An Acyclic Zincagermylene: Rapid Activation of Dihydrogen at Sub-Ambient Temperature

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Electronic Supplementary Information (30 pages)

Contents

1. Experimental

General considerations.

All manipulations were carried out using standard Schlenk and glove box techniques under an atmosphere of high purity dinitrogen. Pentane was distilled over Na/K alloy (50:50), while hexane was distilled over molten potassium. ^{1}H, ^{13}C{^{1}H}, ^{29}Si{^{1}H} and ^{11}B{^{1}H} NMR spectra were recorded on either Bruker DPX300 or Bruker AvanceIII 400 spectrometers and were referenced to the resonances of the solvent used, external $SiMe_4$, or external $BF_3.OEt_2$. Mass spectra were collected using an Agilent Technologies 5975D inert MSD with a solid state probe. FTIR spectra were collected for solid samples on an Agilent Cary 630 attenuated total reflectance (ATR) spectrometer. The microanalysis were carried out at the Science Centre, London Metropolitan University. Melting points were determined in sealed glass capillaries under dinitrogen, and are uncorrected. (TBoN)GeCl[1] and L*Zn−Mg(^{Mes}Nacnac)[2] were prepared by literature methods. All other reagents were used as received.

:Ge(ZnL*)(TBoN) 2. A solution of (TBoN)GeCl (1.00 g, 1.71 mmol) in hexane (30 mL) was added to a suspension of L*Zn−Mg(^{Mes}Nacnac) **1** (1.74 g, 1.71 mmol) in hexane (20 mL) at -80 °C over 5 min. The reaction mixture was warmed to room temperature and stirred for 2 hrs, affording a dark green solution. Volatiles were removed *in vacuo* and the residue was extracted with hexane (30 mL). The dark green extract was filtered and the filtrate concentrated (to *ca.* 10 mL), affording dark blue crystals of **2** overnight at -25 °C (1.48 g, 71 %). N.B. Crystals of **2** used for the X-ray diffraction experiment were grown from a pentane solution. M.p. 182-184 °C; ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ = -0.03 (s, 9H, Si(CH_3)$_3$), 1.20-1.28 (overlapping m, 45H, Si{CH(CH$_3$)$_2$}$_3$, Si{CH(CH_3)$_2$}$_3$, CH(CH_3)$_2$), 1.93 (s, 3H, ArCH_3), 3.04 (br., 2H, CH(CH$_3$)$_2$), 3.56 (br., 2H, CH(CH$_3$)$_2$), 6.18 (s, 2H, {N(Dip)C(H)}$_2$), 6.65 (s, 2H, Ph$_2$CH), 6.96-7.33 (m, 28H, ArH); ^{13}C{^{1}H} NMR (75 MHz,C_6D_6, 298 K): δ = 5.1 (Si(CH$_3$)$_3$), 14.9 (Si{CH(CH$_3$)$_2$}$_3$), 16.3 (Si{CH(CH_3)$_2$}$_3$), 19.6 (br., CH(CH$_3$)$_2$), 21.1 (ArCH$_3$), 28.6 (CH(CH$_3$)$_2$), 51.8 (Ph$_2C$H), 118.9 ({N(Dip)C(H)}$_2$), 124.1, 126.5, 128.6, 128.7, 129.5, 130.1, 130.2, 130.5, 139.5, 142.0, 145.3, 147.6 (Ar-*C);* ^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 298 K): δ = 1.83, 1.66; ^{11}B{^{1}H} NMR (128 MHz, C_6D_6, 298 K): δ = 23.2; UV/vis (hexane) [λ_{max}, nm (ε, M^{-1} cm^{-1})]: 590 (141); IR ν/cm^{-1} (ATR): 1599 (w), 1523 (m), 1492 (m), 1240 (m), 1202 (m), 1177 (m), 1117 (m), 1075 (m), 1029 (m), 970 (w), 758 (m), 732 (m), 703 (s), 679 (m); MS/EI *m/z* (%): 595.5 (L*H$^+$, 19.6), 552.4 (L*H-Pr^{i+}, 57.7), 475.5 (TBoNH$^+$, 9.3), 167.1 (Ph$_2$CH$^+$, 100); anal. calcd. for $C_{71}H_{93}BGeN_4Si_2Zn$: C 70.62 %, H 7.76 %, N 4.64 %, found: C 70.44 %, H 7.65 %, N 4.75 %.

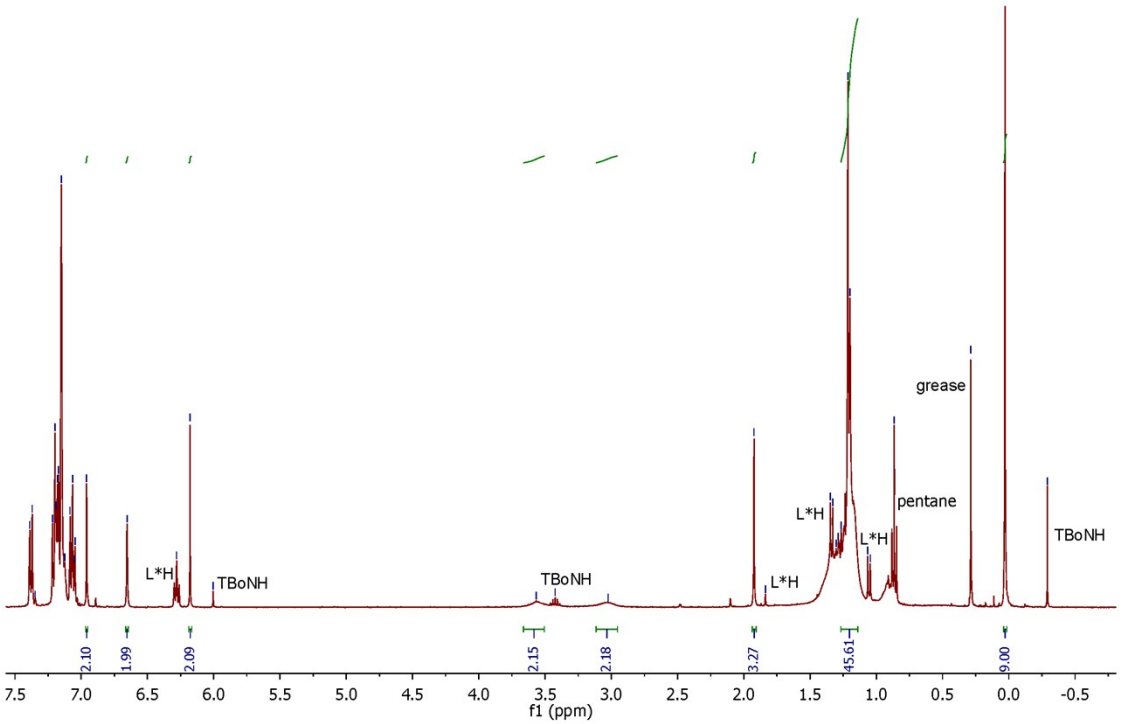


Figure S1. ^{1}H NMR spectrum (C_6D_6, 298 K) of compound **2**. Resonances arising from pentane of crystallisation, silicone grease and minor secondary amine decomposition products marked.

Ge(H)$_2$(ZnL*)(TBoN) 3. A suspension of **2** (1.00 g, 0.83 mmol) in hexane (30 mL) was stirred rapidly under an atmosphere of H_2. The green suspension turned yellow within 2 mins and was stirred for a further 20 mins. Volatiles were then removed *in vacuo* and the residue extracted with hexane (30 mL). The yellow extract was filtered and the filtrate concentrated (to *ca.* 10 mL), affording colorless crystals of **3** overnight at -25 °C (821 mg, 82 %). N.B. Exposure of a C_6D_6 benzene solution of **2** to an atmosphere of H_2 led to the near quantitative formation of **3** in less that 5 secs (as determined by ^{1}H NMR spectroscopy). M.p. 196-200 °C; ^{1}H NMR (400 MHz, C_6D_6, 298 K) δ = -0.14 (s, 9H, Si(CH_3)$_3$), 1.18-1.24 (overlapping m, 33H, Si{CH(CH$_3$)$_2$}$_3$, Si{CH(CH_3)$_2$}$_3$, CH(CH_3)$_2$), 1.39 (d, J = 6.7 Hz, 12H, CH(CH_3)$_2$) 1.82 (s, 3H, ArCH_3), 3.46 (br., 4H, CH(CH$_3$)$_2$), 3.88 (s, 2H, GeH_2) 6.12 (s, 2H, {N(Dip)C(H)}$_2$), 6.58 (s, 2H, Ph$_2$CH), 6.88-7.33 (m, 28H, ArH); ^{13}C{^{1}H} NMR (75 MHz, C_6D_6, 298 K): δ = 3.5 (Si(CH$_3$)$_3$), 14.9 (Si{CH(CH$_3$)$_2$}), 16.2 (Si{CH(CH_3)$_2$}), 19.5 (br., CH(CH$_3$)$_2$), 21.1 (ArCH$_3$), 28.6 ((CH(CH$_3$)$_2$) 51.5 (Ph$_2$$C$H), 118.6 ({N(Dip)$C$(H)}$_2$), 123.9, 126.6, 127.9, 128.3, 128.4, 129.5, 129.6, 130.5, 140.8, 141.4, 145.3, 146.9 (Ar-C); ^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 298 K): δ = 3.31, 4.50; ^{11}B{^{1}H} NMR (128 MHz, C_6D_6, 298 K): δ = 23.6; IR ν/cm^{-1} (Nujol): 2054 (s, GeH str.), 1995 (s, Ge-H str.), 1253 (m), 1227 (w), 1208 (w), 1179 (w), 1155 (w), 1110 (w), 1075 (w), 1029 (w), 805 (m), 759 (m), 738 (m), 699 (m), 655 (m); MS/EI *m/z* (%): 595.5 (L*H$^+$, 8.2), 552.4 (L*H-Pr^{i+}, 35.1), 475.5 (TBoNNH$^+$, 42.3), 386.3 ((BoN)$^+$, 13.9) 167.1 (Ph$_2$CH$^+$, 100), 73 ((TMS)$^+$, 20.5). N.B. a reproducible microanalysis could

not be obtained for the compound as it consistently crystallised with small amounts of L*H and TBoNH (*ca.* 5%) which could not be separated by fractional crystallisation. N.B. The di-deuteride analogue of **3**, *viz.* **3-D**, was prepared by treating a C_6D_6 solution of **2** with an excess of D_2 gas at 20 °C. ^{2}H NMR (C_6D_6, 61.4 MHz, 298 K): δ = 3.86 ppm. Any kinetic isotope effect relating to the rate of the deuteration *vs.* hydrogenation reactions was not determined.

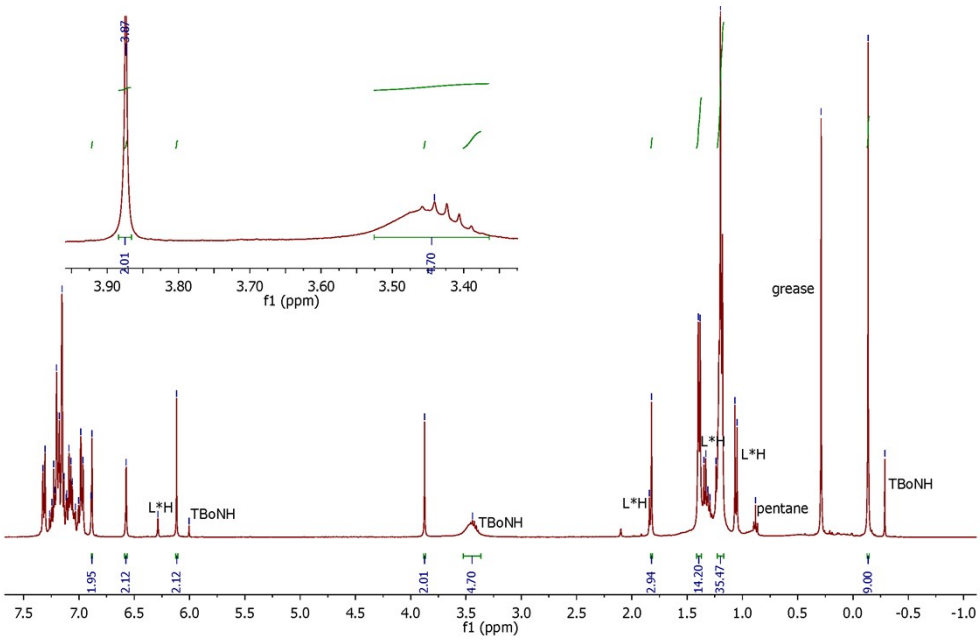


Figure S2. ^{1}H NMR spectrum (C_6D_6, 298 K) of compound **3**. Resonances arising from pentane of crystallisation, silicone grease and minor secondary amine decomposition products marked.

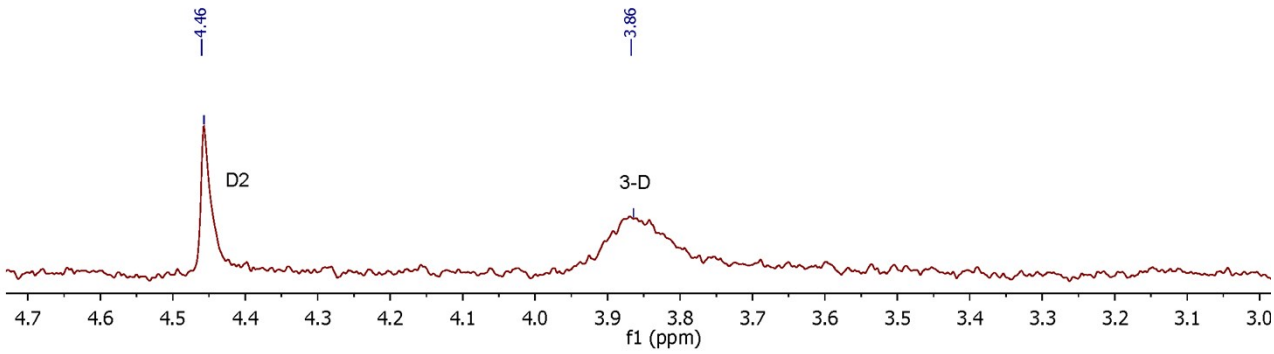


Figure S3. ^{2}H NMR spectrum (C_6D_6, 298 K) of compound **3-D** prepared *in situ* from the reaction of **2** with D_2.

