Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Activation of Non-Polar Bonds by an Electron-Rich Gallagermylene

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V. References

I. Experimental Section

General Procedure. All experiments were performed in a glovebox or using standard Schlenkline techniques under argon atmosphere. Toluene and *n*-hexane were dried using an mBraun Solvent Purification System (SPS), degassed and stored in Schlenk flasks under argon atmosphere. Deuterated solvents were stored over molecular sieves (4 Å) and degassed prior to use. The anhydrous nature of the solvents was verified by Karl Fischer titration. LGa(μ–Cl)GeDMP (**1**) was synthesized according to literature procedure.[1]

Spectroscopic methods. ^{1}H (400 MHz) and ^{13}C{^{1}H} (100 MHz) NMR spectra were recorded using a Ascend™ 400 spectrometer. The spectra were referenced to internal C_6D_5H (^{1}H: δ = 7.16, C_6D_6) or to natural-abundance carbon resonances C_6D_6 (^{13}C: δ = 128.06, C_6D_6). IR spectra were recorded with an ALPHA-T FT-IR spectrometer equipped with a single reflection ATR sampling module. The IR spectrometer was placed in a glovebox to guarantee measurements under inert gas conditions.

Synthesis of L(Cl)GaGe(H)$_2$Ar^{Mes} 2. A solution of **1** (43 mg, 0.047 mmol) in 0.5 mL of benzene-d_6 in a *J*-Young NMR tube was degassed at –196 °C and then exposed to a hydrogen solution (1 atm) at r.t., upon which the initially dark red solution immediately turned colourless. The solution was transferred into a Schlenk tube and concentrated in vacuo until incipient crystallization. Colourless crystals of **2** were obtained upon storage at 6 °C. Yield: 29 mg, 0.032 mmol, 68 %, m.p. 213-214 °C. **^{1}H NMR (400 MHz, C_6D_6, 298 K): δ [ppm] =** 7.19 – 7.13 (m, 9H, Ar*H*, overlapping with solvent), 7.10 (dd, $^{3}J_{HH}$ = 7.7, 1.7 Hz, 2H, Ar*H*), 7.03 (dd, $^{3}J_{HH}$ = 7.5, 1.7 Hz, 3H, Ar*H*), 6.81 (s, 4H, Ar*H*), 6.71 (d, $^{3}J_{HH}$ = 7.5 Hz, 2H, Ar*H*), 4.90 (s, 1H, γ-C*H*), 3.64 (sept, $^{3}J_{HH}$ = 6.7 Hz, 2H, C*H*(CH$_3$)$_2$), 3.33 (s, 2H, Ge*H*), 2.92 (sept, $^{3}J_{HH}$ = 6.8 Hz, 2H, C*H*(CH$_3$)$_2$), 2.33 (s, 6H, *p*-CH$_3$), 1.93 (s, 12H, *o*-CH$_3$), 1.45 (s, 6H, NCCH$_3$), 1.19 (d, $^{3}J_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 1.10 (d, $^{3}J_{HH}$ = 6.6 Hz, 6H, CH(CH$_3$)$_2$), 1.07 (d, $^{3}J_{HH}$ = 6.8 Hz, 6H, CH(CH$_3$)$_2$), 0.94 (d, $^{3}J_{HH}$ = 6.7 Hz, 6H, CH(CH$_3$)$_2$). **^{13}C NMR (101 MHz, C_6D_6, 298 K): δ [ppm] =** 169.21 (NCCH$_3$), 150.03, 146.05, 143.17, 142.01, 141.50, 136.18, 136.11, 129.60, 129.14, 129.01, 127.84, 125.23, 124.19, 99.27 (γ-*C*), 29.52 (*C*H(CH$_3$)$_2$), 28.27 (*C*H(CH$_3$)$_2$), 27.83 (CH(*C*H$_3$)$_2$), 25.05 (CH(*C*H$_3$)$_2$), 24.30 (CH(*C*H$_3$)$_2$), 24.18 (NC*C*H$_3$), 23.89 (CH(*C*H$_3$)$_2$), 21.76 (*p*-CH$_3$), 21.49 (*o*-CH$_3$). **IR(ATR): *ν* [cm^{-1}]** = 2967, 2917, 2863, 2051, 2019, 1942, 1518, 1439, 1380, 1315, 1259, 1177, 1102, 1021, 934, 869, 848, 798, 759, 717, 639, 532, 444.

Synthesis of L(Cl)Ga(P$_4$)GeAr^{Mes} 3. P_4 (3.3 mg, 0.026 mmol) was added to a solution of **1** (24 mg, 0.026 mmol) in 0.5 mL of benzene-d_6 in a *J*-Young NMR tube. The dark red solution turned yellow and was stirred for ten minutes. The solution was transferred into a Schlenk tube and the solvent was removed in vacuo. The residue was dissolved in 1 mL of boiling *n*-hexane and crystallised at r. t. The yellow crystals were washed with *n*-hexane (3x 0.2 mL) and dried in vacuo. Yield: 15 mg, 0.015 mmol, 55 %), m.p. 285 °C. **^{1}H-NMR (400 MHz, C_6D_6, 298 K): δ [ppm] =** 7.27 – 7.12 (m, 9H, Ar*H*, overlapping with solvent), 7.01 (dd, $^{3}J_{HH}$ = 7.7, 1.5 Hz, 1H, Ar*H*), 6.98 (t, $^{3}J_{HH}$ = 7.7 Hz, 1H, Ar*H*), 6.89 (t, $^{3}J_{HH}$ = 7.7 Hz, 1H,m Ar*H*), 6.75 (dd, $^{3}J_{HH}$ = 7.7, 1.3 Hz, 1H, Ar*H*), 6.70 (s, 2H, Ar*H*), 6.68 (s, 1H, Ar*H*), 4.81 (s, 1H, γ-C*H*), 3.95 (sept, $^{3}J_{HH}$ = 6.7 Hz, 1H, C*H*(CH$_3$)$_2$), 3.55 (sept, $^{3}J_{HH}$ = 6.7 Hz, 1H, C*H*(CH$_3$)$_2$), 3.11 (sept, $^{3}J_{HH}$ = 6.9 Hz, 1H), 2.68 (sept, $^{3}J_{HH}$ = 6.8 Hz, 1H, C*H*(CH$_3$)$_2$), 2.40 (s, 6H, Mes-CH$_3$), 2.35 (s, 6H, Mes-CH$_3$), 2.15 (d, $^{3}J_{HH}$ = 6.6 Hz, 3H, CH(CH$_3$)$_2$), 1.54 (s, 3H, NCCH$_3$), 1.46 (d, $^{3}J_{HH}$ = 6.8 Hz, 3H, CH(CH$_3$)$_2$), 1.43 (s, 3H, NCCH$_3$), 1.33 (d, $^{3}J_{HH}$ = 6.8 Hz, 3H, CH(CH$_3$)$_2$), 1.16 (d, $^{3}J_{HH}$ = 6.9 Hz, 3H, CH(CH$_3$)$_2$), 1.14 (d, $^{3}J_{HH}$ =6.7 Hz, 3H, CH(CH$_3$)$_2$), 1.10 (d, $^{3}J_{HH}$ = 6.9 Hz, 3H, CH(CH$_3$)$_2$), 0.96 (d, $^{3}J_{HH}$ = 6.8 Hz, 3H, CH(CH$_3$)$_2$), 0.90 (d, $^{3}J_{HH}$ = 6.8 Hz, 3H, CH(CH$_3$)$_2$). **^{13}C-NMR (101 MHz, C_6D_6, 298 K): δ [ppm] =** 169.8 (NCCH$_3$), 169.6 (NCCH$_3$), 146.3 (Ar), 146.3 (Ar), 143.4 (Ar), 143.1 (Ar), 143.0 (Ar), 142.0 (Ar), 141.9 (Ar), 141.7 (Ar), 138.0 (Ar), 137.4 (Ar), 136.9 (Ar), 136.6 (Ar), 131.3 (Ar), 129.8 (Ar), 128.9 (Ar), 126.3 (Ar), 125.9

(Ar), 125.2 (Ar), 125.2 (Ar), 124.6 (Ar), 97.8 (γ-<u>C</u>), 32.2 (<u>C</u>H(CH$_3$)$_2$), 30.3 (<u>C</u>H(CH$_3$)$_2$), 29.6 (<u>C</u>H(CH$_3$)$_2$), 28.9 (CH(<u>C</u>H$_3$)$_2$), 28.1 (<u>C</u>H(CH$_3$)$_2$), 27.8 (CH(<u>C</u>H$_3$)$_2$), 26.0 (CH(<u>C</u>H$_3$)$_2$), 25.4 (CH(<u>C</u>H$_3$)$_2$), 25.2 (CH(<u>C</u>H$_3$)$_2$), 24.5 (CH(<u>C</u>H$_3$)$_2$), 24.2 (NC<u>C</u>H$_3$), 24.0 (NC<u>C</u>H$_3$), 23.3 (CH(<u>C</u>H$_3$)$_2$), 21.8 (Mes-<u>C</u>H$_3$), 21.2 (Mes-<u>C</u>H$_3$), 14.6 (CH(<u>C</u>H$_3$)$_2$). **^{31}P-NMR (162 MHz, C$_6$D$_6$, 298 K): δ [ppm] =** 198.49 (dd, J_{PP} = 141.9, 23.4 Hz), -72.30 (dd, J_{PP} = 63.9, 36.0 Hz), -175.48 (ddd, J_{PP} = 174.0, 157.0, 140.6 Hz), -231.38 (dd, J_{PP} = 173.8, 35.3 Hz). **IR(ATR): *ν*[cm^{-1}]:** 2963, 2917, 2863, 1611, 1529, 1439, 1384, 1313, 1260, 1179, 1098, 1020, 941, 867, 848, 796, 778, 759, 740, 709, 641, 575, 529, 513, 438.

