Electronic Supplementary Material (ESI) for Chemical Communications.

Symmetric and non-symmetric bis-metallylene iron complexes, precursors of iron germanide nanoparticles

Alexandre Sodreau,[a,b] Nicolas Lentz,[a] Maria Frutos,[a] Sonia Mallet-Ladeira,[c] Céline Nayral,[b] Fabien Delpech,*[b] David Madec*[a]

[a]*Laboratoire Hétérochimie Fondamentale et Appliquée (UMR 5069), Université de Toulouse, CNRS, 118 Route de Narbonne, F-31062 Toulouse, France.*

[b]*LPCNO, Université de Toulouse, CNRS, INSA, UPS, 135 avenue de rangueil, 31077 Toulouse Cedex 09, France.*

[c]*Université de Toulouse, UPS, Institut de Chimie de Toulouse, ICT-FR2599, 118 Route de Narbonne, F-31062 Toulouse, France.*

General procedure:

Iron complexes:

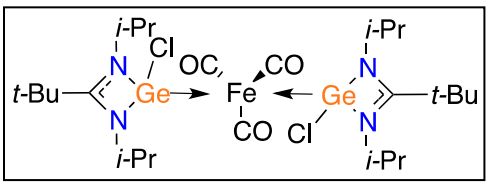
All manipulations with air-sensitive materials were performed in a dry and oxygen-free atmosphere of argon by using standard Schlenk-line and glovebox techniques. Solvents were purified with the MBraun SBS-800 purification system. All reagents were obtained from commercial suppliers unless otherwise statement. NMR spectra were recorded with the following spectrometers: ^{1}H, Bruker Avance II 300 (300.18 MHz); ^{13}C, Bruker Avance II 300 (75.48 MHz) at 298 K, ^{29}Si, Bruker Avance II 300 (59.63 MHz) at 298 K, ^{13}C, Bruker Avance II 300 (111.92 MHz) at 298 K. Mass spectra were measured on a Maldi micro MX microMass in an anthracene matrix (ratio product/matrix: 1/100), on a electrospray ionization HR Xevo G2 QToF Waters, and on a desorption chemical ionization GCT Premier Waters with methane as vector gas. For these two last analyses, products have been dissolved in THF in a ratio 1/10000. Melting points were measured with a capillary electrothermal apparatus. IR spectra were measured in dichloromethane solution under argon atmosphere on a Varian 640-IR FT-IR spectrometer. Single-crystal X-ray data were collected at low temperature (193(2)K) on a Bruker-AXS APEX II Quazar diffractometer equipped with a 30W air-cooled microfocus source or on a Bruker-AXS PHOTON100 D8 VENTURE diffractometer, using MoKα radiation (λ= 0.71037 Å). The structure were solved by the direct method (SHELXS-97)[1] or by intrinsic phasing method (SHELXT)[2] and refined by full-matrix least-squares method on F2.[3] All non-H atoms were refined with anisotropic displacement parameters.

Nanoparticles:

[1] G. M. Sheldrick *Acta Cryst.* **2008**, A64, 112.
[2] G. M. Sheldrick *Acta Cryst*. **2015**, A71, 3–8.
[3] G. M. Sheldrick *Acta Cryst.* **2015**, C71, 3–8.

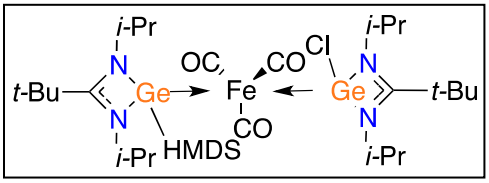
All manipulations with air-sensitive product have been done in dry and oxygen-free atmosphere by using Fisher-Porter reactor, standard Schlenk-line and glovebox techniques. 1-Octadecene (90%) were purchased from Sigma-aldrich, degassed by argon bubbling and dried on molecular sieves. Transmission electron microscopy (TEM) samples were prepared in glovebox by evaporation, under high vacuum, of a drop of iron germanium nanoparticles in 1-octadecene on a TEM carbon-covered copper grid. Images were recorded on a Jeol JEM-1011 apparatus (100 kV, resolution of 4.5 Å) and high resolution TEM pictures were recorded on a Jeol JEM-2100F-EDS apparatus (200kV, resolution of 2.3 Å). The size distribution was determined by measuring over 300 particules. Powder XRD measurements were performed on a PANalytical Empyrean diffractometer using Co-Kα radiation (λ=0.1789 nm) at 45 kV and 35mA.

Synthesis of 2a



[{iPrNC(tBu)NiPr}GeCl]$_2$Fe(CO)$_3$. To a solution of **1a** (635 mg, 1.38 mmol) in 9 mL of THF was added a solution of chlorogermylene (565 mg, 1.94 mmol) in 9 mL of THF. The resulting solution was irradiated under UV-a light (λ = 365nm) for 18 hours. Then solvent was removed under reduced pressure and the solid obtained was washed by 30 mL of cool pentane. The yellow solid was collected and dried under reduced pressure to give 450 mg (45%) of **2a**. Yellow crystals were obtained by diffusion of pentane to a concentrated solution of **2a** in THF at -30°C. Melting point: 203-208°C. ^{1}H NMR (THF-d8, 300 MHz): δ 1.38 (d, $^3J_{H-H}$ = 6.3Hz, 12H, 2*CH*Me$_2$*); 1.39 (d, $^3J_{H-H}$ = 6.3Hz, 12H, 2*CH*Me$_2$*); 1.475 (s, 18H, 2*C*Me$_3$*); 4.42 (sept, $^3J_{H-H}$ = 6.3Hz, 4H, C*H*Me$_2$). ^{13}C{^{1}H} NMR (THF-d8, 75.48 MHz): δ 24.8 (CH*Me$_2$*); 25.2 (CH*Me$_2$*); 29.2 (C*Me$_3$*); 39.9 (*C*Me$_3$); 49.8 (*C*HMe$_2$); 177.0 (N-*C*-N); 215.1 (*C*O). HRMS (ESI) ($C_{25}H_{46}FeGe_2N_4O_3$): [M]$^+$: Calculated: 724.0841 g/mol. Found: 724.0828 g/mol. IR (in CH_2Cl_2, cm^{-1}): υ = 1883

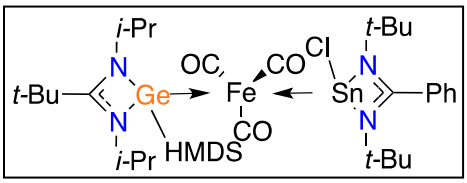
Synthesis of 2b



[{iPrNC(tBu)NiPr}Ge{N(TMS)$_2$}] [{iPrNC(tBu)NiPr}GeCl] Fe(CO)$_3$ 2b. To a solution of **1b** (500 mg, 0.86 mmol) in THF (9 mL) was added a solution of chlorogermylene (349 mg, 1.19 mmol) in THF (9 mL). The resulting solution was irradiated under UV-a light (λ = 365nm) for 18 hours. Then solvent was removed under reduced pressure and the solid obtained was washed by 30 mL of pentane. The white solid was collected and dried under reduced pressure to give 422 mg (57%) of **2b**. Colorless crystals were obtained by diffusion of pentane to a concentrated solution of **2b** in THF at -30°C. Melting point: 163-165°C. ^{1}H NMR (THF-d8, 300 MHz): δ 0.39 (s, 18H, N*(TMS)$_2$*); 1.39 (d, $^3J_{H-H}$ = 6.3Hz, 6H, Ge(Cl)CH*Me$_2$*); 1.395 (d, $^3J_{H-H}$ = 6.3Hz, 6H, Ge(Cl)CH*Me$_2$*); 1.40 (d, $^3J_{H-H}$ = 6.3Hz, 6H, Ge(HMDS)CH*Me$_2$*); 1.51 (d, $^3J_{H-H}$ = 6.3Hz, 6H, Ge(HMDS)CH*Me$_2$*); 1.475 (s, 9H, C*Me$_3$*); 1.48 (s, 9H, C*Me$_3$*); 4.41 (sept, $^3J_{H-H}$ = 6.3Hz, 4H, C*H*Me$_2$). ^{13}C{^{1}H} NMR (THF-d8, 75.48 MHz): δ 7.5 (*N(TMS)$_2$*); 24.6 (CH*Me$_2$*); 24.8 (CH*Me$_2$*); 25.2 (CH*Me$_2$*); 26.3 (CH*Me$_2$*); 29.3 (C*Me$_3$*); 30.0 (C*Me$_3$*); 39.7 (*C*Me$_3$); 39.8 (*C*Me$_3$); 49.2 (*C*HMe$_2$); 49.5 (*C*HMe$_2$); 172.1 (N-*C*-N); 176.8 (N-*C*-N);

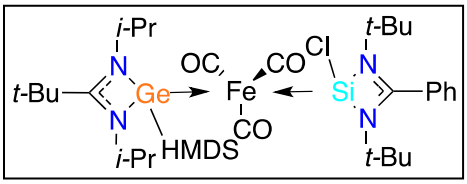
217.2 (*C*O). HRMS (ESI) ($C_{31}H_{64}FeGe_2N_5O_3Si_2$): $[M]^+$: Calculated: 848.2106 g/mol Found: 848.2104 g/mol. IR (in CH_2Cl_2, cm^{-1}): υ = 1863.

Synthesis of 3



[{tBuNC(Ph)NtBu}SnCl][{iPrNC(tBu)NiPr}Ge{N(TMS)$_2$}]Fe(CO)$_3$ 3. 10 ml of THF were added to a solid mixture of **1b** (300 mg, 0.51 mmol) and chlorostannylene (276 mg, 0.72 mmol). The solution was irradiated for 18 hours under UV-A (λ = 365nm) light. Then the solvent was removed under reduced pressure and the resulting solid was washed with heptane (10 mL) and pentane (10 mL). After evaporation of volatiles under reduced pressure, the final product was obtained as an orange solid (205 mg, 43% yield). Melting point: 111-113°C ^{1}H NMR (THF-d8, 300 MHz): δ 0.42 (s, 18H, N(*TMS*)$_2$); 1.125 (s, 18H, 2*(Sn)C*Me*$_3$); 1.44 (d, $^3J_{H\text{-}H}$ = 6.3Hz, 6H, CH*Me*$_2$); 1.50 (s, 18H, (Ge)C*Me*$_3$); 1.55 (d, $^3J_{H\text{-}H}$ = 6.3Hz, 6H, CH*Me*$_2$); 4.455 (sept, $^3J_{H\text{-}H}$ = 6.3Hz, 4H, C*H*Me$_2$); 7.46 (multi, 5H, *Ph*). ^{13}C{^{1}H} NMR (THF-d8, 75.48 MHz): δ 7.5 (N(*TMS*)$_2$); 24.6 (CH*Me*$_2$); 26.2 (CH*Me*$_2$); 30.0 ((Ge)C*Me*$_3$); 32.6 ((Sn)C*Me*$_3$); 39.7 ((Ge)*C*Me$_3$); 49.3 ((Ge)*C*Me$_3$); 55.0 ((Sn)*C*Me$_3$); 121.2-128.9-130.1-130.2-130.8-135.8 (*Ph*); 172.5 ((Ge)N-*C*-N); 173.3 ((Sn)N-*C*-N); 216.4 (*C*O). ^{119}Sn NMR (THF-d8, 111.92 MHz): δ 250.3 (s, N-Sn-N). MS (Maldi-TOF): 908.4 $[M - Cl]^+$; 809.3 $[M – (Ph, tBu)]^+$; 756.3 $[M – [CO, HMDS]^+$. IR (in CH_2Cl_2, cm^{-1}): υ = 1948.3, 1872.5,1860.9.

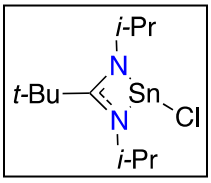
Synthesis of 4



[{tBuNC(Ph)NtBu}SiCl][{iPrNC(tBu)NiPr}Ge{N(TMS)$_2$}]Fe(CO)$_3$ 4. 10 ml of THF were added to a solid mixture of **1b** (300 mg, 0.51 mmol) and chlorosilylene (77 mg, 0.26 mmol). The solution was irradiated for 18 hours under UV-A (λ = 365nm) light. Then the solvent was removed under reduced pressure and the resulting solid was washed with heptane (10mL) and pentane (10mL). After evaporation of volatiles under reduced pressure, the product 3d was obtained as an orange solid (83 mg, 38% yield). Yellow-orange crystals were obtained by diffusion of pentane to a concentrated solution of **4** in THF at -30°C. Melting point: 103-104°C. ^{1}H NMR (THF-d8, 300 MHz): δ 0.39 (s, 18H, N(*TMS*)$_2$); 1.262 (s, 18H, C*Me*$_3$); 1.41 (d, $^3J_{H\text{-}H}$ = 6.3Hz, 6H, CH*Me*$_2$); 1.48 (s, 9H, C*Me*$_3$); 1.52

(d, $^{3}J_{H-H}$ = 6.3Hz, 6H, CH*Me*$_2$); 4.41 (sept, $^{3}J_{H-H}$ = 6.3Hz, 4H, C*H*Me$_2$); 7.49 – 7.63 (multi, 5H, *Ph*). $^{13}C\{^{1}H\}$ NMR (THF-d8, 75.48 MHz): δ 7.6 (N*(TMS)*$_2$); 24.6 (CH*Me*$_2$); 26.5 (CH*Me*$_2$); 30.1 ((Ge)C*Me*$_3$); 31.8 ((Si)C*Me*$_3$); 39.8 ((Ge)*C*Me$_3$); 49.1 (*C*HMe$_2$); 56.0 ((Si)*C*Me$_3$); 129.0-129.3-130.0-130.1-131.6-131.8 (*Ph*); 171.8 (N-*C*-N); 171.9 (N-*C*-N); 218.2 (*C*O). ^{29}Si NMR (THF-d8, 59.63 MHz): δ 83.3 (s, N-Si-N). HRMS (ESI) ($C_{35}H_{67}FeClGeN_5O_3Si_3$): $[M]^+$: Calculated: 847.2603 g/mol Found: 847.2643 g/mol IR (in CH_2Cl_2, cm^{-1}): υ = 1940.2, 1861.9, 1844.3.

Synthesis of 5



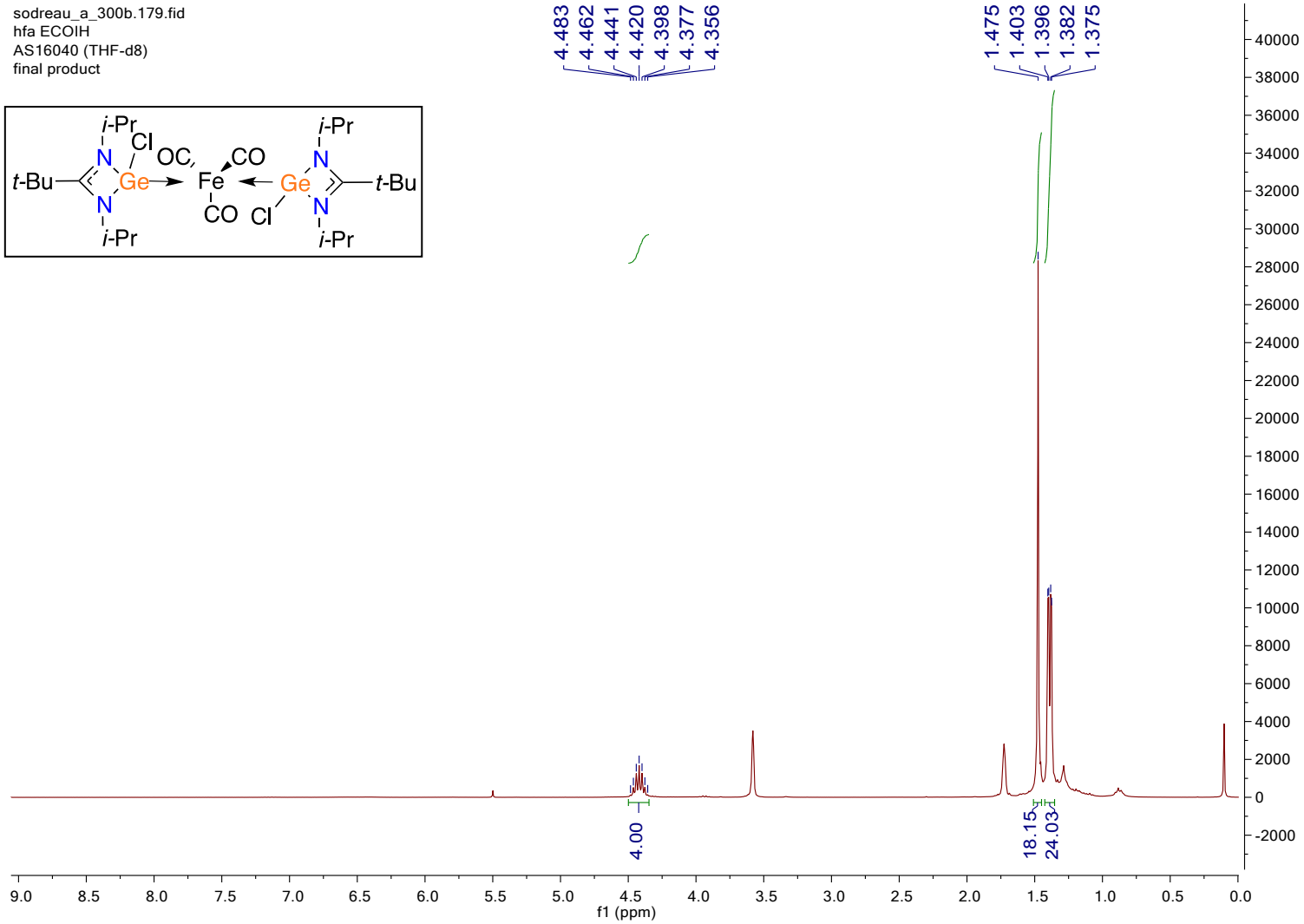
[{iPrNC(tBu)NiPr}SnCl] 5. To a solution of diisopropylcarbodiimide in 25 mL of diethyl ether (1 mL, 6.40 mmol) at -80°C was dropwise added a solution of tert-butyllithium (4 mL, 6.40 mmol, 1.6 mol.L^{-1} in hexanes). The solution was stirred at -80°C for 30 min. The cool bath was removed, and the mixture was stirred for 3h30 at room temperature. Then solid tin(II) chloride (1.744 g, 12.8 mmol) was added to the previous solution at -80°C and the mixture was stirring overnight at room temperature. After solvent evaporation, the resulting solid was extracted with 30 mL of pentane. Finally, pentane was removed under reduced pressure to give 1.95 g (91%) of a white-grey solid. ^{1}H NMR (THF-d8, 300 MHz): δ 1.16 (d, $^{3}J_{H-H}$ = 6.3Hz, 12H, CH*Me*$_2$); 1.41 (s, 9H, C*Me*$_3$); 4.54 (sept, $^{3}J_{H-H}$ = 6.3Hz, 2H, C*H*Me$_2$). $^{13}C\{^{1}H\}$ NMR (THF-d8, 75.48 MHz): δ 26.7 (C*Me*$_3$); 30.1 (CH*Me*$_2$); 43.5 (*C*Me$_3$); 47.7 (*C*HMe$_2$); 180.5 (N-*C*-N). ^{119}Sn NMR (THF-d8, 111.92 MHz): δ 49.4 (N-Sn-N).

Attempts to crystallize of **5** afford to the formation of **6** which could be explained by the very sensitive character of **5**, that further reacts with traces of dioxygen in solution during cristallization.

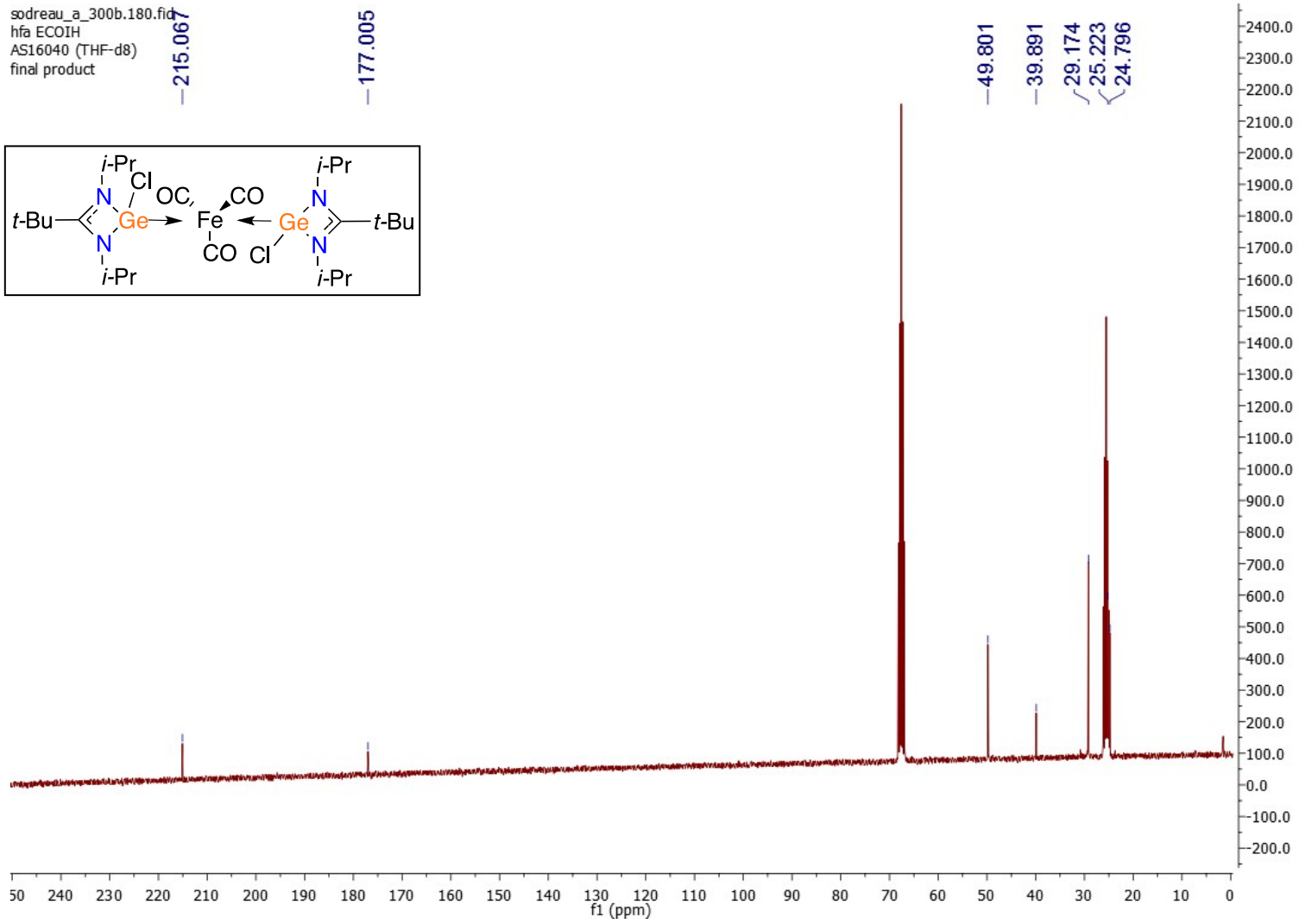
Synthesis of NPs from 2a

Into the core of a 100 mL double envelop Fisher-Porter were added **2a** (100 mg, 0.17 mmol). Then, 1-octadecene (ODE) (10 mL) was poured and Fisher-Porter was sealed in the glove box. 1-octadecene was also used as a heating solvent was introduced in the second envelop. The mixture was warming up to 300°C using a heating mental under magnetic stirring and a probe positioned in ODE leading the heating ratio at 5K.min^{-1}. The mixture moves to black colour at 200°C, the solution was stirred for 16 hours. After, the black solution was diluted by 20 mL of mesitylene and then centrifuged two times during 15 minutes (15000 RPM). Between two

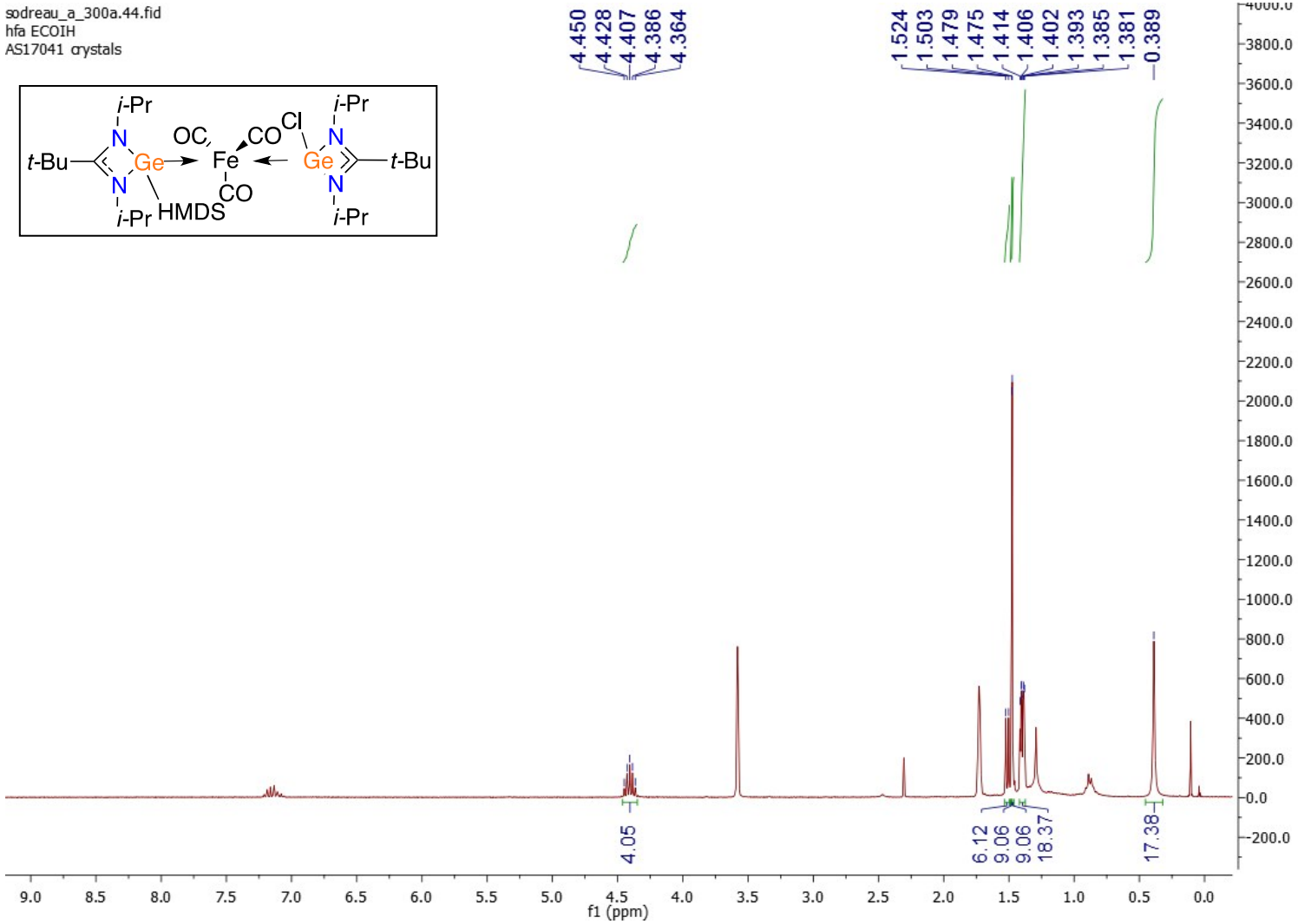
runs the supernatant was eliminated and 30 mL of clean mesitylene was added. Finally, last drops of solvent were removed under vacuum to give 34 mg of a nanoparticles as a black powder



