

Electronic Supplemental Information For

Yttrium germole dianion complexes with Y–Ge bonds

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1. DFT Calculations

Computational Details

All computations reported in this article were performed employing DFT method implemented in the Gaussian 09 suite of programs.^[S1] Geometry optimizations were carried out using gradient-corrected BP86 functional^[S2,S3] in conjunction with the Ahlrichs' split valence plus polarization (def2-SVP) basis set^[S4,S5] for all the atoms along with the corresponding effective core potential (ECP) for yttrium atom. BP86 is composed of Becke's 1988 exchange and Perdew's 1986 correlation functionals. No symmetry constraints were imposed during geometry optimizations. Frequency calculations were accomplished at the same level on the optimized geometries to characterize the nature of stationary points. All of the structures were verified as true minima on the potential energy surface in the absence of imaginary frequency. Single-point calculations were performed on the optimized geometries using BP86 functional in combination with the def2-TZVP basis set^[S4,S5] for all the atoms along with the corresponding ECP for yttrium atom. Tight wave function convergence criteria and "ultrafine" (99,950) grid were used in numerical integration during single-point calculations. Additionally, to incorporate the London dispersion effects, we used Grimme's D3 empirical corrections.^[S6] Natural bond orbital (NBO)^[S7,S8] analysis was performed at the BP86-D3/def2-TZVP//BP86/def2-SVP level using the NBO Version 3.1 program. Wiberg bond indices (WBI) were calculated at the same level of theory.^[S9] Furthermore, to gain insight into the bonding scenario of the complexes, EDA (energy decomposition analysis), which was originally developed by Morokuma^[S10] and later modified by Ziegler and Rauk,^[S11] calculations were performed in conjunction with the NOCV (natural orbital for chemical valence)^[S12] method using the ADF 2019.302 program package.^[S13] EDA-NOCV calculations were performed at the BP86-D3/TZ2P level on the optimized geometries at the BP86/def2-SVP level without any frozen core approximation and also no symmetry constraints were imposed during the calculations. Scalar relativistic effects were considered using zeroth-order regular approximation (ZORA).^[S14] EDA allows partitioning the instantaneous interaction energy (ΔE_{int}) between the fragments (A and B) in the molecule AB into three chemically meaningful terms (eq 1):

$$\Delta E_{\text{int}} = \Delta E_{\text{elstat}} + \Delta E_{\text{Pauli}} + \Delta E_{\text{orb}} \quad (1)$$

In eq 1, ΔE_{elstat} denotes the quasiclassical Coulomb interaction energy between frozen charge densities of the fragments in the geometry of the adduct. ΔE_{Pauli} corresponds to the Pauli

repulsion between the fragments and accounts for the four-electron destabilizing interaction between the occupied orbitals. The stabilizing orbital interaction term ΔE_{orb} represents the interaction between the occupied and virtual orbitals of the two fragments. Since the dispersion corrected functional is used, the dispersion term, ΔE_{disp} , which represents the dispersion interaction between the two fragments, is added to the ΔE_{int} . The ΔE_{orb} term can be further partitioned into the contributions of the orbitals belonging to different irreducible representations of the interacting system. The EDA-NOCV method merges charge (NOCV) and energy (EDA) partitioning schemes to decompose the deformation density ($\Delta\rho$) into different components of the chemical bond. The bond dissociation energy (ΔE) between the interacting fragments is given by eq 2.

$$\Delta E = -D_e = \Delta E_{\text{int}} + \Delta E_{\text{prep}} \quad (2)$$

The destabilizing preparation energy term ΔE_{prep} is defined as the energy required to promote the fragments A and B from their equilibrium geometry and ground electronic state to the geometry and the electronic state in the molecule AB. The deformation density plots were rendered using ADF-GUI interface.^[S15] Furthermore, QTAIM (quantum theory of atoms in molecules) calculations were performed in the AIMALL Version 17.01.25 software package^[S16] to characterize the electron distribution around selected bonds in the chemical species by applying Bader's AIM (atoms-in-molecules) theory.^[S17] Importantly, any two bonded atoms are connected through a bond path where the electron density [$\rho(\mathbf{r})$] shows the maximum value. The bond critical point (BCP) is characterized by a point on the bond path where the gradient [$\nabla\rho(\mathbf{r})$] of the electron density is equal to zero. The magnitude of the electron density and its Laplacian [$\nabla^2\rho(\mathbf{r})$] at the BCP convey important information about the strength and type of chemical bond. The Laplacian indicates whether the electron density is locally concentrated [$\nabla^2\rho(\mathbf{r}) < 0$] or depleted [$\nabla^2\rho(\mathbf{r}) > 0$]. The extent to which density is preferentially accumulated in a given plane containing the bond path is denoted by the term ellipticity (ϵ). Orbital diagrams were rendered in Chemcraft^[S18] and optimized geometries were prepared using the CYLview^[S19] visualization software.