II. Spectroscopic Characterization

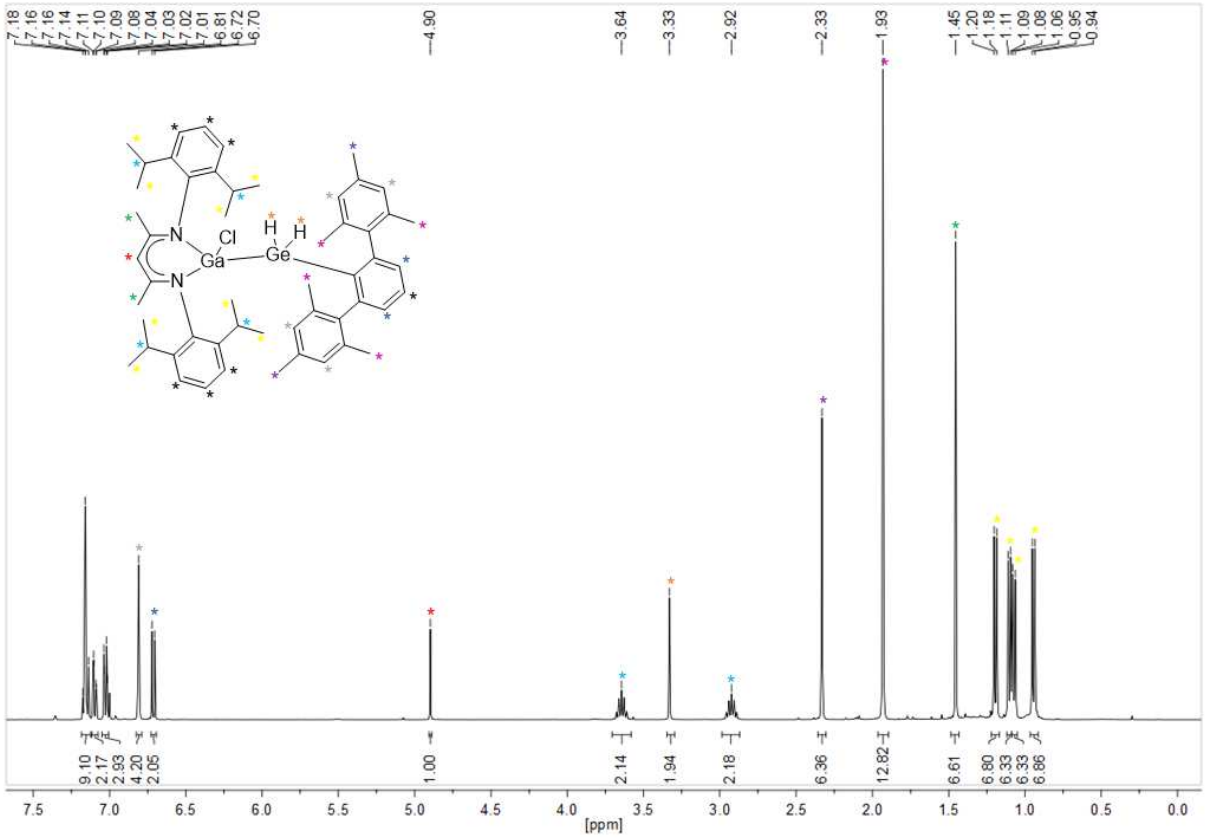


Figure S4: ^{1}H NMR spectrum of **2** in C_6D_6.

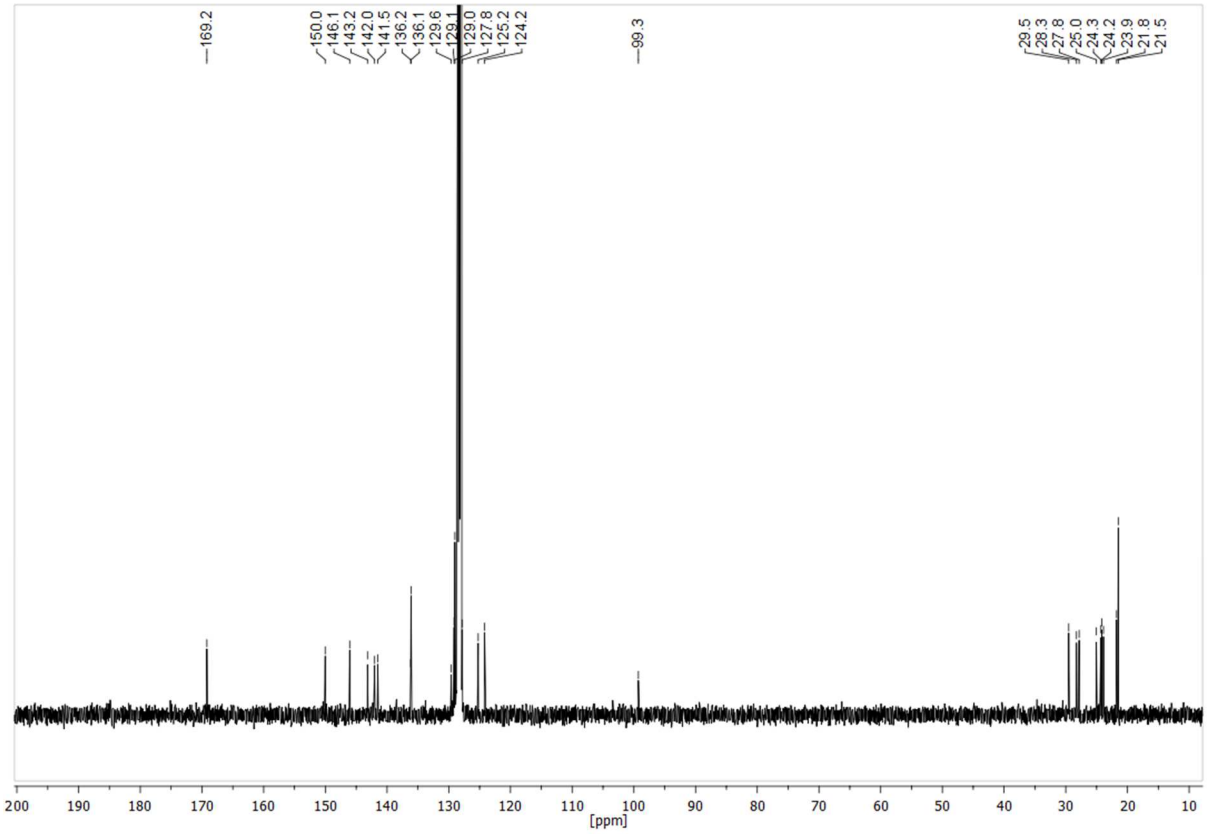


Figure S5: ^{13}C NMR spectrum of **2** in C_6D_6.

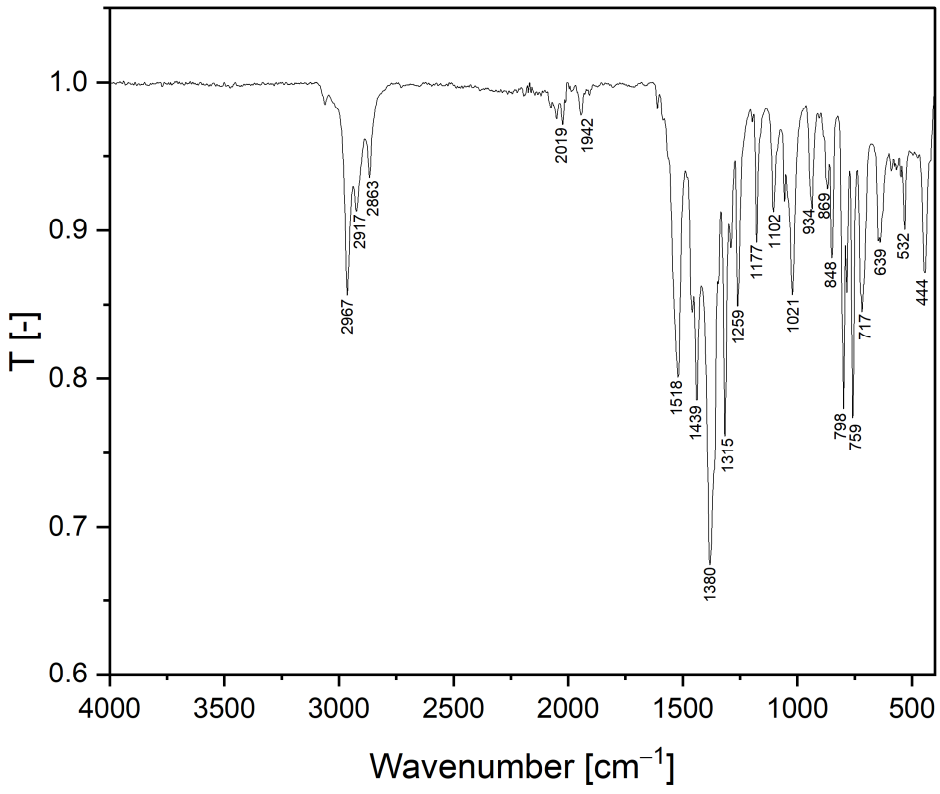


Figure S6: IR spectrum of **2**.