2. X-Ray Crystallography

Crystals of **2**, **3** and :Ge(ZnL*)(L) **1S** suitable for X-ray structural determination were mounted in silicone oil. Crystallographic measurements were made using the Australian Synchrotron (λ = 0.71090 Å). The software package Blu-Ice[3] was used for synchrotron data acquisition, while the program XDS[4] was employed for synchrotron data reduction. All structures were solved by direct methods and refined on F^2 by full matrix least squares (SHELX97[5]) using all unique data. Hydrogen atoms are included in calculated positions (riding model), except the hydride hydrogens of **3**, the atomic displacement parameters of which were refined isotropically. 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. Crystal structure and refinement data for **2**, **3** and :Ge(ZnL*)(L) **1S**.

	2·(pentane)$_{0.6}$	**3**	**1S**
empirical formula	$C_{74}H_{100.2}BGeN_4Si_2Zn$	$C_{71}H_{93}BGeN_4Si_2Zn$	$C_{78}H_{84}GeN_2Si_2Zn$
formula weight	1250.73	1209.46	1243.61
crystal system	monoclinic	triclinic	monoclinic
space group	$P2_1/n$	P-1	$P2_1/c$
a (Å)	12.268(3)	12.899(3)	15.104(3)
b (Å)	40.891(8)	15.071(3)	19.536(4)
c (Å)	14.886(3)	19.496(4)	23.139(5)
α (°)	90	82.02(3)	90
β (°)	90	88.06(3)	106.57(3)
γ (°)	90	65.04(3)	90
V (Å^3)	7323(3)	3401.4(12)	6544(2)
Z	4	2	4
T (K)	100(2)	100(2)	100(2)
ρ_{calcd} (g·cm^3)	1.134	1.181	1.262
μ (mm^{-1})	0.812	0.871	0.908
F(000)	2669	1288	2624
reflns collected	104463	57853	51132
unique reflns	13594	12638	11422
R_{int}	0.1637	0.0877	0.0340
R1 [I > 2σ(I)]	0.0556	0.0541	0.0476
wR2 (all data)	0.1462	0.1387	0.1129
largest peak and hole (e·Å^{-3})	1.11, -1.10	1.12, -0.98	0.75, -0.67
CCDC no.	1576729	1576728	1576727

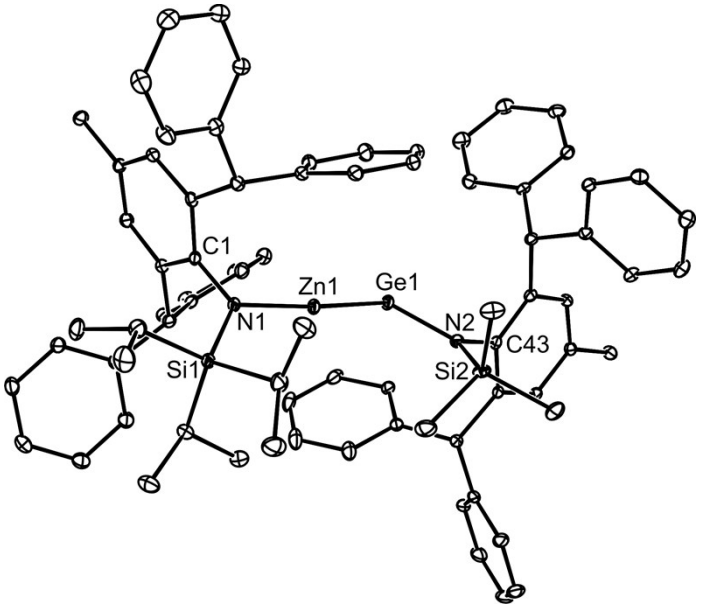


Figure S4. ORTEP diagram of :Ge(ZnL*)(L) **1S** (20% thermal ellipsoids; hydrogen atoms omitted). Zn(1)-N(1) 1.902(2), Zn(1)-Ge(1) 2.4950(9), Ge(1)-N(2) 1.860(3), N(1)-Zn(1)-Ge(1) 156.31(8), N(2)-Ge(1)-Zn(1) 110.69(8).

3. Computational Studies

Geometry optimizations without symmetry restrictions were carried out with the Gaussian 09[6] optimizer in association with Turbomole 6.6[7] energies and gradients. The calculations were performed for all molecules using the BP86[8] functional with def2-TZVPP[9] basis set and dispersion correction by Grimme[10] with Becke-Johnson damping D3(BJ) in conjunction with the resolution-of-identity (RI)[11] approximation (termed as RI-BP86+D3(BJ)/def2-TZVPP). Frequency results were examined to confirm stationary points as transition states (only one imaginary frequency) or minima (no imaginary frequencies). The RI-BP86+D3(BJ)/def2-TZVPP calculated frequencies were used to obtain zero-point energy-corrected enthalpies and free energies at 298.15 K and 1 atm. For comparision, different functions, such B3LYP,[12] and M06-2X,[13] were also examined for the first H_2 activation step by using the def2-TZVPP basis set. For the key H_2 activation step, solvent effects were also estimated by single-point calculations with different functions (i.e., BP86, B3LYP, and M06-2X) at the RI-BP86+D3(BJ)/def2-TZVPP optimized geometries in the gas phase by means of the SMD[14] method with Gaussian 09 and COSMO[15] method with Turbomole 6.6,[7] using the experimental solvent (toluene, $\varepsilon = 2.37$) .

The orbital interactions have been investigated with the EDA-NOCV method[16] which combines the energy decomposition analysis (EDA)[17] with the natural orbital for chemical valence (NOCV)[18,19] method. The interaction energy between the fragments ΔE_{int} which are calculated with

the frozen geometry is decomposed into four main components ΔE_{elstat} (electrostatic interactions), ΔE_{Pauli} (Pauli repulsion), ΔE_{disp} (dispersion interactions), and ΔE_{orb} (orbital interactions). The latter term can be separated into contributions which come from pairwise orbital interactions, which makes it possible to identify the dominant orbitals of the interactions in the transition state. For a detailed description of the method[20-22], we refer to the literature. The EDA-NOCV calculations were carried out with the program package ADF.[23,24] We analyzed the electron density distribution with the QTAIM (Quantum Theory of Atoms in Molecules) method that was developed by Bader.[25] Wiberg bond index P and partial charges q were obtained from a single-point calculation of the molecules with BP86/def2-TZVPP basis sets by using NBO 6.0[26] as implemented with Gaussian 09 program.[6]

All energies discussed in this study are ΔG values at 298 K and 1 atm at the RI-BP86+D3(BJ)/def2-TZVPP unless specified; the electronic energies without zero point corrections are also given for reference.

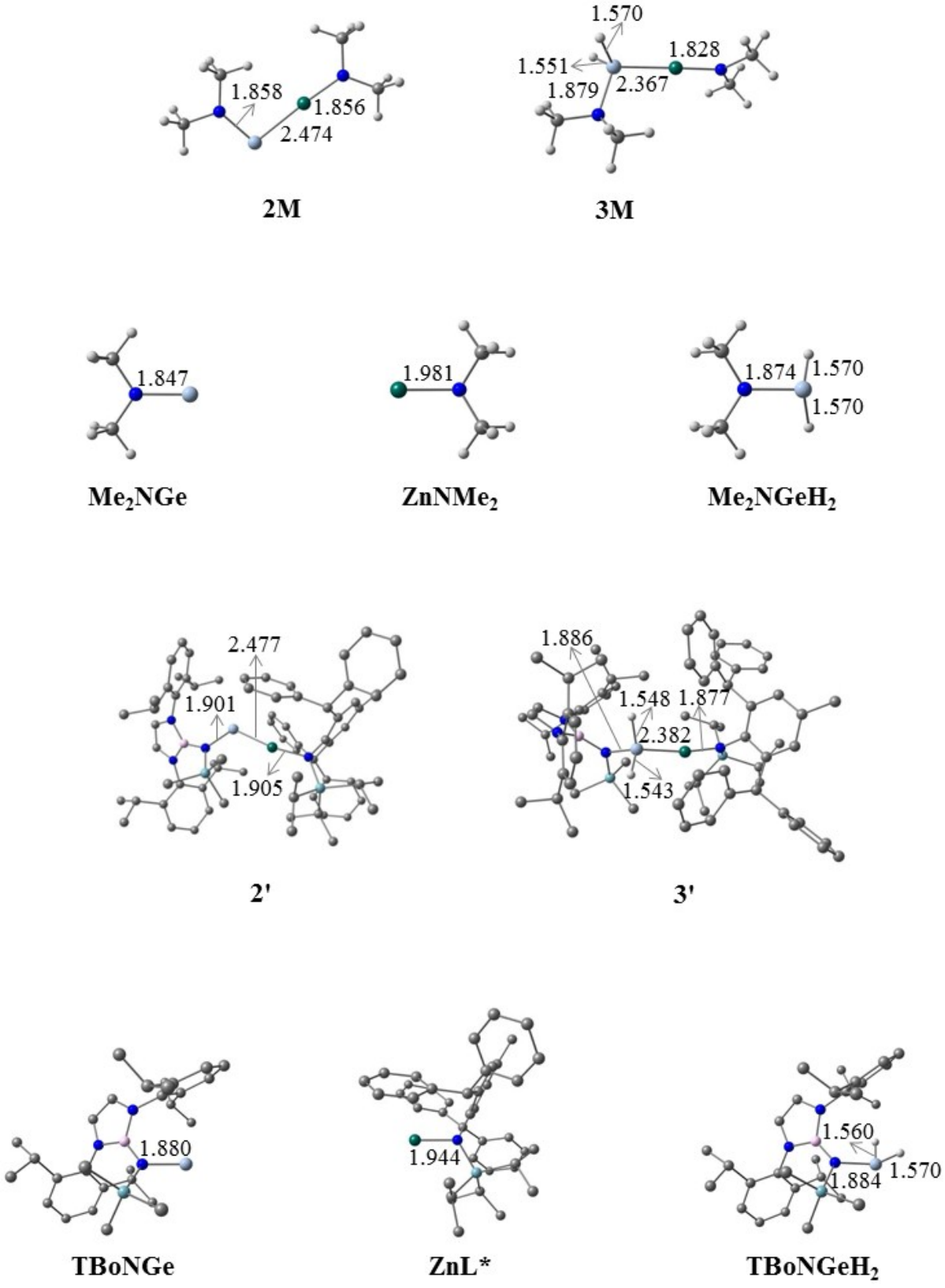


Figure S5. Optimized structures of **2', 2M, 3', 3M** and fragments after breaking the Ge-Zn bond calculated at the BP86-D3(BJ)/def2-TZVPP level. Non-hydride hydrogens are omitted for clarity. Bond distance in Å, angles in degrees.