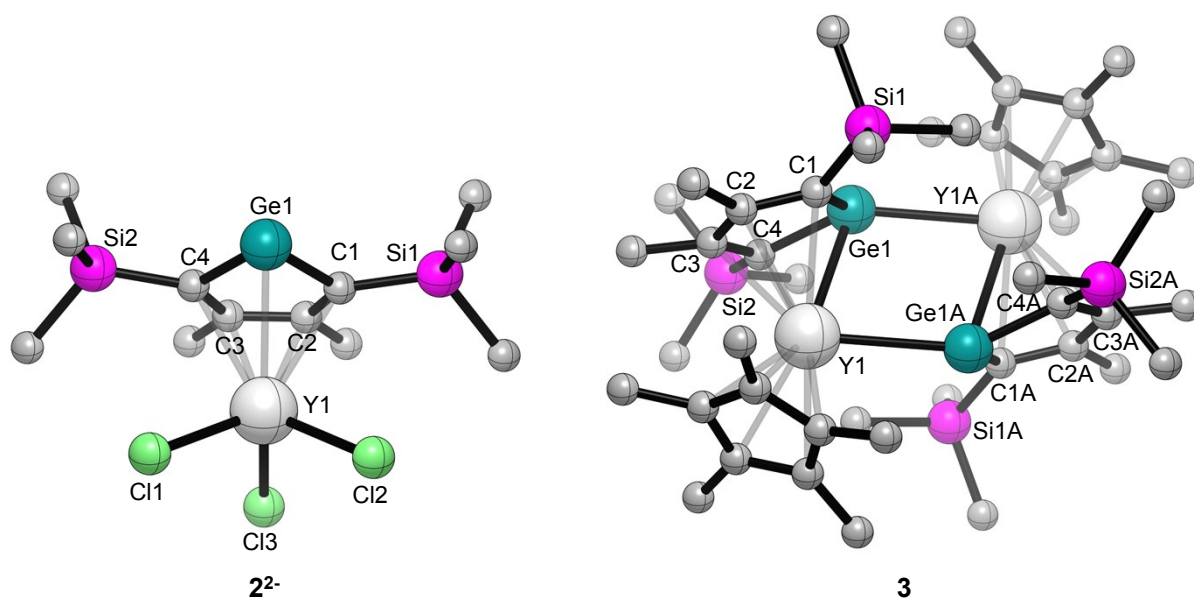


Fig. S1. Optimized geometries of the complexes **2²⁻** and **3** in singlet ground electronic states at the BP86/def2-SVP level of theory. Hydrogen atoms are omitted for clarity.

Table S1. Selected geometrical parameters of the complexes **2²⁻** and **3** in singlet ground electronic states at BP86/def2-SVP level of theory. Bond distances (d) are in angstroms (Å) and bond angles (∠) are in degrees (°).

Compound	Geometrical Parameter	Crystal Structure	Calculated
2²⁻	d (Y1–Ge1)	3.0024(4)	3.040
	d (Y1–C1)	2.654(3)	2.732
	d (Y1–C2)	2.608(3)	2.703
	d (Y1–C3)	2.610(3)	2.703
	d (Y1–C4)	2.670(2)	2.732
	d (Y1–Cl1)	2.5657(7)	2.590
	d (Y1–Cl2)	2.5777(7)	2.590
	d (Y1–Cl3)	2.5795(7)	2.602
	d (C1–Si1)	1.836(3)	1.859
	d (C4–Si2)	1.837(3)	1.859
	∠C4–Ge1–C1	85.26(11)	84.5
	∠Y1–Ge1–C1	60.47(7)	61.7
	∠Ge1–Y1–Cl1	105.356(18)	101.9

	\angle Ge1-Y1-Cl2	102.480(18)	101.9
	\angle Ge1-Y1-Cl3	146.12(2)	143.0
	\angle Y1-C1-Si1	124.66(12)	124.1
	\angle Ge1-C1-Si1	119.55(13)	120.2
3	d (Ge1–Ge1A)	3.630(5)	3.659
	d (Y1–Y1A)	4.668(5)	4.811
	d (Ge1–Y1A)	2.9512(6)	3.039
	d (Y1–Ge1A)	2.9513(6)	3.039
	d (Y1–Ge1)	2.9610(6)	3.005
	d (Y1–C1)	2.674(5)	2.702
	d (Y1–C2)	2.674(4)	2.680
	d (Y1–C3)	2.646(4)	2.669
	d (Y1–C4)	2.647(4)	2.683
	d (Y1A–Ge1A)	2.9610(6)	3.005
	d (Y1A–C1A)	2.674(5)	2.702
	d (Y1A–C2A)	2.674(4)	2.680
	d (Y1A–C3A)	2.646(4)	2.669
	d (Y1A–C4A)	2.647(4)	2.683
	\angle Y1-Ge1-Y1A	104.241(18)	105.5
	\angle Ge1-Y1-Ge1A	75.760(18)	74.5
	\angle Y1-Ge1A-Y1A	104.241(18)	105.5
	\angle Ge1-Y1A-Ge1A	75.760(18)	74.5

