A Crystalline T-shaped Planar Group 14 Anion

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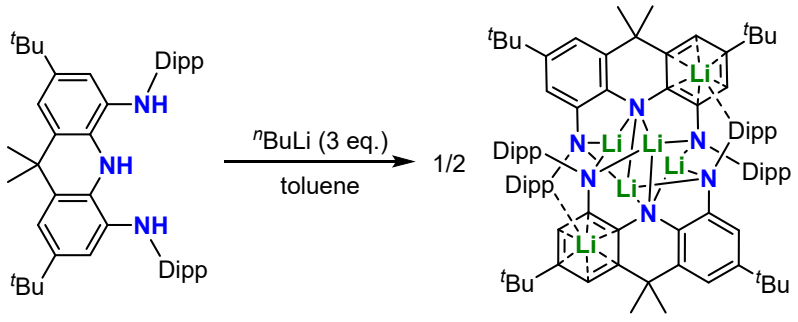
Contents

1. Synthesis of new compounds and their NMR spectra

General considerations: All reactions and product manipulations were conducted under a dry dinitrogen atmosphere with rigid exclusion of air and moisture using standard Schlenk techniques, or in a glove box. All glasswares were oven dried. Organic solvents were distilled under nitrogen from purple sodium benzophenone ketyl and vacuum transferred from the same prior to use. Commercially available reagents were purchased from Energy Chemical and used as received. ^{1}H, ^{13}C{^{1}H}, DEPT135, ^{7}Li and ^{77}Se{^{1}H} NMR spectra were obtained with a Bruker AVIII 400 MHz BBFO1 spectrometer and Agilent VNMRS-300 spectrometer at 298 K. Chemical shifts (δ) are given in p.p.m. Coupling constants J are given in Hz. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad signal. UV-vis spectra were recorded on the Lambda 750 spectrometer at room temperature. EPR spectra were obtained using JEOL JES-X320 X-band variable-temperature apparatus. Electrospray ionization (ESI) mass spectra were obtained with the Waters Q-Tof Premier Mass Spectrometer. Element analyses were performed on an Elementar Vario EL III instrument. Compound **1** was synthesized according to the literature procedure.[S1]

Synthesis of compound 2

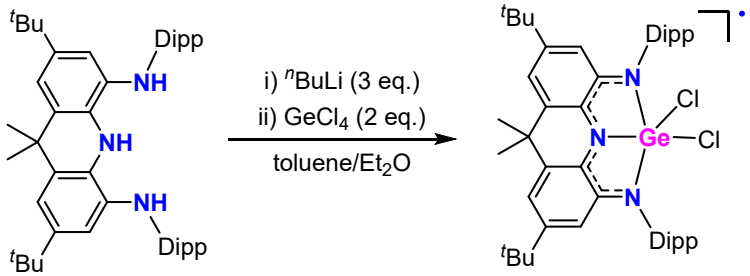


1 **2** (64%)

A hexane solution of ^{n}BuLi (0.9 ml, 1.6 M, 1.44 mmol) was added dropwise into a toluene/Et_2O (30 mL/0.5 mL) solution of **1** (302 mg, 0.45 mmol) at –78 °C and the reaction mixture was stirred for 4 hours. After removal of the solvent under vacuum, the residue was washed with cooled hexane (10 ml) to afford **2** as a yellow powder (193 mg, 64%). ^{1}H NMR (C_6D_6, 300 MHz, 298 K): δ 7.03–6.97 (m, 4H, Ar-*H*), 6.92

(d, J = 6.0 Hz, 2H, Ar-*H*), 6.86 (d, J = 6.0 Hz, 2H, Ar-*H*), 6.81 (s, 2H, Ar-*H*), 6.70 (d, J = 6.0 Hz, 2H, Ar-*H*), 6.46 (s, 2H, Ar-*H*), 6.43–6.38 (m, 2H, Ar-*H*), 6.14 (s, 2H, Ar-*H*), 6.01 (s, 2H, Ar-*H*), 3.34 (br, 2H, $(CH_3)_2CH$), 3.23 (br, 2H, $(CH_3)_2CH$), 2.94 (br, 2H, $(CH_3)_2CH$), 2.71 (br, 2H, $(CH_3)_2CH$), 1.95 (s, 6H, $C(CH_3)_2$), 1.68 (d, J = 6.0 Hz, 6H, $(CH_3)_2CH$), 1.59 (s, 6H, $C(CH_3)_2$), 1.42 (s, 18H, $C(CH_3)_3$), 1.38 (d, 6H, $(CH_3)_2CH$), 1.28 (d, 12H, $(CH_3)_2CH$), 1.05 (d, J = 6.0 Hz, 6H, $(CH_3)_2CH$), 0.98 (s, 18H, $C(CH_3)_3$), 0.73 (d, J = 6.0 Hz, 6H, $(CH_3)_2CH$), 0.64 (d, J = 6.0 Hz, 6H, $(CH_3)_2CH$), 0.16 (d, J = 6.0 Hz, 6H, $(CH_3)_2CH$); Attempts to collect the $^{13}C\{^1H\}$ NMR spectrum of compound **2** failed due to its bad solubility in C_6D_6 and C_7D_8 after isolation and unstability in THF-D_8; ^7Li NMR (C_6D_6, 156 MHz, 298 K): 1.96 (S, 2Li), 0.49 (br, 2Li), -0.62 (br, 2Li). HRMS (ESI): m/z calcd for $C_{94}H_{125}Li_6N_6$: 1380.0891 $[(M+H)]^+$; found: 1380.0926. Elemental analysis for $C_{94}H_{120}Li_6N_6$ (%): Calculated: C 82.07; H 8.79, N 6.11; Found: C 82.19, H 8.83, N 5.99.

Synthesis of compound 3

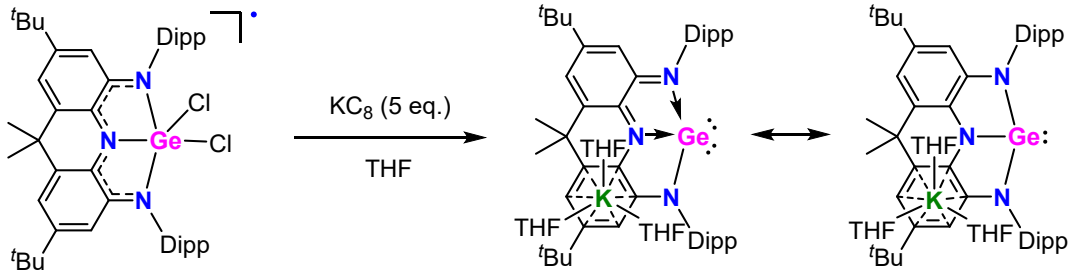


1 **3** (61%)

A hexane solution of ^{n}BuLi (4.0 ml, 1.6 M, 6.4 mmol) was added dropwise into a mixture tolene/Et_2O (50 mL/1.5 mL) solution of **1** (1.34 g, 2.0 mmol) at –78 °C and the reaction mixture was slowly warm up to 10 °C. The toluene solution (20 ml) of $GeCl_4$ (0.86 g, 4.0 mmol) was added dropwise at –78 °C. After slowly warming up to room temperature and stirred overnight, the solvent was removed under vacuum and the resulting residue was extracted with hexane (20 ml). After filtration and removal of the solvent, **3** was obtained as a purple powder (1.0 g, 61%). Single crystals of **3** suitable for X-ray diffraction studies were grown from its saturated hexane solution at room temperature. UV-vis (toluene): λ_{max} = 580 and 400 nm. HRMS (ESI): m/z calcd

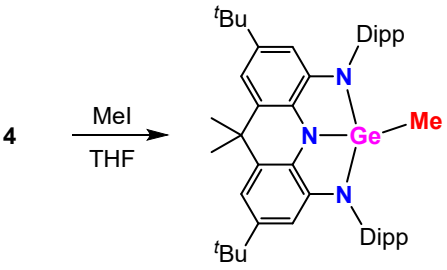
for $C_{47}H_{62}Cl_2N_3Ge$: 812.3533 $[(M)]^+$; found: 812.3532. Elemental analysis for $C_{47}H_{64}Cl_2GeN_3$ (%): Calculated: C 69.30, H 7.92, N 5.16; Found: C 69.13, H 7.83, N 5.36.

Synthesis of compound 4



Potassium graphite (0.82 g, 6.1 mmol) was slowly added to a THF (100 ml) solution of **3** (0.97 g, 1.2 mmol) at –30 °C. The reaction mixture was slowly warmed up to room temperature and stirred overnight. After filtration, the solvent was removed under vacuum and the residue was washed with cooled hexane (5 ml) to afford **4** as a yellow powder (0.69 g, 58%). Single crystals of **4** suitable for X-ray diffraction studies were grown from its saturated THF solution at –30 °C. ^{1}H NMR (THF-d_8, 300 MHz, 298 K): δ 7.04 (d, *J* = 7.5 Hz, 4H, Dipp-*m*-C*H*), 6.91–6.84 (m, 2H, Dipp-*p*-C*H*), 6.58 (s, 2H, Me_2CCCH), 5.94 (s, 2H, DippNCC*H*), 3.60–3.56 (m, 12H, THF-CH_2), 3.14 (sep, *J* = 9.2 Hz, 4H, $(CH_3)_2CH$), 1.75–1.71 (m, 12H, THF-CH_2), 1.68 (s, 6H, $C(CH_3)_2$), 1.21 (s, 18H, $C(CH_3)_3$), 1.04 (d, *J* = 7.5 Hz, 12H, $(CH_3)_2CH$), 1.00 (d, *J* = 7.5 Hz, 12H, $(CH_3)_2CH$); ^{13}C{^{1}H} NMR (THF-d_8, 100 MHz, 298 K): δ 146.91 (Ar-*C*), 146.09 (Ar-*C*), 144.45 (Ar-*C*), 140.84 (Ar-*C*), 131.59 (Ar-*C*), 127.32 (Ar-*C*), 122.37 (Dipp-*p*-CH), 122.27 (Dipp-*m*-CH), 104.59 (Me_2CCCH), 103.06 (DippNCCH), 68.02 (THF-CH_2), 37.64 ($(CH_3)_2C$), 34.94 ($(CH_3)_3C$), 34.40 ($(CH_3)_2C$), 32.55 ($(CH_3)_3C$), 27.97 ($(CH_3)_2CH$), 26.76 ($(CH_3)_2CH$), 26.14 (THF-CH_2), 24.99 ($(CH_3)_2CH$). UV-vis (THF): λ_{max} = 309 and 396 (shoulder) nm. HRMS (ESI): m/z calcd for $C_{47}H_{62}N_3Ge$: 742.4156 $[(M\text{-}K)]^-$; found: 742.4142. Elemental analysis for $C_{59}H_{86}GeKN_3O_3$ (%): Calculated: C 71.07, H 8.69, O 4.81, N 4.21; Found: C 70.68, H 8.71, O 4.79, N 4.72.

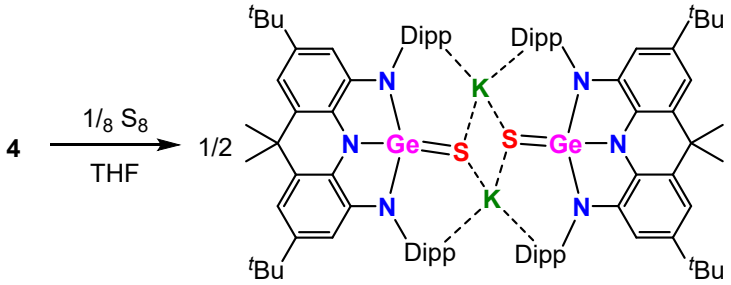
Synthesis of compound 5



5 (70%)

MeI (20 µl, 45.6 mg, 0.32 mmol) was slowly added to a THF (5 ml) solution of **4** (0.32 g, 0.32 mmol) at room temperature and stirred for 20 mins. Then the solvent was removed under vacuum and the residue was washed with hexane to afford **6** as a yellow powder (0.17 g, 70%). Single crystals of **5** suitable for X-ray diffraction studies were grown from its saturated hexane solution at room temperature. ^{1}H NMR (C_6D_6, 300 MHz, 298 K): δ 7.22 (br, 8H, Ar-*H*), 6.51 (s, 2H, DippNCC*H*), 3.20 (sept, J = 8.0 Hz, 4H, $(CH_3)_2CH$), 1.86 (s, 6H, $(CH_3)_2C$), 1.31 (s, 18H, $(CH_3)_3C$), 1.12 (d, J = 9.0 Hz, 12H, $(CH_3)_2CH$), 1.07 (d, J = 9.0 Hz, 12H, $(CH_3)_2CH$), 0.78 (s, 3H, $GeCH_3$); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz, 298 K): δ 147.77 (Ar-*C*), 145.07 (Ar-*C*), 138.96 (Ar-*C*), 138.25 (Ar-*C*), 132.79 (Ar-*C*), 132.78 (Ar-*C*), 127.63 (Dipp-*CH*), 124.50 (Dipp-*CH*), 110.81 (Me_2CCCH), 109.06 (DippNCCH), 39.47 ($(CH_3)_2C$), 35.17 ($(CH_3)_3C$), 32.18 ($(CH_3)_2C$), 28.77 ($(CH_3)_3CH$), 28.76 ($(CH_3)_3CH$), 27.19 ($(CH_3)_3C$), 25.99 ($(CH_3)_3CH$), 24.17 ($(CH_3)_3CH$), -1.47 ($Ge\text{-}CH_3$). UV-vis (THF): λ_{max} = 324 nm. HRMS (ESI): m/z calcd for $C_{48}H_{66}N_3Ge$: 758.4469 $[(M+H)]^+$; found: 758.4490. Elemental analysis for $C_{48}H_{65}GeN_3$ (%): Calculated: C 76.19, H 8.66, N 5.55; Found: C 76.31, H 8.72, N 5.46.

