Synthesis, Characterization, and Electronic Structures of a Methyl Germyliumylidene Ion and Germylone-Group VI Metal Complexes

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Supporting Information

Contents

1. Synthesis of compounds 2–5 and their spectral data

General considerations: All reactions were performed under an atmosphere of argon or nitrogen by using standard Schlenk or dry box techniques; solvents were dried over Na metal, K metal or CaH_2. Reagents were of analytical grade, obtained from commercial suppliers and used without further purification. ^{1}H and ^{13}C NMR spectra were obtained with a Bruker AVIII 400MHz BBFO1 spectrometer at 298 K unless otherwise stated. NMR multiplicities are abbreviated as follows: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad signal. Coupling constants *J* are given in Hz. Electrospray ionization (ESI) mass spectra were obtained at the Mass Spectrometry Laboratory at the Division of Chemistry and Biological Chemistry, Nanyang Technological University. Melting points were measured with a OpticMelt Stanford Research System. IR spectra were measured with the Bruker Alpha-FT-IR Spectrometer with an ECO-ATR module. UV-Vis spectra were measured with Cary 100 Bio UV-Visible spectrophotometer. Compound **1** was synthesized following the reported procedure.[S1]

Compound 2: MeOTf (25 mg, 0.152 mmol) was added to a toluene solution of compound **1** (70 mg, 0.148 mmol) at room temperature. After 1 h with stirring, the solvent was removed under vacuum, and the residue was washed with hexane (3 × 2 mL) to afford **2** as red solid (65%). Single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from a saturated toluene solution of **2** at room temperature.

M.p.:65 ^{o}C (decomposed); ^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ 6.57 (s, 1H, *Ar*), 6.55 (s, 1H, *Ar*), 5.00–4.93 (m, 1H, NCH_2), 4.86–4.79 (m, 1H, NCH_2), 4.70–4.61 (m, 1H, NCH_2), 4.31–4.23 (m, 1H, NCH_2), 2.24 (s, 3H, Ar-CH_3), 2.08 (s, 3H, Ar-CH_3), 2.01–1.99 (m, 6H, Ar-CH_3 & Ad-C*H*), 1.93–1.86 (m, 6H, Ad-CH_2), 1.41 (d, *J* = 12.7 Hz, 3H, Ad-CH_2), 1.35 (d, *J* = 12.1 Hz, 3H, Ad-CH_2), 1.12 (s, 9H, C(CH_3)$_3$), 0.77 (s, 3H, Ge-CH_3); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz, 298 K): δ 206.0 ($C_{carbene}$), 165.7 (*C*=N), 137.2 (C_{Ar}), 135.9 (C_{Ar}), 131.5 (C_{Ar}), 130.6 (C_{Ar}), 129.0 (C_{Ar}H), 128.8 (C_{Ar}H), 58.7 (Ad-*q*), 50.4 (N*C*H$_2$), 49.3 (N*C*H$_2$), 40.1 (Ad-*C*H$_2$), 39.2 (*C*(CH$_3$)$_3$), 34.9 (Ad-*C*H$_2$), 28.8 (Ad-*C*H), 27.8 (C(*C*H$_3$)$_3$), 20.0 (Ar-*C*H$_3$), 18.9 (Ar-*C*H$_3$), 18.3 (Ar-*C*H$_3$), 6.7 (Ge–*C*H$_3$), The signal for *C*F$_3$ could not be detected, presumably due to an overlap with other peaks; ^{19}F NMR (376 MHz, CDCl$_3$): δ −77.6. HRMS (ESI): *m/z* calcd for $C_{28}H_{42}GeN_3$: 494.2591 [(*M–OTf*)]$^{+}$; found: 494.2585.

General procedure for the synthesis of compound 3–5.

The respective M(CO)$_5$(thf) (M = Cr, Mo, W) was prepared by UV-irradiation of the corresponding M(CO)$_6$ in THF.[S2] A THF solution of the freshly prepared M(CO)$_5$(thf) was added dropwise to a THF solution of compound **1** at room temperature. After 2 hours, the resulting solution was concentrated under reduced pressure and stored at –26 ^{o}C to afford red crystals. Compound **3–5** are tharmally stable in THF, benzene and toluene solvents, and even under heating condition at 80 ^{o}C for several hours, no decomposition was detected. However, they rapidly decompose upon exposure to air.

Compound 3: Quantity used: $Cr(CO)_6$ (46 mg, 0.210 mmol), compound **1** (100 mg, 0.209 mmol), THF (15 mL); yield (40 %). M.p.:92 ^{o}C (decomposed); ^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ 6.78 (s, 2H, *Ar*), 3.50 (t, *J* = 7.3 Hz, 2H, NCH_2), 2.99 (t, *J* = 7.3 Hz, 2H, NCH_2), 2.13 (m, 12H, Ar-CH_3 & Ad-C*H*), 2.03 (m, 6H, Ad-CH_2), 1.75 (d, *J* = 11.9 Hz, 3H, Ad-CH_2), 1.62 (d, *J* = 12.1 Hz, 3H, Ad-CH_2), 0.77 (s, 9H, C(CH_3)$_3$); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz, 298 K): 225.9 (*C*O), 218.6 (*C*O), 195.5 ($C_{carbene}$), 145.1 (*C*=N), 140.2 (C_{Ar}), 136.8 (C_{Ar}), 133.9 (C_{Ar}), 129.7 (C_{Ar}H), 54.7 (Ad-*q*), 49.9 (N*C*H$_2$), 46.8 (N*C*H$_2$), 39.7 (Ad-*C*H$_2$), 38.6 (*C*(CH$_3$)$_3$), 36.7 (Ad-*C*H$_2$), 29.8 (Ad-*C*H), 29.1 (C(*C*H$_3$)$_3$), 21.0 (Ar-*C*H$_3$), 19.0 (Ar-*C*H$_3$); IR ν/cm^{-1} (solid): 2048 (s), 1976 (m), 1917 (s), 1899 (s); UV-Vis (ε, in THF): λ = 402 nm (10800), 465 nm (8950); HRMS (ESI): *m/z* calcd for $C_{32}H_{40}CrGeN_3O_5$: 672.1585 [(*M*+*H*)]$^{+}$; found: 672.1594.

Compound 4: Quantity used: $Mo(CO)_6$ (56 mg, 0.210 mmol), compound **1** (100 mg, 0.209 mmol), THF (15 mL); yield (36 %). M.p.:95 ^{o}C (decomposed); ^{1}H NMR (C_6D_6, 400 MHz, 298 K): δ 6.79 (s, 2H, *Ar*), 3.53 (t, *J* = 7.3 Hz, 2H, NCH_2), 2.99 (t, *J* = 7.3 Hz, 2H, NCH_2), 2.15 (m, 6H, Ar-CH_3 & Ad-C*H*), 2.12 (s, 6H, Ar-CH_3), 2.05 (m, 6H, Ad-CH_2), 1.75 (d, *J* = 11.9 Hz, 3H, Ad-CH_2), 1.63 (d, *J* = 12.1 Hz, 3H, Ad-CH_2), 0.77 (s, 9H, C(CH_3)$_3$); ^{13}C{^{1}H} NMR (C_6D_6, 100 MHz, 298 K): 213.7 (*C*O), 206.7 (*C*O), 190.9 ($C_{carbene}$), 143.6 (*C*=N), 140.6 (C_{Ar}), 136.7 (C_{Ar}), 133.7 (C_{Ar}), 129.7 (C_{Ar}H), 54.5 (Ad-*q*), 49.9 (N*C*H$_2$), 46.9 (N*C*H$_2$), 39.6 (Ad-*C*H$_2$), 38.3 (*C*(CH$_3$)$_3$), 36.7 (Ad-*C*H$_2$), 29.8 (Ad-*C*H), 29.1 (C(*C*H$_3$)$_3$), 21.0 (Ar-*C*H$_3$), 18.9 (Ar-*C*H$_3$); IR ν/cm^{-1} (solid): 2061 (s), 1985 (m), 1923 (s), 1897 (s); UV-Vis (ε, in THF): λ = 327 nm

(15700), 430 nm (11100); HRMS (ESI): *m/z* calcd for $C_{32}H_{40}MoGeN_3O_5$: 718.1234 $[(M+H)]^+$; found: 718.1251.

Compound 5: Quantity used: $W(CO)_6$ (73 mg, 0.208 mmol), compound **1** (100 mg, 0.209 mmol), THF (15 mL); yield (32 %). M.p.:105 ^oC (decomposed); ^1H NMR (C_6D_6, 400 MHz, 298 K): δ 6.78 (s, 2H, *Ar*), 3.51 (t, *J* = 7.3 Hz, 2H, NCH_2), 2.99 (t, *J* = 7.3 Hz, 2H, NCH_2), 2.15 (m, 6H, Ar-CH_3 & Ad-C*H*), 2.11 (s, 6H, Ar-CH_3), 2.05 (m, 6H, Ad-CH_2), 1.75 (d, *J* = 11.9 Hz, 3H, Ad-CH_2), 1.63 (d, *J* = 12.2 Hz, 3H, Ad-CH_2), 0.76 (s, 9H, C(CH_3)$_3$); $^{13}C\{^1H\}$ NMR (C_6D_6, 100 MHz, 298 K): 201.9 (*C*O), 197.5 (*C*O), 188.0 ($C_{carbene}$), 143.7 (*C*=N), 140.4 (C_{Ar}), 136.8 (C_{Ar}), 133.8 (C_{Ar}), 129.7 (C_{Ar}H), 54.5 (Ad-*q*), 49.9 (N*C*H$_2$), 47.0 (N*C*H$_2$), 39.7 (Ad-*C*H$_2$), 38.3 (*C*(CH$_3$)$_3$), 36.7 (Ad-*C*H$_2$), 29.8 (Ad-*C*H), 29.1 (C(*C*H$_3$)$_3$), 21.0 (Ar-*C*H$_3$), 19.0 (Ar-*C*H$_3$); IR v/cm^{-1} (solid): 2059 (s), 1978 (m), 1917 (s), 1895 (s); UV-Vis (ε, in THF): λ = 328 nm (13300), 434 nm (8910); HRMS (ESI): *m/z* calcd for $C_{32}H_{40}WGeN_3O_5$: 804.1689 $[(M+H)]^+$; found: 804.1710.

