Supplementary Information

Yinhuan Li, Guorong Zhen, Lu Huang, Rong Zhang, Liliang Wang, Fan Qi, Mitsuo Kira, and Zhifang Li**

College of Material, Chemistry and Chemical Engineering, Key Laboratory of Organosilicon Chemistry and Material Technology, Ministry of Education, Hangzhou Normal University, Hangzhou, Zhejiang, 311121, P. R. China

Table of Contents

1. General Information

All reactions were performed under an atmosphere of argon by using standard Schlenk or dry box techniques; solvents were dried over Na metal under nitrogen atmosphere. All the starting materials were synthesized following literature procedures.[1-3] ^{1}H, ^{13}C, and ^{29}Si NMR spectra were obtained with a Bruker AV 400 instrument at 400 MHz (^{1}H NMR), and 101 MHz (^{13}C NMR), as well Bruker AV 500 instrument at 500 MHz (^{1}H NMR), 126 MHz (^{13}C NMR), and 99 MHz (^{29}Si NMR) at 298 K. The ^{1}H and ^{13}C NMR chemical shifts were referenced to residual ^{1}H and ^{13}C of the solvents: C_6D_6 (^{1}H δ 7.16 and ^{13}C δ 128.0) and THF-d_8 (δ 3.58, 1.73 for ^{1}H and δ 67.21, 25.31 for ^{13}C). NMR multiplicities are abbreviated as follows: s = singlet, brs = broad singlet, d = doublet, dt = doublet of triplets, t = triplet, and m = multiplet. Coupling constants J are given in Hz. Electrospray ionization (ESI) mass spectra were obtained at the Mass Spectrometry Laboratory at Hangzhou Normal University with a Bruker Daltonics MicroQtof spectrometer. Melting points were measured with an OpticMelt Stanford Research System. Sampling of air-sensitive compounds was carried out using a MBRAUN's MB-10-G glove box. UV-vis spectrum was recorded on a Shimadzu UV-1800 spectrophotometer.

2. Experimental Procedures

a) Synthesis of gold(I) complex 2a and 2b

In a glove box, THTAuCl (85.80 mg, 0.27 mmol) was added into a toluene (10 mL) solution of dialkylsilylene **1a** (100 mg, 0.27 mmol) and the mixture was stirred at room temperature for 30 min. The solvent was removed under vacuum to afford the residue that was extracted with hexane (5 mL) for 3 times. The residual solvent was concentrated under vacuum affording a silylgold(I) complex **2a** as an off-white powder (131 mg, 70 %); mp. 132.3 ºC (dec.); ^{1}H NMR (400 MHz, C_6D_6) δ 2.41 (t, SCH_2CH$_2$, $^{1}J_{H\text{-}H}$ = 6.4 Hz, 4H), 2.24–2.20 (m, ring-CH_2, 2H), 2.04–2.01 (m, ring-CH_2, 2H), 1.23–1.20 (m, SCH$_2$CH_2 ,4H), 0.54 (s, SiCH_3, 18H), 0.53 (s, SiCH_3, 18H); ^{13}C NMR (126 MHz, C_6D_6) δ 36.62 (ring-C^q), 33.40 (SCH$_2$CH$_2$), 30.20 (SCH$_2$$CH_2$), 19.92 (ring-$CH_2$), 4.99 (Si$CH_3$); ^{29}Si NMR (99 MHz, C_6D_6) δ 63.77, 4.20, 1.98. HRMS (ESI): m/z calcd for [$C_{20}H_{48}AuClSSi_5$]: 692.1677; [(M–Cl)]$^{+}$, found: 657.1979.

In a glove box, THTAuCl (154 mg, 0.48 mmol) was added into a THF (10 mL) solution of dialkylgermylene **1b** (200 mg, 0.48 mmol) and the mixture was further stirred at room temperature for 30 min. The solvent was removed under vacuum giving a germylgold(I) complex **2b** (329 mg, 93 %) as a white powder; mp. 114.4 ºC (dec.); ^{1}H NMR (400 MHz, C_6D_6) δ 2.38–2.36 (t, SCH_2CH$_2$, $^{1}J_{H\text{-}H}$ = 4 Hz, 4H), 2.33–2.31 (m, ring-CH_2, 2H), 2.10–2.06 (m, ring-CH_2, 2H), 1.21–1.19 (m, SCH$_2$CH_2 ,4H), 0.57 (s, SiCH_3, 18H), 0.49 (s,

SiCH_3, 18H); ^{13}C NMR (126 MHz, C_6D_6) δ 36.89 (ring-C^q), 34.37 (S$CH_2$$CH_2$), 30.17 (S$CH_2$$CH_2$), 25.07 (ring-$CH_2$), 4.78 (Si$CH_3$), 4.65 (Si$CH_3$); ^{29}Si NMR (99 MHz, C_6D_6) δ 4.47, 2.15: HRMS (ESI): m/z calcd for $C_{20}H_{48}AuGeClSSi_4$: 738.1114; $[(M–Cl)]^+$, found: 703.1429.

b) Synthesis of [(R$_2$Si)Au)]$_3^-$·K$^+$(THF) 3a and [(R$_2$Ge)Au)]$_3^-$·K$^+$(18-Crown-6) 3b

2a (100 mg, 0.145 mmol) and KC_8 (0.28 mmol, 39 mg) were mixed in THF (10 mL). The mixture was stirred at ambient temperature for 12 h. The solvent was removed under vacuum to afford the residue that was washed with hexane (5 mL) for 3 times. Extracting from the residue with ether (20 mL) followed by concentration under vacuum gave **3a** (55 mg, 65 %) as a blue solid. **3a**: mp. 271.6 ºC (dec.); ^{1}H NMR (400 MHz, THF-d_8) δ 3.63–3.61 (m, OC$H_2$$CH_2$, 8H), 2.27 (brs, ring-C$H_2$, 12H), 1.79–1.77 (m, OCH_2CH_2, 8H), 0.18 (s, SiCH_3, 108H); ^{13}C NMR (101 MHz, THF-d_8) δ 68.03 (O$CH_2$$CH_2$), 36.52 (ring-$C^q$), 32.96 ($OCH_2$$CH_2$), 26.19 (ring-$CH_2$), 5.42 (Si$CH_3$); ^{29}Si NMR (99 MHz, THF-d_8) δ 333.46, –0.18; HRMS (ESI): m/z calcd for $[C_{48}H_{120}Au_3Si_{15}]^-$: 1707.4926 $[(M–K)]^-$, found: 1707.4906.

2b (100 mg, 0.135 mmol), and KC_8 (0.15 mmol, 21 mg) were mixed in THF (10 mL). The mixture was stirred at ambient temperature for 12 h, 18-Crown-6 (0.14 mmol, 37 mg) was subsequently added to the mixture. The solvent was removed under vacuum to afford the residue that was washed with hexane (5 mL) for 3 times. Extracting from the residue with toluene (20 mL) followed by concentration under vacuum gave **3b** (65 mg, 67 %) as a blue solid. **3b**: mp. 247.4 ºC (dec.); ^{1}H NMR (400 MHz, THF-d_8) δ 3.63 (s, 18-Crown-6, 24H), 2.43 (s, ring-CH_2, 12H), 0.15 (s, SiCH_3, 108H); ^{13}C NMR (101 MHz, THF-d_8) δ 70.99 (18-Crown-6), 39.17 (ring-C^q), 37.31 (ring-CH_2), 5.13 (SiCH_3); ^{29}Si NMR (99 MHz, THF-d_8) δ –0.22; HRMS (ESI): m/z calcd for $[C_{48}H_{120}Au_3Ge_3Si_{12}]^-$: 1843.3290 $[(M–K)]^-$, found: 1843.3260.

