73.1 (GeO*C*(CH$_3$)$_3$), 74.4 (SiO*C*(CH$_3$)$_3$), 126.4, 126.9, 128.9, 129.7, 130.5, 131.1, 131.2, 133.0, 142.6, 144.6, 145.4, 145.5 (Ar-*C*); ^{29}Si{^{1}H} NMR (C_6D_6, 80 MHz, 298 K), δ = -96.2; IR, ν/cm^{-1} (ATR): 3059 (w), 3025 (w), 1947 (w), 1810(w), 1598 (m), 1361 (m), 1238 (m), 1182 (s), 1049 (s), 1020 (s), 901 (m), 842 (m), 744 (m); MS/EI *m/z* (%): 831.7 (M$^+$, 1), 757.6 (M$^+$-OBu^t, 3), 167.2 (Ph$_2$C$^+$, 100); anal. calc. for $C_{49}H_{63}GeNO_4Si$: C, 70.84 %; H, 7.64 %; N, 1.69 %; found: C, 71.11 %; H, 7.51 %; N, 1.73 %.

Synthesis of ^{tBuO}L†GeH, 4. To a colourless solution of **2** (200 mg, 0.23 mmol) in toluene (20 cm^3) was added HBcat (23 μL, 0.24 mmol) at ambient temperature, with stirring. The reaction mixture immediately became pale yellow in colour. The mixture was then stirred for 2 h, after which time all volatiles are removed *in vacuo* and the residue extracted into warm hexane (30 cm^3). The extract was filtered, and the filtrate concentrated to incipient crystallisation, before being stored at 6 ºC for 2 days to yield **4** as small pale yellow plates (80 mg, 44 %). M.p.: 97-102 ºC (melt), 148-153 ºC (decomp.); ^{1}H NMR (C_6D_6, 400 MHz, 298 K), δ = 1.01 (d, $^{3}J_{HH}$ = 6.8 Hz, 6H, CH(C*H*$_3$)$_2$), 1.48 (s, 27H, OC(C*H*$_3$)$_3$), 2.60 (sept, $^{3}J_{HH}$ = 6.8 Hz, 1H, C*H*(CH$_3$)$_2$), 6.51 (s, 2H, Ph$_2$C*H*), 6.75 (m, 2H, *p*-Ar*H*), 7.01-7.55 (m, 20H, Ar-*H*), 10.02 (v br, 1H, Ge*H*); ^{13}C{^{1}H}NMR (C_6D_6, 75.5 MHz, 298 K), δ = 24.5 (CH(*C*H$_3$)$_2$), 32.4 (*C*H(CH$_3$)$_2$), 32.6 (OC(*C*H$_3$)$_3$), 52.3 (Ph$_2$*C*H), 74.7 (O*C*(CH$_3$)$_3$), 122.3, 126.3, 126.4, 127.4, 129.1, 129.3, 130.7, 143.1, 144.9, 145.6, 146.5, 148.6 (Ar-*C*); ^{29}Si{^{1}H} NMR (C_6D_6, 80MHz, 298K), δ = -93.1; IR, ν/cm^{-1} (Nujol): 3061 (w), 3026 (w), 2057 (br m, Ge-H), 1599 (w), 1521 (w), 1326 (m), 1237 (m), 1182 (s), 1065 (s), 1041 (s), 925 (s), 871 (m), 742 (s); MS/EI *m/z* (%): 713.7 (L$^{\dagger+}$, 10), 167.2 (Ph$_2$C$^+$, 100); anal. calc. for $C_{47}H_{59}GeNO_3Si$: C, 71.76 %; H, 7.56 %; N, 1.78 %; found: C, 71.66 %; H, 7.67 %; N, 1.83 %.

Synthesis of ^{tBuO}L*GeH, 5. This compound was prepared following a method similar to that used for **4**, but using **3** (250 mg, 0.30 mmol) and HBcat (34 μL, 0.32 mmol). The product was isolated as pale-yellow crystalline blocks, grown by slow-cooling of a concentrated hexane solution to -25 ºC (110 mg, 48 %). M.p.: 155-160 ºC (decomp.); ^{1}H NMR (C_6D_6, 400 MHz, 298 K), δ = 1.49 (s, 27H, OC(C*H*$_3$)$_3$), 2.00 (s, 3H, *p*-C*H*$_3$), 6.50 (s, 2H, Ph$_2$C*H*), 6.92-7.54 (m, 22H, Ar-*H*), 10.00 (v br, 1H, Ge*H*); ^{13}C{^{1}H}NMR (C_6D_6, 75.5 MHz, 298 K), δ = 21.4 (*p*-*C*H$_3$), 32.6 (OC(*C*H$_3$)$_3$), 52.1 (Ph$_2$*C*H), 74.7 (O*C*(CH$_3$)$_3$), 122.4, 126.4, 127.5, 128.8, 129.1, 129.3, 130.0, 130.5, 130.8, 144.8, 145.3, 145.5 (Ar-*C*); ^{29}Si{^{1}H} NMR (C_6D_6, 80 MHz, 298 K), δ = -94.0; UV/vis (toluene, 298 K), λ_{max}, nm (ε,

$Lcm^{-1}mol^{-1}$): 330 (700); IR, ν/cm^{-1} (Nujol): 3060 (w), 3026 (w), 2083 (w, Ge-H), 1597 (m), 1386 (m), 1363 (m), 1181 (s), 1039 (s), 925 (s), 853 (m), 737 (m); MS/EI *m/z* (%): 757.6 (M^+, <1), 167.2 (Ph_2C^+, 100); anal. calc. for $C_{45}H_{55}GeNO_3Si$: C, 71.24 %; H, 7.31 %; N, 1.85 %; found: C, 71.05 %; H, 7.20 %; N, 1.93 %.

2. X-Ray Crystallography

Crystals of **3**·(hexane), **4**·(hexane), **5**, ^{tBuO}L*H, and ^{tBuO}L*Li(THF)·(THF) suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were carried out with either a Bruker Apex X8 diffractometer using a graphite monochromator with Mo Kα radiation (λ = 0.71073 Å), or the MX1 beamline of the Australian Synchrotron (λ = 0.7109 Å). The software package Blu-Ice[4] was used for synchrotron data acquisition, while the program XDS[5] was employed for synchrotron data reduction. All structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX97)[6] using all unique data. Hydrogen atoms are included in calculated positions (riding model), except for the amino proton of ^{tBuO}L*H, and the hydride ligand of **4**, the positional and displacement parameters of which were freely refined. The hydride ligand of **5** could not be located from difference maps, and was not included in a calculated position. Crystal data, details of data collections and refinements for all structures can be found in their CIF files and are summarized in Table S1.

Table S1. Summary of Crystallographic Data for **3**·(hexane), **4**·(hexane), **5**, ^{tBuO}L*H, and ^{tBuO}L*Li(THF)·(THF)

	3	**4**	**5**	^{tBuO}L*H	^{tBuO}L*Li(THF)
empirical formula	$C_{55}H_{77}GeNO_4Si$	$C_{50}H_{66}GeNO_3Si$	$C_{45}H_{55}GeNO_3Si$	$C_{45}H_{55}NO_3Si$	$C_{53}H_{70}LiNO_5Si$
formula weight	916.86	829.72	758.58	685.99	836.13
crystal system	triclinic	triclinic	monoclinic	monoclinic	monoclinic
space group	*P*-1	*P*-1	$P2_1/n$	$P2_1/n$	$P2_1/c$
a (Å)	11.9476(4)	10.074(2)	10.7047(5)	12.369(3)	11.531(2)
b (Å)	13.7236(5)	14.516(3)	21.7462(9)	21.768(4)	24.287(5)
c (Å)	16.2518(5)	18.777(4)	17.0790(7)	14.724(3)	17.056(3)
α (deg.)	81.454(3)	109.23(3)	90	90	90
β (deg)	83.839(2)	96.79(3)	92.615(2)	96.32(3)	98.37(3)
γ (deg.)	80.731(3)	97.99(3)	90	90	90
vol (Å^3)	2591.21(14)	2527.7(9)	3971.6(3)	3940.3(14)	4725.7(16)
Z	2	2	4	4	4
ρ (calcd) (g.cm^{-3})	1.175	1.090	1.269	1.156	1.175
μ (mm^{-1})	0.658	0.666	0.842	0.099	0.097
F(000)	984	886	1608	1480	1808
T (K)	123(2)	100(2)	150(2)	100(2)	100(2)
reflections collected	26342	9771	52358	27068	35498
unique reflections	9642	9771	7760	6763	8997
R_{int}	0.0248	0.0000	0.1433	0.0783	0.0932
R1 indices [$I>2\sigma(I)$]	0.0488	0.0716	0.0772	0.0530	0.0654
*w*R2 indices (all data)	0.1344	0.2099	0.2110	0.1350	0.1841
CCDC No.	1048745	1048746	1048747	1048748	1048749