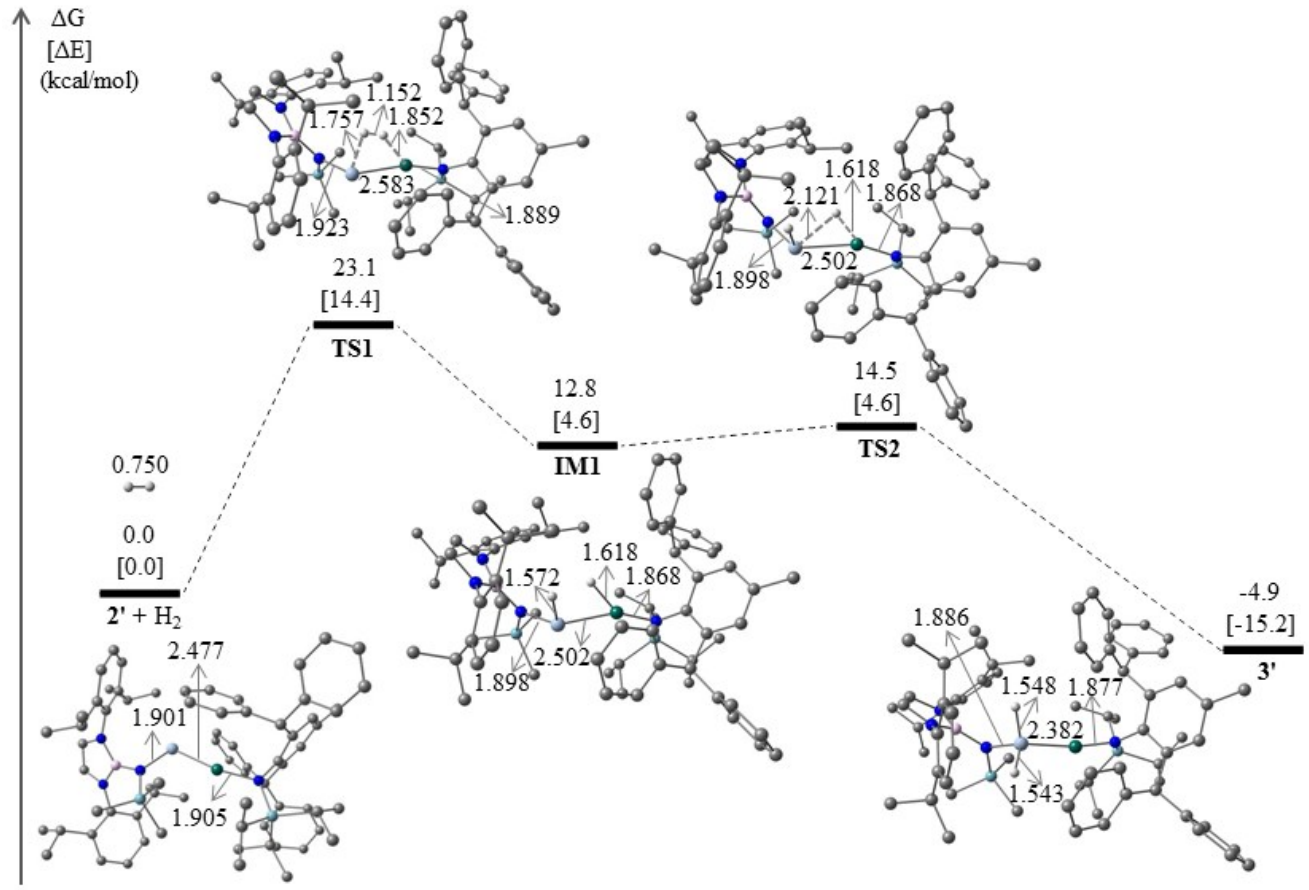
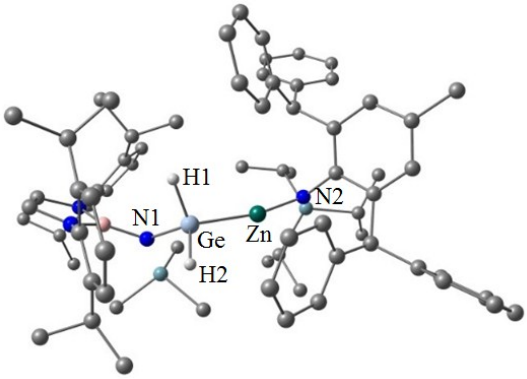
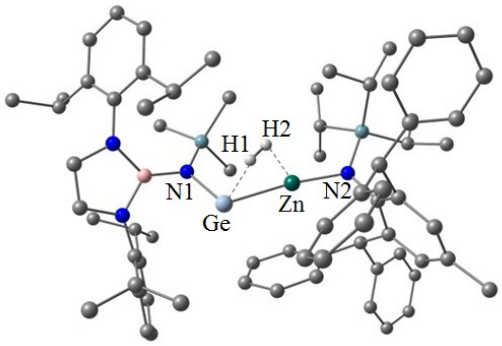


Figure S6. Computed energy profile for the reaction of **2'** with H_2 at the RI-BP86+(D3BJ)/def2-TZVPP level of theory. Key bond distances are given in Å. Non-hydride hydrogens have been omitted for clarity.



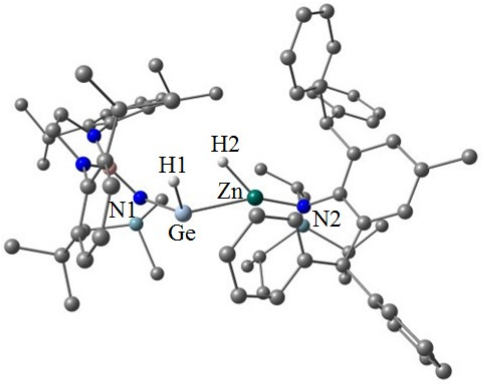
GeH1 = 1.552, GeH2 = 1.546, H1H2 = 2.494
GeZn = 2.382, GeN1 = 1.889, ZnN2 = 1.882

H_2Ge(TBoN)(ZnL*) **A**



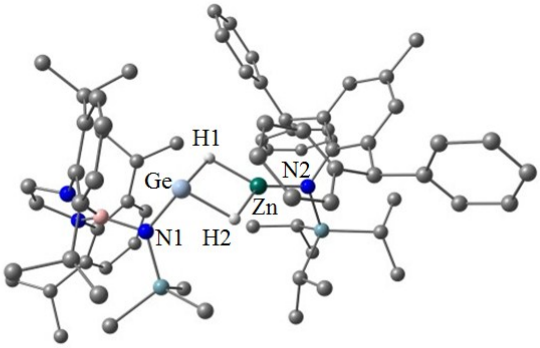
GeH1 = 2.553, ZnH2 = 2.889, H1H2 = 0.780
GeZn = 2.487, GeN1 = 1.914, ZnN2 = 1.906

(TBoN)Ge(μ-H_2)ZnL* **B**



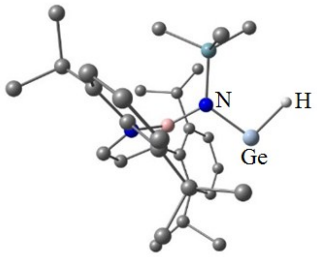
GeH1 = 1.573, ZnH2 = 1.632, H1H2 = 2.229
GeZn = 2.497, GeN1 = 1.900, ZnN2 = 1.873

(TBoN)Ge(H)Zn(H)L* **C**



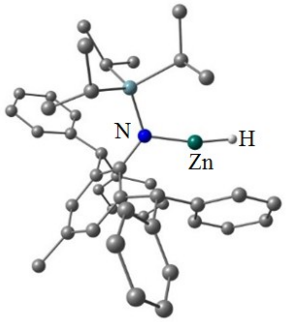
GeH1 = 1.908, GeH2 = 1.782
ZnH1 = 1.718, ZnH2 = 1.794
GeZn = 2.734, GeN1 = 1.929, ZnN2 = 1.890

(TBoN)Ge(μ-$H)_2$ZnL* **D**



GeN = 1.880
GeH = 1.630
∠NGeH = 94.4

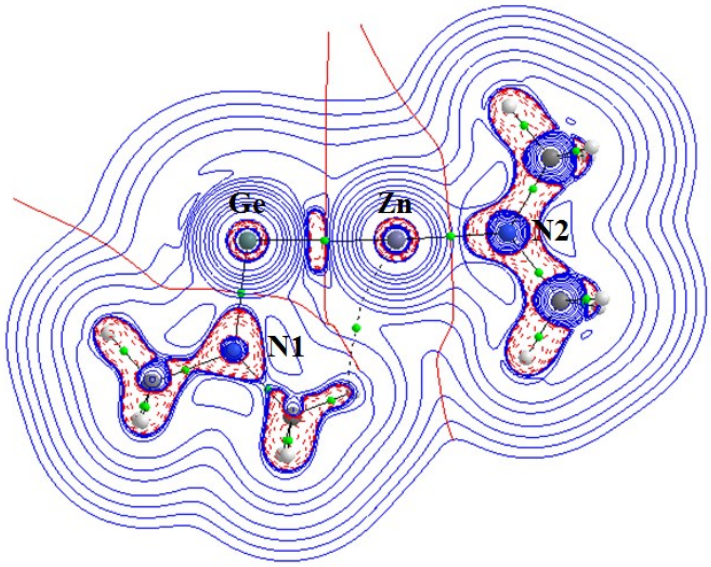
(TBoN)GeH



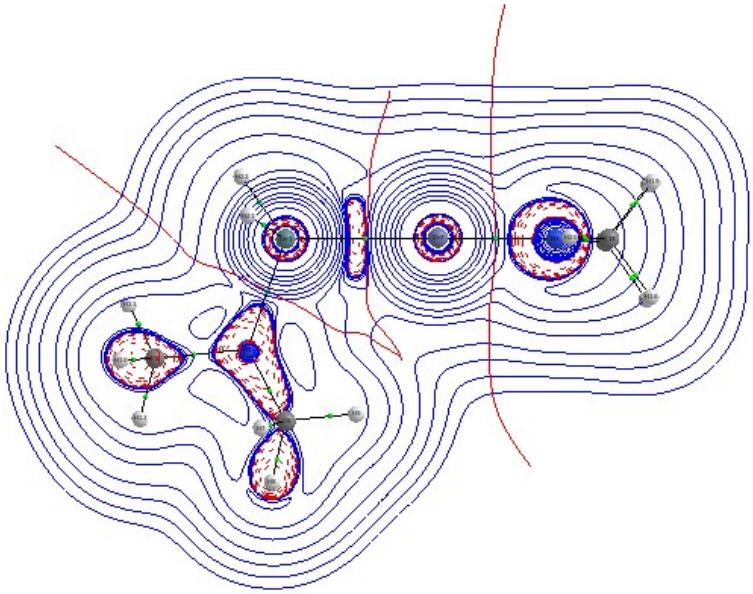
ZnN = 1.874
ZnH = 1.531
∠NZnH = 167.1

L*ZnH

Figure S7. Optimized structures of isomers of H_2Ge(TBoN)(ZnL*) (**3'**) and fragments after breaking the Ge-Zn bond calculated at the BP86-D3(BJ)/def2-SVP level. Non-hydride hydrogens are omitted for clarity. Bond distance in Å, angles in degrees.



(a) Me_2NGe-$ZnNMe_2$ (**2M**)



(b) $Me_2NGe(H_2)$-$ZnNMe_2$ (**3M**)

Figure S8. Laplacian distribution$\nabla^2\rho(r)$ of (a) **2M** and (b) of **3M** in the Ge-Zn-N plane. Dashed red lines indicate areas of charge concentration ($\nabla^2\rho(r) < 0$) while blue lines show areas of charge depletion ($\nabla^2\rho(r) > 0$) at the BP86/def2-TZVPP level. The solid lines connecting the atomic nuclei are the bond paths. Solid red lines indicate the zero-flux surfaces. Green dots are bond critical points.

Table S2. Calculated NBO partial charges q and Wiberg bond orders P of the zinca-germanium bonded compounds **2'**, **3'**, **2M** and **3M** at the BP86/def2-TZVPP level.

	q(Ge)	q(Zn)	q(GeN1R_2)	q(ZnN2R_2)	P(Ge-Zn)
2-M	0.23	0.91	-0.20	0.20	0.81
3-M	0.30	1.12	-0.41[a]	0.41	0.69
2'	0.28	1.04	-0.28	0.28	0.77
3'	0.37	1.19	-0.41[a]	0.41	0.68

[a]Inclusive of hydridic hydrogen atoms at Ge.

Table S3. EDA-NOCV results at the BP86+D3(BJ)/TZ2P+ level of theory for **2'** and **3'**. The interacting fragments are in the electronic doublet (D) states. Energy values are given in kcal/mol.

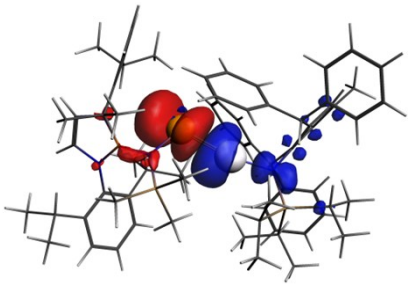
	2'	**3'**
Fragments	R_2NGe (D) + ZnL(D)	R_2NGeH_2 (D) + ZnL(D)
ΔE_{int}	-81.2	-88.0
ΔE_{Pauli}	161.2	160.2
ΔE_{elstat}[a]	-120.4 (49.7 %)	-124.3 (50.1 %)
ΔE_{orb}[a]	-81.6 (33.7 %)	-87.8 (35.4 %)
ΔE_{disp}[a]	-40.4 (16.6 %)	-36.0 (14.5 %)
$\Delta E_{\rho 1}$ [b]	-30.8 (37.7 %)	-46.5 (53.0 %)
$\Delta E_{\rho 2}$ [b]	-30.2 (37.0 %)	-25.5 (29.0 %)
$\Delta E_{\rho 3}$ [b]	-4.7 (5.8 %)	-2.7 (3.1 %)
$\Delta E_{\rho 4}$ [b]	-3.3 (4.0 %)	-2.2 (2.5 %)
ΔE_{rest}	-12.6 (15.5 %)	-10.9 (12.4 %)

[a]The values in parentheses give the percentage contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb} + \Delta E_{disp}$.

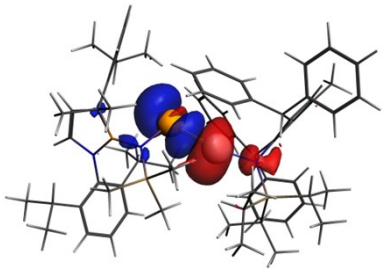
[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}

Figure S9. Plot of deformation densities $\Delta\rho_{1\text{-}4}$ of the pairwise orbital interactions between the two fragments in **2'** and **3'**, associated interaction energies ΔE_{orb} (in kcal/mol) and eigenvalues ν. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue.