3. Experimental Spectra (^{1}H, ^{13}C, ^{29}Si, NMR Spectra)

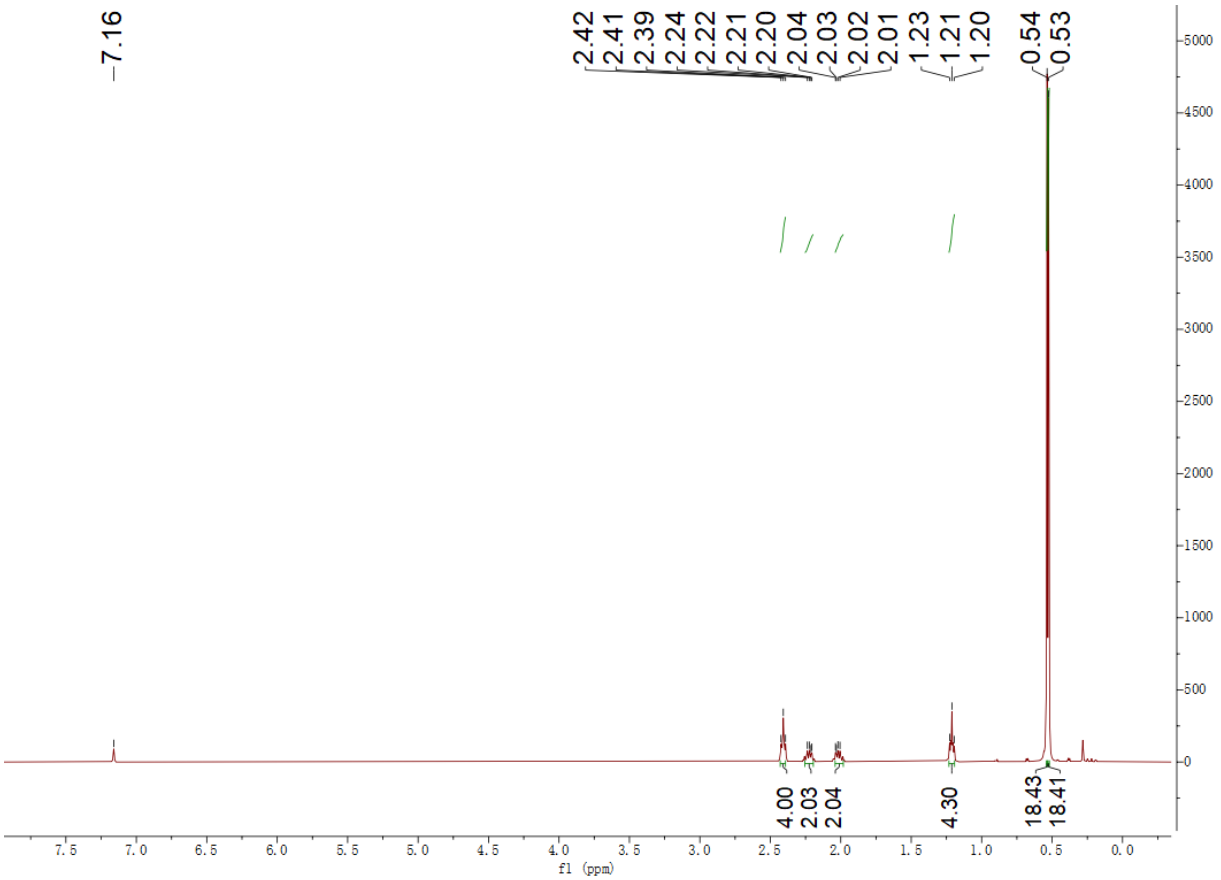


Figure S1. ^{1}H NMR spectrum of **2a** in C_6D_6

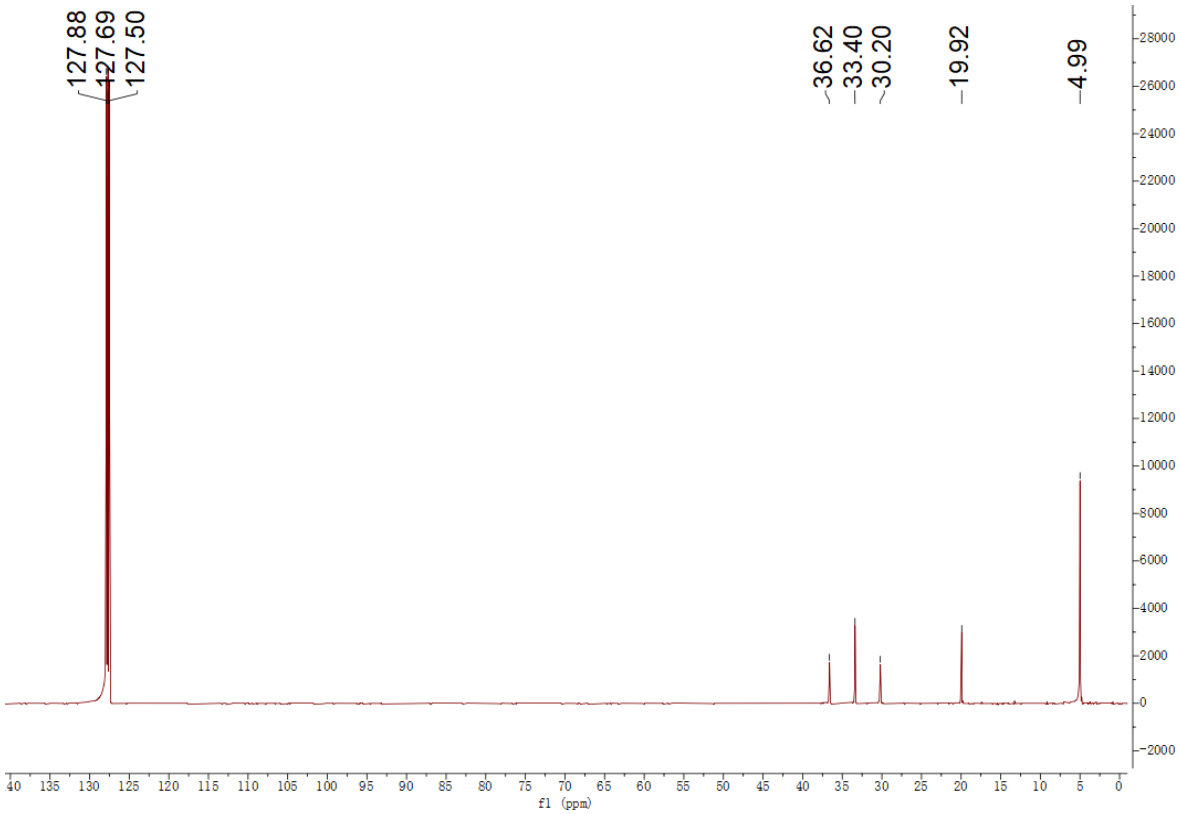


Figure S2. ^{13}C NMR spectrum of **2a** in C_6D_6

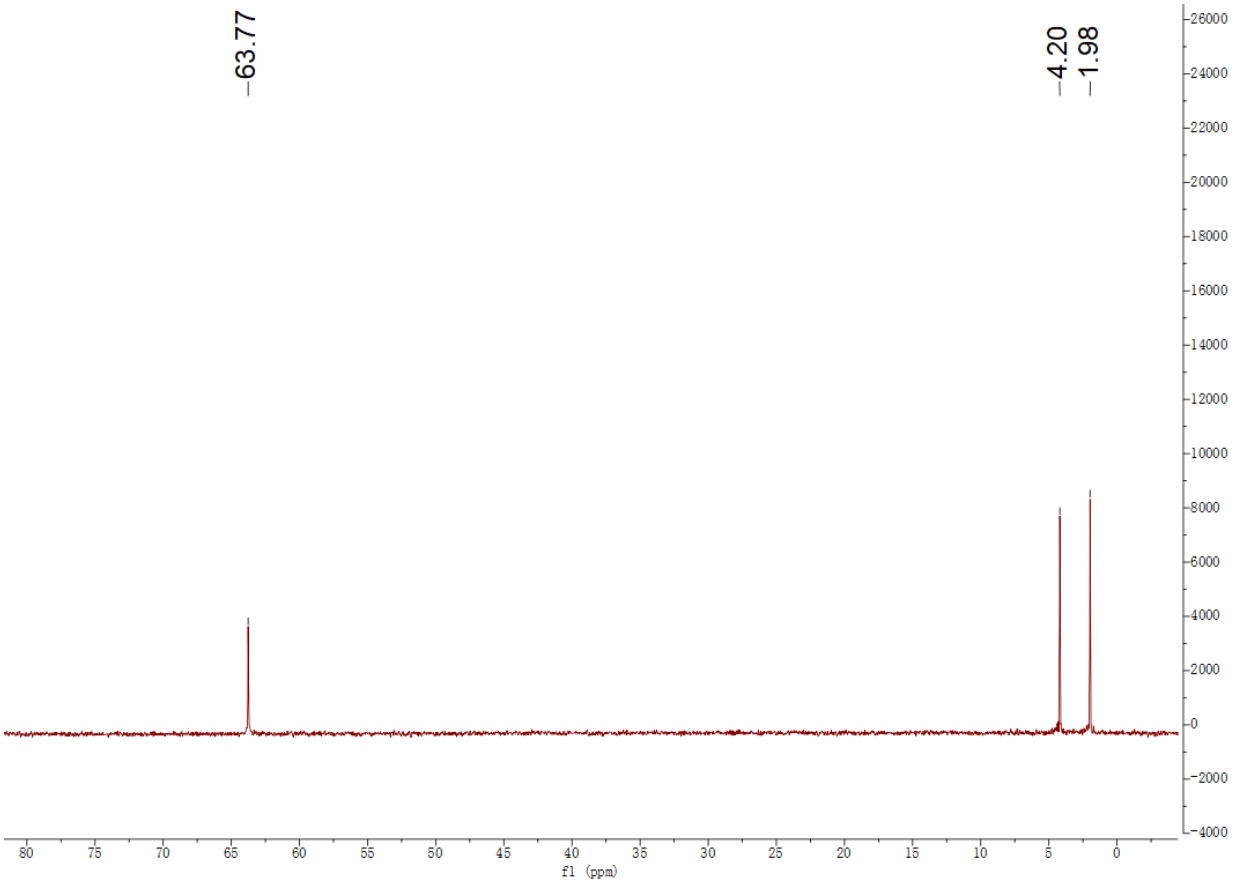


Figure S3. ^{29}Si NMR spectrum of **2a** in C_6D_6

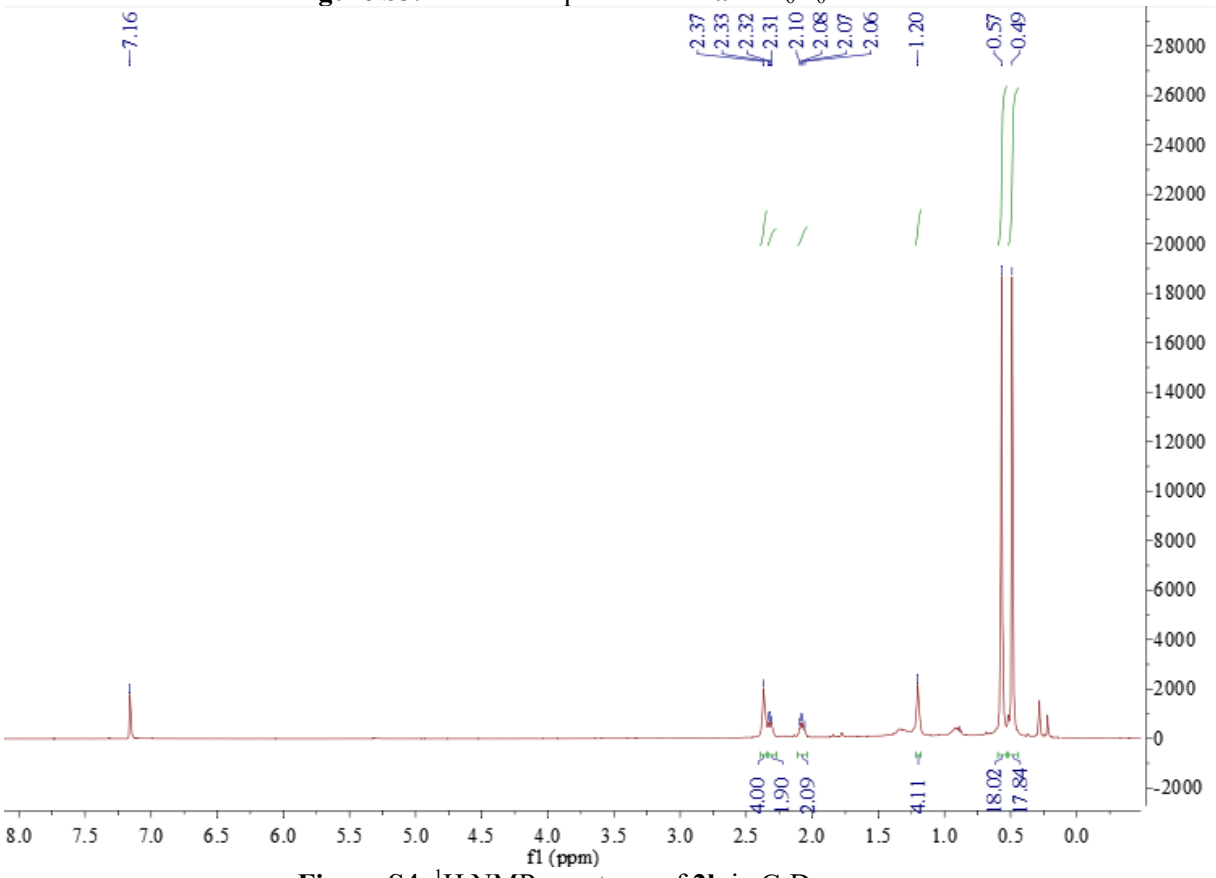


Figure S4. ^{1}H NMR spectrum of **2b** in C_6D_6

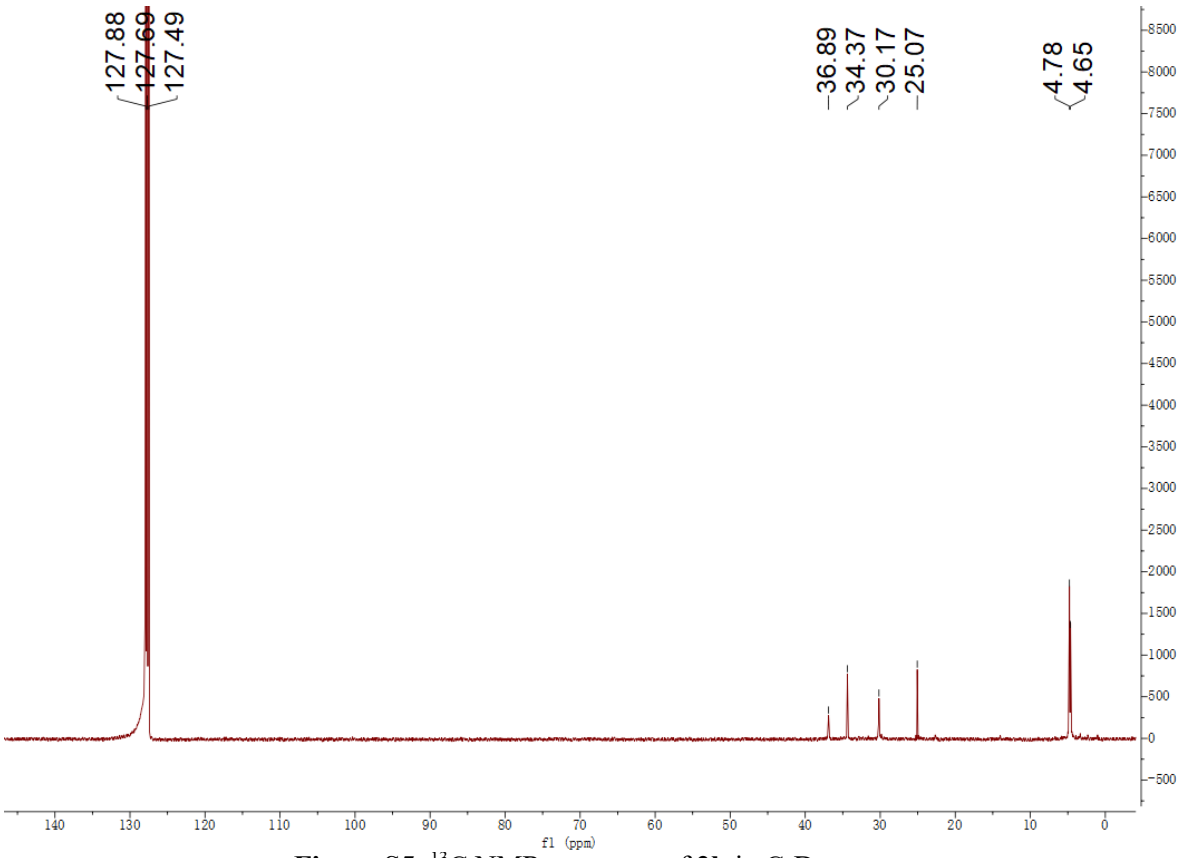


Figure S5. ^{13}C NMR spectrum of **2b** in C_6D_6

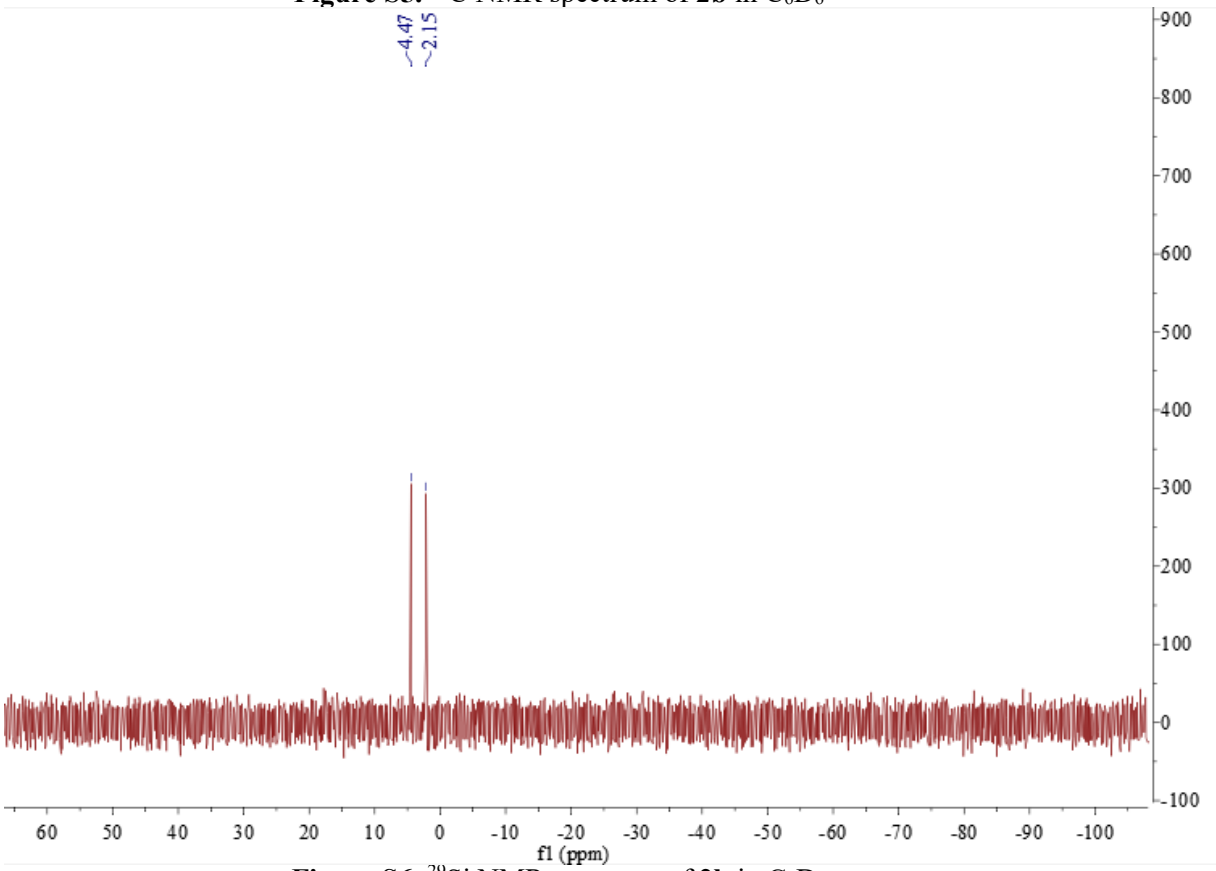


Figure S6. ^{29}Si NMR spectrum of **2b** in C_6D_6

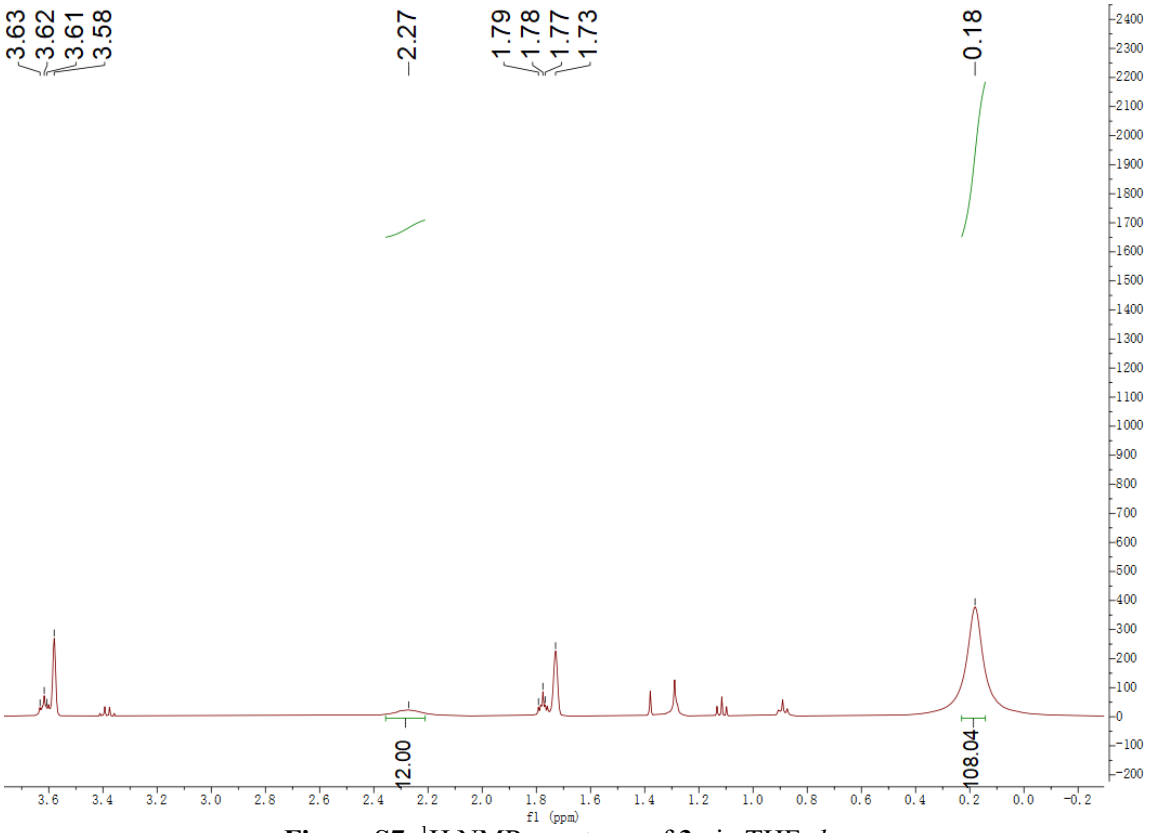


Figure S7. ^{1}H NMR spectrum of **3a** in THF-d_8

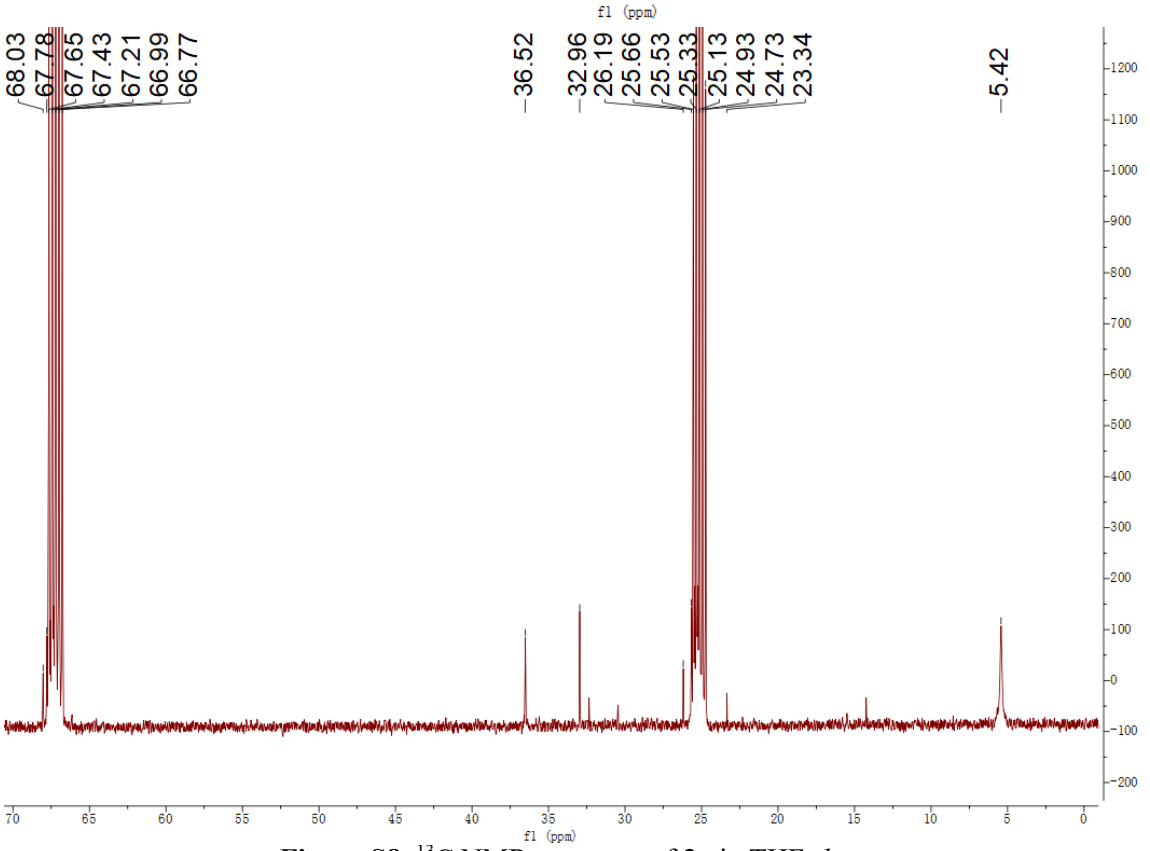


Figure S8. ^{13}C NMR spectrum of **3a** in THF-d_8

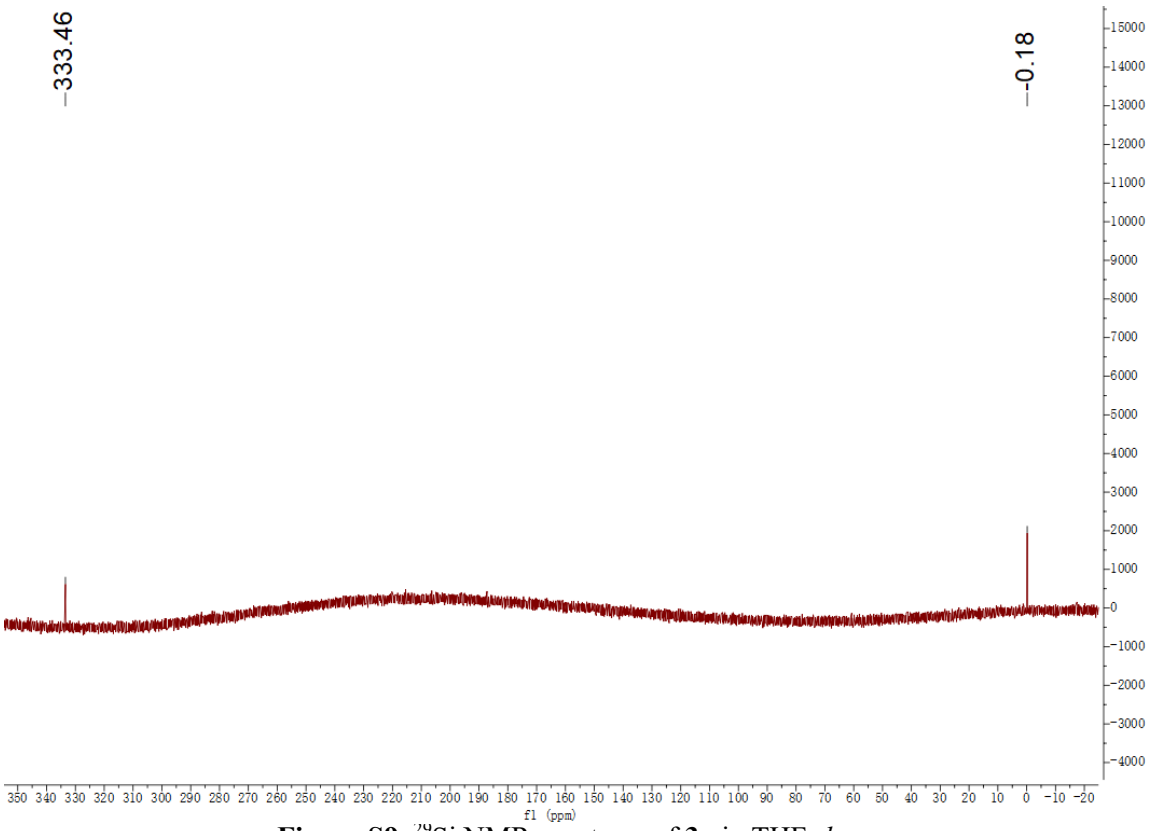


Figure S9. ^{29}Si NMR spectrum of **3a** in THF-d_8