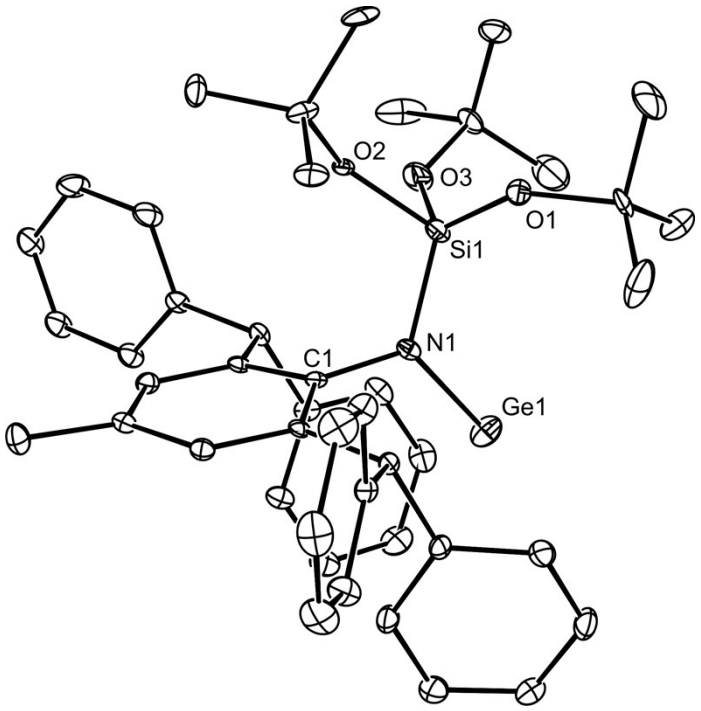

Fig. S1 Molecular structure of **5** (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Ge(1)-N(1) 1.877(4), N(1)-C(1) 1.427(6), Si(1)-N(1) 1.730(4), C(1)-N(1)-Si(1) 118.7(3), C(1)-N(1)-Ge(1) 119.9(3), Si(1)-N(1)-Ge(1) 120.5(2).

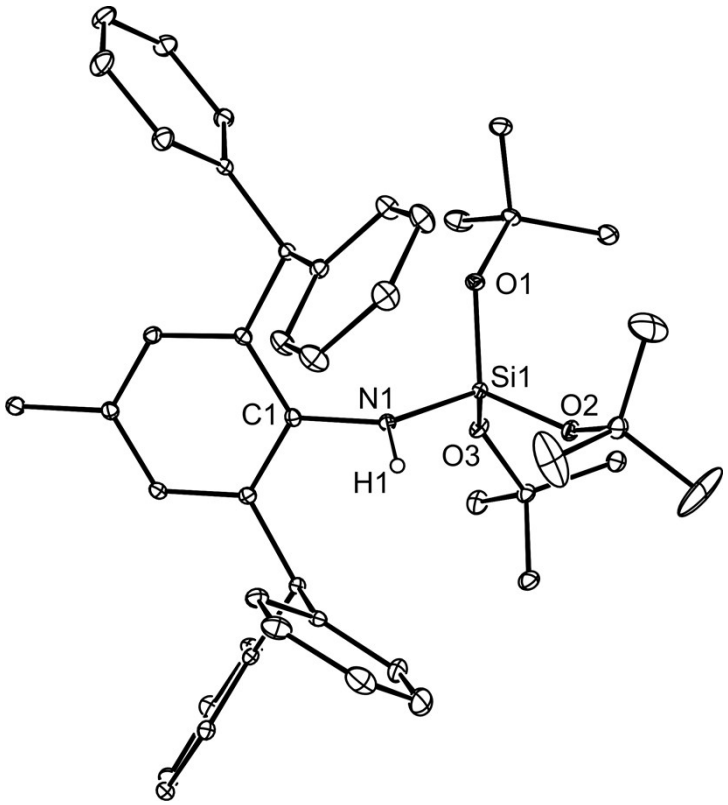

Fig. S2 Molecular structure of ^{tBuO}L*H (25% thermal ellipsoids; hydrogen atoms, except H(1), omitted). Selected bond lengths (Å) and angles (º): Si(1)-N(1) 1.7129(14), N(1)-C(1) 1.4288(18), C(1)-N(1)-Si(1) 131.18(10).

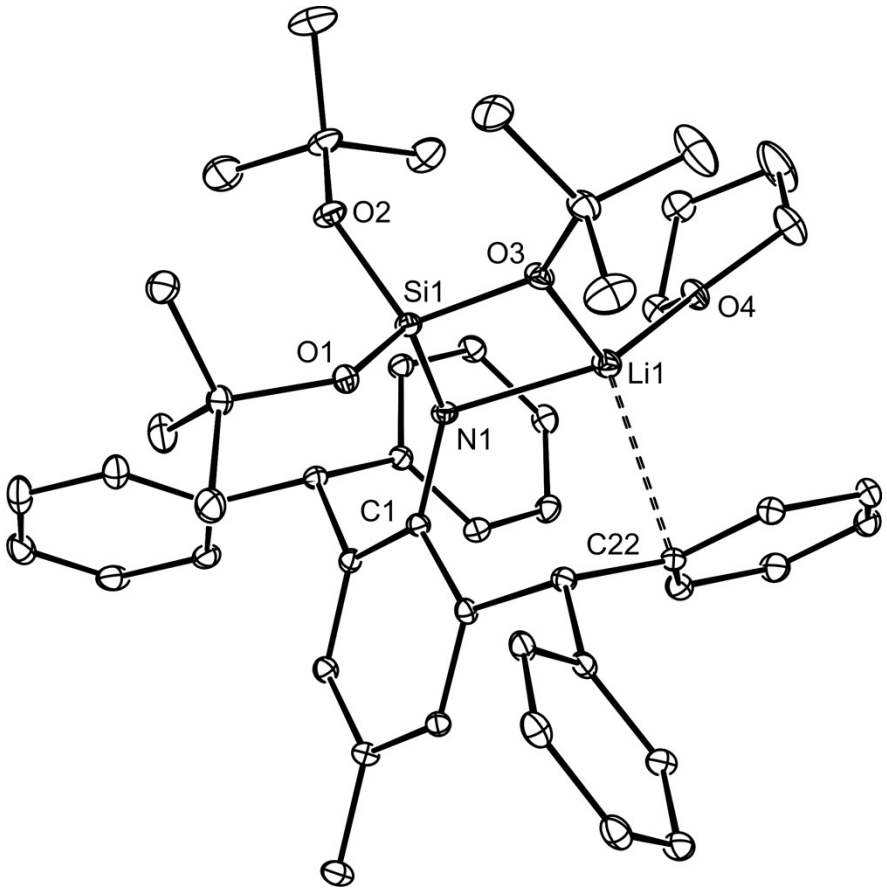

Fig. S3 Molecular structure of ^{tBuO}L*Li(THF) (25% thermal ellipsoids; hydrogen atoms omitted). Selected bond lengths (Å) and angles (º): Li(1)-O(4) 1.883(5), Li(1)-O(3) 1.980(5), Li(1)-C(22) 2.523(5), N(1)-Li(1) 2.029(5), O(3)-Li(1)-N(1) 79.35(17), O(4)-Li(1)-C(22) 114.6(2), C(1)-N(1)-Si(1) 127.70(16), C(1)-N(1)-Li(1) 120.4(2), Si(1)-N(1)-Li(1) 89.41(15).