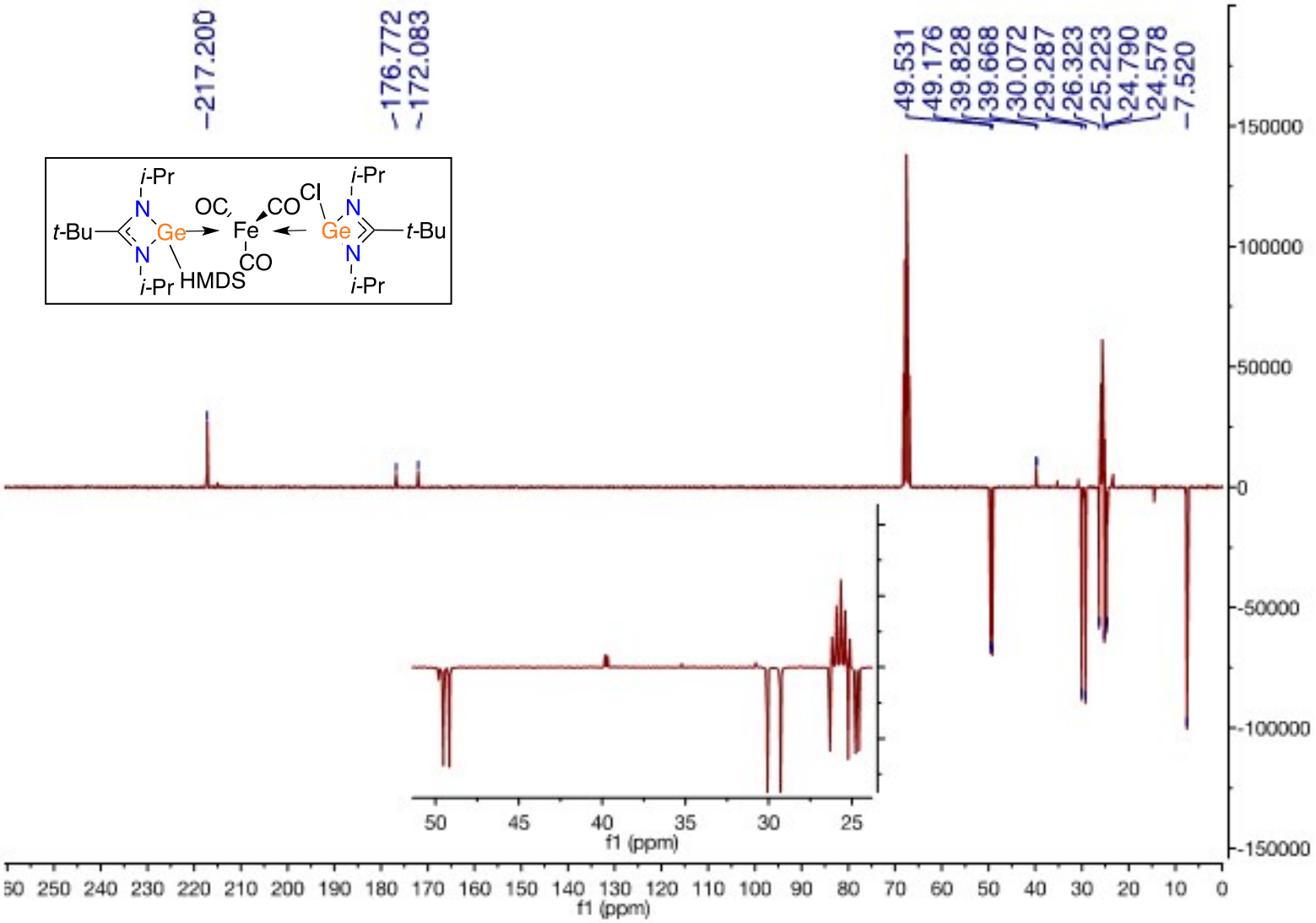
^{1}H NMR spectrum of compound **2a** (THF-d8, 300 MHz)



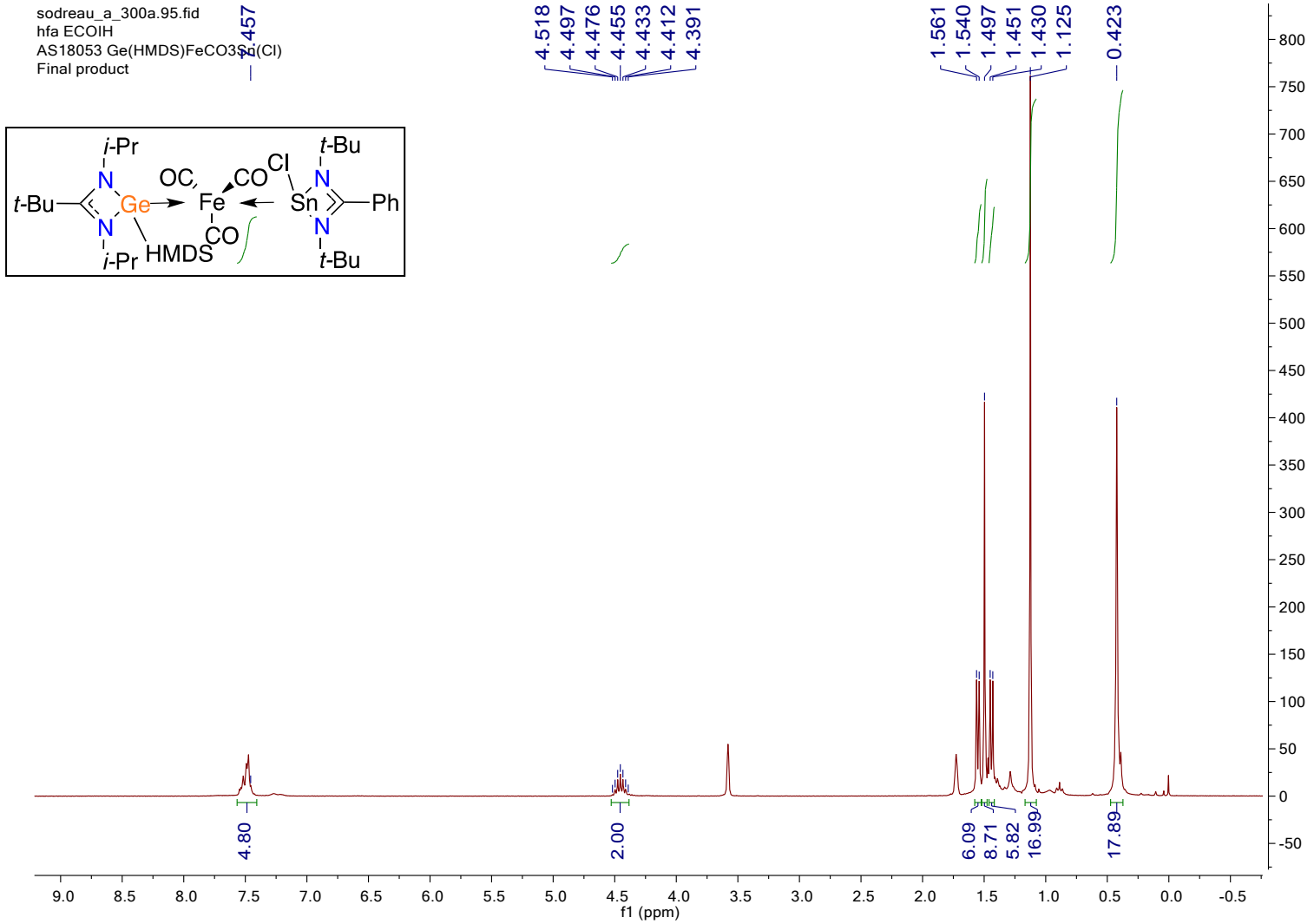
^{13}C NMR spectrum of compound **2a** (THF-d8, 75.48 MHz)



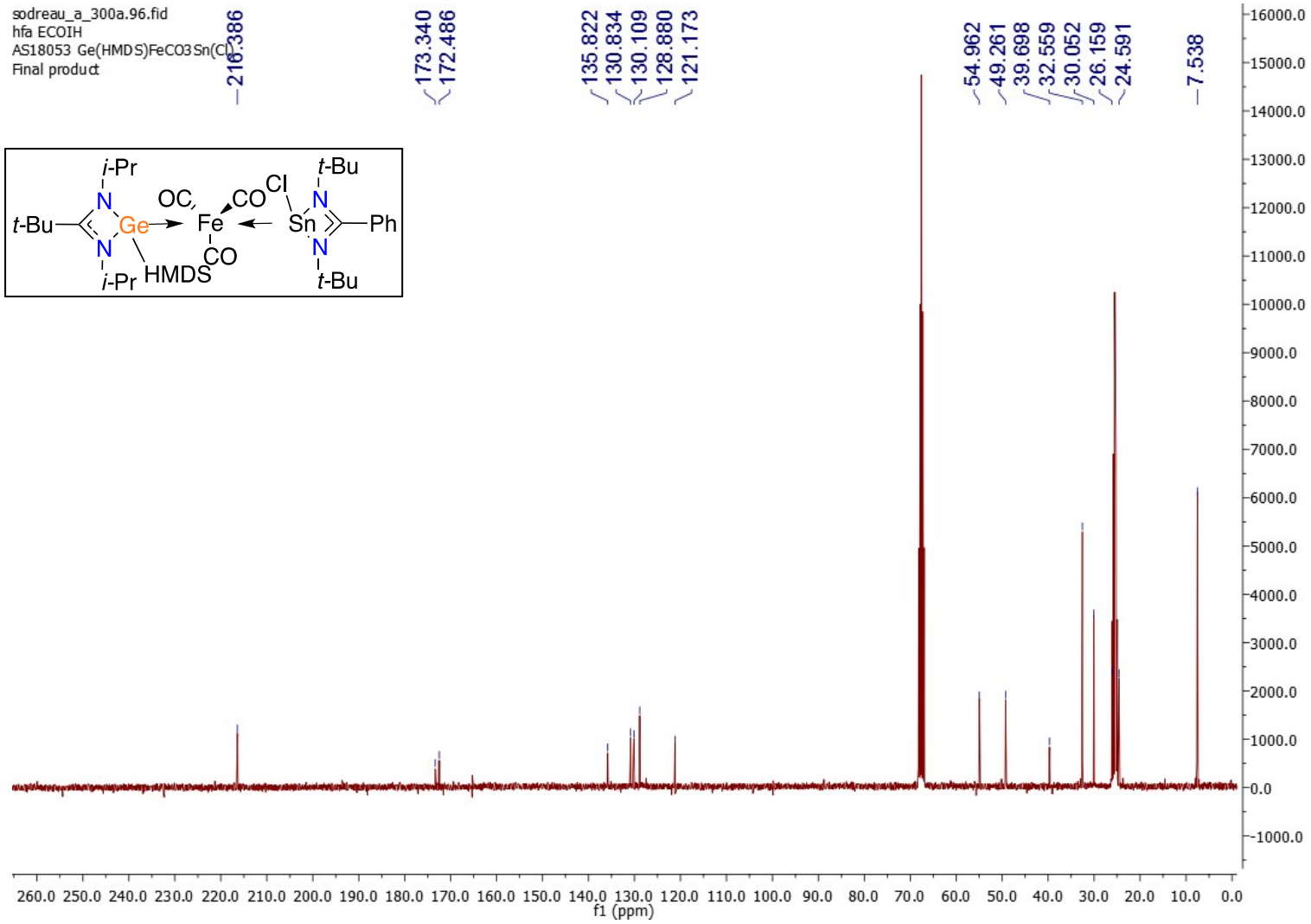
^{1}H NMR spectrum of compound **2b** (THF-d8, 300 MHz)



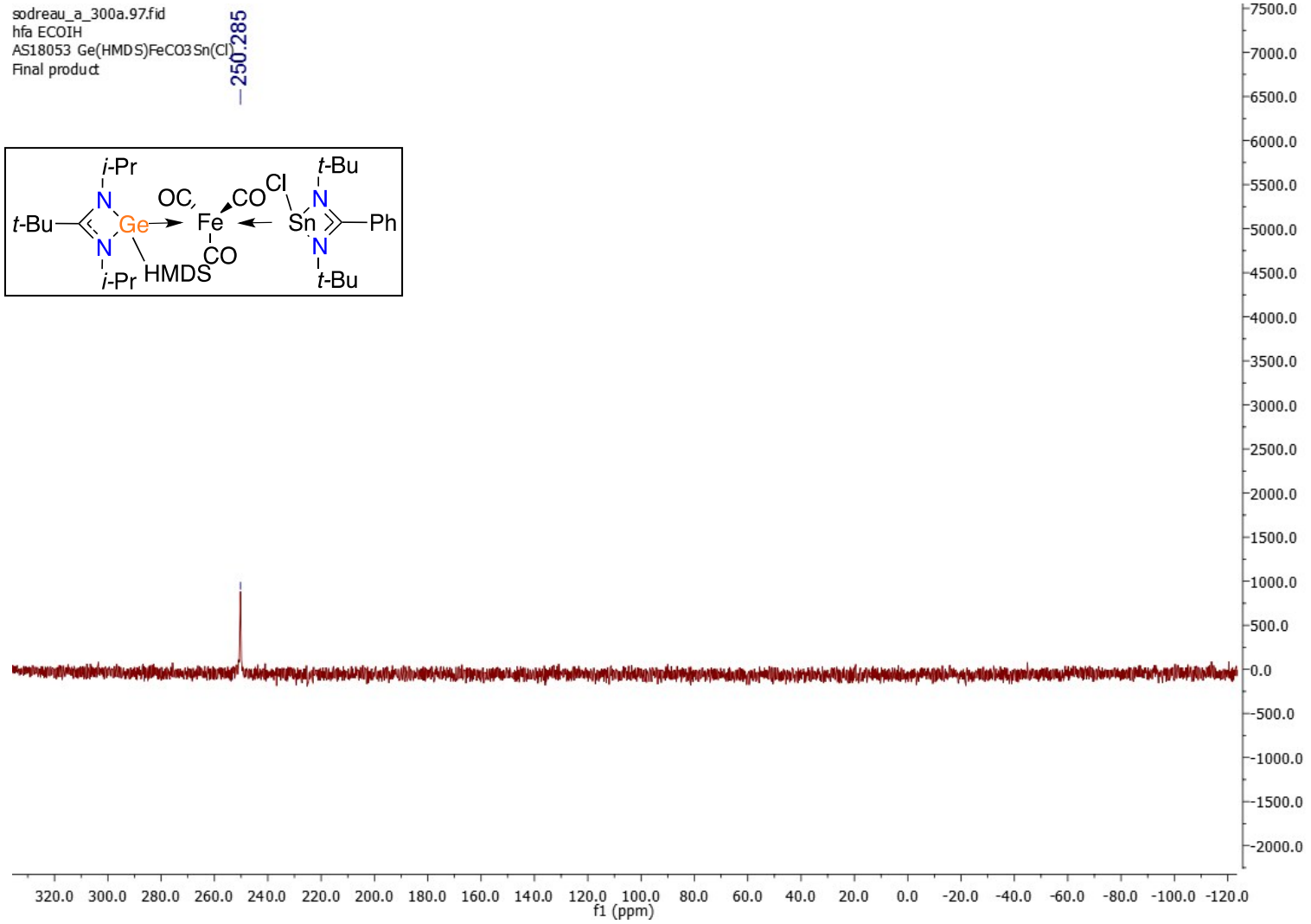
^{13}C NMR spectrum of compound **2b** (THF-d8, 75.48 MHz)



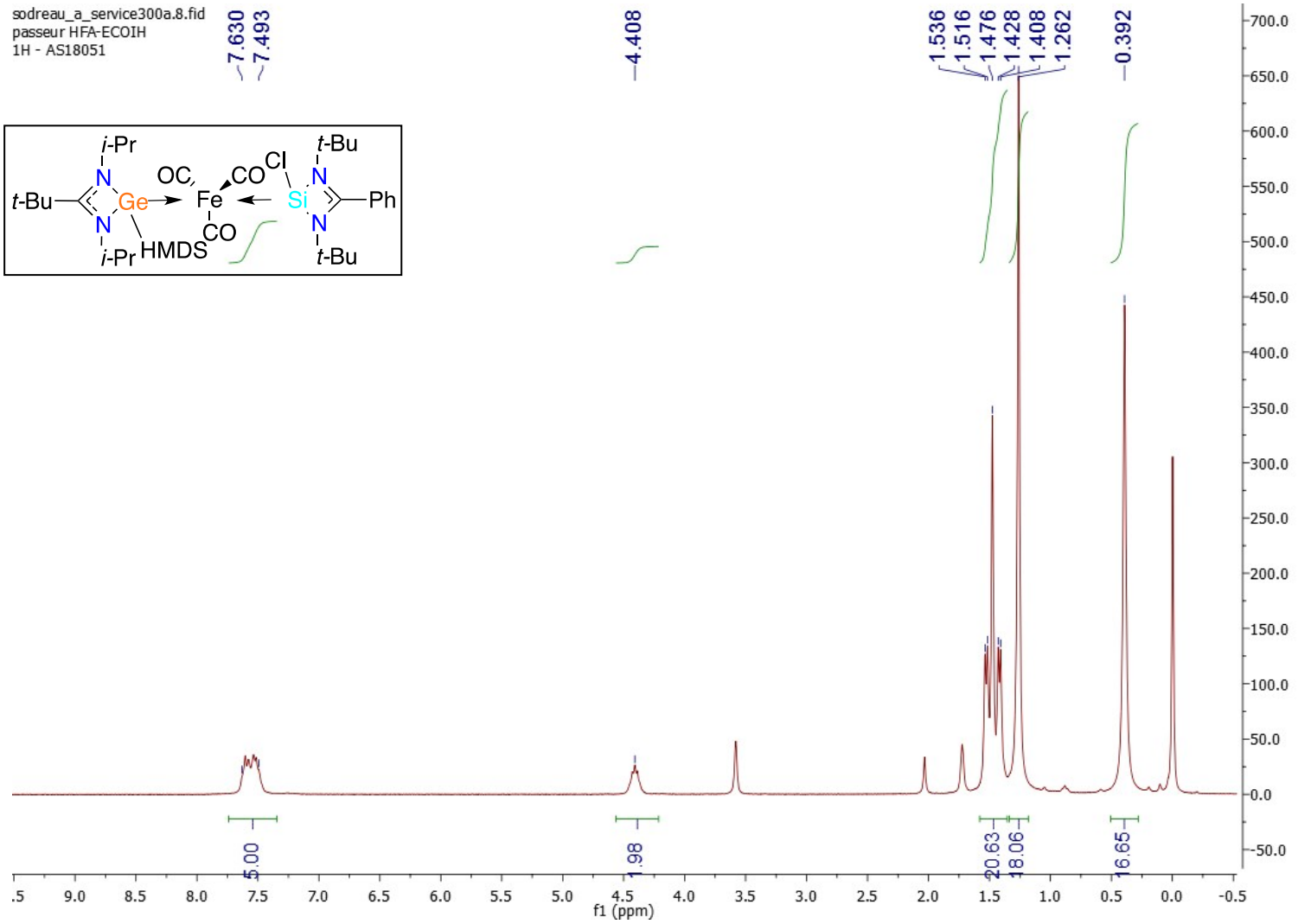
^{1}H NMR spectrum of compound **3** (THF-d8, 300 MHz)



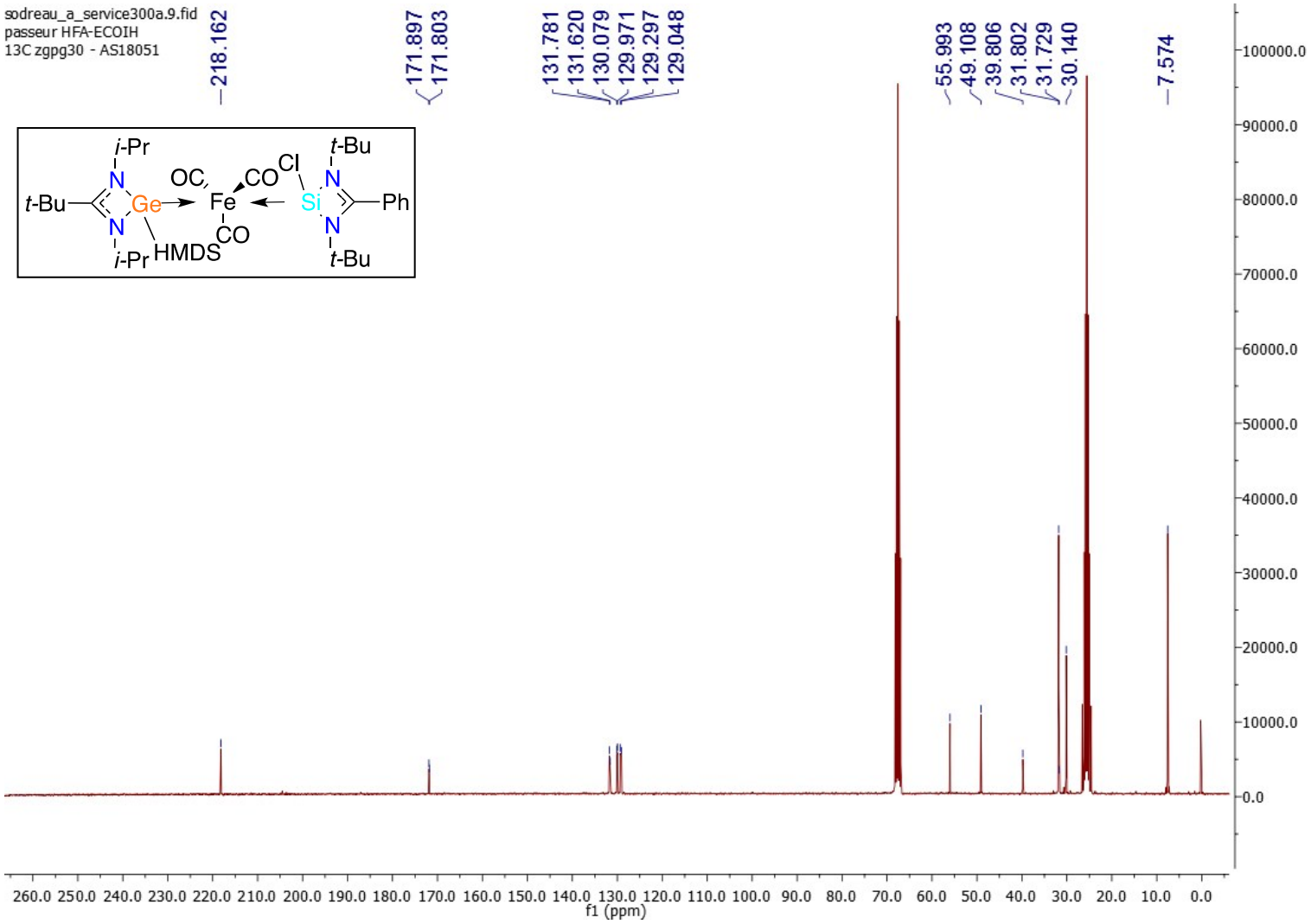
^{13}C NMR spectrum of compound **3** (THF-d8, 75.48 MHz)



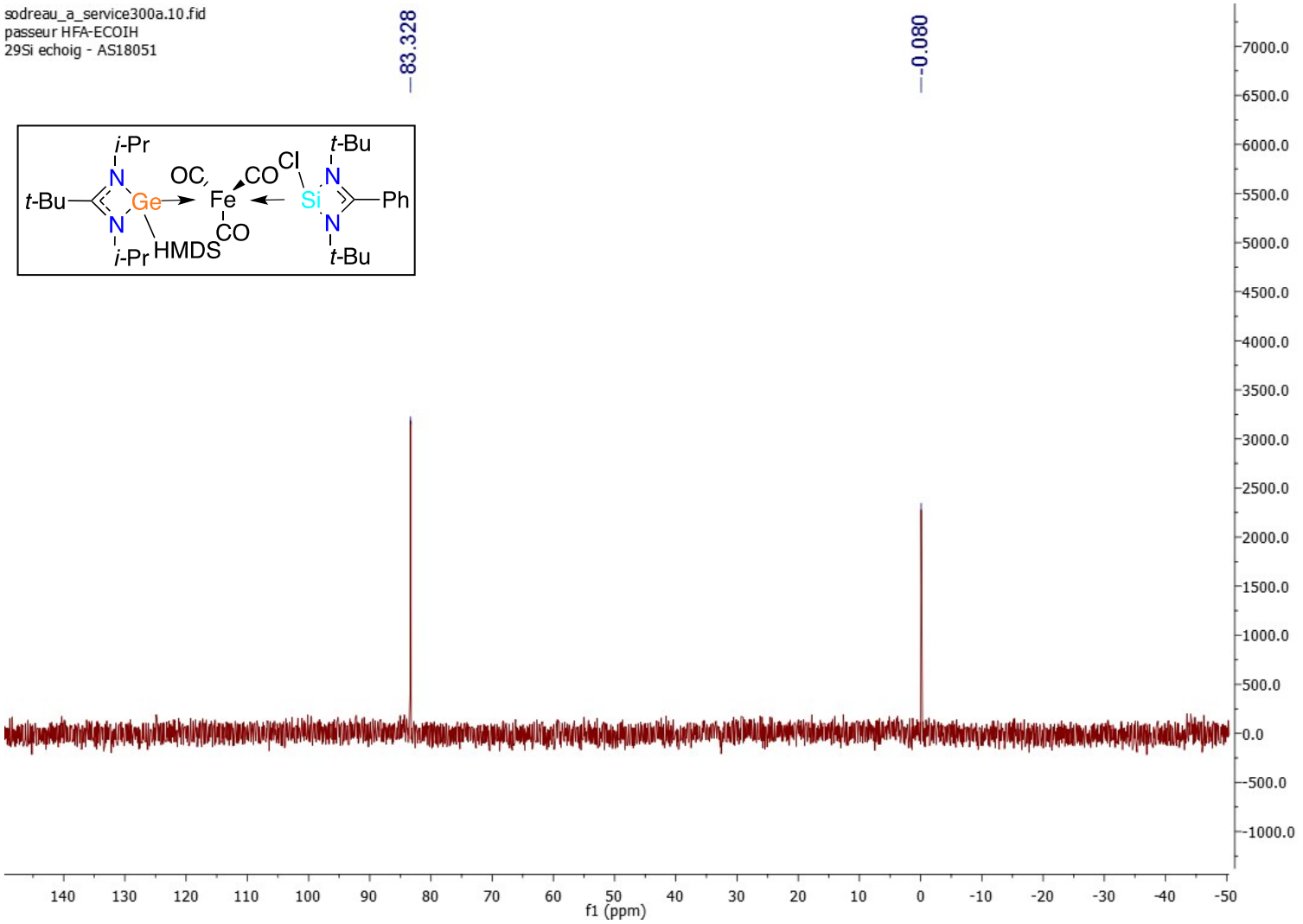
^{119}Sn NMR spectrum of compound **3** (THF-d8, 111.92 MHz)



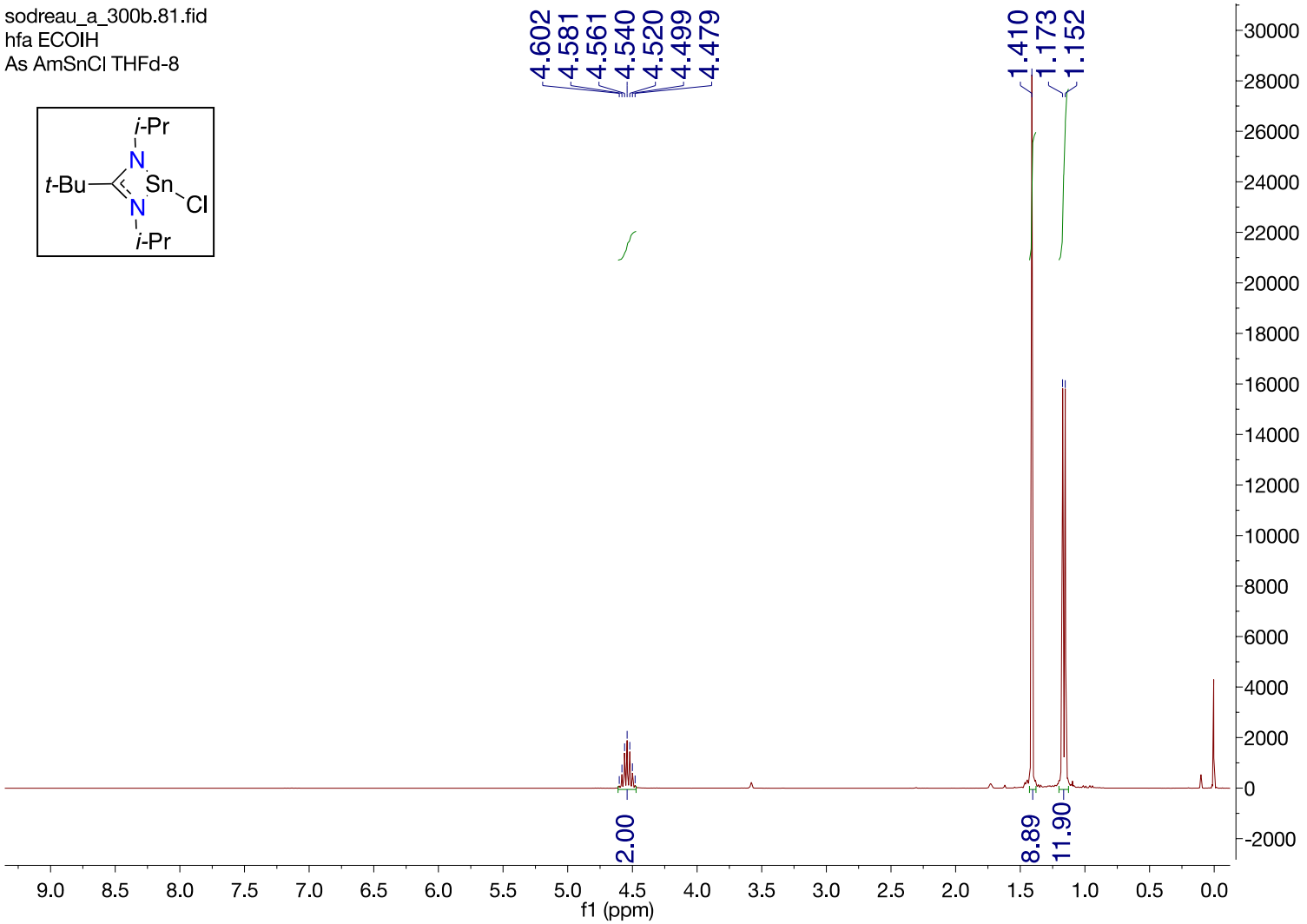
^{1}H NMR spectrum of compound **4** (THF-d8, 300 MHz)