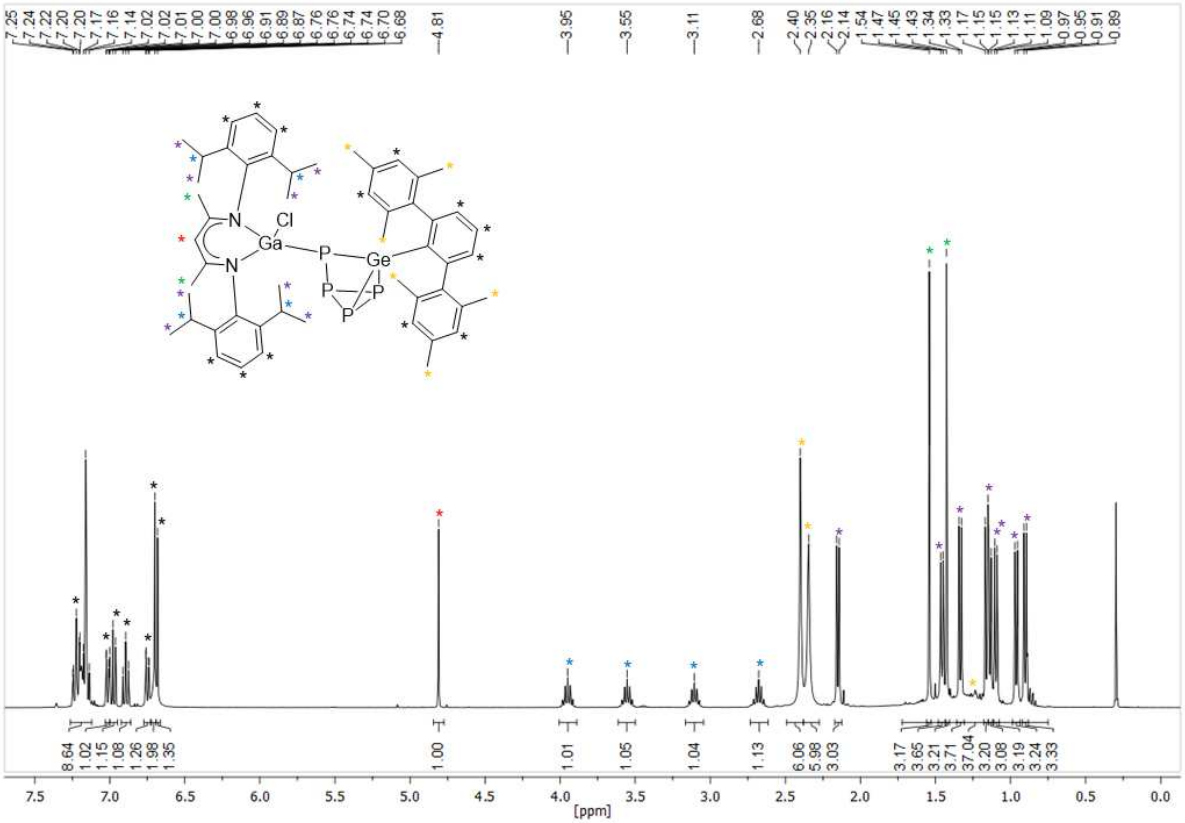


Figure S7. ^{1}H NMR spectrum of **3** in C_6D_6.

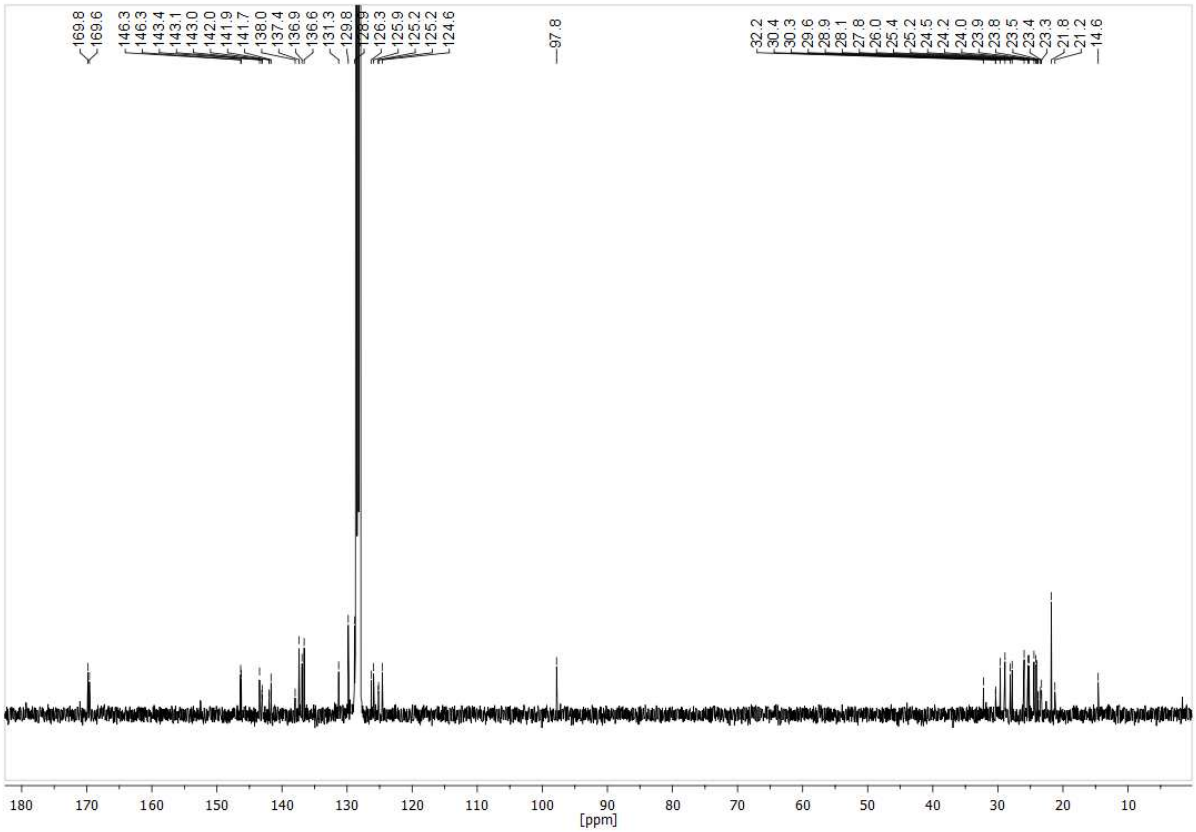


Figure S8. ^{13}C NMR spectrum of **3** in C_6D_6.

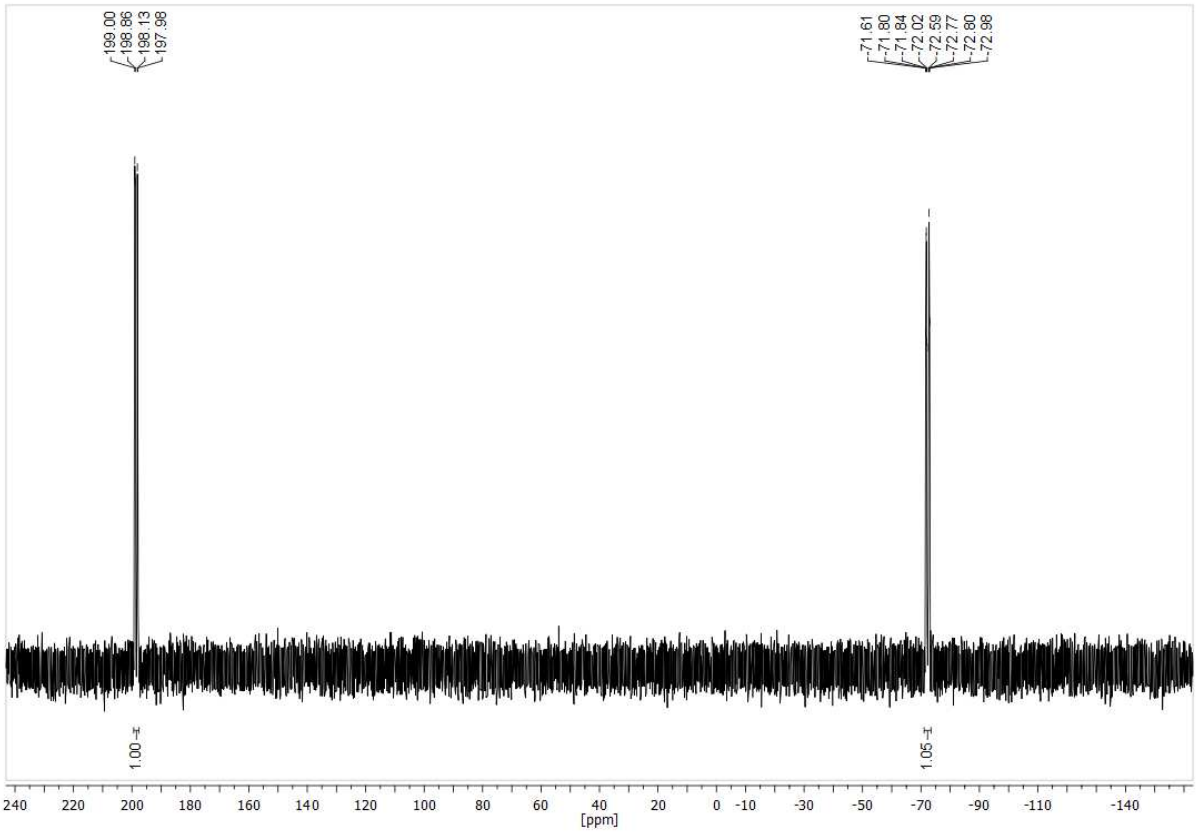


Figure S9. ^{31}P NMR spectrum (low field) of **3** in C_6D_6.