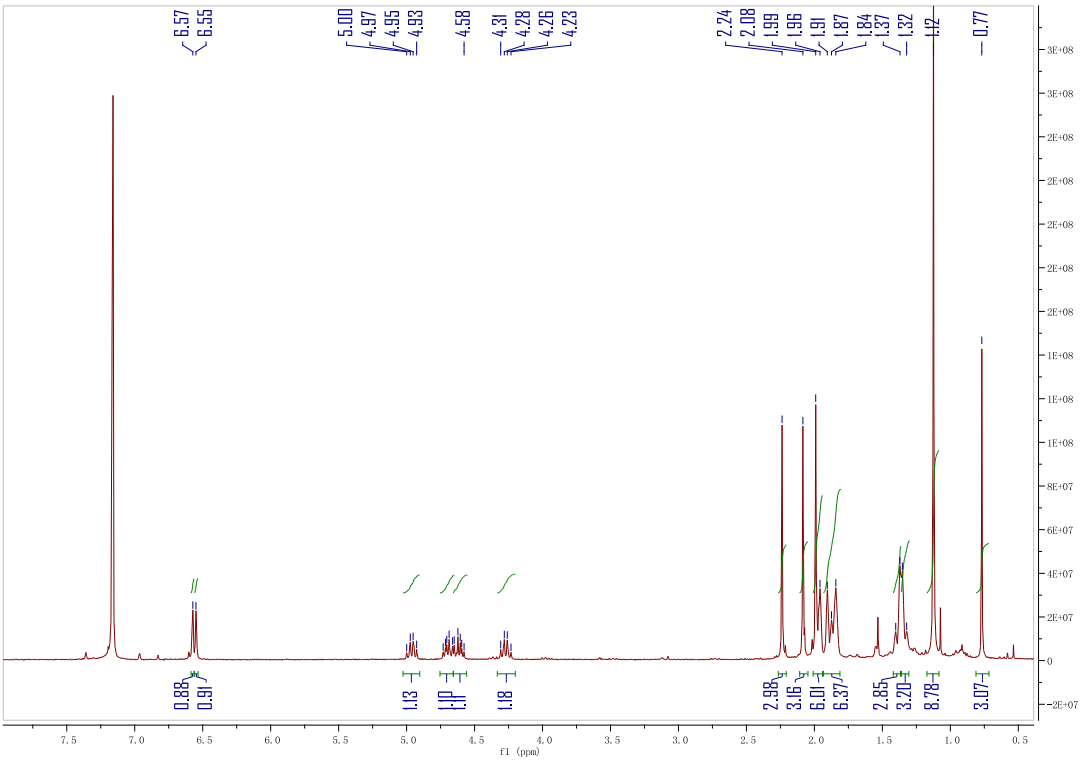


Figure S1: ^{1}H NMR spectrum of **2**.

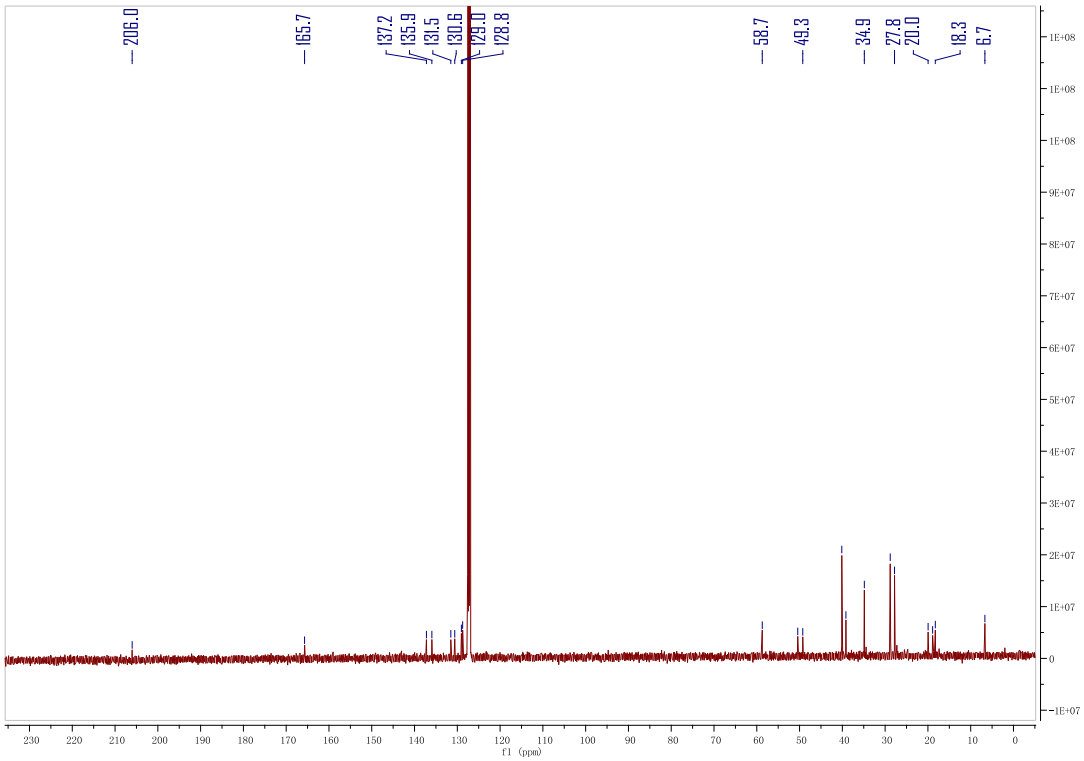


Figure S2: ^{13}C NMR spectrum of **2**.

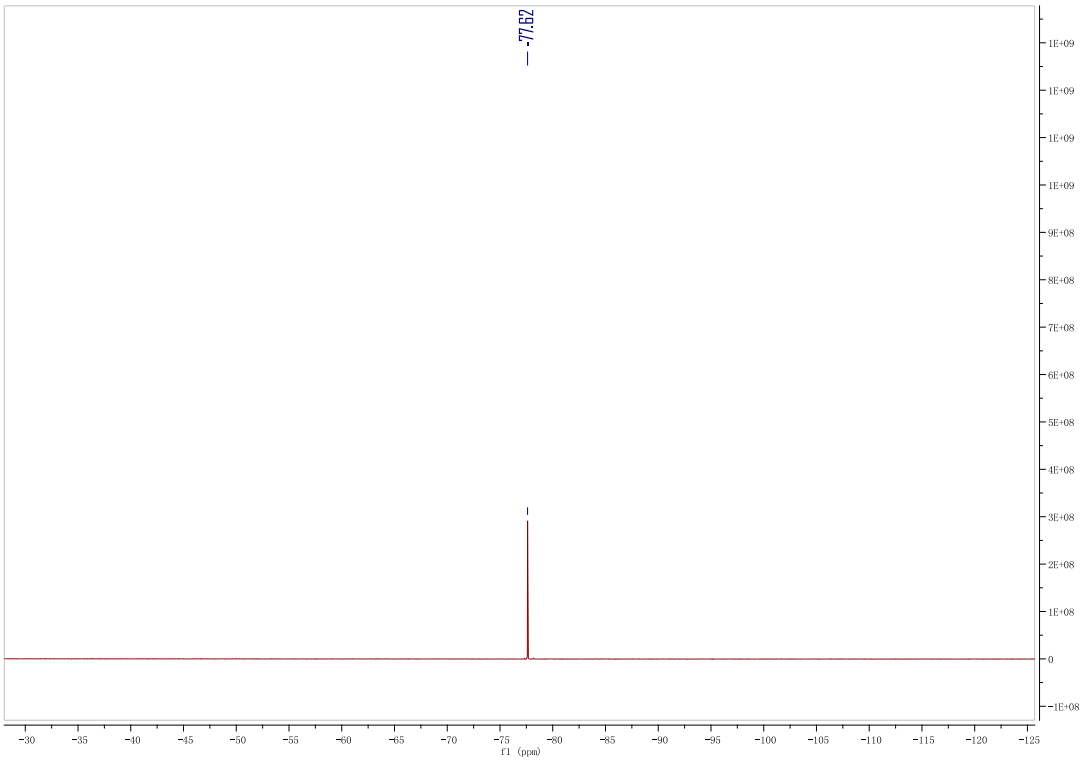


Figure S3: ^{19}F NMR spectrum of **2**.

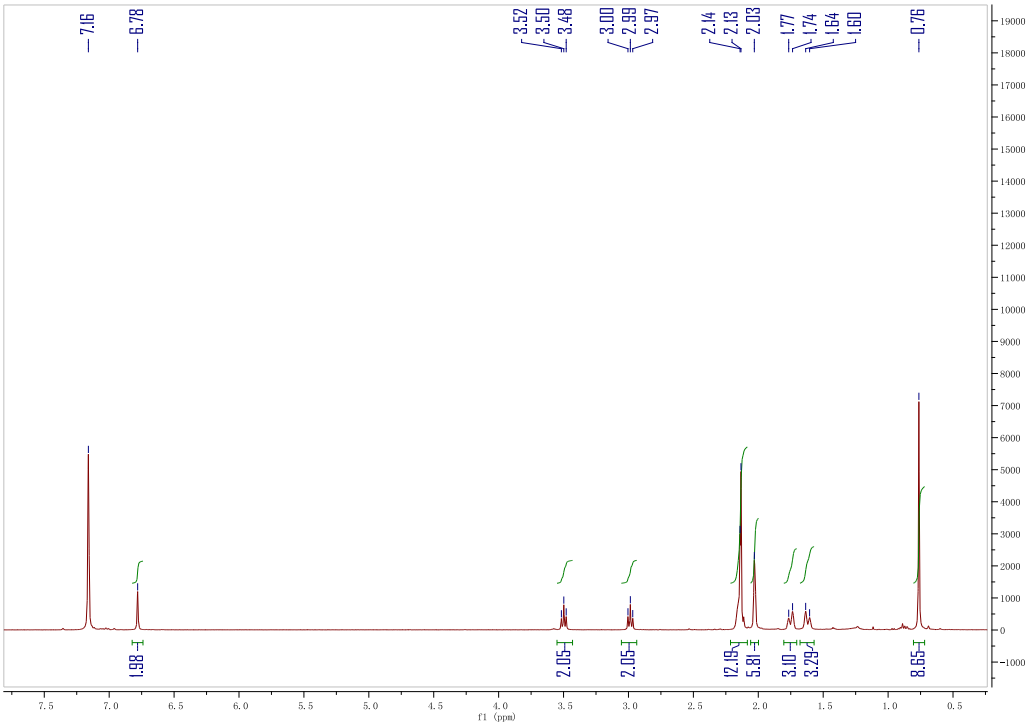


Figure S4: ^{1}H NMR spectrum of **3**.

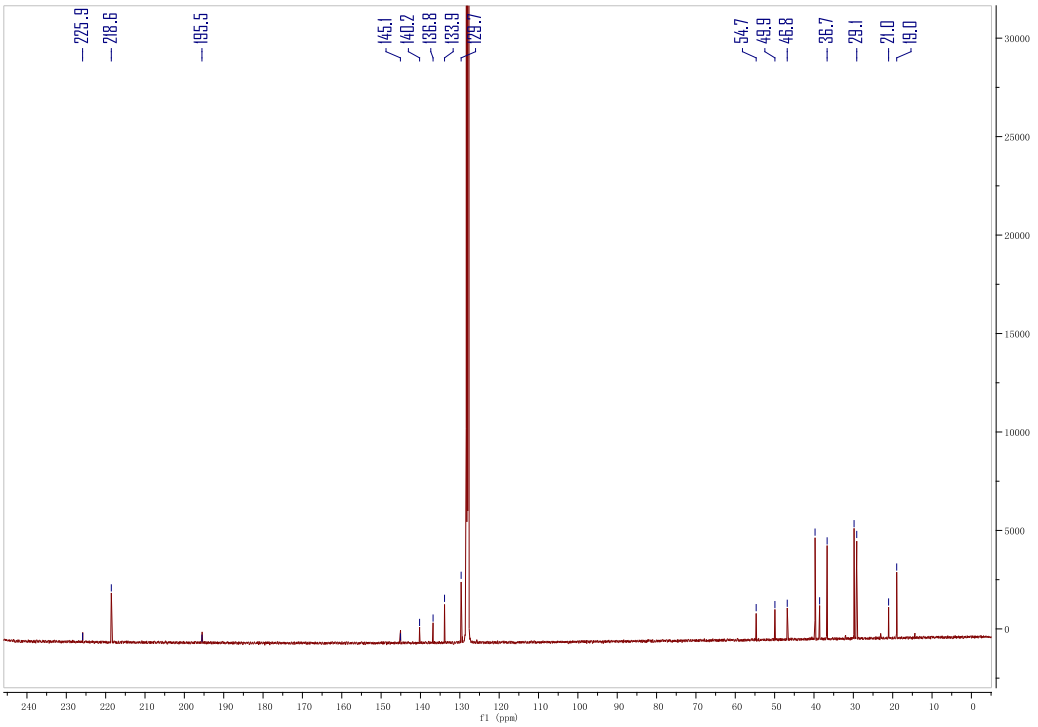


Figure S5: ^{13}C NMR spectrum of **3**.