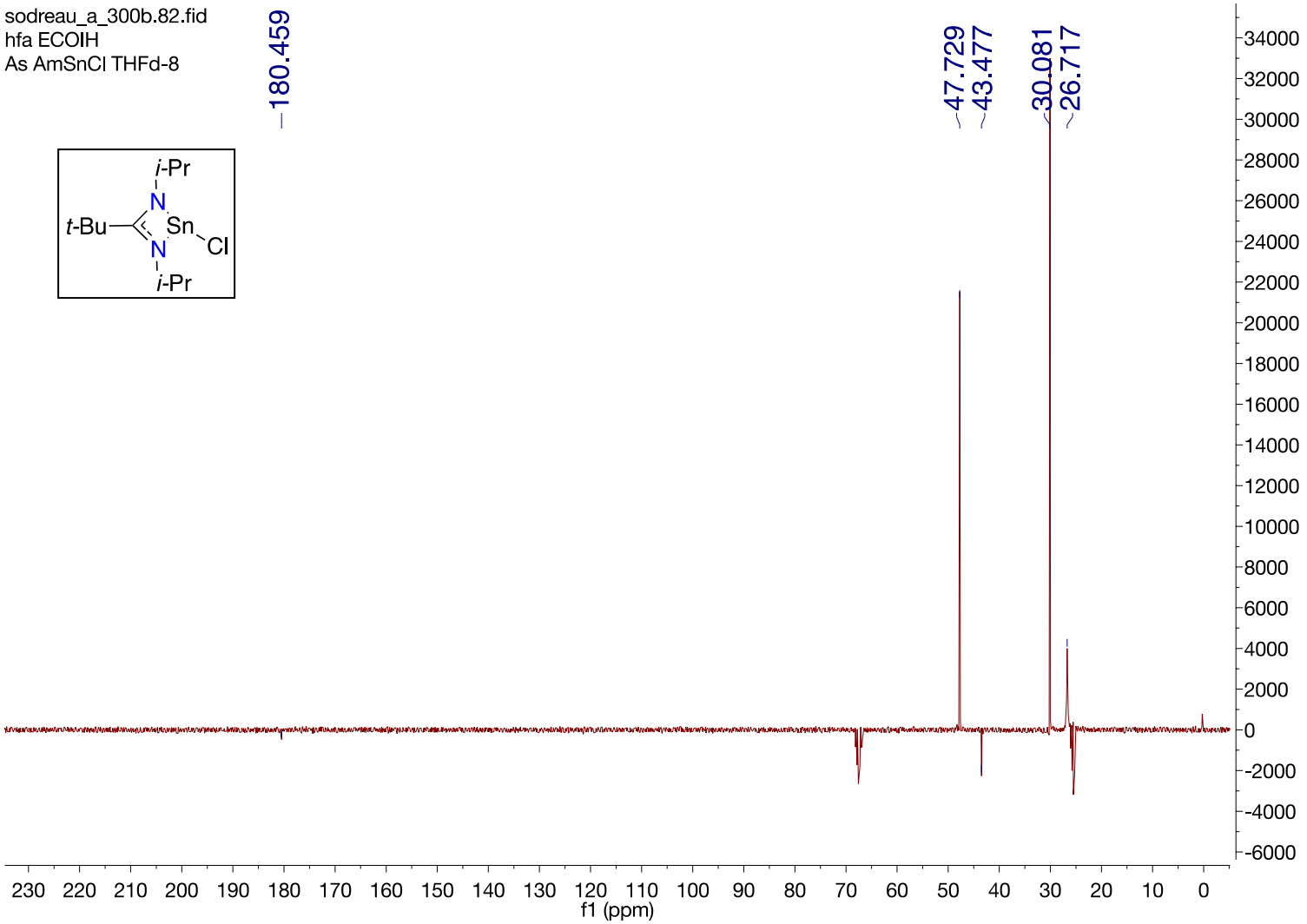
^{13}C NMR spectrum of compound **4** (THF-d8, 75.48 MHz)



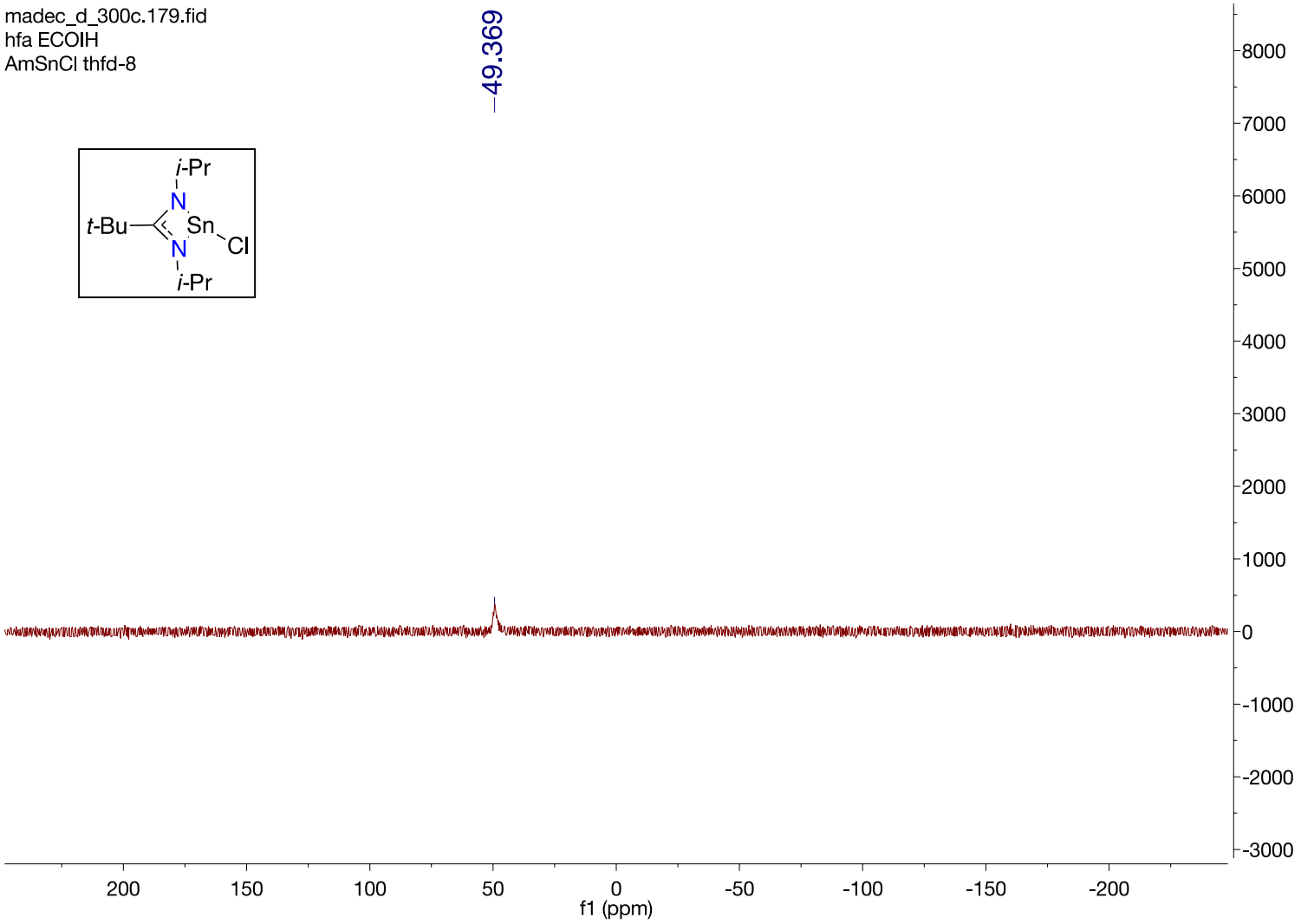
^{29}Si NMR spectrum of compound **4** (THF-d8, 59.63 MHz)



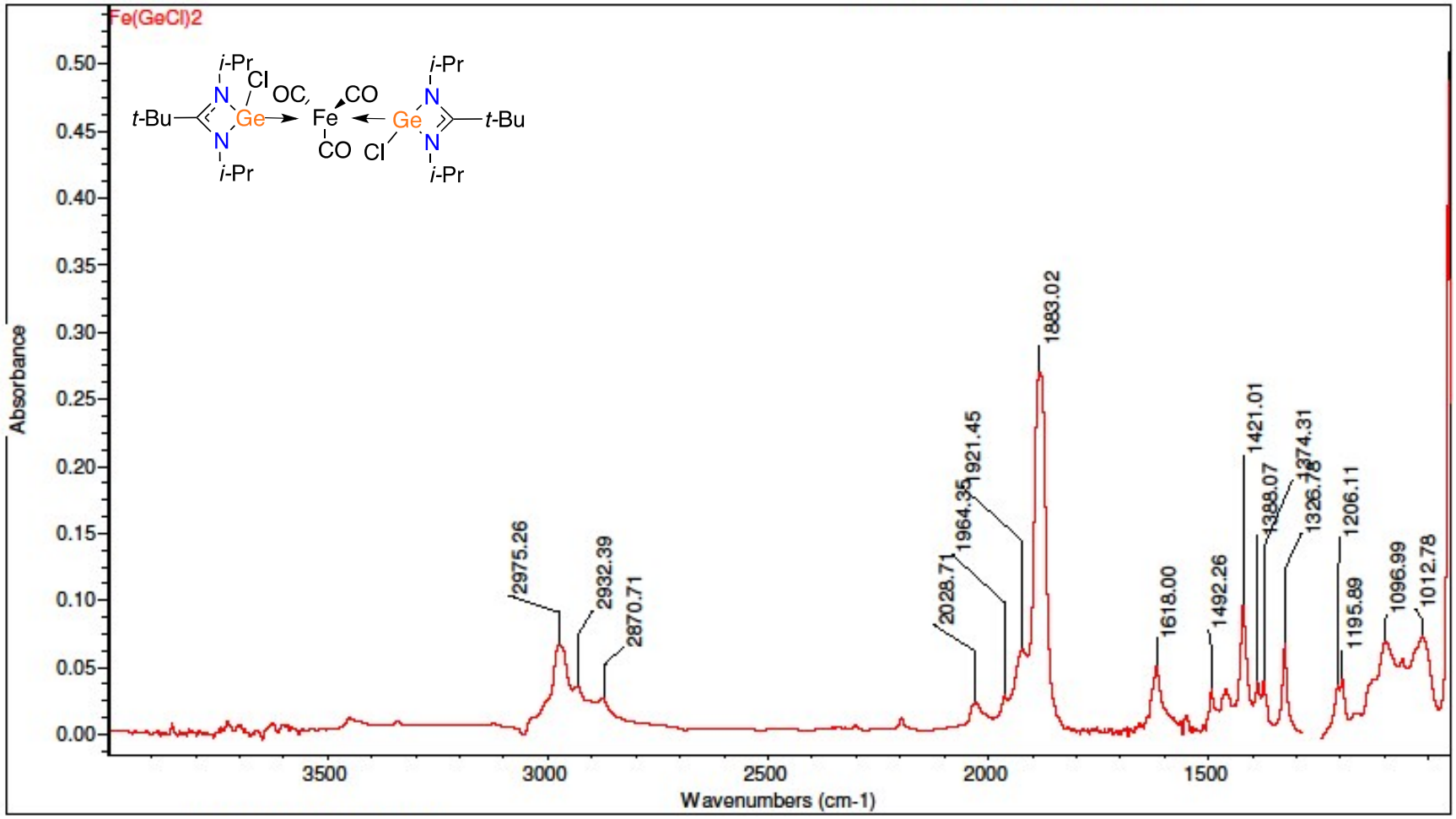
^{1}H NMR spectrum of compound **5** (THF-d8, 300 MHz)



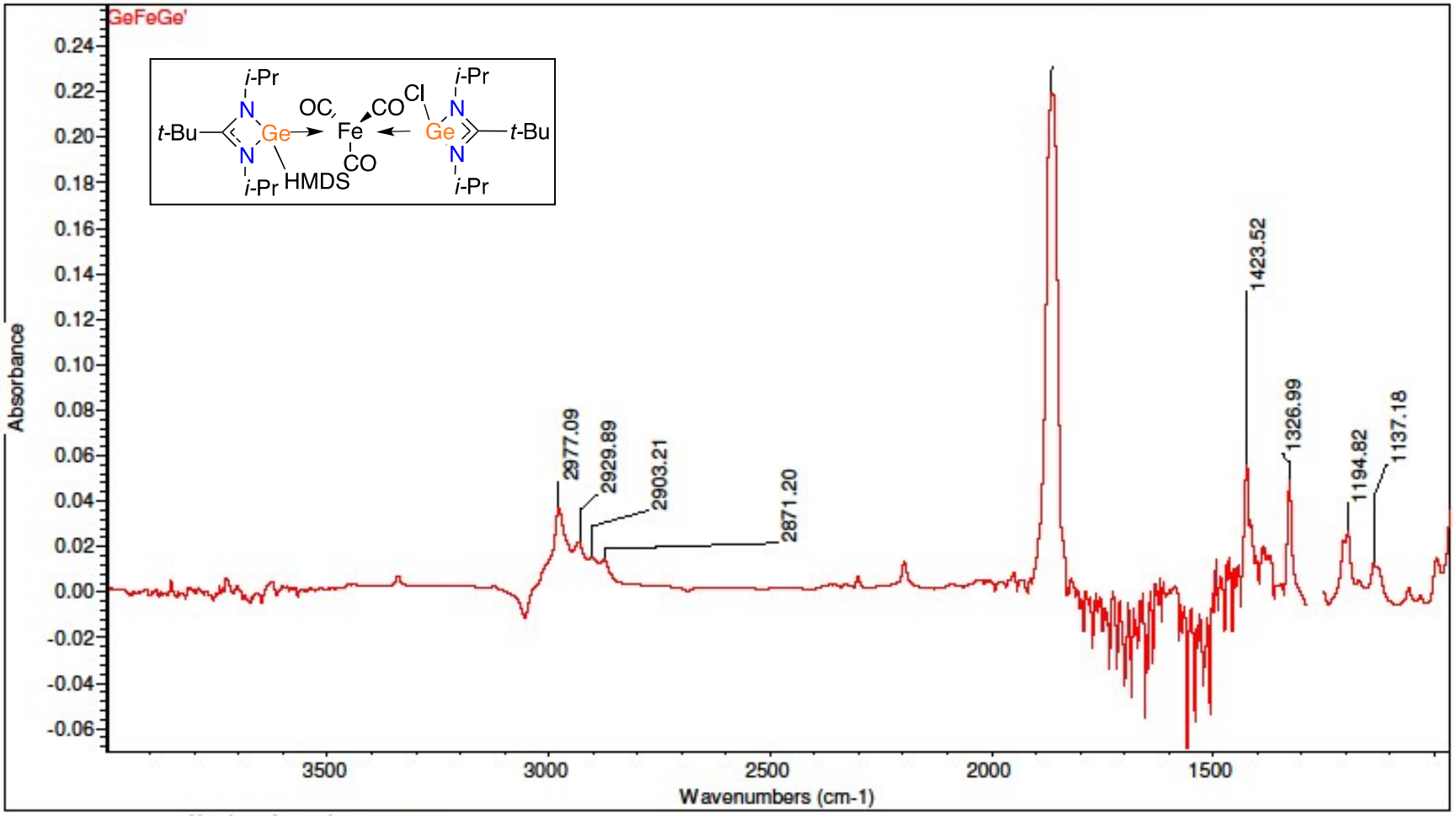
^{13}C NMR spectrum of compound **5** (THF-d8, 75.48 MHz)



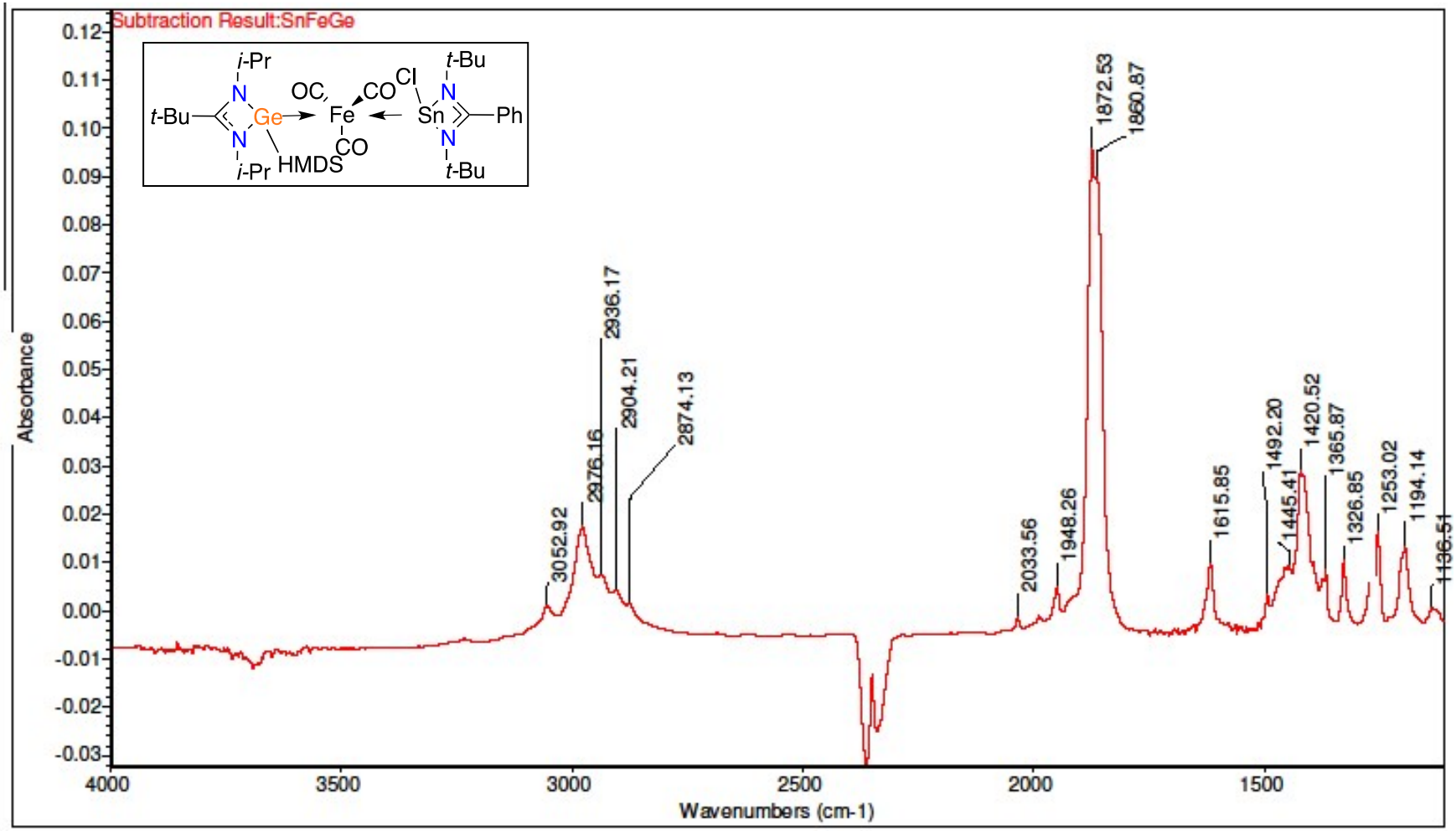
^{119}Sn NMR spectrum of compound **5** (THF-d8, 111.92 MHz)



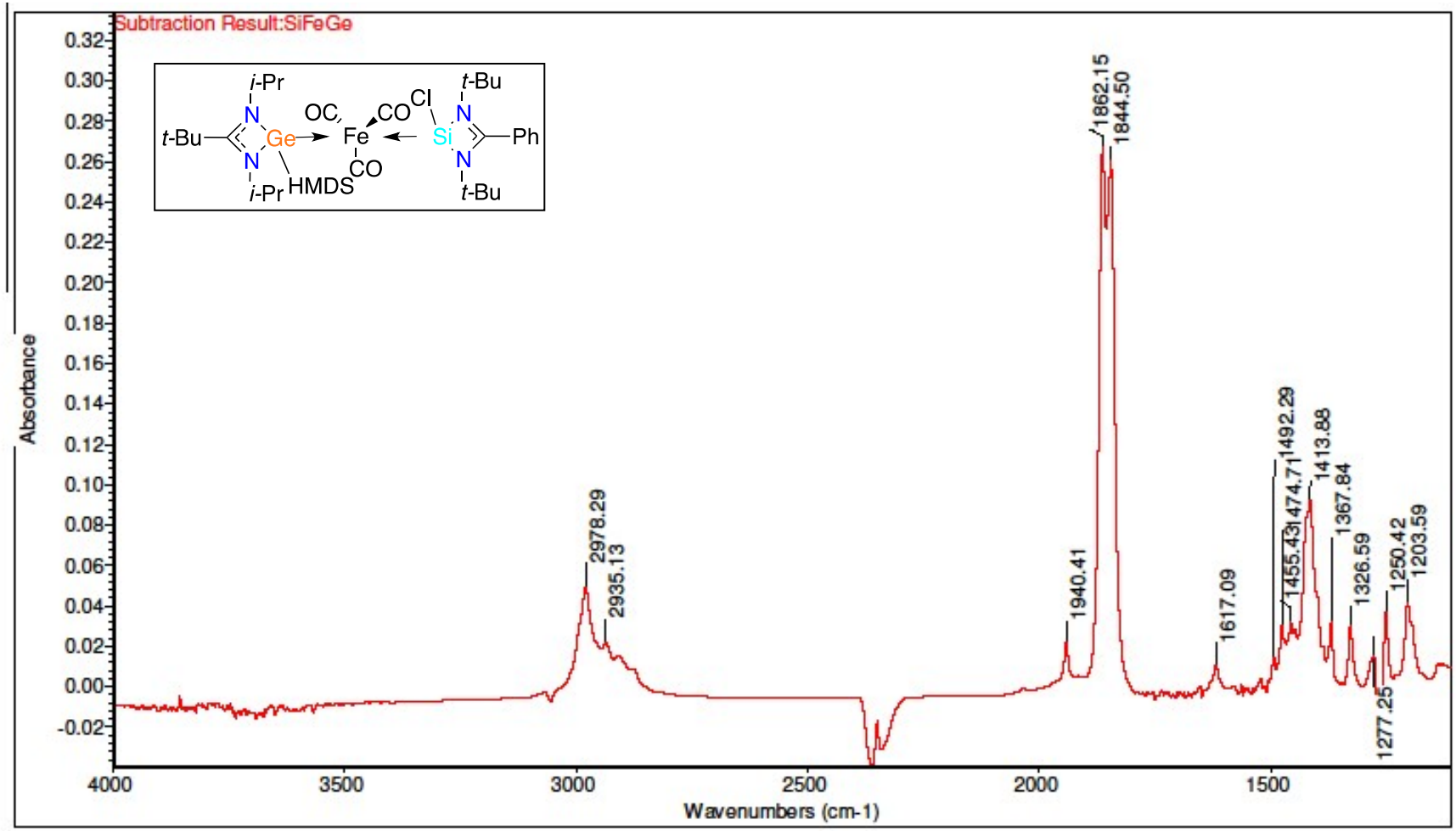
IR spectrum of compound **2a**



IR spectrum of compound **2b**



IR spectrum of compound **3**



IR spectrum of compound **4**

In table S1 are summarized selected NMR and IR data for compounds **1a**, **1b**, **2a**, **2b**, **3** and **4**. Slight variations are observed for central *ipso* carbons of the amidinate systems and CO resonances in ^{13}C NMR spectra. IR spectra of **2a** and **2b** show only one band for CO stretching frequencies, while two separate bands can be observed for **3** and **4**.

Compound	^{13}C C *ipso* (δ/ppm)[a]	^{13}C CO (δ/ppm)[a]	$^{119}Sn/^{29}Si$ (δ/ppm)[a]	IR υ(CO)[b] cm^{-1}
1a	179.5	214.6	-	2043, 1949,1931
1b	174.0	217.0	-	2036, 1959, 1922
2a	177.0	215.1	-	1883
2b	176.8/172.1	217.2	-	1863
3	173.3/172.5	216.4	250.3	1872, 1861
4	171.9/171.8	218.2	83.3	1862, 1844

Table S1. ^{13}C, ^{119}Sn, ^{29}Si NMR and IR data for compounds **1a**, **1b**, **2a**, **2b**, **3** and **4**.

Crystal data and structure refinement of compound **2a**

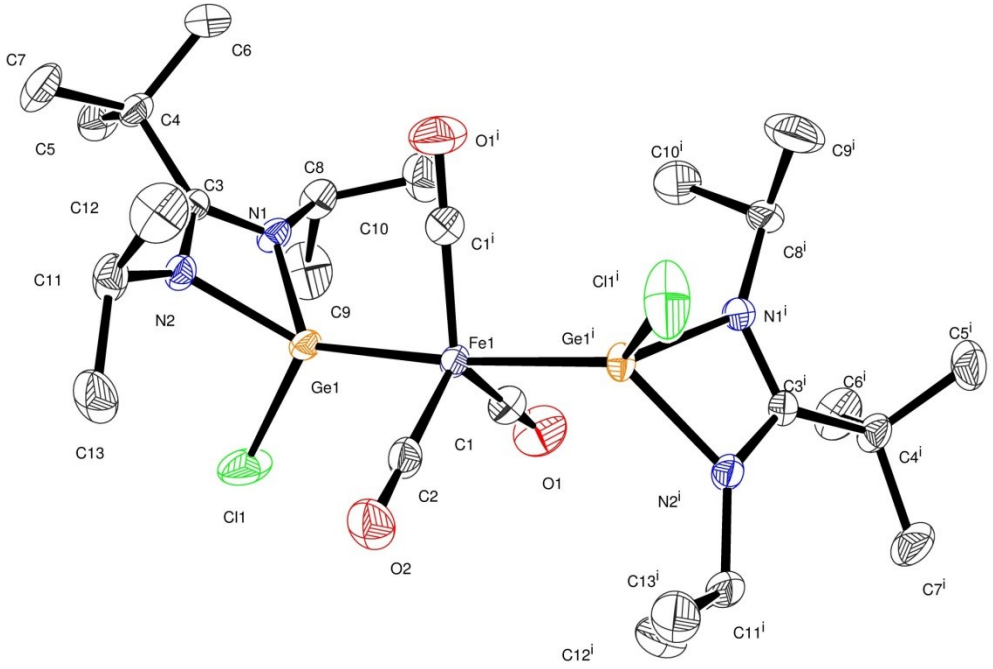


Table S2. Crystal data and structure refinement for AS16038.