3. Computational Studies

Standard molecular orbital theory calculations were performed using GAUSSIAN09.[7] Geometry optimizations and subsequent frequency calculations were performed at M062X/cc-pVDZ.[8,9] The rationale for using M062X in this work lies in improved performance of this meta-GGA functional for non-covalent interactions.[10] Recently M062X was shown to perform reliably for semi-Coulombic systems such as ionic liquids accounting for non-negligible dispersion interactions. Improved electronic energies were carried out with M062X/cc-pVTZ.[9] Standard physical chemistry formulae were used to calculate Gibbs free energies at 298.15 K as discussed elsewhere.[11]

Table S2. Gibbs free energies of dimerization (in kcal mol^{-1}) calculated at the M062X/cc-pVTZ level of theory

Dimers	**ΔG**
^{tBuO}L*(H)Ge=Ge(H)^{tBuO}L*	3.1
L"(H)Ge=Ge(H)L"	-8.3
^{tBuO}L*Ge(μ-H)$_2$Ge^{tBuO}L*	16.5

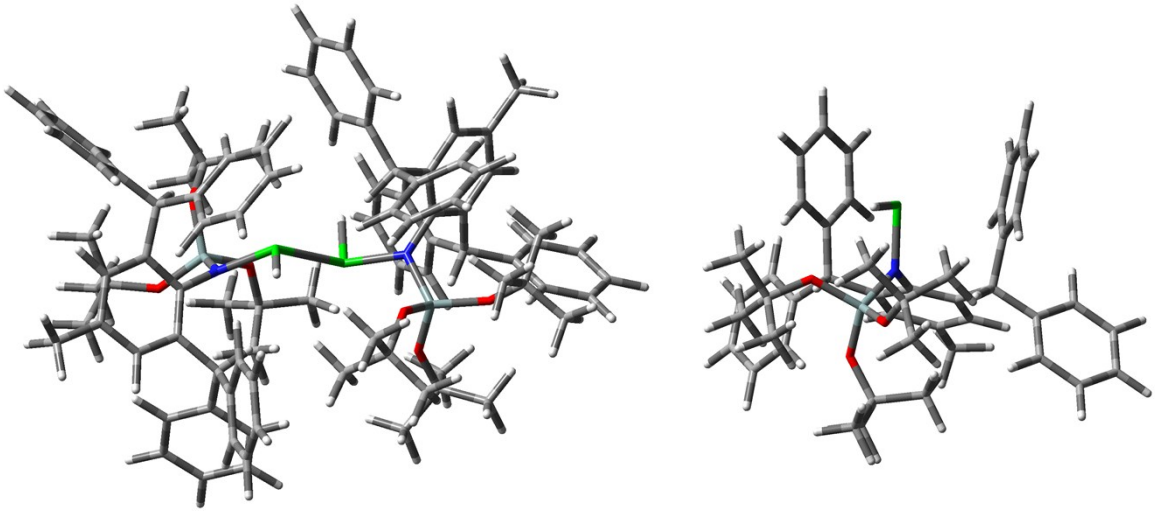

Figure S4. M062X/cc-pVDZ optimized structures of ^{tBuO}L*(H)Ge=Ge(H)^{tBuO}L* and :Ge(H)^{tBuO}L*.

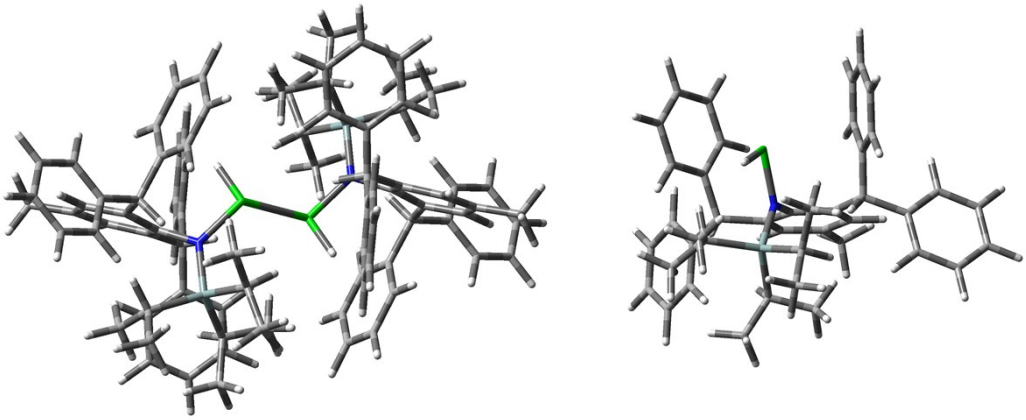

Figure S5. M062X/cc-pVDZ optimized structures of L"(H)Ge=Ge(H)L" and :Ge(H)L".

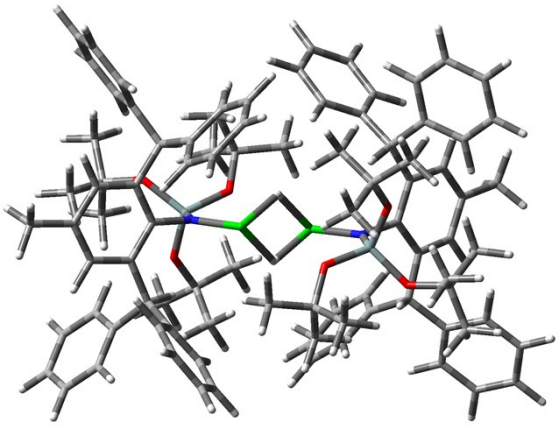

Figure S6. M062X/cc-pVDZ optimized structure of ^{tBuO}L*Ge(μ-H)$_2$Ge^{tBuO}L*.

Table S3. Geometrical parameters of optimized structures.

	^{tBuO}L*(H)Ge=Ge(H)^{tBuO}L*	L"(H)Ge=Ge(H)L"	^{tBuO}L*Ge(μ-H)$_2$Ge^{tBuO}L*	:Ge(H)^{tBuO}L*	:Ge(H)L"
(Ge-H), Å	1.567	1.567	1.796	1.611	1.616
	1.569	1.567	1.794		
(Ge-Ge), Å	2.546	2.545	2.955		
(Ge-N), Å	1.908	1.875	1.948	1.915	1.893
	1.893	1.875	1.936		
∠(HGeN)	98.2	98.7	100	91.7	92.2
	99.8	98.7	101		

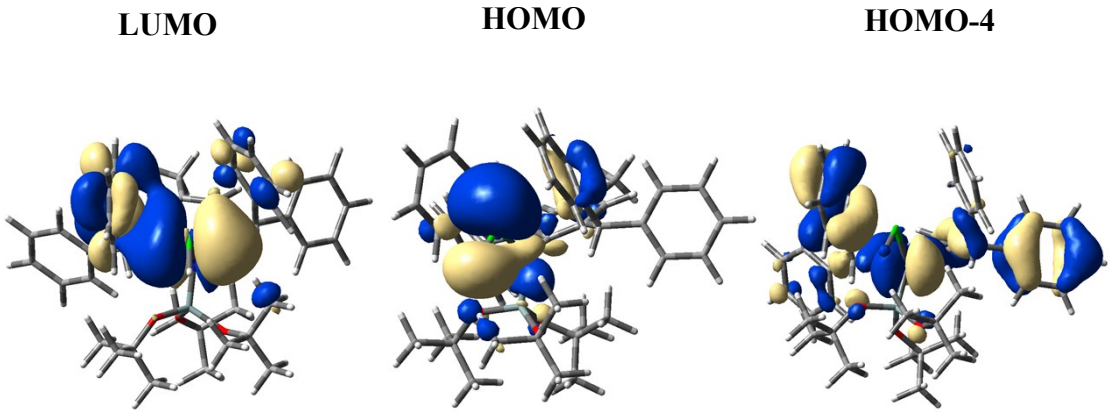

Figure S7. Selected Molecular Orbitals of :Ge(H)^{tBuO}L*.

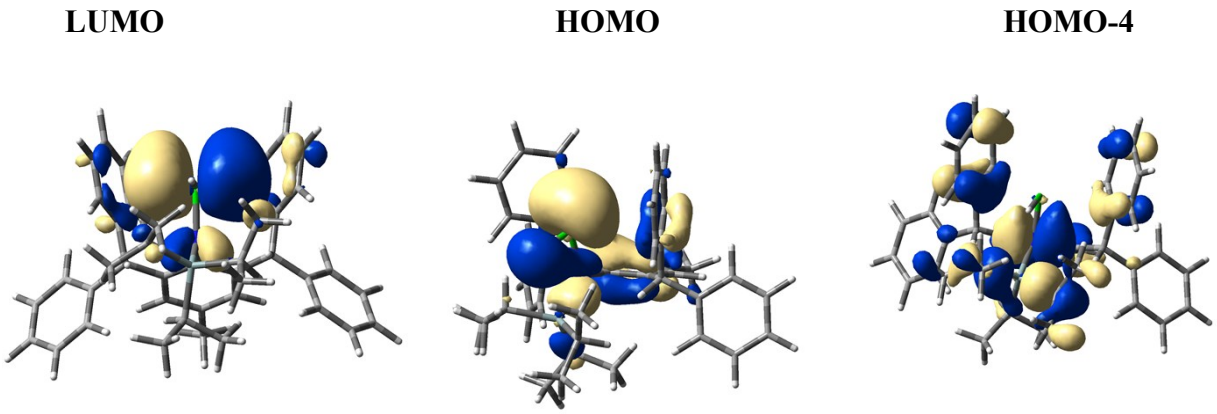

Figure S8. Selected Molecular Orbitals of :Ge(H)L".