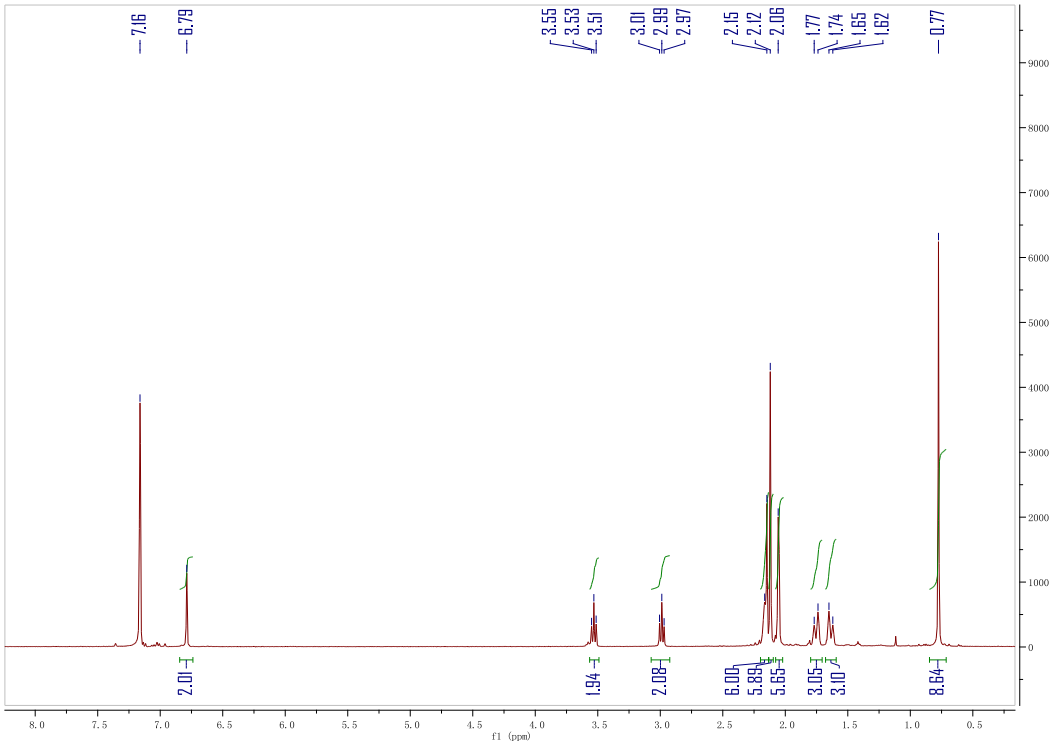


Figure S6: ^{1}H NMR spectrum of **4**.

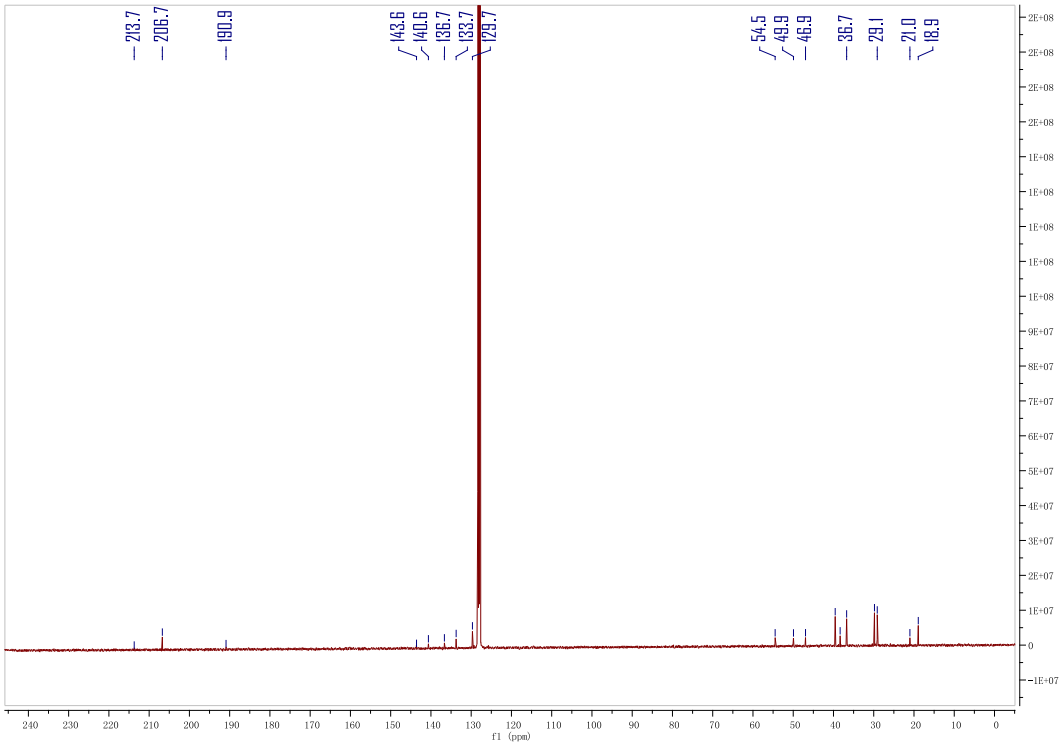


Figure S7: ^{13}C NMR spectrum of **4**.

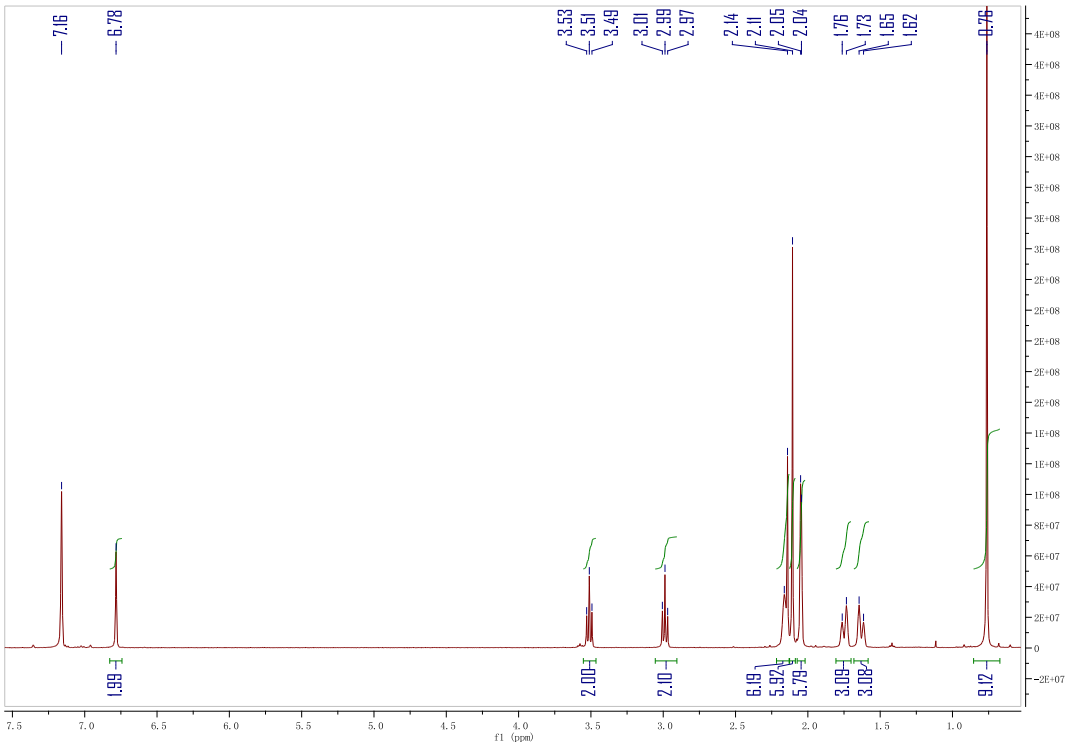


Figure S8: ^{1}H NMR spectrum of **5**.

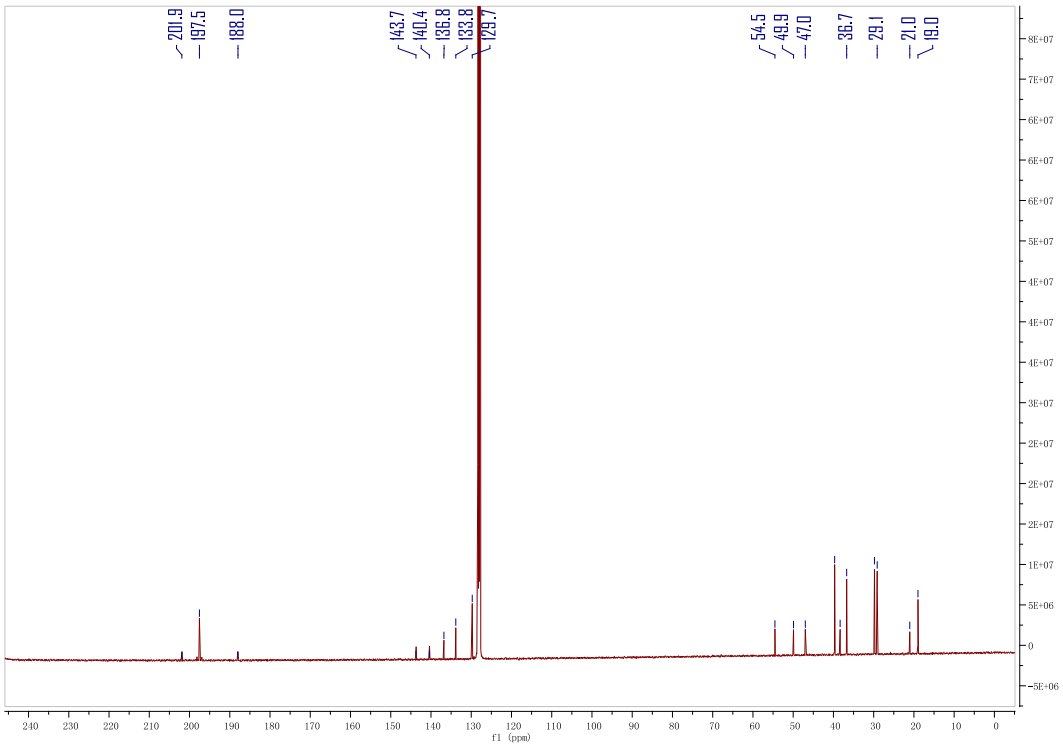


Figure S9: ^{13}C NMR spectrum of **5**.

2. Crystal structure parameters

X-ray data collection and structural refinement. Intensity data for compounds **2–5** was collected using a Bruker APEX II diffractometer. The structures were solved by direct phase determination (SHELX-2013) and refined for all data by full-matrix least squares methods on F^2.[S3] All non-hydrogen atoms were subjected to anisotropic refinement. The hydrogen atoms were generated geometrically and allowed to ride in their respective parent atoms; they were assigned appropriate isotropic thermal parameters and included in the structure-factor calculations. CCDC; 1429594-1429597 contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from the Cambridge Crystallography Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Table S1 Crystallographic data for compounds 2–5.