Identification code	AS16038
Empirical formula	C25 H46 Cl2 Fe Ge2 N4 O3
Formula weight	722.59
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P 21 21 2
Unit cell dimensions	a = 11.1361(5) A alpha = 90 deg. b = 15.7091(8) A beta = 90 deg. c = 9.5057(5) A gamma = 90 deg.
Volume	1662.91(14) A^3
Z, Calculated density	2, 1.443 Mg/m^3
Absorption coefficient	2.417 mm^-1
F(000)	744

Crystal size	0.220 x 0.140 x 0.120 mm
Theta range for data collection	3.102 to 32.577 deg.
Limiting indices	-16<=h<=16, -23<=k<=23, -14<=l<=14
Reflections collected / unique	78732 / 6060 [R(int) = 0.0305]
Completeness to theta = 25.242	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6060 / 0 / 177
Goodness-of-fit on F^2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0184, wR2 = 0.0423
R indices (all data)	R1 = 0.0214, wR2 = 0.0438
Absolute structure parameter	0.089(7)
Largest diff. peak and hole	0.229 and -0.424 e.A^-3

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for AS16038. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	4268(2)	5847(1)	7015(2)	27(1)
C(2)	5000	5000	4263(3)	24(1)
C(3)	2849(1)	2857(1)	7294(2)	19(1)
C(4)	2689(2)	2000(1)	8030(2)	25(1)
C(5)	1445(2)	1956(1)	8731(2)	37(1)
C(6)	3700(2)	1916(1)	9126(2)	41(1)
C(7)	2768(2)	1228(1)	7047(2)	40(1)
C(8)	2510(2)	3852(1)	9402(2)	28(1)
C(9)	1357(2)	4373(2)	9420(3)	53(1)
C(10)	3546(2)	4354(2)	10031(2)	41(1)
C(11)	3433(2)	2495(1)	4722(2)	30(1)
C(12)	4773(2)	2294(2)	4749(3)	45(1)
C(13)	3090(2)	2984(2)	3398(2)	42(1)
N(1)	2796(1)	3610(1)	7951(2)	22(1)
N(2)	3096(1)	3020(1)	5941(1)	22(1)
O(1)	3801(2)	6401(1)	7602(2)	47(1)
O(2)	5000	5000	3052(2)	39(1)
Cl(1)	1574(1)	4745(1)	5572(1)	50(1)
Fe(1)	5000	5000	6133(1)	18(1)
Ge(1)	3296(1)	4236(1)	6292(1)	20(1)

Table S4. Bond lengths [A] and angles [deg] for AS16038.

C(1)-O(1)	1.157(2)
C(1)-Fe(1)	1.7719(18)
C(2)-O(2)	1.151(3)
C(2)-Fe(1)	1.778(2)
C(3)-N(1)	1.339(2)
C(3)-N(2)	1.340(2)
C(3)-C(4)	1.528(2)
C(4)-C(7)	1.534(3)
C(4)-C(5)	1.538(3)
C(4)-C(6)	1.540(3)
C(5)-H(5A)	0.9800
C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-N(1)	1.466(2)
C(8)-C(10)	1.519(3)
C(8)-C(9)	1.522(3)
C(8)-H(8)	1.0000
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-N(2)	1.471(2)
C(11)-C(13)	1.523(3)
C(11)-C(12)	1.526(3)
C(11)-H(11)	1.0000
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
N(1)-Ge(1)	1.9405(14)
N(2)-Ge(1)	1.9521(13)
Cl(1)-Ge(1)	2.1869(5)
Fe(1)-Ge(1)#1	2.25010(18)
Fe(1)-Ge(1)	2.25012(18)
O(1)-C(1)-Fe(1)	179.17(19)
O(2)-C(2)-Fe(1)	180.0
N(1)-C(3)-N(2)	106.74(13)
N(1)-C(3)-C(4)	124.01(14)
N(2)-C(3)-C(4)	129.22(14)
C(3)-C(4)-C(7)	114.27(15)
C(3)-C(4)-C(5)	110.09(14)
C(7)-C(4)-C(5)	106.28(16)
C(3)-C(4)-C(6)	107.44(14)

C(7)-C(4)-C(6)	107.58(17)
C(5)-C(4)-C(6)	111.20(17)
C(4)-C(5)-H(5A)	109.5
C(4)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(4)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(4)-C(6)-H(6A)	109.5
C(4)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(4)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(4)-C(7)-H(7A)	109.5
C(4)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(4)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(1)-C(8)-C(10)	109.90(15)
N(1)-C(8)-C(9)	109.45(17)
C(10)-C(8)-C(9)	110.95(17)
N(1)-C(8)-H(8)	108.8
C(10)-C(8)-H(8)	108.8
C(9)-C(8)-H(8)	108.8
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(2)-C(11)-C(13)	107.71(16)
N(2)-C(11)-C(12)	110.60(16)
C(13)-C(11)-C(12)	111.28(18)
N(2)-C(11)-H(11)	109.1
C(13)-C(11)-H(11)	109.1
C(12)-C(11)-H(11)	109.1
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(3)-N(1)-C(8)	132.71(14)
C(3)-N(1)-Ge(1)	93.21(10)

C(8)-N(1)-Ge(1)	134.04(11)
C(3)-N(2)-C(11)	134.50(14)
C(3)-N(2)-Ge(1)	92.65(10)
C(11)-N(2)-Ge(1)	130.90(11)
C(1)-Fe(1)-C(1)#1	123.52(12)
C(1)-Fe(1)-C(2)	118.24(6)
C(1)#1-Fe(1)-C(2)	118.24(6)
C(1)-Fe(1)-Ge(1)#1	87.47(6)
C(1)#1-Fe(1)-Ge(1)#1	88.88(6)
C(2)-Fe(1)-Ge(1)#1	93.859(9)
C(1)-Fe(1)-Ge(1)	88.88(6)
C(1)#1-Fe(1)-Ge(1)	87.47(6)
C(2)-Fe(1)-Ge(1)	93.859(9)
Ge(1)#1-Fe(1)-Ge(1)	172.282(18)
N(1)-Ge(1)-N(2)	67.04(6)
N(1)-Ge(1)-Cl(1)	100.81(5)
N(2)-Ge(1)-Cl(1)	101.76(5)
N(1)-Ge(1)-Fe(1)	124.56(5)
N(2)-Ge(1)-Fe(1)	127.33(4)
Cl(1)-Ge(1)-Fe(1)	121.588(16)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,z

Table S5. Anisotropic displacement parameters (A^2 x 10^3) for AS16038.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	28(1)	24(1)	29(1)	0(1)	2(1)	0(1)
C(2)	24(1)	24(1)	26(1)	0	0	-7(1)
C(3)	18(1)	18(1)	19(1)	2(1)	-1(1)	-3(1)
C(4)	33(1)	17(1)	25(1)	4(1)	-1(1)	-4(1)
C(5)	40(1)	34(1)	36(1)	8(1)	8(1)	-12(1)
C(6)	48(1)	30(1)	44(1)	11(1)	-14(1)	2(1)
C(7)	62(1)	18(1)	40(1)	-1(1)	5(1)	-9(1)
C(8)	37(1)	25(1)	22(1)	-3(1)	10(1)	-2(1)
C(9)	41(1)	62(2)	55(1)	-19(1)	16(1)	11(1)
C(10)	49(1)	48(1)	25(1)	-8(1)	-1(1)	-8(1)
C(11)	41(1)	27(1)	22(1)	-6(1)	4(1)	-10(1)
C(12)	45(1)	45(1)	44(1)	-7(1)	15(1)	5(1)
C(13)	55(1)	53(1)	19(1)	-2(1)	-1(1)	-18(1)
N(1)	28(1)	17(1)	20(1)	1(1)	6(1)	-2(1)
N(2)	28(1)	19(1)	18(1)	0(1)	1(1)	-6(1)
O(1)	55(1)	35(1)	51(1)	-9(1)	10(1)	13(1)
O(2)	45(1)	49(1)	23(1)	0	0	-10(1)
Cl(1)	27(1)	45(1)	79(1)	33(1)	-10(1)	-1(1)
Fe(1)	19(1)	15(1)	19(1)	0	0	-2(1)
Ge(1)	19(1)	17(1)	22(1)	5(1)	0(1)	-3(1)

Crystal data and structure refinement of compound **2b**

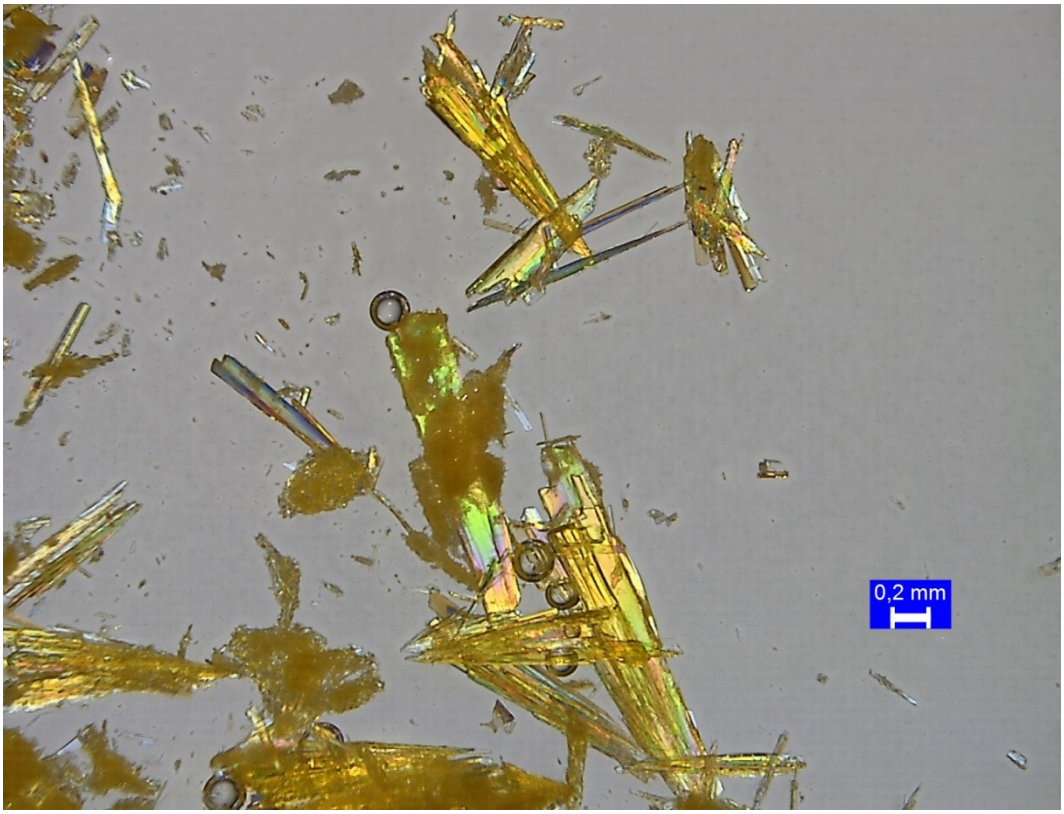


Figure S1 : Sample

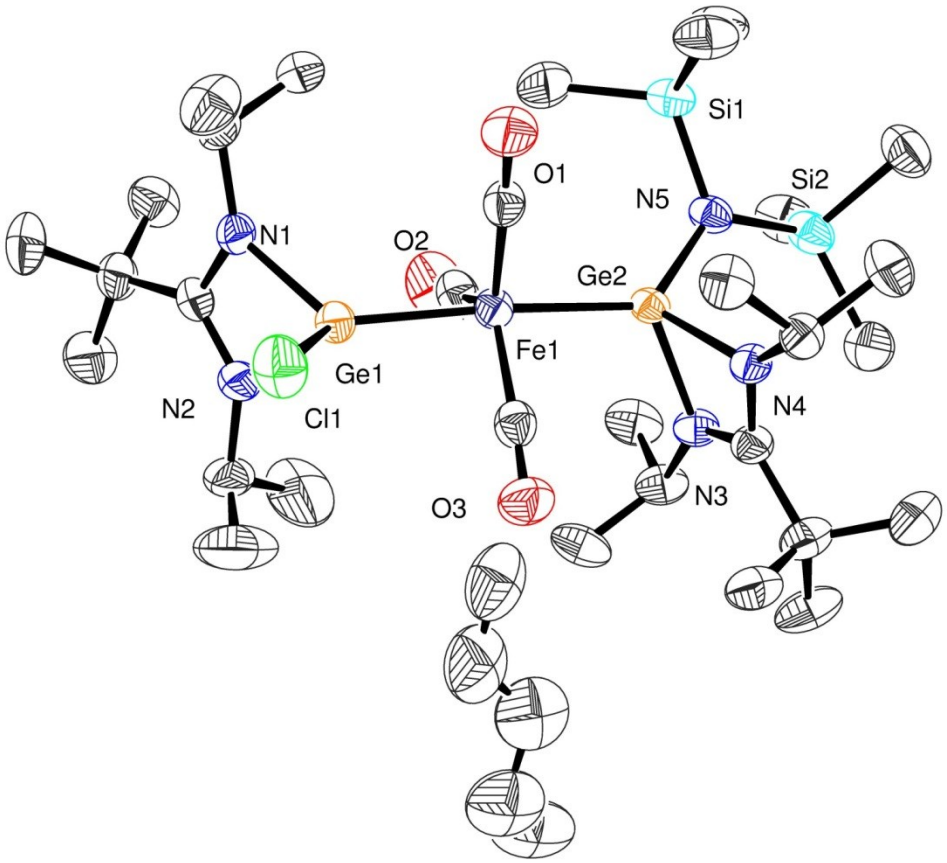


Figure S2 : Asymmetric Unit

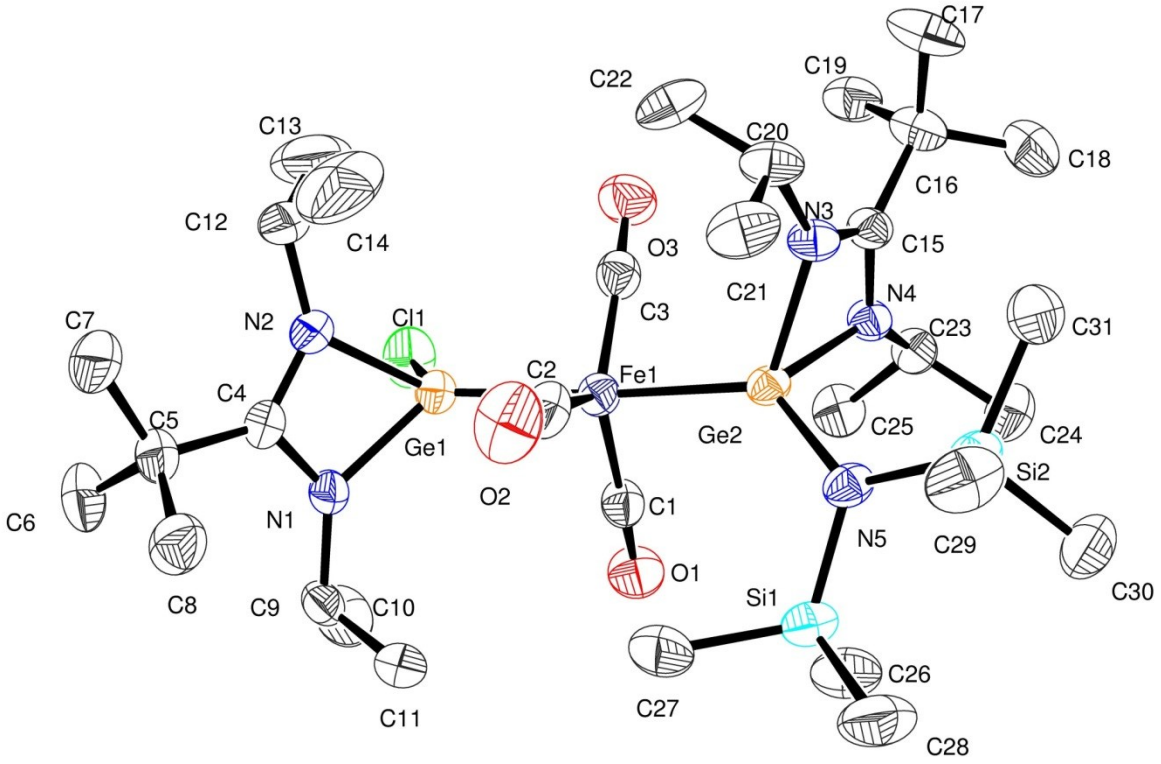


Figure S3 : Compound

Table S6. Crystal data and structure refinement for AS17041.

Identification code	AS17041
Empirical formula	C31 H64 Cl Fe Ge2 N5 O3 Si2, 0.5(C5 H12)
Formula weight	883.65
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, C 2/c
Unit cell dimensions	a = 44.814(2) A alpha = 90 deg. b = 9.9093(4) A beta = 107.296(2) deg. c = 21.2706(10) A gamma = 90 deg.

Volume	9018.7(7) A^3
Z, Calculated density	8, 1.302 Mg/m^3
Absorption coefficient	1.789 mm^-1
F(000)	3720
Crystal size	0.120 x 0.100 x 0.040 mm
Theta range for data collection	3.510 to 25.349 deg.
Limiting indices	-53<=h<=53, -11<=k<=11, -25<=l<=25
Reflections collected / unique	104234 / 8212 [R(int) = 0.0829]
Completeness to theta = 25.242	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8212 / 34 / 474
Goodness-of-fit on F^2	1.092
Final R indices [I>2sigma(I)]	R1 = 0.0383, wR2 = 0.1026
R indices (all data)	R1 = 0.0644, wR2 = 0.1158
Largest diff. peak and hole	0.569 and -0.490 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for as_a.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	6783(1)	4088(4)	7041(2)	38(1)
C(2)	6371(1)	2128(4)	6055(2)	48(1)
C(3)	6498(1)	5049(4)	5644(2)	39(1)
C(4)	7092(1)	703(4)	5689(2)	35(1)
C(5)	7162(1)	-781(4)	5580(2)	44(1)
C(6)	7519(1)	-977(5)	5755(3)	64(1)
C(7)	7020(1)	-1277(4)	4871(2)	64(1)
C(8)	7020(1)	-1662(4)	6014(2)	56(1)
C(9)	7353(1)	855(4)	6946(2)	40(1)
C(10)	7604(1)	1876(5)	7245(2)	65(1)
C(11)	7136(1)	670(5)	7371(2)	58(1)
C(12)	6790(1)	1644(5)	4547(2)	56(1)
C(13)	6881(2)	2964(6)	4299(3)	107(2)
C(14)	6445(1)	1444(9)	4389(3)	120(3)
C(15)	5814(1)	6411(4)	5791(2)	35(1)
C(16)	5683(1)	7635(4)	5347(2)	48(1)
C(17)	5409(1)	7279(5)	4728(2)	69(2)
C(18)	5552(1)	8713(5)	5725(2)	66(1)
C(19)	5951(1)	8241(4)	5125(2)	53(1)
C(20)	5595(1)	4334(4)	5057(2)	45(1)
C(21)	5526(1)	2925(4)	5263(2)	55(1)
C(22)	5783(1)	4254(5)	4569(2)	58(1)
C(23)	6159(1)	7642(4)	6805(2)	37(1)
C(24)	6003(1)	7848(4)	7341(2)	54(1)
C(25)	6505(1)	7377(4)	7108(2)	47(1)
C(26)	6365(1)	4169(5)	8335(2)	65(1)
C(27)	6356(1)	1579(5)	7567(2)	62(1)
C(28)	5873(1)	2033(5)	8178(2)	71(2)
C(29)	5262(1)	2613(5)	6857(2)	62(1)
C(30)	5482(1)	5022(5)	7778(2)	61(1)
C(31)	5271(1)	5386(5)	6359(2)	55(1)
C(32)	5273(5)	810(20)	3505(11)	116(6)
C(33)	5170(6)	840(20)	2812(10)	130(5)
C(34)	4857(6)	1160(20)	2433(9)	124(5)
C(35)	4789(6)	1300(20)	1686(11)	132(6)
C(36)	4494(5)	914(18)	1323(8)	137(6)
N(1)	7177(1)	1306(3)	6279(1)	35(1)
N(2)	6937(1)	1620(3)	5261(2)	42(1)
N(3)	5762(1)	5089(3)	5649(1)	35(1)
N(4)	6017(1)	6479(3)	6390(1)	33(1)
N(5)	5889(1)	3848(3)	7034(1)	35(1)
O(1)	6948(1)	4296(3)	7566(1)	53(1)
O(2)	6264(1)	1047(3)	5941(2)	71(1)
O(3)	6480(1)	5876(3)	5254(2)	57(1)
Si(1)	6114(1)	2972(1)	7739(1)	43(1)
Si(2)	5501(1)	4189(1)	7001(1)	44(1)
Cl(1)	7326(1)	4298(1)	5870(1)	58(1)
Fe(1)	6539(1)	3747(1)	6238(1)	32(1)

Ge(1)	6948(1)	2933(1)	5951(1)	35(1)
Ge(2)	6092(1)	4515(1)	6442(1)	29(1)

Table S8. Bond lengths [A] and angles [deg] for as_a.

C(1)-O(1)	1.158(4)
C(1)-Fe(1)	1.766(4)
C(2)-O(2)	1.170(5)
C(2)-Fe(1)	1.766(4)
C(3)-O(3)	1.153(5)
C(3)-Fe(1)	1.777(4)
C(4)-N(2)	1.327(5)
C(4)-N(1)	1.339(5)
C(4)-C(5)	1.535(5)
C(5)-C(7)	1.533(6)
C(5)-C(8)	1.539(6)
C(5)-C(6)	1.546(6)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-N(1)	1.473(5)
C(9)-C(10)	1.508(6)
C(9)-C(11)	1.521(6)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-N(2)	1.466(5)
C(12)-C(14)	1.494(7)
C(12)-C(13)	1.511(7)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-N(4)	1.330(4)
C(15)-N(3)	1.349(5)
C(15)-C(16)	1.542(5)
C(16)-C(19)	1.538(6)
C(16)-C(17)	1.550(6)
C(16)-C(18)	1.554(6)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800

C(19)-H(19C)	0.9800
C(20)-N(3)	1.466(5)
C(20)-C(22)	1.522(6)
C(20)-C(21)	1.523(6)
C(20)-H(20)	1.0000
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-N(4)	1.475(4)
C(23)-C(25)	1.516(5)
C(23)-C(24)	1.517(6)
C(23)-H(23)	1.0000
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-H(25A)	0.9800
C(25)-H(25B)	0.9800
C(25)-H(25C)	0.9800
C(26)-Si(1)	1.852(4)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-Si(1)	1.857(5)
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-Si(1)	1.872(5)
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800
C(28)-H(28C)	0.9800
C(29)-Si(2)	1.867(4)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-Si(2)	1.871(4)
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-Si(2)	1.870(4)
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-C(33)	1.41(2)
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(34)	1.431(15)
C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900
C(34)-C(35)	1.533(19)
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-C(36)	1.37(2)
C(35)-H(35A)	0.9900
C(35)-H(35B)	0.9900

C(36)-H(36A)	0.9800
C(36)-H(36B)	0.9800
C(36)-H(36C)	0.9800
N(1)-Ge(1)	1.927(3)
N(2)-Ge(1)	1.950(3)
N(3)-Ge(2)	1.967(3)
N(4)-Ge(2)	1.973(3)
N(5)-Si(2)	1.751(3)
N(5)-Si(1)	1.767(3)
N(5)-Ge(2)	1.881(3)
Cl(1)-Ge(1)	2.2156(11)
Fe(1)-Ge(1)	2.2458(6)
Fe(1)-Ge(2)	2.3007(6)

O(1)-C(1)-Fe(1)	178.6(4)
O(2)-C(2)-Fe(1)	178.9(5)
O(3)-C(3)-Fe(1)	177.5(4)
N(2)-C(4)-N(1)	106.3(3)
N(2)-C(4)-C(5)	129.9(3)
N(1)-C(4)-C(5)	123.8(3)
C(7)-C(5)-C(4)	114.3(3)
C(7)-C(5)-C(8)	106.5(4)
C(4)-C(5)-C(8)	108.3(3)
C(7)-C(5)-C(6)	107.1(4)
C(4)-C(5)-C(6)	109.0(3)
C(8)-C(5)-C(6)	111.6(4)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(1)-C(9)-C(10)	108.7(3)
N(1)-C(9)-C(11)	110.8(3)
C(10)-C(9)-C(11)	111.2(4)
N(1)-C(9)-H(9)	108.7
C(10)-C(9)-H(9)	108.7
C(11)-C(9)-H(9)	108.7
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5

H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(2)-C(12)-C(14)	110.4(4)
N(2)-C(12)-C(13)	107.0(4)
C(14)-C(12)-C(13)	113.9(5)
N(2)-C(12)-H(12)	108.5
C(14)-C(12)-H(12)	108.5
C(13)-C(12)-H(12)	108.5
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
N(4)-C(15)-N(3)	106.6(3)
N(4)-C(15)-C(16)	125.1(3)
N(3)-C(15)-C(16)	128.2(3)
C(19)-C(16)-C(15)	107.7(3)
C(19)-C(16)-C(17)	108.7(4)
C(15)-C(16)-C(17)	113.7(3)
C(19)-C(16)-C(18)	110.0(4)
C(15)-C(16)-C(18)	111.0(3)
C(17)-C(16)-C(18)	105.7(4)
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5
C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(16)-C(19)-H(19A)	109.5
C(16)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(16)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
N(3)-C(20)-C(22)	111.5(3)
N(3)-C(20)-C(21)	108.4(3)
C(22)-C(20)-C(21)	110.6(4)
N(3)-C(20)-H(20)	108.8
C(22)-C(20)-H(20)	108.8
C(21)-C(20)-H(20)	108.8
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5

C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
N(4)-C(23)-C(25)	108.9(3)
N(4)-C(23)-C(24)	110.0(3)
C(25)-C(23)-C(24)	110.2(3)
N(4)-C(23)-H(23)	109.2
C(25)-C(23)-H(23)	109.2
C(24)-C(23)-H(23)	109.2
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5
H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
Si(1)-C(26)-H(26A)	109.5
Si(1)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
Si(1)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
Si(1)-C(27)-H(27A)	109.5
Si(1)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
Si(1)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
Si(1)-C(28)-H(28A)	109.5
Si(1)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
Si(1)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
Si(2)-C(29)-H(29A)	109.5
Si(2)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
Si(2)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
Si(2)-C(30)-H(30A)	109.5
Si(2)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
Si(2)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
Si(2)-C(31)-H(31A)	109.5

Si(2)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
Si(2)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(33)-C(32)-H(32A)	109.5
C(33)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(33)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(32)-C(33)-C(34)	123.8(17)
C(32)-C(33)-H(33A)	106.4
C(34)-C(33)-H(33A)	106.4
C(32)-C(33)-H(33B)	106.4
C(34)-C(33)-H(33B)	106.4
H(33A)-C(33)-H(33B)	106.5
C(33)-C(34)-C(35)	117.6(19)
C(33)-C(34)-H(34A)	107.9
C(35)-C(34)-H(34A)	107.9
C(33)-C(34)-H(34B)	107.9
C(35)-C(34)-H(34B)	107.9
H(34A)-C(34)-H(34B)	107.2
C(36)-C(35)-C(34)	114.9(19)
C(36)-C(35)-H(35A)	108.6
C(34)-C(35)-H(35A)	108.6
C(36)-C(35)-H(35B)	108.6
C(34)-C(35)-H(35B)	108.5
H(35A)-C(35)-H(35B)	107.5
C(35)-C(36)-H(36A)	109.5
C(35)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(35)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(4)-N(1)-C(9)	133.5(3)
C(4)-N(1)-Ge(1)	93.6(2)
C(9)-N(1)-Ge(1)	132.7(2)
C(4)-N(2)-C(12)	134.8(3)
C(4)-N(2)-Ge(1)	92.9(2)
C(12)-N(2)-Ge(1)	132.2(3)
C(15)-N(3)-C(20)	134.2(3)
C(15)-N(3)-Ge(2)	93.1(2)
C(20)-N(3)-Ge(2)	130.6(3)
C(15)-N(4)-C(23)	131.5(3)
C(15)-N(4)-Ge(2)	93.4(2)
C(23)-N(4)-Ge(2)	134.5(2)
Si(2)-N(5)-Si(1)	116.07(17)
Si(2)-N(5)-Ge(2)	125.33(17)
Si(1)-N(5)-Ge(2)	118.15(16)
N(5)-Si(1)-C(26)	110.08(19)
N(5)-Si(1)-C(27)	114.75(19)
C(26)-Si(1)-C(27)	109.9(2)
N(5)-Si(1)-C(28)	113.45(19)
C(26)-Si(1)-C(28)	107.5(2)
C(27)-Si(1)-C(28)	100.7(2)
N(5)-Si(2)-C(29)	111.1(2)
N(5)-Si(2)-C(31)	118.46(17)