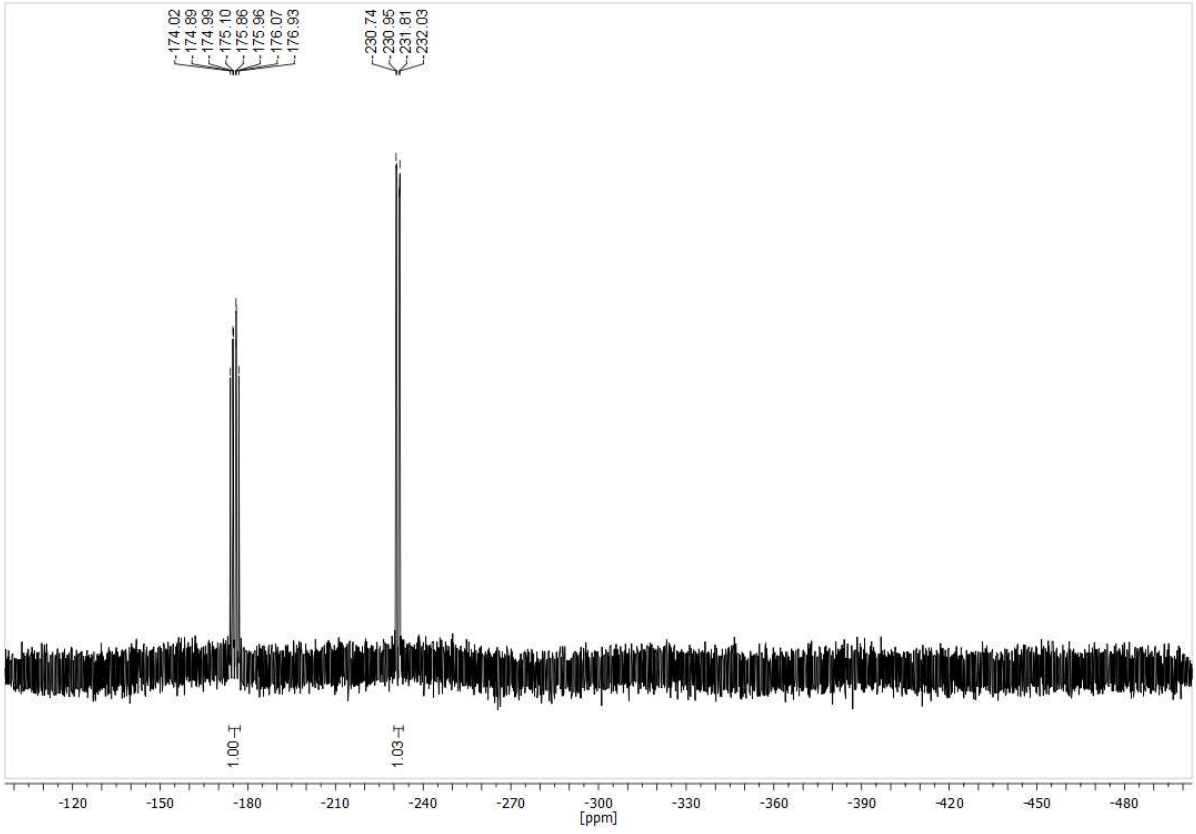


Figure S10. ^{31}P NMR spectrum (high field) of **3** in C_6D_6.

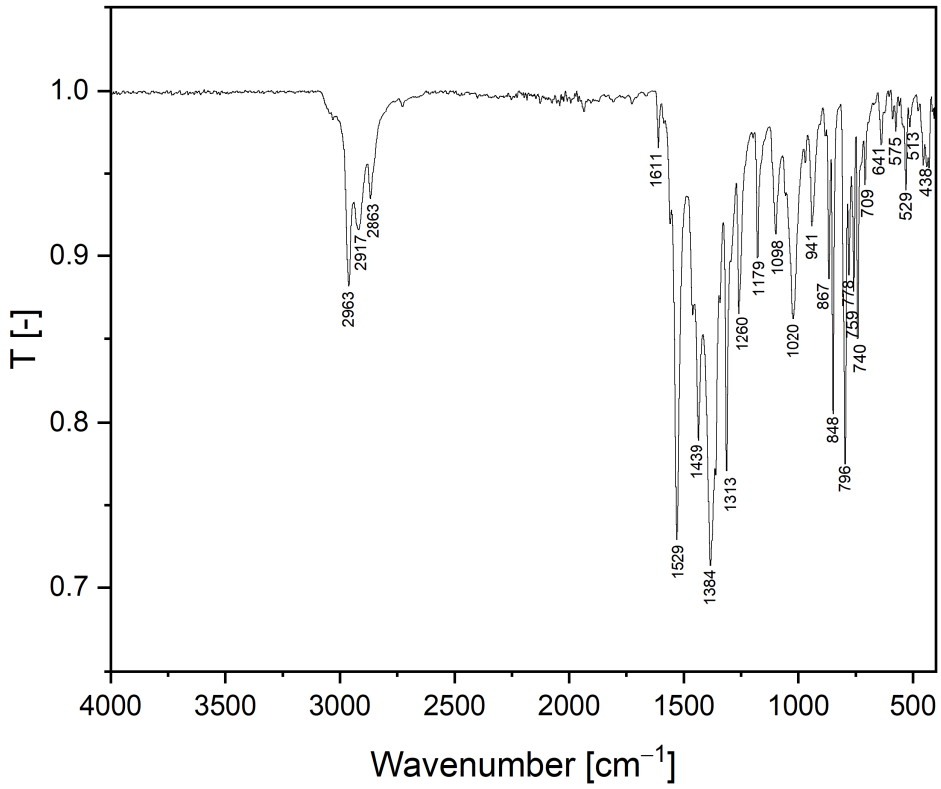


Figure S11. IR spectrum of **3**.

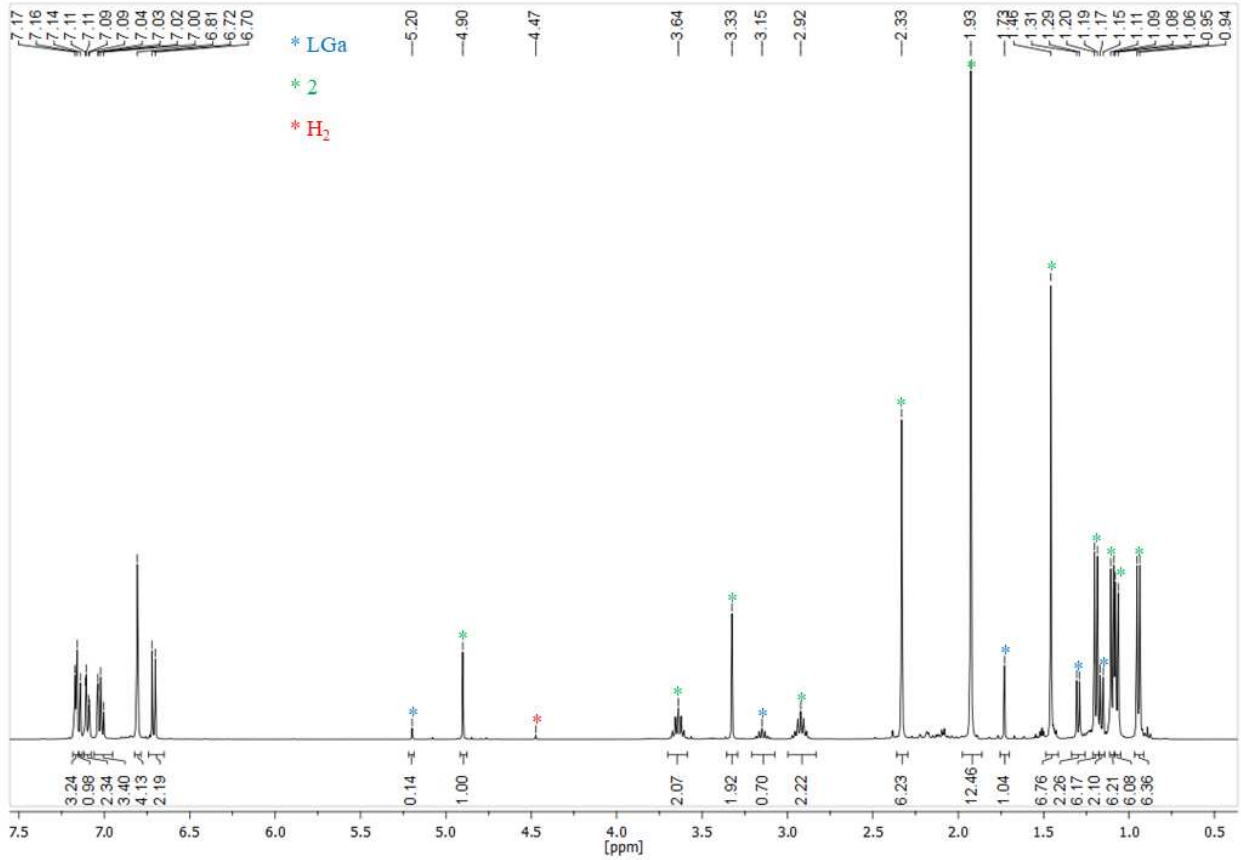


Figure S12. Initial *in situ* ^{1}H NMR spectrum of **1** and H_2 at r.t.