Table S4. Electronic energies (given in Hartrees) calculated at the M062X/cc-pVTZ level of theory, and zero-point vibrational energies (ZPVE given in Hartrees) calculated at M062X/cc-pVDZ.

Molecule	E(M062X)	ZPVE
:Ge(H)^{tBuO}L*	-8789.934859	1.795795
:Ge(H)L"	-8102.405468	1.599944
^{tBuO}L*(H)Ge=Ge(H)^{tBuO}L*	-8789.913609	1.795747
L"(H)Ge=Ge(H)L"	-4394.955500	0.89694
^{tBuO}L*Ge(μ-H)$_2$Ge^{tBuO}L*	-4051.180999	0.798835

Table S5. Cartesian coordinates of geometry optimized molecules

^{tBuO}L*(H)Ge=Ge(H)^{tBuO}L*

H	-2.35093000	-2.69993400	7.04455100
H	-2.39310600	-0.53354300	5.80311800
H	-2.74733400	2.57854400	4.36857800
H	-1.07007700	4.23415800	3.54400900
C	-2.48544800	-2.68814900	5.96215300
C	-2.51028100	-1.47661700	5.26632500
C	-2.70507700	2.83632200	3.30872200
C	-1.76740400	3.76223300	2.84991000
H	-2.65008400	-4.83066000	5.79061300
C	-2.64949200	-3.87738300	5.25994000
H	-4.31214600	1.49678500	2.78469400
H	-7.94113100	4.86443300	1.42763800
C	-3.59039600	2.23027000	2.41753400
C	-2.68188600	-1.46625100	3.88742100
H	-6.01256400	3.38168100	1.87898000
H	-2.70786400	-0.51407200	3.35214500
H	3.42100800	3.79154300	5.98188500
C	-1.72312600	4.08321600	1.49340800
H	-1.00541700	4.81298700	1.12206600
C	-7.44192400	4.36091300	0.59856200
H	1.35091600	2.55317900	5.35344100
C	-2.81518600	-3.86505400	3.87111200
C	-6.35988000	3.52067300	0.85313600
C	3.18462400	3.61389300	4.93194100
H	-5.42627300	-2.71707500	2.54151300
C	-6.36481700	-0.94109300	1.78017100
H	-6.90110300	1.01834200	1.06291700
C	-2.81522700	-2.66145100	3.16378400
C	-3.54980900	2.53856000	1.05014300
Si	3.19366400	-0.89015700	1.39899100
C	2.02575200	2.92317200	4.57973900
H	4.95962900	4.59922000	4.19652000
C	-5.30599100	-1.82886100	1.91509900
C	-6.11874400	0.25803400	1.09863700
C	-2.60331000	3.46869000	0.60229700
H	-2.93762500	-4.80966100	3.34136600
C	4.04450400	4.06724800	3.93166900
H	-1.35018300	0.38672600	1.88600200
H	-8.72301800	5.23048100	-0.90818800
H	8.62638400	-2.06512200	-0.00261300
C	-7.87953500	4.56802900	-0.70979900
H	6.22521500	-1.40099400	0.05255900
C	-5.70335600	2.86267200	-0.19403400
C	-4.89024700	0.52172500	0.50147300
C	-4.06608800	-1.62087700	1.29045300
C	-4.52359800	1.93028600	0.04219800
H	-2.56062800	3.71963400	-0.46138300
C	1.72698700	2.69572300	3.23661600
C	-2.93491600	-2.57862000	1.63390300

C	8.12924900	-1.74123200	-0.91900600
H	0.82455600	2.14479100	2.96076700
C	3.74284200	3.83860400	2.58992100
C	-3.87943400	-0.47952600	0.49058500
C	6.78315500	-1.38446600	-0.88652800
H	-1.99935100	-2.12146900	1.27226100
Ge	-1.14285700	0.58030700	0.34275200
N	2.65331200	0.16595300	0.11244500
C	2.57424300	3.15851700	2.22545100
H	-5.06082400	-3.86098900	0.35421900
C	-7.22156600	3.93366500	-1.76119800
H	4.42701700	4.19207300	1.81651800
H	-3.98615000	1.86157200	-0.91145600
C	-6.14160400	3.09012500	-1.50201000
H	4.17825000	-1.24557600	-1.22840700
C	-3.00268000	-3.94946600	0.97940400
H	9.89329200	-1.96688300	-2.14815200
C	-4.15217000	-4.46098800	0.37861900
C	8.83950700	-1.68711200	-2.11869600
N	-2.69499500	-0.29048900	-0.30263500
H	1.40767800	2.16623800	0.78329500
Ge	0.99618900	-0.34091600	-0.68517800
H	-7.54401700	4.10004200	-2.79010400
C	3.48763500	1.17453000	-0.46013600
H	-0.93852200	-4.34480900	1.45627700
C	6.11828800	-0.97569800	-2.04914900
C	-1.84439700	-4.74020900	0.98784300
H	-5.61413100	2.60274700	-2.32323600
C	2.15324300	2.97269900	0.77745700
C	4.65262400	-0.55944800	-1.94305300
H	4.45934100	-2.80783200	-3.42619800
C	4.51248700	0.84663200	-1.37926200
C	3.28241000	2.53619300	-0.14499300
C	-4.14309500	-5.72686500	-0.21452600
H	-5.05061100	-6.10428800	-0.68879100
H	2.02069700	5.60926000	1.74370100
C	8.18964700	-1.27433300	-3.27965700
C	5.35497000	1.84638900	-1.86515900
C	-1.83382800	-6.00363200	0.40745100
H	6.15636900	1.56824500	-2.55381100
C	4.11965000	3.51262700	-0.69468400
C	3.93734600	-1.97797500	-3.90752100
C	6.83851100	-0.92485700	-3.24681600
C	-2.98756400	-6.50183500	-0.20323000
C	5.18843300	3.18895900	-1.52609900
H	1.11702300	0.49893400	-2.00354600
C	3.91523700	-0.72414100	-3.27512400
H	3.91775800	4.56333400	-0.47055700
Si	-2.82340000	-0.50106200	-2.04485000
H	-0.91953400	-6.59922200	0.42250900
C	1.44817100	4.20219400	0.20936200
C	1.47968100	5.46323600	0.80803100
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H	-2.98179500	-7.48906200	-0.66692100
H	3.39369200	-3.14743100	-5.63014700
H	6.33877800	-0.61408800	-4.16621400
C	3.35019500	-2.16629700	-5.15472100
H	0.71985000	3.06080800	-1.46407500
C	3.25617200	0.32681300	-3.91927900
C	0.73272900	4.04413300	-0.98626500
H	0.83541000	7.51914800	0.71153600
C	0.80211200	6.54133000	0.22876100
H	3.21087000	1.30894400	-3.44738700
C	2.71270200	-1.10289200	-5.79715100
C	2.65906800	0.13786800	-5.16932800
C	0.04726700	5.11131200	-1.55674500
C	0.07771800	6.36928000	-0.94736300
H	2.25614900	-1.24584300	-6.77755500
H	2.15556000	0.97606300	-5.65352900
H	-0.51226700	4.96391900	-2.48289200
H	-0.45879300	7.20859200	-1.39128600
O	2.92598000	-2.46539200	0.92357800
O	2.19621500	-0.56872100	2.69510700
O	4.81668800	-0.72456200	1.70055700
C	5.65395700	0.09708600	2.53842400
C	4.87989600	0.64362100	3.73174000
C	6.77619800	-0.82515800	3.00762400
C	6.21462100	1.23565200	1.69127000
H	4.00624000	1.22464800	3.40694800
H	4.52856000	-0.17346800	4.37638400