Synthesis of compound 6

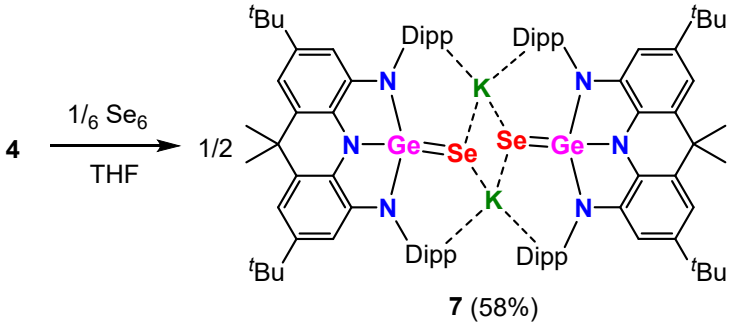


6 (62%)

S_8 (6.4 mg, 0.025 mmol) was slowly added to a THF (5 ml) solution of **4** (0.20 g, 0.20

mmol) at room temperature. After stirring overnight, the solvent was removed under vacuum and the residue was washed with hexane to afford **6** as a yellow powder (0.10 g, 62%). Single crystals of **6** suitable for X-ray diffraction studies were grown from its saturated hexane/THF solution at room temperature. ^{1}H NMR (THF-d_8 , 300 MHz, 298K): δ 7.14 (s, 6H, Dipp-C*H*), 6.64 (s, 2H, Me_2CCCH) , 5.83 (s, 2H, DippNCC*H*), 3.31 (sept, J = 8.8 Hz, 4H, $(CH_3)_2CH$), 1.69 (s, 6H, $C(CH_3)_2$), 1.23 (d, J = 6.8 Hz, 12H, $(CH_3)_2CH$), 1.10 (s, 18H, CH_3), 0.90 (d, J = 6.7 Hz, 12H, $(CH_3)_2CH$); ^{13}C{^{1}H} NMR (THF-d_8, 100 MHz, 298K): δ 149.70 (Ar-*C*), 143.50 (Ar-*C*), 142.55 (Ar-*C*), 140.82 (Ar-*C*), 135.38 (Ar-*C*), 131.86 (Ar-*C*), 125.70 (Dipp-*C*H), 123.84 (Dipp-*C*H), 108.08 (Me_2CCCH), 107.96 (DippNC*C*H), 39.33 ($(CH_3)_2C$), 35.07 ($(CH_3)_3C$), 32.20 ($(CH_3)_3CH$), 29.06 ($(CH_3)_2C$), 25.97 ($(CH_3)_3C$), 25.65 ($(CH_3)_3CH$), 24.64 ($(CH_3)_3CH$). UV-vis (THF): λ_{max} = 332 and 344 nm. HRMS (ESI): m/z calcd for $C_{47}H_{62}N_3GeS$: 774.3865 [(*M*-*K*)]$^-$; found: 774.3876. Elemental analysis for $C_{94}H_{124}Ge_2K_2N_6S_2$ (%): Calculated: C 69.45, H 7.69, N 5.17; Found: C 69.65, H 7.68, N 4.72.

Synthesis of compound 7



Se_6 (16 mg, 0.033 mmol) was added into a THF (3 ml) solution of **4** (0.20 g, 0.20 mmol) and the mixture was stirred at 90 °C for 12 h. After cooling down to room temperature, the solvent was removed under vacuum to afford **7** as a yellow powder (0.10 g, 58%). Single crystals of **7** suitable for X-ray diffraction studies were grown from its saturated hexane/THF solution at room temperature. ^{1}H NMR (THF-d_8 , 400 MHz, 298 K): δ 7.18 (br, 6H, Dipp-C*H*), 6.68 (s, 2H, Me_2CCCH), 5.85 (s, 2H, DippNCC*H*), 3.32 (sept, J = 6.8 Hz, 4H, $(CH_3)_2CH$), 1.71 (s, 6H, CH_3), 1.29 (d, J = 6.8 Hz, 12H, CH_3), 1.14 (s, 18H, CH_3), 0.93 (d, J = 6.8 Hz, 12H, CH_3); ^{13}C{^{1}H}

NMR (THF-d_8, 100 MHz, 298 K): δ 149.63 (Ar-*C*), 143.26 (Ar-*C*), 142.46 (Ar-*C*), 140.82 (Ar-*C*), 135.47 (Ar-*C*), 131.62 (Ar-*C*), 125.62 (Dipp-*C*H), 123.79 (Dipp-*C*H), 108.15 (DippNC*C*H), 107.92 (Me_2CC*C*H), 39.20 (($CH_3)_2$*C*), 35.05 (($CH_3)_3$*C*), 32.19 (($CH_3)_2$C), 29.14 (($CH_3)_3$C), 26.11 (($CH_3)_3$*C*H), 25.64 (($CH_3)_3$CH), 24.84 (($CH_3)_3$CH); ^{77}Se NMR (THF-d_8, 114 MHz, 298 K): -271.93 (s). UV-vis (THF): λ_{max} = 333 and 344 nm. HRMS (ESI): m/z calcd for $C_{47}H_{62}N_3GeSe$: 822.3321 $[(M\text{-}K)]^-$; found: 822.3338. Elemental analysis for $C_{94}H_{124}Ge_2K_2N_6Se_2$ (%): Calculated: C 65.66, H 7.27, N 4.89; Found: C 65.79, H 7.43, N 4.51.

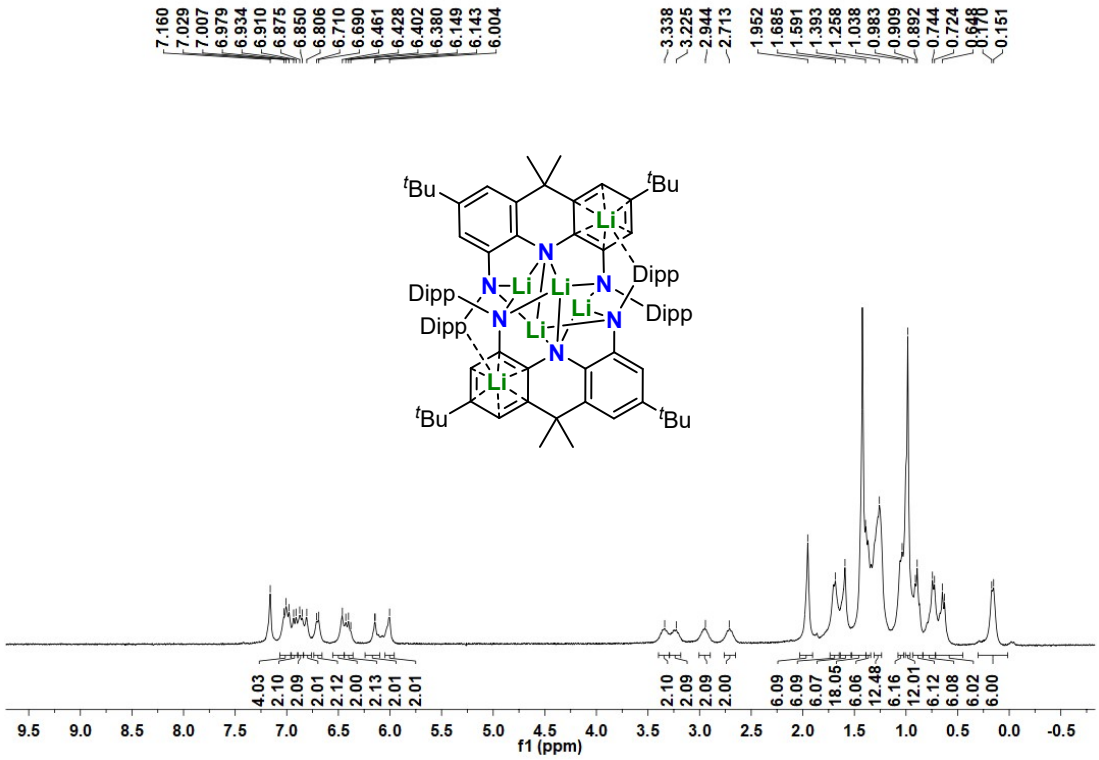


Fig. S1 ^{1}H NMR spectrum of **2** in C_6D_6 at 298 K.

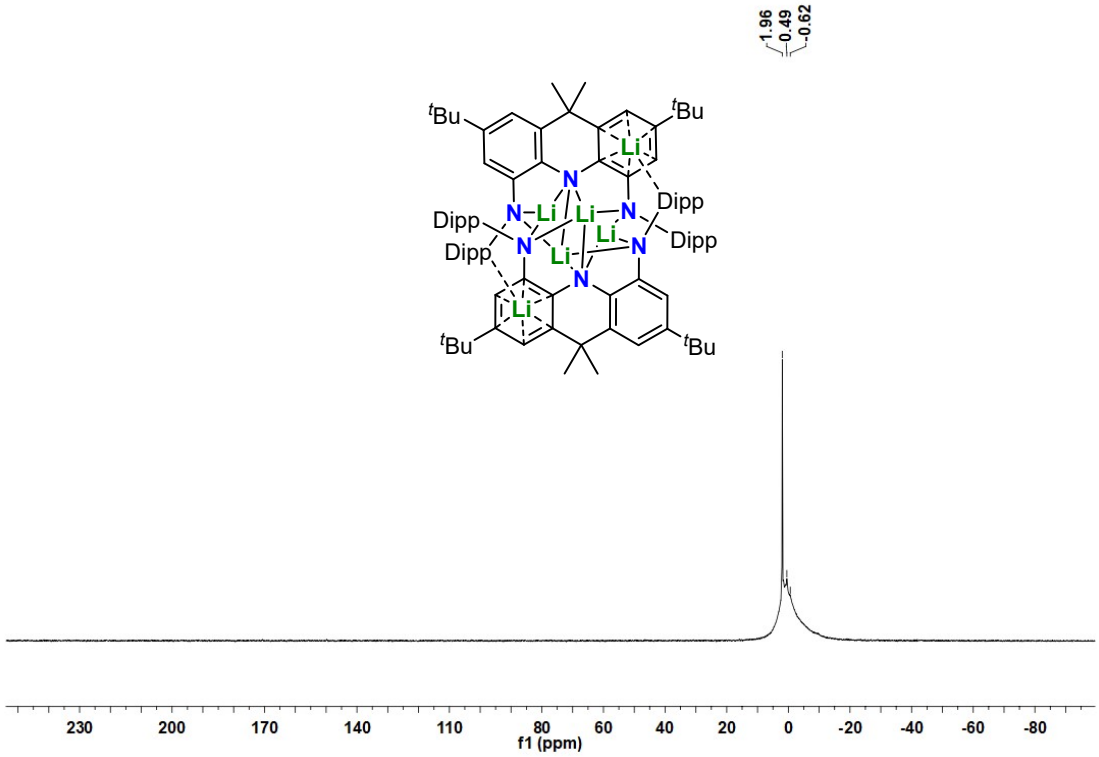


Fig. S2 ^{7}Li NMR spectrum of **2** in C_6D_6 at 298 K.

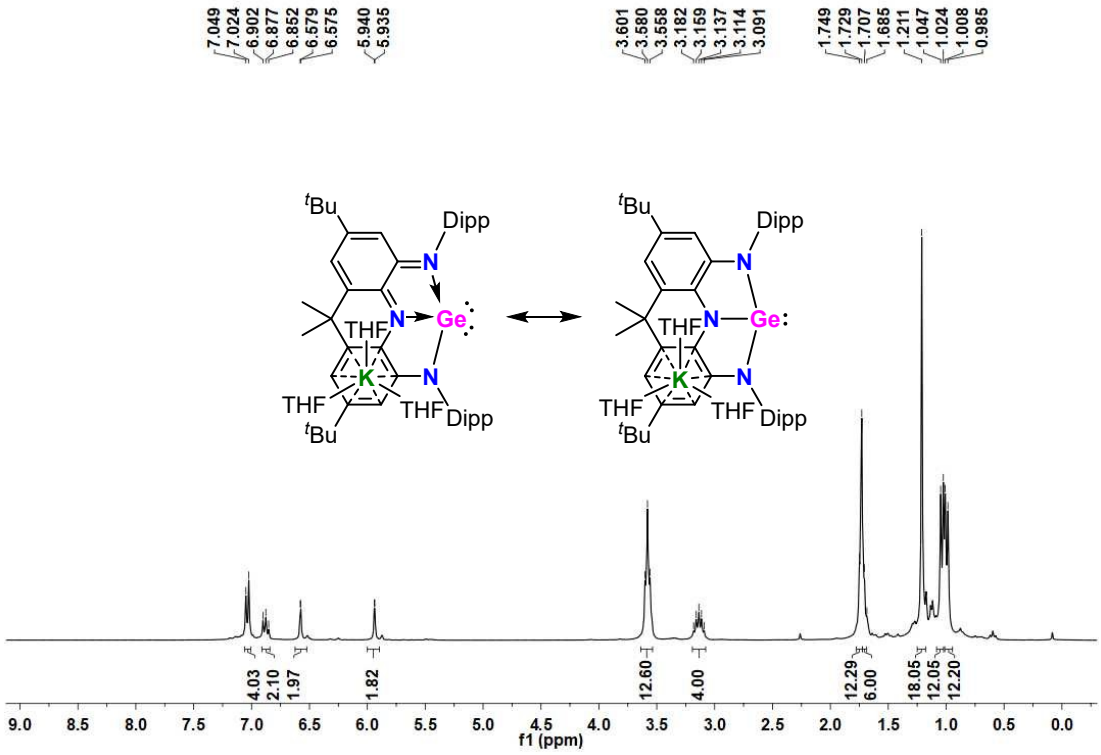


Fig. S3 ^{1}H NMR spectrum of **4** in THF-D_8 at 298 K.

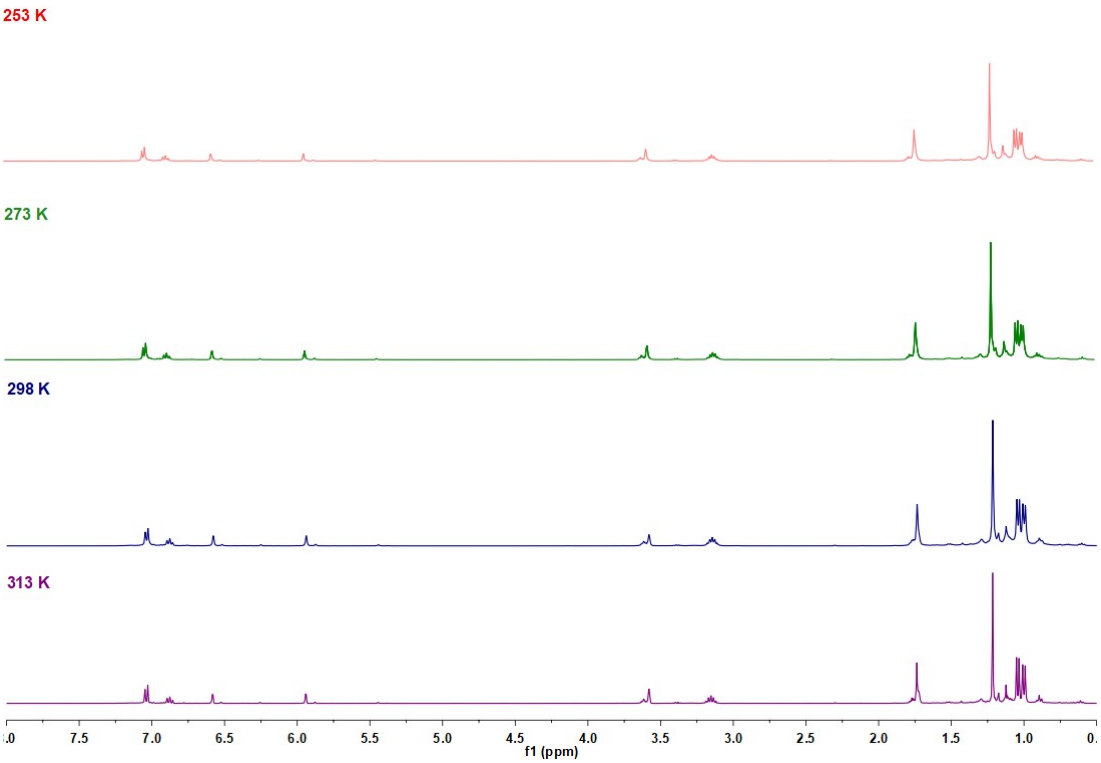


Fig. S4 VT-^{1}H NMR spectrum of **4** in THF-D_8.