Table S2. NPA charges (in e) on selected atoms in the complexes **2²⁻** and **3** at the BP86-D3/def2-TZVP//BP86/def2-SVP level.

Complex	Atom	NPA Charge
2²⁻	Ge1	+0.477

	Y1	+0.921
	Cl1	-0.523
	Cl2	-0.523
	Cl3	-0.534
3	Ge1	+0.692
	Y1	+1.117
	Ge1A	+0.692
	Y1A	+1.117

Table S3. EDA results of 2^{2-} at the BP86-D3/TZ2P(ZORA)//BP86/def2-SVP level.^[a]

Complex	Fragments
2^{2-}	germole dianion ring (α) + YCl_3 (β)
ΔE_{int}	-141.2
ΔE_{Pauli}	94.9
$\Delta E_{\text{elstat}}^{\text{[b]}}$	-125.5 (53.1%)
$\Delta E_{\text{orb}}^{\text{[b]}}$	-96.6 (40.9%)
$\Delta E_{\text{disp}}^{\text{[b]}}$	-14.1 (6.0%)
$\Delta E_{\text{prep}}(\alpha)^{\text{[b]}}$	3.5
$\Delta E_{\text{prep}}(\beta)$	17.8
ΔE_{prep}	21.3
$\Delta E(-D_e)$	-119.9

^[a]Energy values are given in kcal mol⁻¹. ^[b]Percentage contribution to the total attractive interactions $\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$. ^[c] $\Delta E_{\text{prep}}(\alpha)$ and $\Delta E_{\text{prep}}(\beta)$ are the preparation energies of the germole dianion ring (α) and YCl_3 (β) fragments, respectively.

Table S4. EDA results of **3** at the BP86-D3/TZ2P(ZORA)//BP86/def2-SVP level.^[a]

Complex	Fragments	
3	η^5 -germole-Y-Cp* + η^5 -germole-Y-Cp*	η^1 -germole-Y-Cp* + η^1 -germole-Y-Cp*
ΔE_{int}	-97.4	-218.7
ΔE_{Pauli}	142.7	416.7
$\Delta E_{\text{elstat}}^{[b]}$	-113.7 (47.3%)	-323.5 (50.9%)
$\Delta E_{\text{orb}}^{[b]}$	-87.5 (36.5%)	-270.8 (42.6%)
$\Delta E_{\text{disp}}^{[b]}$	-38.9 (16.2%)	-41.1 (6.5%)

^[a]Energy values are given in kcal mol⁻¹. ^[b]Percentage contribution to the total attractive interactions $\Delta E_{\text{elstat}} + \Delta E_{\text{orb}} + \Delta E_{\text{disp}}$. Cp* = pentamethylcyclopentadienyl.

Table S5. Topological parameters of selected bonds at (3, -1) BCPs in **3** at the BP86-D3/def2-TZVP//BP86/def2-SVP level.

Complex	Bond	$\rho(\mathbf{r})^{[a]}$	$[\nabla^2\rho(\mathbf{r})]^{[b]}$	$\epsilon^{[c]}$
3	Ge1-Y1A	0.031	+0.032	0.167
	Ge1A-Y1	0.031	+0.032	0.167
	Ge1-Ge1A	0.015	+0.014	4.156

^[a]Electron density at BCP ($e/\text{\AA}^3$). ^[b]Laplacian at BCP ($e/\text{\AA}^5$). ^[c]Ellipticity.