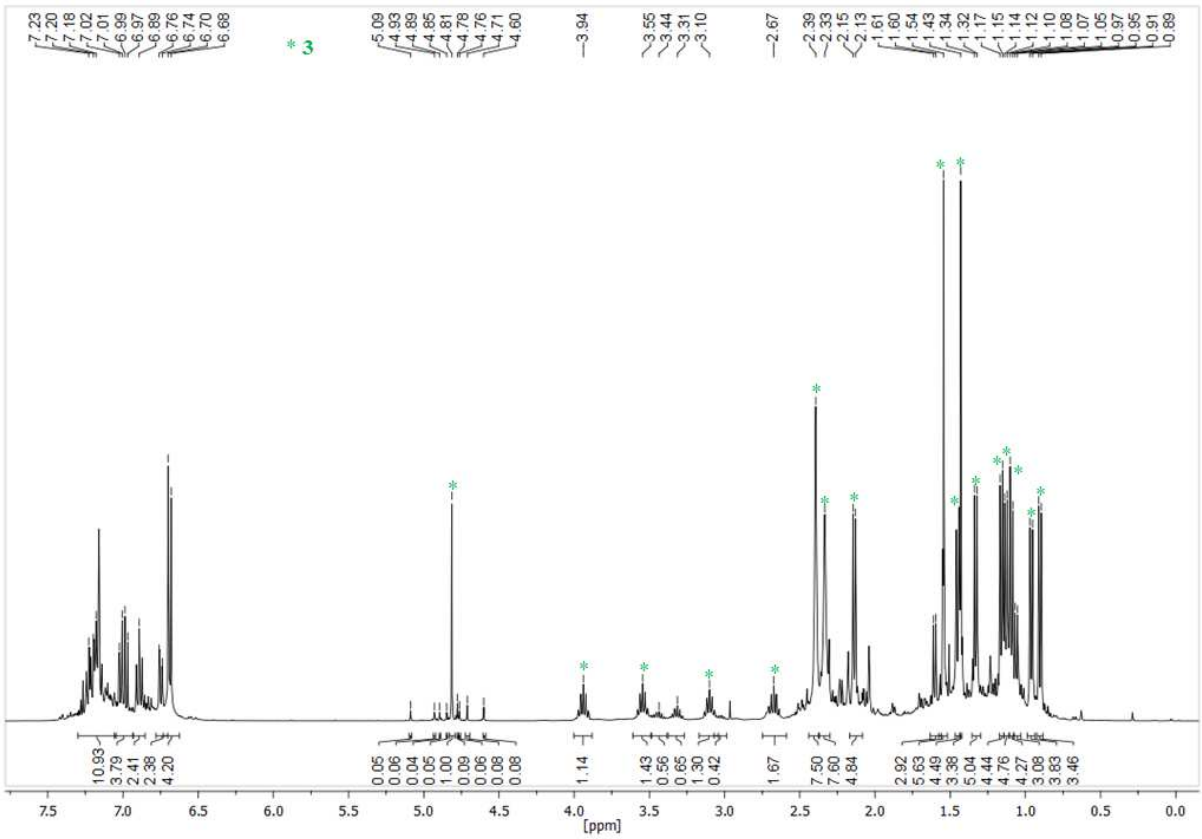


Figure S13. Initial *in situ* ^{1}H NMR spectrum of **1** and P_4 at r.t.

III. Crystallographic Data

Single-crystal X-ray analyses. The crystals were mounted on nylon loops in inert oil. Data were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (monochromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) at 100(2) K. The structures were solved by Direct Methods (SHELXS-2013)[2] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-2017).[3,4] Absorption corrections were performed semi-empirically from equivalent reflections on basis of multi-scans (Bruker AXS APEX3). Hydrogen atoms were refined using a riding model or rigid methyl groups.

In **2** an isopropyl group is disordered over two positions. Its displacement parameters were restrained with RIGU and SIMU and those of C15 and C15' constrained to be equal due to the atoms' close proximity (EADP).

In **3** also an isopropyl group is disordered over two positions. In this case its bond lengths were restrained to be equal (SADI) and RIGU restraints were applied to the displacement parameters of the disordered atoms.

CCDC-2321151 (**2**), and -2321152 (**3**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S3. Crystallographic details of compounds **2** and **3**.

Identification code	**2 (ab_316m2)**	**3 (ab_255am3)**
Empirical formula	$C_{56}H_{71}ClGaGeN_2$	$C_{53}H_{66}ClGaGeN_2P_4$
M	949.90	1032.71
Crystal size [mm]	0.281 × 0.140 × 0.139	0.604 × 0.300 × 0.172
T [K]	100(2)	100(2)
Crystal system	triclinic	monoclinic
Space group	$P\bar{1}$	$C2/c$
a [Å]	11.3222(11)	45.016(4)
b [Å]	12.2948(12)	10.0401(8)
c [Å]	20.0701(19)	23.3390(18)
α [°]	98.212(4)	90
β [°]	91.794(4)	102.560(4)
γ [°]	114.236(4)	90
V [Å^3]	2508.9(4)	10296.0(14)
Z	2	8
D_{calc} [g·cm^{-3}]	1.257	1.332
μ(MoK_α [mm^{-1}])	1.226	1.320
Transmissions	0.75/0.64	0.75/0.59
F(000)	1002	4304
Index ranges	$-17 \le h \le 17$	$-81 \le h \le 81$
	$-18 \le k \le 18$	$-18 \le k \le 18$
	$-30 \le l \le 30$	$-42 \le l \le 42$
θ_{max} [°]	32.829	40.401
Reflections collected	191527	387884
Independent reflections	18497	32569
R_{int}	0.0918	0.0585
Refined parameters	598	596
R_1 [$I > 2\sigma(I)$]	0.0424	0.0413
wR_2 [all data]	0.1106	0.1064
GooF	1.025	1.113
$\Delta\rho_{final}$ (max/min) [e·Å^{-3}]	1.189/-0.586	1.995/-0.688

IV. Quantum Chemical Calculations

All computations including geometry optimization and single-point computations were performed using ORCA 5.0.4[5] at the def2-TZVPP level of theory (def2-QZVP for E>Ne)[7] using the atom-pairwise dispersion correction based on tight binding partial charges (D4)[8,9] with the PBE0[10,11] functional. As in our previous studies[1] the geometry optimization for **1** resulted in a shift of the Cl towards the Ge center, resulting in structure **1_opt**. Frequency computations were performed to verify the nature of the stationary point. Natural bond orbital analysis was performed using the NBO program package (version 7.0.10).[6]

Table S4. NBO analysis of **1_opt** and **A-C** including the natural atomic partial charges Q [e], Wiberg bond indices (WBI) [a.u.], Mayer bond orders (MBO) [a.u.] and orbital character of the Ge lone-pair [%].

	Q(Ge)	Q(E)	WBI (Ge–E)	MBO (Ge–E)	Orbital character Ge lone pair s	p
A	+1.13	–0.55	0.60	0.94	83.3	16.6
B	+0.78	C: –0.50 Si: –0.60	C: 0.66 Si: 0.92	C: 1.00 Si: 0.92	79.9	20.0
C	+0.41	N: –1.37 Zn: 1.03	N: 0.55 Zn: 0.81	N: 1.12 Zn: 0.90	86.3	13.6
1_opt	+0.45	C: –0.48 Ga: 1.23 Cl: –0.55	C: 0.69 Ga: 1.00 Cl: 0.40	C: 0.99 Ga: 0.89 Cl: 0.46	83.5	16.5

Table S5. Comparison of the computed electronic properties of acyclic germylenes **A-C** and **1_opt** in H_2 activation. The root mean square deviation (RMSD) from the experimental structure is given in %.