C(29)-Si(2)-C(31)	104.2(2)
N(5)-Si(2)-C(30)	110.84(18)
C(29)-Si(2)-C(30)	109.8(2)
C(31)-Si(2)-C(30)	101.8(2)
C(1)-Fe(1)-C(2)	119.26(19)
C(1)-Fe(1)-C(3)	116.92(18)
C(2)-Fe(1)-C(3)	123.70(19)
C(1)-Fe(1)-Ge(1)	90.66(12)
C(2)-Fe(1)-Ge(1)	86.72(13)
C(3)-Fe(1)-Ge(1)	89.36(12)
C(1)-Fe(1)-Ge(2)	94.47(12)
C(2)-Fe(1)-Ge(2)	90.19(14)
C(3)-Fe(1)-Ge(2)	88.90(12)
Ge(1)-Fe(1)-Ge(2)	174.83(3)
N(1)-Ge(1)-N(2)	66.79(13)
N(1)-Ge(1)-Cl(1)	101.63(10)
N(2)-Ge(1)-Cl(1)	101.34(11)
N(1)-Ge(1)-Fe(1)	126.26(9)
N(2)-Ge(1)-Fe(1)	127.22(10)
Cl(1)-Ge(1)-Fe(1)	120.43(4)
N(5)-Ge(2)-N(3)	106.58(13)
N(5)-Ge(2)-N(4)	105.96(13)
N(3)-Ge(2)-N(4)	66.08(12)
N(5)-Ge(2)-Fe(1)	129.24(10)
N(3)-Ge(2)-Fe(1)	114.11(9)
N(4)-Ge(2)-Fe(1)	117.36(9)

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for as_a. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	35(2)	38(2)	41(2)	-5(2)	9(2)	2(2)
C(2)	51(3)	49(3)	45(3)	-10(2)	18(2)	0(2)
C(3)	32(2)	44(2)	42(2)	-4(2)	11(2)	0(2)
C(4)	36(2)	35(2)	36(2)	-6(2)	15(2)	0(2)
C(5)	51(2)	35(2)	48(3)	-4(2)	18(2)	7(2)
C(6)	59(3)	59(3)	80(4)	-8(3)	30(3)	20(2)
C(7)	92(4)	46(3)	52(3)	-16(2)	20(3)	7(3)
C(8)	73(3)	44(2)	55(3)	-5(2)	25(2)	-3(2)
C(9)	40(2)	37(2)	36(2)	-2(2)	2(2)	11(2)
C(10)	54(3)	59(3)	65(3)	-15(2)	-7(2)	1(2)
C(11)	69(3)	63(3)	42(3)	15(2)	18(2)	26(2)
C(12)	80(3)	54(3)	29(2)	-1(2)	8(2)	20(2)
C(13)	180(7)	85(4)	46(3)	16(3)	18(4)	16(4)
C(14)	69(4)	224(8)	50(3)	-38(4)	-9(3)	9(5)
C(15)	28(2)	44(2)	31(2)	3(2)	5(2)	2(2)
C(16)	48(2)	45(2)	42(2)	8(2)	0(2)	4(2)
C(17)	56(3)	71(3)	57(3)	20(3)	-17(2)	3(2)
C(18)	65(3)	60(3)	70(3)	15(3)	18(3)	22(2)
C(19)	62(3)	47(3)	45(3)	12(2)	9(2)	2(2)
C(20)	40(2)	54(3)	31(2)	-3(2)	-8(2)	-8(2)
C(21)	59(3)	59(3)	38(2)	-14(2)	0(2)	-21(2)
C(22)	70(3)	72(3)	27(2)	-10(2)	9(2)	-18(3)
C(23)	40(2)	32(2)	36(2)	-8(2)	6(2)	-3(2)
C(24)	60(3)	55(3)	50(3)	-16(2)	21(2)	-4(2)
C(25)	40(2)	46(2)	49(3)	-13(2)	3(2)	-12(2)
C(26)	67(3)	77(3)	38(3)	1(2)	-4(2)	-5(3)
C(27)	76(3)	52(3)	60(3)	22(2)	24(3)	10(2)
C(28)	71(3)	91(4)	51(3)	26(3)	19(3)	-4(3)
C(29)	49(3)	84(3)	53(3)	0(3)	14(2)	-26(2)
C(30)	57(3)	81(3)	51(3)	-9(2)	26(2)	0(3)
C(31)	33(2)	78(3)	55(3)	5(2)	14(2)	1(2)
C(32)	104(11)	84(12)	141(13)	-34(11)	10(11)	9(10)
C(33)	161(9)	76(9)	150(12)	-34(10)	44(11)	10(8)
C(34)	162(9)	62(8)	136(12)	-27(7)	28(10)	-28(7)
C(35)	186(12)	68(9)	138(12)	5(8)	40(11)	-22(8)
C(36)	211(15)	79(10)	115(11)	9(9)	37(12)	-44(12)
N(1)	38(2)	32(2)	33(2)	-4(1)	9(1)	5(1)
N(2)	55(2)	40(2)	30(2)	-2(2)	12(2)	10(2)
N(3)	31(2)	40(2)	28(2)	-1(1)	0(1)	-5(1)
N(4)	30(2)	35(2)	29(2)	-4(1)	2(1)	0(1)
N(5)	31(2)	45(2)	28(2)	-1(1)	7(1)	-6(1)
O(1)	45(2)	62(2)	41(2)	-11(2)	-4(1)	-3(1)
O(2)	86(3)	42(2)	89(3)	-24(2)	33(2)	-25(2)
O(3)	63(2)	53(2)	57(2)	17(2)	21(2)	5(2)
Si(1)	45(1)	50(1)	31(1)	4(1)	9(1)	-4(1)

Si(2)	35(1)	62(1)	36(1)	-3(1)	12(1)	-7(1)
Cl(1)	59(1)	48(1)	76(1)	1(1)	33(1)	-7(1)
Fe(1)	33(1)	31(1)	31(1)	-4(1)	7(1)	-1(1)
Ge(1)	40(1)	32(1)	33(1)	-2(1)	12(1)	3(1)
Ge(2)	28(1)	34(1)	23(1)	-3(1)	4(1)	-3(1)

Crystal data and structure refinement of compound **3**

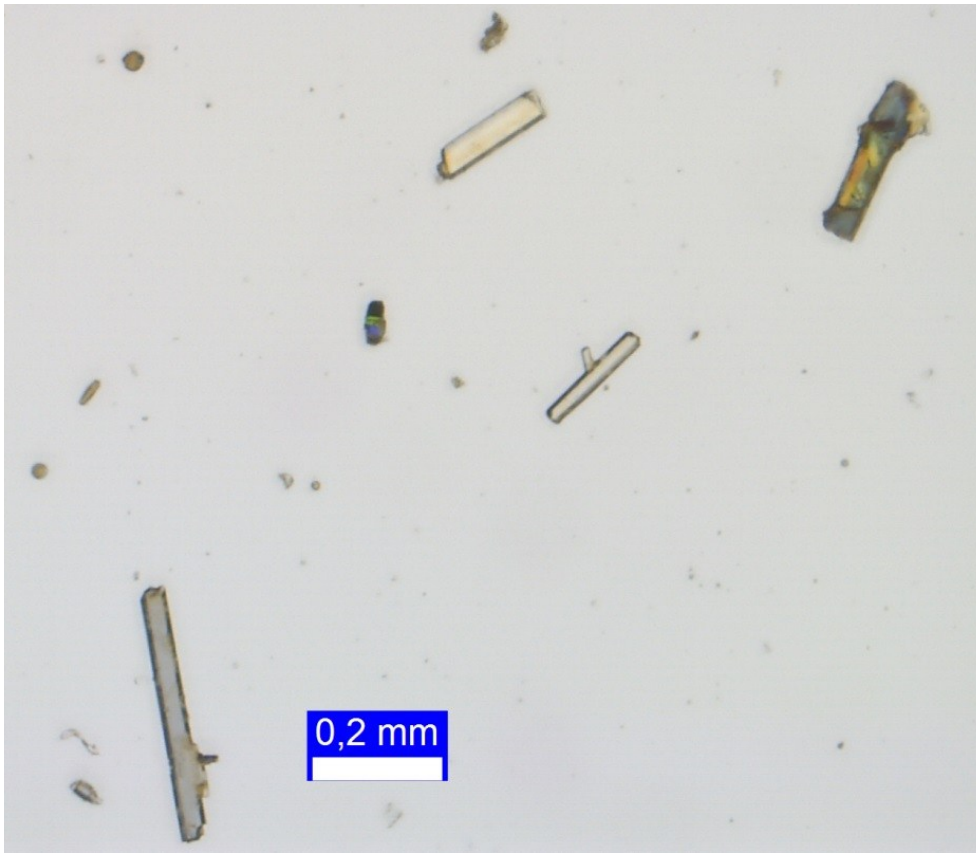


Figure S4 : Sample

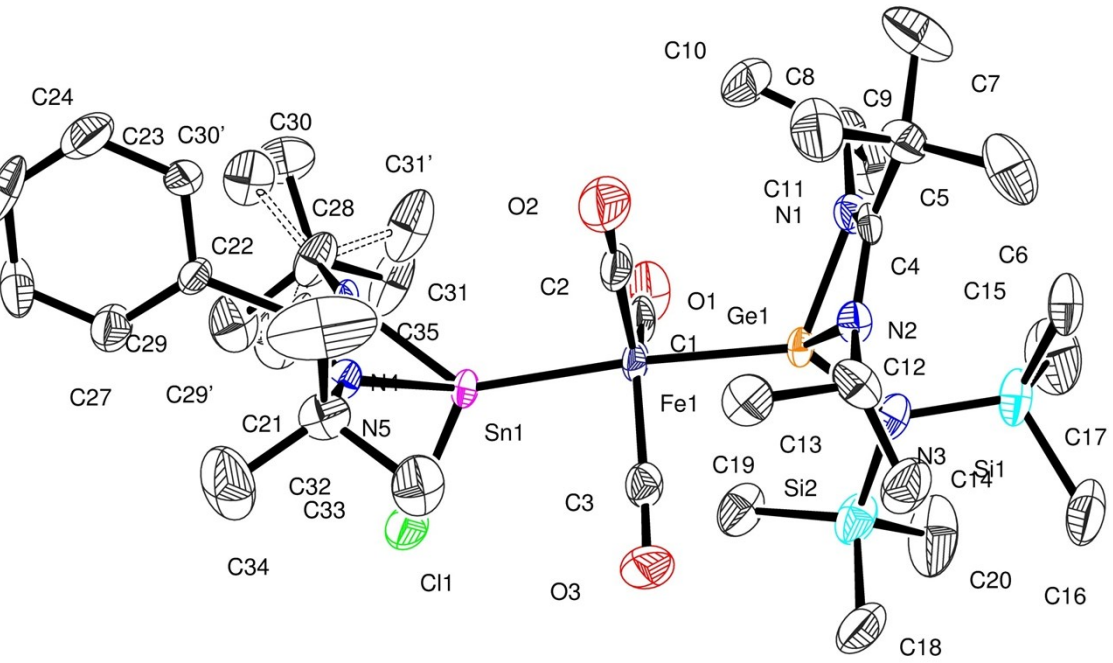


Figure S5 : One molecule of the asymmetric Unit

Table S10. Crystal data and structure refinement for AS18045.

Identification code	AS18045
Empirical formula	C35 H64 Cl Fe Ge N5 O3 Si2 Sn
Formula weight	941.71
Temperature	193(2) K
Wavelength	0.71073 A

Crystal system, space group	Monoclinic, P c
Unit cell dimensions	a = 10.8967(4) A alpha = 90 deg. b = 33.0836(13) A beta = 105.207(2) deg. c = 13.0091(6) A gamma = 90 deg.
Volume	4525.6(3) A^3
Z, Calculated density	4, 1.382 Mg/m^3
Absorption coefficient	1.672 mm^-1
F(000)	1944
Crystal size	0.200 x 0.080 x 0.080 mm
Theta range for data collection	3.481 to 25.680 deg.
Limiting indices	-13<=h<=13, -40<=k<=39, -14<=l<=15
Reflections collected / unique	38811 / 14165 [R(int) = 0.0370]
Completeness to theta = 25.242	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	14165 / 260 / 1022
Goodness-of-fit on F^2	1.050
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.1047
R indices (all data)	R1 = 0.0538, wR2 = 0.1109
Absolute structure parameter	-0.007(8)
Largest diff. peak and hole	2.876 and -0.591 e.A^-3

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for as18045_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	3584(8)	6724(3)	8431(7)	36(2)
C(2)	4605(8)	6161(3)	7031(7)	36(2)
C(3)	2410(8)	5847(3)	7868(7)	34(2)
C(4)	2656(7)	6511(2)	4650(6)	26(2)
C(5)	3164(9)	6495(3)	3652(7)	36(2)
C(6)	2088(13)	6415(4)	2638(8)	66(3)
C(7)	3850(14)	6878(4)	3431(10)	74(4)
C(8)	4175(11)	6146(4)	3799(9)	60(3)
C(9)	3393(9)	7206(3)	5502(8)	42(2)
C(10)	4776(9)	7169(3)	6156(10)	60(3)
C(11)	2675(11)	7487(3)	6054(9)	54(3)
C(12)	1693(9)	5796(2)	4584(7)	37(2)
C(13)	2626(9)	5494(2)	5218(8)	40(2)
C(14)	386(10)	5695(3)	4645(10)	55(3)
C(15)	-80(9)	6906(3)	3909(8)	50(3)
C(16)	-2205(10)	6608(4)	4736(9)	65(3)
C(17)	-989(14)	7435(4)	5408(12)	87(5)
C(18)	-1102(10)	6056(4)	7088(9)	66(3)
C(19)	754(10)	6596(4)	8679(8)	54(3)
C(20)	-1548(12)	6955(5)	7375(10)	94(5)
C(21)	7217(7)	5676(3)	10008(6)	26(2)
C(22)	8544(7)	5523(2)	10442(7)	26(2)
C(23)	9486(8)	5633(3)	9947(8)	37(2)
C(24)	10742(9)	5525(3)	10403(10)	51(3)
C(25)	11072(9)	5322(3)	11326(9)	51(3)
C(26)	10155(10)	5208(3)	11833(8)	50(3)
C(27)	8900(9)	5313(3)	11380(8)	42(2)
N(4)	6824(6)	6036(2)	10176(6)	29(2)
C(28)	7426(9)	6347(3)	10961(9)	45(2)
C(29)	7670(20)	6150(5)	12113(11)	57(5)
C(30)	8631(16)	6519(6)	10823(17)	61(5)
C(31)	6400(14)	6657(5)	10982(19)	64(5)
C(29')	7050(50)	6284(16)	12030(30)	66(9)
C(30')	8830(20)	6403(14)	11140(50)	52(10)
C(31')	6740(50)	6729(9)	10410(40)	68(10)
C(32)	6231(9)	5049(2)	8946(8)	38(2)
C(33)	4832(10)	4980(3)	8318(9)	52(3)
C(34)	6585(14)	4716(3)	9779(12)	86(5)
C(35)	7023(15)	5039(4)	8159(13)	100(6)
C(36)	3562(9)	9145(3)	3082(8)	39(2)
C(37)	5751(9)	8857(3)	2213(7)	35(2)
C(38)	4761(8)	8282(3)	3642(7)	37(2)
C(39)	3838(8)	8479(2)	-147(7)	30(2)
C(40)	4323(10)	8498(3)	-1173(7)	39(2)
C(41)	5278(11)	8851(3)	-1051(9)	55(3)
C(42)	3166(11)	8558(4)	-2161(8)	58(3)
C(43)	4993(12)	8114(3)	-1402(9)	58(3)

C(44)	2805(9)	9180(2)	-239(7)	38(2)
C(45)	3703(10)	9495(2)	400(8)	47(3)
C(46)	1423(10)	9261(4)	-199(11)	65(3)
C(47)	4733(9)	7806(2)	736(8)	37(2)
C(48)	6081(10)	7885(3)	1314(10)	55(3)
C(49)	4134(12)	7515(3)	1365(9)	52(3)
N(8)	1598(6)	8291(2)	1474(6)	32(2)
Si(4)	665(3)	8016(1)	413(2)	48(1)
C(50)	-913(17)	8313(8)	-56(14)	48(2)
C(51)	1310(20)	7965(9)	-764(15)	50(1)
C(52)	300(30)	7488(5)	763(18)	50(2)
C(50')	-1056(18)	8177(13)	-30(20)	48(2)
C(51')	1140(30)	8006(12)	-854(18)	50(2)
C(52')	710(40)	7464(6)	870(20)	49(2)
C(53)	74(11)	8922(3)	2228(10)	60(3)
C(54)	1911(9)	8391(3)	3890(8)	48(3)
C(55)	-362(10)	8028(4)	2608(9)	67(3)
C(56)	8322(7)	9345(2)	5255(6)	22(2)
C(57)	9669(8)	9478(2)	5659(7)	29(2)
C(58)	10546(9)	9358(3)	5138(9)	45(2)
C(59)	11833(10)	9463(3)	5582(10)	56(3)
C(60)	12212(9)	9679(3)	6507(9)	51(3)
C(61)	11308(9)	9809(3)	6978(9)	51(3)
C(62)	10048(9)	9710(3)	6566(8)	41(2)
N(9)	7379(6)	9555(2)	4671(6)	27(2)
C(63)	7342(9)	9945(2)	4112(8)	39(2)
C(64)	8290(20)	9975(8)	3450(20)	52(4)
C(65)	7650(30)	10282(5)	4968(18)	48(5)
C(66)	5968(16)	9996(9)	3430(20)	45(5)
C(64')	7890(40)	9867(10)	3150(20)	46(5)
C(65')	8020(40)	10288(8)	4790(30)	48(6)
C(66')	5910(20)	10038(12)	3630(30)	43(5)
N(10)	7931(7)	8972(2)	5466(6)	27(2)
C(67)	8502(9)	8672(3)	6279(8)	39(2)
C(68)	9620(20)	8471(8)	5970(30)	39(6)
C(69)	8970(40)	8862(9)	7395(15)	57(7)
C(70)	7490(30)	8353(8)	6280(30)	35(6)
C(68')	9820(20)	8536(12)	6310(40)	53(8)
C(69')	8440(50)	8855(10)	7368(18)	57(8)
C(70')	7590(30)	8310(8)	6040(30)	32(7)
N(1)	2724(6)	6817(2)	5351(5)	28(2)
N(2)	2017(6)	6209(2)	4973(5)	26(1)
N(3)	388(6)	6670(2)	6265(6)	34(2)
N(5)	6264(6)	5449(2)	9443(5)	25(2)
N(6)	3152(6)	8770(2)	154(6)	31(2)
N(7)	3962(7)	8179(2)	554(6)	30(2)
O(1)	3662(7)	7030(2)	8803(6)	54(2)
O(2)	5319(7)	6109(3)	6525(6)	61(2)
O(3)	1735(7)	5585(2)	7938(6)	53(2)
O(4)	2877(7)	9403(2)	3125(6)	53(2)
O(5)	6466(7)	8924(2)	1729(6)	56(2)
O(6)	4827(7)	7971(2)	4034(6)	54(2)
Si(1)	-639(3)	6891(1)	5140(2)	42(1)
Si(2)	-327(2)	6564(1)	7307(2)	46(1)
Si(3)	871(2)	8410(1)	2502(2)	39(1)
Fe(1)	3490(1)	6237(1)	7788(1)	25(1)
Fe(2)	4652(1)	8762(1)	2992(1)	26(1)
Ge(1)	2034(1)	6485(1)	6325(1)	23(1)

Ge(2)	3232(1)	8498(1)	1526(1)	24(1)
Sn(1)	4900(1)	5931(1)	9317(1)	23(1)
Sn(2)	6024(1)	9071(1)	4536(1)	23(1)
Cl(1)	4163(2)	5719(1)	10806(2)	50(1)
Cl(2)	5232(2)	9284(1)	5997(2)	51(1)

Table S12. Bond lengths [A] and angles [deg] for as18045_a.

C(1)-O(1)	1.114(10)
C(1)-Fe(1)	1.804(9)
C(2)-O(2)	1.157(11)
C(2)-Fe(1)	1.770(9)
C(3)-O(3)	1.155(10)
C(3)-Fe(1)	1.770(9)
C(4)-N(2)	1.348(10)
C(4)-N(1)	1.351(10)
C(4)-C(5)	1.540(11)
C(5)-C(7)	1.536(14)
C(5)-C(6)	1.541(15)
C(5)-C(8)	1.571(13)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-N(1)	1.467(10)
C(9)-C(11)	1.512(14)
C(9)-C(10)	1.529(13)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-N(2)	1.466(10)
C(12)-C(14)	1.486(14)
C(12)-C(13)	1.508(12)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-Si(1)	1.857(11)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-Si(1)	1.895(12)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-Si(1)	1.890(12)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-Si(2)	1.870(12)
C(18)-H(18A)	0.9800

C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-Si(2)	1.866(10)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-Si(2)	1.876(12)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-N(4)	1.302(10)
C(21)-N(5)	1.335(10)
C(21)-C(22)	1.496(10)
C(22)-C(27)	1.369(12)
C(22)-C(23)	1.395(11)
C(23)-C(24)	1.388(13)
C(23)-H(23)	0.9500
C(24)-C(25)	1.339(15)
C(24)-H(24)	0.9500
C(25)-C(26)	1.386(15)
C(25)-H(25)	0.9500
C(26)-C(27)	1.383(13)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
N(4)-C(28)	1.477(11)
N(4)-Sn(1)	2.129(6)
C(28)-C(30)	1.486(16)
C(28)-C(30')	1.50(2)
C(28)-C(31)	1.523(14)
C(28)-C(31')	1.55(2)
C(28)-C(29')	1.56(3)
C(28)-C(29)	1.591(17)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(29')-H(29D)	0.9800
C(29')-H(29E)	0.9800
C(29')-H(29F)	0.9800
C(30')-H(30D)	0.9800
C(30')-H(30E)	0.9800
C(30')-H(30F)	0.9800
C(31')-H(31D)	0.9800
C(31')-H(31E)	0.9800
C(31')-H(31F)	0.9800
C(32)-N(5)	1.471(10)
C(32)-C(35)	1.503(14)
C(32)-C(34)	1.522(15)
C(32)-C(33)	1.545(13)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800

C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-O(4)	1.143(10)
C(36)-Fe(2)	1.764(9)
C(37)-O(5)	1.145(10)
C(37)-Fe(2)	1.787(9)
C(38)-O(6)	1.144(10)
C(38)-Fe(2)	1.786(9)
C(39)-N(7)	1.330(10)
C(39)-N(6)	1.340(10)
C(39)-C(40)	1.560(11)
C(40)-C(43)	1.534(13)
C(40)-C(41)	1.545(12)
C(40)-C(42)	1.559(15)
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-N(6)	1.462(10)
C(44)-C(45)	1.519(13)
C(44)-C(46)	1.544(13)
C(44)-H(44)	1.0000
C(45)-H(45A)	0.9800
C(45)-H(45B)	0.9800
C(45)-H(45C)	0.9800
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800
C(47)-N(7)	1.475(10)
C(47)-C(48)	1.487(14)
C(47)-C(49)	1.517(12)
C(47)-H(47)	1.0000
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-H(49A)	0.9800
C(49)-H(49B)	0.9800
C(49)-H(49C)	0.9800
N(8)-Si(4)	1.739(7)
N(8)-Si(3)	1.768(7)
N(8)-Ge(2)	1.894(6)
Si(4)-C(51')	1.853(17)
Si(4)-C(51)	1.854(14)
Si(4)-C(52)	1.875(14)
Si(4)-C(50')	1.888(18)
Si(4)-C(52')	1.919(17)
Si(4)-C(50)	1.934(15)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800

C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(50')-H(50D)	0.9800
C(50')-H(50E)	0.9800
C(50')-H(50F)	0.9800
C(51')-H(51D)	0.9800
C(51')-H(51E)	0.9800
C(51')-H(51F)	0.9800
C(52')-H(52D)	0.9800
C(52')-H(52E)	0.9800
C(52')-H(52F)	0.9800
C(53)-Si(3)	1.894(11)
C(53)-H(53A)	0.9800
C(53)-H(53B)	0.9800
C(53)-H(53C)	0.9800
C(54)-Si(3)	1.864(11)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-Si(3)	1.875(10)
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-N(9)	1.306(10)
C(56)-N(10)	1.359(9)
C(56)-C(57)	1.489(11)
C(57)-C(58)	1.367(12)
C(57)-C(62)	1.376(12)
C(58)-C(59)	1.413(14)
C(58)-H(58)	0.9500
C(59)-C(60)	1.368(16)
C(59)-H(59)	0.9500
C(60)-C(61)	1.358(15)
C(60)-H(60)	0.9500
C(61)-C(62)	1.376(13)
C(61)-H(61)	0.9500
C(62)-H(62)	0.9500
N(9)-C(63)	1.475(10)
N(9)-Sn(2)	2.155(6)
C(63)-C(64)	1.506(16)
C(63)-C(65')	1.51(2)
C(63)-C(66)	1.537(17)
C(63)-C(64')	1.545(19)
C(63)-C(65)	1.551(17)
C(63)-C(66')	1.55(2)
C(64)-H(64A)	0.9800
C(64)-H(64B)	0.9800
C(64)-H(64C)	0.9800
C(65)-H(65A)	0.9800
C(65)-H(65B)	0.9800
C(65)-H(65C)	0.9800
C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800

C(64')-H(64D)	0.9800
C(64')-H(64E)	0.9800
C(64')-H(64F)	0.9800
C(65')-H(65D)	0.9800
C(65')-H(65E)	0.9800
C(65')-H(65F)	0.9800
C(66')-H(66D)	0.9800
C(66')-H(66E)	0.9800
C(66')-H(66F)	0.9800
N(10)-C(67)	1.463(10)
N(10)-Sn(2)	2.138(7)
C(67)-C(68')	1.49(2)
C(67)-C(70)	1.526(17)
C(67)-C(68)	1.531(18)
C(67)-C(70')	1.535(18)
C(67)-C(69)	1.542(19)
C(67)-C(69')	1.56(2)
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800
C(70)-H(70C)	0.9800
C(68')-H(68D)	0.9800
C(68')-H(68E)	0.9800
C(68')-H(68F)	0.9800
C(69')-H(69D)	0.9800
C(69')-H(69E)	0.9800
C(69')-H(69F)	0.9800
C(70')-H(70D)	0.9800
C(70')-H(70E)	0.9800
C(70')-H(70F)	0.9800
N(1)-Ge(1)	1.969(7)
N(2)-Ge(1)	1.978(6)
N(3)-Si(1)	1.751(8)
N(3)-Si(2)	1.767(8)
N(3)-Ge(1)	1.877(7)
N(5)-Sn(1)	2.157(6)
N(6)-Ge(2)	1.980(7)
N(7)-Ge(2)	1.970(7)
Fe(1)-Ge(1)	2.2869(14)
Fe(1)-Sn(1)	2.3957(12)
Fe(2)-Ge(2)	2.2897(14)
Fe(2)-Sn(2)	2.3955(13)
Sn(1)-Cl(1)	2.389(2)
Sn(2)-Cl(2)	2.391(2)

O(1)-C(1)-Fe(1)	177.5(9)
O(2)-C(2)-Fe(1)	179.0(9)
O(3)-C(3)-Fe(1)	178.0(9)
N(2)-C(4)-N(1)	106.7(7)
N(2)-C(4)-C(5)	124.4(7)
N(1)-C(4)-C(5)	128.9(7)
C(7)-C(5)-C(4)	115.4(8)
C(7)-C(5)-C(6)	106.2(9)

C(4)-C(5)-C(6)	111.5(8)
C(7)-C(5)-C(8)	105.5(9)
C(4)-C(5)-C(8)	108.6(7)
C(6)-C(5)-C(8)	109.3(8)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(1)-C(9)-C(11)	107.6(8)
N(1)-C(9)-C(10)	112.7(8)
C(11)-C(9)-C(10)	110.1(9)
N(1)-C(9)-H(9)	108.8
C(11)-C(9)-H(9)	108.8
C(10)-C(9)-H(9)	108.8
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(2)-C(12)-C(14)	109.8(8)
N(2)-C(12)-C(13)	111.2(7)
C(14)-C(12)-C(13)	109.8(8)
N(2)-C(12)-H(12)	108.6
C(14)-C(12)-H(12)	108.6
C(13)-C(12)-H(12)	108.6
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5

Si(1)-C(15)-H(15A)	109.5
Si(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
Si(1)-C(16)-H(16A)	109.5
Si(1)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
Si(1)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
Si(1)-C(17)-H(17A)	109.5
Si(1)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
Si(1)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
Si(2)-C(18)-H(18A)	109.5
Si(2)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
Si(2)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
Si(2)-C(19)-H(19A)	109.5
Si(2)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
Si(2)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
Si(2)-C(20)-H(20A)	109.5
Si(2)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
Si(2)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N(4)-C(21)-N(5)	111.3(6)
N(4)-C(21)-C(22)	125.0(7)
N(5)-C(21)-C(22)	123.6(7)
C(27)-C(22)-C(23)	118.2(8)
C(27)-C(22)-C(21)	121.9(7)
C(23)-C(22)-C(21)	119.5(7)
C(24)-C(23)-C(22)	119.9(9)
C(24)-C(23)-H(23)	120.1
C(22)-C(23)-H(23)	120.1
C(25)-C(24)-C(23)	121.0(9)
C(25)-C(24)-H(24)	119.5
C(23)-C(24)-H(24)	119.5
C(24)-C(25)-C(26)	120.4(9)
C(24)-C(25)-H(25)	119.8
C(26)-C(25)-H(25)	119.8
C(27)-C(26)-C(25)	119.0(9)
C(27)-C(26)-H(26)	120.5
C(25)-C(26)-H(26)	120.5
C(22)-C(27)-C(26)	121.6(9)
C(22)-C(27)-H(27)	119.2
C(26)-C(27)-H(27)	119.2
C(21)-N(4)-C(28)	130.3(7)