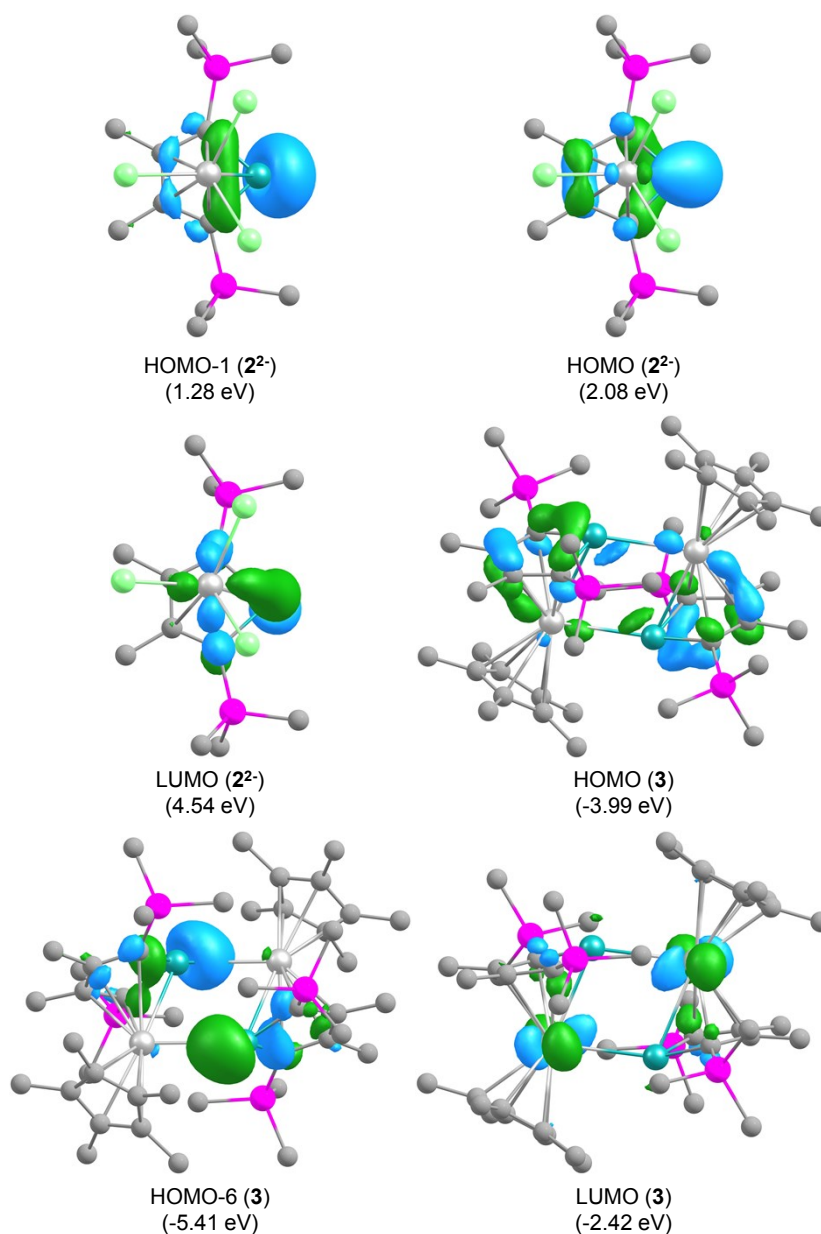


Fig. S2. Selected KS-MOs of the complexes 2^{2-} and 3 (isosurface = 0.06 a.u.). The orbital energies are shown in parentheses. Hydrogen atoms are omitted for clarity.

Table S6. Absolute energies (in hartrees) of the complexes 2^{2-} and 3 at the BP86/def2-SVP level. E_e = Electronic energy at 298 K, H_{298} = gas-phase enthalpy at 298 K, G_{298} = gas-phase Gibbs free energy at 298 K.

Complex	E_e	G_{298}	H_{298}	No. of imaginary frequency
2^{2-}	-4546.34368878	-4546.094714	-4545.997085	0
3	-7111.20752061	-7110.264704	-7110.069521	0

Cartesian coordinates of 2²⁻ and 3

Table S7. Cartesian coordinates (in Å) of the optimized structures at the BP86/def2-SVP level of theory.

2 ²⁻			
C	1.3401370	-0.9765380	0.268460
C	0.7193860	-0.6103650	1.515980
C	-0.7192990	-0.6103740	1.515997
C	-1.3400780	-0.9765480	0.268501
C	1.4691550	-0.3036540	2.805152
H	1.1797040	0.6835190	3.229010
H	2.5656200	-0.2863620	2.645949
H	1.2625130	-1.0728780	3.588788
C	-1.4690340	-0.3035750	2.805175
H	-1.1796660	0.6836910	3.228866
H	-1.2622310	-1.0726430	3.588915
H	-2.5655010	-0.2864620	2.646022
C	4.3562290	0.1830420	0.499076
H	4.0351480	1.1316730	0.016946
H	5.3992680	-0.0439320	0.178823
H	4.3668400	0.3437700	1.598593
C	3.4987270	-1.4447880	-1.915306
H	2.8575060	-2.2414080	-2.348270
H	4.5667790	-1.6989300	-2.103035
H	3.2585980	-0.4976670	-2.442986
C	3.7965430	-2.8164020	0.823097
H	3.6727300	-2.7445710	1.926036
H	4.8736140	-3.0101110	0.611964
H	3.2103440	-3.6974810	0.482502
C	-3.4985540	-1.4438730	-1.915536
H	-3.2588440	-0.4962580	-2.442521
H	-4.5664750	-1.6983910	-2.103480
H	-2.8569210	-2.2398700	-2.349037
C	-4.3565890	0.1820090	0.500002
H	-4.3675160	0.3417140	1.599668
H	-5.3994920	-0.0449670	0.179305
H	-4.0356900	1.1311680	0.018792
C	-3.7959210	-2.8173930	0.822025
H	-3.2092390	-3.6980300	0.481132
H	-4.8728590	-3.0114760	0.610535
H	-3.6724140	-2.7460390	1.925028
Cl	-1.9980170	2.3347480	-1.517646
Cl	1.9969360	2.3341430	-1.519530
Cl	0.0006900	2.8768000	1.925403
Ge	0.0000360	-1.5421760	-1.095142
Si	3.1561300	-1.2161190	-0.050454
Si	-3.1560250	-1.2163650	-0.050538