H	5.53406900	1.29981900	4.32469800
H	7.47606600	-0.28101400	3.65842300
H	6.35733300	-1.67414500	3.56790100
H	7.33568000	-1.21636100	2.14425800
H	6.92462100	1.83033000	2.28636400
H	6.73702200	0.83972300	0.80787200
H	5.40699800	1.89707100	1.34685800
C	1.60394600	-1.45305700	3.66219000
C	0.48169200	-2.23701400	2.99069900
C	2.63785200	-2.40877800	4.25038200
C	1.04357200	-0.54633800	4.75153500
H	-0.24827000	-1.53177700	2.56992100
H	0.88487100	-2.85131300	2.17316200
H	-0.04008800	-2.87689300	3.72017700
H	3.44539800	-1.86274200	4.75752600
H	2.15865000	-3.07527400	4.98264100
H	3.07124000	-3.02687200	3.45429600
H	0.56441400	-1.14575700	5.53988800
H	1.85364600	0.05572000	5.18966700
H	0.28923900	0.13297400	4.32401700
C	3.57033600	-3.72221800	0.69038200
C	3.87967000	-3.84374000	-0.80150000
C	4.85935100	-3.87560900	1.49562900
C	2.55031100	-4.78871600	1.08915000
H	3.00912200	-3.52020800	-1.39219500
H	4.74941800	-3.22787400	-1.07158500
H	4.11620300	-4.88654000	-1.06050400
H	4.66985800	-3.85579500	2.57774700
H	5.32633700	-4.84077300	1.24861300
H	5.56606800	-3.07128500	1.25546400
H	2.94921500	-5.79567300	0.89847000
H	2.29949500	-4.70851100	2.15693700
H	1.62788600	-4.65387600	0.50293800
O	-1.37954300	-1.06532000	-2.67446800
O	-3.06204300	1.02202000	-2.69752400
O	-4.03410500	-1.57450600	-2.39962400
C	-2.55201500	1.62451900	-3.90061700
C	-3.35216100	2.91066300	-4.08083900
C	-1.07390400	1.94162000	-3.69589800
C	-2.75708200	0.69962700	-5.09622000
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H	-3.27278500	3.53731900	-3.17954900
H	-2.97661800	3.48039300	-4.94325400
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H	-0.67797500	2.52355900	-4.54236100
H	-0.95927800	2.53057900	-2.77275600
H	-2.37529600	1.17374900	-6.01256400
H	-2.21837700	-0.24457100	-4.94244600
H	-3.82671400	0.48514000	-5.24108700
C	-5.41078100	-1.53820600	-2.81359400
C	-5.95220800	-0.11575200	-2.86744400
C	-5.48105600	-2.19102600	-4.19147300
C	-6.19060600	-2.36031300	-1.79391400
H	-5.88864600	0.35254400	-1.87547600
H	-5.38895700	0.49770000	-3.58395700
H	-7.01036600	-0.13348800	-3.16754600
H	-5.09848800	-3.22088000	-4.14505100
H	-6.52075500	-2.21942300	-4.54903900
H	-4.87620600	-1.62568100	-4.91592200
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H	-5.79108900	-3.38425200	-1.76257400
H	-6.09581700	-1.90945600	-0.79434000
C	-1.02213200	-2.42917600	-3.01915100
C	-1.35282800	-3.34829300	-1.85354600
C	-1.76560100	-2.84476300	-4.28722200
C	0.47682500	-2.43163000	-3.30083200
H	-0.87079200	-2.96434600	-0.94033900
H	-2.43914100	-3.40877000	-1.68723800
H	-0.97499600	-4.36451600	-2.04221600
H	-1.42033600	-2.25356300	-5.14884600
H	-1.56465400	-3.90482300	-4.50184300
H	-2.84641100	-2.71077300	-4.16161500
H	0.75756900	-3.35528200	-3.82914100
H	0.75490500	-1.57241200	-3.92786100
H	1.06409600	-2.39658100	-2.37033300
C	-7.71752800	-1.22747400	2.37525100
H	-8.15535700	-0.32387500	2.82211700
H	-8.41532900	-1.58060100	1.59980700
H	-7.65563800	-2.00360100	3.14947700
C	6.12473600	4.24483400	-2.05188900

H	7.05604200	4.26814900	-1.46477400
H	6.40130500	4.04594600	-3.09669800
H	5.66928400	5.24274000	-1.99828700

L"(H)Ge=Ge(H)L"

H	0.32294900	-4.63104500	-5.72844900
H	0.75358900	-2.21160200	-5.28989900
H	2.52337900	2.28466200	-4.47323800
H	-2.44035000	1.67725700	-5.19760700
H	1.74729800	4.50820800	-3.67728200
H	-3.11234400	-0.87840700	-5.04350600
H	-1.69365300	-1.94234300	-4.97699800
H	-1.48036600	-0.18000100	-4.98725700
C	0.69073800	-4.30556700	-4.75445600
H	-2.30391500	3.39543700	-4.77859900
C	0.92954100	-2.95120100	-4.50724500
C	-2.11085300	-0.99401300	-4.60155700
H	-5.01043800	0.65661100	-4.67241400
C	-2.74046800	2.43444200	-4.45831200
H	-3.83288100	2.53841400	-4.51668700
C	2.77894700	2.62431400	-3.46839000
C	2.33942100	3.86834900	-3.02095000
H	0.76012100	-6.29607600	-3.92953600
H	-5.12395800	-0.97961200	-3.99575000
H	-6.50376900	0.13511800	-3.86810700
C	0.93535200	-5.23458800	-3.74829200
C	-5.40327600	0.07198600	-3.82597100
H	3.86314000	0.82140600	-2.98988900
H	8.59878200	3.30116400	-2.34296500
H	-0.29423500	1.24671900	-3.55974300
H	-0.31496500	3.02034700	-3.40559200
C	3.53843300	1.80163800	-2.63480400
C	1.39909100	-2.53962600	-3.26459400
H	6.32104400	2.34248900	-2.46722900
H	1.59633900	-1.48107900	-3.07949900
H	-2.25436800	6.73991000	-2.98197000
C	-0.72760800	2.08721500	-2.98947900
C	-2.25505400	2.09783200	-3.04045700
C	2.66513500	4.29041400	-1.73121200
C	-2.14331300	-1.01286200	-3.06648200
H	-5.06707100	2.75648800	-2.84943000
H	-2.12569100	-3.18862100	-3.02006400
H	2.33172400	5.26444000	-1.36820100
C	8.09911900	2.97682400	-1.42908600
H	-3.74896100	-2.48849200	-2.79015200
H	-0.10029900	5.71772300	-2.25005400
H	-1.09070700	-0.94353800	-2.72666800
C	1.41040500	-4.81956700	-2.50054400
C	6.82045400	2.42908500	-1.49975800
C	-2.24328900	5.99279200	-2.18744100
H	4.28364900	-3.60520700	-2.36561800
C	5.61933500	-1.94038000	-2.10412400
H	-2.60547900	2.91166800	-2.38467100
C	-2.67801000	-2.35395600	-2.55619000
H	6.62014700	-0.06494200	-1.78848300
C	-4.89383300	0.59002800	-2.47428300
C	1.64454400	-3.46756100	-2.24117500
H	-6.55539100	1.97996700	-2.26415800
C	3.87479200	2.21531500	-1.34162000
C	-5.45705800	1.98614200	-2.16628900
Si	-2.99074700	0.51118200	-2.28153000
C	-1.03784700	5.41982900	-1.77692300
H	-0.36073400	2.01574900	-1.95359800
H	-4.37792500	6.04984600	-1.87996500
C	4.43770400	-2.63745900	-1.88006500
C	5.72928100	-0.65360200	-1.56345300
C	3.43053200	3.47157100	-0.90432300
H	1.59682500	-5.56155800	-1.72337100
C	-3.43079900	5.60521400	-1.57100000
H	1.43659500	0.23513200	-1.74254100
H	9.73270900	3.55704500	-0.13922700
H	-8.55094000	-2.85110100	-1.93745400
C	8.73387900	3.12281600	-0.19554800
H	-5.30641700	-0.07334200	-1.70234400
H	-6.28426800	-1.87903200	-1.80886100
H	-2.55516000	-2.45053700	-1.46713500