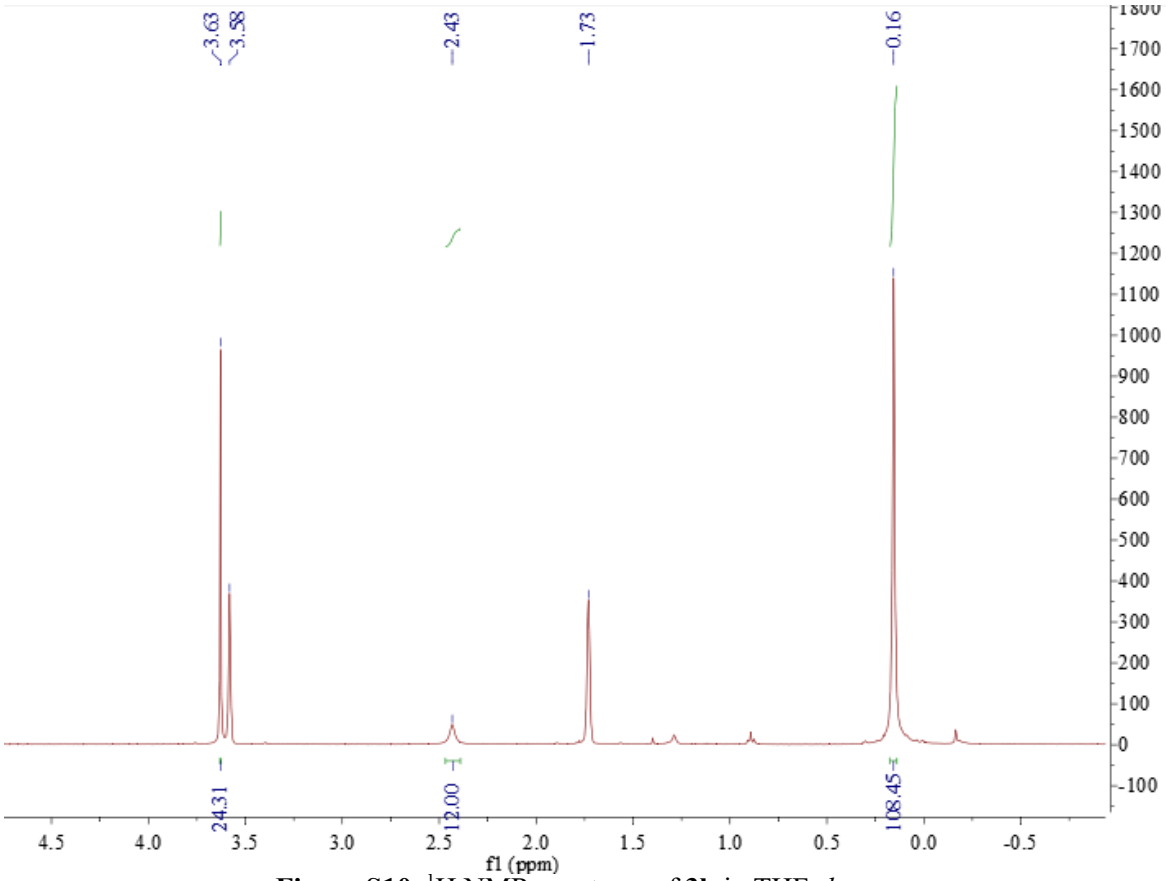


Figure S10. ^{1}H NMR spectrum of **3b** in THF-d_8

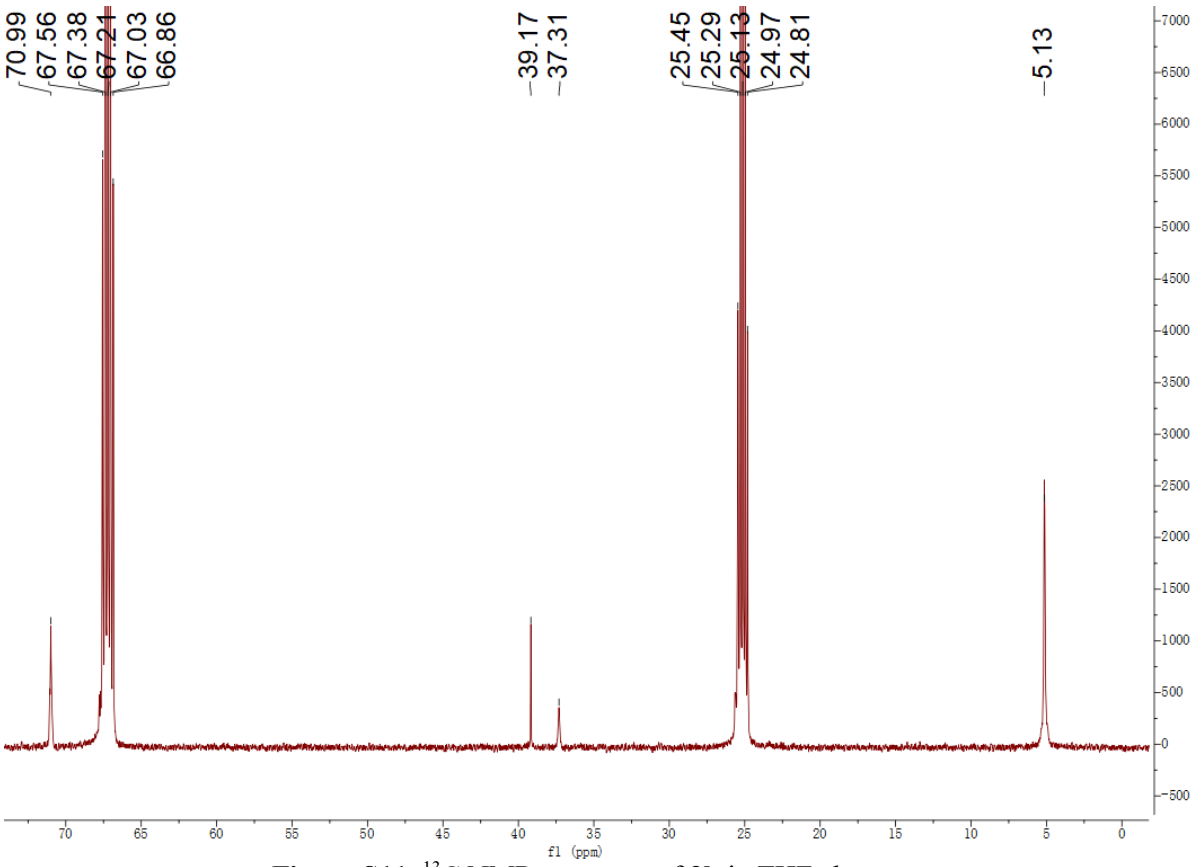


Figure S11. ^{13}C NMR spectrum of **3b** in THF-d_8

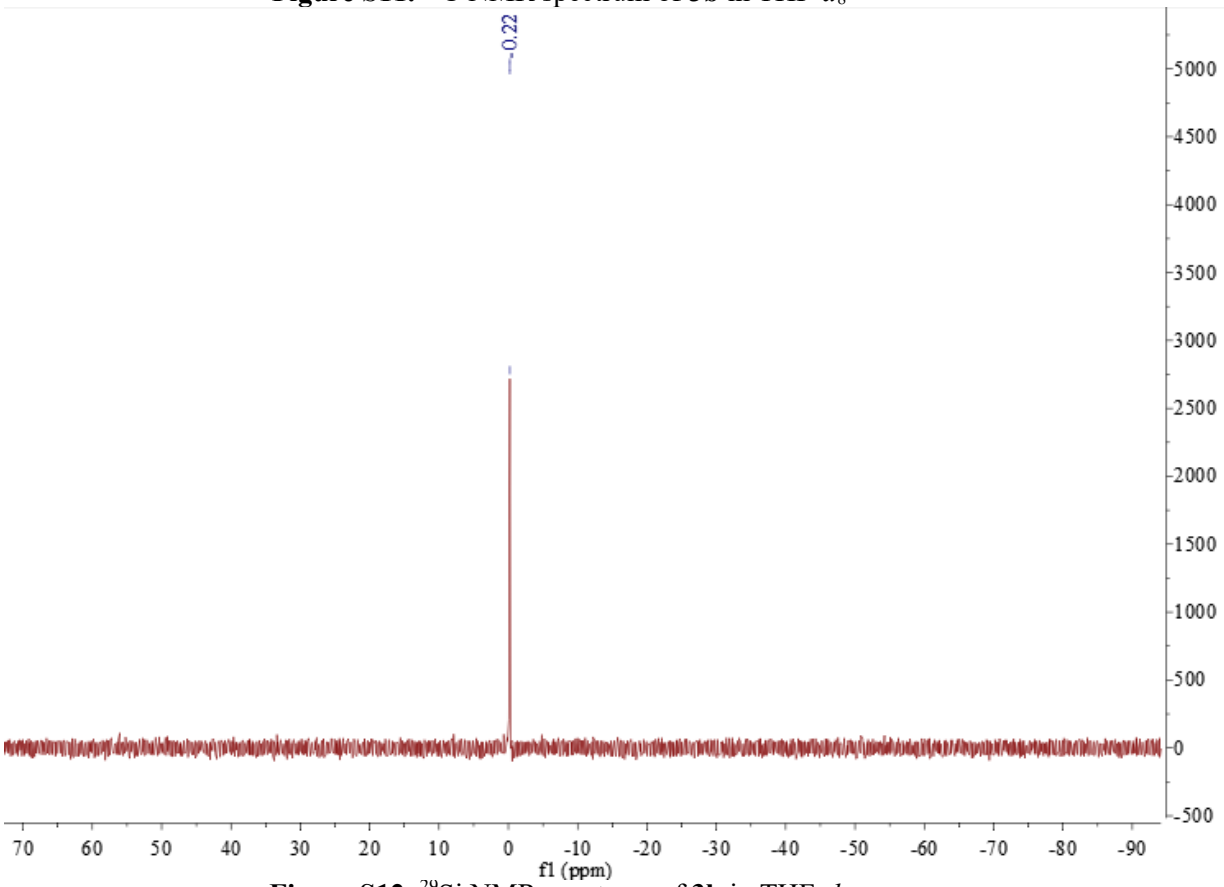


Figure S12. ^{29}Si NMR spectrum of **3b** in THF-d_8

UV-visible spectroscopy

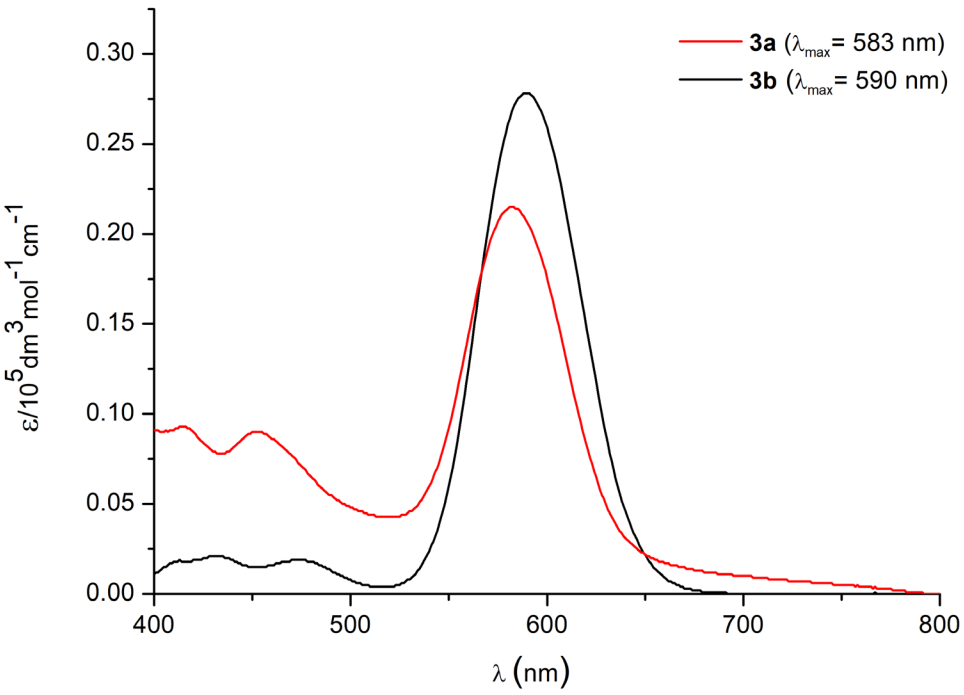


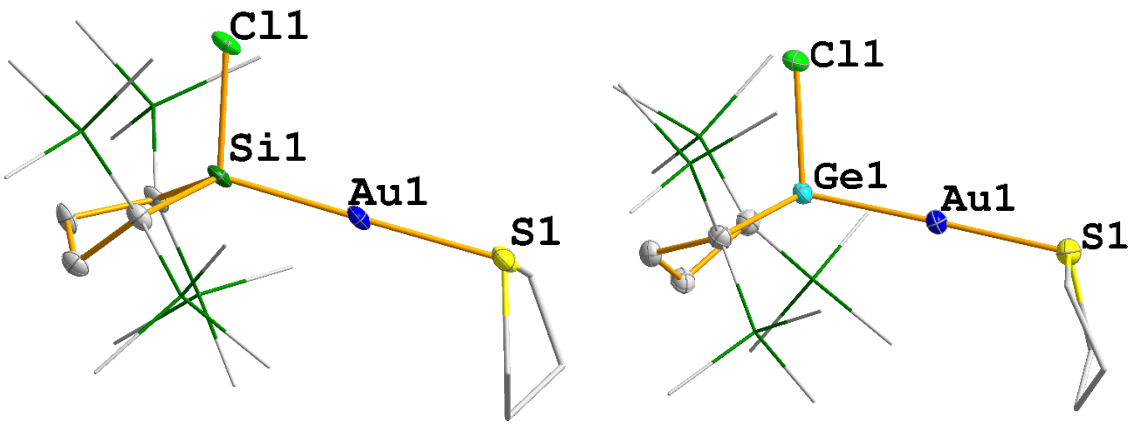
Figure S13. UV-visible spectrum of **3a** in ether (ε = 21500 M^{-1}•cm^{-1}) and **3b** in THF (ε = 27800 M^{-1}•cm^{-1}).

Crystallographic details

X-ray data collection and structural refinement. Intensity data for compounds **2a**, **2b**, **3a** and **3b** were collected using a 'Bruker D8 VENTURE' diffractometer. The crystal was kept at 100.0 K during data collection. The structure was solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL[4, 5] refinement package using Least Squares minimisation. All non-hydrogen atoms