C(21)-N(4)-Sn(1)	95.0(5)
C(28)-N(4)-Sn(1)	132.3(6)
N(4)-C(28)-C(30)	115.5(11)
N(4)-C(28)-C(30')	116(2)
N(4)-C(28)-C(31)	106.7(8)
C(30)-C(28)-C(31)	114.8(12)
N(4)-C(28)-C(31')	100.3(17)
C(30')-C(28)-C(31')	109(2)
N(4)-C(28)-C(29')	110.5(18)
C(30')-C(28)-C(29')	112(2)
C(31')-C(28)-C(29')	108(2)
N(4)-C(28)-C(29)	107.5(9)
C(30)-C(28)-C(29)	109.6(12)
C(31)-C(28)-C(29)	101.6(12)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(28)-C(31)-H(31A)	109.5
C(28)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(28)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(29')-H(29D)	109.5
C(28)-C(29')-H(29E)	109.5
H(29D)-C(29')-H(29E)	109.5
C(28)-C(29')-H(29F)	109.5
H(29D)-C(29')-H(29F)	109.5
H(29E)-C(29')-H(29F)	109.5
C(28)-C(30')-H(30D)	109.5
C(28)-C(30')-H(30E)	109.5
H(30D)-C(30')-H(30E)	109.5
C(28)-C(30')-H(30F)	109.5
H(30D)-C(30')-H(30F)	109.5
H(30E)-C(30')-H(30F)	109.5
C(28)-C(31')-H(31D)	109.5
C(28)-C(31')-H(31E)	109.5
H(31D)-C(31')-H(31E)	109.5
C(28)-C(31')-H(31F)	109.5
H(31D)-C(31')-H(31F)	109.5
H(31E)-C(31')-H(31F)	109.5
N(5)-C(32)-C(35)	111.4(8)
N(5)-C(32)-C(34)	111.5(9)
C(35)-C(32)-C(34)	112.7(11)
N(5)-C(32)-C(33)	105.7(7)
C(35)-C(32)-C(33)	107.5(10)
C(34)-C(32)-C(33)	107.5(8)
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5

H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(32)-C(35)-H(35A)	109.5
C(32)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(32)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
O(4)-C(36)-Fe(2)	177.7(9)
O(5)-C(37)-Fe(2)	178.6(8)
O(6)-C(38)-Fe(2)	178.3(8)
N(7)-C(39)-N(6)	107.6(7)
N(7)-C(39)-C(40)	128.4(7)
N(6)-C(39)-C(40)	124.0(7)
C(43)-C(40)-C(41)	107.7(8)
C(43)-C(40)-C(42)	105.5(9)
C(41)-C(40)-C(42)	111.5(8)
C(43)-C(40)-C(39)	114.6(7)
C(41)-C(40)-C(39)	108.3(7)
C(42)-C(40)-C(39)	109.2(8)
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(40)-C(43)-H(43A)	109.5
C(40)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(40)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
N(6)-C(44)-C(45)	112.0(8)
N(6)-C(44)-C(46)	108.4(7)
C(45)-C(44)-C(46)	110.8(9)
N(6)-C(44)-H(44)	108.5
C(45)-C(44)-H(44)	108.5
C(46)-C(44)-H(44)	108.5
C(44)-C(45)-H(45A)	109.5
C(44)-C(45)-H(45B)	109.5
H(45A)-C(45)-H(45B)	109.5
C(44)-C(45)-H(45C)	109.5
H(45A)-C(45)-H(45C)	109.5
H(45B)-C(45)-H(45C)	109.5

C(44)-C(46)-H(46A)	109.5
C(44)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(44)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
N(7)-C(47)-C(48)	112.3(7)
N(7)-C(47)-C(49)	108.0(7)
C(48)-C(47)-C(49)	110.3(9)
N(7)-C(47)-H(47)	108.7
C(48)-C(47)-H(47)	108.7
C(49)-C(47)-H(47)	108.7
C(47)-C(48)-H(48A)	109.5
C(47)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(47)-C(48)-H(48C)	109.5
H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(47)-C(49)-H(49A)	109.5
C(47)-C(49)-H(49B)	109.5
H(49A)-C(49)-H(49B)	109.5
C(47)-C(49)-H(49C)	109.5
H(49A)-C(49)-H(49C)	109.5
H(49B)-C(49)-H(49C)	109.5
Si(4)-N(8)-Si(3)	115.6(3)
Si(4)-N(8)-Ge(2)	124.5(4)
Si(3)-N(8)-Ge(2)	119.8(4)
N(8)-Si(4)-C(51')	118.3(12)
N(8)-Si(4)-C(51)	115.7(9)
N(8)-Si(4)-C(52)	114.3(8)
C(51)-Si(4)-C(52)	105.4(10)
N(8)-Si(4)-C(50')	115.0(11)
C(51')-Si(4)-C(50')	102.7(12)
N(8)-Si(4)-C(52')	106.7(10)
C(51')-Si(4)-C(52')	105.6(13)
C(50')-Si(4)-C(52')	107.9(10)
N(8)-Si(4)-C(50)	105.8(8)
C(51)-Si(4)-C(50)	106.6(9)
C(52)-Si(4)-C(50)	108.7(7)
Si(4)-C(50)-H(50A)	109.5
Si(4)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
Si(4)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
Si(4)-C(51)-H(51A)	109.5
Si(4)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
Si(4)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
Si(4)-C(52)-H(52A)	109.5
Si(4)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
Si(4)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
Si(4)-C(50')-H(50D)	109.5

Si(4)-C(50')-H(50E)	109.5
H(50D)-C(50')-H(50E)	109.5
Si(4)-C(50')-H(50F)	109.5
H(50D)-C(50')-H(50F)	109.5
H(50E)-C(50')-H(50F)	109.5
Si(4)-C(51')-H(51D)	109.5
Si(4)-C(51')-H(51E)	109.5
H(51D)-C(51')-H(51E)	109.5
Si(4)-C(51')-H(51F)	109.5
H(51D)-C(51')-H(51F)	109.5
H(51E)-C(51')-H(51F)	109.5
Si(4)-C(52')-H(52D)	109.5
Si(4)-C(52')-H(52E)	109.5
H(52D)-C(52')-H(52E)	109.5
Si(4)-C(52')-H(52F)	109.5
H(52D)-C(52')-H(52F)	109.5
H(52E)-C(52')-H(52F)	109.5
Si(3)-C(53)-H(53A)	109.5
Si(3)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53B)	109.5
Si(3)-C(53)-H(53C)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
Si(3)-C(54)-H(54A)	109.5
Si(3)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
Si(3)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
Si(3)-C(55)-H(55A)	109.5
Si(3)-C(55)-H(55B)	109.5
H(55A)-C(55)-H(55B)	109.5
Si(3)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
N(9)-C(56)-N(10)	111.1(7)
N(9)-C(56)-C(57)	126.9(7)
N(10)-C(56)-C(57)	122.0(7)
C(58)-C(57)-C(62)	119.6(8)
C(58)-C(57)-C(56)	119.4(8)
C(62)-C(57)-C(56)	120.9(7)
C(57)-C(58)-C(59)	118.3(10)
C(57)-C(58)-H(58)	120.8
C(59)-C(58)-H(58)	120.8
C(60)-C(59)-C(58)	121.7(9)
C(60)-C(59)-H(59)	119.1
C(58)-C(59)-H(59)	119.1
C(61)-C(60)-C(59)	118.3(9)
C(61)-C(60)-H(60)	120.8
C(59)-C(60)-H(60)	120.8
C(60)-C(61)-C(62)	121.1(10)
C(60)-C(61)-H(61)	119.5
C(62)-C(61)-H(61)	119.5
C(61)-C(62)-C(57)	120.8(9)
C(61)-C(62)-H(62)	119.6
C(57)-C(62)-H(62)	119.6
C(56)-N(9)-C(63)	131.8(7)
C(56)-N(9)-Sn(2)	94.0(4)

C(63)-N(9)-Sn(2)	132.8(6)
N(9)-C(63)-C(64)	113.9(10)
N(9)-C(63)-C(65')	115.3(15)
N(9)-C(63)-C(66)	106.2(12)
C(64)-C(63)-C(66)	111.7(14)
N(9)-C(63)-C(64')	106.7(12)
C(65')-C(63)-C(64')	111.3(16)
N(9)-C(63)-C(65)	107.6(11)
C(64)-C(63)-C(65)	108.0(12)
C(66)-C(63)-C(65)	109.3(13)
N(9)-C(63)-C(66')	105.5(16)
C(65')-C(63)-C(66')	111.9(18)
C(64')-C(63)-C(66')	105.5(18)
C(63)-C(64)-H(64A)	109.5
C(63)-C(64)-H(64B)	109.5
H(64A)-C(64)-H(64B)	109.5
C(63)-C(64)-H(64C)	109.5
H(64A)-C(64)-H(64C)	109.5
H(64B)-C(64)-H(64C)	109.5
C(63)-C(65)-H(65A)	109.5
C(63)-C(65)-H(65B)	109.5
H(65A)-C(65)-H(65B)	109.5
C(63)-C(65)-H(65C)	109.5
H(65A)-C(65)-H(65C)	109.5
H(65B)-C(65)-H(65C)	109.5
C(63)-C(66)-H(66A)	109.5
C(63)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(63)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
C(63)-C(64')-H(64D)	109.5
C(63)-C(64')-H(64E)	109.5
H(64D)-C(64')-H(64E)	109.5
C(63)-C(64')-H(64F)	109.5
H(64D)-C(64')-H(64F)	109.5
H(64E)-C(64')-H(64F)	109.5
C(63)-C(65')-H(65D)	109.5
C(63)-C(65')-H(65E)	109.5
H(65D)-C(65')-H(65E)	109.5
C(63)-C(65')-H(65F)	109.5
H(65D)-C(65')-H(65F)	109.5
H(65E)-C(65')-H(65F)	109.5
C(63)-C(66')-H(66D)	109.5
C(63)-C(66')-H(66E)	109.5
H(66D)-C(66')-H(66E)	109.5
C(63)-C(66')-H(66F)	109.5
H(66D)-C(66')-H(66F)	109.5
H(66E)-C(66')-H(66F)	109.5
C(56)-N(10)-C(67)	131.7(7)
C(56)-N(10)-Sn(2)	93.2(5)
C(67)-N(10)-Sn(2)	132.7(5)
N(10)-C(67)-C(68')	116.6(17)
N(10)-C(67)-C(70)	107.3(15)
N(10)-C(67)-C(68)	108.8(13)
C(70)-C(67)-C(68)	108.8(14)
N(10)-C(67)-C(70')	104.6(14)
C(68')-C(67)-C(70')	109.7(17)

N(10)-C(67)-C(69)	112.2(13)
C(70)-C(67)-C(69)	110.2(16)
C(68)-C(67)-C(69)	109.4(15)
N(10)-C(67)-C(69')	106.4(15)
C(68')-C(67)-C(69')	111.2(17)
C(70')-C(67)-C(69')	107.8(17)
C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(67)-C(69)-H(69A)	109.5
C(67)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(67)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(67)-C(70)-H(70A)	109.5
C(67)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5
C(67)-C(70)-H(70C)	109.5
H(70A)-C(70)-H(70C)	109.5
H(70B)-C(70)-H(70C)	109.5
C(67)-C(68')-H(68D)	109.5
C(67)-C(68')-H(68E)	109.5
H(68D)-C(68')-H(68E)	109.5
C(67)-C(68')-H(68F)	109.5
H(68D)-C(68')-H(68F)	109.5
H(68E)-C(68')-H(68F)	109.5
C(67)-C(69')-H(69D)	109.5
C(67)-C(69')-H(69E)	109.5
H(69D)-C(69')-H(69E)	109.5
C(67)-C(69')-H(69F)	109.5
H(69D)-C(69')-H(69F)	109.5
H(69E)-C(69')-H(69F)	109.5
C(67)-C(70')-H(70D)	109.5
C(67)-C(70')-H(70E)	109.5
H(70D)-C(70')-H(70E)	109.5
C(67)-C(70')-H(70F)	109.5
H(70D)-C(70')-H(70F)	109.5
H(70E)-C(70')-H(70F)	109.5
C(4)-N(1)-C(9)	133.3(7)
C(4)-N(1)-Ge(1)	93.1(5)
C(9)-N(1)-Ge(1)	131.6(6)
C(4)-N(2)-C(12)	132.9(7)
C(4)-N(2)-Ge(1)	92.8(5)
C(12)-N(2)-Ge(1)	133.1(5)
Si(1)-N(3)-Si(2)	114.2(4)
Si(1)-N(3)-Ge(1)	124.4(4)
Si(2)-N(3)-Ge(1)	120.8(4)
C(21)-N(5)-C(32)	132.4(7)
C(21)-N(5)-Sn(1)	92.7(4)
C(32)-N(5)-Sn(1)	134.1(6)
C(39)-N(6)-C(44)	132.7(7)
C(39)-N(6)-Ge(2)	92.3(5)
C(44)-N(6)-Ge(2)	133.0(5)
C(39)-N(7)-C(47)	133.3(7)

C(39)-N(7)-Ge(2)	93.0(5)
C(47)-N(7)-Ge(2)	130.9(6)
N(3)-Si(1)-C(15)	116.7(4)
N(3)-Si(1)-C(17)	111.0(5)
C(15)-Si(1)-C(17)	105.1(6)
N(3)-Si(1)-C(16)	110.9(5)
C(15)-Si(1)-C(16)	104.4(5)
C(17)-Si(1)-C(16)	108.1(6)
N(3)-Si(2)-C(19)	115.3(4)
N(3)-Si(2)-C(18)	109.6(4)
C(19)-Si(2)-C(18)	110.1(5)
N(3)-Si(2)-C(20)	111.1(5)
C(19)-Si(2)-C(20)	101.1(6)
C(18)-Si(2)-C(20)	109.3(7)
N(8)-Si(3)-C(54)	116.5(4)
N(8)-Si(3)-C(55)	112.2(5)
C(54)-Si(3)-C(55)	99.9(5)
N(8)-Si(3)-C(53)	109.3(4)
C(54)-Si(3)-C(53)	110.1(5)
C(55)-Si(3)-C(53)	108.3(6)
C(3)-Fe(1)-C(2)	119.5(4)
C(3)-Fe(1)-C(1)	125.6(4)
C(2)-Fe(1)-C(1)	114.9(4)
C(3)-Fe(1)-Ge(1)	89.1(3)
C(2)-Fe(1)-Ge(1)	90.9(3)
C(1)-Fe(1)-Ge(1)	90.5(3)
C(3)-Fe(1)-Sn(1)	86.2(3)
C(2)-Fe(1)-Sn(1)	91.0(3)
C(1)-Fe(1)-Sn(1)	92.6(3)
Ge(1)-Fe(1)-Sn(1)	175.27(6)
C(36)-Fe(2)-C(38)	124.7(4)
C(36)-Fe(2)-C(37)	118.3(4)
C(38)-Fe(2)-C(37)	117.0(4)
C(36)-Fe(2)-Ge(2)	90.5(3)
C(38)-Fe(2)-Ge(2)	90.2(3)
C(37)-Fe(2)-Ge(2)	90.1(3)
C(36)-Fe(2)-Sn(2)	85.4(3)
C(38)-Fe(2)-Sn(2)	91.9(3)
C(37)-Fe(2)-Sn(2)	92.1(3)
Ge(2)-Fe(2)-Sn(2)	175.94(6)
N(3)-Ge(1)-N(1)	108.3(3)
N(3)-Ge(1)-N(2)	109.2(3)
N(1)-Ge(1)-N(2)	66.6(3)
N(3)-Ge(1)-Fe(1)	126.7(2)
N(1)-Ge(1)-Fe(1)	115.9(2)
N(2)-Ge(1)-Fe(1)	114.59(19)
N(8)-Ge(2)-N(7)	108.5(3)
N(8)-Ge(2)-N(6)	108.3(3)
N(7)-Ge(2)-N(6)	66.1(3)
N(8)-Ge(2)-Fe(2)	126.3(2)
N(7)-Ge(2)-Fe(2)	116.1(2)
N(6)-Ge(2)-Fe(2)	116.0(2)
N(4)-Sn(1)-N(5)	61.0(2)
N(4)-Sn(1)-Cl(1)	96.7(2)
N(5)-Sn(1)-Cl(1)	95.26(18)
N(4)-Sn(1)-Fe(1)	134.11(18)
N(5)-Sn(1)-Fe(1)	130.90(18)
Cl(1)-Sn(1)-Fe(1)	121.28(7)

N(10)-Sn(2)-N(9)	61.6(2)
N(10)-Sn(2)-Cl(2)	95.44(19)
N(9)-Sn(2)-Cl(2)	95.61(19)
N(10)-Sn(2)-Fe(2)	135.20(17)
N(9)-Sn(2)-Fe(2)	130.50(19)
Cl(2)-Sn(2)-Fe(2)	121.10(7)

Symmetry transformations used to generate equivalent atoms:

Table S13. Anisotropic displacement parameters (A^2 x 10^3) for as18045_a.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	33(5)	36(5)	26(5)	5(4)	-13(4)	1(4)
C(2)	26(4)	50(5)	26(5)	4(4)	-3(4)	5(4)
C(3)	35(5)	37(5)	25(5)	-2(4)	-1(4)	-2(4)
C(4)	24(4)	29(4)	20(4)	8(3)	-3(3)	5(3)
C(5)	42(5)	34(4)	34(5)	3(4)	15(4)	2(4)
C(6)	97(10)	75(8)	24(6)	5(5)	15(6)	13(7)
C(7)	110(11)	72(8)	52(8)	17(6)	40(8)	-9(8)
C(8)	56(7)	85(8)	45(7)	10(6)	22(6)	24(6)
C(9)	47(6)	32(4)	37(5)	3(4)	-4(4)	-14(4)
C(10)	38(6)	60(7)	72(8)	3(6)	-3(6)	-20(5)
C(11)	74(8)	28(5)	52(7)	-5(5)	0(6)	-1(5)
C(12)	59(6)	27(4)	23(5)	-4(4)	10(4)	-3(4)
C(13)	42(5)	26(4)	52(6)	-6(4)	12(5)	4(4)
C(14)	42(6)	38(5)	71(8)	-2(5)	-6(5)	-7(5)
C(15)	42(6)	54(6)	44(6)	6(5)	-6(5)	21(5)
C(16)	37(6)	106(10)	45(7)	5(7)	-2(5)	19(6)
C(17)	94(10)	71(8)	93(11)	8(8)	19(9)	48(8)
C(18)	33(6)	121(10)	40(6)	0(7)	3(5)	-22(6)
C(19)	40(6)	91(8)	31(6)	-12(5)	9(5)	-2(6)
C(20)	63(8)	169(15)	54(8)	-2(9)	23(7)	58(9)
C(21)	11(3)	48(5)	16(4)	-12(4)	-2(3)	7(3)
C(22)	17(4)	30(4)	30(5)	0(4)	3(3)	0(3)
C(23)	26(4)	41(5)	48(6)	17(4)	16(4)	6(4)
C(24)	28(5)	55(6)	74(8)	-2(6)	19(5)	0(5)
C(25)	23(5)	53(6)	68(8)	-21(6)	-5(5)	20(4)
C(26)	48(6)	60(6)	37(6)	12(5)	3(5)	26(5)
C(27)	33(5)	59(6)	33(5)	6(5)	8(4)	6(4)
N(4)	20(3)	26(3)	30(4)	6(3)	-12(3)	-5(3)
C(28)	32(5)	41(5)	55(6)	-21(4)	-3(4)	1(4)
C(29)	66(11)	60(9)	35(8)	-11(7)	-5(7)	-4(8)
C(30)	57(9)	48(11)	75(12)	-14(8)	12(8)	-28(8)
C(31)	41(8)	45(8)	89(12)	-39(8)	-15(8)	17(6)
C(29')	69(16)	55(15)	63(15)	-18(14)	-6(14)	-3(14)
C(30')	54(16)	21(17)	70(19)	-18(15)	-5(15)	-13(14)
C(31')	47(17)	53(16)	87(19)	-38(16)	-15(16)	12(15)
C(32)	42(5)	28(4)	45(6)	-10(4)	15(4)	-1(4)
C(33)	59(7)	39(5)	48(7)	-12(5)	-4(5)	-6(5)
C(34)	95(10)	35(6)	100(11)	13(6)	-23(9)	-7(6)
C(35)	121(13)	90(9)	118(14)	-76(10)	86(12)	-46(9)
C(36)	37(5)	37(5)	40(6)	5(4)	6(4)	3(4)
C(37)	38(5)	33(4)	31(5)	-3(4)	7(4)	-9(4)
C(38)	34(5)	39(5)	34(6)	0(4)	2(4)	-4(4)
C(39)	36(5)	27(4)	28(5)	-6(3)	12(4)	-16(4)

C(40)	54(6)	38(5)	27(5)	-1(4)	16(4)	-13(4)
C(41)	72(7)	50(6)	58(7)	-11(5)	45(6)	-28(5)
C(42)	76(8)	74(7)	26(5)	-5(5)	17(5)	-18(6)
C(43)	87(8)	51(6)	54(7)	-10(5)	47(7)	-9(6)
C(44)	56(6)	29(4)	31(5)	12(4)	18(4)	0(4)
C(45)	69(7)	27(4)	53(7)	0(4)	28(6)	-6(4)
C(46)	45(6)	66(7)	82(9)	27(7)	10(6)	21(6)
C(47)	49(6)	22(4)	45(6)	-4(4)	22(5)	0(4)
C(48)	42(6)	42(5)	79(9)	0(5)	12(6)	8(5)
C(49)	86(8)	28(5)	55(7)	4(4)	41(6)	2(5)
N(8)	21(3)	50(4)	29(4)	2(3)	12(3)	-20(3)
Si(4)	44(2)	66(2)	35(2)	-3(1)	10(1)	-30(1)
C(50)	43(3)	66(3)	35(3)	-3(3)	12(2)	-31(2)
C(51)	46(3)	66(3)	36(3)	-4(2)	8(2)	-29(2)
C(52)	44(3)	66(3)	38(3)	-4(2)	10(2)	-30(2)
C(50')	43(3)	66(3)	35(3)	-3(3)	11(2)	-31(3)
C(51')	46(3)	66(3)	36(3)	-4(2)	9(2)	-29(2)
C(52')	44(3)	66(3)	37(3)	-4(2)	10(2)	-30(3)
C(53)	52(7)	67(7)	61(8)	12(6)	18(6)	19(6)
C(54)	44(6)	70(7)	37(6)	4(5)	22(5)	-3(5)
C(55)	46(6)	112(10)	48(7)	8(7)	19(6)	-24(7)
C(56)	24(4)	19(3)	29(4)	-9(3)	15(4)	-6(3)
C(57)	24(4)	28(4)	37(5)	-6(4)	14(4)	-6(3)
C(58)	42(5)	49(5)	51(6)	-5(5)	25(5)	2(5)
C(59)	33(5)	66(7)	79(9)	4(6)	32(6)	0(5)
C(60)	29(5)	60(6)	65(8)	13(6)	12(5)	-18(5)
C(61)	43(6)	54(6)	53(7)	-11(5)	8(5)	-27(5)
C(62)	38(5)	45(5)	47(6)	-13(4)	23(5)	-11(4)
N(9)	26(4)	24(3)	32(4)	2(3)	9(3)	-3(3)
C(63)	49(5)	23(3)	52(5)	7(3)	25(4)	2(3)
C(64)	56(9)	38(8)	68(9)	16(7)	28(7)	-4(7)
C(65)	52(10)	23(6)	69(9)	6(6)	13(8)	2(7)
C(66)	57(7)	34(7)	48(9)	9(7)	20(7)	9(6)
C(64')	52(10)	33(9)	60(10)	10(8)	29(8)	-4(8)
C(65')	55(11)	22(7)	67(10)	8(8)	18(9)	-8(8)
C(66')	57(8)	26(8)	49(10)	1(8)	17(8)	9(7)
N(10)	31(4)	24(3)	29(4)	4(3)	13(3)	2(3)
C(67)	40(5)	36(4)	34(5)	16(4)	-3(4)	-3(4)
C(68)	19(9)	31(10)	60(15)	4(10)	-2(9)	-5(8)
C(69)	69(17)	63(11)	31(10)	14(9)	0(10)	-15(13)
C(70)	34(10)	36(10)	35(13)	-2(9)	14(8)	-2(8)
C(68')	27(11)	41(13)	68(17)	8(12)	-26(11)	0(10)
C(69')	66(17)	66(12)	31(11)	19(10)	-4(11)	-27(14)
C(70')	34(11)	24(10)	37(14)	12(10)	7(10)	7(9)
N(1)	31(4)	30(3)	22(4)	0(3)	3(3)	-2(3)
N(2)	28(4)	24(3)	25(4)	-1(3)	2(3)	3(3)
N(3)	26(4)	39(4)	36(4)	-10(3)	4(3)	5(3)
N(5)	23(3)	22(3)	29(4)	-5(3)	4(3)	2(3)
N(6)	34(4)	31(4)	28(4)	4(3)	11(3)	-5(3)
N(7)	34(4)	28(3)	31(4)	0(3)	11(3)	-9(3)
O(1)	67(5)	36(4)	47(5)	-18(3)	-7(4)	3(3)
O(2)	45(4)	91(6)	52(5)	12(4)	19(4)	11(4)
O(3)	50(4)	49(4)	54(5)	-1(4)	4(4)	-23(4)
O(4)	49(4)	50(4)	56(5)	-5(4)	6(4)	19(4)
O(5)	52(5)	73(5)	51(5)	-4(4)	27(4)	-18(4)

O(6)	73(5)	32(4)	51(5)	12(3)	6(4)	-2(3)
Si(1)	35(1)	48(2)	35(2)	-3(1)	-4(1)	17(1)
Si(2)	30(1)	74(2)	33(2)	-8(1)	9(1)	6(1)
Si(3)	33(1)	55(2)	34(2)	7(1)	15(1)	-2(1)
Fe(1)	22(1)	29(1)	18(1)	0(1)	-6(1)	1(1)
Fe(2)	27(1)	26(1)	24(1)	-1(1)	5(1)	-2(1)
Ge(1)	22(1)	25(1)	16(1)	-2(1)	-3(1)	1(1)
Ge(2)	26(1)	25(1)	21(1)	0(1)	8(1)	-4(1)
Sn(1)	19(1)	28(1)	17(1)	-1(1)	-3(1)	2(1)
Sn(2)	24(1)	25(1)	22(1)	0(1)	8(1)	-2(1)
Cl(1)	32(1)	86(2)	32(1)	12(1)	12(1)	1(1)
Cl(2)	40(1)	83(2)	36(1)	-13(1)	22(1)	-1(1)