Y	-0.0000520	1.3597520	-0.188838
3			
C	0.880428	2.450044	-0.523725
C	0.808748	3.510675	0.439787
C	-0.403936	3.568745	1.218288
C	-1.396227	2.551474	0.946998
C	1.834508	4.629627	0.499960
H	2.817814	4.309552	0.106108
H	1.998608	5.022833	1.523649
H	1.499270	5.493836	-0.117424
C	-0.689067	4.780259	2.089060
H	0.223746	5.220344	2.531013
H	-1.384448	4.554220	2.919739
H	-1.162305	5.582922	1.479767
C	3.940001	2.376072	-1.553234
H	4.262029	3.408002	-1.299299
H	4.538338	2.057220	-2.433940
H	4.215839	1.718011	-0.704472
C	1.667207	0.672038	-2.839584
H	1.757171	-0.177896	-2.123261
H	2.338319	0.454521	-3.696166
H	0.632698	0.738964	-3.242896
C	1.764320	3.724939	-3.215181
H	0.706414	3.733341	-3.550629
H	2.411870	3.613527	-4.111975
H	1.980760	4.717895	-2.767486
C	-4.274259	1.311833	0.900561
H	-4.182707	1.175719	-0.195128
H	-5.340469	1.527223	1.127559
H	-4.018859	0.351288	1.387592
C	-3.941759	4.334549	0.778953
H	-3.449560	5.255688	1.152239
H	-5.021870	4.405344	1.032091
H	-3.850376	4.329496	-0.327777
C	-3.451886	2.809075	3.414777
H	-3.028421	1.915654	3.919337
H	-4.541389	2.828912	3.635540
H	-3.007312	3.707737	3.890418
C	2.915062	0.502422	3.329979
C	2.977821	1.935110	3.237417
C	1.883385	2.475778	4.002841
C	1.135575	1.373166	4.547022
C	1.782562	0.153125	4.140918
C	3.975054	-0.463514	2.871243
H	4.680142	-0.696724	3.702179
H	4.585938	-0.053773	2.042380
H	3.545447	-1.427243	2.528882
C	4.125794	2.722664	2.655959

H	4.955870	2.819695	3.392487
H	3.828432	3.750120	2.369339
H	4.556929	2.241620	1.753968
C	1.730888	3.912113	4.430205
H	2.298730	4.098872	5.370615
H	0.677119	4.187267	4.633824
H	2.124321	4.624261	3.677285
C	-0.004384	1.498029	5.528451
H	0.372166	1.680985	6.560650
H	-0.623095	0.579238	5.571603
H	-0.684669	2.340421	5.284987
C	1.490153	-1.238586	4.643505
H	1.522036	-1.997367	3.833030
H	0.498479	-1.311262	5.132921
H	2.243488	-1.547047	5.403432
Ge	-0.840276	1.496408	-0.633736
Si	2.074267	2.322807	-1.961426
Si	-3.192446	2.742491	1.518290
Y	0.755849	1.264558	1.901633
C	-0.880428	-2.450044	0.523725
C	-0.808748	-3.510675	-0.439787
C	0.403936	-3.568745	-1.218288
C	1.396227	-2.551474	-0.946998
C	-1.834508	-4.629627	-0.499960
H	-2.817814	-4.309552	-0.106108
H	-1.998608	-5.022833	-1.523649
H	-1.499270	-5.493836	0.117424
C	0.689067	-4.780259	-2.089060
H	-0.223746	-5.220344	-2.531013
H	1.384448	-4.554220	-2.919739
H	1.162305	-5.582922	-1.479767
C	-3.940001	-2.376072	1.553234
H	-4.262029	-3.408002	1.299299
H	-4.538338	-2.057220	2.433940
H	-4.215839	-1.718011	0.704472
C	-1.667207	-0.672038	2.839584
H	-1.757171	0.177896	2.123261
H	-2.338319	-0.454521	3.696166
H	-0.632698	-0.738964	3.242896
C	-1.764320	-3.724939	3.215181
H	-0.706414	-3.733341	3.550629
H	-2.411870	-3.613527	4.111975
H	-1.980760	-4.717895	2.767486
C	4.274259	-1.311833	-0.900561
H	4.182707	-1.175719	0.195128
H	5.340469	-1.527223	-1.127559
H	4.018859	-0.351288	-1.387592
C	3.941759	-4.334549	-0.778953
H	3.449560	-5.255688	-1.152239
H	5.021870	-4.405344	-1.032091
H	3.850376	-4.329496	0.327777