Compounds	**2**•$(C_6H_6)_1$	**3**•$(THF)_1$	**4**•$(THF)_1$	**5**•$(THF)_1$
Formula	$C_{35}H_{48}F_3GeN_3O_3S$	$C_{36}H_{47}CrGeN_3O_6$	$C_{36}H_{47}GeMoN_3O_6$	$C_{36}H_{47}GeWN_3O_6$
Fw	720.41	742.35	786.29	874.20
Cryst syst	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P 1 21/n 1	P 1 21/c 1	P 1 21/c 1	P 1 21/c 1
Size (mm^3)	0.120 x 0.180 x 0.320	0.180 x 0.200 x 0.200	0.100 x 0.120 x 0.180	0.060 x 0.080 x 0.120
T, K	103(2)	103(2)	103(2)	133(2)
a, Å	11.7454(9)	10.2157(3)	10.3172(9)	10.3691(5)
b, Å	24.4796(19)	22.5884(5)	22.6231(18)	22.6170(7)
c, Å	13.3037(10)	15.2996(5)	15.3939(12)	15.3476(7)
α, deg	90	90	90	90
β, deg	115.166(2)	97.6480(13)	97.423(3)	97.055(3)
γ, deg	90	90	90	90
V, $Å^3$	3462.0(5)	3499.07(17)	3562.9(5)	3572.0(3)
Z	4	4	4	4
d_{calcd} $g·cm^{-3}$	1.382	1.409	1.466	1.626
μ, mm^{-1}	1.000	1.218	1.244	4.107
Refl collected	40551	46257	32532	50991
T_{max}/T_{min}	0.8890/0.7400	0.8110/0.7930	0.8860/0.8070	0.7910/ 0.6380
N_{measd}	8645	11215	7754	9666
[R_{int}]	0.0751	0.0561	0.1085	0. 0879
R [I>2sigma(I)]	0.0482	0.0403	0.0512	0.0416
R_w[I>2sigma(I)]	0.1075	0.0894	0.1292	0.0885
GOF	1.025	1.017	1.024	1.001
Largest diff. peak/hole[$e·Å^{-3}$]	1.357/-0.664	1.325/-1.138	0.849/-1.298	1.397/-1.289

3. UV -Vis spectra

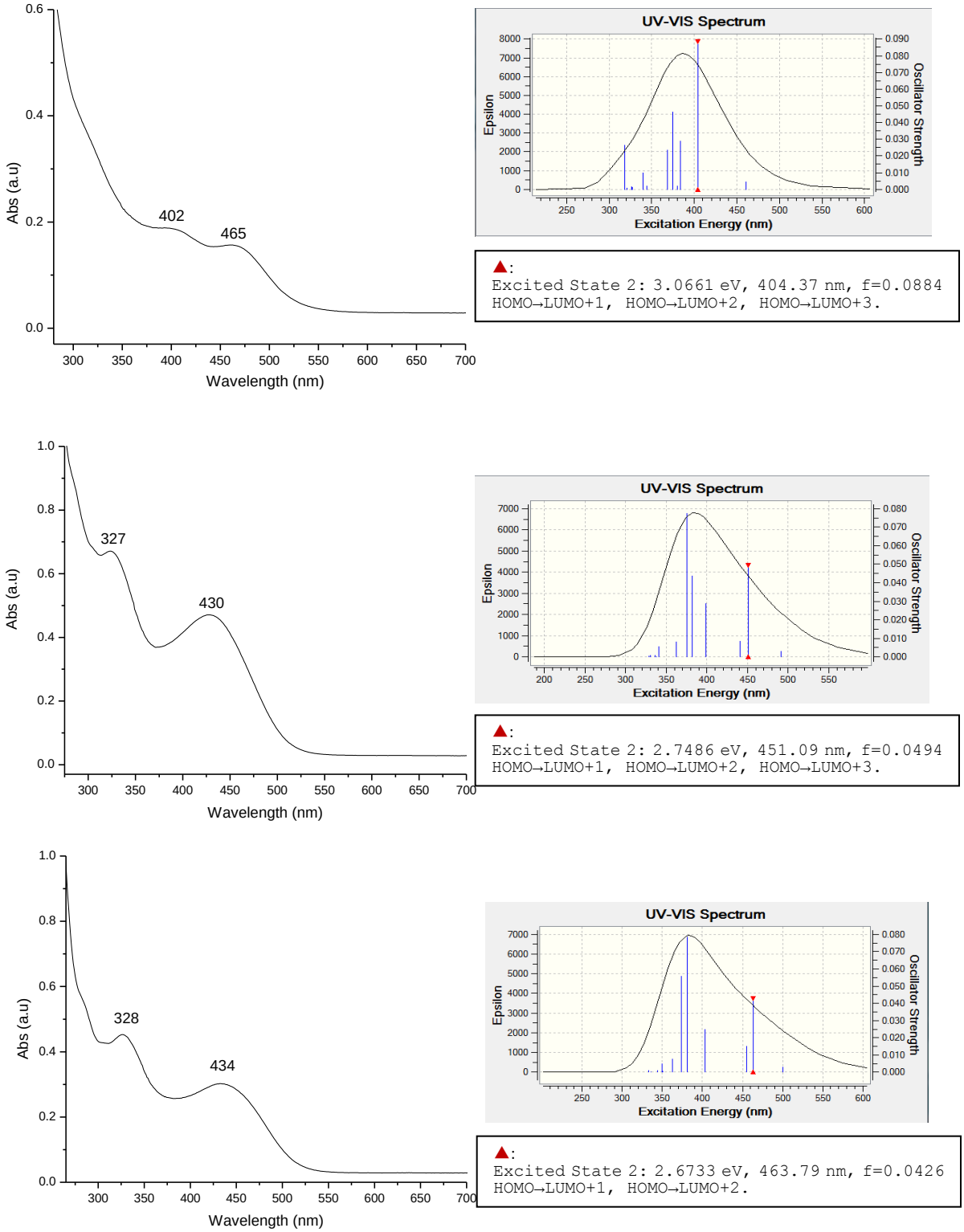


Figure S10. UV-Vis spectra of **3** (top), **4** (middle) and **5** (bottom) in THF, and TDDFT calculation results with assignments of the 2nd excited states.

4. IR spectra

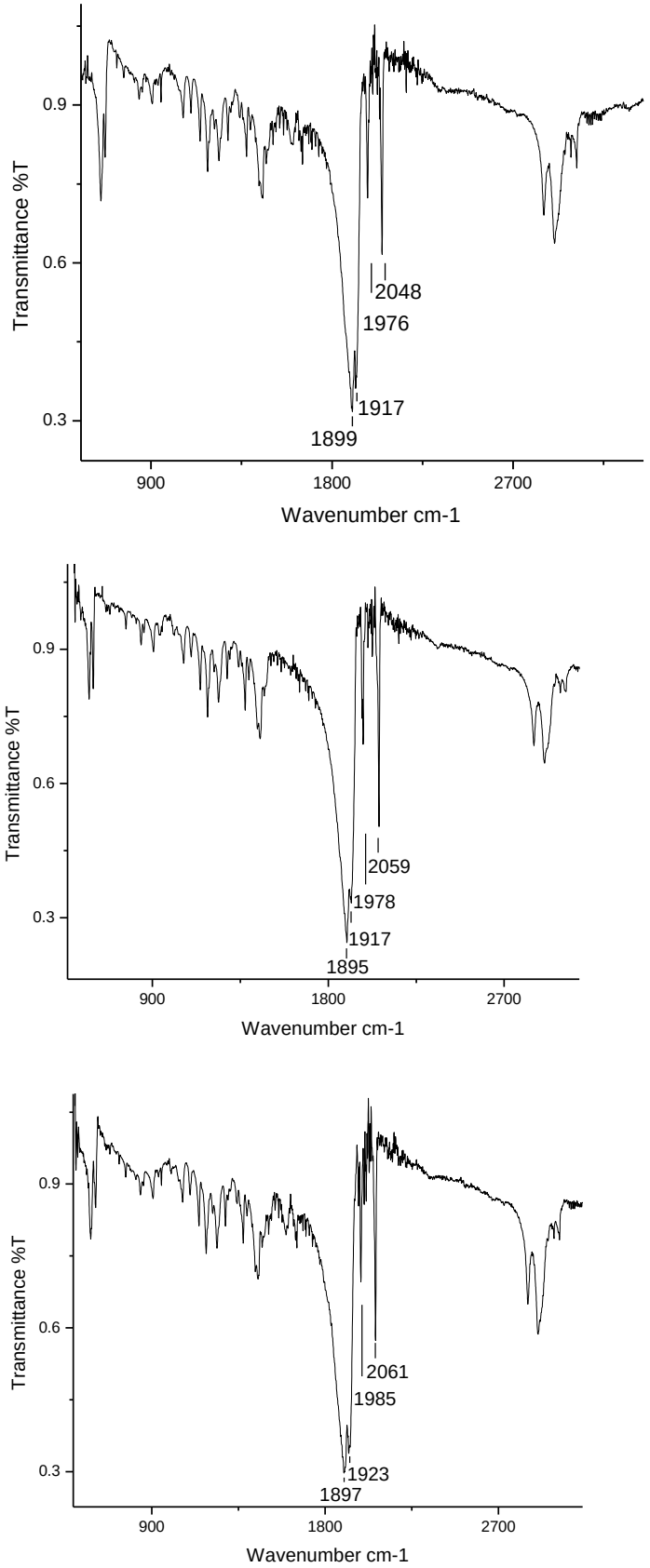
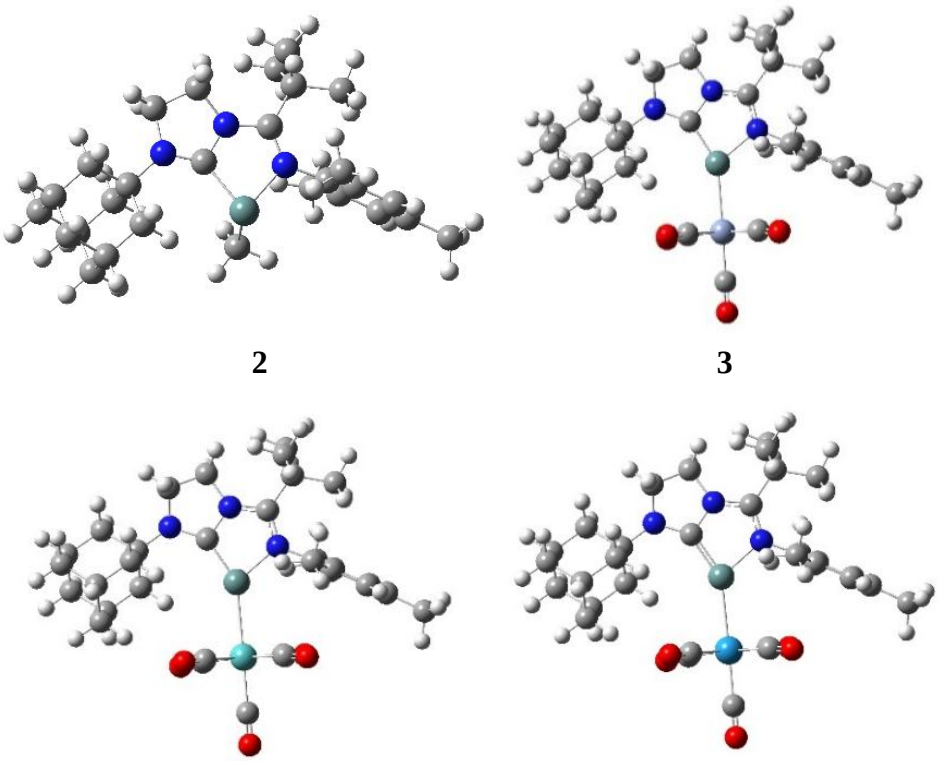


Figure S11. The IR spectra of **3** (top), **4** (middle) and **5** (bottom) in the solid state.