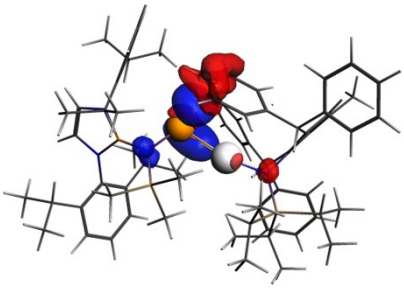
2'



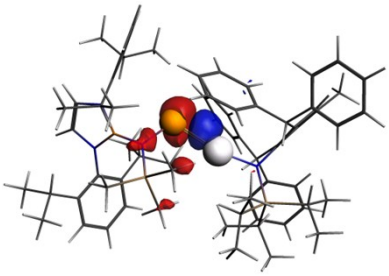
$\Delta E_{\rho 1}$ = -30.8 kcal/mol, ν_1= ±0.546



$\Delta E_{\rho 2}$ = -30.2 kcal/mol, ν_2 = ±0.537

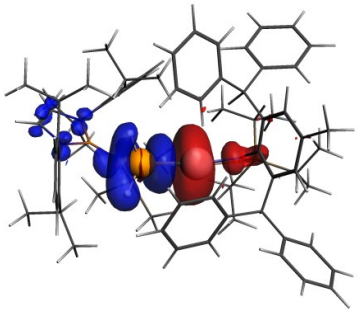


$\Delta E_{\rho 3}$ = -4.7 kcal/mol, ν_3= ±0.257

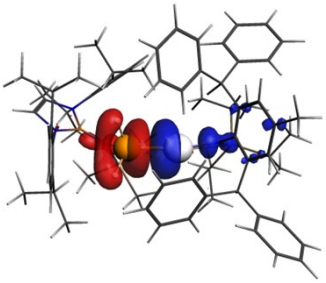


$\Delta E_{\rho 4}$ = -3.3 kcal/mol, ν_4= ±0.161

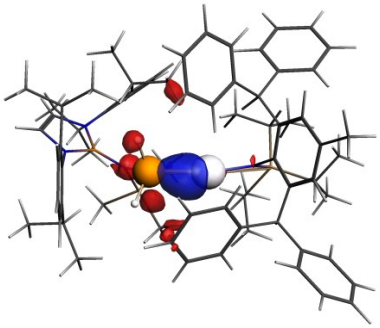
3'



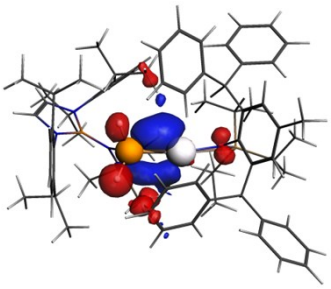
$\Delta E_{\rho 1}$ = -46.5 kcal/mol, ν_1= ±0.612



$\Delta E_{\rho 2}$ = -25.5 kcal/mol, ν_2 = ±0.440



$\Delta E_{\rho 3}$ = -2.7 kcal/mol, ν_3= ±0.129



$\Delta E_{\rho 4}$ = -2.2 kcal/mol, ν_4= ±0.132

Table S4. Bond dissociation energies D_e (kcal/mol) for the dissociation reactions of **2M**, **3M**, **2'** and **3'** yielding fragments in the doublet (D) state at the BP86+D3(BJ)/def2-TZVPP level of theory.

	D_e
2M → Me_2NGe (D) + $ZnNMe_2$ (D)	52.1
3M → Me_2NGeH_2 (D) + $ZnNMe_2$ (D)	59.6
2' → TBoNGe (D) + ZnL* (D)	72.8
3' → $TBoNGeH_2$ (D) + ZnL* (D)	80.7

Table S5. Computed barriers of **TS1** with different methods, using the def2-TZVPP basis set at the BP86+(D3BJ)/def2-TZVPP optimized geometry. The single point and COSMO calculations were conducted by using the Gauss-Turbomole program, the SMD solvent model is used by Gaussian program.

Methods	Gas phase			COSMO			SMD		
	BP86 +(D3BJ)	B3LYP +(D3BJ)	M06-2X +(D3ABC)	BP86 +(D3BJ)	B3LYP +(D3BJ)	M06-2X +(D3ABC)	BP86	B3LYP	M06-2X
ΔG [ΔE]	23.1 [14.4]	25.6 [16.9]	23.9 [15.1]	23.1 [14.4]	25.6 [16.9]	23.9 [15.2]	18.6 [9.8]	21.5 [12.8]	22.5 [13.8]

Table S6. H_2 activation barriers computed using different functions, BP86, B3LYP, and M06-2X at the RI-BP86+D3(BJ)/def2-TZVPP optimized geometries. Solvent effects were also estimated by single-point calculations with different functionals by means of the SMD and COSMO methods, using the experimental solvent (toluene, ε = 2.37).

	Functions	H_2	**2'**	**TS1**
Gas phase	BP86+(D3BJ)	-1.177952843123	-7443.402147967	-7444.557196886
	B3LYP+(D3BJ)	-1.173495008828	-7440.479412888	-7441.626044061
	M06-2X+(D3ABC)	-1.168929581656	-7440.929598965	-7442.074402912
COSMO	BP86+(D3BJ)	-1.178124496909	-7443.410419158	-7444.565578892
	B3LYP+(D3BJ)	-1.173674543359	-7440.487640145	-7441.634384013
	M06-2X+(D3ABC)	-1.169125533954	-7440.939229720	-7442.084207894
SMD	BP86	-1.17742919028	-7442.68983045	-7443.85158822
	B3LYP	-1.17953103297	-7442.35979311	-7443.51897664
	M06-2X	-1.16822932549	-7440.95691959	-7442.10320819

Table S7. Relative energies (ΔE, ΔE_o, ΔG, in kcal/mol) for **A-D**, and ((TBoN)GeH + L*ZnH) (see Figure S7) at the BP86+D3(BJ)/def2-SVP level of theory.

Energy	**A**	**B**	**C**	**D**	(TBoN)GeH + L*ZnH
ΔE	0.0	20.7	20.0	14.5	52.2
ΔE_o	0.0	18.3	19.1	13.6	49.1
ΔG	0.0	18.0	18.0	13.5	32.1

Table S8. EDA-NOCV results at the BP86+D3(BJ)/TZ2P+ level of theory of Me_2NGe-$ZnNMe_2$ using different electronic states (singlet:S; doublet: D, triplet: T) of the fragments Me_2NGe and $ZnNMe_2$. The smaller ΔE_{orb} value suggests that the description in terms of dative bonding is more favorable. Energy values are given in kcal/mol.

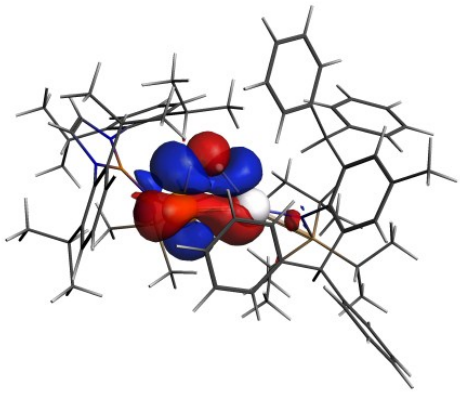
	TS1	
Fragments	**2** (S) + H_2 (S)	**2** (T) + H_2 (T)
ΔE_{int}	-32.5	-180.1
ΔE_{Pauli}	139.5	105.2
ΔE_{disp}	-3.6	-3.6
ΔE_{elstat}[a]	-65.4 (38.8 %)	-103.5 (36.7 %)
ΔE_{orb}[a]	-103.0 (61.2 %)	-178.2 (63.3 %)
$\Delta E_{\rho 1}$ [b]	-92.5.2 (89.8%)	
$\Delta E_{\rho 2}$ [b]	-7.7 (7.5%)	
ΔE_{rest}	-2.8 (2.7%)	

[a]The values in parentheses give the percentage contribution to the total attractive interactions ΔE_{elstat} + ΔE_{orb}.

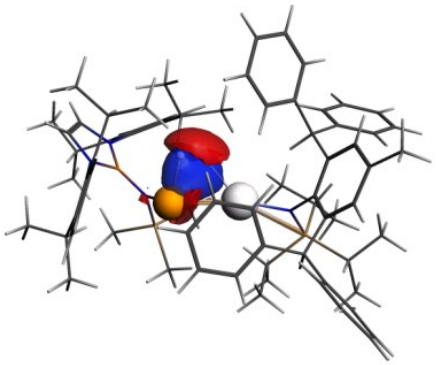
[b]The values in parentheses give the percentage contribution to the total orbital interactions ΔE_{orb}

Figure S10. Plot of deformation densities $\Delta\rho_{1\text{-}2}$ of the pairwise orbital interactions between the two fragments in **TS1**, associated interaction energies ΔE_{orb} (in kcal/mol) and eigenvalues ν. The eigenvalues ν indicate the size of the charge flow, and the direction of charge flow is red→blue. Shape of the most important interacting occupied and vacant orbitals of fragments**.**

TS1



$\Delta E_{\rho 1}$ = -92.5 kcal/mol, ν_1= ±1.463



$\Delta E_{\rho 2}$ = -7.6 kcal/mol, ν_2 = ±0.169

Table S9. Coordinates and energies (in hartree) of the calculated structures at the BP86-D3(BJ)/def2-TZVPP level.

H_2

Energy = -1.177952843123

H	-2.0277411	1.3206099	0.0000000
H	-1.2780585	1.3206099	0.0000000

2'

Energy = -7443.402147967

Ge	3.7342231	26.7722171	7.2737304
Zn	3.3342461	25.4725541	9.3435604
Si	4.8773054	28.8186886	9.5687232
Si	2.4584658	24.4954279	12.2704979
N	3.6102407	30.5951379	6.7154821
N	5.1476916	29.3369112	5.5734955
N	2.6539843	24.1758527	10.5621574
N	4.4505270	28.4157011	7.9053766
C	6.0300481	28.3286966	5.0878722
C	2.6674089	20.6682695	9.2949402
H	3.3755422	19.8434923	9.2005969
C	3.8480385	31.1752155	5.4602337
H	3.3410103	32.0771657	5.1430674
C	3.1178365	21.8883607	9.7945760
C	4.7568798	30.4280546	4.7822587
H	5.1782127	30.5939410	3.7985925
C	4.6024215	22.1641791	9.9827805
H	4.7089410	22.7611705	10.8997258
C	2.2143484	22.9745598	9.9629611
C	5.0961951	23.0496840	8.8401272
C	2.6253999	31.0713970	7.6323394
C	1.3434826	20.4891714	8.8673887
C	5.6211519	27.5048234	4.0176674
C	-0.2036033	24.3538963	7.8149615
C	0.9093189	22.8293724	9.4313740
C	5.4347133	20.9083660	10.1638463
C	6.5365782	26.5723192	3.5096936
H	6.2410459	25.9343887	2.6764513
C	4.4908943	23.0136677	7.5710657
H	3.6616058	22.3284834	7.3980259
C	2.8191839	32.2973873	8.3106030
C	4.9361224	23.8434659	6.5407048
H	4.4572182	23.7985908	5.5627314
C	4.2269941	27.5938854	3.4209620
H	3.6318523	28.2522158	4.0681388
C	7.3064786	28.1834106	5.6801401
C	3.9829668	33.2215293	7.9898121
H	4.7468008	32.6273654	7.4671109
C	-1.4486929	24.6570642	7.2551062
H	-2.3421627	24.6228066	7.8763973
C	6.1623495	23.9368266	9.0413334
H	6.6529837	23.9695784	10.0143260
C	7.8058193	26.4350777	4.0629732
H	8.5027111	25.7005777	3.6592514
C	0.5019485	21.6017397	8.8940296
H	-0.4986123	21.5257377	8.4629314
C	3.8833347	25.6965876	12.6826339
H	3.8661994	26.4126010	11.8374166
C	2.5946104	22.8431091	13.2176199
H	3.4412915	22.3234921	12.7349173
C	1.4689324	30.2892020	7.8575572
C	6.0466619	27.5210184	10.2622824
H	5.6276701	26.5074073	10.2471712
H	6.3021096	27.7621851	11.3041089
H	6.9773778	27.5024857	9.6797118
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H	0.0600227	24.6296299	12.0999890
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H	6.1772223	20.8159725	8.1418561
C	6.5883831	24.7915359	8.0206161
H	7.3995959	25.4948625	8.2040024
C	3.3459278	28.9717317	10.6395860
H	2.7647403	29.8619975	10.3652305
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H	3.2387390	28.2969596	1.6084339
H	4.8376797	27.5733538	1.3230175
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H	2.0882600	28.7137200	6.5609488
C	3.5379613	26.2225460	3.4059715
H	4.0484901	25.5141205	2.7387288
H	2.5002659	26.3213950	3.0587570
H	3.5228209	25.8036852	4.4206700
C	-1.6945770	22.9161437	10.8478505
H	-1.1471568	21.9792876	10.7637121
C	4.6270505	33.8469114	9.2362055
H	3.9512703	34.5656221	9.7201233
H	5.5361116	34.3951632	8.9539254
H	4.9015918	33.0877992	9.9772467
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H	3.0657171	33.9386857	6.1224448
H	4.3720768	34.9740234	6.7429247
H	2.7739299	34.9768082	7.5268800
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H	9.1650109	27.0962805	5.5917779
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H	1.8969902	24.1024808	7.3829137
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H	6.8786365	30.3165492	9.3617187
H	5.7560109	30.8982796	10.6035237
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H	0.4639739	27.0099475	7.2098588
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H	0.9927533	26.0224055	14.6739331
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C	1.3508276	21.9564042	13.0329905
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H	1.1552029	21.7366968	11.9765697
H	0.4502177	22.4346467	13.4438628
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H	-0.3764128	27.0556962	11.9564588
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H	1.3027012	27.4250504	12.3870267
C	0.7491898	31.9031718	9.5290307
H	0.0272330	32.2184356	10.2824303
C	0.2058406	29.4296172	5.8707812
H	-0.7535810	29.8022484	6.2577906
H	0.0056336	28.5467356	5.2478528
H	0.6440155	30.2119761	5.2370467
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H	8.6668589	27.4846616	8.0039363
H	9.0102835	29.1323342	8.5723137
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H	2.1466046	23.5272804	15.2553844
H	3.8735722	23.5405086	14.8714439
H	3.0445869	22.0043068	15.1828357
C	3.7206015	26.5205820	13.9667958
H	3.6788555	25.8796057	14.8585730
H	2.8075948	27.1285163	13.9551765
H	4.5733354	27.2058807	14.0992126
C	-2.8110131	22.9919822	11.6858912
H	-3.1330154	22.1057064	12.2330270
C	8.0458577	30.4979471	6.3522517
H	8.9153580	30.4823930	5.6794929
H	8.2857060	31.1472281	7.2061153
H	7.2013302	30.9438788	5.8135535
C	5.4426604	20.2777431	11.4163244
H	4.8701409	20.7167971	12.2352266
C	6.1612461	19.1008628	11.6206728
H	6.1573919	18.6267338	12.6023996