were subjected to anisotropic refinement. The hydrogen atoms were located at calculated positions or found in the *F*map. CCDC: 2160631, 2160633, 2160634 and 2160632 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_reCquest/cif.

Table S1. X-ray data for **2a**, **2b**, **3a** and **3b**

Compounds	**2a**	**2b**	**3a**	**3b**
Formula	$C_{20}H_{48}AuClSSi_5$	$C_{20}H_{48}AuClGeSSi_4$	$C_{56}H_{134}Au_3KO_2Si$	$C_{68}H_{160}Au_3Ge_3K$
Fw	693.51	738.01	1890.97	2290.80
Crystsyst	monoclinic	monoclinic	orthorhombic	monoclinic
Space group	$P2_1/c$	$P2_1/c$	Pccn	$P2_1/n$
Size (mm^3) space group	0.41 × 0.35 × 0.34	0.28 × 0.22 × 0.16	0.31 × 0.26 × 0.14	0.16 × 0.08 × 0.06
T/K	100	100	200	200
a, Å	9.9342(3)	9.9388(3)	18.0257(7)	23.1810(5)
b, Å	27.1838(8)	27.3687(10)	19.7111(8)	19.2043(4)
c, Å	11.0297(3)	11.0478(4)	28.0391(10)	23.5947(5)
α, deg	90	90	90	90
β, deg	103.5240(10)	103.247(2)	90.3640(10)	106.2360(10)
γ, deg	90	90	90	90