C	3.451886	-2.809075	-3.414777
H	3.028421	-1.915654	-3.919337
H	4.541389	-2.828912	-3.635540
H	3.007312	-3.707737	-3.890418
C	-2.915062	-0.502422	-3.329979
C	-2.977821	-1.935110	-3.237417
C	-1.883385	-2.475778	-4.002841
C	-1.135575	-1.373166	-4.547022
C	-1.782562	-0.153125	-4.140918
C	-3.975054	0.463514	-2.871243
H	-4.680142	0.696724	-3.702179
H	-4.585938	0.053773	-2.042380
H	-3.545447	1.427243	-2.528882
C	-4.125794	-2.722664	-2.655959
H	-4.955870	-2.819695	-3.392487
H	-3.828432	-3.750120	-2.369339
H	-4.556929	-2.241620	-1.753968
C	-1.730888	-3.912113	-4.430205
H	-2.298730	-4.098872	-5.370615
H	-0.677119	-4.187267	-4.633824
H	-2.124321	-4.624261	-3.677285
C	0.004384	-1.498029	-5.528451
H	-0.372166	-1.680985	-6.560650
H	0.623095	-0.579238	-5.571603
H	0.684669	-2.340421	-5.284987
C	-1.490153	1.238586	-4.643505
H	-1.522036	1.997367	-3.833030
H	-0.498479	1.311262	-5.132921
H	-2.243488	1.547047	-5.403432
Ge	0.840276	-1.496408	0.633736
Si	-2.074267	-2.322807	1.961426
Si	3.192446	-2.742491	-1.518290
Y	-0.755849	-1.264558	-1.901633

2. NMR spectra of K₂2, 3 and 4

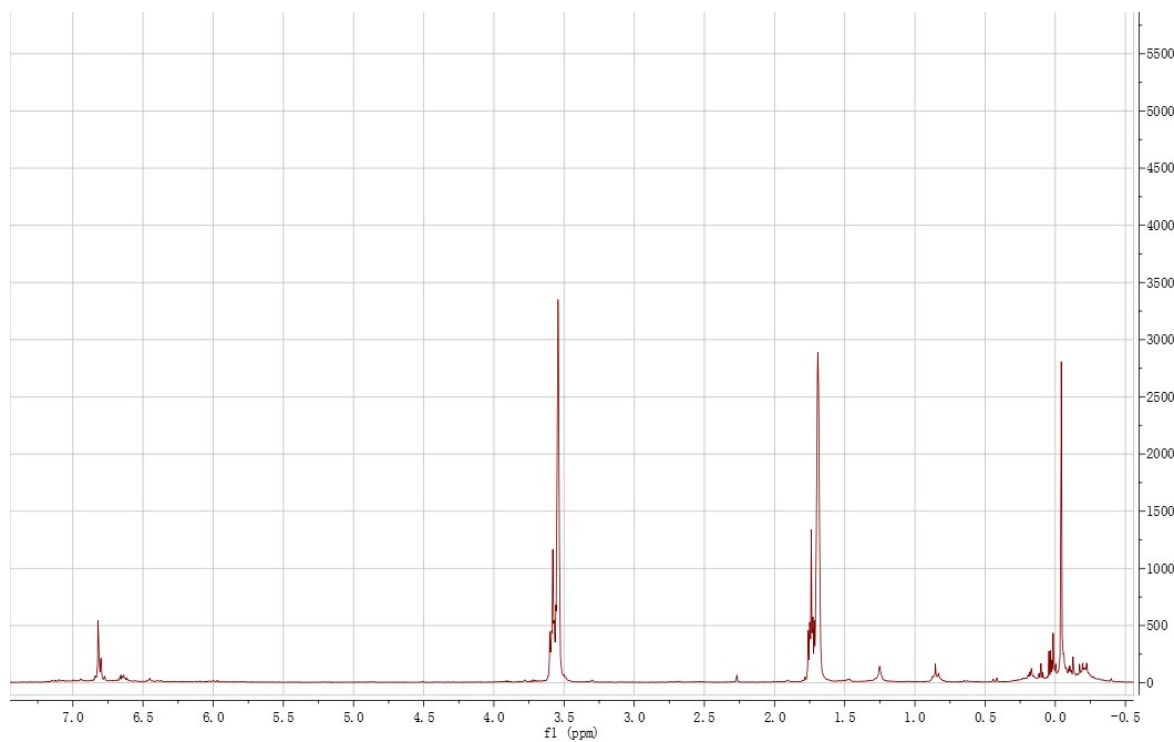


Fig. S3. ¹H NMR spectrum of K₂2 in d₈-THF.