5. Theoretical calculation

Gaussian 09 was used for all density functional theory (DFT) calculations.[S4] Geometry optimization, frequency calculations, natural bond orbital (NBO) analysis, TDDFT and NICS calculations of compound **2**–**5** were performed at the B3LYP/6-311G(d,p) level of theory, with the LANL2TZ(f) pseudo-potential applied for the metal atoms.

Figure S12. Calculated optimized structures for **2, 3**, **4** and **5**.



2 **3**

4 **5**

2

Ge	-0.160593	-1.079018	-0.603191
C	0.828228	0.643073	-0.133302
H	2.322121	-1.657319	-0.469518
N	-0.048857	1.707194	-0.038006
N	-1.722820	0.202143	-0.093956
N	2.078088	1.078868	-0.135769
C	3.152109	-1.063385	-0.863137
H	-1.820359	-0.221594	2.420471
C	0.702593	2.981516	-0.181708
C	-1.434255	1.467019	-0.010778
C	-3.010452	-0.452295	-0.029616
C	2.131806	2.538925	0.118045
C	3.319484	0.234473	-0.050772
H	2.923844	-0.824363	-1.906165
C	4.437284	-1.915184	-0.768683
C	-2.868873	-0.493889	2.528218
H	0.357675	3.750664	0.499973
H	0.611703	3.339677	-1.208207

C	-2.391802	2.673552	0.155468
C	-3.515835	-0.861763	1.213322
C	-3.664876	-0.782627	-1.232643
H	2.849028	3.029482	-0.534576
H	2.418203	2.720336	1.158264
C	3.610301	-0.116143	1.428231
C	4.516281	1.023093	-0.631812
C	5.622756	-1.123190	-1.347085
H	4.284893	-2.832213	-1.344641
C	4.712878	-2.263099	0.707321
H	-3.387004	0.351841	2.994126
H	-2.928642	-1.326163	3.232255
C	-2.150379	3.310012	1.549546
C	-2.166985	3.709541	-0.981150
C	-3.889176	2.300964	0.092849
C	-4.706363	-1.595053	1.229751
C	-4.850946	-1.509929	-1.154030
C	-3.142804	-0.343333	-2.579883
H	2.761905	-0.668110	1.845145
H	3.727870	0.799709	2.017789
C	4.898124	-0.964317	1.514940
H	4.312251	1.292279	-1.674176
H	4.671726	1.950720	-0.073301
C	5.801345	0.173675	-0.538851
H	6.535527	-1.724750	-1.299638
H	5.448153	-0.892966	-2.403710
H	3.887546	-2.853414	1.120665
H	5.611895	-2.882225	0.782754

H	-2.791486	4.188529	1.649155
H	-1.124405	3.633316	1.722439
H	-2.417196	2.611244	2.344578
H	-2.171621	3.231907	-1.964376
H	-1.254815	4.291867	-0.882799
H	-2.994575	4.420484	-0.962348
H	-4.176345	1.874972	-0.867547
H	-4.456238	3.225156	0.223524
H	-4.194231	1.616035	0.879217
H	-5.106581	-1.907835	2.189079
C	-5.390029	-1.931994	0.064411
H	-5.369301	-1.755027	-2.075354
H	-3.822362	-0.659076	-3.371647
H	-2.158768	-0.768198	-2.794203
H	-3.044278	0.745026	-2.645830
H	5.088329	-1.204000	2.565057
C	6.081727	-0.163571	0.938486
H	6.630258	0.756961	-0.949552
C	-6.657347	-2.748435	0.106971
H	7.003238	-0.747998	1.019771
H	6.238143	0.754438	1.515969
H	-7.380463	-2.398981	-0.633393
H	-7.128559	-2.704718	1.090291
H	-6.448734	-3.800500	-0.113370
C	-0.044664	-2.092758	1.145730
H	0.742209	-2.842446	1.040237
H	0.152115	-1.486199	2.028033
H	-0.989348	-2.624690	1.272764

3

Ge	0.097271	-0.050560	-0.028143
Cr	0.289847	-2.612021	-0.042388
C	-0.936568	1.515844	-0.178296
C	-2.293230	3.370262	0.091746
C	-0.927213	3.859774	-0.351041
C	1.247163	2.515332	-0.078392
C	2.154386	3.766960	0.032578
C	1.868385	4.484933	1.379002
C	1.927036	4.728731	-1.165279
C	3.671551	3.473072	0.026101
C	2.924312	0.681195	0.033288

C	3.515144	0.365308	1.266754
C	2.845593	0.670417	2.585108
C	4.785296	-0.217752	1.264719
C	5.469891	-0.501267	0.085455
C	6.820782	-1.174353	0.107973
C	4.848470	-0.186219	-1.124634
C	3.582854	0.394844	-1.177629
C	2.964881	0.727180	-2.513492
C	-3.464831	1.135705	-0.099785
C	-3.696784	0.800330	1.395944
C	-3.341352	-0.178950	-0.891466

C	-4.706566	1.895024	-0.631247
C	-5.979241	1.041677	-0.471985
C	-6.190490	0.726032	1.021906
C	-4.974475	-0.054905	1.556013
C	-4.827585	-1.365632	0.760133
C	-4.610122	-1.039933	-0.730525
C	-5.827031	-0.266789	-1.267557
C	1.633205	-2.544126	-1.404459
C	1.627969	-2.567914	1.323043
C	0.394177	-4.473392	-0.029184
C	-1.028322	-2.669645	1.332933
C	-1.028560	-2.734718	-1.419164
N	-2.264177	1.970544	-0.336580
N	-0.105161	2.650323	-0.151644
N	1.587311	1.213362	-0.011097
O	2.420394	-2.567829	-2.236130
O	2.407083	-2.625140	2.161131
O	0.454986	-5.621137	-0.019886
O	-1.795973	-2.739716	2.182793
O	-1.797673	-2.870512	-2.258603
H	-2.401697	3.471127	1.184023
H	-3.089692	3.930653	-0.393598
H	-0.936309	4.118251	-1.413236
H	-0.577045	4.706309	0.228599
H	0.828663	4.783535	1.507710
H	2.482084	5.387454	1.448956
H	2.129001	3.835766	2.217514
H	2.082441	4.206881	-2.112829
H	2.656785	5.540452	-1.109729
H	0.942347	5.187962	-1.191282
H	3.993073	2.858599	0.862893
H	4.187391	4.433551	0.105512
H	4.004508	2.997461	-0.895032
H	3.145706	1.656308	2.959855
H	3.133621	-0.065410	3.337196
H	1.758334	0.667667	2.503243
H	5.241562	-0.468577	2.217324
H	7.317426	-1.040865	1.071210
H	7.476909	-0.778173	-0.671047
H	6.722141	-2.251157	-0.065552
H	5.355934	-0.412777	-2.057227
H	3.481178	0.199178	-3.315777
H	3.027304	1.800197	-2.727568
H	1.908057	0.456060	-2.549828
H	-3.798685	1.725072	1.975517
H	-2.829231	0.265346	1.793734
H	-2.482525	-0.746090	-0.529634
H	-3.156244	0.047527	-1.946145
H	-4.846287	2.829858	-0.080021
H	-4.542811	2.155380	-1.682956
H	-6.834058	1.610561	-0.853362
H	-7.103617	0.135394	1.155720
H	-6.325664	1.655206	1.588208
H	-5.118898	-0.283161	2.617227
H	-3.992352	-1.951545	1.150983
H	-5.728972	-1.977251	0.880547
H	-4.476652	-1.965846	-1.297541
H	-6.733877	-0.874342	-1.172827
H	-5.697535	-0.047229	-2.333455

4

Ge	0.075470	0.135497	-0.033753
Mo	0.322265	-2.563713	-0.041460
C	-0.980550	1.686098	-0.187211
C	-2.370499	3.517999	0.063972
C	-1.009095	4.028054	-0.371177
C	1.185921	2.718917	-0.079494
C	2.074255	3.983427	0.030056
C	1.770113	4.704848	1.370638
C	1.840228	4.935991	-1.173625
C	3.594776	3.708349	0.034152
C	2.886792	0.904998	0.040725
C	3.548055	0.620029	-1.169192
C	2.924300	0.937912	-2.505879
C	4.819927	0.052861	-1.114120
C	5.444391	-0.251669	0.097192
C	6.803454	-0.907995	0.122201
C	4.755194	0.025772	1.275180
C	3.478363	0.594337	1.275001
C	2.800242	0.887642	2.591630
C	-3.496535	1.256683	-0.105344
C	-4.760786	1.998432	-0.607390
C	-6.015642	1.121937	-0.432493

C	-6.194264	0.788986	1.061857
C	-4.955013	0.025485	1.566739
C	-3.696232	0.904617	1.391052
C	-3.365141	-0.048667	-0.913253
C	-4.615761	-0.932775	-0.735291
C	-5.856113	-0.176824	-1.242206
C	-4.798721	-1.275111	0.756227
C	1.744109	-2.478003	-1.544845
C	1.802975	-2.506456	1.402049
C	-1.066144	-2.658803	1.479133
C	-1.139847	-2.732957	-1.489865
C	0.469194	-4.567216	-0.031524
N	1.544546	1.422629	-0.006618
N	-0.168515	2.833606	-0.159673
N	-2.314586	2.115415	-0.353408
O	2.519577	-2.478083	-2.386857
O	2.603103	-2.551080	2.219939
O	-1.814411	-2.734390	2.344498
O	-1.933039	-2.879988	-2.303812
O	0.548220	-5.714440	-0.025959
H	-2.489887	3.624838	1.154540
H	-3.172206	4.061468	-0.431933
H	-1.014491	4.281089	-1.434727
H	-0.677580	4.883514	0.206492
H	0.726691	4.995151	1.488432
H	2.375169	5.613082	1.441597
H	2.028824	4.062087	2.214662
H	2.009366	4.412542	-2.117925
H	2.556875	5.759288	-1.117366
H	0.848543	5.379566	-1.207450
H	3.918406	3.102481	0.876535
H	4.098924	4.675210	0.111013
H	3.938704	3.230942	-0.882048
H	3.459631	0.429798	-3.308613
H	2.951449	2.013024	-2.716361
H	1.876741	0.632414	-2.545248
H	5.330341	-0.170623	-2.045854
H	6.718869	-1.985557	-0.053897
H	7.295592	-0.770363	1.087134
H	7.456855	-0.501895	-0.654012
H	5.212768	-0.219621	2.228518
H	3.065204	1.886348	2.958803
H	3.114693	0.168591	3.349559
H	1.713647	0.846099	2.510217
H	-4.621590	2.270489	-1.659723
H	-4.906570	2.925891	-0.045348
H	-6.886770	1.679592	-0.792936
H	-6.335659	1.710205	1.639486
H	-7.094208	0.180893	1.206324
H	-5.075854	-0.214874	2.628205
H	-2.812454	0.382142	1.769246
H	-3.803591	1.822788	1.980075
H	-2.488545	-0.606368	-0.578548
H	-3.207749	0.193646	-1.969092
H	-4.477926	-1.851389	-1.312840
H	-6.750229	-0.801014	-1.135548
H	-5.750745	0.053718	-2.308426
H	-5.685408	-1.905459	0.888381
H	-3.945378	-1.848761	1.126118