Crystal data and structure refinement of compound **4**

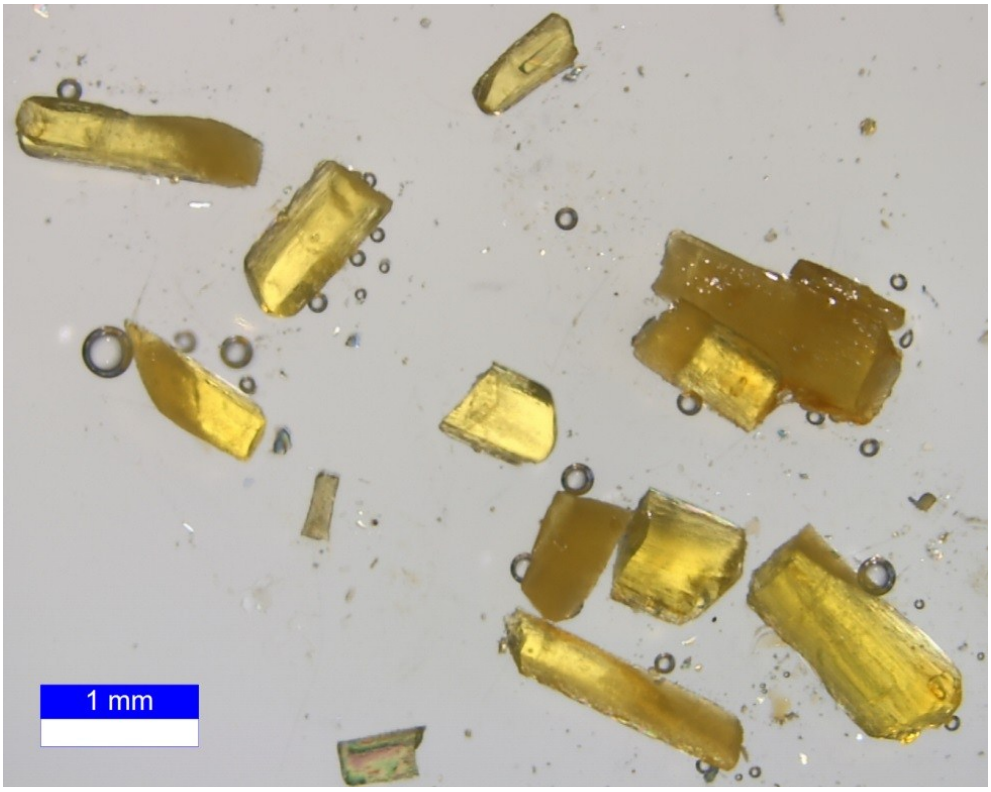


Figure S6 : Sample

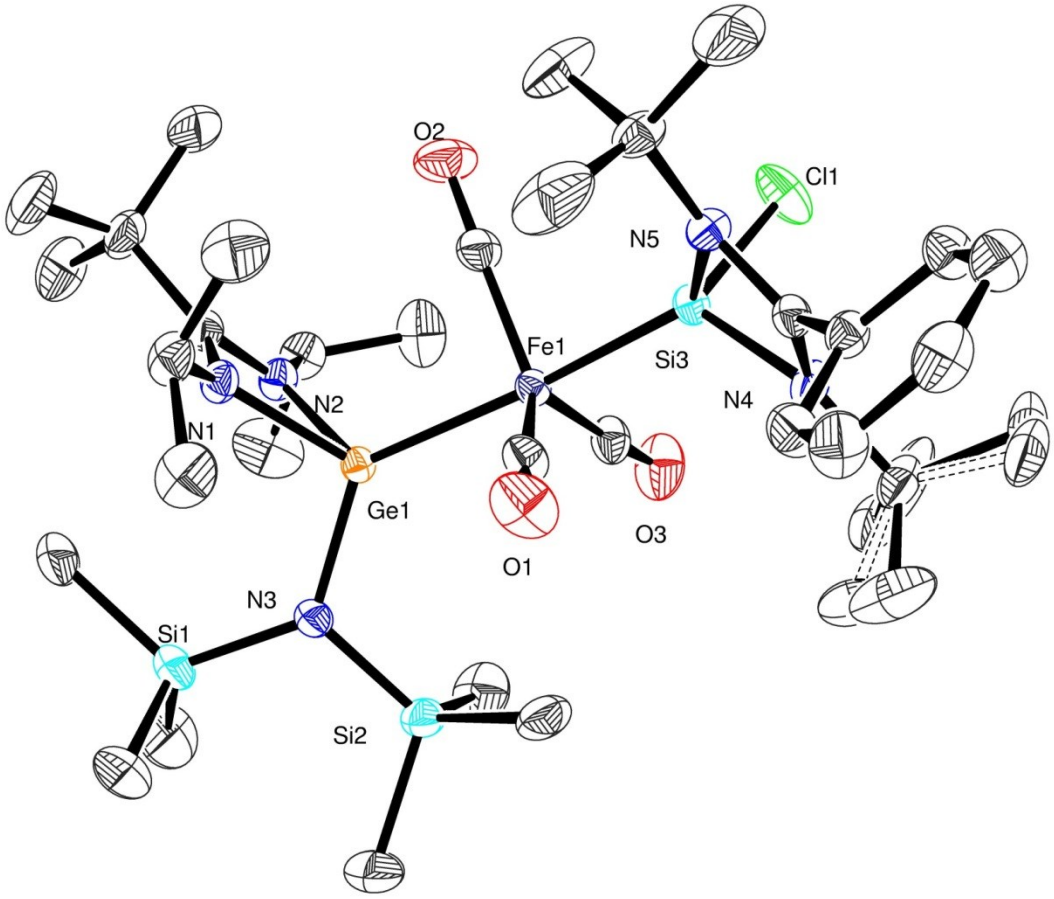


Figure S7 : Asymmetric Unit

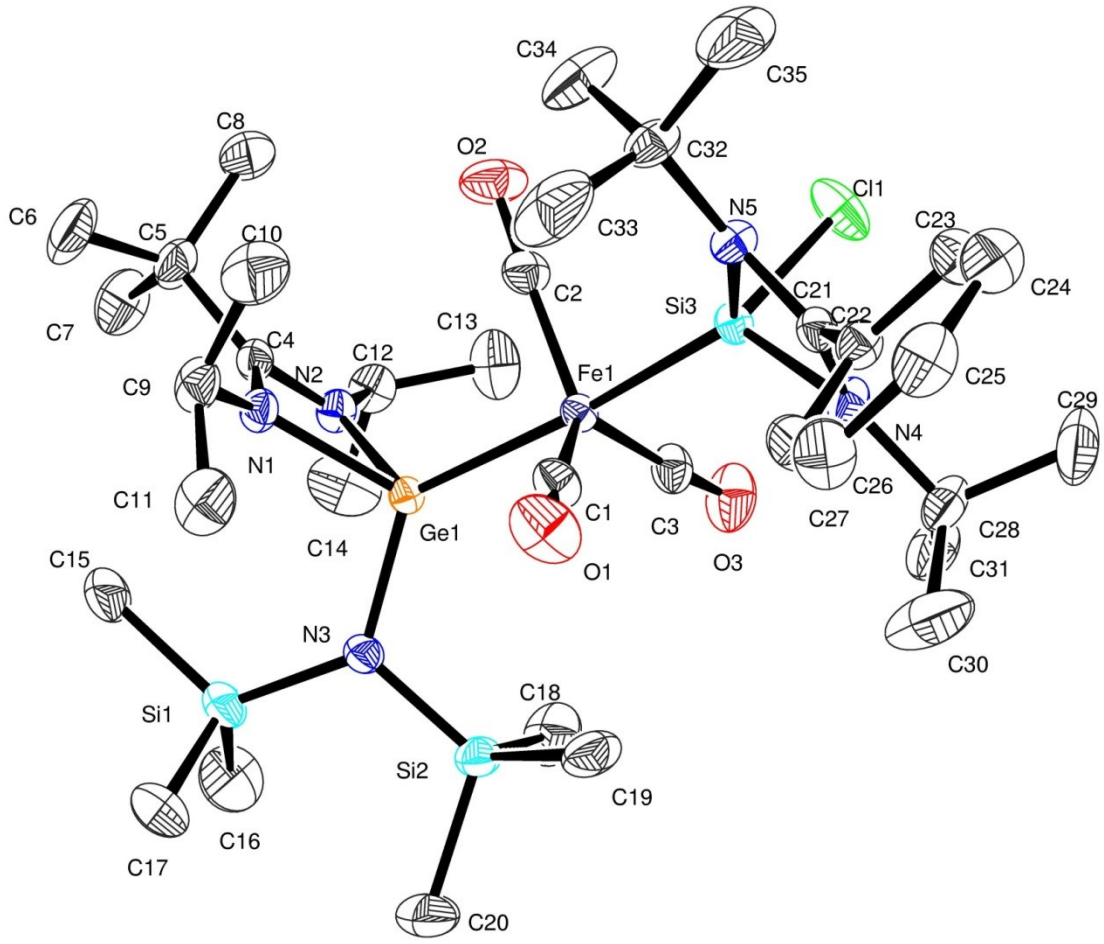


Table S14. Crystal data and structure refinement for AS18046.

Identification code	AS18046
Empirical formula	C35 H64 Cl Fe Ge N5 O3 Si3
Formula weight	851.09
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/c
Unit cell dimensions	a = 23.0059(14) A alpha = 90 deg. b = 9.9312(6) A beta = 101.860(2) deg. c = 19.8961(13) A gamma = 90 deg.

Volume	4448.7(5) A^3
Z, Calculated density	4, 1.271 Mg/m^3
Absorption coefficient	1.179 mm^-1
F(000)	1800
Crystal size	0.500 x 0.340 x 0.220 mm
Theta range for data collection	2.937 to 32.031 deg.
Limiting indices	-34<=h<=34, -14<=k<=14, -29<=l<=29
Reflections collected / unique	181117 / 15462 [R(int) = 0.0348]
Completeness to theta = 25.242	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	15462 / 63 / 487
Goodness-of-fit on F^2	1.126
Final R indices [I>2sigma(I)]	R1 = 0.0344, wR2 = 0.0827
R indices (all data)	R1 = 0.0457, wR2 = 0.0928
Largest diff. peak and hole	0.630 and -0.498 e.A^-3

Table S15. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for as18046_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	2633(1)	5681(2)	5916(1)	28(1)
C(2)	2892(1)	2592(2)	5845(1)	28(1)
C(3)	3238(1)	3908(2)	7157(1)	28(1)
C(4)	1451(1)	1640(2)	5799(1)	24(1)
C(5)	1239(1)	346(2)	5395(1)	35(1)
C(6)	833(1)	609(3)	4693(1)	55(1)
C(7)	873(1)	-540(3)	5796(2)	56(1)
C(8)	1786(1)	-432(2)	5272(1)	48(1)
C(9)	1192(1)	3561(2)	4916(1)	32(1)
C(10)	1655(1)	3476(3)	4469(1)	50(1)
C(11)	1048(1)	5029(2)	5034(1)	45(1)
C(12)	1947(1)	573(2)	6939(1)	30(1)
C(13)	2613(1)	695(2)	7222(1)	46(1)
C(14)	1609(1)	596(3)	7519(1)	58(1)
C(15)	311(1)	2891(3)	6260(1)	49(1)
C(16)	512(1)	3706(3)	7702(2)	61(1)
C(17)	241(1)	5805(3)	6545(2)	56(1)
C(18)	2181(1)	4509(3)	8326(1)	51(1)
C(19)	2325(1)	6789(2)	7361(1)	43(1)
C(20)	1265(1)	6694(3)	7943(2)	57(1)
C(21)	3977(1)	6530(2)	5462(1)	21(1)
C(22)	4059(1)	7780(2)	5083(1)	23(1)
C(23)	4559(1)	7950(2)	4803(1)	28(1)
C(24)	4598(1)	9066(2)	4390(1)	34(1)
C(25)	4148(1)	10002(2)	4268(1)	37(1)
C(26)	3657(1)	9856(2)	4566(1)	38(1)
C(27)	3610(1)	8740(2)	4976(1)	32(1)
N(4)	4039(1)	6363(1)	6141(1)	25(1)
C(28)	4296(1)	7267(2)	6721(1)	33(1)
C(29)	4948(4)	7500(17)	6710(7)	57(3)
C(30)	3985(7)	8657(10)	6682(6)	69(3)
C(31)	4236(4)	6580(11)	7383(4)	43(2)
C(29')	4855(4)	7933(10)	6613(6)	45(2)
C(30')	3824(4)	8299(12)	6800(6)	68(3)
C(31')	4450(7)	6343(11)	7350(4)	73(3)
C(32)	3574(1)	4993(2)	4438(1)	28(1)
C(33)	3030(1)	5823(3)	4127(1)	65(1)
C(34)	3406(1)	3515(2)	4423(1)	50(1)
C(35)	4062(1)	5165(3)	4032(1)	70(1)
Fe(1)	2878(1)	4123(1)	6288(1)	18(1)
Ge(1)	1930(1)	3607(1)	6423(1)	17(1)
N(1)	1400(1)	2926(1)	5586(1)	23(1)
N(2)	1738(1)	1665(1)	6457(1)	23(1)
N(3)	1437(1)	4515(1)	6920(1)	23(1)
N(5)	3787(1)	5347(1)	5173(1)	22(1)
O(1)	2494(1)	6710(2)	5658(1)	48(1)
O(2)	2910(1)	1574(2)	5567(1)	47(1)

O(3)	3490(1)	3714(2)	7715(1)	47(1)
Si(1)	674(1)	4245(1)	6855(1)	33(1)
Si(2)	1790(1)	5563(1)	7597(1)	28(1)
Si(3)	3714(1)	4676(1)	6015(1)	19(1)
Cl(1)	4449(1)	3396(1)	6269(1)	41(1)

Table S16. Bond lengths [A] and angles [deg] for as18046_a.

C(1)-O(1)	1.159(2)
C(1)-Fe(1)	1.7579(17)
C(2)-O(2)	1.158(2)
C(2)-Fe(1)	1.7613(17)
C(3)-O(3)	1.158(2)
C(3)-Fe(1)	1.7693(17)
C(4)-N(2)	1.338(2)
C(4)-N(1)	1.343(2)
C(4)-C(5)	1.542(2)
C(5)-C(6)	1.535(3)
C(5)-C(8)	1.538(3)
C(5)-C(7)	1.549(3)
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-N(1)	1.464(2)
C(9)-C(10)	1.524(3)
C(9)-C(11)	1.524(3)
C(9)-H(9)	1.0000
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-N(2)	1.462(2)
C(12)-C(14)	1.518(3)
C(12)-C(13)	1.523(3)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-Si(1)	1.871(2)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-Si(1)	1.879(3)
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-Si(1)	1.877(2)
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-Si(2)	1.863(2)
C(18)-H(18A)	0.9800

C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-Si(2)	1.859(2)
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-Si(2)	1.881(2)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-N(4)	1.3382(19)
C(21)-N(5)	1.3416(19)
C(21)-C(22)	1.485(2)
C(22)-C(23)	1.388(2)
C(22)-C(27)	1.389(2)
C(23)-C(24)	1.394(2)
C(23)-H(23)	0.9500
C(24)-C(25)	1.377(3)
C(24)-H(24)	0.9500
C(25)-C(26)	1.387(3)
C(25)-H(25)	0.9500
C(26)-C(27)	1.393(3)
C(26)-H(26)	0.9500
C(27)-H(27)	0.9500
N(4)-C(28)	1.485(2)
N(4)-Si(3)	1.8307(14)
C(28)-C(29')	1.501(7)
C(28)-C(31)	1.515(8)
C(28)-C(29)	1.522(8)
C(28)-C(30')	1.524(8)
C(28)-C(31')	1.534(7)
C(28)-C(30)	1.549(8)
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(29')-H(29D)	0.9800
C(29')-H(29E)	0.9800
C(29')-H(29F)	0.9800
C(30')-H(30D)	0.9800
C(30')-H(30E)	0.9800
C(30')-H(30F)	0.9800
C(31')-H(31D)	0.9800
C(31')-H(31E)	0.9800
C(31')-H(31F)	0.9800
C(32)-N(5)	1.485(2)
C(32)-C(34)	1.517(3)
C(32)-C(33)	1.521(3)
C(32)-C(35)	1.522(3)
C(33)-H(33A)	0.9800
C(33)-H(33B)	0.9800
C(33)-H(33C)	0.9800
C(34)-H(34A)	0.9800

C(34)-H(34B)	0.9800
C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
Fe(1)-Si(3)	2.1734(5)
Fe(1)-Ge(1)	2.3098(3)
Ge(1)-N(3)	1.8817(13)
Ge(1)-N(1)	1.9691(13)
Ge(1)-N(2)	1.9834(13)
N(3)-Si(1)	1.7530(14)
N(3)-Si(2)	1.7624(14)
N(5)-Si(3)	1.8417(13)
Si(3)-Cl(1)	2.0920(6)

O(1)-C(1)-Fe(1)	177.03(16)
O(2)-C(2)-Fe(1)	178.38(19)
O(3)-C(3)-Fe(1)	176.49(18)
N(2)-C(4)-N(1)	106.57(13)
N(2)-C(4)-C(5)	124.37(15)
N(1)-C(4)-C(5)	129.06(15)
C(6)-C(5)-C(8)	107.75(19)
C(6)-C(5)-C(4)	113.66(16)
C(8)-C(5)-C(4)	108.74(15)
C(6)-C(5)-C(7)	105.82(19)
C(8)-C(5)-C(7)	110.22(19)
C(4)-C(5)-C(7)	110.57(17)
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(1)-C(9)-C(10)	111.72(16)
N(1)-C(9)-C(11)	108.20(15)
C(10)-C(9)-C(11)	110.12(19)
N(1)-C(9)-H(9)	108.9
C(10)-C(9)-H(9)	108.9
C(11)-C(9)-H(9)	108.9
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5

C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
N(2)-C(12)-C(14)	109.65(16)
N(2)-C(12)-C(13)	110.75(14)
C(14)-C(12)-C(13)	110.55(19)
N(2)-C(12)-H(12)	108.6
C(14)-C(12)-H(12)	108.6
C(13)-C(12)-H(12)	108.6
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
Si(1)-C(15)-H(15A)	109.5
Si(1)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
Si(1)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
Si(1)-C(16)-H(16A)	109.5
Si(1)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
Si(1)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
Si(1)-C(17)-H(17A)	109.5
Si(1)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
Si(1)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
Si(2)-C(18)-H(18A)	109.5
Si(2)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
Si(2)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
Si(2)-C(19)-H(19A)	109.5
Si(2)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
Si(2)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
Si(2)-C(20)-H(20A)	109.5
Si(2)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
Si(2)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5

H(20B)-C(20)-H(20C)	109.5
N(4)-C(21)-N(5)	106.39(13)
N(4)-C(21)-C(22)	128.12(14)
N(5)-C(21)-C(22)	125.37(13)
C(23)-C(22)-C(27)	120.44(15)
C(23)-C(22)-C(21)	120.50(15)
C(27)-C(22)-C(21)	118.93(14)
C(22)-C(23)-C(24)	119.51(17)
C(22)-C(23)-H(23)	120.2
C(24)-C(23)-H(23)	120.2
C(25)-C(24)-C(23)	120.22(17)
C(25)-C(24)-H(24)	119.9
C(23)-C(24)-H(24)	119.9
C(24)-C(25)-C(26)	120.30(17)
C(24)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9
C(25)-C(26)-C(27)	120.02(18)
C(25)-C(26)-H(26)	120.0
C(27)-C(26)-H(26)	120.0
C(22)-C(27)-C(26)	119.47(17)
C(22)-C(27)-H(27)	120.3
C(26)-C(27)-H(27)	120.3
C(21)-N(4)-C(28)	130.70(14)
C(21)-N(4)-Si(3)	91.10(10)
C(28)-N(4)-Si(3)	138.18(11)
N(4)-C(28)-C(29')	111.7(5)
N(4)-C(28)-C(31)	108.1(4)
N(4)-C(28)-C(29)	108.4(5)
C(31)-C(28)-C(29)	110.3(6)
N(4)-C(28)-C(30')	108.0(4)
C(29')-C(28)-C(30')	111.6(5)
N(4)-C(28)-C(31')	105.1(4)
C(29')-C(28)-C(31')	108.6(5)
C(30')-C(28)-C(31')	111.6(6)
N(4)-C(28)-C(30)	113.2(5)
C(31)-C(28)-C(30)	108.7(6)
C(29)-C(28)-C(30)	108.0(6)
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(28)-C(31)-H(31A)	109.5
C(28)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(28)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(28)-C(29')-H(29D)	109.5
C(28)-C(29')-H(29E)	109.5
H(29D)-C(29')-H(29E)	109.5

C(28)-C(29')-H(29F)	109.5
H(29D)-C(29')-H(29F)	109.5
H(29E)-C(29')-H(29F)	109.5
C(28)-C(30')-H(30D)	109.5
C(28)-C(30')-H(30E)	109.5
H(30D)-C(30')-H(30E)	109.5
C(28)-C(30')-H(30F)	109.5
H(30D)-C(30')-H(30F)	109.5
H(30E)-C(30')-H(30F)	109.5
C(28)-C(31')-H(31D)	109.5
C(28)-C(31')-H(31E)	109.5
H(31D)-C(31')-H(31E)	109.5
C(28)-C(31')-H(31F)	109.5
H(31D)-C(31')-H(31F)	109.5
H(31E)-C(31')-H(31F)	109.5
N(5)-C(32)-C(34)	106.27(14)
N(5)-C(32)-C(33)	110.52(16)
C(34)-C(32)-C(33)	109.4(2)
N(5)-C(32)-C(35)	111.48(16)
C(34)-C(32)-C(35)	108.1(2)
C(33)-C(32)-C(35)	111.0(2)
C(32)-C(33)-H(33A)	109.5
C(32)-C(33)-H(33B)	109.5
H(33A)-C(33)-H(33B)	109.5
C(32)-C(33)-H(33C)	109.5
H(33A)-C(33)-H(33C)	109.5
H(33B)-C(33)-H(33C)	109.5
C(32)-C(34)-H(34A)	109.5
C(32)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(32)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(32)-C(35)-H(35A)	109.5
C(32)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(32)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(1)-Fe(1)-C(2)	125.84(8)
C(1)-Fe(1)-C(3)	124.29(9)
C(2)-Fe(1)-C(3)	109.43(9)
C(1)-Fe(1)-Si(3)	83.99(6)
C(2)-Fe(1)-Si(3)	89.19(5)
C(3)-Fe(1)-Si(3)	90.87(5)
C(1)-Fe(1)-Ge(1)	90.87(5)
C(2)-Fe(1)-Ge(1)	88.87(5)
C(3)-Fe(1)-Ge(1)	97.09(5)
Si(3)-Fe(1)-Ge(1)	172.000(15)
N(3)-Ge(1)-N(1)	105.90(6)
N(3)-Ge(1)-N(2)	106.58(6)
N(1)-Ge(1)-N(2)	65.89(6)
N(3)-Ge(1)-Fe(1)	129.82(4)
N(1)-Ge(1)-Fe(1)	114.43(4)
N(2)-Ge(1)-Fe(1)	116.25(4)
C(4)-N(1)-C(9)	133.50(14)
C(4)-N(1)-Ge(1)	93.48(9)
C(9)-N(1)-Ge(1)	130.70(11)

C(4)-N(2)-C(12)	131.14(14)
C(4)-N(2)-Ge(1)	93.01(10)
C(12)-N(2)-Ge(1)	134.23(11)
Si(1)-N(3)-Si(2)	116.38(8)
Si(1)-N(3)-Ge(1)	126.15(8)
Si(2)-N(3)-Ge(1)	116.84(7)
C(21)-N(5)-C(32)	129.95(13)
C(21)-N(5)-Si(3)	90.52(9)
C(32)-N(5)-Si(3)	137.41(11)
N(3)-Si(1)-C(15)	117.86(8)
N(3)-Si(1)-C(17)	110.72(10)
C(15)-Si(1)-C(17)	104.35(12)
N(3)-Si(1)-C(16)	110.97(10)
C(15)-Si(1)-C(16)	102.56(13)
C(17)-Si(1)-C(16)	109.85(14)
N(3)-Si(2)-C(19)	114.81(8)
N(3)-Si(2)-C(18)	109.66(10)
C(19)-Si(2)-C(18)	109.01(12)
N(3)-Si(2)-C(20)	113.73(10)
C(19)-Si(2)-C(20)	102.08(11)
C(18)-Si(2)-C(20)	107.05(13)
N(4)-Si(3)-N(5)	71.50(6)
N(4)-Si(3)-Cl(1)	103.64(5)
N(5)-Si(3)-Cl(1)	102.68(5)
N(4)-Si(3)-Fe(1)	123.69(5)
N(5)-Si(3)-Fe(1)	124.73(5)
Cl(1)-Si(3)-Fe(1)	119.86(2)

Symmetry transformations used to generate equivalent atoms:

Table S17. Anisotropic displacement parameters (A^2 x 10^3) for as18046_a.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	24(1)	27(1)	34(1)	5(1)	9(1)	1(1)
C(2)	29(1)	26(1)	32(1)	-1(1)	14(1)	-4(1)
C(3)	25(1)	34(1)	26(1)	3(1)	6(1)	-5(1)
C(4)	20(1)	22(1)	28(1)	-2(1)	3(1)	-2(1)
C(5)	34(1)	26(1)	43(1)	-10(1)	-1(1)	-6(1)
C(6)	54(1)	45(1)	54(1)	-19(1)	-16(1)	-7(1)
C(7)	54(1)	39(1)	74(2)	-11(1)	9(1)	-25(1)
C(8)	47(1)	32(1)	62(1)	-20(1)	7(1)	2(1)
C(9)	32(1)	36(1)	23(1)	2(1)	-6(1)	2(1)
C(10)	61(1)	64(2)	25(1)	4(1)	9(1)	-1(1)
C(11)	51(1)	35(1)	40(1)	10(1)	-8(1)	9(1)
C(12)	37(1)	20(1)	32(1)	8(1)	6(1)	-1(1)
C(13)	41(1)	43(1)	49(1)	25(1)	-4(1)	0(1)
C(14)	75(2)	52(1)	55(1)	25(1)	34(1)	8(1)
C(15)	23(1)	49(1)	76(2)	-18(1)	13(1)	-7(1)
C(16)	53(1)	75(2)	65(2)	0(1)	36(1)	-18(1)
C(17)	36(1)	56(2)	73(2)	-13(1)	3(1)	21(1)
C(18)	57(1)	64(2)	29(1)	2(1)	3(1)	-5(1)
C(19)	51(1)	29(1)	54(1)	-16(1)	24(1)	-13(1)
C(20)	50(1)	58(2)	71(2)	-32(1)	29(1)	-3(1)
C(21)	19(1)	22(1)	23(1)	1(1)	6(1)	-2(1)
C(22)	26(1)	20(1)	24(1)	1(1)	6(1)	-4(1)
C(23)	29(1)	27(1)	31(1)	5(1)	10(1)	-1(1)
C(24)	42(1)	32(1)	32(1)	5(1)	15(1)	-10(1)
C(25)	46(1)	26(1)	35(1)	9(1)	5(1)	-8(1)
C(26)	36(1)	25(1)	51(1)	7(1)	4(1)	2(1)
C(27)	30(1)	26(1)	43(1)	2(1)	12(1)	0(1)
N(4)	27(1)	28(1)	20(1)	-1(1)	4(1)	-10(1)
C(28)	39(1)	39(1)	23(1)	-7(1)	7(1)	-17(1)
C(29)	39(3)	96(8)	39(4)	-18(5)	10(3)	-38(4)
C(30)	97(7)	48(4)	56(4)	-22(3)	3(5)	12(4)
C(31)	51(4)	56(3)	23(2)	-8(2)	11(2)	-22(3)
C(29')	46(3)	49(4)	39(3)	-8(2)	7(2)	-28(3)
C(30')	62(4)	83(6)	62(4)	-50(4)	22(3)	-9(3)
C(31')	111(8)	74(5)	23(2)	7(3)	-14(4)	-60(5)
C(32)	41(1)	28(1)	18(1)	-2(1)	9(1)	-8(1)
C(33)	82(2)	61(2)	37(1)	-10(1)	-24(1)	17(1)
C(34)	86(2)	32(1)	31(1)	-8(1)	11(1)	-19(1)
C(35)	87(2)	90(2)	46(1)	-33(1)	45(1)	-45(2)
Fe(1)	18(1)	18(1)	20(1)	1(1)	6(1)	-1(1)
Ge(1)	17(1)	17(1)	19(1)	1(1)	4(1)	-1(1)
N(1)	21(1)	24(1)	22(1)	0(1)	0(1)	0(1)
N(2)	25(1)	18(1)	26(1)	2(1)	4(1)	-2(1)
N(3)	20(1)	23(1)	26(1)	-2(1)	8(1)	-1(1)
N(5)	28(1)	21(1)	18(1)	1(1)	7(1)	-3(1)
O(1)	49(1)	32(1)	63(1)	20(1)	16(1)	11(1)

O(2)	62(1)	28(1)	59(1)	-13(1)	34(1)	-9(1)
O(3)	44(1)	65(1)	27(1)	9(1)	-4(1)	-10(1)
Si(1)	21(1)	37(1)	44(1)	-5(1)	12(1)	-1(1)
Si(2)	30(1)	28(1)	29(1)	-6(1)	12(1)	-3(1)
Si(3)	18(1)	20(1)	19(1)	3(1)	5(1)	-1(1)
Cl(1)	27(1)	50(1)	50(1)	20(1)	14(1)	16(1)

Crystal data and structure refinement of compound **6**

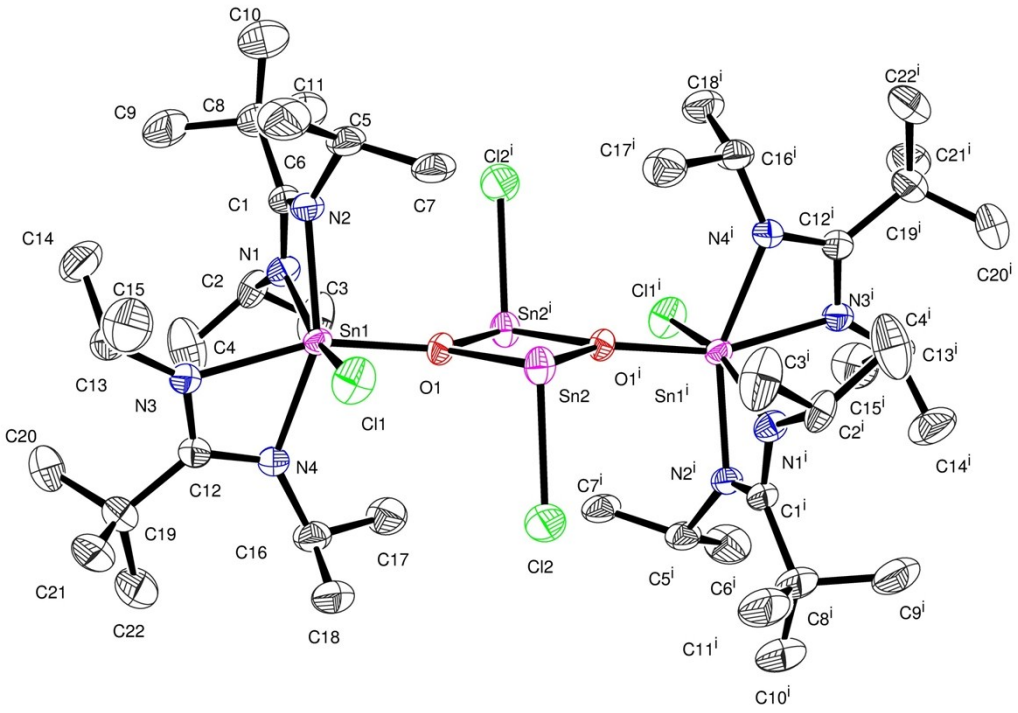


Figure S8: Molecular structure of **6**. Hydrogen atoms have been omitted for clarity. Selected bond distances [Å] and bond angles [deg]: N1-Sn1 2.195(2); N2-Sn1 2.164(2); N3-Sn1 2.203(2); N4-Sn1 2.167(2); Cl1-Sn1 2.448(1); Sn1-O1 2.030(2); Sn2-O1 2.127(2); Sn2-O1^{i} 2.158(2); Cl2-Sn2 2.475(1); N1-C1-N2 110.8(2); N2-Sn1-N1 60.49(9); Sn1-O1-Sn2 124.26(10); Sn2-O1-Sn2^{i} 102.82(8); O1-Sn2-O1^{i} 77.18(8).