V, A^3	2895.97(15)	2925.17(18)	9962.5(7)	10084.9(4)
Z	4	4	4	4
d_{calcd} g·cm^{-3}	1.591	1.676	1.261	1.509
μ, mm^{-1}	13.093	13.676	10.454	11.065
Refl collected	28935	29027	124978	97309
N_{measd}	28935	29027	124978	97309
[R int]	0.0729	0.0772	0.0915	0.0714
R [I>2sigma(I)]	0.0727	0.0760	0.0834	0.0386
R_w [I>2sigma(I)]	0.1908	0.1981	0.2461	0.0959
GOF	1.139	1.134	1.058	1.034
Largest diff. peak/ hole [e. $Å^{-3}$]	6.97 and -2.00	8.05 and -2.54	2.80 and -1.88	2.21 and -1.38

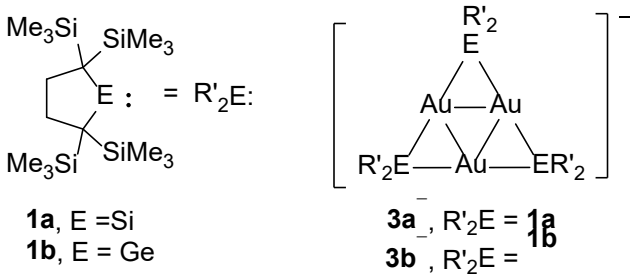


2a **2b**

Figure S14. Solid structures of **2**. Thermal ellipsoids are shown at the 50% probability level. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and bond angles [º]: **2a**: Au1-S1 2.4101(18), Au1-Si1 2.3097(18), Cl1-Si1 2.134(2); Si1-Au1-S1 178.49(6), Cl1-Si1-Au1 103.75(8). **2b**: Au1-Ge1 2.3773(8), Au1-S1 2.3633(19), Ge1-Cl1 2.2441(19); S1-Au1-Ge1 178.27(6), Cl1-Ge1-Au1 103.78(6).