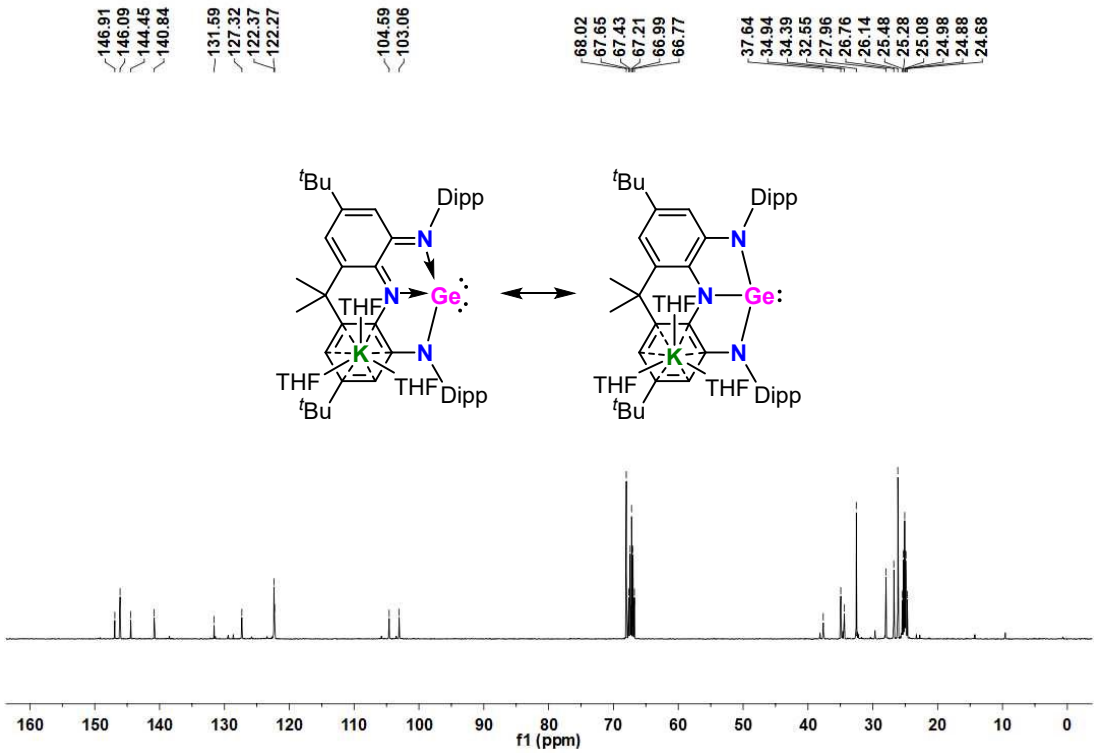


Fig. S5 $^{13}C\{^{1}H\}$ NMR spectrum of **4** in THF-D_8 at 298 K.

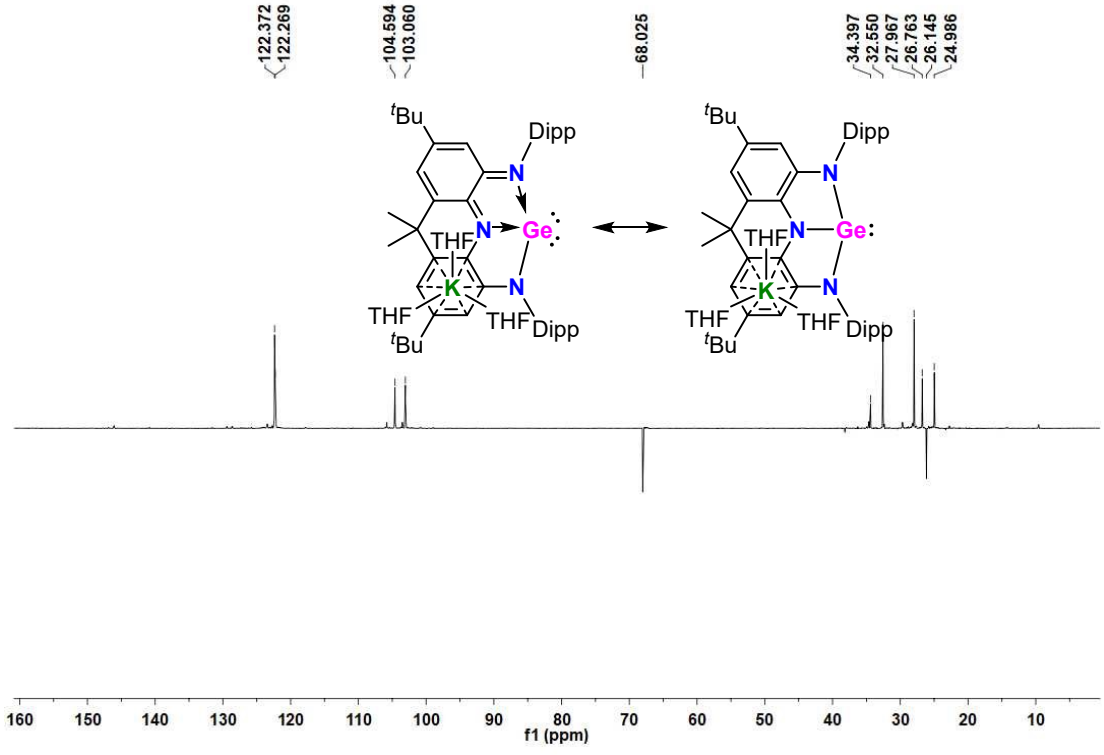


Fig. S6 ^{13}C(DEPT135) NMR spectrum of **4** in THF-D_8 at 298 K.

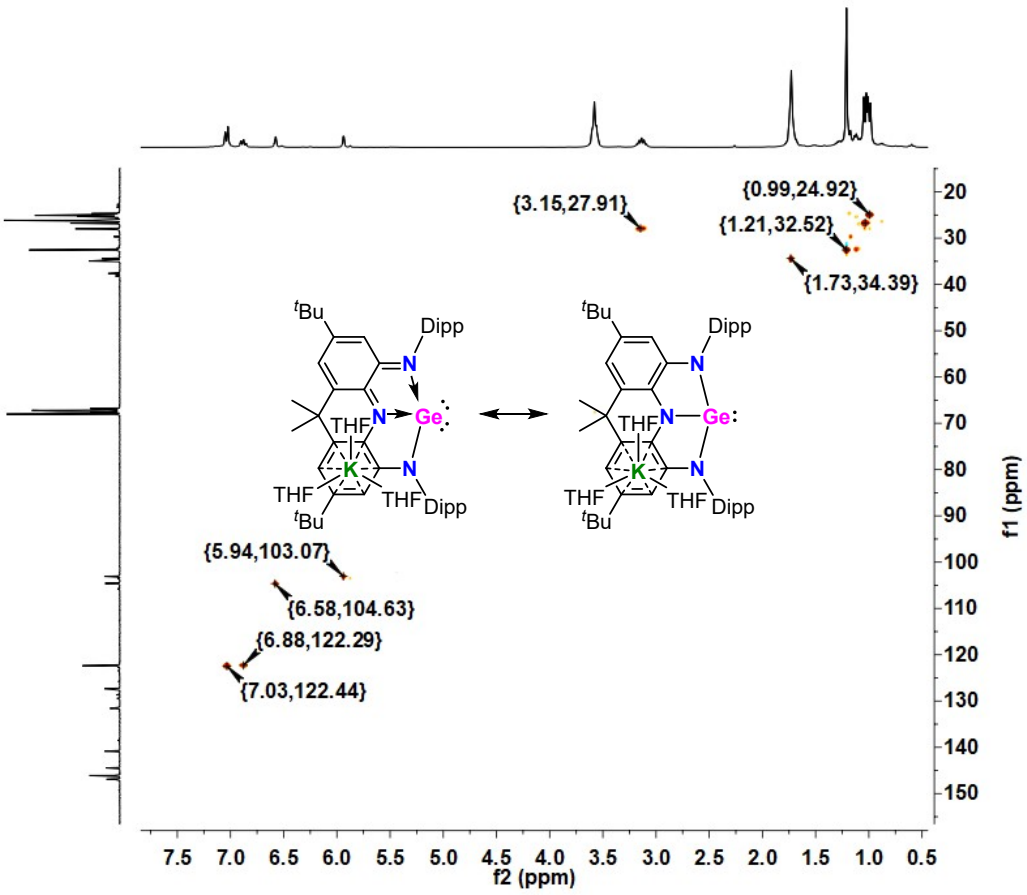


Fig. S7 The HSQC spectrum of **4** in THF-D_8 at 298 K.

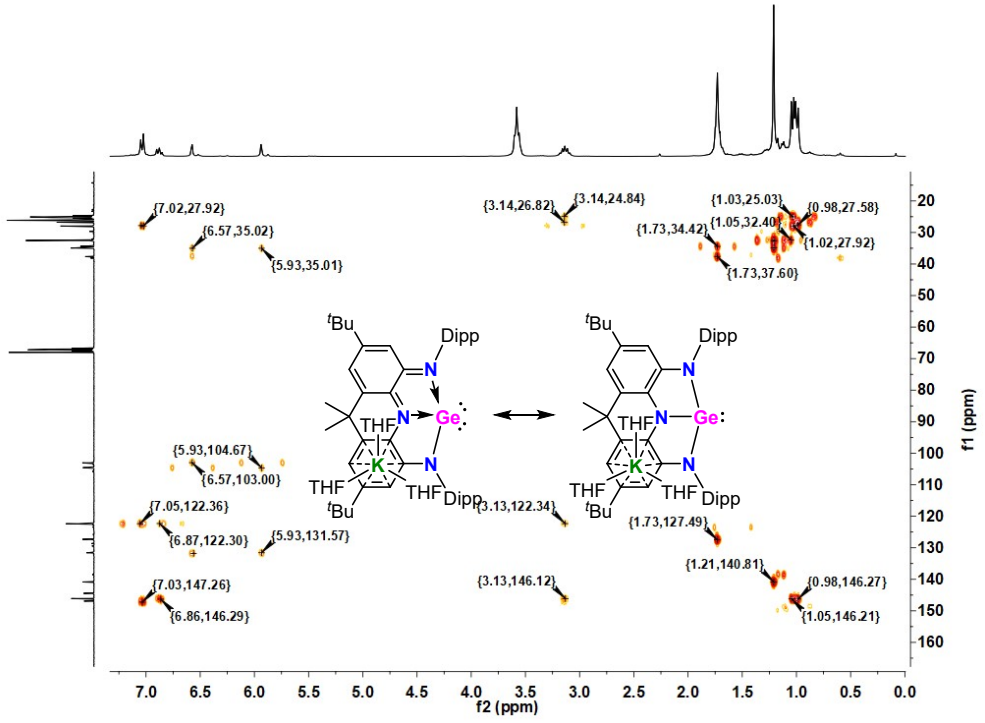


Fig. S8 The HMBC spectrum of **4** in THF-D_8 at 298 K.

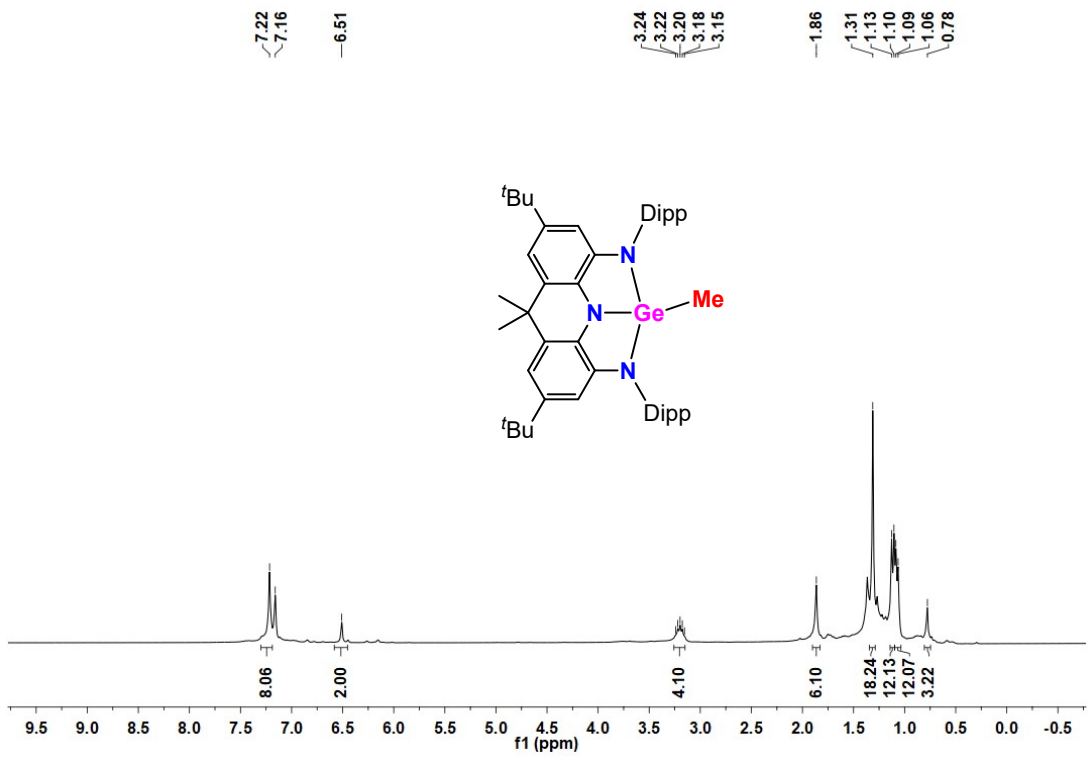


Fig. S9 ^{1}H NMR spectrum of **5** in C_6D_6 at 298 K.