C	6.15621900	2.00107000	-0.34297600
H	-5.21743000	2.30032600	-1.13913100
C	4.72602000	-0.09426200	-0.77648300
C	3.42391000	-2.13684300	-1.05237800
C	4.76060200	1.38951500	-0.40698300
H	3.71193500	3.81776400	0.09281900
C	-1.02919200	4.45575300	-0.77342000
C	2.14424200	-2.94839500	-0.89024800
C	-8.07411500	-2.72495200	-0.96455700
H	-0.08477000	3.99568900	-0.46606000
C	-3.41932400	4.63883400	-0.56281600
C	3.59324900	-0.88256500	-0.42984000
C	-6.79571200	-2.17156200	-0.88928800
H	1.36455200	-2.25971800	-0.53454500
Ge	1.14740400	0.50159500	-0.22591900
N	-2.63209700	0.37909500	-0.50711600
C	-2.22150500	4.03933300	-0.16589600
H	4.35850900	-4.33104100	0.10197200
C	8.07411500	2.72496600	0.96454400
H	-4.35851000	4.33103900	-0.10211100
H	4.32494100	1.50014100	0.59331400
C	6.79570100	2.17160100	0.88928300
H	-4.32495400	-1.50009900	-0.59331200
C	2.22150700	-4.03932900	0.16583500
H	-9.73268000	-3.55710200	0.13920200
C	3.41933500	-4.63884900	0.56269600
C	-8.73386000	-3.12285400	0.19552700
N	2.63211800	-0.37912800	0.50716600
H	-1.36456300	2.25974800	0.53457400
Ge	-1.14742000	-0.50166500	0.22601700
H	8.55093400	2.85113700	1.93744100
C	-3.59324800	0.88257600	0.42985000
H	0.08478000	-3.99569100	0.46606700
C	-6.15622400	-2.00105700	0.34297200
C	1.02921100	-4.45576700	0.77338200
H	5.21748900	-2.30045000	1.13923400
H	6.28424400	1.87911900	1.80886400
C	-2.14426800	2.94843500	0.89022500
C	-4.76061600	-1.38948300	0.40698500
H	-3.71177900	-3.81765200	-0.09288300
C	-4.72603900	0.09429300	0.77647400
C	-3.42393600	2.13688100	1.05234100
C	3.43083800	-5.60526800	1.57084100
H	4.37797300	-6.04991600	1.87975900
H	5.30646500	0.07324200	1.70231100
H	2.55521000	2.45046600	1.46725500
H	-1.59667700	5.56161000	1.72319900
H	6.55544700	-1.98004300	2.26425100
C	-8.09909300	-2.97688600	1.42906600
C	-5.72932500	0.65365900	1.56339200
C	1.03789400	-5.41988700	1.77684500
C	5.45711500	-1.98621700	2.16637700
H	-6.62020500	0.06501400	1.78840500
C	-4.43776100	2.63752800	1.87997300
C	-3.43043000	-3.47147900	0.90428200
C	-6.82044100	-2.42912200	1.49974600
C	2.24334600	-5.99287000	2.18730100
C	-5.61939600	1.94045700	2.10402200
H	-1.43661300	-0.23516400	1.74263100
C	-3.87478800	-2.21527100	1.34161700
C	4.89389700	-0.59008400	2.47429500
H	-4.28372500	3.60529800	2.36548900
Si	2.99080900	-0.51125200	2.28157400
H	0.10036000	-5.71780700	2.24998500
H	0.36079500	-2.01589200	1.95371100
C	-1.64463500	3.46765500	2.24115500
C	-1.41040200	4.81966000	2.50044600
H	2.60558100	-2.91174600	2.38469300
C	2.67803300	2.35387900	2.55631100
H	-8.59874300	-3.30126800	2.34293700
H	5.06711900	-2.75652900	2.84955300
H	2.25444800	-6.74002200	2.98179800
H	3.74897400	2.48844800	2.79030400
H	-2.33150800	-5.26429000	1.36811600
H	-6.32102300	-2.34254900	2.46721500
H	2.12567300	3.18851800	3.02018100
H	1.09076200	0.94341900	2.72678300
C	-2.66499600	-4.29030100	1.73115900
C	2.14337300	1.01276000	3.06657900
C	2.25516100	-2.09792800	3.04050300

C	0.72771300	-2.08735100	2.98957700
H	6.50384800	-0.13508900	3.86807400
H	-1.59669800	1.48123300	3.07963900
C	5.40335500	-0.07195900	3.82594300
C	-3.53849200	-1.80162200	2.63482600
C	-1.39937200	2.53977700	3.26467100
H	5.12403800	0.97965100	3.99565300
H	0.31511200	-3.02049900	3.40569800
H	-0.76012800	6.29621800	3.92938900
C	-0.93543700	5.23473200	3.74821000
H	-3.86328300	-0.82143000	2.98994500
H	0.29433500	-1.24687600	3.55986700
C	-2.33935100	-3.86826700	3.02092400
H	5.01052200	-0.65652600	4.67242900
H	3.83306200	-2.53848900	4.51666200
C	2.74064200	-2.43455500	4.45833000
C	-2.77897500	-2.62428000	3.46840100
C	2.11095600	0.99387600	4.60165500
C	-0.92991700	2.95140400	4.50734100
H	2.30413600	-3.39557300	4.77861100
C	-0.69101300	4.30576700	4.75447200
H	-1.74720500	-4.50810800	3.67725000
H	3.11245700	0.87823500	5.04357100
H	1.69379500	1.94221100	4.97712900
H	1.48046100	0.17987400	4.98735900
H	2.44052400	-1.67739800	5.19765400
H	-2.52345900	-2.28465200	4.47327000
H	-0.75411900	2.21184900	5.29007000
H	-0.32329700	4.63128500	5.72847900
C	-6.73686200	2.52589900	2.92668800
H	-7.56426100	2.85842600	2.28090800
H	-7.14681200	1.78354500	3.62611100
H	-6.39224900	3.39285600	3.50557800
C	6.73677400	-2.52580200	-2.92684200
H	7.14682200	-1.78337900	-3.62613400
H	7.56411600	-2.85851200	-2.28108400
H	6.39209800	-3.39263700	-3.50587800

^{tBuO}L*Ge(μ-H)$_2$Ge^{tBuO}L*

H	8.71024800	-5.60571600	-1.32143400
H	6.47511300	-6.47871800	-1.99647600
C	5.72871000	0.47409000	-2.99439700
H	5.95444800	-1.65852000	-2.91423800
C	7.82618700	-4.97023500	-1.25788700
C	6.57851700	-5.45533500	-1.63300500
H	5.36229800	2.56386300	-2.71614400
C	5.42866200	-0.79590500	-2.49989300
H	1.77884000	-3.76856900	-4.66879500
C	5.07785500	1.55375000	-2.41440400
H	8.90039200	-3.25115000	-0.50851400
H	4.77809900	6.99574800	0.39897000
H	3.46952600	-2.32453400	-3.57497000
H	7.05674600	6.25255300	1.08753100
C	7.93100700	-3.65516700	-0.80419300
H	4.48562900	-5.05422000	-1.86311600
C	5.44546400	-4.64155100	-1.55458500
H	3.63752000	3.26462300	-3.57891600
H	2.09811400	4.62654500	-4.91972600
C	5.06841400	5.94903400	0.29711100
C	6.34220300	5.53596000	0.68086600
C	1.92774400	-3.83077100	-3.58959300
C	2.87422600	-3.01476700	-2.97484200
C	6.80051600	-2.84781800	-0.72835700
C	5.53098400	-3.32224200	-1.09475800
H	3.16983200	5.38653000	-0.53305700
H	7.68533700	3.85027800	0.82253900
C	6.69205700	4.19523900	0.53070200
C	4.15592300	5.03363800	-0.22844800
C	2.72075500	3.62802600	-3.11868700
C	1.84942900	4.40247700	-3.88123700
C	4.51339300	-1.00021900	-1.46763400
H	0.45306200	-5.38533100	-3.31849100
C	4.10239900	1.39990000	-1.41913900
H	6.90887500	-1.81893900	-0.38690700
C	1.17973000	-4.73178300	-2.83215000
C	5.77589300	3.28168700	0.01293100