Theoretical calculations

Theoretical calculations were performed for the following anions **3a**$^-$ – **3b**$^-$ with the Gaussian 16 program package.[6] The structures phase were optimized using a dispersion-corrected DFT method at the M062X/Def2SVP.[7] All of the structures obtained herein were verified by examination of their Hessian matrix as minima (all frequencies real). The solvent effects on the relative stability of the compounds were not evaluated. The AIM charges[8, 9] of the atoms were calculated using the grid-based method implemented in Multiwfn 3.8dev.[10]



Wiberg Bond Index of 3a

Au-Au	0.1597
Au-Si	0.5430
Si-Si	0.2622

Wiberg Bond Index of 3b

Au-Au	0.1661
Au-Ge	0.5438
Ge-Ge	0.2514

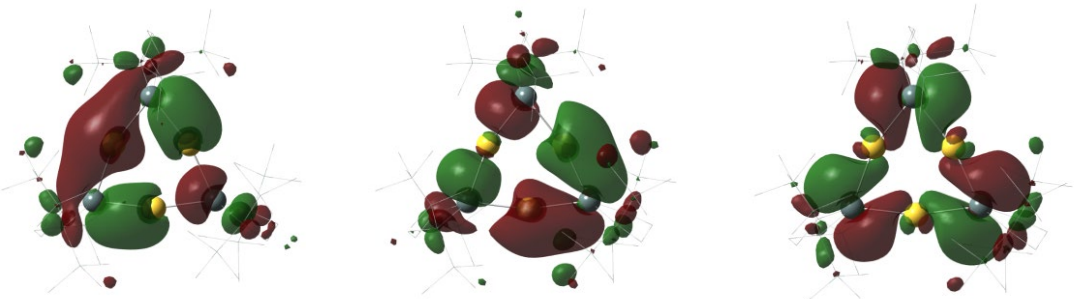


Figure S15. Calculated frontier molecular orbitals of **3b**$^-$ (HOMO: highest occupied molecular orbital, LUMO: lowest unoccupied molecular orbital). The HOMO and HOMO' are degenerate.

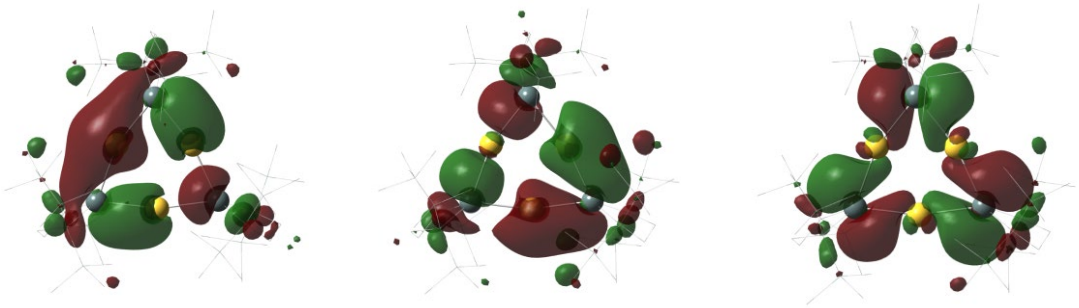


Figure S16. Calculated frontier molecular orbitals of **IV**$^{-}$ (HOMO: highest occupied molecular orbital, LUMO: lowest unoccupied molecular orbital).

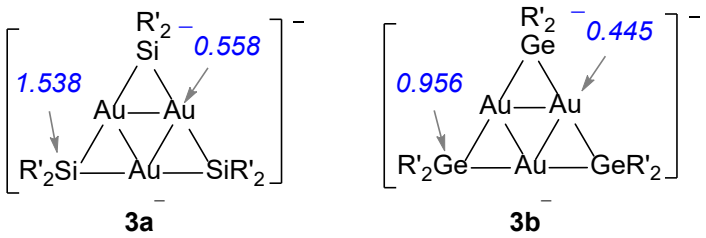


Figure S17. Calculated effective atomic charges of in **3a**$^{-}$ and **3b**$^{-}$. The effective atomic charges of all atoms were calculated using the AIM method.

Charge of 3a

Element	Natural charge	AIM charge
Au	–0.147	–0.558
Si	0.803	1.538

Charge of 3b

Element	Natural charge	AIM charge
Au	–0.153	–0.445
Ge	0.672	0.956

Coordinates of optimized geometries

3a$^-$

Au	-0.12081620	1.71163175	0.00019626
Au	-1.42096044	-0.95974208	-0.00153108
Au	1.54193272	-0.75130319	0.00073821
Si	2.34221712	1.58138982	0.00054125
Si	-2.54130821	1.23724605	-0.00057272
Si	0.19858418	-2.81912967	-0.00032849
C	3.53631271	2.15458449	1.41866761
C	3.32099421	2.47540156	-1.41663330
Si	2.58105118	2.81188049	2.92818900
C	1.29679715	1.60661034	3.58205634
C	3.74864058	3.26995215	4.35930879
C	1.66350574	4.42198417	2.57646290
Si	4.73157452	0.76837236	2.01234696
C	6.33819923	1.55710782	2.65854123
C	5.33142274	-0.49010547	0.74460644
C	4.02508168	-0.31914423	3.37860921
C	0.48415678	-4.11280940	-1.41790809
C	0.09708214	-4.14014493	1.41736732
Si	1.14344471	-3.64218239	2.92748292
C	0.95425007	-4.88186419	4.35898187
C	2.99710246	-3.65467702	2.57792065
C	0.74238040	-1.92698614	3.58047161
Si	3.57519617	1.34407892	-2.92620173
C	1.97791328	0.60239432	-3.58002022
C	4.72689090	-0.10800189	-2.57522165
C	4.43624981	2.25695285	-4.35682019
Si	-1.70136601	-4.48193687	2.01069526
C	-2.29040937	-3.32915646	3.37948343
C	-1.82141446	-6.26830550	2.65468328
C	-3.09096408	-4.37002183	0.74299415
Si	2.48182129	4.10204688	-2.01060928
C	1.53750653	5.12819750	-0.74341709
C	1.21047841	3.85481973	-3.37861742
C	3.81441301	5.29774727	-2.65501577
H	1.42083466	0.11226768	-2.77511670
H	2.22613469	-0.15692991	-4.32975192
H	1.31154890	1.32394737	-4.04946530
C	0.64300714	-5.42460810	0.72154396
C	4.37591615	3.26966710	0.72333886
H	-1.74048026	-3.40881397	4.32014085
H	-3.34277192	-3.56218701	3.57817458
H	-2.24482199	-2.29638902	3.02888915
C	4.66833516	2.83802613	-0.72034021
C	0.12348679	-5.46113747	-0.72237369
H	1.74068789	-5.40941976	0.69560981
H	0.37020685	-6.34216134	1.25848954
H	0.73843006	4.54293644	-0.28298709
H	1.07774992	5.96889034	-1.27815479
H	2.16900900	5.53847344	0.04707487
H	5.33363893	1.96485194	-0.69440261
H	5.22219039	3.61901393	-1.25697125
H	0.63609406	1.26984701	2.77676916
H	0.68282848	2.12169986	4.32902076
H	1.71730819	0.72081889	4.05496632
H	3.81383934	4.21260473	0.69698642
H	5.30664697	3.49226860	1.26077742
H	-0.05373058	-4.91691471	4.78259163
H	1.64482095	-4.59286897	5.16118424

H	1.22378770	-5.89536778	4.03878145
H	6.95657867	1.92172963	1.83004785
H	6.91363207	0.78169190	3.17957388
H	6.17801346	2.38511839	3.35418848
H	3.36472041	-4.63496117	2.25954888
H	3.50987642	-3.39311684	3.51103283
H	3.27308474	-2.91361511	1.82528976
H	4.28294998	2.41519446	4.78427668
H	3.15280290	3.72458912	5.16070052
H	4.49156045	4.00972893	4.03813532
H	5.72495090	0.20640805	-2.25511054
H	4.83834553	-0.67282550	-3.50829763
H	4.31188043	-0.78201724	-1.82337692
H	4.49006257	-1.01182702	0.28304625
H	5.93865723	-1.23158485	1.27897946
H	5.94884008	-0.05709528	-0.04489257
H	3.84329950	3.07265089	-4.78080267
H	4.63490689	1.53511741	-5.15896773
H	5.40030500	2.66898962	-4.03556541
H	0.78329360	-1.18641243	2.77531167
H	1.49400472	-1.65337326	4.32909719
H	-0.23602567	-1.84778371	4.05113498
H	3.81785365	0.19583069	4.31960142
H	4.75157619	-1.11533341	3.57736400
H	3.10791534	-0.79378040	3.02473487
H	2.32769148	5.23075609	2.25684712
H	1.17993700	4.73624557	3.50890382
H	0.88421900	4.28782001	1.82375674
H	1.61151040	3.47134950	-4.31971648
H	0.74435767	4.82682630	-3.57660257
H	0.42639505	3.18170177	-3.02703456
H	4.38380211	5.73388601	-1.82595581
H	3.31058842	6.12199238	-3.17523318
H	4.52246736	4.84013760	-3.35107869
H	-1.81176213	-6.98553885	1.82572154
H	-2.78183137	-6.38051108	3.17321266
H	-1.02550056	-6.54265151	3.35212042
H	-3.12109798	-3.38004965	0.28244992
H	-4.03692704	-4.52496729	1.27706424
H	-3.02515840	-5.12034841	-0.04735510
C	-3.80378275	1.63799969	-1.41844287
C	-3.63574716	1.98499950	1.41677287
Si	-2.94978707	2.42288441	-2.92753331
Si	-4.79331330	0.09820998	-2.01235427
C	-4.79131637	2.62430946	-0.72296789
Si	-3.72807265	0.82868391	2.92613173
Si	-3.03269415	3.71289320	2.01123675
C	-5.02060163	2.15517373	0.72044727
C	-1.50849029	1.41000231	-3.58038310
C	-4.16989842	2.71218388	-4.35903443
C	-2.26728547	4.14579235	-2.57546323
C	-6.49461249	0.65390742	-2.65850133
C	-5.21076599	-1.23181781	-0.74447610
C	-3.94116923	-0.87991875	-3.37822135
H	-4.36675599	3.63664868	-0.69601972
H	-5.74388216	2.71477173	-1.26060575
C	-2.04219825	0.31866028	3.57956277
C	-4.66491632	-0.77056665	2.57514412
C	-4.70724811	1.61084556	4.35820735
C	-2.24358904	4.86263299	0.74388985
C	-1.73711345	3.64448095	3.37700122
C	-4.51930117	4.70889277	2.65826273