TS1

Energy = -7444.557196886

Ge	0.2362223	-2.3680334	0.1825951
Zn	-0.8945237	-0.1286055	-0.4306884
Si	-2.2634628	-3.1807720	1.9712152
Si	-3.5263733	1.4911671	-1.1857632
N	0.4021347	-3.0873042	4.3101028
N	1.6449818	-4.0856542	2.6605510
N	-1.7879214	1.3022545	-1.2810404
N	-0.5290325	-2.9475084	1.8483486
C	2.2062092	-4.5283762	1.4294712
C	0.0495686	2.9655801	-4.0691719
H	0.2321076	2.8029386	-5.1320343
C	1.5488004	-3.6780859	4.8700032
H	1.7596772	-3.6105974	5.9289501
C	-0.6789969	2.0145418	-3.3574675
C	2.2868169	-4.2617061	3.8935322
H	3.2173599	-4.8089620	3.9779781
C	-1.0431373	0.6771520	-3.9815205
H	-2.0450462	0.4082149	-3.6187952
C	-0.9629128	2.2170387	-1.9784133
C	-0.1041103	-0.4255989	-3.4948680
C	-0.4651531	-2.2700066	5.0966295
C	0.5846751	4.1043830	-3.4504588
C	3.3798594	-3.9150893	0.9363507
C	1.0290682	3.3983061	0.7360262
C	-0.3429729	3.3124605	-1.3317302
C	-1.1071133	0.7178433	-5.4990392
C	3.9101331	-4.3755326	-0.2753119
H	4.8204817	-3.9209867	-0.6670131
C	1.1051027	-0.1491308	-2.8378537
H	1.3772014	0.8867229	-2.6346117
C	-1.2215986	-2.8454441	6.1422933
C	1.9819915	-1.1835717	-2.4898844
H	2.9201312	-0.9502140	-1.9870785
C	4.0605712	-2.7802453	1.6815606
H	3.3688237	-2.4388722	2.4634185
C	1.5565290	-5.5588201	0.7088015
C	-1.1293007	-4.3201285	6.5038046
H	-0.6207947	-4.8366665	5.6770016
C	1.5603213	4.3839329	1.5724983
H	0.9539171	5.2495081	1.8357298
C	-0.4212555	-1.7643669	-3.7727140
H	-1.3532016	-1.9908406	-4.2924785
C	3.2823739	-5.3867673	-0.9972342
H	3.7051264	-5.7264926	-1.9431971
C	0.4163334	4.2277468	-2.0719191
H	0.9032432	5.0500476	-1.5433757
C	-4.1423445	-0.3031657	-0.9761862
H	-3.4757292	-0.7121013	-0.1879587
C	-4.1458981	2.3184498	-2.7894982
H	-3.5662409	1.8333799	-3.5913975
C	-0.5266777	-0.8800997	4.8262182
C	-2.9176984	-3.5785980	0.2490770
H	-2.6769081	-2.8099454	-0.4956761
H	-4.0125058	-3.6781543	0.2717987
H	-2.5004863	-4.5298344	-0.1093176
C	-4.0090504	2.5601670	0.3131040
H	-3.3766771	3.4551058	0.1976090
C	0.0120642	0.4305587	-6.2917484
H	0.9437010	0.1299104	-5.8122328
C	0.4501988	-2.7950169	-3.4250597

H	0.1839485	-3.8285343	-3.6463086
C	-3.1222926	-1.6510982	2.6333398
H	-2.9513130	-1.5275004	3.7104611
H	-4.2065415	-1.6905771	2.4558838
H	-2.7363002	-0.7501238	2.1376182
C	-0.0571490	0.5189275	-7.6837364
H	0.8244369	0.2925756	-8.2839417
C	-0.3925001	3.4381932	0.1778960
H	-0.8827817	2.5144725	0.5315396
C	-1.2497934	4.5727090	0.7119172
C	5.3517911	-3.2632763	2.3634396
H	5.1596833	-4.1016849	3.0445745
H	5.8098775	-2.4501885	2.9435548
H	6.0829233	-3.6021777	1.6153506
C	1.6601549	-2.5085221	-2.7857226
H	2.3328225	-3.3135915	-2.4940081
C	0.3178197	-0.2534741	3.7277414
H	0.1810308	-0.8768124	2.8321666
C	4.3545389	-1.5794627	0.7717268
H	5.0856624	-1.8264481	-0.0108253
H	4.7702348	-0.7535382	1.3649579
H	3.4353400	-1.2263594	0.2867292
C	-1.7739217	5.5813953	-0.1031796
H	-1.5377379	5.5883720	-1.1656376
C	-2.5070223	-4.9724508	6.7033116
H	-3.0073642	-4.5854725	7.6017979
H	-2.3948378	-6.0575778	6.8337605
H	-3.1684766	-4.7971923	5.8472992
C	-0.2834468	-4.5153647	7.7763220
H	0.7166792	-4.0757511	7.6787285
H	-0.1667610	-5.5841793	8.0038429
H	-0.7715526	-4.0350420	8.6364371
C	2.1078774	-5.9619079	-0.5123905
H	1.6206908	-6.7477433	-1.0874991
C	1.8394852	2.3002745	0.4032438
H	1.4492514	1.5357083	-0.2705079
C	-2.6165399	-4.6626021	3.0701718
H	-2.3914998	-5.6053906	2.5538370
H	-3.6748011	-4.6852066	3.3656625
H	-2.0117204	-4.6266618	3.9830070
C	-3.9130772	-1.1382357	-2.2444829
H	-4.2538371	-2.1756210	-2.1045580
H	-2.8499484	-1.1774308	-2.5176089
H	-4.4627192	-0.7285801	-3.1042725
C	2.8568812	4.2624272	2.0847671
H	3.2510160	5.0409478	2.7385050
C	1.3365504	5.1383230	-4.2461516
H	1.9169960	4.6771388	-5.0564099
H	2.0254572	5.7088720	-3.6100813
H	0.6457888	5.8580627	-4.7122747
C	3.1271943	2.1712171	0.9152655
H	3.7296168	1.3028212	0.6506170
C	3.6421456	3.1545603	1.7666259
H	4.6489072	3.0578805	2.1725967
C	-1.5889997	4.5725572	2.0747418
H	-1.1936611	3.7865670	2.7188255
C	-0.1156850	1.1634019	3.3519198
H	-1.1829283	1.2087437	3.1008398
H	0.4594576	1.5032147	2.4825987
H	0.0765563	1.8805772	4.1637223
C	-1.2506435	0.8915706	-8.3059294
H	-1.3067843	0.9565261	-9.3924707
C	0.3204395	-6.2294971	1.2804125
H	-0.2684800	-5.4420536	1.7663449
C	-5.4640041	3.0481438	0.3769979
H	-6.1793370	2.2170149	0.4472236
H	-5.7374489	3.6467318	-0.5010250
H	-5.6134185	3.6844712	1.2637443
C	-1.3835027	-0.0943086	5.6040323
H	-1.4572442	0.9728752	5.4056061
B	0.4156343	-3.3283183	2.8722149
C	-2.0592110	-2.0110537	6.8954169
H	-2.6536290	-2.4407210	7.7016863
C	-3.8090434	3.8187256	-2.8395098
H	-4.1291437	4.2551648	-3.7991217
H	-2.7320620	3.9992125	-2.7359655
H	-4.3171822	4.3758109	-2.0400068
C	-3.6046874	1.8827238	1.6254521
H	-3.6797417	2.5782556	2.4749287
H	-2.5656334	1.5228572	1.5922128
H	-4.2426871	1.0171982	1.8506013
C	-2.1477272	-0.6499072	6.6290657
H	-2.8103284	-0.0174892	7.2201917
C	1.8175670	-0.2577266	4.0747470
H	2.0062441	0.3634110	4.9623263
H	2.3930959	0.1651238	3.2391421
H	2.1931736	-1.2673868	4.2791519
C	-0.5749317	-6.8762484	0.2213176
H	-0.8238875	-6.1690921	-0.5818781
H	-1.5140779	-7.2129119	0.6809461
H	-0.1043879	-7.7583452	-0.2362675
C	-2.9640315	6.5399046	1.7770249
H	-3.6359668	7.2943259	2.1859602
C	-2.4364807	5.5431674	2.6041732
H	-2.6955716	5.5166678	3.6628993
C	-5.6333049	2.0767358	-3.0921878
H	-6.2842720	2.4965859	-2.3135873
H	-5.8715663	1.0080935	-3.1774270
H	-5.9169815	2.5549731	-4.0436625
C	-5.5774555	-0.4656675	-0.4592420
H	-6.3117283	-0.0477461	-1.1618441
H	-5.7259374	0.0314846	0.5072754
H	-5.8233859	-1.5311910	-0.3261705
C	-2.6265764	6.5560520	0.4236953
H	-3.0357029	7.3241966	-0.2328643
C	0.7126340	-7.2447051	2.3683087
H	1.3233484	-8.0536605	1.9422180
H	-0.1854638	-7.6926291	2.8167220
H	1.2877290	-6.7634453	3.1690533
C	-2.2996917	1.0871272	-6.1344324
H	-3.1791475	1.3118326	-5.5293373
C	-2.3745693	1.1737470	-7.5250878
H	-3.3135329	1.4587375	-8.0001625
H	1.3773219	-1.2272308	0.8791220
H	0.5352389	-0.4617153	0.6986711

IM1

Energy = -7444.572730059

Ge	-2.1202202	-0.2713777	1.0434537
Zn	0.3791723	-0.2891489	1.1652655
Si	-2.8471612	-0.8182575	-1.9763701
Si	2.6924557	-2.0018012	-0.1167538
N	-3.8592509	2.5087112	-1.5797877

N	-4.8230696	1.8016226	0.3788986
N	2.1077286	-0.9966780	1.1909524
N	-2.9544410	0.2556599	-0.5778738
C	-5.1010794	1.2352116	1.6560940
C	3.7824025	-1.0970077	4.5190560
H	3.8165063	-1.7511939	5.3909413
C	-4.8824034	3.3977081	-1.2090559
H	-5.1127752	4.2741906	-1.8004538
C	2.9355213	-1.4245010	3.4617067
C	-5.4458359	2.9831362	-0.0479022
H	-6.2571692	3.4289169	0.5143760
C	1.9289183	-2.5582457	3.5769379
H	1.9078750	-3.0733808	2.6054491
C	2.8980279	-0.6072623	2.2991797
C	0.5117232	-2.0264429	3.7890883
C	-2.9820127	2.8023871	-2.6676106
C	4.5645104	0.0663700	4.5062769
C	-4.7768195	1.9662655	2.8211816
C	2.9167973	2.9675383	1.8780487
C	3.5979391	0.6218430	2.3300343
C	2.3040718	-3.5904461	4.6243722
C	-5.0703193	1.3953581	4.0653121
H	-4.8352114	1.9492603	4.9749571
C	0.2408383	-0.6723164	4.0468950
H	1.0694652	0.0334530	4.1197263
C	-3.4748929	2.8141569	-3.9906957
C	-1.0712987	-0.2353782	4.2719893
H	-1.2629682	0.8182695	4.4713367
C	-4.0995038	3.3263063	2.7580100
H	-3.8550796	3.5287713	1.7080232
C	-5.6630790	-0.0582321	1.7342937
C	-4.9388905	2.5735112	-4.3206185
H	-5.4212905	2.1621443	-3.4228073
C	3.6495198	4.1556295	1.8058615
H	4.5965846	4.1699853	1.2674387
C	-0.5646082	-2.9261781	3.7558637
H	-0.3663592	-3.9821496	3.5689318
C	-5.6312673	0.1240934	4.1607247
H	-5.8455282	-0.3076321	5.1387497
C	4.4162602	0.9325816	3.4234849
H	4.9331911	1.8944658	3.4318770
C	1.1172078	-2.8854550	-0.7293582
H	0.3864824	-2.0536020	-0.8287225
C	4.0194420	-3.1869363	0.5675875
H	3.6163325	-3.5300879	1.5345866
C	-1.6255369	3.1029784	-2.3877441
C	-2.5549505	-2.5746452	-1.3679442
H	-1.6140944	-2.6883094	-0.8181499
H	-2.5229548	-3.2582763	-2.2291361
H	-3.3686942	-2.9027405	-0.7071233
C	3.4188206	-0.9162311	-1.5000164
H	4.1091753	-0.2486371	-0.9608871
C	1.8797992	-3.4772209	5.9549403
H	1.2296686	-2.6497752	6.2398241
C	-1.8701211	-2.4909412	3.9735845
H	-2.6929302	-3.2046432	3.9327632
C	-1.4418924	-0.3318295	-3.1199180
H	-1.6559649	0.5905710	-3.6736973
H	-1.2360335	-1.1312202	-3.8464908
H	-0.5245436	-0.1609775	-2.5405136
C	2.2752778	-4.4140292	6.9119130
H	1.9360615	-4.3099087	7.9427845
C	3.3813458	1.6593044	1.2438830
H	2.5342314	1.2880194	0.6424921
C	4.5276697	1.8204328	0.2609650
C	-5.0416403	4.4388541	3.2445895
H	-5.9749357	4.4544604	2.6666905
H	-4.5613184	5.4221369	3.1456361
H	-5.3076023	4.2961569	4.3019405
C	-2.1314063	-1.1412221	4.2310747
H	-3.1529382	-0.7939947	4.3798913
C	-1.1123317	3.1818162	-0.9584969
H	-1.4679880	2.2840434	-0.4309377
C	-2.7773797	3.3507182	3.5407482
H	-2.9327933	3.1611246	4.6123905
H	-2.3005229	4.3357108	3.4405117
H	-2.0835134	2.5941575	3.1512821
C	5.7899866	1.2543628	0.4638636
H	5.9861722	0.6977677	1.3785489
C	-5.1268415	1.5717248	-5.4706881
H	-4.7904529	1.9933799	-6.4279426
H	-6.1894428	1.3152928	-5.5808151
H	-4.5669243	0.6463383	-5.2950435
C	-5.6430466	3.8985511	-4.6661574
H	-5.5485119	4.6357877	-3.8592095
H	-6.7130003	3.7316421	-4.8537149
H	-5.2034209	4.3418722	-5.5710798
C	-5.9104998	-0.5993020	3.0018683
H	-6.3420107	-1.5958718	3.0839652
C	1.7002901	2.9748090	2.5788785
H	1.1178447	2.0544418	2.6481133
C	-4.4954293	-0.8187918	-2.8822976
H	-5.2370950	-1.4174747	-2.3369450
H	-4.3842369	-1.2596646	-3.8827004
H	-4.9027604	0.1914351	-3.0010287
C	0.5568381	-3.8588088	0.3173000
H	-0.3556673	-4.3547420	-0.0488015
H	0.2935511	-3.3429441	1.2494383
H	1.2800652	-4.6510973	0.5602088
C	3.1722458	5.3252189	2.4075511
H	3.7574996	6.2426048	2.3389978
C	5.5062863	0.3798638	5.6386677
H	5.1046994	0.0360159	6.6011936
H	5.6996776	1.4579022	5.7108865
H	6.4768643	-0.1200758	5.4957480
C	1.2175011	4.1371603	3.1735970
H	0.2635234	4.1190148	3.7005757
C	1.9548718	5.3230262	3.0885842
H	1.5811605	6.2365181	3.5508492
C	4.2917862	2.5213986	-0.9324826
H	3.3101712	2.9659600	-1.1000650
C	0.4125633	3.1820138	-0.8533554
H	0.8563777	2.3271787	-1.3789123
H	0.7086878	3.1290999	0.2007407
H	0.8506376	4.1030685	-1.2654692
C	3.0992645	-5.4824234	6.5506884
H	3.4046851	-6.2166371	7.2960445
C	-6.0419643	-0.8047554	0.4687576
H	-5.2929927	-0.5437740	-0.2871080
C	4.2401684	-1.6225226	-2.5882992
H	3.6423802	-2.3478849	-3.1572941
H	5.1011239	-2.1593566	-2.1698207
H	4.6340459	-0.8864842	-3.3070585
C	-0.7717296	3.3589913	-3.4656781