	E_{HOMO} [eV]	E_{LUMO} [eV]	$\Delta E_{HOMO-LUMO}$ [eV]	$\angle_{exp.}$ (E–Ge–E) [°]	$\angle_{calc.}$ (E–Ge–E) [°]	RMSD
A[12]	–5.25	–1.96	3,29	114.4	114.6	0.57
B[13]	–5.26	–2.13	3.13	112.7	111.9	0.10
C[14]	–5.15	–1.64	3.51	110.7	107.2	0.44
1_opt[1]	–4.98	–1.32	3.67	103.97, 113.4	98.2, 111.5	0.44

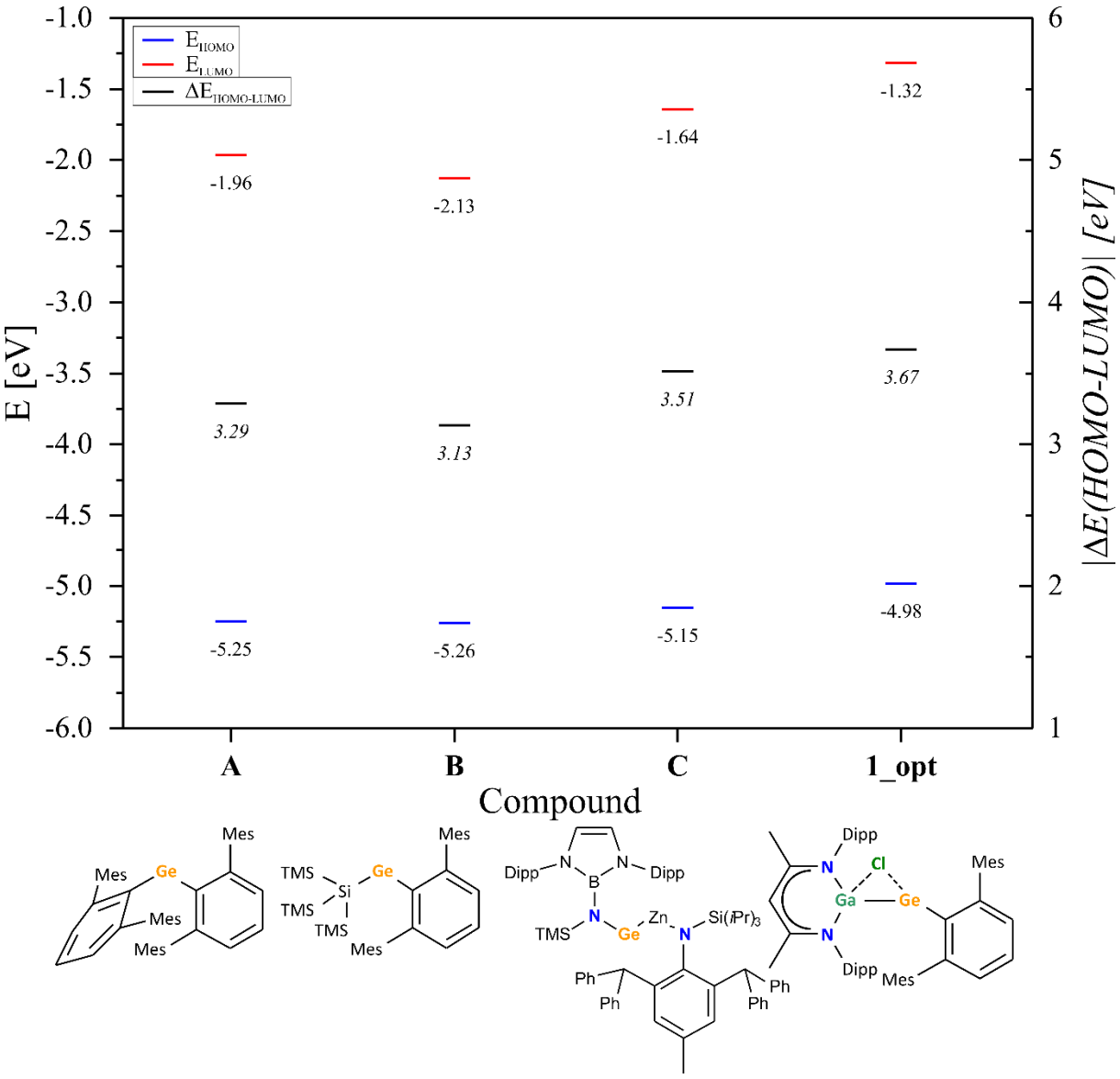
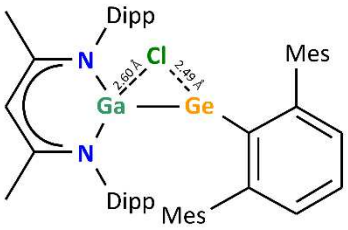
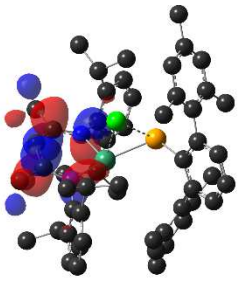


Figure S14. Comparison of frontier orbital energies (E_{HOMO}, E_{LUMO}) [eV] and the energy gap ($E_{HOMO-LUMO}$) [eV] of **A-C** and **1_opt**.

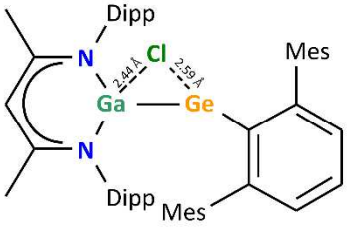


1

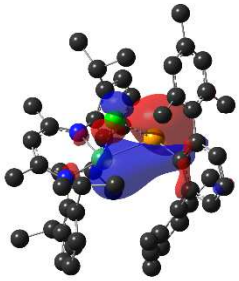


-1.32 eV

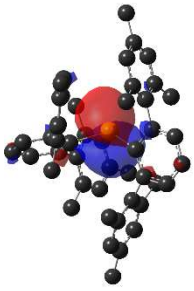
1_opt



1_opt

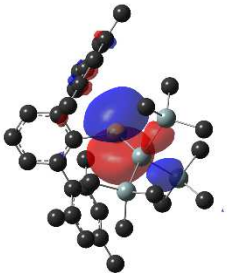


-4.98 eV



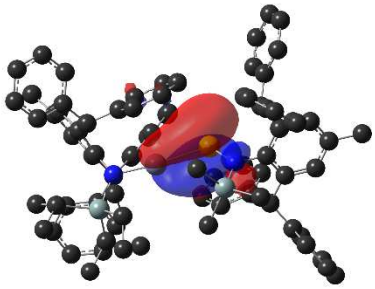
-1.96 eV

A



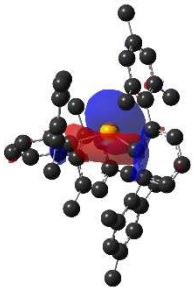
-2.13 eV

B

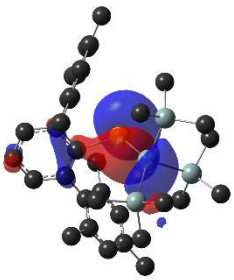


-1.64 eV

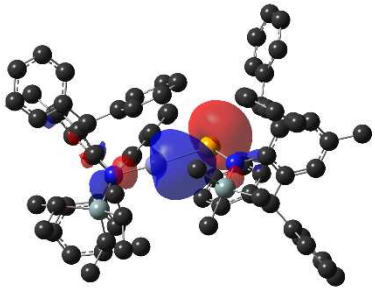
C



-5.25 eV



-5.26 eV



-5.15 eV

Figure S15. Frontier orbitals of **A**, **B**, **C** and **1_opt** (isovalue 0.03). The hydrogens are omitted for clarity.

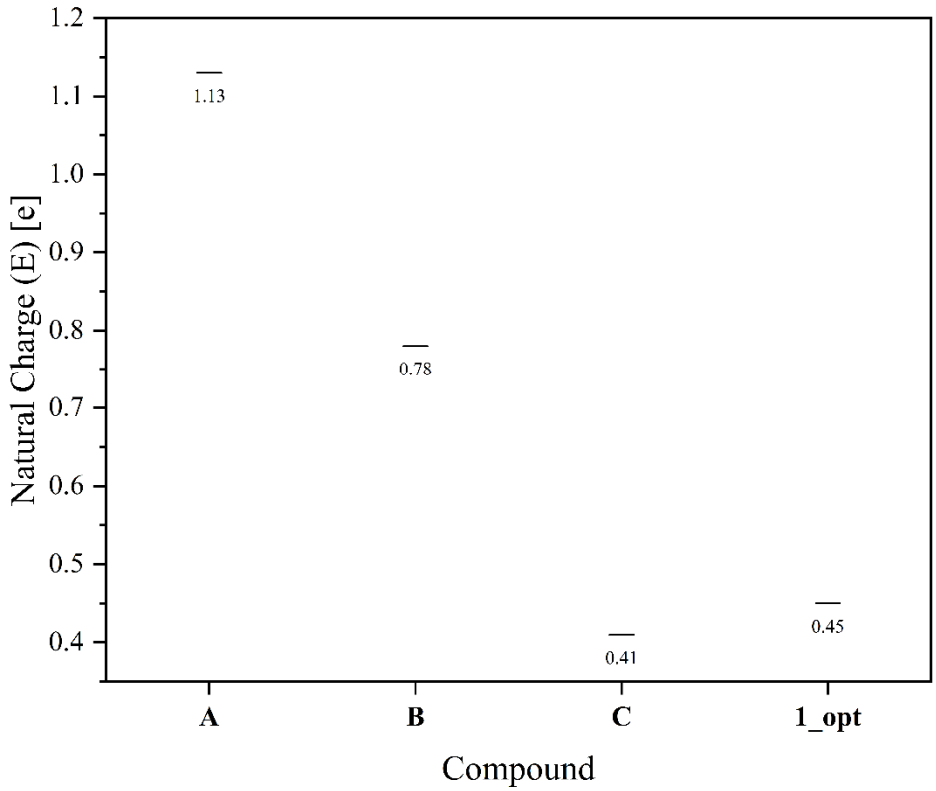


Figure S16. Comparison of the computed natural partial charge [e] of the Ge atom in **A**-**C** and **1_opt**.

Table S4. Cartesian coordinates [Å] of computed compounds **A**, **B**, **C** and **1_opt** with the corresponding final single point energies (FSPE) [Ha].