H	-5.55658628	1.19713614	0.69382950
H	-5.67884088	2.85033805	1.25730458
H	-0.80707528	1.17037709	-2.77475673
H	-0.97314473	2.00588138	-4.32778679
H	-1.79995090	0.47343560	-4.05250354
H	-4.57834365	1.79067873	-4.78410127
H	-3.64388941	3.24631107	-5.16025872
H	-5.00974934	3.33980515	-4.03800277
H	-3.03795152	4.85356705	-2.25531098
H	-1.83274875	4.52492917	-3.50792826
H	-1.47666173	4.12191631	-1.82295654
H	-7.15768946	0.92882640	-1.82995902
H	-6.95590735	-0.19487458	-3.17874307
H	-6.45231911	1.49565502	-3.35480452
H	-4.30467142	-1.62914634	-0.28169542
H	-5.70631603	-2.05203108	-1.27905746
H	-5.88425590	-0.89001247	0.04402467
H	-3.80722464	-0.34109899	-4.31911283
H	-4.54903980	-1.76988463	-3.57738676
H	-2.96690190	-1.22157954	-3.02362603
H	-1.42138625	-0.08838460	2.77497570
H	-2.18162453	-0.46795547	4.32929117
H	-1.48387938	1.12654003	4.04928868
H	-5.69725106	-0.59922589	2.25509156
H	-4.69593562	-1.34558566	3.50811076
H	-4.15964041	-1.37984885	1.82327458
H	-4.23375970	2.50103565	4.78253332
H	-4.80192376	0.86761300	5.15982429
H	-5.71987958	1.88410917	4.03845367
H	-1.37165717	4.39533583	0.28090803
H	-1.90429666	5.75846015	1.27911379
H	-2.92795667	5.18205006	-0.04460307
H	-2.07892765	3.20754317	4.31815654
H	-1.41066021	4.67167984	3.57572414
H	-0.86744595	3.08776777	3.02292372
H	-5.14507154	5.06150955	1.83011561
H	-4.13570751	5.59528644	3.17885297
H	-5.15534221	4.15578748	3.35445301
Si	-0.62148194	-3.76612260	-2.92817956
Si	2.31292822	-4.19924174	-2.01083673
C	-0.26171273	-4.96823722	-4.35901325
C	-2.45516360	-4.03690829	-2.57786538
C	-0.46371232	-2.01201393	-3.58208005
C	2.73515684	-2.97446067	-3.37874284
C	2.68204655	-5.95118539	-2.65488306
C	3.67357687	-3.89482862	-0.74319429
H	-0.96547802	-5.59987547	-0.69666454
H	0.52219491	-6.33131961	-1.25946578
H	0.74163914	-4.86356452	-4.78206060
H	-0.98523582	-4.77792726	-5.16164913
H	-0.38845878	-6.00916168	-4.03844147
H	-2.68216909	-5.05853323	-2.25818886
H	-2.99964942	-3.85067269	-3.51110974
H	-2.83182104	-3.34085549	-1.82589752
H	-0.60762312	-1.28397855	-2.77730781
H	-1.24610692	-1.84640316	-4.33086909
H	0.49404835	-1.79696130	-4.05277446
H	2.20227503	-3.12950362	-4.31979237
H	3.80988801	-3.05734778	-3.57708789
H	2.54500839	-1.95861633	-3.02726091
H	2.77276783	-6.66245931	-1.82568306
H	3.64893352	-5.92778899	-3.17299568

H	1.93280769	-6.33475180	-3.35250863
H	3.56613374	-2.91041633	-0.28232225
H	4.63163281	-3.91642582	-1.27775749
H	3.71334667	-4.64725217	0.04693772

3b^{-}

Au	0.91803300	1.49443200	-0.00258800
Au	-1.74349600	0.04665700	0.00405400
Au	0.83389500	-1.53879300	-0.00126700
Ge	2.86477700	-0.07854600	-0.00549300
Ge	-1.36569100	2.51878400	0.00519800
Ge	-1.49889300	-2.44216100	0.00022200
C	-2.41451300	-3.49943000	1.45306200
C	-2.03422700	-3.73765700	-1.44938200
C	-2.24125100	3.62832700	-1.43349400
C	-1.80759000	3.84190100	1.46265000
Si	-1.26217600	-3.66341800	2.95712800
C	-0.55272800	-2.02399200	3.55212500
C	0.22014300	-4.78104000	2.62294300
C	-2.13020700	-4.48804700	4.43600300
Si	-4.05415500	-2.68128500	2.00826300
C	-3.81154500	-1.32531000	3.29209200
C	-5.11402100	-1.83291200	0.70018800
C	-5.20054700	-4.01859900	2.72627900
Si	-0.56621500	-4.83406000	-2.00427400
C	0.53447000	-4.01174800	-3.29277100
C	0.67045100	-5.39314600	-0.69602700
C	-1.24550000	-6.46155400	-2.71705200
Si	-2.70057500	-2.78291600	-2.95329200
C	-4.36473500	-1.96183300	-2.61620700
C	-3.04666300	-3.93034000	-4.43102300
C	-1.55817600	-1.41045600	-3.54911700
Si	-1.10331300	3.72804400	-2.95441700
C	-0.48894000	2.05221100	-3.55324600
C	-1.94542600	4.59552700	-4.42352100
C	0.43948100	4.76632900	-2.63946400
Si	-3.93051800	2.90122700	-1.96640600
C	-5.01739900	2.10882500	-0.64574800
C	-5.01126400	4.29995000	-2.66906900
C	-3.77867200	1.53518100	-3.25411100
C	-2.70220800	-4.84940900	0.73630800
C	-3.10909800	-4.60065700	-0.72900300
C	-2.44315300	4.99118400	-0.71235600
C	-2.84315300	4.76399400	0.75821700
C	2.05501500	0.50168500	3.54855000
Si	3.82823300	0.70885700	2.95070900
C	4.25221600	-0.35494100	1.43229800
C	4.05801500	2.55357700	2.63350600
C	4.98096200	0.35026800	4.42153000
Si	4.36606000	-2.19008200	1.96723000
C	5.55866700	0.07725700	0.70825400
C	4.24259700	0.12188300	-1.46482100
C	3.07249300	-2.67044000	3.24845000
C	4.15734400	-3.51753900	0.64505700
C	6.10056800	-2.52016300	2.67452900
C	5.53374300	-0.38460400	-0.76164800
Si	3.73492200	-0.91494700	-2.97593300
Si	4.45247600	1.94721400	-2.00190300
C	1.96877500	-0.60741000	-3.54987400
C	3.86420000	-2.77055300	-2.66355700
C	4.88268800	-0.62111700	-4.46476300
C	3.17199500	2.50482000	-3.26561500
C	4.33990600	3.28489500	-0.67807200

C	6.19244600	2.17757800	-2.73562400
Si	-2.50430000	2.92552800	2.97636400
Si	-0.27244000	4.85408100	1.99704500
C	-1.43115200	1.49147500	3.55598900
C	-2.76532600	4.08617200	4.46141400
C	-4.21682700	2.19925600	2.66334800
C	0.97064400	5.35490700	0.67140200
C	-0.85077300	6.51200000	2.72855100
C	0.80147900	3.96299900	3.26134100
H	1.34083600	0.59778500	2.72426500
H	-1.26009400	-0.75255800	-2.72628800
H	0.87724500	-4.36141900	1.85875900
H	0.91390200	-3.06708100	-2.89490800
H	2.07672800	-2.45596600	2.85165100
H	3.15992000	-3.09950800	-1.89705500
H	-0.12249500	-1.44895200	2.72578400
H	0.25319800	-2.23880200	4.26282500
H	-1.27559700	-1.38405200	4.05692600
H	-0.06350200	-5.79575700	2.32707900
H	0.79411100	-4.85270100	3.55442400
H	-2.95311400	-3.89437600	4.84564100
H	-1.39308800	-4.63435100	5.23558000
H	-2.52456700	-5.47401000	4.16298300
H	-3.43233400	-1.66709500	4.25823800
H	-4.78113800	-0.84211400	3.45739200
H	-3.13256000	-0.56742600	2.89318800
H	-4.57620900	-0.99806700	0.24387200
H	-5.99877100	-1.42844000	1.20812900
H	-5.45772900	-2.50145700	-0.09139200
H	-5.63053700	-4.63027000	1.92436400
H	-6.03275200	-3.52608200	3.24445500
H	-4.70632100	-4.68772700	3.43536400
H	0.05563300	-3.82241000	-4.25660900
H	1.39798800	-4.66458900	-3.46360000
H	1.17981600	-4.53500300	-0.25015500
H	1.42445900	-6.01028000	-1.20113600
H	0.22839600	-5.99073700	0.10332700
H	-1.60090500	-7.11702200	-1.91325300
H	-0.43024500	-6.98608400	-3.23080300
H	-2.06343100	-6.32324000	-3.42903800
H	-5.14262200	-2.67091000	-2.31683300
H	-4.68981700	-1.48220900	-3.54702400
H	-4.28248600	-1.18587700	-1.85271200
H	-2.14646400	-4.40314600	-4.83519100
H	-3.50339800	-3.33830500	-5.23401000
H	-3.75389400	-4.72269800	-4.15847600
H	-2.10536300	-0.80315600	-4.27895500
H	-0.64811600	-1.76533100	-4.03072600
H	-0.08366200	1.45519800	-2.72994700
H	0.32172900	2.22329100	-4.27051800
H	-1.24926400	1.45175300	-4.05146000
H	-2.81047400	4.05160300	-4.81464700
H	-1.21519000	4.69314100	-5.23665200
H	-2.27408000	5.60495400	-4.14897000
H	0.21199700	5.79486000	-2.34272900
H	1.00902000	4.80612600	-3.57547900
H	1.07927100	4.31379900	-1.87948700
H	-4.51965100	1.24405900	-0.19960100
H	-5.92984500	1.75490100	-1.14234200
H	-5.31287700	2.79221200	0.15249500
H	-5.39302100	4.93614200	-1.86186700
H	-5.87823500	3.85421300	-3.17241600

H	-4.49159000	4.93894200	-3.38791200
H	-3.39022600	1.85583300	-4.22374000
H	-4.77545300	1.10752400	-3.41060300
H	-3.13957300	0.73941500	-2.86301700
H	-1.80359700	-5.48017400	0.74063400
H	-3.47944300	-5.43226200	1.24927500
H	-4.07663600	-4.08177900	-0.73338500
H	-3.28050400	-5.55790400	-1.24030500
H	-1.51046200	5.57003400	-0.72900900
H	-3.19324900	5.61725100	-1.21486200
H	-3.83817100	4.30006500	0.77569200
H	-2.95371000	5.72891800	1.27186600
H	1.84150700	1.29953600	4.26870600
H	1.85997900	-0.44957000	4.04235000
H	5.07745400	2.81562500	2.33401500
H	3.83851200	3.07941100	3.57023500
H	3.36285100	2.91967000	1.87563900
H	4.88419900	-0.66637000	4.81448500
H	4.73896000	1.04743400	5.23356200
H	6.03052300	0.51054800	4.14755700
H	5.65641400	1.17072100	0.72302700
H	6.45631800	-0.31026800	1.20952200
H	3.18037200	-2.17908300	4.21852600
H	3.13682300	-3.75308300	3.40489400
H	3.16141500	-3.46720700	0.19755300
H	4.25692200	-4.49176300	1.14051700
H	4.90150600	-3.46865700	-0.15211100
H	6.84080900	-2.57822900	1.86777500
H	6.09383700	-3.49218100	3.18319000
H	6.43658300	-1.76416000	3.38897100
H	5.56783500	-1.48184700	-0.77745200
H	6.44402900	-0.04909000	-1.27744200
H	1.25691800	-0.68678700	-2.72170600
H	1.71092000	-1.37751400	-4.28571400
H	1.81741700	0.36272700	-4.02125200
H	4.87150800	-3.08943100	-2.37847400
H	3.60382800	-3.28096700	-3.59835100
H	4.83678200	0.39996300	-4.85537300
H	4.58764900	-1.30244300	-5.27267900
H	5.92597800	-0.84087700	-4.20882900
H	3.23609700	2.00984100	-4.23771200
H	3.30078600	3.58180600	-3.42205600
H	2.16989200	2.35221200	-2.85628000
H	3.34903500	3.29446100	-0.21679100
H	4.49052500	4.25092200	-1.17666500
H	5.09077200	3.19260900	0.10892400
H	6.94689900	2.19622400	-1.94029700
H	6.23235300	3.14712100	-3.24754600
H	6.47456800	1.40214800	-3.45267000
H	-1.17143800	0.82461700	2.72734700
H	-2.00487800	0.90853600	4.28525700
H	-0.50203500	1.79655000	4.03558900
H	-1.83546400	4.50885700	4.85389900
H	-3.24108600	3.51616600	5.26932500
H	-3.43344900	4.91595500	4.20184500
H	-4.95778500	2.95117000	2.37482400
H	-4.55521600	1.73850100	3.59893900
H	-4.18956800	1.42001900	1.89924300
H	1.42181100	4.47410900	0.20745500
H	1.76791500	5.92200000	1.16859900
H	0.54921100	5.98588900	-0.11340500
H	-1.17802500	7.19170000	1.93293700