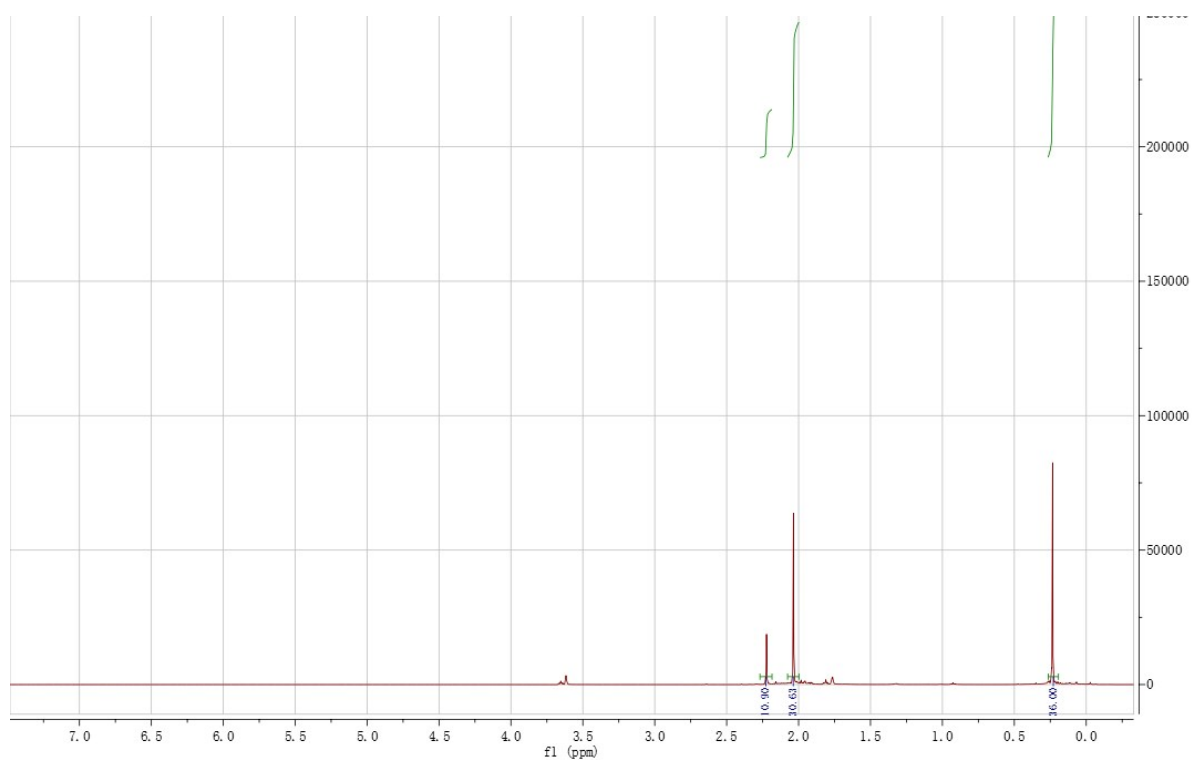


Fig. S4. ¹H NMR spectrum of 3 in d₈-THF.