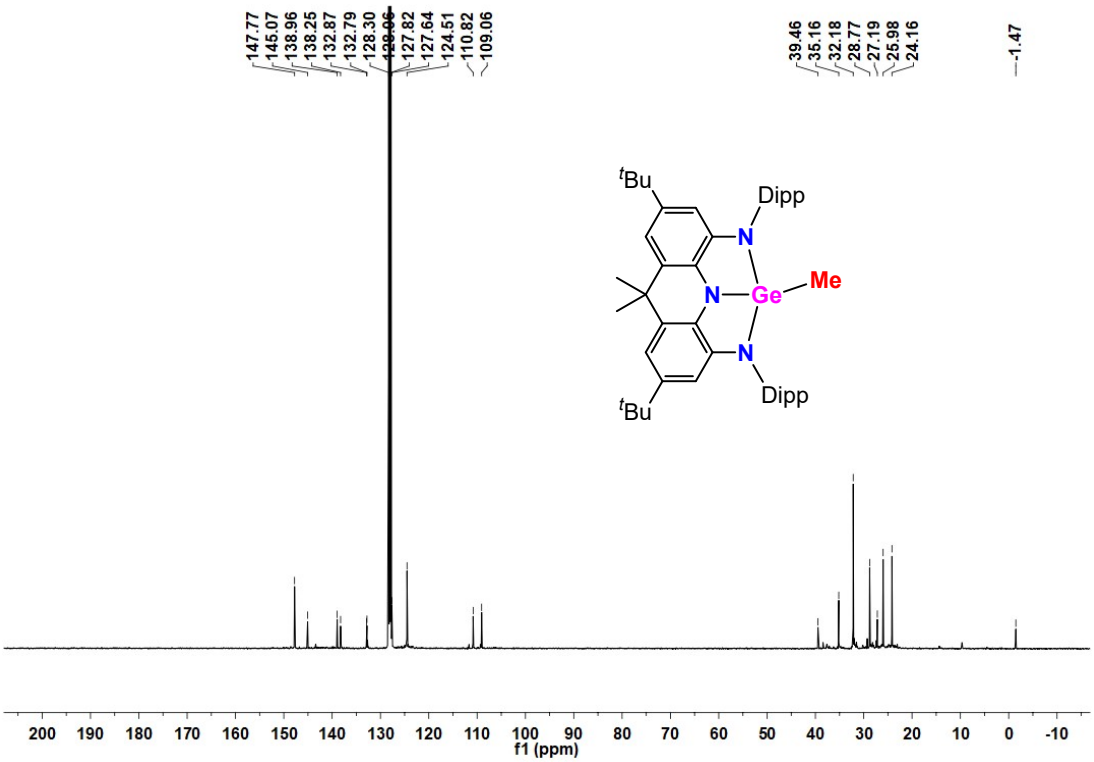


Fig. S10 ^{13}C{^{1}H} NMR spectrum of **5** in C_6D_6 at 298 K.

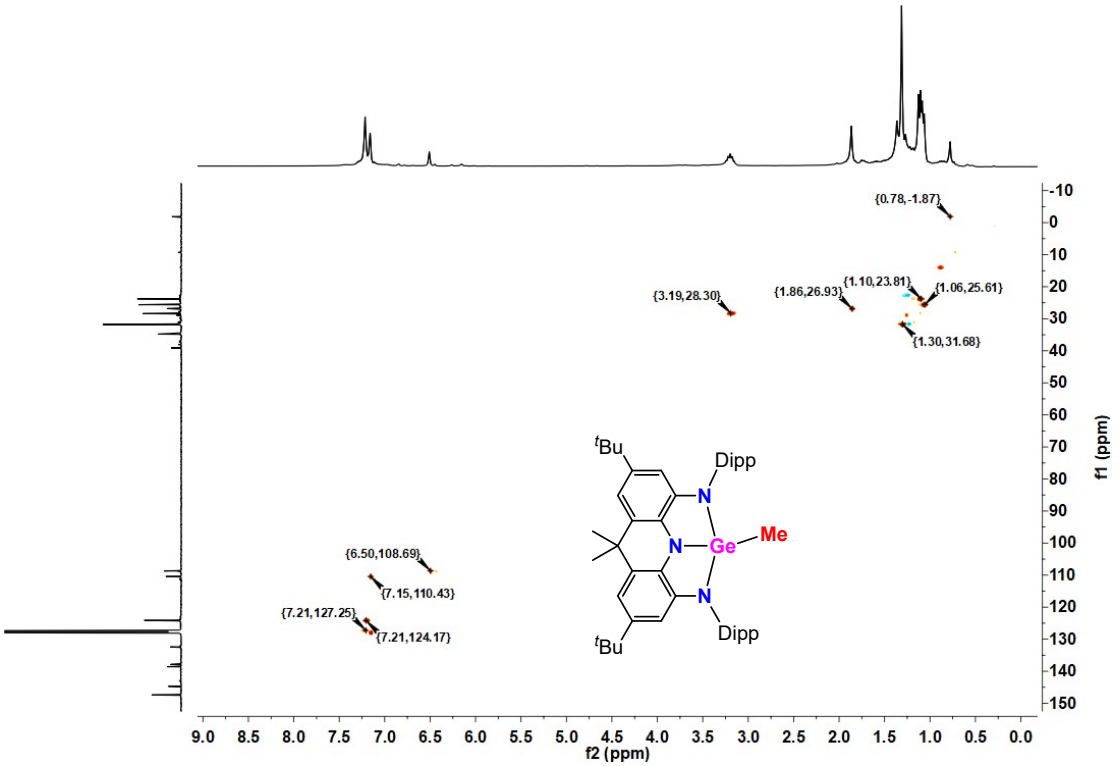


Fig. S11 The HSQC spectrum of **5** in C_6D_6 at 298 K.

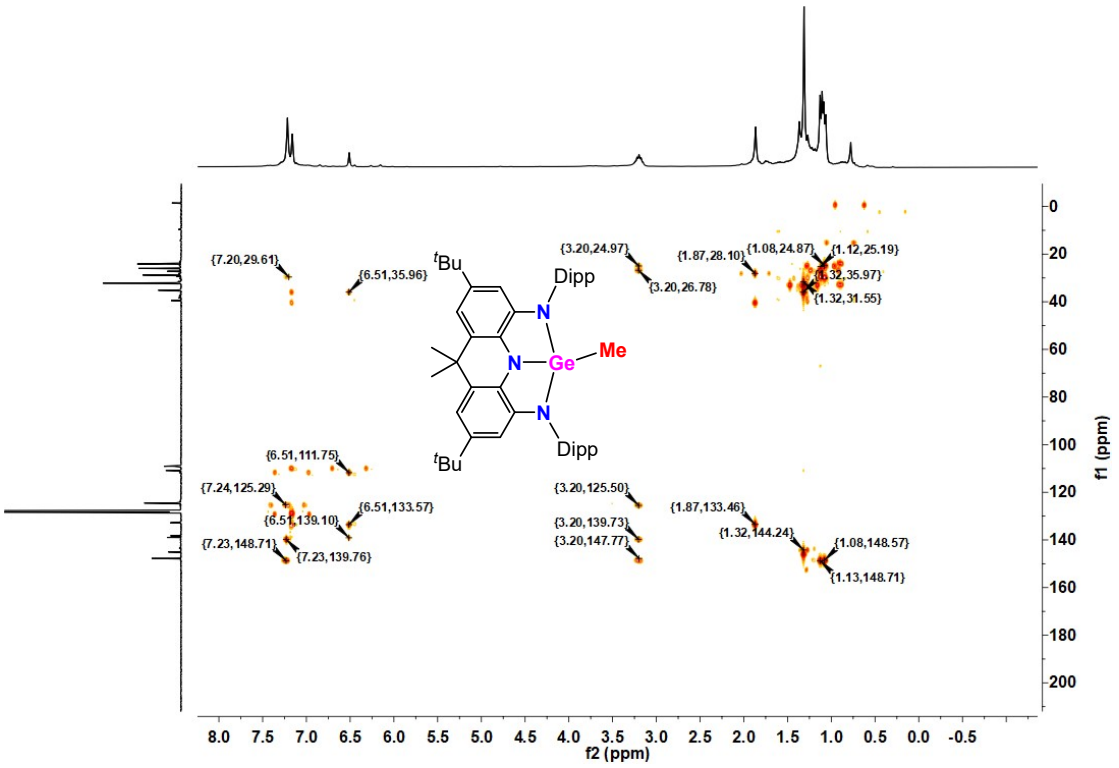


Fig. S12 The HMBC spectrum of **5** in C_6D_6 at 298 K.

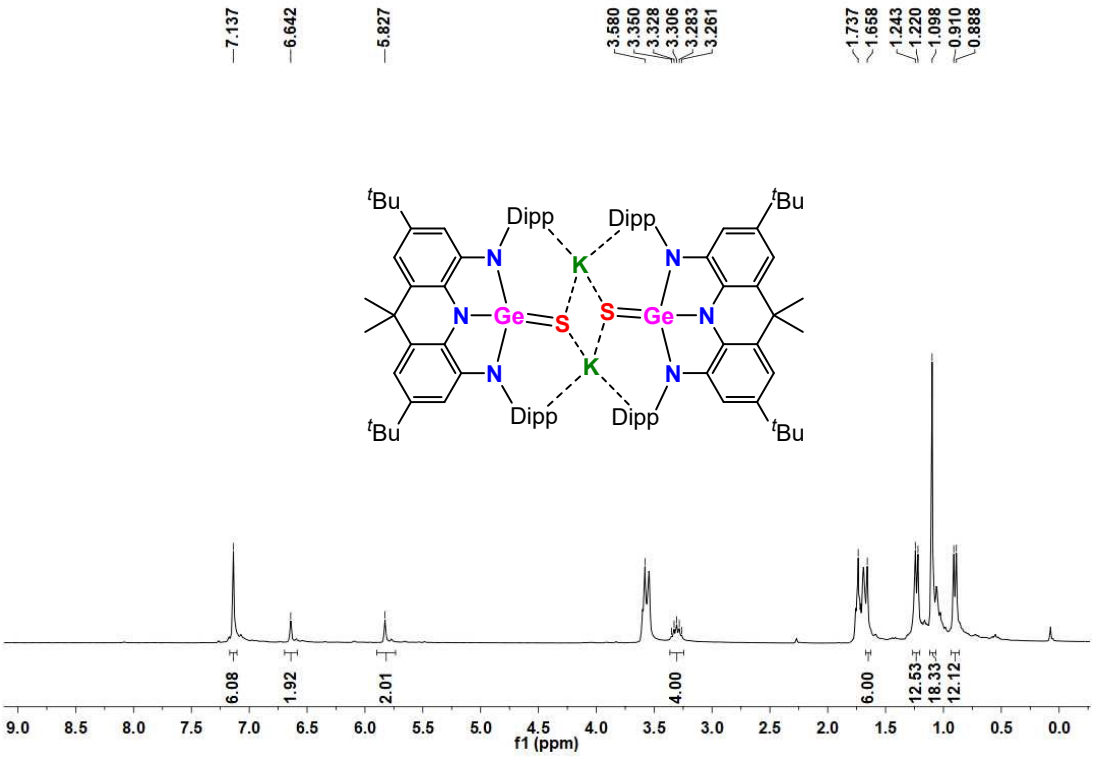


Fig. S13 ^{1}H NMR spectrum of **6** in THF-D_8 at 298 K.

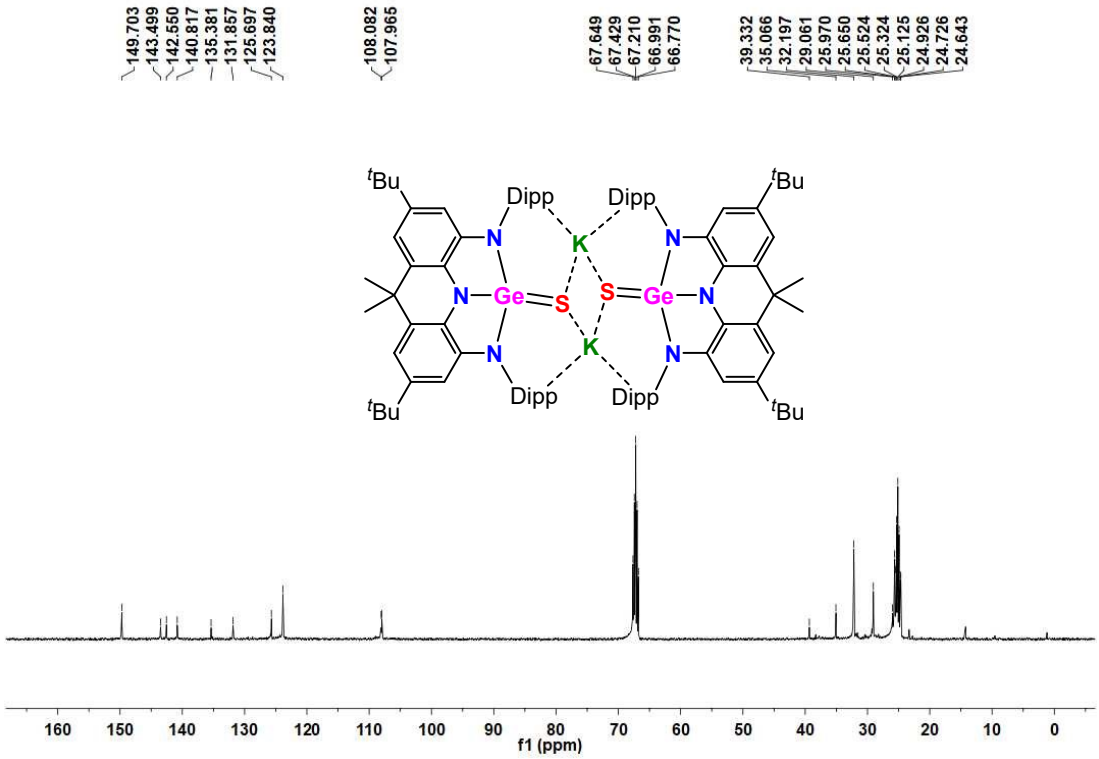


Fig. S14 ^{13}C{^{1}H} NMR spectrum of **6** in THF-D_8 at 298 K.