H	-0.00289500	6.98733400	3.23723800
H	-1.66793200	6.41375800	3.44789000
H	0.33038000	3.80072000	4.23387200
H	1.70661300	4.56103900	3.41631600
H	1.11372100	2.99787700	2.85398100

IV^{-}

Au	-1.93566300	0.37999300	-0.06337800
Au	0.60528200	-1.77262700	-0.11533200
Au	1.22552300	1.39601600	0.05480700
Sn	-1.00202800	2.89492500	0.09982200
Sn	-2.02728000	-2.30370500	-0.13626600
Sn	3.04278400	-0.60213300	-0.00785500
C	-1.24454700	4.57180100	-1.34495400
C	-1.76950300	4.25270900	1.68963900
C	4.64832600	-0.76123900	-1.54722700
C	4.58653500	-1.05865300	1.53750500
Si	0.43361600	5.34262900	-1.80245900
C	1.71984700	5.49170200	-0.42462200
C	1.35840600	4.36890400	-3.13590100
C	0.16542500	7.12321000	-2.40547900
Si	-2.09123600	3.90374900	-2.90532000
C	-2.08000700	5.15768500	-4.33326100
C	-3.91819200	3.50761200	-2.62771300
C	-1.32446600	2.28456800	-3.51554000
Si	-3.55668300	3.80011800	2.16902900
C	-4.40304400	5.32063700	2.93035800
C	-4.71890300	3.26072100	0.77852600
C	-3.65586100	2.35912000	3.39246400
Si	-0.65105600	4.11466000	3.21533600
C	-1.38619200	4.97404000	4.74308200
C	-0.25308000	2.32037700	3.65983600
C	1.02643200	4.94720500	2.96299100
Si	5.00414700	0.46767000	2.58910300
C	3.50211100	1.52000800	3.04246300
C	6.24229500	1.61176700	1.73072000
C	5.85768900	0.01555900	4.22496600
Si	3.94046100	-2.47704300	2.62084400
C	5.29951700	-3.22761200	3.71635300
C	3.35633000	-3.98176800	1.62811900
C	2.51172200	-1.89270900	3.71026700
C	-2.11302900	5.56563700	-0.51951700
C	-1.71110100	5.63348200	0.97390000
C	5.79024900	-1.53986100	0.67481300
C	5.94428400	-0.81716400	-0.68534100
H	-2.07063800	6.58536100	-0.94321100
H	-3.17603200	5.27106200	-0.56924300
H	-2.35504000	6.37604000	1.47894500
H	-0.68808900	6.04519100	1.02985500
H	1.38782200	6.09908600	0.42781200
H	2.61218100	5.97610200	-0.85427500
H	2.02470300	4.50109400	-0.05232500
H	2.31241000	4.88473900	-3.33041400
H	0.82430900	4.26865600	-4.09062400
H	1.59750500	3.35966200	-2.76103000
H	-0.11313200	7.77784300	-1.56493100
H	-0.61657500	7.20332600	-3.17326900
H	1.10534100	7.51142000	-2.82863800
H	-1.06781600	5.42391800	-4.67045200
H	-2.59294300	6.08604200	-4.03513400
H	-2.62368500	4.73569500	-5.19326100

H	-4.33393900	3.14337900	-3.58102200
H	-4.50973800	4.38188400	-2.31645600
H	-4.05098800	2.71102200	-1.88099400
H	-1.82561000	1.97922800	-4.44847800
H	-1.48792300	1.48241900	-2.77575100
H	-0.24610400	2.34137600	-3.71200200
H	-4.61461000	6.07235500	2.15388300
H	-3.80248300	5.80094200	3.71507300
H	-5.36736200	5.01976800	3.36949200
H	-4.38581400	2.31772300	0.31802900
H	-4.84235600	4.01200500	-0.01288700
H	-5.70950000	3.08200800	1.22817300
H	-3.14818700	2.53467500	4.35083600
H	-3.23786200	1.44489700	2.93903100
H	-4.72041400	2.16538700	3.59924700
H	-0.67368500	4.89639900	5.57956500
H	-2.34146000	4.53964800	5.07110500
H	-1.55140700	6.04463500	4.54227500
H	0.36627400	1.86490400	2.86882300
H	-1.13599400	1.68423400	3.80126200
H	0.33709600	2.29995400	4.59035700
H	1.60356200	4.83628400	3.89509900
H	0.94831700	6.02264600	2.74234400
H	1.59923400	4.46513000	2.15785600
H	6.74400300	-1.43585600	1.22726300
H	5.69152800	-2.62025900	0.46932000
H	2.64374200	0.91416400	3.36740400
H	3.16715300	2.12857600	2.18799000
H	3.76798200	2.20344300	3.86509200
H	6.49820200	2.42958900	2.42282600
H	5.82217400	2.06221500	0.82193400
H	7.17423400	1.08948700	1.46483000
H	5.17595600	-0.47625300	4.93425600
H	6.21514800	0.94566400	4.69485700
H	6.72607100	-0.64274300	4.07022900
H	5.56208400	-2.61512700	4.58743900
H	6.21563200	-3.39822200	3.12841100
H	4.95431100	-4.20839900	4.08031900
H	2.83109700	-4.65626200	2.32407200
H	4.21483700	-4.53823200	1.22161100
H	2.66014600	-3.74646500	0.80924200
H	1.70081100	-1.45856400	3.10006700
H	2.83044500	-1.13461500	4.44151900
H	2.09172300	-2.74478800	4.26702000
C	-2.86853200	-3.66048900	1.41709000
C	-3.30934000	-3.34683500	-1.63088400
Si	4.42229700	-2.30955500	-2.62201200
Si	4.63009200	0.81605100	-2.60226600
H	6.77090500	-1.30331500	-1.23870900
H	6.29903000	0.20799900	-0.47987100
Si	-1.62407600	-5.00791500	1.92111100
Si	-3.33929900	-2.61986700	2.93194100
C	-4.08261500	-4.27569100	0.66216100
C	-0.52904500	-5.72691700	0.55725800
C	-0.36193000	-4.41583200	3.20051300
C	-2.56379800	-6.50133800	2.62357500
C	-3.80667900	-3.69328200	4.42908100
C	-4.85725900	-1.53636100	2.62521200
C	-1.97232500	-1.41964600	3.45426700
H	-4.43697600	-5.19939500	1.15419600
H	-4.93921400	-3.57980200	0.69216800
C	-3.78020000	-4.59095300	-0.82279700

H	-1.09077500	-6.20098600	-0.25847600
H	0.11009100	-6.49880600	1.01681700
H	0.13288800	-4.95859400	0.12779200
H	0.31581500	-5.25645700	3.41991000
H	-0.79242300	-4.06899500	4.14987100
H	0.24711600	-3.60120500	2.77430500
H	-3.09562900	-7.03643200	1.82142300
H	-3.29844100	-6.22235500	3.39185500
H	-1.84678400	-7.20688800	3.07224600
H	-2.98013700	-4.32500700	4.78531100
H	-4.65428800	-4.35203100	4.18112200
H	-4.11952000	-3.04323100	5.26143300
H	-5.06788800	-0.97911600	3.55231500
H	-5.75769800	-2.11546200	2.36999600
H	-4.67704200	-0.79981600	1.82810000
H	-2.31094000	-0.85948500	4.34138800
H	-1.77879900	-0.68370300	2.65494400
H	-1.01728100	-1.90090000	3.70127500
H	-4.67751400	-5.04914000	-1.27680100
H	-3.00407600	-5.37604100	-0.84953100
Si	-4.78971400	-2.25923300	-2.13660800
Si	-2.26831300	-3.75391200	-3.16213900
C	-6.18082900	-3.36779000	-2.80306500
C	-5.61760000	-1.23228100	-0.78200400
C	-4.34817600	-0.96699400	-3.44713700
C	-3.31963300	-4.33826200	-4.63374800
C	-1.20149600	-2.29288400	-3.71273200
C	-1.05055400	-5.16718700	-2.86018100
H	-6.64814900	-3.93438100	-1.98251000
H	-5.83672800	-4.08576400	-3.56010000
H	-6.96300900	-2.73789400	-3.25555100
H	-4.93460600	-0.46821600	-0.38001900
H	-6.00386900	-1.83022800	0.05417800
H	-6.47211400	-0.70931600	-1.24217700
H	-3.95971500	-1.38159400	-4.38736500
H	-3.60585400	-0.25708300	-3.04625900
H	-5.26033800	-0.39381700	-3.67695700
H	-2.65459800	-4.59798900	-5.47259900
H	-4.03346000	-3.58163100	-4.98980200
H	-3.88926600	-5.24239100	-4.36568600
H	-1.75730200	-1.35653100	-3.85053100
H	-0.70429500	-2.54034100	-4.66454100
H	-0.40974900	-2.10771400	-2.96784400
H	-0.50219100	-5.34727500	-3.79887300
H	-1.54122200	-6.10938500	-2.57232500
H	-0.31234700	-4.90699100	-2.08814300
C	2.63372100	-2.63201200	-3.13946900
C	5.02792200	-3.87436300	-1.74902900
C	5.44631800	-2.23325300	-4.21991300
H	2.10425200	-1.71720000	-3.44258900
H	2.05974500	-3.08438800	-2.31573700
H	2.61845700	-3.33222600	-3.99031900
H	4.91864500	-4.72558300	-2.43960900
H	4.43406700	-4.09405700	-0.85138500
H	6.08816400	-3.80637800	-1.46038800
H	5.04237500	-1.50589900	-4.93956500
H	5.42143000	-3.22560700	-4.69762900
H	6.49844700	-1.97533600	-4.02504900
C	6.19332600	0.98569000	-3.66816200
C	4.66523700	2.41222500	-1.57954600
C	3.10996900	0.87365100	-3.72260000
H	6.21519200	0.31748100	-4.53774000

H	7.09362700	0.79133700	-3.06346900
H	6.25871100	2.02327000	-4.03276200
H	4.40172200	3.24538500	-2.25157500
H	5.67877900	2.61002900	-1.19866300
H	3.95424400	2.43232400	-0.73995000
H	2.18068600	0.78041700	-3.13472600
H	3.11797000	0.07363300	-4.47821700
H	3.07558500	1.83886100	-4.25154900

References

1. R. Uson, A. Laguna, M. Laguna, D. A. Briggs, H. H. Murray and J. P. Fackler Jr., in *Inorg. Synth.*, 1989, **17**, 85-91.
2. M. Kira, S. Ishida, T. Iwamoto and C. Kabuto, *J. Am. Chem. Soc.*, 1999, **121**, 9722-9723.
3. M. Kira, S. Ishida, T. Iwamoto, M. Ichinohe, C. Kabuto, L. Ignatovich, and H. Sakurai, *Chem. Lett.*, 1999, **28**, 263-264.
4. G. Sheldrick, *Acta Crystallogr. A.*, 2015, **71**, 3-8.
5. G. Sheldrick, *Acta Crystallogr. A.*, 2008, **64**, 112-122.
6. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, *Journal*, 2016.
7. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
8. R. F. W. Bader, *Chem. Rev.*, 1991, **91**, 893-928.
9. R. F. W. Bader, *Atoms in molecules : a quantum theory*, Clarendon, Oxford, 2003.
10. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, **33**, 580-592.