MesTerphGe (**A**)				MesTerphGeHypsi (**B**)			
Ge	5.169160	31.691471	6.234271	Ge	6.964405	12.479172	1.988653
C	4.155578	33.050920	5.145701	Si	9.390041	12.265045	2.068912
C	6.182870	30.331942	5.145930	Si	10.187194	14.288506	1.146670
C	4.464167	34.359581	5.563203	C	11.665648	14.007020	0.014807
C	3.037545	32.877298	4.317408	C	8.831730	15.129534	0.155569
C	5.874541	29.023261	5.563547	C	10.775075	15.441151	2.511942
C	7.301086	30.505717	4.317936	Si	10.862688	11.496551	3.733098
C	3.725663	35.450670	5.123381	C	12.630569	11.923273	3.238931
C	5.601068	34.622871	6.488437	C	10.548104	12.273394	5.416320
C	2.320203	33.989362	3.873435	C	10.755889	9.622214	3.854451
C	2.435976	31.575332	3.924972	Si	9.560497	10.759964	0.248058
C	6.613539	27.932321	5.124183	C	11.349823	10.268548	–0.076114
C	4.737426	28.759645	6.488417	C	8.588829	9.194566	0.607599
C	8.018989	29.393814	3.874471	C	8.856008	11.531204	–1.317195
C	7.902169	31.807747	3.924945	C	6.142366	12.312641	3.796410
C	2.657296	35.270629	4.264696	C	5.738156	11.136782	4.435568
H	3.994501	36.443191	5.467952	C	4.992986	11.217020	5.609063
C	5.446131	34.479252	7.876901	C	4.632627	12.442899	6.144429
C	6.792931	35.147205	5.968935	C	5.002821	13.609611	5.495000
H	1.460323	33.828122	3.232895	C	5.741908	13.543970	4.321329
C	2.487068	31.157304	2.591241	C	6.089466	14.783230	3.575297
C	1.609634	30.903239	4.836256	C	5.249622	15.233916	2.542433
C	7.682201	28.112519	4.265897	C	4.009047	14.480091	2.175363
H	6.344853	26.939780	5.468817	C	5.559085	16.424005	1.895744
C	4.891861	28.903128	7.876937	C	6.657160	17.191256	2.259025
C	3.545877	28.235038	5.968434	C	7.458274	16.742608	3.301645
H	8.878999	29.555221	3.234141	C	7.198257	15.550685	3.962036
C	7.849284	32.225899	2.591330	C	8.062738	15.103344	5.098421
C	8.729723	32.479626	4.835214	C	6.989799	18.452891	1.526237
H	2.077339	36.118669	3.920700	C	6.050999	9.801631	3.867801
C	6.530437	34.745661	8.703535	C	7.010003	8.986906	4.482418
C	4.133775	34.080665	8.472489	C	7.722180	9.442075	5.719823
C	7.843912	35.417925	6.833042	C	7.274701	7.731726	3.951067
C	6.910599	35.462053	4.511455	C	6.595905	7.249669	2.839785
C	1.703563	30.083900	2.184080	C	5.617795	8.053579	2.273434
C	3.324583	31.886537	1.584618	C	5.331984	9.322028	2.764681
C	0.817073	29.858726	4.380646	C	4.233785	10.127650	2.135564
C	1.531775	31.321496	6.273171	C	6.930234	5.914283	2.252057
H	8.262562	27.264592	3.922302	H	12.482286	13.508464	0.540277
C	3.807408	28.636114	8.703198	H	12.037502	14.972724	–0.341144
C	6.203809	29.302307	8.473042	H	11.409142	13.407096	–0.859381
C	2.494802	27.963601	6.832191	H	7.970545	15.366981	0.782554
C	3.428605	27.920782	4.510785	H	9.204918	16.062007	–0.278850
C	8.632450	33.299155	2.183196	H	8.483879	14.492449	–0.659335
C	7.010091	31.496677	1.586145	H	9.989417	15.630164	3.240994
C	9.521811	33.524117	4.378668	H	11.080670	16.400882	2.084736
C	8.809270	32.061040	6.271942	H	11.634165	15.022479	3.039699
C	7.743461	35.194813	8.200013	H	12.881971	11.507020	2.261857
H	6.414252	34.617848	9.775013	H	12.791744	13.001813	3.196747
H	3.311644	34.651542	8.037150	H	13.331614	11.509738	3.970231
H	4.135718	34.237134	9.551182	H	9.523616	12.125567	5.760258
H	3.926319	33.021448	8.284617	H	10.738259	13.348290	5.384944
H	8.765590	35.820345	6.425749	H	11.219907	11.836527	6.160847
C	0.844503	29.435706	3.058752	H	9.726808	9.273411	3.933266
H	1.750613	29.763040	1.147846	H	11.309356	9.262617	4.726635
H	4.203337	32.337651	2.042151	H	11.194121	9.158971	2.968129
H	2.758150	32.697371	1.117294	H	11.980325	11.131494	–0.293020
H	3.649082	31.213884	0.789392	H	11.781485	9.740905	0.776236
H	0.152994	29.364233	5.082321	H	11.391496	9.595314	–0.937728
H	0.682955	30.847794	6.766398	H	7.523834	9.405146	0.724286
H	1.436888	32.403959	6.373587	H	8.924688	8.713034	1.527293
H	2.428738	31.023920	6.827565	H	8.700046	8.479415	–0.213077
C	2.594760	28.186458	8.199247	H	7.822968	11.850329	–1.163511
H	3.923212	28.763808	9.774732	H	9.431226	12.399414	–1.642925
H	7.026578	28.732972	8.036915	H	8.867382	10.798271	–2.129241
H	6.202051	29.144376	9.551525	H	4.678982	10.300435	6.096401
H	6.410019	30.362022	8.286579	H	4.048908	12.487327	7.055951
H	1.573418	27.560864	6.424551	H	4.707026	14.576346	5.888244
C	9.492765	33.947157	3.056827	H	3.465702	14.993459	1.382655
H	8.584101	33.620104	1.147050	H	3.346968	14.372578	3.037266
H	6.129815	31.049375	2.044540	H	4.245077	13.471306	1.827394

H	7.574216	30.682836	1.121269	H	4.912311	16.768069	1.095337
H	6.687923	32.168221	0.789054	H	8.309383	17.340652	3.610185
H	10.186779	34.018561	5.079542	H	8.894280	15.790004	5.255660
H	9.657304	32.536414	6.764902	H	7.493106	15.040847	6.028034
H	8.906670	30.978731	6.371806	H	8.466685	14.106905	4.912936
H	7.911903	32.356216	6.826917	H	7.504030	19.165369	2.172543
C	8.912603	35.433503	9.104430	H	6.094070	18.931769	1.128786
C	0.004543	28.282742	2.603701	H	7.650508	18.241417	0.680319
C	1.425461	27.947021	9.103264	H	8.565736	8.791136	5.948075
C	10.332230	35.100064	2.600715	H	8.088909	10.463401	5.615818
H	9.530436	34.533946	9.184774	H	7.053212	9.437364	6.583682
H	8.590514	35.697319	10.112708	H	8.028533	7.110056	4.424166
H	9.551141	36.233936	8.727618	H	5.053914	7.683147	1.423033
H	–0.242765	28.362773	1.544287	H	4.629228	10.926718	1.500025
H	–0.926675	28.221539	3.168967	H	3.607649	10.605433	2.890558
H	0.532540	27.333778	2.742316	H	3.603953	9.493820	1.511097
H	0.806832	28.846076	9.183114	H	6.056807	5.451507	1.790392
H	1.747371	27.683747	10.111739	H	7.693830	6.017386	1.475222
H	0.787747	27.145948	8.726412	H	7.321603	5.231489	3.007390
H	10.579952	35.018940	1.541476	FSPE	–4522.322923634767		
H	11.263214	35.162461	3.166225				
H	9.803609	36.048873	2.738007				
H	2.449164	27.504962	4.284889				
H	4.186654	27.197633	4.204205				
H	3.571748	28.810338	3.894925				
H	7.890275	35.877503	4.285908				
H	6.152949	36.185724	4.205115				
H	6.767095	34.572869	3.895155				
FSPE	–3934.605091174609						