H	0.2778654	3.5738213	-3.2769101
B	-3.7895447	1.4415067	-0.5886887
C	-2.5795143	3.0912554	-5.0331764
H	-2.9433731	3.0967872	-6.0605796
C	5.3428895	-2.4619677	0.8663328
H	6.0760901	-3.1588415	1.3028403
H	5.2040992	-1.6377469	1.5766846
H	5.7909158	-2.0420601	-0.0451036
C	2.3269157	-0.0383148	-2.1209158
H	2.7578921	0.7551356	-2.7500290
H	1.7153848	0.4574271	-1.3514854
H	1.6457281	-0.6247200	-2.7530607
C	-1.2377595	3.3492433	-4.7794045
H	-0.5523931	3.5490011	-5.6032548
C	-1.6781023	4.4082181	-0.2195904
H	-1.3352305	5.3356574	-0.7006609
H	-1.3214195	4.4135060	0.8197797
H	-2.7744826	4.4145774	-0.2091550
C	-6.0162727	-2.3270219	0.6225897
H	-5.0561223	-2.6707547	1.0317838
H	-6.1600296	-2.8053430	-0.3559449
H	-6.8172063	-2.6922742	1.2812964
C	6.5366387	2.0497260	-1.6992140
H	7.3102739	2.1271343	-2.4629778
C	5.2825839	2.6344716	-1.9049213
H	5.0747378	3.1716561	-2.8306088
C	4.2537331	-4.4346541	-0.2986793
H	4.6112048	-4.1748782	-1.3042789
H	3.3403908	-5.0325957	-0.4187175
H	5.0167623	-5.0851408	0.1583657
C	1.2129382	-3.5491643	-2.1092166
H	1.9498346	-4.3639858	-2.1159160
H	1.5008491	-2.8370012	-2.8921515
H	0.2425231	-3.9832193	-2.3967594
C	6.7870855	1.3648779	-0.5101404
H	7.7597895	0.9032228	-0.3393210
C	-7.4047758	-0.3164233	-0.0512459
H	-8.2002795	-0.5356704	0.6754271
H	-7.6577126	-0.8144424	-0.9981144
H	-7.3910067	0.7662552	-0.2298332
C	3.1286283	-4.6666789	4.2731603
H	3.4653817	-4.7648268	3.2400456
C	3.5241593	-5.6069874	5.2253826
H	4.1621461	-6.4406812	4.9313336
H	-2.5269929	0.9550174	1.9390442
H	-0.4810198	1.0754212	1.0436281

TS2

Energy = -7444.572712976

Ge	-1.6638640	-0.4639075	0.8162734
Zn	0.7319223	-0.2799273	0.1201083
Si	-3.3720614	0.3071656	-1.7193013
Si	2.4017032	-1.0074145	-2.4509374
N	-4.0159003	2.9951540	0.4280381
N	-4.3146582	1.4033336	2.0536892
N	2.3338523	-0.7417997	-0.7225990
N	-2.9545571	0.6372279	-0.0347572
C	-4.1874888	0.3070475	2.9545125
C	5.0006892	-2.1105458	1.4930429
H	5.2855650	-3.0722263	1.9211002
C	-4.8075910	3.5201112	1.4635501
H	-5.1711525	4.5389807	1.4370781
C	3.8390311	-2.0298240	0.7271077
C	-4.9770316	2.5814401	2.4265904
H	-5.5301387	2.6485367	3.3554231
C	2.8717623	-3.1993214	0.6334768
H	2.5094949	-3.2384345	-0.4040914
C	3.4630819	-0.7957081	0.1298036
C	1.6295456	-2.9665604	1.4928162
C	-3.5375125	3.8268850	-0.6296681
C	5.7927420	-0.9839228	1.7553616
C	-3.4575522	0.4786510	4.1523937
C	3.5293474	2.5866330	1.3624631
C	4.1961131	0.3617082	0.4829612
C	3.5196980	-4.5386881	0.9339702
C	-3.3556020	-0.6085536	5.0285246
H	-2.8034337	-0.4912499	5.9617250
C	1.5253722	-1.9001053	2.4014725
H	2.3661506	-1.2152113	2.5194906
C	-4.4430751	4.3698537	-1.5673272
C	0.3823365	-1.7478917	3.1975340
H	0.3186389	-0.9159219	3.8977148
C	-2.7648395	1.7883284	4.4949561
H	-2.8688830	2.4569035	3.6314866
C	-4.7630039	-0.9382853	2.6183536
C	-5.9442571	4.1485833	-1.4790332
H	-6.1216832	3.3360111	-0.7603753
C	4.2662736	3.7499576	1.6021759
H	4.9869765	4.0909692	0.8596721
C	0.5582704	-3.8679038	1.3978143
H	0.6321928	-4.7067095	0.7048563
C	-3.9231881	-1.8414854	4.7163356
H	-3.8267051	-2.6792631	5.4074525
C	5.3419650	0.2472836	1.2804632
H	5.8810733	1.1569742	1.5530364
C	0.6664007	-1.6858503	-2.8580985
H	-0.0090450	-0.9760061	-2.3328578
C	3.8096718	-2.2348041	-2.8310124
H	3.7242285	-3.0098871	-2.0518205
C	-2.1510040	4.1123676	-0.6994133
C	-2.9931683	-1.4975973	-2.0928907
H	-1.9306396	-1.7441393	-1.9887773
H	-3.2884377	-1.7253397	-3.1277221
H	-3.5570526	-2.1645418	-1.4267639
C	2.6946820	0.6412101	-3.3535267
H	3.5590070	1.0693578	-2.8222690
C	3.5554382	-5.0650052	2.2320406
H	3.0697671	-4.5213200	3.0426342
C	-0.5810843	-3.7129462	2.1846022
H	-1.4064881	-4.4181089	2.0874372
C	-2.3961700	1.3875945	-2.9023621
H	-2.7271828	2.4331544	-2.8807792
H	-2.4881173	1.0171222	-3.9336900
H	-1.3306272	1.3750188	-2.6358296
C	4.1989356	-6.2764750	2.4930972
H	4.2175025	-6.6706845	3.5093894
C	3.6900932	1.7408151	0.1022285
H	2.6743683	1.5850281	-0.2994742
C	4.4591000	2.4298919	-1.0113838
C	-3.4309831	2.4699789	5.7005839
H	-4.5001386	2.6435412	5.5220233
H	-2.9565672	3.4394567	5.9067474
H	-3.3408990	1.8495735	6.6039597

C	-0.6763138	-2.6499409	3.0886248
H	-1.5743916	-2.5133581	3.6894590
C	-1.1848996	3.6022605	0.3582777
H	-1.3930964	2.5317855	0.5044852
C	-1.2596275	1.5991377	4.7388771
H	-1.0640055	0.9419922	5.5981143
H	-0.7882461	2.5701794	4.9456717
H	-0.7757558	1.1664228	3.8534230
C	5.6855471	1.9613281	-1.4925883
H	6.1386305	1.0825380	-1.0371715
C	-6.5602699	3.7425022	-2.8271668
H	-6.5412649	4.5757695	-3.5431480
H	-7.6107535	3.4505941	-2.6919397
H	-6.0249535	2.8991573	-3.2775913
C	-6.6493429	5.4093140	-0.9454551
H	-6.2509566	5.7210372	0.0279593
H	-7.7281170	5.2318838	-0.8331589
H	-6.5127431	6.2488915	-1.6420074
C	-4.6083263	-2.0044586	3.5129016
H	-5.0429126	-2.9734771	3.2716017
C	2.6074155	2.1675725	2.3349385
H	2.0261777	1.2599154	2.1645068
C	-5.2235921	0.5397152	-1.9517078
H	-5.7772780	-0.3078955	-1.5262454
H	-5.4736489	0.5962916	-3.0202516
H	-5.5882244	1.4533544	-1.4693705
C	0.4308074	-3.0734145	-2.2451255
H	-0.5800196	-3.4442746	-2.4764054
H	0.5266440	-3.0542749	-1.1521219
H	1.1442184	-3.8136769	-2.6358793
C	4.0777117	4.4835069	2.7786797
H	4.6608732	5.3892646	2.9469654
C	7.0674754	-1.1000945	2.5485288
H	6.9831247	-1.8631575	3.3337710
H	7.3319178	-0.1457664	3.0218779
H	7.9099130	-1.3922277	1.9025579
C	2.4112595	2.8971685	3.5042264
H	1.6801092	2.5570930	4.2375880
C	3.1485846	4.0643298	3.7310080
H	2.9980652	4.6403835	4.6438858
C	3.8852935	3.5558230	-1.6231391
H	2.9286371	3.9281777	-1.2552043
C	0.2845088	3.7160634	-0.0474305
H	0.4773830	3.2366892	-1.0154201
H	0.9131113	3.2309390	0.7084092
H	0.6109321	4.7646056	-0.1128896
C	4.8141282	-6.9828159	1.4570163
H	5.3129147	-7.9305865	1.6591419
C	-5.5780204	-1.0857982	1.3468428
H	-5.1052005	-0.4459967	0.5934748
C	3.0743489	0.5716676	-4.8397547
H	2.2856634	0.1117180	-5.4511805
H	3.9956841	-0.0021340	-5.0018952
H	3.2481098	1.5844461	-5.2366739
C	-1.6942774	4.9060476	-1.7567921
H	-0.6317971	5.1237096	-1.8415848
B	-3.6805453	1.6139620	0.7545433
C	-3.9339871	5.1702729	-2.5996057
H	-4.6196505	5.5904935	-3.3353078
C	5.1973195	-1.5901397	-2.6723955
H	5.9918717	-2.3311801	-2.8549994
H	5.3453298	-1.1860560	-1.6633796
H	5.3463815	-0.7663544	-3.3844151
C	1.5099185	1.5884159	-3.1346686
H	1.7542926	2.6157975	-3.4440530
H	1.2135704	1.6322911	-2.0756722
H	0.6273085	1.2740660	-3.7090940
C	-2.5726327	5.4287887	-2.7046605
H	-2.1923223	6.0423225	-3.5215516
C	-1.4000568	4.3057335	1.7107790
H	-1.1861698	5.3804926	1.6204472
H	-0.7160385	3.8857774	2.4613950
H	-2.4274025	4.1921205	2.0769197
C	-5.5893771	-2.5096497	0.7863872
H	-4.5690818	-2.9008188	0.6697742
H	-6.0729062	-2.5206098	-0.2000031
H	-6.1490465	-3.2049892	1.4282523
C	5.7279172	3.6956014	-3.1836435
H	6.2131346	4.1774024	-4.0323363
C	4.5091843	4.1825115	-2.6993220
H	4.0402954	5.0475331	-3.1689538
C	3.6767370	-2.9384231	-4.1909200
H	3.7010129	-2.2255022	-5.0260650
H	2.7413941	-3.5081689	-4.2722736
H	4.5084527	-3.6449542	-4.3436934
C	0.2636088	-1.6578741	-4.3381816
H	0.9086984	-2.3079518	-4.9451555
H	0.3184198	-0.6483984	-4.7633990
H	-0.7706368	-2.0148608	-4.4632994
C	6.3148039	2.5872271	-2.5730575
H	7.2633262	2.1974049	-2.9429005
C	-7.0063224	-0.5572594	1.5634227
H	-7.5299451	-1.1511463	2.3263793
H	-7.5836963	-0.6121157	0.6295241
H	-6.9914186	0.4894230	1.8929586
C	4.1383100	-5.2564507	-0.0974632
H	4.1176630	-4.8559205	-1.1122434
C	4.7802684	-6.4688504	0.1580623
H	5.2518601	-7.0151868	-0.6590336
H	-1.6870880	0.1896247	2.2461486
H	-0.0452556	0.9031683	0.9042537