5

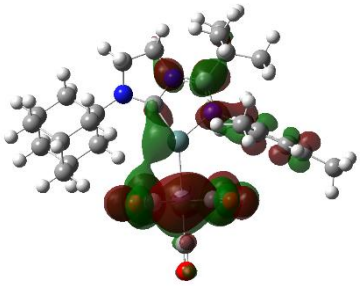
W	0.324024	-2.332169	-0.032048
Ge	0.050471	0.333801	-0.034959
C	1.800853	-2.257768	1.393930
C	1.733412	-2.233919	-1.526442
C	0.491009	-4.327208	-0.011947
C	-1.128515	-2.530760	-1.466985
C	-1.051638	-2.427447	1.481954
C	-1.030741	1.861827	-0.187454
C	-2.445525	3.672621	0.068575
C	-1.092704	4.202761	-0.368589
C	1.121296	2.926084	-0.079399
C	1.991136	4.203402	0.030785
C	1.676319	4.920020	1.371627
C	1.742633	5.152039	-1.173008
C	3.515662	3.951573	0.035055
C	-3.541439	1.396565	-0.105368
C	-3.730173	1.030604	1.388983
C	-3.397929	0.099342	-0.923981
C	-4.816572	2.127009	-0.596269
C	-6.060040	1.234263	-0.422681
C	-6.228091	0.887923	1.069834
C	-4.977708	0.135417	1.563481

C	-4.809550	-1.157096	0.742317
C	-4.636978	-0.801111	-0.747211
C	-5.888492	-0.056228	-1.243120
C	2.850830	1.138692	0.038913
C	3.516080	0.864744	-1.171257
C	2.887596	1.172417	-2.508140
C	4.797300	0.319266	-1.116127
C	5.427204	0.026330	0.095229
C	6.796846	-0.607453	0.120378
C	4.733943	0.292766	1.273344
C	3.447530	0.839022	1.273268
C	2.764905	1.120352	2.590200
N	-2.370813	2.271738	-0.351767
N	-0.234263	3.020567	-0.159211
N	1.499811	1.634742	-0.008258
O	2.609669	-2.289073	2.207046
O	2.511291	-2.220427	-2.369107
O	0.582342	-5.475602	-0.000399
O	-1.924054	-2.692753	-2.278959
O	-1.802569	-2.498033	2.348479
H	-2.564252	3.775625	1.159574
H	-3.255682	4.205487	-0.424859
H	-1.103383	4.455672	-1.432086
H	-0.772428	5.062606	0.208778
H	1.943713	4.280753	2.215599
H	0.629116	5.196341	1.489553
H	2.268999	5.836307	1.442714
H	0.743432	5.578125	-1.208550
H	1.922533	4.631856	-2.117104
H	2.444633	5.987752	-1.115300

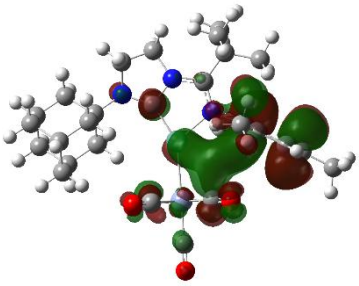
H	4.004806	4.926240	0.110125
H	3.866699	3.477740	-0.880204
H	3.848675	3.352556	0.878668
H	-3.845280	1.942755	1.985872
H	-2.839408	0.514771	1.759571
H	-2.512946	-0.449261	-0.597097
H	-3.248282	0.351432	-1.978667
H	-4.971497	3.048226	-0.026460
H	-4.685566	2.408537	-1.647181
H	-6.939206	1.784345	-0.775135
H	-7.120135	0.268165	1.213631
H	-6.377921	1.803033	1.655038
H	-5.090602	-0.114396	2.623580
H	-3.948133	-1.723588	1.104249
H	-5.688278	-1.798775	0.873072
H	-4.489991	-1.713415	-1.332328
H	-5.790464	0.183819	-2.307949
H	-6.774497	-0.692037	-1.137624
H	2.904964	2.247095	-2.722160
H	1.842993	0.857128	-2.546179
H	3.426633	0.666390	-3.309634
H	5.311045	0.103520	-2.047808
H	7.289487	-0.455493	1.082902
H	7.441211	-0.196048	-0.660537
H	6.728895	-1.687366	-0.048217
H	5.195726	0.055323	2.226635
H	3.081226	0.397522	3.343665
H	1.678731	1.073629	2.506698
H	3.024268	2.117964	2.964166

Figure S13. Plots of the frontier orbitals of compounds **3**, **4** and **5**. Orbital energies (in eV) are shown in parentheses.

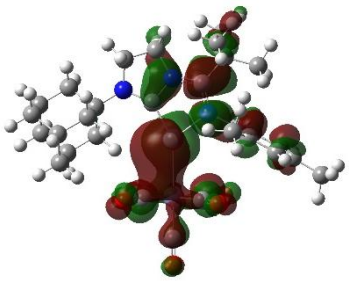
Compound 3:



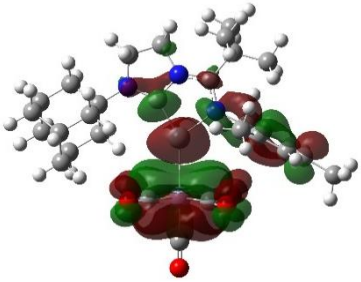
LUMO+3 (-0.3954)



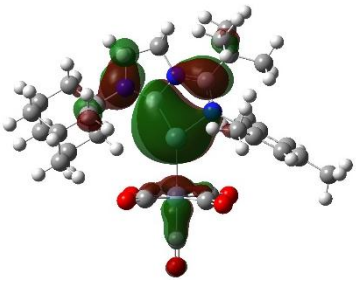
LUMO+2 (-0.4144)



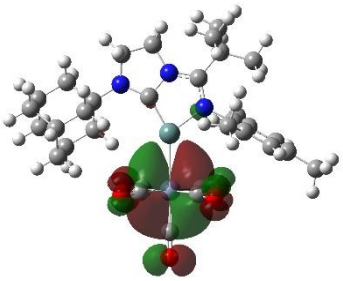
LUMO+1 (-0.7070)



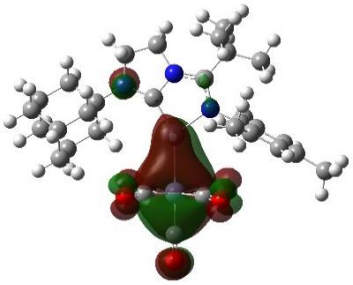
LUMO (-0.8419)



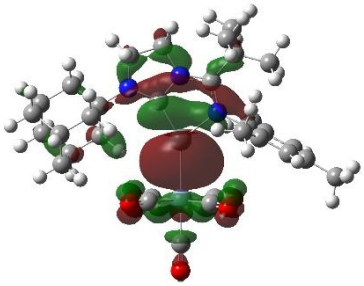
HOMO (-4.2776)



HOMO-1 (-5.7519)

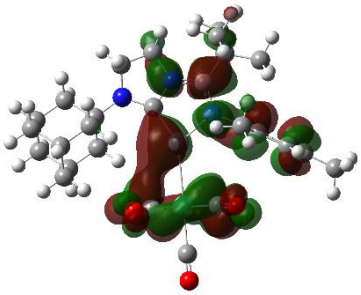


HOMO-2 (-5.8934)

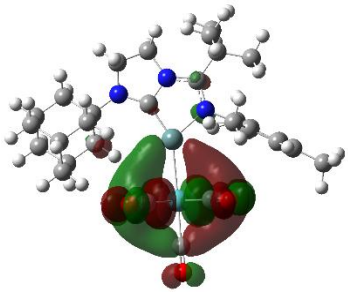


HOMO-7(-7.4761)

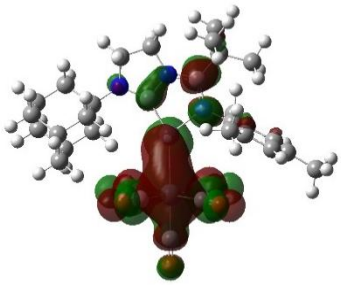
Compound 4:



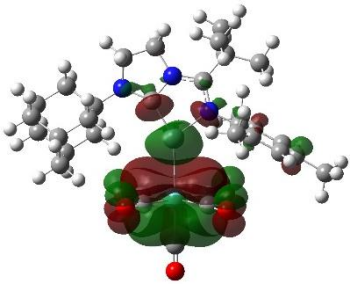
LUMO+3 (-0.5864)



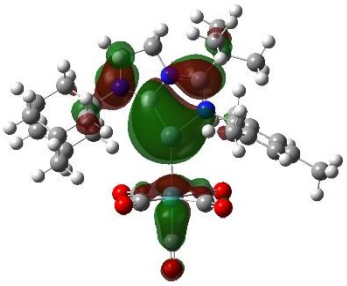
LUMO+2 (-0.7758)



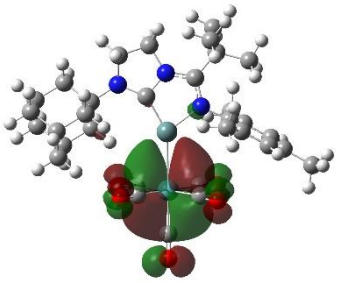
LUMO+1 (-0.9578)



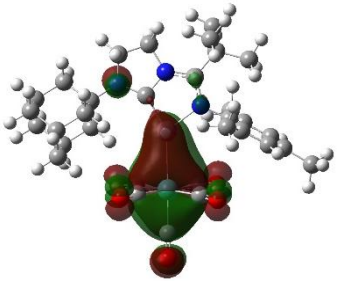
LUMO (-1.0735)



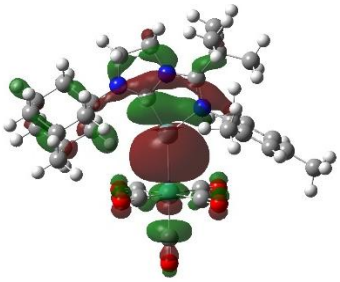
HOMO (-4.2719)



HOMO-1 (-5.7130)

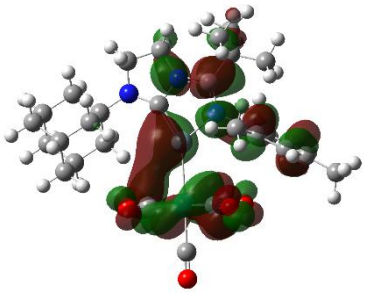


HOMO-2 (-5.8627)

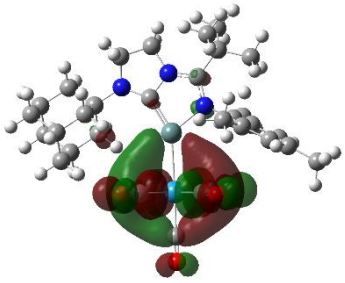


HOMO-7(-7.4807)

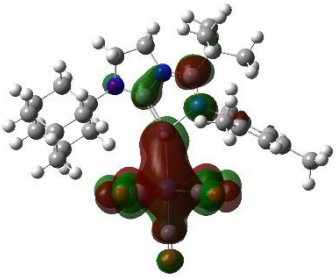
Compound 5:



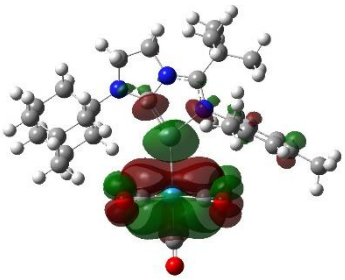
LUMO+3 (-0.6455)



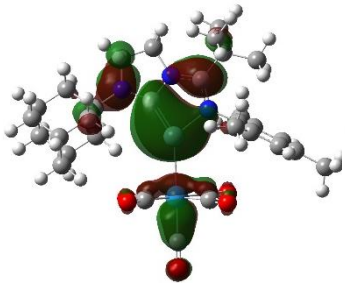
LUMO+2 (-0.8912)



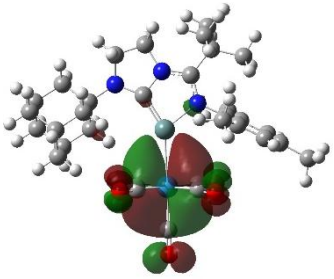
LUMO+1 (-1.0572)



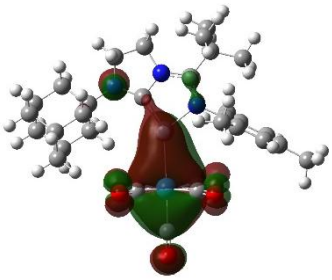
LUMO (-1.1557)



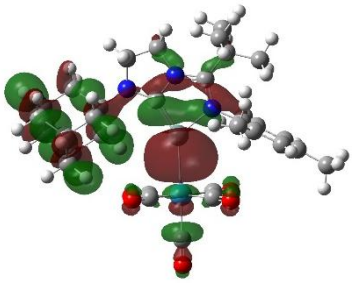
HOMO (-4.3095)



HOMO-1 (-5.6861)



HOMO-2 (-5.8646)



HOMO-7 (-7.7052)

Figure S14. Calculated NICS values for **1, 3**, **4** and **5**.