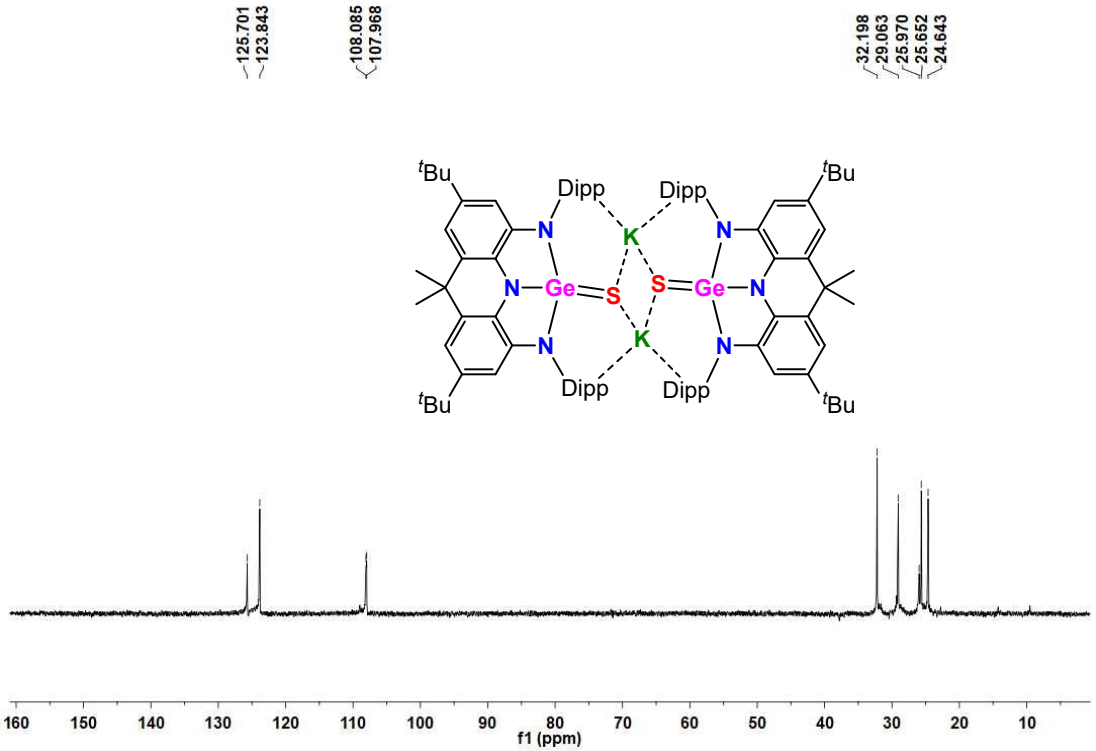


Fig. S15 ^{13}C(DEPT135) NMR spectrum of **6** in THF-D_8 at 298 K.

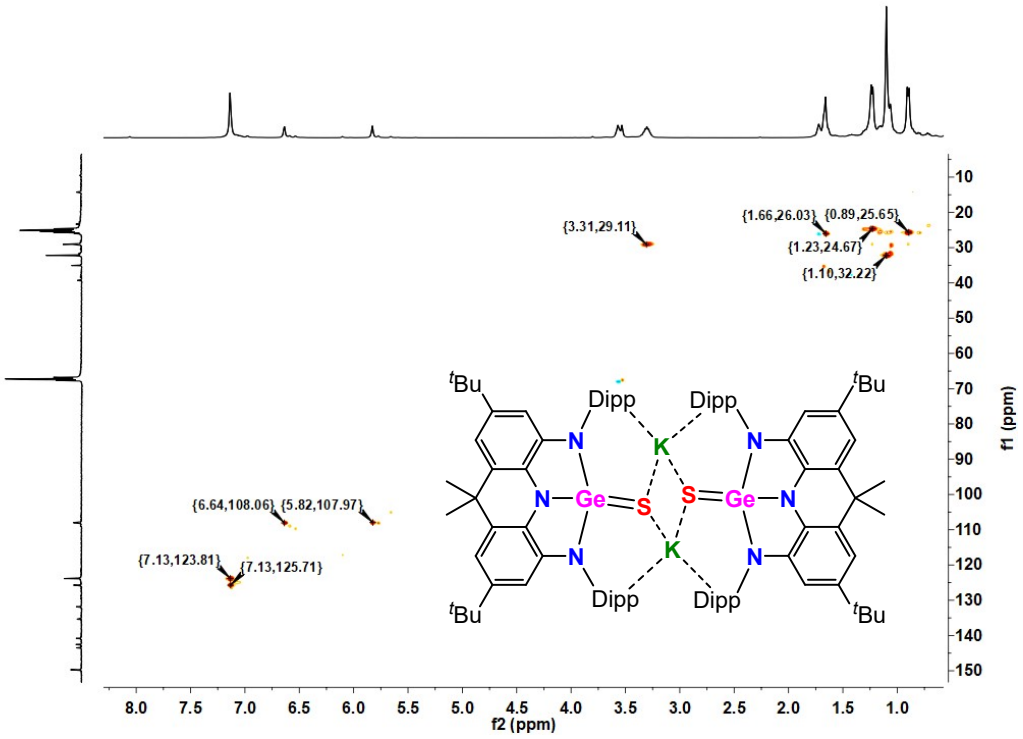


Fig. S16 The HSQC spectrum of **6** in THF-D_8 at 298 K.

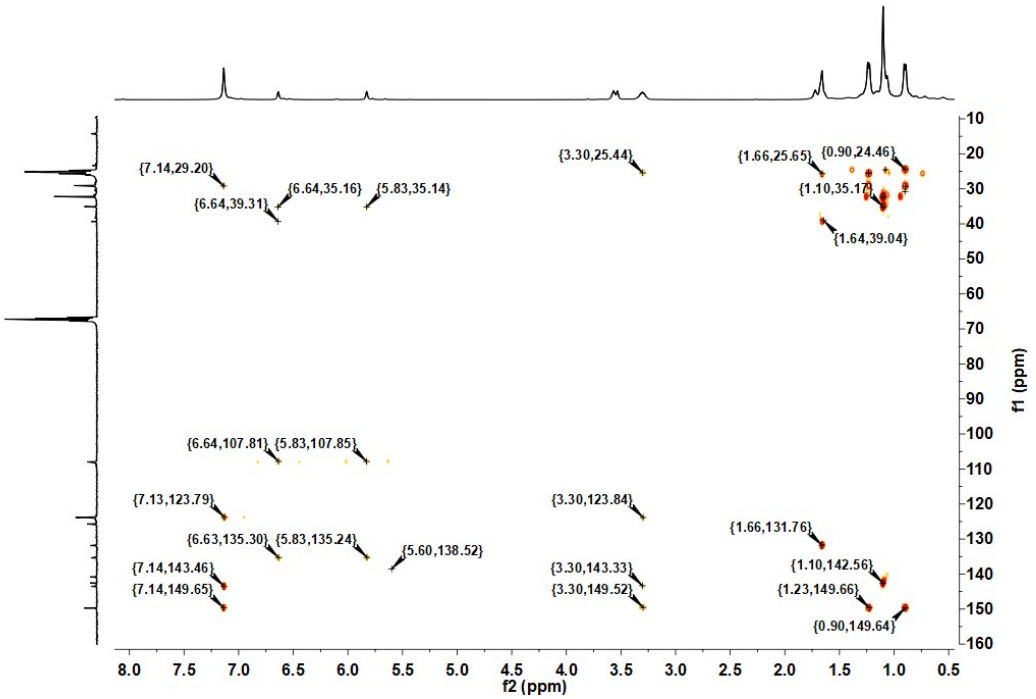


Fig. S17 The HMBC spectrum of **6** in THF-D_8 at 298 K.

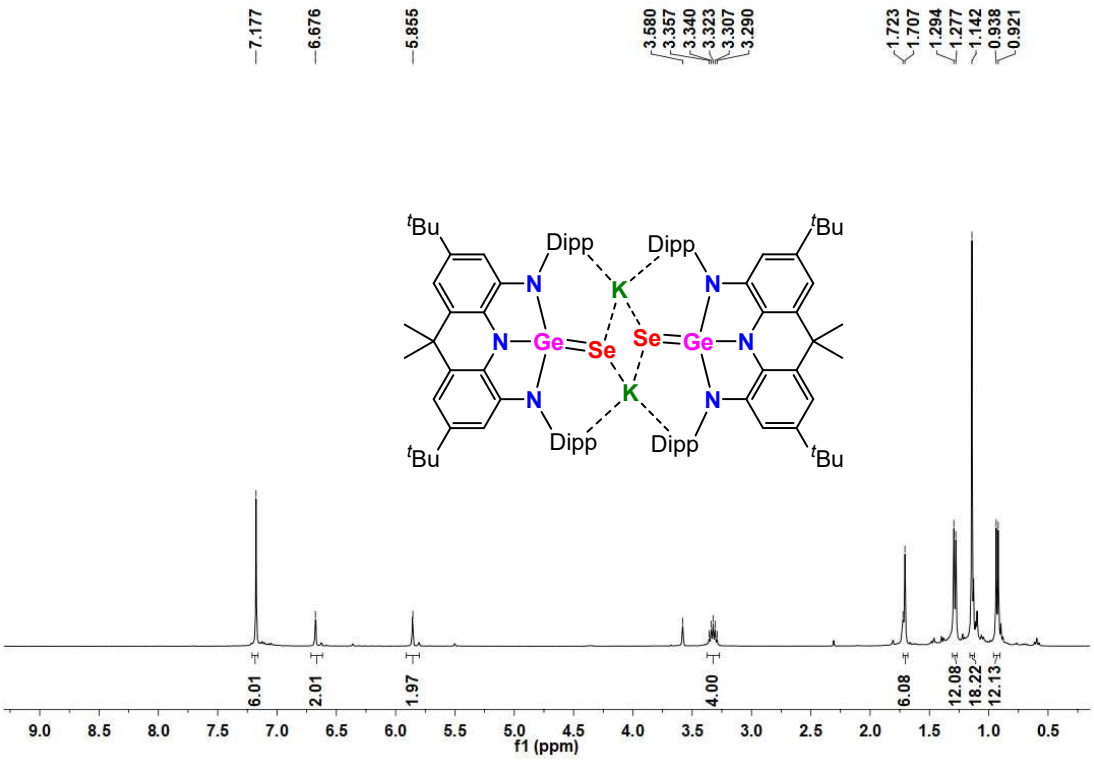


Fig. S18 ^{1}H NMR spectrum of **7** in THF-D_8 at 298 K.

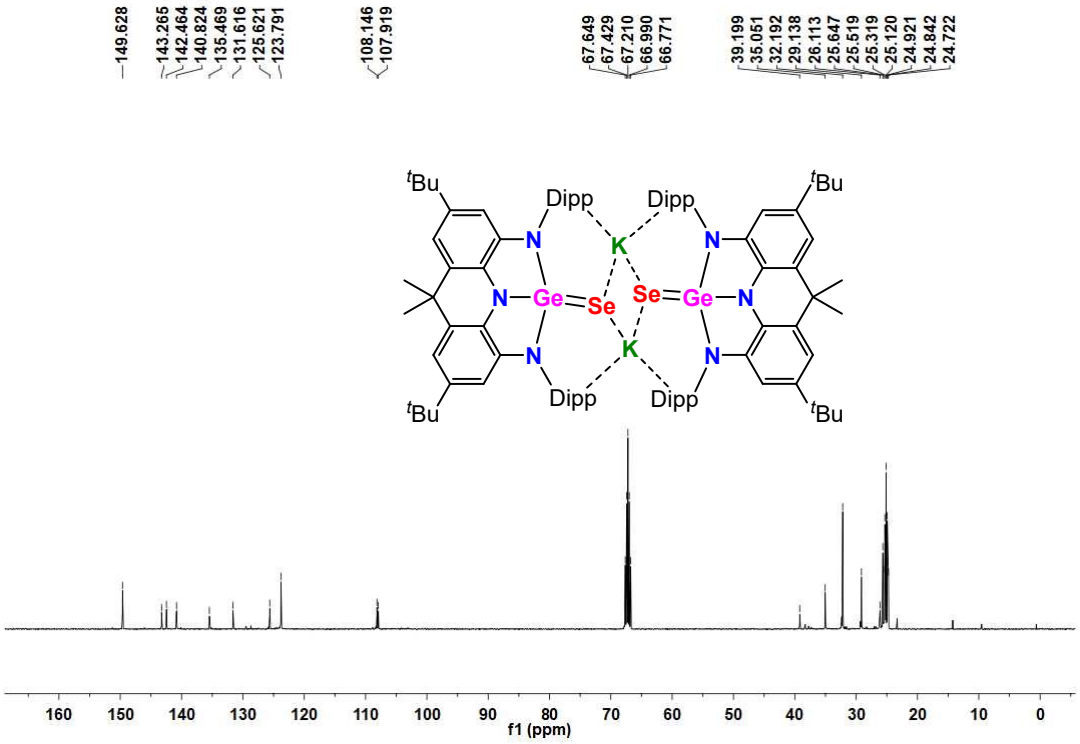


Fig. S19 $^{13}C\{^{1}H\}$ NMR spectrum of **7** in THF-D_8 at 298 K.

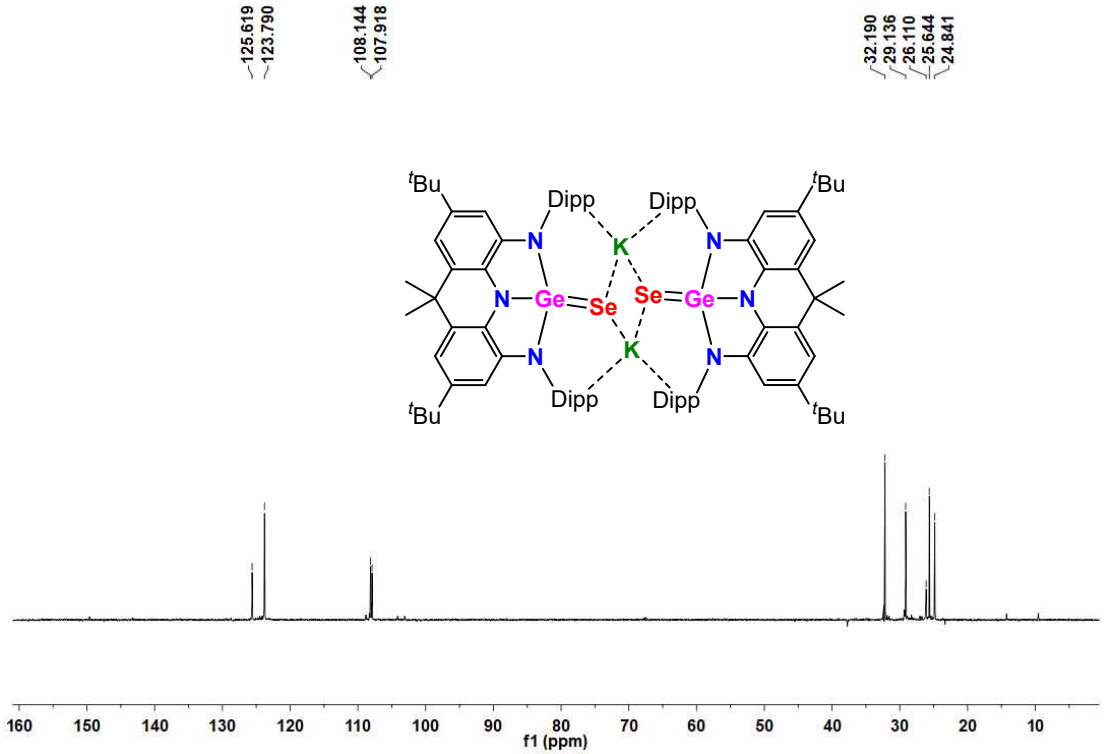


Fig. S20 ^{13}C(DEPT135) NMR spectrum of **7** in THF-D_8 at 298 K.