3'

Energy = -7444.604285227

Ge	0.8256577	0.6180449	0.0133242
Zn	-0.0124248	-0.7948933	1.7380823
Si	1.5801752	2.8085151	2.1089729
Si	-1.2416926	-1.3636997	4.6345209
N	-0.1174834	4.6457041	-0.3103649
N	1.2154126	3.5519391	-1.8250204
N	-0.9214861	-1.8667013	2.9819177
N	0.9499199	2.4302883	0.5214408
C	1.8619729	2.5416843	-2.5970143
C	-1.0078996	-5.5142024	2.2020284
H	-0.3490841	-6.3785651	2.2945002
C	-0.0532648	5.3916922	-1.4988099
H	-0.5735374	6.3353321	-1.6097393
C	-0.5334027	-4.2613055	2.5844049
C	0.7352337	4.7429697	-2.3937346
H	1.0223415	5.0454719	-3.3936658
C	0.9288629	-4.0407710	2.9324803
H	0.9611313	-3.3371089	3.7761312
C	-1.3778693	-3.1218452	2.5033849

C	1.6526233	-3.3558514	1.7757238
C	-1.1496806	4.8115895	0.6591261
C	-2.2922983	-5.6846216	1.6649634
C	1.1492423	1.9041649	-3.6360959
C	-3.5370467	-1.9355455	0.0090363
C	-2.6391985	-3.2742115	1.8836941
C	1.6420469	-5.3058463	3.3763695
C	1.7938002	0.8912826	-4.3580343
H	1.2582665	0.3880263	-5.1637655
C	1.1657545	-3.4022760	0.4594159
H	0.2213599	-3.9077425	0.2585277
C	-1.1098459	5.8789623	1.5776046
C	1.8944350	-2.8378339	-0.5936211
H	1.5011135	-2.8853059	-1.6089533
C	-0.2875123	2.2697419	-3.9757056
H	-0.6463450	2.9696583	-3.2103991
C	3.1818882	2.1580560	-2.2704652
C	-0.0301008	6.9433118	1.5111253
H	0.7568425	6.5658053	0.8428582
C	-4.7282567	-1.7847005	-0.7053016
H	-5.6776039	-1.7673677	-0.1719347
C	2.8760923	-2.7085726	2.0103759
H	3.2724464	-2.6732455	3.0257992
C	3.0950925	0.5046246	-4.0516618
H	3.5779712	-0.2905468	-4.6203782
C	-3.0681930	-4.5422339	1.4705398
H	-4.0313497	-4.6288705	0.9633117
C	0.2176949	-0.2121782	5.0561404
H	0.2968540	0.4392231	4.1638101
C	-1.2977248	-2.9185437	5.7417324
H	-0.4621939	-3.5429335	5.3825632
C	-2.1994922	3.8618900	0.6809594
C	2.7237107	1.4115564	2.6621968
H	2.2206209	0.4479082	2.8152322
H	3.1953947	1.6822420	3.6182050
H	3.5226415	1.2498738	1.9258516
C	-2.9039134	-0.4404950	4.7269329
H	-3.5957489	-1.1339677	4.2214709
C	2.3625484	-6.1067772	2.4817053
H	2.4522153	-5.7989753	1.4398729
C	3.6015179	-2.1428003	0.9620309
H	4.5467993	-1.6411822	1.1681648
C	0.2059598	3.0334156	3.3652093
H	-0.3293954	3.9773093	3.2045022
H	0.5869480	3.0219495	4.3960386
H	-0.5360555	2.2307818	3.2685670
C	2.9691952	-7.2890994	2.9129663
H	3.5262188	-7.9005099	2.2026832
C	-3.4633253	-2.0519701	1.5312861
H	-2.8603139	-1.1909102	1.8665642
C	-4.7907600	-1.9136492	2.2568516
C	-0.3666522	2.9861308	-5.3336585
H	0.2671941	3.8823310	-5.3520583
H	-1.3998321	3.2923835	-5.5491886
H	-0.0315323	2.3251003	-6.1458919
C	3.1171977	-2.2135147	-0.3469623
H	3.6763456	-1.7631749	-1.1660914
C	-2.3569431	2.8353163	-0.4281652
H	-1.3693368	2.6551254	-0.8717386
C	-1.2165816	1.0495518	-3.9476997
H	-0.9374205	0.3041926	-4.7059894
H	-2.2534440	1.3534595	-4.1475832
H	-1.1931530	0.5598878	-2.9666157
C	-5.3362171	-2.9237571	3.0565281
H	-4.8191638	-3.8771854	3.1441171
C	0.6009867	7.2294461	2.8810839
H	-0.1160252	7.7090176	3.5618591
H	1.4570883	7.9093083	2.7722901
H	0.9546835	6.3077028	3.3584388
C	-0.5856137	8.2379938	0.8918021
H	-1.0115261	8.0571865	-0.1036124
H	0.2062781	8.9939076	0.7944600
H	-1.3826260	8.6578792	1.5222675
C	3.7790082	1.1338433	-3.0118857
H	4.7942123	0.8207258	-2.7725316
C	-2.3308415	-1.9702107	-0.7093631
H	-1.3930446	-2.1220502	-0.1715548
C	2.6419318	4.3604176	2.0119445
H	3.6020633	4.1475545	1.5230080
H	2.8589579	4.7450456	3.0183974
H	2.1493500	5.1590190	1.4444832
C	1.5467753	-0.9695940	5.1775027
H	2.3841617	-0.2750604	5.3467258
H	1.7734103	-1.5363250	4.2653860
H	1.5361949	-1.6803625	6.0159219
C	-4.7114088	-1.6448703	-2.0979341
H	-5.6516809	-1.5232802	-2.6363500
C	-2.7987508	-7.0512843	1.2864991
H	-3.2191077	-7.5729209	2.1602654
H	-1.9921571	-7.6829042	0.8908669
H	-3.5905757	-6.9884368	0.5290334
C	-2.3076374	-1.8318396	-2.0929271
H	-1.3559459	-1.8530597	-2.6230630
C	-3.5046215	-1.6610539	-2.7968627
H	-3.4928632	-1.5458973	-3.8802947
C	-5.4658389	-0.6834629	2.1900061
H	-5.0438716	0.1176347	1.5832026
C	-2.8852378	1.4815443	0.0400617
H	-2.2472223	1.0578179	0.8277064
H	-2.9066985	0.7707437	-0.7944824
H	-3.9077423	1.5516930	0.4358886
C	2.8666654	-7.6855509	4.2477224
H	3.3430235	-8.6058141	4.5855236
C	3.9235572	2.8603102	-1.1485607
H	3.1841801	3.0524289	-0.3617536
C	-3.4805655	-0.1900641	6.1286425
H	-2.8367237	0.4650833	6.7314242
H	-3.6229463	-1.1223116	6.6893925
H	-4.4653580	0.2977343	6.0530149
C	-3.1599658	3.9607634	1.6923400
H	-3.9637746	3.2270554	1.7416271
B	0.7010635	3.4492822	-0.4651916
C	-2.1125281	5.9539830	2.5545511
H	-2.0941469	6.7689270	3.2782349
C	-2.5849069	-3.7407473	5.5573622
H	-2.5602386	-4.6420529	6.1905606
H	-2.7180310	-4.0673782	4.5194261
H	-3.4777432	-3.1660091	5.8409313
C	-2.8832192	0.8575067	3.9121077
H	-3.9011058	1.2490587	3.7637695
H	-2.4449698	0.7176884	2.9128518
H	-2.3024852	1.6440051	4.4131499
C	-3.1156905	4.9920385	2.6294330
H	-3.8713900	5.0498449	3.4128919

C	-3.2471553	3.4161430	-1.5419928
H	-4.2550126	3.6336648	-1.1598134
H	-3.3407561	2.6990984	-2.3693556
H	-2.8225051	4.3476413	-1.9379691
C	5.0357452	2.0156176	-0.5226475
H	4.6609874	1.0276406	-0.2204926
H	5.4299507	2.5188002	0.3709252
H	5.8811667	1.8658179	-1.2095943
C	-7.1754680	-1.4833856	3.7014282
H	-8.0919488	-1.3153184	4.2667633
C	-6.6435972	-0.4670552	2.9015319
H	-7.1432554	0.5000560	2.8404563
C	-1.0468404	-2.6308799	7.2313297
H	-1.8208012	-1.9788021	7.6580401
H	-0.0772726	-2.1464821	7.4061438
H	-1.0572723	-3.5676400	7.8114709
C	0.0009176	0.7162538	6.2584475
H	-0.1417333	0.1498570	7.1890079
H	-0.8748144	1.3632352	6.1264864
H	0.8751814	1.3701486	6.4058620
C	-6.5171398	-2.7107333	3.7740435
H	-6.9159792	-3.5088904	4.4004490
C	4.4576680	4.2226839	-1.6218548
H	5.1938141	4.0917929	-2.4280574
H	4.9468072	4.7554481	-0.7938853
H	3.6437658	4.8548527	-1.9984006
C	1.5483783	-5.7115272	4.7144415
H	0.9889291	-5.0947713	5.4196920
C	2.1541134	-6.8901416	5.1496957
H	2.0730231	-7.1871068	6.1955297
H	2.2181215	0.1901088	-0.4956152
H	-0.1300585	0.6017351	-1.2040217

2M

Energy = -4126.255976129

Ge	3.4756984	26.8279839	6.9170582
Zn	3.0058252	25.3980715	8.8796615
N	2.6228471	24.2568442	10.2921132
N	4.1835565	28.2761174	7.8417567
C	4.6309342	29.4326823	7.0684210
C	4.3863317	28.4810528	9.2689636
H	5.4542961	28.6474364	9.4970140
H	3.8310907	29.3675940	9.6239555
H	4.0425361	27.6071444	9.8331684
H	5.7048910	29.6272647	7.2347918
H	4.4690593	29.2583462	5.9981063
H	4.0793581	30.3422468	7.3641448
C	2.9056956	24.5714657	11.6749150
C	2.0100242	22.9561724	10.1326892
H	3.3706185	25.5642582	11.7664002
H	1.9872587	24.5768757	12.2978424
H	3.5985482	23.8375146	12.1362829
H	2.6579219	22.1410345	10.5163231
H	1.0466915	22.8804154	10.6782442
H	1.8060526	22.7438359	9.0731352

3M

Energy = -4127.460653252

Ge	3.090810000	27.110809000	7.348815000
Zn	2.657179000	25.529716000	9.056556000
N	2.345779000	24.324103000	10.394841000
N	4.172786000	28.466129000	8.072376000
C	4.430565000	29.587045000	7.176765000
C	5.386264000	28.012672000	8.736573000
H	6.173698000	27.654130000	8.039531000
H	5.821434000	28.838760000	9.324019000
H	5.155808000	27.193467000	9.434210000
H	5.142283000	29.347623000	6.357989000
H	3.492972000	29.932852000	6.721365000
H	4.858237000	30.428623000	7.748001000
C	1.488823000	24.591841000	11.532128000
C	2.936368000	23.001818000	10.438038000
H	1.057127000	25.600997000	11.475015000
H	0.646985000	23.872892000	11.592022000
H	2.041830000	24.520894000	12.490421000
H	3.556998000	22.856938000	11.345314000
H	2.164737000	22.205793000	10.445439000
H	3.581956000	22.826453000	9.565852000
H	3.777836000	26.476281000	6.088378000
H	1.839380000	27.858096000	6.817567000

Me_2NGe

Energy = -2211.902580591

Ge	3.5371138	26.7591316	7.0536191
N	4.2067570	28.3016205	7.8170328
C	4.6450825	29.4583252	7.0453084
C	4.3516707	28.4912635	9.2550769
H	5.4058626	28.6789847	9.5256082
H	3.7608781	29.3576007	9.6018122
H	4.0072400	27.5965668	9.7876903
H	5.7095215	29.6813372	7.2368521
H	4.5144507	29.2645958	5.9738359
H	4.0633642	30.3573672	7.3152237

$ZnNMe_2$

Energy = -1914.270290759

Zn	3.4762882	25.1374354	8.8785090
N	2.3728767	24.3750054	10.3357634
C	2.8920522	24.5676089	11.6817165
C	1.9299568	23.0032362	10.1347860
H	3.2746678	25.5902182	11.8074250
H	2.0698878	24.4265940	12.4098248
H	3.6939672	23.8579248	11.9681325
H	2.6968673	22.2368692	10.3657126
H	1.0691989	22.8001427	10.8009270
H	1.5915120	22.8523825	9.1000780

Me_2NGeH_2

Energy = -2213.095377271

Ge	2.7837567	27.3964125	7.5957668
N	4.4059354	28.3340026	7.5773481
C	4.4382606	29.7402204	7.2222977
C	5.5016954	27.9226450	8.4344350
H	6.4642811	28.0950283	7.9222409
H	5.5294739	28.4858034	9.3863437
H	5.4249356	26.8530711	8.6655051
H	5.3696613	29.9680715	6.6753179
H	3.5908815	29.9893927	6.5718168
H	4.4063539	30.4019563	8.1084316