LZnTBoN (**C**)							
Zn	–0.608738	4.451200	8.188739	C	–2.320508	6.149388	11.137908
N	–2.365276	4.163055	7.532568	C	–1.393834	1.563398	9.119959
Ge	1.280382	5.232985	9.614172	C	–1.258098	2.311397	10.287295
N	2.833380	5.116544	8.585116	C	–0.284512	0.860473	8.654957
Si	–2.686527	4.326440	5.832195	C	–3.596732	6.473919	4.048180
C	–4.169316	3.241630	5.343186	C	–1.823381	7.026262	5.735904
C	–1.079618	3.752696	4.986432	C	4.079643	9.137834	7.883673
C	–3.032805	6.149177	5.428468	C	–6.682223	2.877403	11.088820
Si	3.009643	4.607916	6.907268	C	–0.855746	2.248537	5.106614
C	2.459364	2.836526	6.702790	C	–0.882194	4.211951	3.545158
C	2.027048	5.705953	5.741157	C	6.545938	2.782417	8.978289
C	4.809568	4.734245	6.419423	C	7.315427	1.891706	8.240905
C	–3.379097	3.876448	8.462754	C	5.171510	1.751244	13.688578
C	3.967484	5.615854	9.286666	C	–6.749521	7.696834	7.203119
C	–3.668564	2.534465	8.804751	C	–3.280021	0.062346	8.435289
C	–4.731160	2.232665	9.636110	C	–4.021055	–0.428523	7.364958
C	–2.705676	1.458151	8.362606	C	–3.118143	–0.745821	9.555413
C	2.117584	8.166896	9.155006	C	–0.046921	2.352171	10.971133
C	2.138967	8.539575	10.497121	C	–3.683971	8.175888	12.415564
C	0.885997	8.082933	8.507342	C	–5.503306	3.791142	5.846144
C	3.388813	7.888266	8.387512	C	–4.253432	2.925699	3.850772
C	–4.100061	4.877892	9.136325	C	–1.977800	6.496746	12.430198
C	4.736882	4.795326	10.117896	C	–4.591309	–1.690188	7.411423
C	4.297201	6.979064	9.186185	C	–4.428332	–2.485807	8.536230
C	5.388387	7.480941	9.872936	C	–2.663996	7.515136	13.079424
C	6.162834	6.675090	10.700340	C	–5.056378	9.385238	7.270780
C	5.806504	5.343532	10.819522	C	5.041325	9.002241	6.883893
C	4.417177	3.329456	10.284554	C	3.803540	10.410317	8.365305
C	–4.656975	7.240540	8.322193	C	4.478248	11.518667	7.868791
C	–5.925654	6.841451	7.923111	C	–3.688957	–2.008903	9.607416
C	–4.240390	8.529015	7.987766	C	–0.292055	8.369122	9.183862
C	–3.693893	6.330935	9.054545	C	–0.257477	8.753427	10.512882
C	5.607852	0.229526	8.462960	C	4.194939	2.335812	14.476496
C	6.850511	0.614199	7.978050	C	0.964516	8.840203	11.165341
C	4.846881	1.120580	9.198900	C	3.305000	3.236010	13.903997
C	5.299941	2.410958	9.465809	C	1.047553	1.646520	10.497079
C	–5.142130	4.535376	9.993768	C	0.921582	0.902138	9.331851
C	–5.512122	3.224028	10.221604	C	5.436452	11.370694	6.880912
C	7.345107	7.233930	11.430514	C	–6.319714	8.969967	6.871437
C	4.370952	2.952169	11.754502	C	5.714718	10.103181	6.386211
C	5.257525	2.055647	12.335458	H	5.635744	8.531848	9.769107
C	3.396745	3.543078	12.558574	H	5.231051	–0.767021	8.265556
C	–3.345653	6.804164	10.457534	H	3.883055	0.811467	9.586317
C	–4.022269	7.823313	11.113820	H	–5.666653	5.331124	10.513404

H	7.131700	8.225767	11.833219	H	5.218608	5.727753	6.610786
H	8.206223	7.336072	10.763869	H	4.909456	4.528740	5.350226
H	7.642244	6.587274	12.256739	H	5.423029	4.012153	6.959055
H	3.403799	3.188362	9.897905	H	4.125592	2.094326	15.530200
H	–3.811811	6.410157	6.153212	H	7.449150	–0.077917	7.398588
H	3.084751	7.333123	7.499126	H	1.766052	0.344863	8.945798
H	–6.488163	1.980337	11.679539	H	3.086546	8.578452	11.020821
H	–7.573785	2.680015	10.486288	H	–3.551950	–2.623598	10.489127
H	–6.923160	3.691700	11.773561	H	–0.376824	0.259283	7.757443
H	–0.288580	4.238734	5.579179	H	–4.704064	10.378213	7.018001
H	–4.944722	1.193685	9.858958	H	5.266388	8.014957	6.495869
H	6.916245	3.782534	9.162961	H	3.091947	2.173532	7.296347
H	6.020736	1.585339	11.727971	H	2.544928	2.536152	5.655125
H	–6.270199	5.843643	8.157342	H	1.425558	2.679846	7.013258
H	–2.114667	2.847593	10.677705	H	0.998887	9.126525	12.209562
H	–2.764698	6.349554	8.475174	H	0.035684	2.926884	11.885853
H	8.282405	2.205089	7.865780	H	–6.960034	9.634707	6.304574
H	–4.824157	8.347154	10.608893	H	–5.724343	4.771342	5.416851
H	–3.995436	2.293807	5.867091	H	–5.519102	3.894370	6.930978
H	–1.784761	5.345708	10.644171	H	–6.323049	3.121399	5.565345
H	–5.161659	–2.054727	6.565396	H	–1.021933	6.881937	5.006674
H	–1.165990	5.979906	12.927581	H	–1.403843	6.814544	6.724796
H	–3.256465	8.865937	8.292400	H	–2.090448	8.087655	5.718173
H	3.050338	10.543492	9.131306	H	1.030935	5.933526	6.123859
H	6.370236	4.701430	11.488356	H	1.901716	5.204349	4.777949
H	–2.465705	1.648977	7.314860	H	2.537175	6.652911	5.549559
H	–2.535822	–0.384507	10.394692	H	–3.794292	7.547514	3.961460
H	–1.237457	8.287541	8.664262	H	–4.539578	5.958857	3.860110
H	5.873300	1.050081	14.124430	H	–2.909771	6.206023	3.242778
H	–1.178021	8.965352	11.041388	H	5.960661	12.235518	6.492911
H	0.854919	7.812119	7.458467	H	–5.107011	2.270221	3.648085
H	2.709404	4.258723	12.116345	H	–3.360517	2.421691	3.478305
H	–4.228205	8.971149	12.911217	H	–4.393498	3.826463	3.249928
H	1.981200	1.667025	11.045343	H	0.079734	3.859049	3.158225
H	2.538136	3.702775	14.511090	H	–0.892360	5.298022	3.452182
H	–2.402606	7.790979	14.093819	H	–1.656584	3.819564	2.882668
H	4.247068	12.503089	8.257985	H	6.457326	9.973722	5.607937
H	–4.154305	0.189486	6.483890	H	–1.637075	1.678579	4.598082
H	–7.731368	7.357290	6.895350	H	–0.833925	1.924733	6.147603
H	–4.870752	–3.473797	8.574660	H	0.099784	1.958215	4.658734
FSPE	–7564.943275946212						

ab_167 (**1_opt**)							
Ge	10.577324	8.451335	3.568232	C	11.021620	3.863670	5.122959
C	9.063539	7.149313	3.420842	C	12.987492	2.747338	6.192565
Ga	12.060781	7.905563	5.465492	C	8.924409	6.456745	2.205276
Cl	12.537751	6.767304	3.355633	C	8.036035	7.063338	4.370651
N	12.964032	6.807363	6.795302	C	6.959281	6.207725	4.151831
N	13.544966	9.238925	5.332670	C	8.004433	7.927045	5.579514
C	14.767844	8.975156	5.731612	C	6.875680	5.457935	2.991803
C	13.201165	10.482281	4.724919	C	7.846900	5.598441	2.014759
C	14.295359	6.815564	6.919393	C	9.856968	6.691921	1.066752
C	12.208789	5.989920	7.689069	C	7.745098	9.297662	5.455641
C	15.128337	7.774859	6.368107	C	8.147435	7.363717	6.854884
C	15.875707	9.971209	5.559707	C	7.645131	10.075988	6.604952
C	14.945957	5.733448	7.728407	C	7.532875	9.955816	4.123684
C	13.544560	10.753604	3.392701	C	7.787961	9.537799	7.872928
C	12.429207	11.384662	5.476519	C	8.042571	8.175559	7.974196
C	12.022108	12.566931	4.875297	C	7.644004	10.386728	9.098372
C	12.078892	11.094361	6.918905	C	8.401883	5.900345	7.031056
C	12.367612	12.858871	3.567423	C	10.797097	5.726441	0.689326
C	13.120816	11.959190	2.842542	C	9.740414	7.872838	0.317933
C	14.330702	9.801994	2.517617	C	10.607751	8.089933	–0.745218
C	10.844555	11.836230	7.406538	C	8.690827	8.897546	0.622729
C	13.265589	11.380688	7.837355	C	11.583046	7.168529	–1.096814
C	13.529731	9.389827	1.284473	C	11.649262	5.985635	–0.375491
C	15.660349	10.413328	2.076542	C	12.545810	7.451691	–2.208382
C	11.851864	6.527930	8.935642	C	10.883993	4.416230	1.405768
C	11.856455	4.681662	7.336831	H	16.183660	7.653531	6.564898
C	11.134138	5.731370	9.819040	H	16.561756	9.618819	4.786966
C	12.271142	7.918246	9.361714	H	16.445252	10.051725	6.485702
C	10.779442	4.436491	9.486806	H	15.508751	10.953293	5.273658
C	11.138044	3.923635	8.254907	H	14.775125	4.765021	7.254783
C	12.243749	4.068610	6.011509	H	14.520038	5.669047	8.729417
C	11.073765	8.779332	9.741434	H	16.017247	5.901588	7.806390
C	13.280655	7.866303	10.506291	H	11.422871	13.272478	5.434852

H	7.483586	5.318723	6.912608
H	8.803835	5.694444	8.021674
H	9.106698	5.526983	6.290951
H	10.511729	9.007304	–1.317723
H	12.389519	5.238896	–0.645467
H	8.532083	9.549445	–0.236763
H	8.990813	9.528883	1.464862
H	7.739957	8.434590	0.889544
H	12.910618	6.530435	–2.664896
H	13.416456	8.000492	–1.836852
H	12.086620	8.061629	–2.988076
H	10.107697	3.726408	1.061721
H	10.748742	4.547167	2.476490
H	11.851368	3.943485	1.233645
FSPE	–6628.917324079191		

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