	1	3	4	5
NICS(0)	–9.36	–9.79	–9.80	–9.86
NICS(1)	–6.27	–6.15	–6.15	–6.13

Figure S15. NBO result showing the bonding interaction between the Ge and Cr atoms in **3**.

```
     (Occupancy)   Bond orbital/ Coefficients/ Hybrids
-------------------------------------------------------------------------------
    1. (1.79133) BD ( 1)Ge   1 -Cr   2
               ( 64.92%)   0.8058*Ge   1 s( 59.66%)p 0.68( 40.29%)d 0.00(  0.05%)
                                          0.7711 -0.0445 -0.0001  0.0020  0.0008
                                         -0.0002  0.0000  0.0000  0.0000  0.0000
                                          0.0000  0.1051  0.0028  0.0065  0.0005
                                          0.0009  0.0000  0.0000 -0.6257 -0.0079
                                         -0.0049 -0.0017 -0.0024  0.0000  0.0000
                                          0.0142  0.0006  0.0004  0.0001  0.0002
                                          0.0000  0.0000  0.0108  0.0147  0.0002
                                         -0.0019 -0.0008 -0.0001  0.0030  0.0016
                                          0.0001 -0.0016  0.0048 -0.0003  0.0048
                                          0.0102  0.0000
               ( 35.08%)   0.5922*Cr   2 s( 15.46%)p 3.63( 56.09%)d 1.84( 28.45%)
                                               f 0.00(  0.00%)
                                         -0.0020  0.3897 -0.0505  0.0138  0.0029
                                          0.0011  0.0002  0.0000  0.0003 -0.0521
                                          0.0019  0.0012 -0.0001 -0.0024  0.7466
                                         -0.0264  0.0005  0.0009 -0.0001  0.0000
                                         -0.0007  0.0003  0.0000 -0.0489  0.0161
                                          0.0002  0.0085 -0.0013 -0.0006 -0.0037
                                         -0.0026  0.0000 -0.4453  0.0910  0.0063
                                         -0.2687  0.0535  0.0035  0.0000  0.0001
                                         -0.0008 -0.0001  0.0000  0.0003 -0.0010
    2. (1.58324) BD ( 2)Ge   1 -Cr   2
               (  1.67%)   0.1293*Ge   1 s(  0.42%)p99.99( 99.05%)d 1.24(  0.53%)
                                         -0.0641 -0.0044 -0.0072  0.0067  0.0034
                                          0.0007 -0.0001  0.0000  0.0000  0.0000
                                          0.0000 -0.5241 -0.0324 -0.0078 -0.0033
                                          0.0014  0.0000 -0.0003 -0.1467 -0.0015
                                         -0.0077 -0.0002 -0.0002  0.0000  0.0000
                                          0.8319  0.0312  0.0033  0.0012 -0.0011
                                          0.0000  0.0000  0.0007  0.0568 -0.0004
                                         -0.0051  0.0045  0.0001  0.0012 -0.0421
                                          0.0006  0.0089 -0.0109  0.0001  0.0012
                                          0.0041 -0.0002
               ( 98.33%)   0.9916*Cr   2 s(  0.00%)p 1.00(  1.69%)d58.14( 98.31%)
                                               f 0.00(  0.00%)
                                         -0.0002  0.0034 -0.0015  0.0001  0.0004
                                          0.0000  0.0000  0.0000 -0.0013  0.0728
                                         -0.0026 -0.0017 -0.0001 -0.0002  0.0041
                                         -0.0018  0.0002  0.0000  0.0023 -0.1075
                                          0.0016  0.0010  0.0002 -0.5231 -0.0264
                                          0.0000 -0.0468 -0.0013  0.0003  0.8380
                                          0.0410  0.0003  0.0512  0.0035  0.0000
                                         -0.0009  0.0009  0.0000  0.0009  0.0003
                                          0.0001  0.0003 -0.0001 -0.0005 -0.0001
```

Table S2. The NPA charges of **3** calculated at the B3LYP/6-311G(d,p) level of theory, with the LANL2TZ(f) pseudo-potential applied for the Cr atom.

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
Ge	1	1.16572	28.00000	2.81526	0.01902	30.83428
Cr	2	-2.62631	17.95983	8.61342	0.05307	26.62631
C	3	-0.21821	1.99908	4.18238	0.03675	6.21821
C	4	-0.18038	1.99943	4.16410	0.01685	6.18038
C	5	-0.18004	1.99941	4.16423	0.01640	6.18004
C	6	0.44634	1.99903	3.52166	0.03298	5.55366
C	7	-0.06207	1.99935	4.04942	0.01330	6.06207
C	8	-0.57130	1.99943	4.56078	0.01109	6.57130
C	9	-0.57742	1.99944	4.56687	0.01112	6.57742
C	10	-0.58013	1.99945	4.56811	0.01256	6.58013
C	11	0.12865	1.99886	3.85219	0.02029	5.87135
C	12	-0.00752	1.99906	3.99259	0.01587	6.00752
C	13	-0.60024	1.99943	4.59148	0.00933	6.60024
C	14	-0.20829	1.99908	4.19436	0.01484	6.20829
C	15	0.00360	1.99917	3.98265	0.01458	5.99640
C	16	-0.59058	1.99944	4.58229	0.00884	6.59058
C	17	-0.20860	1.99908	4.19466	0.01485	6.20860
C	18	-0.00394	1.99906	3.98914	0.01573	6.00394
C	19	-0.59527	1.99944	4.58660	0.00924	6.59527
C	20	0.19598	1.99927	3.78294	0.02182	5.80402
C	21	-0.41686	1.99933	4.40149	0.01604	6.41686
C	22	-0.40754	1.99933	4.39008	0.01813	6.40754
C	23	-0.40521	1.99934	4.38889	0.01698	6.40521
C	24	-0.19347	1.99942	4.17716	0.01689	6.19347
C	25	-0.39057	1.99941	4.37556	0.01560	6.39057
C	26	-0.19369	1.99942	4.17750	0.01676	6.19369
C	27	-0.39586	1.99940	4.38120	0.01526	6.39586
C	28	-0.19500	1.99941	4.17901	0.01658	6.19500
C	29	-0.38941	1.99941	4.37445	0.01555	6.38941
C	30	0.84444	1.99908	3.10053	0.05595	5.15556
C	31	0.84454	1.99907	3.10048	0.05591	5.15546
C	32	0.84078	1.99890	3.10402	0.05631	5.15922
C	33	0.83992	1.99907	3.10446	0.05655	5.16008
C	34	0.83677	1.99907	3.10771	0.05645	5.16323
N	35	-0.51624	1.99931	5.49484	0.02209	7.51624
N	36	-0.39452	1.99922	5.38331	0.01199	7.39452
N	37	-0.72730	1.99934	5.71014	0.01781	7.72730
O	38	-0.45335	1.99975	6.44250	0.01110	8.45335

O	39	-0.45493	1.99975	6.44407	0.01112	8.45493
O	40	-0.45660	1.99975	6.44619	0.01065	8.45660
O	41	-0.46172	1.99975	6.45083	0.01114	8.46172
O	42	-0.45632	1.99975	6.44551	0.01106	8.45632
H	43	0.17303	0.00000	0.82280	0.00417	0.82697
H	44	0.20707	0.00000	0.79126	0.00167	0.79293
H	45	0.19876	0.00000	0.79810	0.00314	0.80124
H	46	0.20678	0.00000	0.79061	0.00261	0.79322
H	47	0.19132	0.00000	0.80747	0.00122	0.80868
H	48	0.20249	0.00000	0.79552	0.00199	0.79751
H	49	0.20767	0.00000	0.79046	0.00187	0.79233
H	50	0.20614	0.00000	0.79189	0.00197	0.79386
H	51	0.20391	0.00000	0.79409	0.00200	0.79609
H	52	0.19714	0.00000	0.80165	0.00122	0.80286
H	53	0.21499	0.00000	0.78290	0.00211	0.78501
H	54	0.20052	0.00000	0.79739	0.00208	0.79948
H	55	0.21175	0.00000	0.78622	0.00203	0.78825
H	56	0.20262	0.00000	0.79543	0.00195	0.79738
H	57	0.21743	0.00000	0.78103	0.00154	0.78257
H	58	0.22133	0.00000	0.77754	0.00113	0.77867
H	59	0.20098	0.00000	0.79633	0.00268	0.79902
H	60	0.20440	0.00000	0.79434	0.00126	0.79560
H	61	0.20582	0.00000	0.79286	0.00132	0.79418
H	62	0.21459	0.00000	0.78396	0.00146	0.78541
H	63	0.20074	0.00000	0.79657	0.00269	0.79926
H	64	0.21237	0.00000	0.78629	0.00134	0.78763
H	65	0.20063	0.00000	0.79724	0.00213	0.79937
H	66	0.22286	0.00000	0.77584	0.00129	0.77714
H	67	0.19328	0.00000	0.80400	0.00271	0.80672
H	68	0.21420	0.00000	0.78353	0.00228	0.78580
H	69	0.20853	0.00000	0.78776	0.00371	0.79147
H	70	0.21092	0.00000	0.78548	0.00360	0.78908
H	71	0.19372	0.00000	0.80347	0.00281	0.80628
H	72	0.20499	0.00000	0.79169	0.00332	0.79501
H	73	0.20506	0.00000	0.79278	0.00216	0.79494
H	74	0.19875	0.00000	0.79884	0.00241	0.80125
H	75	0.19360	0.00000	0.80432	0.00209	0.80640
H	76	0.20719	0.00000	0.79052	0.00229	0.79281
H	77	0.21027	0.00000	0.78696	0.00277	0.78973
H	78	0.19674	0.00000	0.80073	0.00253	0.80326
H	79	0.21470	0.00000	0.78273	0.00257	0.78530
H	80	0.19792	0.00000	0.79967	0.00241	0.80208
H	81	0.19700	0.00000	0.80096	0.00205	0.80300

==========

* Total *	0.00000	125.93265	221.07634	0.99102	348.00000

Table S3. The NPA charges of **4** calculated at the B3LYP/6-311G(d,p) level of theory, with the LANL2TZ(f) pseudo-potential applied for the Mo atom.