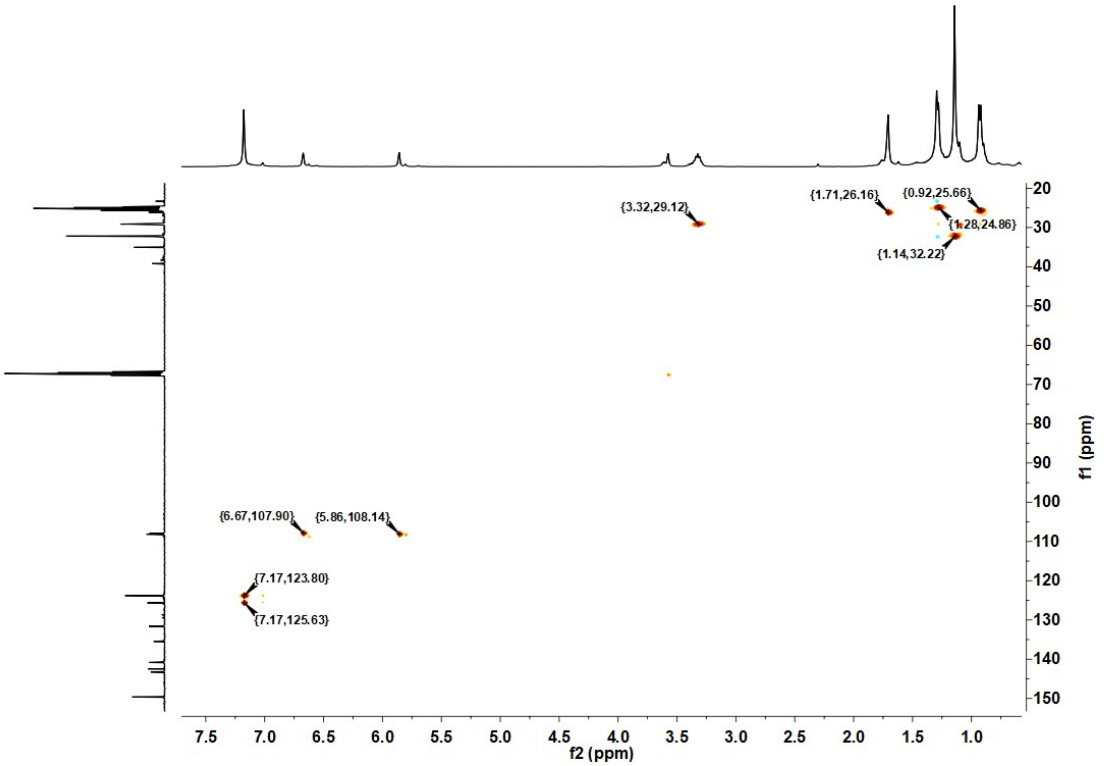


Fig. S21 The HSQC spectrum of **7** in THF-D_8 at 298 K.

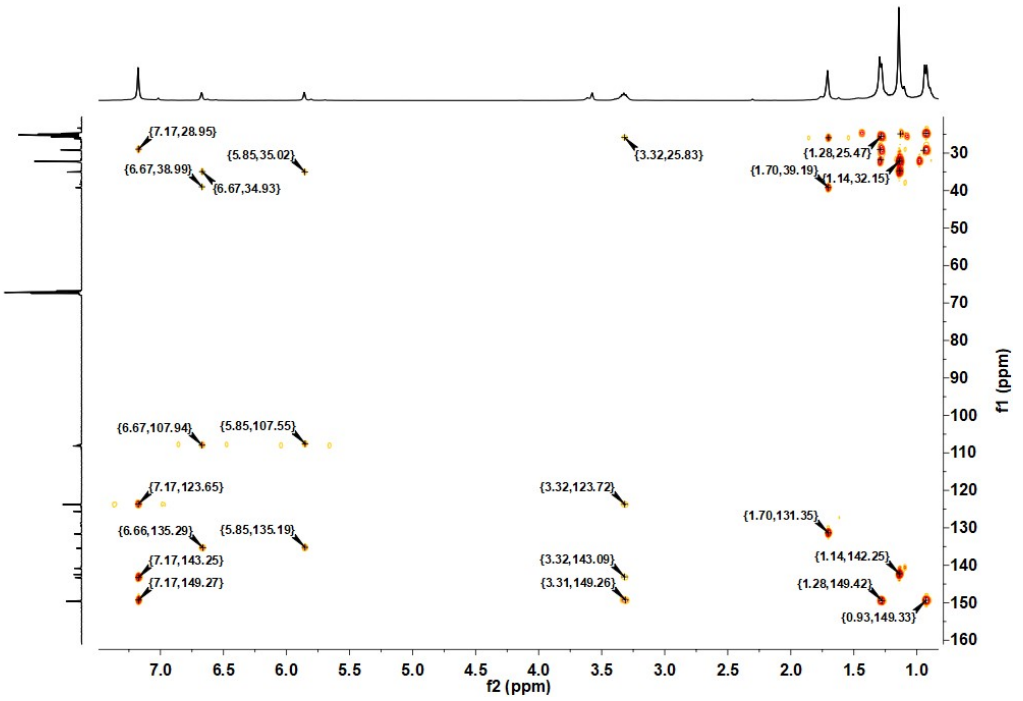


Fig. S22 The HMBC spectrum of **7** in THF-D_8 at 298 K.

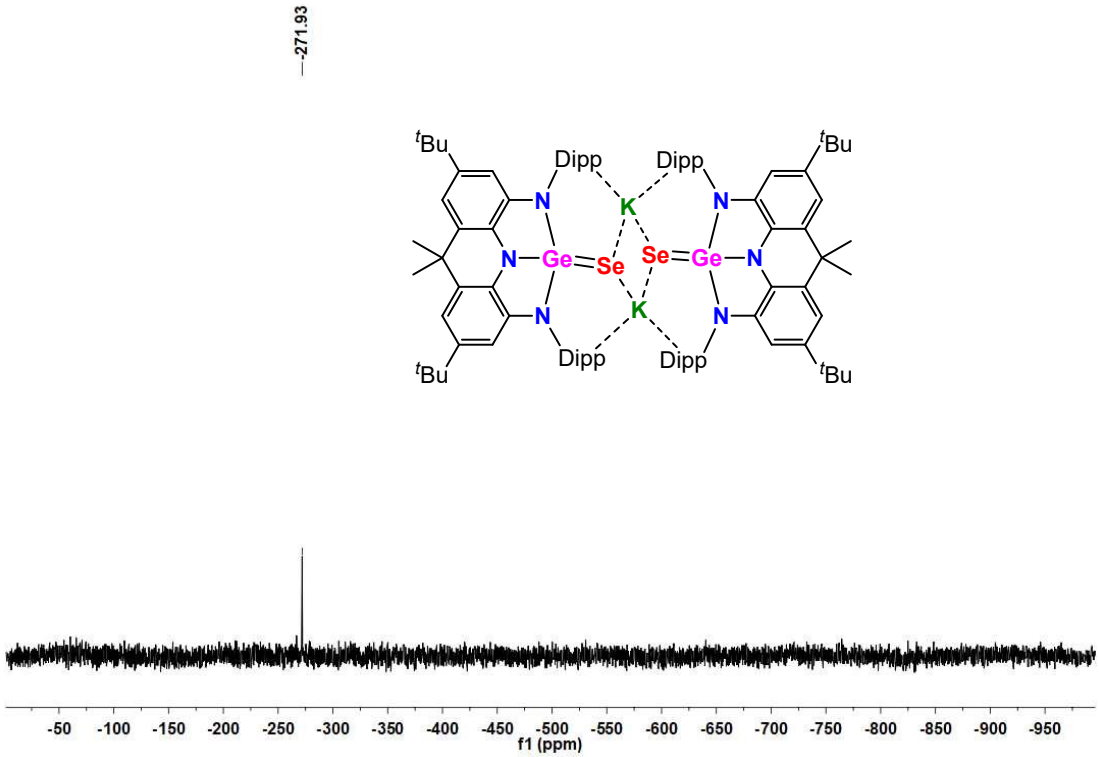


Fig. S23 $^{77}Se\{^{1}H\}$ NMR spectrum of **7** in THF-D_8 at 298 K.

2. Crystal structural parameters

For the single crystal X-ray structure analyses the crystals were each mounted on a glass capillary in perfluorinated oil and measured in a cold N_2 flow. The data for all compounds were collected on a Bruker D8 CMOS detector at low temperatures. The structures were solved by direct methods and all refined on F^2 with the SHELX-2018/3 software package. The positions of the H atoms were calculated and considered isotropically according to a riding model.

Table S1. Summary of data collection and structure refinement.

Compounds	**2**	**3**	**4**
CCDC	2201768	2121988	2121989
Formula	$C_{108.28}H_{157.32}Li_6N_6$	$C_{47}H_{62}Cl_2GeN_3$	$C_{59}H_{86}GeKN_3O_3$
Fw	1584.71	812.554	997.07
Crystal syst	monoclinic	monoclinic	monoclinic
Space group	$P2_1/n$	C2/c	$P2_1/n$
Size, mm^3	0.10 × 0.08 × 0.08	0.15 × 0.12 × 0.11	0.12 × 0.11 × 0.10
T, K	120	120.06	120.00
a, Å	14.4571(7)	31.6991(18)	11.0177(7)
b, Å	42.796(2)	18.5153(9)	21.7711(13)
c, Å	15.4362(9)	15.1604(8)	24.2953(16)
α, deg	90	90	90
β, deg	94.595(3)	94.550(2)	92.991(3)
γ, deg	90	90	90
V, $Å^3$	9519.8(9)	8869.9(8)	5819.7(6)
Z	4	8	4
d_{calcd}, $g•cm^{-1}$	1.106	1.217	1.138
μ, mm^{-1}	0.296	0.846	1.109
Reflections collected	103054	50335	79713
Independent reflections	17456	8708	10641
$[R_{int}]$	0.0861	0.0598	0.0847
R_1[I>2sigma(I)]	0.0639	0.0428	0.0492
wR_2[I>2sigma(I)]	0.1761	0.1101	0.1344
R_1[all data]	0.0975	0.0535	0.0589
wR_2[all data]	0.1958	0.1172	0.1407
GOF	1.048	1.0575	1.026
Largest diff. Peak/hole, $e•Å^{-3}$	0.27/-0.22	0.41/-0.33	0.61/-0.51

Compounds	**5·0.5C_6H_{14}**	**6**	**7**
CCDC	2201769	2121991	2121990
Formula	$C_{51}H_{72}GeN_3$	$C_{108}H_{154}Ge_2K_2N_6O_2S_2$	$C_{114}H_{168}Ge_2K_2N_6O_2Se_2$
Fw	799.70	1856.02	2035.985
Crystal syst	triclinic	triclinic	triclinic
Space group	P-1	P-1	P-1
Size, mm^3	0.14 × 0.13 × 0.12	0.15 × 0.13 × 0.12	0.18× 0.16 × 0.08
T, K	120	120	135.00
a, Å	12.7334(7)	14.1535	14.292(8)
b, Å	13.204(3)	14.2181	14.502(8)
c, Å	14.3960(6)	15.1396	15.149(9)
α, deg	98.596(5)	79.781	70.44(2)
β, deg	101.664(3)	70.505	79.46(2)
γ, deg	96.759(6)	68.035	67.63(2)
V, $Å^3$	2316.3(5)	2658.7	2730(3)
Z	2	1	1
d_{calcd}, $g•cm^{-1}$	1.147	1.159	1.238
μ, mm^{-1}	0.754	1.410	1.655
Reflections collected	37828	7688	8399
Independent reflections	8363	9573	9641
[R_{int}]	0.0424	0.0649	0.0553
R_1[I>2sigma(I)]	0.0383	0.0591	0.0481
wR_2[I>2sigma(I)]	0.0995	0.1839	0.1435
R_1[all data]	0.0398	0.0706	0.0540
wR_2[all data]	0.1008	0.2003	0.1502
GOF	1.054	1.035	1.053
Largest diff. Peak/hole, $e•Å^{-3}$	0.62/-0.37	0.48/-0.62	0.92/-0.52

3. EPR spectrum of 3

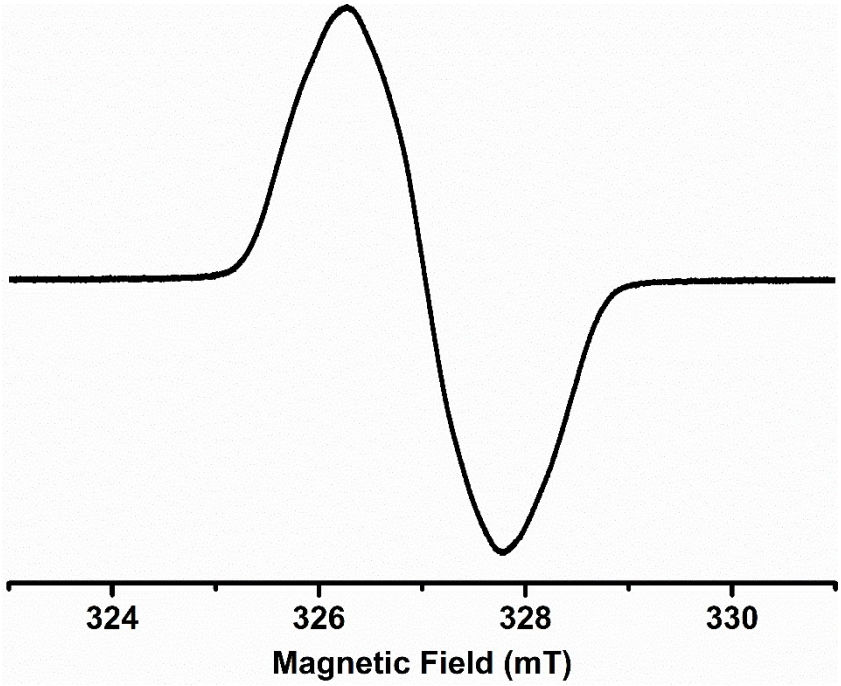


Fig. S24 EPR spectrum of **3** in hexane at room temperature

4. UV-vis spectra

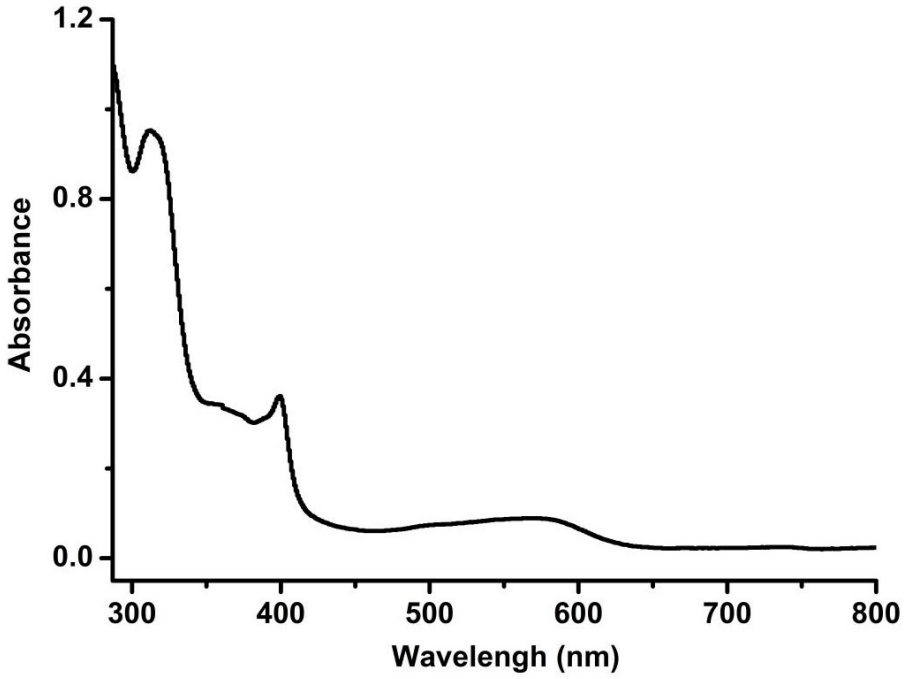


Fig. S25 UV-vis spectrum of **3** in toluene at room temperature.