C	4.48880400	3.67967700	-0.37155400
C	3.09492100	-3.09619700	-1.59558000
C	4.29091200	-2.41806900	-0.94881100
H	6.06925500	2.23979100	-0.09744700
C	3.79657900	0.10717600	-0.93304100
C	3.44916000	2.65259400	-0.85510200
C	2.43704000	3.32553900	-1.78103800
H	-0.00018200	5.52209700	-3.91063400
C	0.67409000	4.89942900	-3.32095400
C	1.35564500	-4.78325600	-1.45070100
C	2.30622500	-3.96753900	-0.83861600
H	4.08667900	-2.33456900	0.12989400
H	0.76209900	-5.47110000	-0.84589000
H	2.89580100	2.34405600	0.03995600
H	2.47765700	-4.04186100	0.23626700
C	1.23006800	3.79267100	-1.24289900
C	0.36556000	4.58448500	-1.99995200
N	2.73193400	-0.10176900	0.02503800
H	0.97342900	3.55451400	-0.20796600
H	-0.55694500	4.95988500	-1.55478400
Si	3.10627800	0.00448400	1.73000300
H	0.01484300	-1.13066000	0.21613500
H	0.01235900	0.96729400	-0.20603200
Si	-2.96558500	-0.31832500	-1.76127900
H	-0.78481100	-5.31949900	3.29564200
H	-1.83788500	-4.28569600	1.30582100
N	-2.66328000	-0.03917800	-0.05823800
C	-1.51234200	-4.51646700	3.42427900
C	-2.09598900	-3.92751700	2.30499200
H	-1.83830300	4.38434800	0.15916900
H	-3.12199500	-2.46080500	0.35654000
H	-0.32330200	5.46290400	1.80660100
H	-3.20119500	2.35154000	-0.35093400
C	-1.85590700	4.07482800	1.20711300
C	-1.02199500	4.69002800	2.13305700
C	-1.87252100	-4.09431400	4.70418600
H	-5.20992600	-2.65712600	-1.07027000
C	-3.82885400	-2.49310200	1.19470500
C	-3.05613800	-2.91493600	2.43864800
C	-5.52502700	-3.45121400	-0.39390300
C	-3.85548500	0.03669200	0.75360600
H	-6.99986400	-4.25259700	-1.74093400
C	-4.88489600	-3.54860600	0.84791500
C	-6.51897700	-4.35034000	-0.76544000
H	-5.02033100	2.84879100	-1.73924600
C	-3.76417300	2.58068400	0.56432500
C	-2.76999900	3.08726800	1.60173700
C	-5.26571900	-4.57818300	1.71247800
C	-1.08060800	4.31664500	3.47869500
C	-6.89739600	-5.37282800	0.10726300
C	-4.46166000	-1.11330200	1.30230600
H	-4.78273300	-4.68487900	2.68470500
H	-0.43586100	4.80316900	4.21234700
H	-7.67738600	-6.08011500	-0.17724800
C	-5.32587000	3.65334200	-1.07040700
C	-6.26721000	-5.48109500	1.34314900
C	-2.78687600	-3.05327500	4.84790100
C	-4.45711300	1.29785600	0.99848700
C	-4.75098300	3.68467500	0.20158800
C	-3.36994400	-2.46367500	3.72471300
H	-6.55237100	-6.27620400	2.03364900
H	-6.69602100	4.56922000	-2.46157900
C	-6.26068700	4.60846600	-1.46107100
C	-2.79803100	2.69970900	2.94273100
C	-1.95579500	3.31150400	3.87544200
H	-3.05688500	-2.69701100	5.84320500
C	-5.12140100	4.70550800	1.08191000
H	-4.66898900	4.75842500	2.07421900
H	-4.09329800	-1.65845400	3.85512300
C	-6.63397800	5.61853400	-0.57385200
C	-5.67776300	-0.99424400	1.98974900
H	-3.48587700	1.91713800	3.26613700
C	-6.06106000	5.66295400	0.69593500
C	-5.65690900	1.37173800	1.70182900
H	-1.99496400	3.00141000	4.92056300
H	-7.36363300	6.37185100	-0.87340300
H	-6.15336700	-1.90297000	2.36773500
H	-6.34250900	6.45299900	1.39371100
H	-6.11654000	2.34987400	1.86107400
C	-6.29972500	0.23200900	2.19133500

C	-7.62613600	0.33919700	2.89611700
H	-8.42654500	0.58355500	2.18095600
H	-7.89257900	-0.60411400	3.39049200
H	-7.61020600	1.13604800	3.65343400
C	6.73241900	0.65453900	-4.10229900
H	7.03385100	1.70599500	-4.19861600
H	7.63322200	0.05065800	-3.92284500
H	6.31078600	0.33474900	-5.06772500
O	-1.62939300	0.24099000	-2.58449700
O	-3.22987000	-1.93179600	-2.08783100
O	-4.33930200	0.50999900	-2.23921000
C	-1.55116900	1.26972000	-3.59322600
C	-2.12641100	2.56950000	-3.03631900
H	-1.66562500	2.77444400	-2.05740700
H	-1.89539200	3.41077900	-3.70662400
H	-3.21534300	2.49273500	-2.91735300
C	-0.07243300	1.43221800	-3.91565900
H	0.47295700	1.84241700	-3.05376500
H	0.36447400	0.45656500	-4.17552400
H	0.05482700	2.12308500	-4.76237300
C	-2.31031800	0.83355600	-4.84526200
H	-1.80418100	-0.00944400	-5.33642200
H	-3.33550900	0.53749700	-4.58510400
H	-2.36065100	1.66613000	-5.56304200
C	-5.64387100	0.18100600	-2.76362500
C	-5.65243000	-1.13021100	-3.54738400
H	-5.48358100	-1.99930600	-2.90500200
H	-6.62833700	-1.24109200	-4.04239800
H	-4.87076500	-1.12339900	-4.32225300
C	-6.61703400	0.12411200	-1.58989300
H	-6.64833600	1.09476300	-1.07329100
H	-7.62974900	-0.12315400	-1.94317600
H	-6.30311800	-0.63862600	-0.86073100
C	-6.03341100	1.30422700	-3.72846100
H	-5.31450800	1.37369500	-4.55747400
H	-7.02663300	1.09604100	-4.15201500
H	-6.08257400	2.27682000	-3.22481300
C	-2.50811800	-3.03602700	-2.65809700
C	-1.39126800	-2.56084600	-3.57814900
H	-1.79816200	-1.87093800	-4.32978100
H	-0.59412600	-2.04252300	-3.02548500
H	-0.95418500	-3.42695300	-4.09470600
C	-1.96063200	-3.87889000	-1.51187200
H	-2.78927300	-4.23007100	-0.87850600
H	-1.43036900	-4.75670900	-1.90550500
H	-1.25154400	-3.29095200	-0.90535000
C	-3.51804400	-3.85818500	-3.45843700
H	-3.90159900	-3.28086700	-4.31103000
H	-3.03562000	-4.76821700	-3.84459400
H	-4.36213300	-4.15807100	-2.82072100
O	1.73182400	-0.43986900	2.56200100
O	3.60456000	1.53747800	2.17353600
O	4.36864800	-1.03548600	2.08898000
C	1.49864800	-1.58421000	3.41602000
C	3.10523100	2.55757600	3.05920900
C	0.11379100	-1.39167700	4.02032700
H	0.01239900	-0.36653100	4.40698500
H	-0.68220300	-1.56447000	3.28361300
H	-0.03226700	-2.09922100	4.84709800
C	2.52906100	-1.66030100	4.54095800
H	3.52871400	-1.84289700	4.13312300
H	2.53633000	-0.73115200	5.12796700
H	2.26852400	-2.49055000	5.21378800
C	2.57266400	1.96943600	4.36481300
H	1.69747400	1.33443000	4.17594400
H	3.34497700	1.37467700	4.87350700
H	2.27764000	2.78964400	5.03612300
C	4.28378800	3.48729100	3.33648700
H	4.66773300	3.90827900	2.39740400
H	3.96607600	4.31351200	3.98977800
H	5.09928300	2.94484000	3.83748900
C	1.99442100	3.32646700	2.35823200
H	1.58053100	4.08228000	3.03885300
H	2.38625000	3.84672400	1.47340000
H	1.17363700	2.64955000	2.06443200
C	5.70177400	-0.80269400	2.58577800
C	5.69208700	-0.16594400	3.97560600
H	5.22747100	-0.82158900	4.72396300
H	6.72926600	0.02643200	4.28946400
H	5.15797100	0.79087200	3.94716600

C	6.33701000	-2.18668200	2.66577800
H	6.30694500	-2.68979000	1.69144700
H	7.38328300	-2.11425200	2.99764800
H	5.78440800	-2.80618400	3.38818100
C	6.44066600	0.12735600	1.62559800
H	7.51992400	0.13556100	1.84084300
H	6.28196800	-0.18461500	0.58247600
H	6.04770400	1.14798300	1.73819600
C	1.57322700	-2.84734500	2.56576700
H	1.33362500	-3.73375800	3.17241800
H	0.85764400	-2.79089800	1.73115600
H	2.59472900	-2.95819800	2.16742400
H	-1.42874200	-4.56317800	5.58376300
Ge	-1.05212500	0.16723000	0.99584100
Ge	1.08302600	-0.33108100	-0.98575200