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
Ge	1	1.15111	28.00000	2.83007	0.01882	30.84889
Mo	2	-2.34130	35.94126	8.36519	0.03485	44.34130
C	3	-0.20646	1.99909	4.17045	0.03692	6.20646
C	4	-0.18053	1.99943	4.16426	0.01683	6.18053
C	5	-0.18014	1.99941	4.16435	0.01638	6.18014
C	6	0.44763	1.99903	3.52076	0.03257	5.55237
C	7	-0.06222	1.99935	4.04957	0.01330	6.06222
C	8	-0.57118	1.99943	4.56067	0.01108	6.57118
C	9	-0.57738	1.99944	4.56683	0.01111	6.57738
C	10	-0.58017	1.99945	4.56820	0.01251	6.58017
C	11	0.13044	1.99886	3.85048	0.02021	5.86956
C	12	-0.00453	1.99906	3.99009	0.01537	6.00453
C	13	-0.59578	1.99944	4.58727	0.00907	6.59578
C	14	-0.20921	1.99908	4.19531	0.01482	6.20921
C	15	0.00324	1.99917	3.98301	0.01459	5.99676
C	16	-0.59058	1.99944	4.58230	0.00884	6.59058
C	17	-0.20831	1.99908	4.19437	0.01486	6.20831
C	18	-0.00813	1.99906	3.99350	0.01557	6.00813
C	19	-0.59984	1.99943	4.59125	0.00915	6.59984
C	20	0.19587	1.99927	3.78299	0.02187	5.80413
C	21	-0.40558	1.99934	4.38928	0.01696	6.40558
C	22	-0.19335	1.99942	4.17704	0.01689	6.19335
C	23	-0.39054	1.99941	4.37553	0.01561	6.39054
C	24	-0.19382	1.99942	4.17765	0.01674	6.19382
C	25	-0.41698	1.99933	4.40160	0.01604	6.41698
C	26	-0.40762	1.99933	4.39045	0.01785	6.40762
C	27	-0.19554	1.99941	4.17955	0.01658	6.19554
C	28	-0.38945	1.99941	4.37449	0.01555	6.38945
C	29	-0.39492	1.99941	4.38028	0.01523	6.39492
C	30	0.78445	1.99918	3.15476	0.06161	5.21555
C	31	0.78295	1.99917	3.15617	0.06171	5.21705
C	32	0.77871	1.99917	3.16055	0.06157	5.22129
C	33	0.77598	1.99917	3.16316	0.06170	5.22402
C	34	0.77082	1.99898	3.16771	0.06250	5.22918

N	35	-0.72126	1.99935	5.70446	0.01746	7.72126
N	36	-0.39440	1.99923	5.38328	0.01190	7.39440
N	37	-0.51480	1.99931	5.49367	0.02182	7.51480
O	38	-0.44799	1.99975	6.43788	0.01037	8.44799
O	39	-0.44955	1.99975	6.43937	0.01044	8.44955
O	40	-0.45477	1.99975	6.44463	0.01040	8.45477
O	41	-0.45156	1.99975	6.44143	0.01039	8.45156
O	42	-0.45558	1.99975	6.44555	0.01028	8.45558
H	43	0.17303	0.00000	0.82278	0.00419	0.82697
H	44	0.20716	0.00000	0.79117	0.00167	0.79284
H	45	0.19874	0.00000	0.79816	0.00310	0.80126
H	46	0.20684	0.00000	0.79056	0.00260	0.79316
H	47	0.19131	0.00000	0.80748	0.00121	0.80869
H	48	0.20256	0.00000	0.79545	0.00199	0.79744
H	49	0.20756	0.00000	0.79057	0.00187	0.79244
H	50	0.20607	0.00000	0.79196	0.00197	0.79393
H	51	0.20398	0.00000	0.79402	0.00200	0.79602
H	52	0.19711	0.00000	0.80167	0.00121	0.80289
H	53	0.21486	0.00000	0.78304	0.00210	0.78514
H	54	0.20062	0.00000	0.79729	0.00208	0.79938
H	55	0.21194	0.00000	0.78605	0.00201	0.78806
H	56	0.21189	0.00000	0.78678	0.00134	0.78811
H	57	0.20067	0.00000	0.79719	0.00214	0.79933
H	58	0.22352	0.00000	0.77526	0.00122	0.77648
H	59	0.20089	0.00000	0.79641	0.00270	0.79911
H	60	0.21460	0.00000	0.78394	0.00146	0.78540
H	61	0.20448	0.00000	0.79426	0.00126	0.79552
H	62	0.20588	0.00000	0.79280	0.00132	0.79412
H	63	0.20122	0.00000	0.79608	0.00269	0.79878
H	64	0.20254	0.00000	0.79549	0.00197	0.79746
H	65	0.21608	0.00000	0.78241	0.00151	0.78392
H	66	0.22189	0.00000	0.77701	0.00109	0.77811
H	67	0.20482	0.00000	0.79185	0.00333	0.79518
H	68	0.19412	0.00000	0.80309	0.00279	0.80588
H	69	0.20514	0.00000	0.79270	0.00216	0.79486
H	70	0.19371	0.00000	0.80421	0.00209	0.80629
H	71	0.19884	0.00000	0.79874	0.00241	0.80116
H	72	0.20736	0.00000	0.79032	0.00231	0.79264
H	73	0.21423	0.00000	0.78372	0.00205	0.78577
H	74	0.19344	0.00000	0.80383	0.00273	0.80656
H	75	0.20959	0.00000	0.78645	0.00396	0.79041
H	76	0.21002	0.00000	0.78658	0.00340	0.78998
H	77	0.21519	0.00000	0.78229	0.00253	0.78481
H	78	0.19798	0.00000	0.79961	0.00242	0.80202

H	79	0.19698	0.00000	0.80097	0.00205	0.80302
H	80	0.19714	0.00000	0.80033	0.00253	0.80286
H	81	0.20829	0.00000	0.78906	0.00265	0.79171
* Total *		0.00000	143.91456	221.09102	0.99442	366.00000

Table S4. The NPA charges of **5** calculated at the B3LYP/6-311G(d,p) level of theory, with the LANL2TZ(f) pseudo-potential applied for the W atom.

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
W	1	-2.18292	67.94744	8.19983	0.03566	76.18292
Ge	2	1.17580	28.00000	2.80553	0.01867	30.82420
C	3	0.74305	1.99910	3.19460	0.06325	5.25695
C	4	0.74476	1.99911	3.19294	0.06319	5.25524
C	5	0.72887	1.99887	3.20830	0.06396	5.27113
C	6	0.73499	1.99909	3.20265	0.06326	5.26501
C	7	0.73775	1.99910	3.20012	0.06303	5.26225
C	8	-0.20138	1.99907	4.16541	0.03690	6.20138
C	9	-0.18045	1.99943	4.16418	0.01684	6.18045
C	10	-0.18009	1.99941	4.16425	0.01643	6.18009
C	11	0.44932	1.99904	3.51948	0.03216	5.55068
C	12	-0.06234	1.99935	4.04969	0.01329	6.06234
C	13	-0.57118	1.99943	4.56069	0.01107	6.57118
C	14	-0.57732	1.99944	4.56677	0.01111	6.57732
C	15	-0.58019	1.99945	4.56821	0.01252	6.58019
C	16	0.19570	1.99927	3.78319	0.02185	5.80430
C	17	-0.41701	1.99933	4.40165	0.01603	6.41701
C	18	-0.40787	1.99933	4.39058	0.01796	6.40787
C	19	-0.40571	1.99934	4.38943	0.01695	6.40571
C	20	-0.19327	1.99942	4.17696	0.01689	6.19327
C	21	-0.39059	1.99941	4.37557	0.01560	6.39059
C	22	-0.19374	1.99942	4.17756	0.01676	6.19374
C	23	-0.39503	1.99941	4.38039	0.01523	6.39503
C	24	-0.19569	1.99941	4.17967	0.01660	6.19569
C	25	-0.38948	1.99941	4.37452	0.01554	6.38948
C	26	0.12911	1.99886	3.85166	0.02036	5.87089
C	27	-0.00451	1.99906	3.98992	0.01553	6.00451
C	28	-0.59567	1.99944	4.58712	0.00911	6.59567
C	29	-0.20871	1.99908	4.19481	0.01482	6.20871
C	30	0.00413	1.99917	3.98213	0.01457	5.99587

C	31	-0.59067	1.99944	4.58239	0.00885	6.59067
C	32	-0.20764	1.99908	4.19369	0.01487	6.20764
C	33	-0.00785	1.99906	3.99305	0.01575	6.00785
C	34	-0.60016	1.99943	4.59154	0.00918	6.60016
N	35	-0.51382	1.99931	5.49255	0.02196	7.51382
N	36	-0.39312	1.99923	5.38210	0.01180	7.39312
N	37	-0.71935	1.99934	5.70289	0.01712	7.71935
O	38	-0.44863	1.99975	6.43777	0.01112	8.44863
O	39	-0.44658	1.99975	6.43582	0.01102	8.44658
O	40	-0.45564	1.99975	6.44516	0.01073	8.45564
O	41	-0.45062	1.99975	6.43977	0.01110	8.45062
O	42	-0.45420	1.99975	6.44335	0.01110	8.45420
H	43	0.17340	0.00000	0.82246	0.00414	0.82660
H	44	0.20767	0.00000	0.79067	0.00166	0.79233
H	45	0.19911	0.00000	0.79780	0.00309	0.80089
H	46	0.20724	0.00000	0.79016	0.00260	0.79276
H	47	0.20776	0.00000	0.79037	0.00186	0.79224
H	48	0.19127	0.00000	0.80753	0.00121	0.80873
H	49	0.20287	0.00000	0.79515	0.00198	0.79713
H	50	0.19709	0.00000	0.80169	0.00121	0.80291
H	51	0.20622	0.00000	0.79182	0.00196	0.79378
H	52	0.20426	0.00000	0.79375	0.00200	0.79574
H	53	0.20084	0.00000	0.79708	0.00208	0.79916
H	54	0.21214	0.00000	0.78585	0.00201	0.78786
H	55	0.21496	0.00000	0.78294	0.00210	0.78504
H	56	0.19345	0.00000	0.80382	0.00273	0.80655
H	57	0.21411	0.00000	0.78378	0.00211	0.78589
H	58	0.20905	0.00000	0.78670	0.00425	0.79095
H	59	0.21002	0.00000	0.78663	0.00335	0.78998
H	60	0.19412	0.00000	0.80309	0.00279	0.80588
H	61	0.20479	0.00000	0.79189	0.00331	0.79521
H	62	0.20518	0.00000	0.79266	0.00216	0.79482
H	63	0.19901	0.00000	0.79858	0.00241	0.80099
H	64	0.19364	0.00000	0.80427	0.00209	0.80636
H	65	0.20767	0.00000	0.79002	0.00231	0.79233
H	66	0.20870	0.00000	0.78851	0.00279	0.79130
H	67	0.19721	0.00000	0.80025	0.00253	0.80279
H	68	0.21587	0.00000	0.78160	0.00252	0.78413
H	69	0.19692	0.00000	0.80103	0.00205	0.80308
H	70	0.19813	0.00000	0.79946	0.00241	0.80187
H	71	0.20067	0.00000	0.79721	0.00212	0.79933
H	72	0.22280	0.00000	0.77599	0.00121	0.77720
H	73	0.21267	0.00000	0.78599	0.00134	0.78733
H	74	0.20112	0.00000	0.79618	0.00270	0.79888

H	75	0.20459	0.00000	0.79415	0.00126	0.79541
H	76	0.20590	0.00000	0.79278	0.00132	0.79410
H	77	0.21498	0.00000	0.78355	0.00146	0.78502
H	78	0.20151	0.00000	0.79580	0.00269	0.79849
H	79	0.21721	0.00000	0.78125	0.00154	0.78279
H	80	0.22104	0.00000	0.77788	0.00108	0.77896
H	81	0.20276	0.00000	0.79529	0.00195	0.79724
* Total *		0.00000	175.92034	221.07352	1.00614	398.00000

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