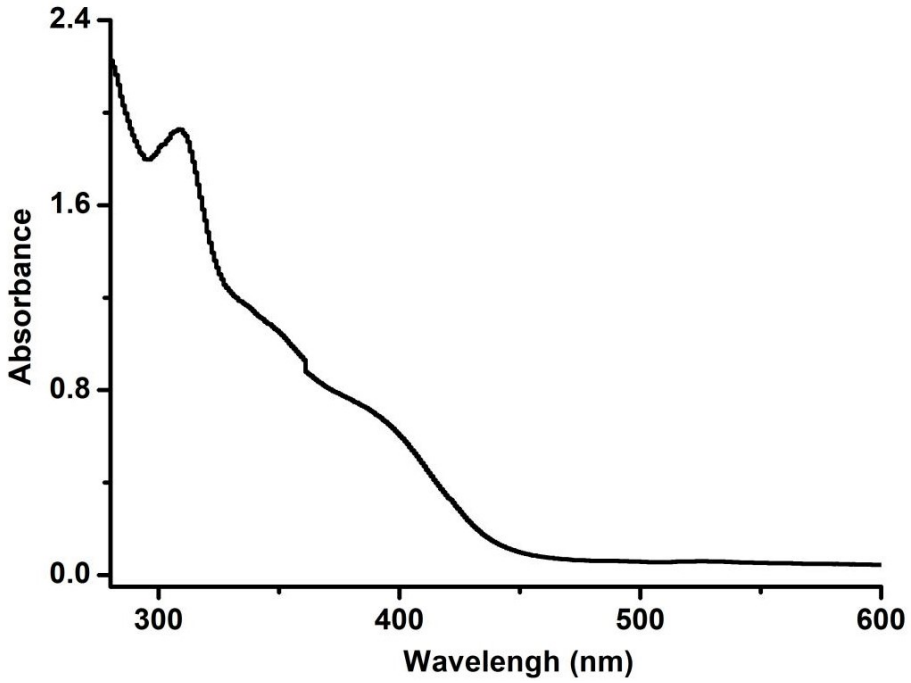


Fig. S26 UV-vis spectrum of **4** in THF at room temperature.

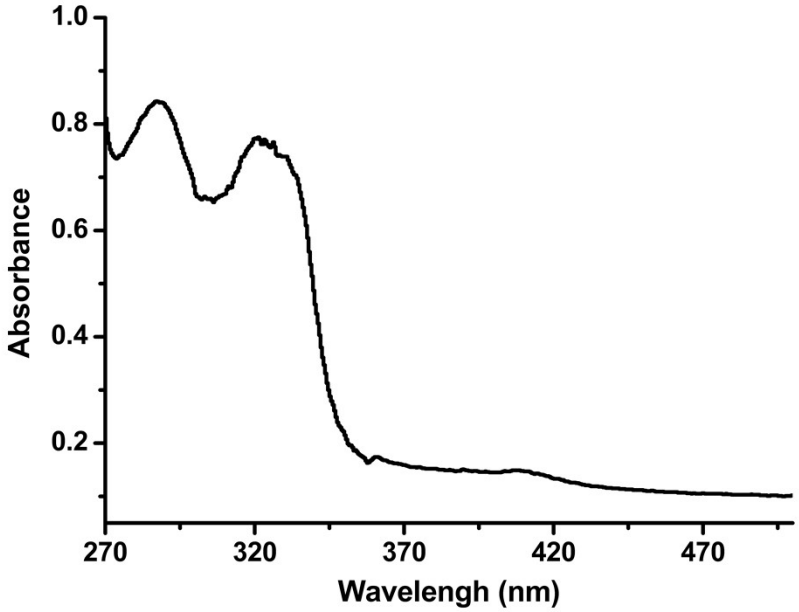


Fig. S27 UV-vis spectrum of **5** in THF at room temperature.

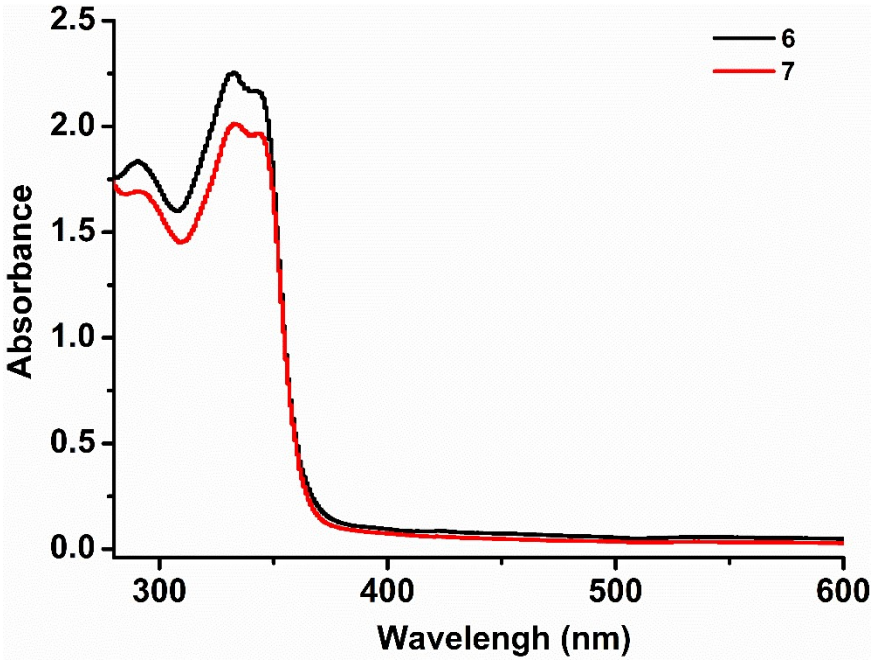


Fig. S28 UV-vis spectrum of **6** and **7** in THF at room temperature.

5. Theoretical calculations

All of the calculations were performed with the Gaussian 16 program.[S2] All of the geometry optimizations were performed at the (U)B3LYP-D3BJ/6-311G(d) level in consideration of the London dispersion and solvent correction.[S3,S4] The natural bond orbital (NBO) analysis[S5] was carried out at the same level. To further figure out the absorption properties of the anionic part of **4**, we also obtained the UV-vis spectrum at the time-dependent DFT (TDDFT)//B3LYP/6-311G(d) level,[S6] which agrees well with the experimental data, and the calculated Kohn-Sham orbitals related to the observed transitions are shown in Table S2 and S3.

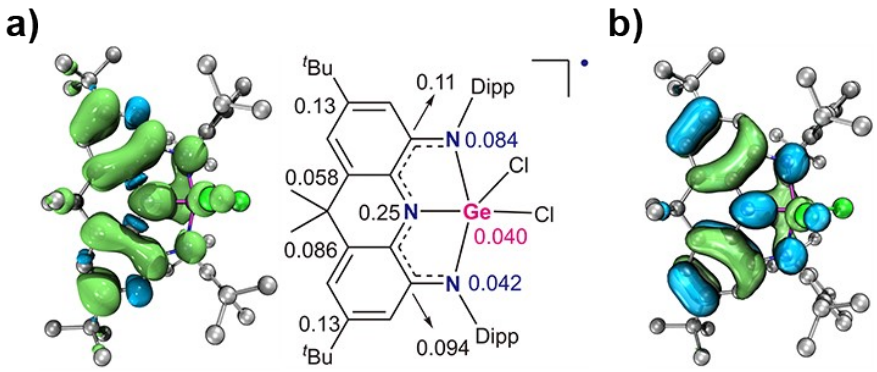


Fig. S29 a) Spin density and b) SOMO of **2** calculated at the UB3LYP-D3BJ/6-311G(d) level.

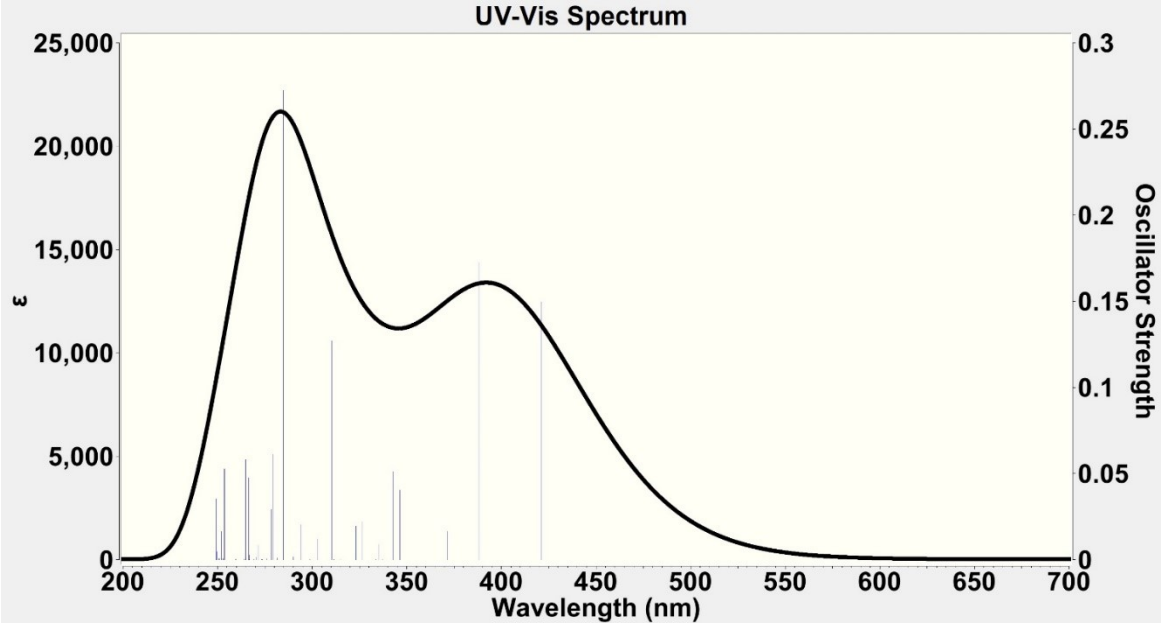


Fig. S30 Calculated UV-vis spectrum of the anionic part of **4** at the time-dependent DFT (TDDFT)//B3LYP/6-311G(d) level.

Table S2 Calculated absorption properties of the anionic part of **4** including wavelength (nm), oscillator strength (*f*) and the related transition nature

Energy / ev	Wavelength / nm	Oscillator strength / *f*	Transition nature
2.9453	420.96	0.1497	HOMO−1→LUMO (0.66256) HOMO→LUMO (-0.22026)
3.1941	388.17	0.1727	HOMO−1→LUMO (0.21830) HOMO→LUMO (0.65781)
3.9927	310.53	0.1272	HOMO→LUMO+5 (0.67687)
4.3542	284.75	0.2724	HOMO−2→LUMO+3 (0.69946)

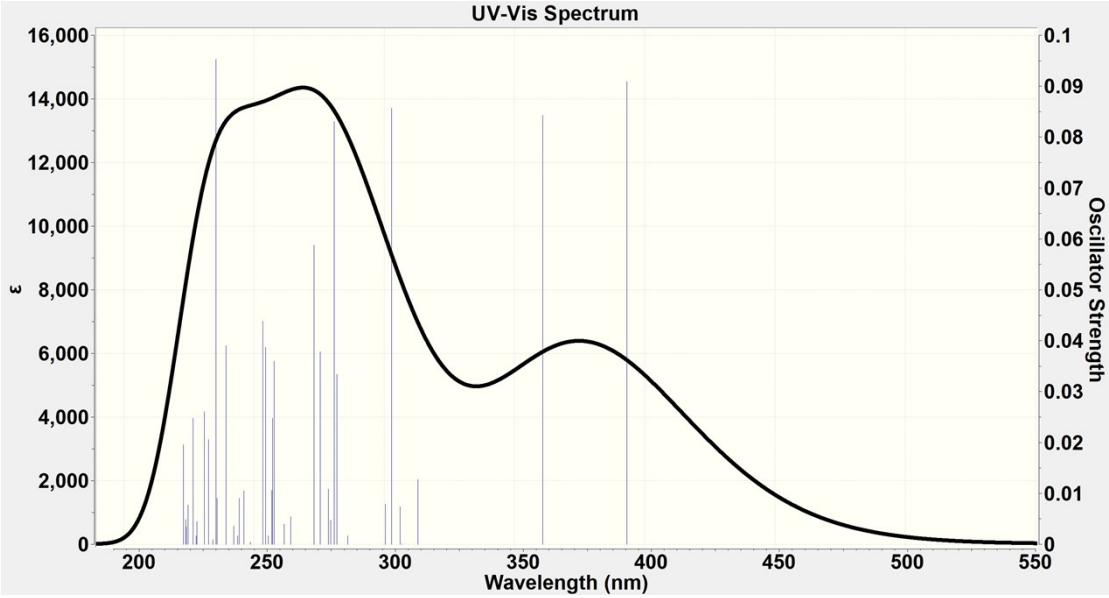


Fig. 31 Calculated UV-vis spectrum of **5** at the time-dependent DFT (TDDFT)//B3LYP/6-311G(d) level.