:Ge(H)^{tBuO}L*

H	-7.119067	-0.607454	-3.506052
H	-6.715042	-2.466310	-1.898264
C	-6.252959	-0.581807	-2.843686
C	-6.024943	-1.622647	-1.944242
H	-5.546212	1.324251	-3.569243
C	-5.371820	0.496993	-2.879799
H	-4.471207	0.154961	4.091939
C	-4.922382	-1.586997	-1.092276
H	-4.763952	-2.397592	-0.378294
H	-3.921816	-2.171947	4.793538
C	-4.009574	-0.536387	3.385418
H	-3.986770	0.899778	1.774992
C	-3.706216	-1.840326	3.777264
C	-4.267150	0.526663	-2.029754
C	-3.727320	-0.114046	2.087291
C	-4.020694	-0.516880	-1.131888
H	-2.952061	3.666559	1.973862
H	-3.584826	1.377820	-2.058117
C	-3.127245	-2.715241	2.860824
C	-3.114970	-0.975882	1.168590
H	-2.889998	2.767869	0.430010
H	-2.885523	-3.736442	3.158312
H	-1.979352	2.177032	1.850994
C	-2.302772	3.077288	1.309287
C	-2.827104	-2.284882	1.569149
C	-2.792834	-0.463729	-0.232367
H	-2.517808	0.595154	-0.121151
H	-2.332811	-2.964689	0.872385
H	-2.147832	5.794214	0.738981
H	-2.681331	-2.472160	-2.099980
H	-0.869073	4.825556	2.808998
H	-2.152018	4.838220	-0.772941
C	-1.094378	3.896663	0.867258
C	-1.547007	5.133666	0.096974
H	0.203454	3.420636	2.548861
C	-1.565679	-1.169234	-0.800433
C	-0.244556	4.302349	2.069675
C	-1.689830	-2.209583	-1.726386
H	-1.486132	2.247379	-1.967349
H	0.134009	1.357322	2.865234
H	-1.769455	-4.333663	-3.311912
H	-1.521074	1.908528	-3.719783
Ge	-0.231202	-0.150892	2.432231
H	-0.669810	5.691158	-0.262575
H	-1.238592	0.573913	-2.574558
O	-0.329472	3.134852	-0.072638
C	-1.040499	1.637548	-2.767402
H	0.561401	4.983458	1.762937
H	-0.398989	-3.653304	-4.214286
N	-0.122877	0.296698	0.572944
C	-0.725576	-4.004940	-3.223367
C	-0.581035	-2.913441	-2.194857
C	-0.284675	-0.798256	-0.342597
H	1.426730	-4.407170	3.246465
H	0.335180	3.998677	-2.363148
H	2.312303	-2.898836	5.016596
Si	0.625266	1.767122	-0.029600
C	1.803059	-3.417930	2.982398
H	0.256046	3.642344	-4.115777

H	-0.107672	-4.877130	-2.966779
C	0.461664	1.893119	-2.850019
C	2.299045	-2.573097	3.975990
H	1.351624	-3.650939	0.884624
C	0.734346	3.361696	-3.165619
C	0.676767	-2.574003	-1.689530
C	0.841493	-1.538263	-0.769938
C	1.767054	-2.997326	1.654906
O	1.121058	1.551035	-1.613899
H	0.618900	1.178789	-4.891997
C	2.766180	-1.306230	3.631553
H	2.087576	4.674051	0.405177
O	1.991503	2.008561	0.902780
H	3.145470	-0.632429	4.401447
H	0.918731	-0.066140	-3.640273
C	1.078435	0.988826	-3.911049
H	1.816372	3.537248	-3.259690
C	2.239526	-1.729191	1.295260
H	1.555428	-3.130520	-2.024432
H	2.364460	3.814277	-1.129744
C	2.739965	-0.887900	2.298231
H	3.043419	3.730285	2.557044
C	2.204751	-1.246500	-0.146435
C	2.807063	4.065113	-0.157400
H	2.328376	-0.157500	-0.107403
H	3.072197	0.115863	2.026908
H	2.159664	1.177260	-3.990870
C	3.161463	2.794358	0.610171
C	3.763028	3.144379	1.967075
H	3.714473	4.662034	-0.330294
H	4.004894	2.228746	2.526565
H	4.047821	-3.313514	0.341028
C	3.371573	-1.749798	-0.984405
H	3.640965	1.650269	-1.160951
H	4.684610	3.731521	1.843082
H	2.958613	-0.272832	-2.484423
C	4.120396	1.936187	-0.213416
C	4.205057	-2.804452	-0.610543
H	4.392059	1.017895	0.329692
C	3.613132	-1.099869	-2.202584
H	5.044056	2.491460	-0.434555
C	5.251228	-3.209697	-1.444897
C	4.652093	-1.502106	-3.033925
H	5.894244	-4.035683	-1.137476
H	4.823308	-0.983808	-3.978814
C	5.476891	-2.564993	-2.656979
H	6.294263	-2.883378	-3.305207

:Ge(H)L"

H	-6.803400	0.187743	-3.752816
H	-6.349946	-1.986774	-2.627074
C	-5.961789	0.090094	-3.066090
C	-5.706200	-1.126910	-2.436354
H	-5.336189	2.145478	-3.279171
C	-5.139538	1.184381	-2.802210
H	-4.456901	-1.141317	3.836833
C	-4.634386	-1.250713	-1.553147
H	-4.452130	-2.203110	-1.051549
H	-3.606807	-3.483177	3.893791
C	-3.884751	-1.537754	2.996910
H	-4.012494	0.292553	1.861263
C	-3.412008	-2.850112	3.027434
C	-4.066613	1.055997	-1.922336
C	-3.627628	-0.729706	1.891366
C	-3.793547	-0.163080	-1.292687
H	-3.430143	1.919255	-1.716038
C	-2.690346	-3.345004	1.943977
C	-2.876896	-1.208532	0.809958
H	-2.316492	-4.369661	1.959165
C	-2.420147	-2.529398	0.845187
C	-2.592512	-0.275021	-0.362588
H	-2.433628	0.721842	0.073639
H	-1.822122	-2.915178	0.017512
H	-2.282726	-1.647368	-2.705935
C	-1.296766	-0.656047	-1.072461
C	-1.319594	-1.400152	-2.254736

H	0.105990	1.002734	3.170604
H	-1.125016	-3.168964	-4.269178
Ge	-0.096301	-0.378478	2.357299
H	-0.159740	-1.894810	-5.038008
N	0.012788	0.504018	0.685146
C	-0.197769	-2.586605	-4.181972
C	-0.148701	-1.828194	-2.881168
C	-0.056266	-0.305909	-0.493306
H	1.864616	-4.457610	2.091988
H	2.923727	-3.472753	4.117087
Si	0.314798	2.281527	0.523113
C	2.250626	-3.437790	2.065736
H	0.654416	-3.273538	-4.275070
C	2.843205	-2.887252	3.200691
H	1.623690	-3.104530	0.027213
C	1.070960	-1.515238	-2.278212
C	1.133673	-0.773918	-1.097741
C	2.122806	-2.681299	0.901439
C	3.329277	-1.580411	3.158997
H	3.796751	-1.140525	4.040993
C	2.601757	-1.367898	0.849392
H	1.999837	-1.854853	-2.742053
C	3.218055	-0.831577	1.987155
C	2.464319	-0.510116	-0.400522
H	2.438079	0.528948	-0.045166
H	3.612253	0.187506	1.948040
H	4.303052	-2.577930	-0.696422
C	3.669295	-0.614354	-1.325658
H	3.318460	1.345329	-2.159926
C	4.494855	-1.740841	-1.369205
C	3.952102	0.454777	-2.185840
C	5.568953	-1.801488	-2.258956
C	5.024029	0.398137	-3.071991
H	6.202436	-2.689419	-2.277710
H	5.227737	1.243523	-3.730504
C	5.836932	-0.735177	-3.113535
H	6.678667	-0.782612	-3.805352
C	0.672912	2.639789	-1.334310
C	1.482486	3.912766	-1.629701
C	-0.614541	2.650641	-2.171000
H	1.264100	1.776862	-1.686066
H	2.541574	3.805851	-1.366192
H	1.435475	4.145410	-2.706482
H	1.097215	4.795211	-1.093930
H	-1.214023	1.740292	-2.028057
H	-1.243230	3.523001	-1.925296
H	-0.371344	2.716665	-3.243734
C	1.797210	2.710968	1.685022
C	1.501348	3.796444	2.726344
C	3.151941	3.012604	1.028402
H	1.913038	1.764402	2.237818
H	0.574634	3.597925	3.283118
H	2.324143	3.860142	3.457449
H	1.412836	4.787376	2.253602
H	3.409027	2.332956	0.200316
H	3.182923	4.039548	0.636123
H	3.956497	2.933414	1.778950
C	-1.334833	3.167497	0.941329
C	-1.267355	4.697611	0.852596
C	-2.043919	2.734420	2.225659
H	-1.971384	2.828666	0.101912
H	-0.812285	5.043124	-0.087685
H	-2.278909	5.132591	0.907762
H	-0.686806	5.122097	1.684465
H	-2.170280	1.642170	2.279330
H	-1.494787	3.043521	3.127627
H	-3.049279	3.186010	2.278427

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