H	3.2713718	25.9078829	7.4878228
H	2.1554509	27.8119046	6.2182369

TBoNGe

Energy = -3689.004165996

Ge	4.5904138	26.8041461	7.3916348
Si	5.0551960	29.0698139	9.6105248
N	3.7157620	30.7320608	6.7502422
N	5.2589284	29.4968795	5.5923646
N	4.6972591	28.5983764	7.9433244
C	5.9972580	28.3848834	5.0929539
C	3.9399467	31.3187323	5.4921931
H	3.4213437	32.2189294	5.1866329
C	4.8550960	30.5840186	4.8069361
H	5.2666381	30.7566349	3.8198038
C	2.6017000	31.0772561	7.5691114
C	5.4216651	27.5580236	4.1006848
C	6.1715535	26.4751662	3.6278373
H	5.7483562	25.8290513	2.8584067
C	2.6068314	32.2827363	8.3012655
C	4.0194272	27.8020875	3.5682360
H	3.5611345	28.5848958	4.1868427
C	7.2739052	28.1068614	5.6367976
C	3.7682913	33.2572255	8.2230553
H	4.6003371	32.7336252	7.7309233
C	7.4293491	26.1866306	4.1522567
H	7.9897653	25.3271155	3.7841076
C	1.5098270	30.1818674	7.6328107
C	5.9633251	27.6651375	10.4660227
H	5.3432037	26.7638972	10.5591833
H	6.2577271	27.9815061	11.4781483
H	6.8742954	27.3867854	9.9189078
C	3.4772871	29.4339277	10.5617970
H	2.9368685	30.3006164	10.1620416
H	3.7088408	29.6323139	11.6186983
H	2.7977871	28.5710441	10.5241371
C	4.0577905	28.3124482	2.1187792
H	4.6517690	29.2317102	2.0325885
H	3.0421611	28.5257171	1.7575357
H	4.5051208	27.5622750	1.4509429
C	1.4480503	28.9207945	6.7881505
H	2.4446272	28.7447682	6.3609319
C	3.1377535	26.5506449	3.6883416
H	3.5029360	25.7307514	3.0541118
H	2.1096855	26.7804469	3.3752996
H	3.1151987	26.1971180	4.7283723
C	4.2429560	33.7094239	9.6119213
H	3.4887138	34.3332131	10.1114773
H	5.1599862	34.3081654	9.5249602
H	4.4540966	32.8511254	10.2610108
C	3.4037755	34.4753778	7.3566120
H	3.0965006	34.1751294	6.3467335
H	4.2607831	35.1571640	7.2651157
H	2.5700006	35.0341415	7.8056609
C	7.9674939	26.9893373	5.1567667
H	8.9469784	26.7491286	5.5675973
C	6.1702770	30.5881172	9.5889049
H	7.1982567	30.3183770	9.3127033
H	6.2057125	31.0592441	10.5813140
H	5.8166720	31.3404819	8.8724163
C	1.0903364	27.6761680	7.6092758
H	1.7761901	27.5569769	8.4594005
H	1.1575896	26.7764515	6.9821460
H	0.0677508	27.7265232	8.0095389
C	7.8735137	29.0313643	6.6782229
H	7.0431061	29.3820858	7.3029117
C	0.4332579	30.5107286	8.4643792
H	-0.4159639	29.8302982	8.5319354
B	4.5484189	29.5500308	6.8604769
C	1.4999026	32.5739203	9.1083037
H	1.4871568	33.4989142	9.6848671
C	0.4238441	31.6944336	9.1984288
H	-0.4237249	31.9321841	9.8413334
C	0.4840134	29.1126325	5.6060662
H	-0.5420679	29.2937404	5.9572916
H	0.4748977	28.2170641	4.9690729
H	0.7873734	29.9694812	4.9901421
C	8.8794980	28.3445503	7.6038749
H	8.4523319	27.4390609	8.0560504
H	9.1694748	29.0262749	8.4151101
H	9.8011430	28.0598346	7.0764397
C	8.4894181	30.2697374	6.0037573
H	9.3212164	29.9801779	5.3457214
H	8.8760619	30.9678404	6.7596290
H	7.7429479	30.8011084	5.3999544

ZnL*

Energy = -3754.282033045

Zn	-7.4843137	-7.2028544	4.7913745
Si	-8.5992334	-8.1300164	7.6015308
N	-8.4186687	-8.4966795	5.9015750
C	-8.4430461	-11.9707602	4.5676110
H	-7.7490390	-12.8061710	4.4667842
C	-7.9824928	-10.7727413	5.1068984
C	-6.5072043	-10.5551163	5.3937269
H	-6.4437003	-10.0013435	6.3429411
C	-8.8699815	-9.6703571	5.2800274
C	-5.8810264	-9.6425407	4.3424310
C	-9.7647804	-12.1202935	4.1233072
C	-11.3957663	-8.2632583	3.2341022
C	-10.1801569	-9.7920856	4.7482215
C	-5.7310121	-11.8459894	5.5754544
C	-6.5102955	-9.3645706	3.1178256
H	-7.4737790	-9.8229872	2.8955119
C	-5.9069184	-8.5161499	2.1795581
H	-6.4149590	-8.3127801	1.2371068
C	-12.5872433	-8.6488335	2.6089606
H	-13.3654664	-9.1369116	3.1961227
C	-4.6349057	-9.0495731	4.6005664
H	-4.1294640	-9.2671125	5.5421146
C	-10.5982624	-11.0030044	4.1864433
H	-11.6053427	-11.0663979	3.7695494
C	-7.1639691	-6.9264972	7.9774007
H	-7.2189461	-6.1908098	7.1449107
C	-8.4516377	-9.7645818	8.5794648
H	-7.5992174	-10.2855894	8.1099229
C	-10.2766006	-7.2901822	7.9222776
H	-10.9911468	-7.9612441	7.4200533
C	-5.0286884	-12.4464958	4.5235698
H	-5.0019014	-11.9574995	3.5496599
C	-4.0358204	-8.2019971	3.6689198
H	-3.0709789	-7.7477004	3.8941176

C	-4.3623427	-13.6598988	4.7129650
H	-3.8203352	-14.1139497	3.8830986
C	-11.0961645	-8.5830754	4.6927079
H	-10.4958980	-7.7466100	5.0825674
C	-12.3380334	-8.6564528	5.5661227
C	-4.6698160	-7.9324417	2.4520000
H	-4.2045470	-7.2658685	1.7266331
C	-12.6644588	-9.7738088	6.3412192
H	-12.0333580	-10.6592796	6.2962858
C	-10.4163349	-7.6163468	2.4678174
H	-9.4829874	-7.3042331	2.9479517
C	-5.7917870	-7.6089290	7.8856830
H	-4.9758533	-6.8815000	8.0207602
H	-5.6425512	-8.0895967	6.9098025
H	-5.6727902	-8.3816040	8.6589620
C	-12.7898215	-8.4013725	1.2487865
H	-13.7237310	-8.7089057	0.7775172
C	-10.2554059	-13.4348572	3.5780167
H	-10.5697683	-14.1076752	4.3911542
H	-9.4684388	-13.9549773	3.0156239
H	-11.1188693	-13.2953600	2.9149455
C	-10.6145695	-7.3633878	1.1116211
H	-9.8428148	-6.8513777	0.5362222
C	-11.8052244	-7.7597462	0.4946832
H	-11.9660237	-7.5630905	-0.5652226
C	-13.1609667	-7.5212213	5.6509900
H	-12.9178241	-6.6441366	5.0498693
C	-4.3878074	-14.2884143	5.9593900
H	-3.8651135	-15.2330754	6.1086695
C	-10.7373625	-7.1838635	9.3836477
H	-10.0608461	-6.5688072	9.9928574
H	-10.8103142	-8.1690732	9.8619952
H	-11.7364878	-6.7229548	9.4363192
C	-9.6874969	-10.6622725	8.4043134
H	-9.5572579	-11.6120434	8.9475151
H	-9.8698382	-10.9048901	7.3504149
H	-10.5951907	-10.1821685	8.7964274
C	-10.3586932	-5.9283689	7.2171875
H	-11.3919124	-5.5486064	7.2142590
H	-10.0250334	-5.9814435	6.1694288
H	-9.7329771	-5.1751474	7.7179056
C	-14.5777287	-8.6184628	7.2762042
H	-15.4393196	-8.6013002	7.9434796
C	-14.2670718	-7.4987000	6.4971131
H	-14.8869424	-6.6036428	6.5544858
C	-8.1125084	-9.5813668	10.0672904
H	-8.8939499	-9.0228142	10.5997483
H	-7.1659829	-9.0451138	10.2151870
H	-8.0178501	-10.5603131	10.5643252
C	-7.2951615	-6.1292861	9.2829949
H	-7.2958456	-6.7888196	10.1617887
H	-8.2183858	-5.5379045	9.3156905
H	-6.4502232	-5.4324435	9.3999663
C	-13.7743439	-9.7551682	7.1917628
H	-14.0043873	-10.6338459	7.7947856
C	-5.7495911	-12.4848967	6.8226251
H	-6.2992682	-12.0263597	7.6464836
C	-5.0842684	-13.6952019	7.0165385
H	-5.1064142	-14.1755992	7.9949201

TBoNGeH$_2$

Energy = -3690.193720390

Ge	0.6240612	0.5641372	-0.0563009
Si	1.4945736	2.6543064	2.1048313
N	-0.2013920	4.5695890	-0.3243978
N	1.1297292	3.5082306	-1.8616469
N	0.9452151	2.3485007	0.4568168
C	1.8684029	2.5658705	-2.6399925
C	-0.1480041	5.3293360	-1.4997032
H	-0.6917146	6.2602299	-1.6009726
C	0.6446626	4.6999172	-2.4077812
H	0.9194056	5.0175696	-3.4059583
C	-1.1679096	4.8180983	0.6947700
C	1.2302401	1.9137158	-3.7177687
C	1.9779263	1.0028982	-4.4743240
H	1.5055270	0.4917778	-5.3135182
C	-1.0382515	5.9402649	1.5376570
C	-0.2298785	2.1634211	-4.0626366
H	-0.6734509	2.7364116	-3.2369273
C	3.2109113	2.2893582	-2.3006129
C	0.1035863	6.9298494	1.3886027
H	0.8499635	6.4726388	0.7235344
C	3.3034985	0.7214180	-4.1573998
H	3.8660222	0.0004679	-4.7509317
C	-2.2525820	3.9186565	0.8250824
C	2.5110446	1.1714879	2.6624977
H	1.9101221	0.2546329	2.7419328
H	2.9340834	1.3720619	3.6576412
H	3.3440022	0.9726272	1.9749563
C	0.0703736	2.8719652	3.3089157
H	-0.4964595	3.7931532	3.1291808
H	0.4457468	2.8962003	4.3426890
H	-0.6285947	2.0280540	3.2244353
C	-0.3597500	3.0031922	-5.3448412
H	0.1755706	3.9573354	-5.2608152
H	-1.4152167	3.2211102	-5.5599218
H	0.0584621	2.4624395	-6.2060139
C	-2.4513822	2.7759089	-0.1564968
H	-1.4612578	2.4629370	-0.5102135
C	-1.0296402	0.8589602	-4.2000521
H	-0.6885776	0.2604350	-5.0561160
H	-2.0937188	1.0839492	-4.3577078
H	-0.9394743	0.2408322	-3.2975019
C	0.7840806	7.2405641	2.7302132
H	0.1190258	7.8085401	3.3953527
H	1.6850314	7.8480096	2.5686381
H	1.0785576	6.3223836	3.2519493
C	-0.3821876	8.2302976	0.7242515
H	-0.8439732	8.0392447	-0.2527757
H	0.4548485	8.9269169	0.5766882
H	-1.1331914	8.7282884	1.3541586
C	3.9084536	1.3544365	-3.0725505
H	4.9426098	1.1198567	-2.8249439
C	2.6040748	4.1732925	2.0914515
H	3.5858380	3.9362698	1.6609385
H	2.7682054	4.5428998	3.1131980
H	2.1687867	4.9905745	1.5032518
C	-3.1114511	1.5395093	0.4591373
H	-2.5706458	1.2046037	1.3542837
H	-3.1067258	0.7155400	-0.2669248
H	-4.1589020	1.7233288	0.7376921
C	3.8771734	3.0225904	-1.1513427
H	3.1107920	3.1536066	-0.3787958

C	-3.1857549	4.1534193	1.8395315
H	-4.0230008	3.4683563	1.9657386
B	0.6301231	3.3850254	-0.4970373
C	-2.0088588	6.1412009	2.5285390
H	-1.9238685	7.0013454	3.1926714
C	-3.0681990	5.2536152	2.6876632
H	-3.8059827	5.4182401	3.4730328
C	-3.2253587	3.2700101	-1.3917373
H	-4.2320131	3.6106436	-1.1096300
H	-3.3295471	2.4607882	-2.1284396
H	-2.7034511	4.1067108	-1.8741474
C	5.0297968	2.2459911	-0.5107603
H	4.7176371	1.2320436	-0.2263295
H	5.3725640	2.7643548	0.3954291
H	5.8970027	2.1614089	-1.1812369
C	4.3285946	4.4249258	-1.5946420
H	5.0909702	4.3557351	-2.3839063
H	4.7605916	4.9770169	-0.7477664
H	3.4840389	5.0073196	-1.9845546
H	2.0004806	-0.1848730	-0.1512242
H	-0.0076637	0.6751918	-1.4782987

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