Table S3 Calculated absorption properties of **5** including wavelength (nm), oscillator strength (*f*) and the related transition nature

Energy / ev	Wavelength / nm	Oscillator strength / *f*	Transition nature
3.1541	393.09	0.0909	HOMO→LUMO (0.69604)
3.4356	360.88	0.0843	HOMO−1→LUMO (0.69684)
4.4149	280.83	0.0831	HOMO→LUMO+5 (0.54044) HOMO→LUMO+6 (0.15389)
4.8940	253.34	0.0438	HOMO-1→LUMO+5 (-0.22852) HOMO-1→LUMO+6 (-2.20759) HOMO-6→LUMO (0.47857) HOMO→LUMO+7 (0.23136)

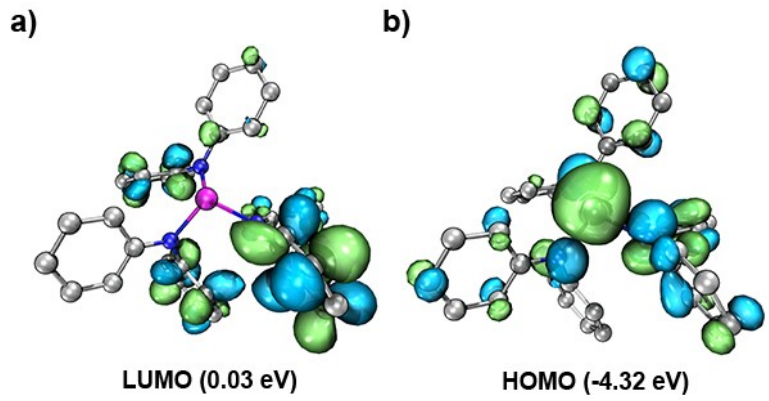


Fig. S32 a) LUMO and b) HOMO of $[Ge(NPh_2)_3]^-$ calculated at the B3LYP-D3BJ/6-311G(d) level in consideration of solvent(THF) correction.

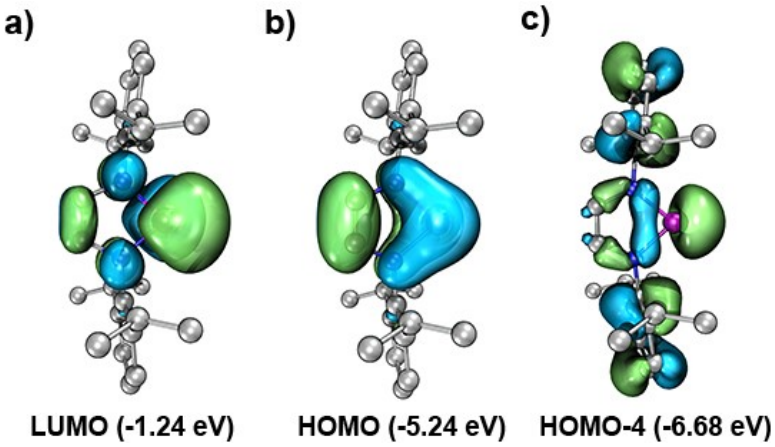


Fig. S33 a) LUMO, b) HOMO, and c) HOMO-1 of $[(DippNCH)_2Ge:]$ calculated at the B3LYP-D3BJ/6-311G(d) level in consideration of solvent(THF) correction.

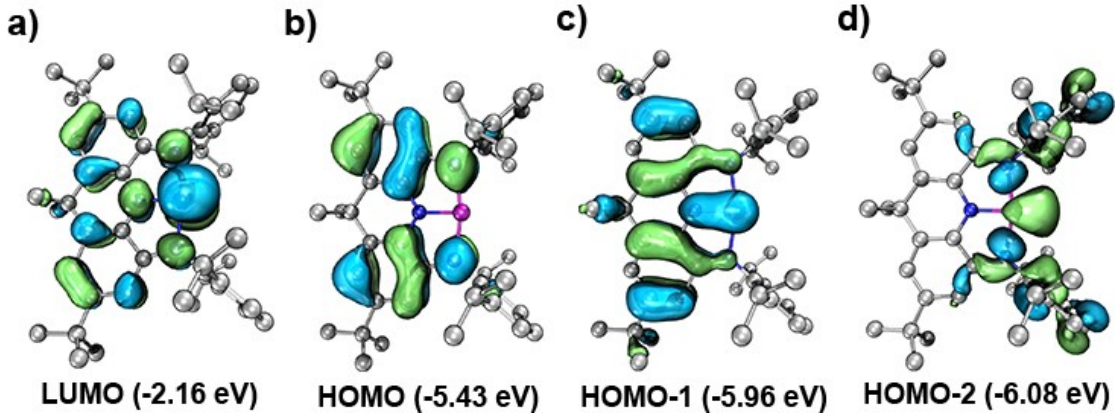


Fig. S34 a) LUMO, b) HOMO, c) HOMO-1, and HOMO-2 of ^{NNN}**LP** calculated at the B3LYP/6-311G(d) level with DFT-D3BJ and THF solvation-corrected..

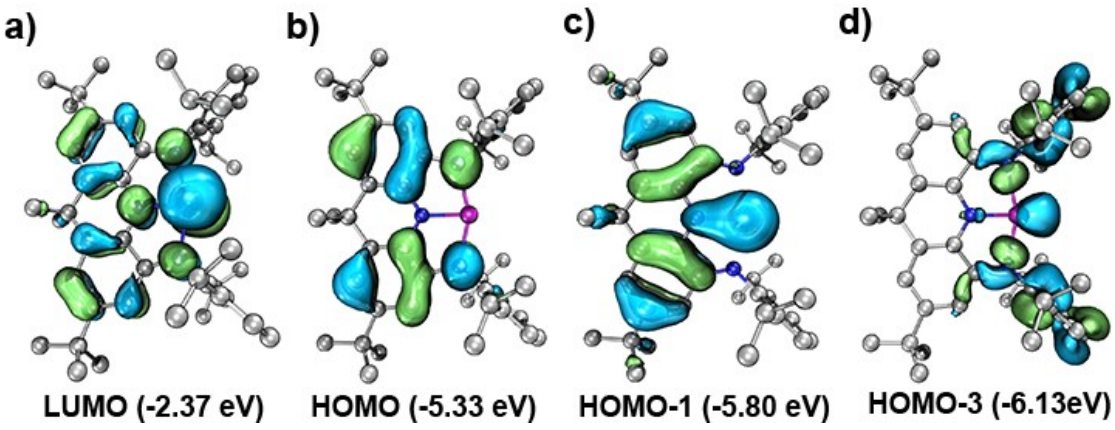
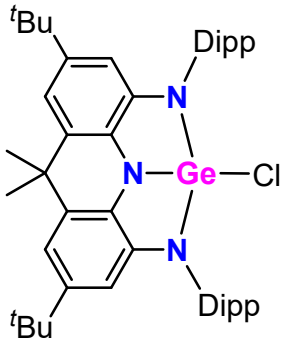


Fig. S35 a) LUMO, b) HOMO, c) HOMO-1, and d) HOMO-3 of ^{NNN}**LAs** calculated at the B3LYP/6-311G(d) level with DFT-D3BJ and THF solvation-corrected..

Coordinates of the studied molecules



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N	0.00700100	0.71569500	-0.52421000
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C	3.56427700	1.13143900	0.00394900
H	4.41598400	0.49103700	0.17731700
C	3.68956400	2.50655200	-0.03125000
C	2.53551400	3.31375900	-0.25402100
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C	1.28215100	2.77337700	-0.45675300
C	1.19007200	1.36843000	-0.45781200
C	-2.29275500	0.54579400	-0.18393700
C	-3.53487900	1.17150300	0.04984500

H	-4.39616800	0.54423000	0.23596900
C	-3.65322700	2.55197700	-0.00720700
C	-2.49946200	3.34451300	-0.24391700
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C	-1.16891800	1.38439700	-0.43505000
C	0.01935500	3.58970000	-0.78260100
C	0.02979600	4.93929000	-0.04945800
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H	-0.87368900	4.40822600	-2.60303900
H	0.00747800	2.89656000	-2.86240500
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H	4.72445800	3.55149800	2.30077000
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H	5.42874900	3.40697800	-1.97290100
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C	-5.95379900	2.71565600	-0.98509900
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H	-6.06902400	1.63014000	-0.99122800
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C	3.04549700	-1.73643200	0.12658700
C	3.41919100	-1.92975800	1.47017700
C	4.41801000	-2.86615500	1.74793000
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C	5.03678000	-3.57877800	0.72962700
H	5.81226800	-4.30038700	0.96560100
C	4.66174700	-3.36766900	-0.59229500
H	5.15384200	-3.92502900	-1.38123200
C	3.66217800	-2.45152600	-0.91891700
C	2.76056700	-1.17495500	2.61394000
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C	3.77582600	-0.34631800	3.41465900
H	4.52348000	-0.98087800	3.89831300
H	3.27000100	0.22475000	4.19857500
H	4.30132200	0.36123600	2.77007300
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H	1.24902300	-2.70807500	2.95729900
H	1.44673100	-1.57978800	4.30395100
H	2.64880900	-2.84427400	4.02220000
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H	2.31629700	-1.70054900	-2.36517000
C	3.19114500	-3.44630700	-3.21301100
H	4.15986900	-3.93554400	-3.35081000
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H	2.50755200	-4.16344800	-2.75500500
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H	-5.87269500	-4.22109600	0.96250900

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C	-3.40677200	-1.93362600	1.49925300
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H	-1.98601300	-0.52903200	2.23634500
C	-1.90604300	-2.25027000	3.49203700
H	-2.56683700	-2.97648400	3.97337500
H	-1.33739600	-1.74273600	4.27633100
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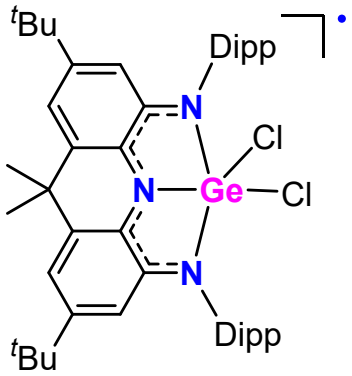

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N	-1.89826700	-0.70760400	-0.10312900

N	1.90436800	-0.68485400	-0.13560600
N	-0.00801200	0.90728400	-0.49473700
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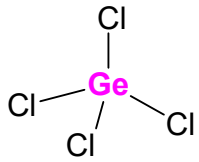

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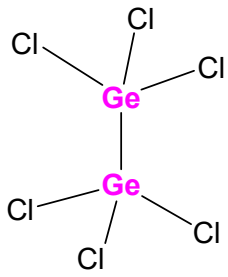

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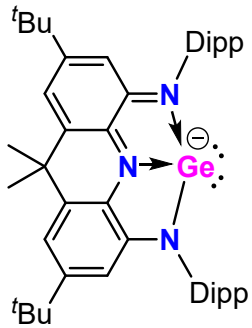

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H	7.22073100	2.71609500	-0.15359100
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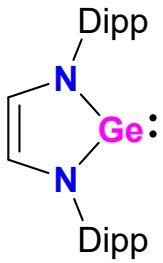

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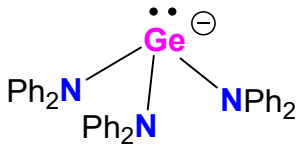

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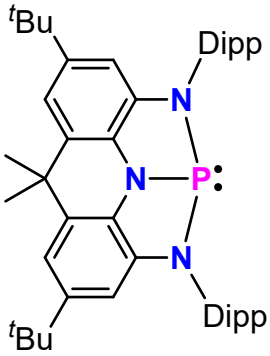

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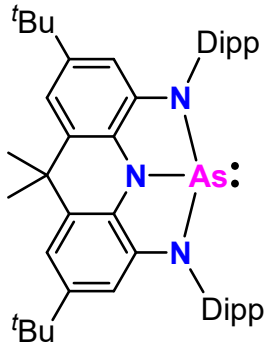

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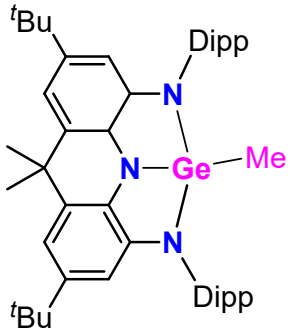

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C	-3.48281500	-1.91816700	-2.39310500
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C	4.83755200	-0.24453300	-2.56320400
H	4.94347300	0.42538800	-1.70876200
H	4.71943800	0.37081600	-3.45969900
H	5.76594900	-0.81346900	-2.66896800
C	3.43424800	-2.06770300	-3.62135800
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H	-4.12953500	-3.39551700	2.76505600
C	-4.78133100	-3.65434400	0.74321500
H	-5.54961500	-4.37414300	1.00657900
C	-2.14649200	-1.55821500	2.53027100
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C	-4.60872800	-0.94342500	-2.77751700
H	-5.58786700	-1.42546800	-2.69844600
H	-4.48569000	-0.59895400	-3.80855200
H	-4.60854800	-0.06692700	-2.12754700
C	-4.60879500	4.00174100	1.86185100
H	-4.23836000	3.38141000	2.68210700

H	-5.53820800	4.47846700	2.18844700
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C	-5.36847600	4.05535300	-0.53798200
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H	-6.31032700	4.53346200	-0.25128900
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C	-5.94347000	2.12047500	0.92103200
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H	2.83564500	-3.84105200	3.74683600
C	5.41429300	3.97230100	-0.05089000
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H	4.74251700	4.76414500	-0.38864600
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H	6.69532200	2.57905700	1.88859000
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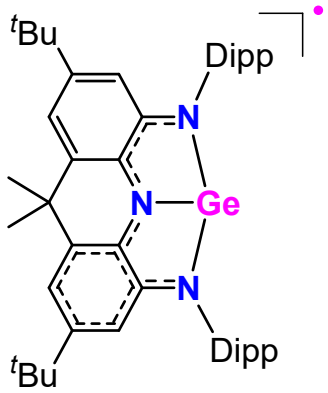

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N	2.06764600	-0.83351200	0.32146400
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C	-3.61179500	1.01654000	-0.21268400
H	-4.46206500	0.37013900	-0.37295600
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C	-1.30255500	2.62690700	0.14426100
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