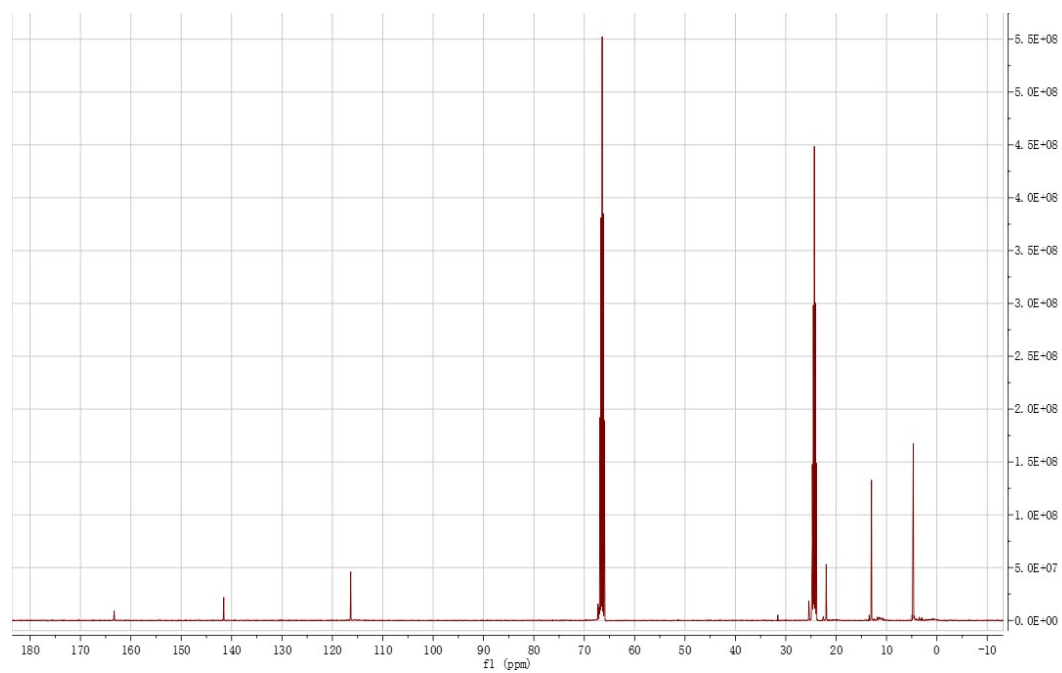


Fig. S5. ^{13}C NMR spectrum of **3** in d_8 -THF.

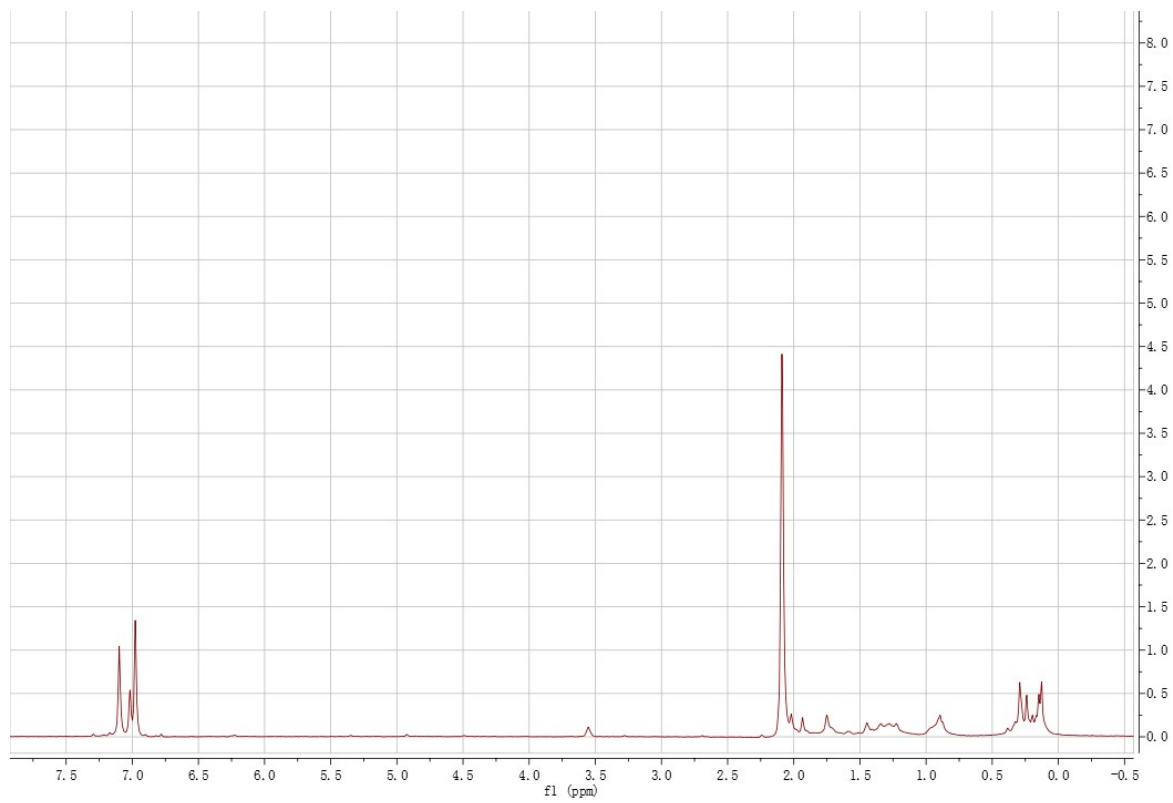


Fig. S6. ^1H NMR spectrum of **4** in d_8 -toluene.

3. Notes and references

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