Table S18. Crystal data and structure refinement of compound 6.

Identification code	Nicolas 1
Empirical formula	C44 H92 Cl4 N8 O2 Sn4
Formula weight	1381.81
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P 21/n
Unit cell dimensions	a = 9.9149(4) A alpha = 90 deg. b = 18.3126(8) A beta = 104.495(2) deg.

	c = 16.2508(7) A gamma = 90 deg.
Volume	2856.7(2) A^3
Z, Calculated density	2, 1.606 Mg/m^3
Absorption coefficient	1.956 mm^-1
F(000)	1392
Crystal size	0.28 x 0.16 x 0.08 mm
Theta range for data collection	3.414 to 30.507 deg.
Limiting indices	-14<=h<=14, -24<=k<=26, -23<=l<=23
Reflections collected / unique	42206 / 8695 [R(int) = 0.0277]
Completeness to theta = 25.242	99.7 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8695 / 198 / 373
Goodness-of-fit on F^2	1.095
Final R indices [I>2sigma(I)]	R1 = 0.0318, wR2 = 0.0817
R indices (all data)	R1 = 0.0423, wR2 = 0.0968
Largest diff. peak and hole	1.397 and -0.740 e.A^-3

Table S19. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for nicolas1_a. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
C(1)	5778(3)	5902(2)	2517(2)	29(1)
N(1)	4698(3)	6218(1)	2717(1)	28(1)
C(2)	3348(6)	6435(4)	2141(5)	34(1)
C(3)	2191(9)	6047(6)	2392(7)	62(2)
C(4)	3133(9)	7246(4)	2161(7)	69(2)
C(2')	3296(19)	6442(13)	2190(20)	41(4)
C(3')	2250(30)	5854(15)	2180(20)	49(5)
C(4')	2710(30)	7119(13)	2501(18)	56(5)
N(2)	6887(2)	5892(1)	3186(2)	27(1)
C(5')	8193(15)	5463(11)	3320(16)	39(3)
C(6')	9470(15)	5938(11)	3644(14)	51(3)
C(7')	8177(14)	4830(7)	3912(14)	40(3)
C(5)	8097(12)	5394(8)	3346(12)	34(2)
C(6)	9403(15)	5828(9)	3367(15)	58(3)
C(7)	8235(14)	4968(10)	4162(10)	44(2)
C(8)	5764(5)	5628(2)	1608(2)	48(1)
C(9)	5577(9)	6328(4)	1016(4)	61(1)
C(10)	7039(9)	5267(5)	1459(4)	66(1)
C(11)	4529(9)	5118(4)	1282(4)	65(1)
C(9')	7110(13)	5878(7)	1377(7)	62(1)
C(10')	5861(16)	4781(6)	1659(7)	65(1)
C(11')	4535(14)	5776(7)	872(6)	65(1)
C(12)	5219(3)	7885(2)	3974(2)	32(1)
C(13)	7295(4)	7994(2)	3342(2)	43(1)
C(14)	7195(6)	7761(3)	2427(3)	65(1)
C(15)	8757(5)	7851(3)	3906(4)	66(1)
C(16)	3598(3)	7431(2)	4839(2)	37(1)
C(17)	2788(4)	6736(2)	4855(3)	47(1)
C(18)	4369(5)	7660(2)	5733(2)	47(1)
C(19)	4864(5)	8715(2)	3918(3)	47(1)
C(20)	4640(6)	8979(2)	2986(3)	62(1)
C(21)	6063(5)	9119(2)	4531(3)	60(1)
C(22)	3530(5)	8950(2)	4163(3)	66(1)
N(3)	6252(3)	7612(1)	3684(2)	30(1)
N(4)	4572(3)	7350(1)	4295(2)	31(1)
Cl(1)	7805(1)	6604(1)	5284(1)	43(1)
Cl(2)	5391(1)	5878(1)	6735(1)	54(1)
Sn(1)	5869(1)	6478(1)	4018(1)	22(1)
Sn(2)	6446(1)	5153(1)	5771(1)	30(1)
O(1)	5261(2)	5606(1)	4609(1)	26(1)

Table S20. Bond lengths [A] and angles [deg] for nicolas1_a.

C(1)-N(1)	1.328(4)
C(1)-N(2)	1.340(4)
C(1)-C(8)	1.556(4)
C(1)-Sn(1)	2.640(3)
N(1)-C(2)	1.482(6)
N(1)-C(2')	1.496(16)
N(1)-Sn(1)	2.195(2)
C(2)-C(3)	1.490(8)
C(2)-C(4)	1.501(8)
C(2)-H(2)	1.0000
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(2')-C(3')	1.491(17)
C(2')-C(4')	1.509(18)
C(2')-H(2')	1.0000
C(3')-H(3D)	0.9800
C(3')-H(3E)	0.9800
C(3')-H(3F)	0.9800
C(4')-H(4D)	0.9800
C(4')-H(4E)	0.9800
C(4')-H(4F)	0.9800
N(2)-C(5)	1.477(10)
N(2)-C(5')	1.483(12)
N(2)-Sn(1)	2.164(2)
C(5')-C(7')	1.509(13)
C(5')-C(6')	1.519(15)
C(5')-H(5')	1.0000
C(6')-H(6A)	0.9800
C(6')-H(6B)	0.9800
C(6')-H(6C)	0.9800
C(7')-H(7A)	0.9800
C(7')-H(7B)	0.9800
C(7')-H(7C)	0.9800
C(5)-C(6)	1.512(11)
C(5)-C(7)	1.514(12)
C(5)-H(5)	1.0000
C(6)-H(6D)	0.9800
C(6)-H(6E)	0.9800
C(6)-H(6F)	0.9800
C(7)-H(7D)	0.9800
C(7)-H(7E)	0.9800
C(7)-H(7F)	0.9800
C(8)-C(10)	1.499(8)
C(8)-C(11')	1.503(12)
C(8)-C(11)	1.526(9)
C(8)-C(9')	1.544(11)
C(8)-C(10')	1.553(11)
C(8)-C(9)	1.586(8)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800

C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(9')-H(9D)	0.9800
C(9')-H(9E)	0.9800
C(9')-H(9F)	0.9800
C(10')-H(10D)	0.9800
C(10')-H(10E)	0.9800
C(10')-H(10F)	0.9800
C(11')-H(11D)	0.9800
C(11')-H(11E)	0.9800
C(11')-H(11F)	0.9800
C(12)-N(3)	1.329(4)
C(12)-N(4)	1.345(4)
C(12)-C(19)	1.558(5)
C(12)-Sn(1)	2.652(3)
C(13)-N(3)	1.468(4)
C(13)-C(14)	1.526(5)
C(13)-C(15)	1.531(7)
C(13)-H(13)	1.0000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-N(4)	1.470(4)
C(16)-C(17)	1.509(5)
C(16)-C(18)	1.523(5)
C(16)-H(16)	1.0000
C(17)-H(17A)	0.9800
C(17)-H(17B)	0.9800
C(17)-H(17C)	0.9800
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(22)	1.535(6)
C(19)-C(21)	1.536(6)
C(19)-C(20)	1.552(6)
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
N(3)-Sn(1)	2.203(2)
N(4)-Sn(1)	2.167(2)
Cl(1)-Sn(1)	2.4483(8)
Cl(2)-Sn(2)	2.4751(10)
Sn(1)-O(1)	2.0303(19)
Sn(2)-O(1)	2.1272(18)
Sn(2)-O(1)#1	2.158(2)

N(1)-C(1)-N(2)	110.8(2)
N(1)-C(1)-C(8)	123.9(3)
N(2)-C(1)-C(8)	125.2(3)
N(1)-C(1)-Sn(1)	56.07(14)
N(2)-C(1)-Sn(1)	54.78(13)
C(8)-C(1)-Sn(1)	175.0(2)
C(1)-N(1)-C(2)	128.2(4)
C(1)-N(1)-C(2')	132.0(13)
C(1)-N(1)-Sn(1)	93.81(17)
C(2)-N(1)-Sn(1)	136.6(3)
C(2')-N(1)-Sn(1)	133.2(12)
N(1)-C(2)-C(3)	109.5(6)
N(1)-C(2)-C(4)	111.3(5)
C(3)-C(2)-C(4)	110.0(6)
N(1)-C(2)-H(2)	108.7
C(3)-C(2)-H(2)	108.7
C(4)-C(2)-H(2)	108.7
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3')-C(2')-N(1)	110.7(19)
C(3')-C(2')-C(4')	106(2)
N(1)-C(2')-C(4')	114.3(18)
C(3')-C(2')-H(2')	108.6
N(1)-C(2')-H(2')	108.6
C(4')-C(2')-H(2')	108.6
C(2')-C(3')-H(3D)	109.5
C(2')-C(3')-H(3E)	109.5
H(3D)-C(3')-H(3E)	109.5
C(2')-C(3')-H(3F)	109.5
H(3D)-C(3')-H(3F)	109.5
H(3E)-C(3')-H(3F)	109.5
C(2')-C(4')-H(4D)	109.5
C(2')-C(4')-H(4E)	109.5
H(4D)-C(4')-H(4E)	109.5
C(2')-C(4')-H(4F)	109.5
H(4D)-C(4')-H(4F)	109.5
H(4E)-C(4')-H(4F)	109.5
C(1)-N(2)-C(5)	128.0(8)
C(1)-N(2)-C(5')	129.4(11)
C(1)-N(2)-Sn(1)	94.83(17)
C(5)-N(2)-Sn(1)	133.0(8)
C(5')-N(2)-Sn(1)	134.3(10)
N(2)-C(5')-C(7')	110.6(11)
N(2)-C(5')-C(6')	111.6(14)
C(7')-C(5')-C(6')	111.1(15)
N(2)-C(5')-H(5')	107.8
C(7')-C(5')-H(5')	107.8

C(6')-C(5')-H(5')	107.8
C(5')-C(6')-H(6A)	109.5
C(5')-C(6')-H(6B)	109.5
H(6A)-C(6')-H(6B)	109.5
C(5')-C(6')-H(6C)	109.5
H(6A)-C(6')-H(6C)	109.5
H(6B)-C(6')-H(6C)	109.5
C(5')-C(7')-H(7A)	109.5
C(5')-C(7')-H(7B)	109.5
H(7A)-C(7')-H(7B)	109.5
C(5')-C(7')-H(7C)	109.5
H(7A)-C(7')-H(7C)	109.5
H(7B)-C(7')-H(7C)	109.5
N(2)-C(5)-C(6)	109.4(10)
N(2)-C(5)-C(7)	111.3(11)
C(6)-C(5)-C(7)	111.2(12)
N(2)-C(5)-H(5)	108.3
C(6)-C(5)-H(5)	108.3
C(7)-C(5)-H(5)	108.3
C(5)-C(6)-H(6D)	109.5
C(5)-C(6)-H(6E)	109.5
H(6D)-C(6)-H(6E)	109.5
C(5)-C(6)-H(6F)	109.5
H(6D)-C(6)-H(6F)	109.5
H(6E)-C(6)-H(6F)	109.5
C(5)-C(7)-H(7D)	109.5
C(5)-C(7)-H(7E)	109.5
H(7D)-C(7)-H(7E)	109.5
C(5)-C(7)-H(7F)	109.5
H(7D)-C(7)-H(7F)	109.5
H(7E)-C(7)-H(7F)	109.5
C(10)-C(8)-C(11)	108.1(5)
C(11')-C(8)-C(9')	109.3(7)
C(11')-C(8)-C(10')	104.5(7)
C(9')-C(8)-C(10')	105.3(8)
C(10)-C(8)-C(1)	119.2(4)
C(11')-C(8)-C(1)	120.6(5)
C(11)-C(8)-C(1)	110.0(4)
C(9')-C(8)-C(1)	109.4(5)
C(10')-C(8)-C(1)	106.5(5)
C(10)-C(8)-C(9)	103.5(5)
C(11)-C(8)-C(9)	108.9(5)
C(1)-C(8)-C(9)	106.7(3)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(8)-C(10)-H(10A)	109.5
C(8)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(8)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(8)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5

C(8)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(8)-C(9')-H(9D)	109.5
C(8)-C(9')-H(9E)	109.5
H(9D)-C(9')-H(9E)	109.5
C(8)-C(9')-H(9F)	109.5
H(9D)-C(9')-H(9F)	109.5
H(9E)-C(9')-H(9F)	109.5
C(8)-C(10')-H(10D)	109.5
C(8)-C(10')-H(10E)	109.5
H(10D)-C(10')-H(10E)	109.5
C(8)-C(10')-H(10F)	109.5
H(10D)-C(10')-H(10F)	109.5
H(10E)-C(10')-H(10F)	109.5
C(8)-C(11')-H(11D)	109.5
C(8)-C(11')-H(11E)	109.5
H(11D)-C(11')-H(11E)	109.5
C(8)-C(11')-H(11F)	109.5
H(11D)-C(11')-H(11F)	109.5
H(11E)-C(11')-H(11F)	109.5
N(3)-C(12)-N(4)	110.4(3)
N(3)-C(12)-C(19)	121.9(3)
N(4)-C(12)-C(19)	127.6(3)
N(3)-C(12)-Sn(1)	55.96(15)
N(4)-C(12)-Sn(1)	54.46(15)
C(19)-C(12)-Sn(1)	177.7(2)
N(3)-C(13)-C(14)	110.8(3)
N(3)-C(13)-C(15)	110.1(3)
C(14)-C(13)-C(15)	110.9(4)
N(3)-C(13)-H(13)	108.3
C(14)-C(13)-H(13)	108.3
C(15)-C(13)-H(13)	108.3
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
N(4)-C(16)-C(17)	111.0(3)
N(4)-C(16)-C(18)	110.7(3)
C(17)-C(16)-C(18)	111.0(3)
N(4)-C(16)-H(16)	108.0
C(17)-C(16)-H(16)	108.0
C(18)-C(16)-H(16)	108.0
C(16)-C(17)-H(17A)	109.5
C(16)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(16)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(16)-C(18)-H(18A)	109.5

C(16)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(16)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(22)-C(19)-C(21)	105.9(4)
C(22)-C(19)-C(20)	104.1(4)
C(21)-C(19)-C(20)	112.4(4)
C(22)-C(19)-C(12)	117.1(3)
C(21)-C(19)-C(12)	107.8(3)
C(20)-C(19)-C(12)	109.7(3)
C(19)-C(20)-H(20A)	109.5
C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(12)-N(3)-C(13)	129.4(3)
C(12)-N(3)-Sn(1)	94.05(18)
C(13)-N(3)-Sn(1)	136.4(2)
C(12)-N(4)-C(16)	127.5(3)
C(12)-N(4)-Sn(1)	95.21(18)
C(16)-N(4)-Sn(1)	135.4(2)
O(1)-Sn(1)-N(2)	98.37(9)
O(1)-Sn(1)-N(4)	102.68(9)
N(2)-Sn(1)-N(4)	152.76(9)
O(1)-Sn(1)-N(1)	97.86(9)
N(2)-Sn(1)-N(1)	60.49(9)
N(4)-Sn(1)-N(1)	99.31(10)
O(1)-Sn(1)-N(3)	161.37(8)
N(2)-Sn(1)-N(3)	100.17(9)
N(4)-Sn(1)-N(3)	60.32(9)
N(1)-Sn(1)-N(3)	92.80(10)
O(1)-Sn(1)-Cl(1)	86.58(6)
N(2)-Sn(1)-Cl(1)	100.45(7)
N(4)-Sn(1)-Cl(1)	97.88(8)
N(1)-Sn(1)-Cl(1)	160.82(7)
N(3)-Sn(1)-Cl(1)	88.34(7)
O(1)-Sn(1)-C(1)	100.19(8)
N(2)-Sn(1)-C(1)	30.39(9)
N(4)-Sn(1)-C(1)	127.01(10)
N(1)-Sn(1)-C(1)	30.12(9)
N(3)-Sn(1)-C(1)	96.70(9)
Cl(1)-Sn(1)-C(1)	130.75(7)
O(1)-Sn(1)-C(12)	132.65(9)
N(2)-Sn(1)-C(12)	127.82(9)

N(4)-Sn(1)-C(12)	30.33(9)
N(1)-Sn(1)-C(12)	96.80(9)
N(3)-Sn(1)-C(12)	29.99(9)
Cl(1)-Sn(1)-C(12)	93.73(7)
C(1)-Sn(1)-C(12)	114.32(9)
O(1)-Sn(2)-O(1)#1	77.18(8)
O(1)-Sn(2)-Cl(2)	97.20(6)
O(1)#1-Sn(2)-Cl(2)	95.80(6)
Sn(1)-O(1)-Sn(2)	124.26(10)
Sn(1)-O(1)-Sn(2)#1	132.53(9)
Sn(2)-O(1)-Sn(2)#1	102.82(8)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1

Table S21. Anisotropic displacement parameters (A^2 x 10^3) for nicolas1_a.

The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
C(1)	39(2)	29(1)	21(1)	-3(1)	10(1)	-1(1)
N(1)	28(1)	35(1)	20(1)	-1(1)	2(1)	0(1)
C(2)	31(2)	48(2)	20(2)	7(2)	0(2)	-3(2)
C(3)	36(3)	86(6)	63(5)	31(4)	6(3)	-7(3)
C(4)	52(4)	56(3)	80(5)	31(3)	-20(3)	2(3)
C(2')	35(6)	50(6)	32(6)	6(6)	-7(6)	2(5)
C(3')	33(7)	54(8)	51(10)	14(7)	-8(7)	-14(6)
C(4')	49(8)	47(7)	55(9)	0(7)	-19(7)	16(7)
N(2)	28(1)	30(1)	25(1)	-2(1)	9(1)	4(1)
C(5')	36(4)	41(5)	43(5)	0(4)	16(4)	10(4)
C(6')	30(4)	66(7)	62(7)	5(6)	18(5)	2(4)
C(7')	32(4)	40(4)	49(7)	-8(4)	12(5)	14(3)
C(5)	30(3)	38(4)	38(3)	-3(3)	16(3)	7(3)
C(6)	36(4)	65(6)	81(8)	-2(6)	27(5)	8(4)
C(7)	45(4)	52(5)	36(5)	4(4)	14(4)	23(4)
C(8)	68(2)	50(2)	27(2)	-12(1)	15(2)	-2(2)
C(9)	91(3)	66(3)	33(2)	-9(2)	28(2)	-5(2)
C(10)	95(3)	69(3)	39(2)	-16(2)	27(2)	2(2)
C(11)	97(3)	64(3)	37(2)	-17(2)	22(2)	-6(2)
C(9')	93(3)	67(3)	35(2)	-12(2)	30(2)	-3(2)
C(10')	96(3)	65(3)	38(2)	-18(2)	26(2)	-3(2)
C(11')	95(3)	67(3)	36(2)	-13(2)	25(2)	-4(2)
C(12)	40(2)	28(1)	29(1)	-2(1)	11(1)	1(1)
C(13)	54(2)	33(2)	51(2)	-10(1)	31(2)	-15(1)
C(14)	95(4)	57(3)	60(3)	-12(2)	54(3)	-24(2)
C(15)	54(2)	62(3)	87(3)	-6(2)	29(2)	-23(2)
C(16)	37(2)	39(2)	41(2)	-6(1)	18(1)	1(1)
C(17)	42(2)	49(2)	57(2)	-7(2)	23(2)	-7(2)
C(18)	63(2)	44(2)	40(2)	-9(2)	23(2)	-1(2)
C(19)	65(2)	29(2)	54(2)	2(1)	28(2)	8(2)
C(20)	90(3)	36(2)	66(3)	17(2)	29(2)	15(2)
C(21)	91(3)	31(2)	65(3)	-16(2)	36(2)	-11(2)
C(22)	81(3)	42(2)	86(3)	11(2)	42(3)	26(2)
N(3)	38(1)	26(1)	32(1)	-3(1)	16(1)	-3(1)
N(4)	36(1)	28(1)	34(1)	2(1)	17(1)	4(1)
Cl(1)	37(1)	55(1)	29(1)	-1(1)	-4(1)	-11(1)
Cl(2)	87(1)	45(1)	30(1)	-3(1)	13(1)	7(1)
Sn(1)	24(1)	24(1)	18(1)	-1(1)	5(1)	1(1)
Sn(2)	27(1)	32(1)	25(1)	5(1)	-2(1)	1(1)
O(1)	28(1)	28(1)	21(1)	5(1)	5(1)	2(1)

Characterization of NPs from 2a

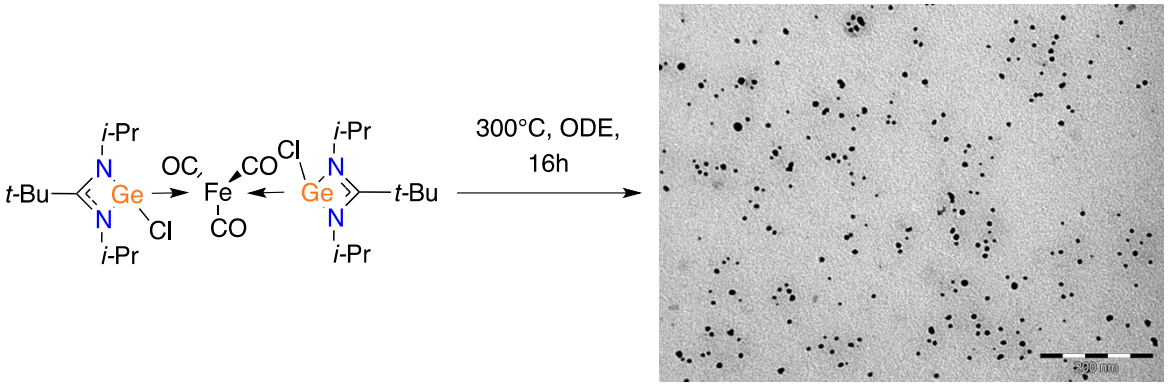
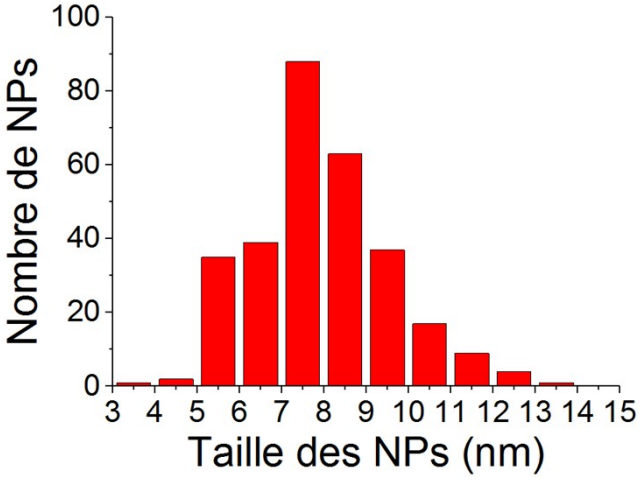


Figure S9: Synthesis of NPs from [{iPrNC(tBu)NiPr}GeCl]$_2$Fe(CO)$_3$.



d = 8.03 ± 1.80 nm

Figure S10: Size distribution of NPs (over 300 NPs count).

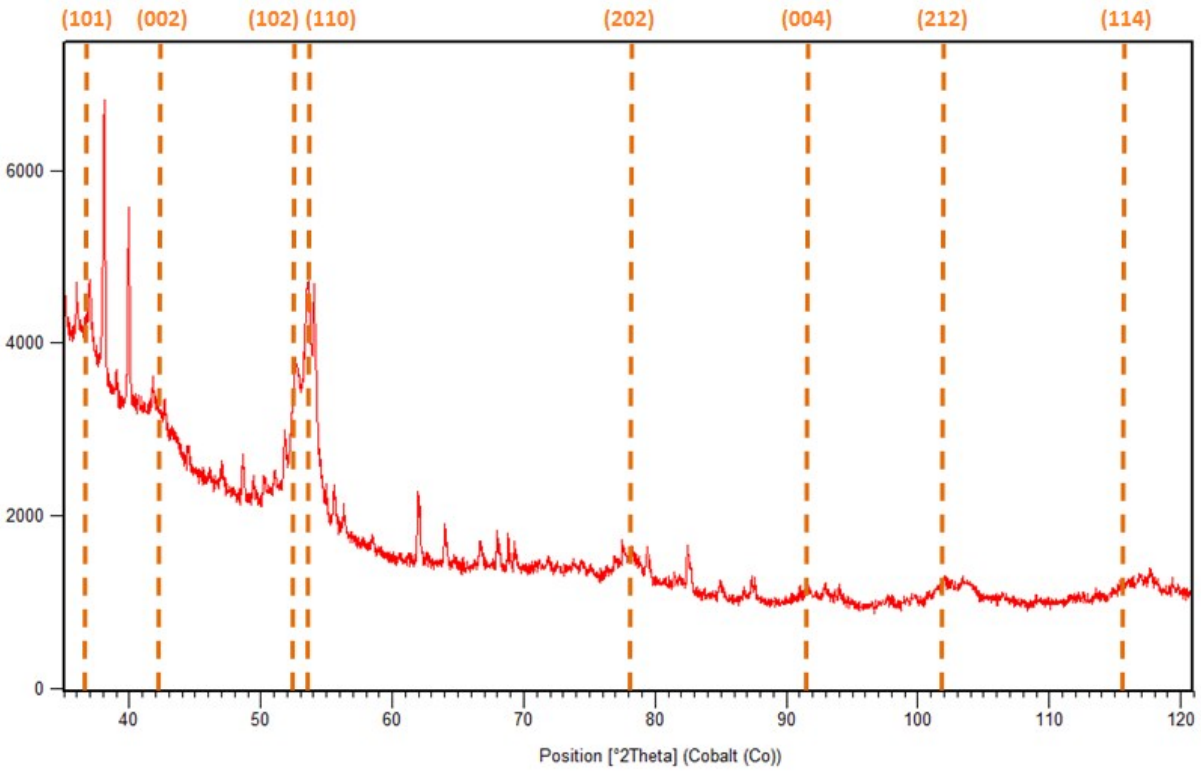


Figure S11: XRD diffractogram of NPs prepared from **2a.**

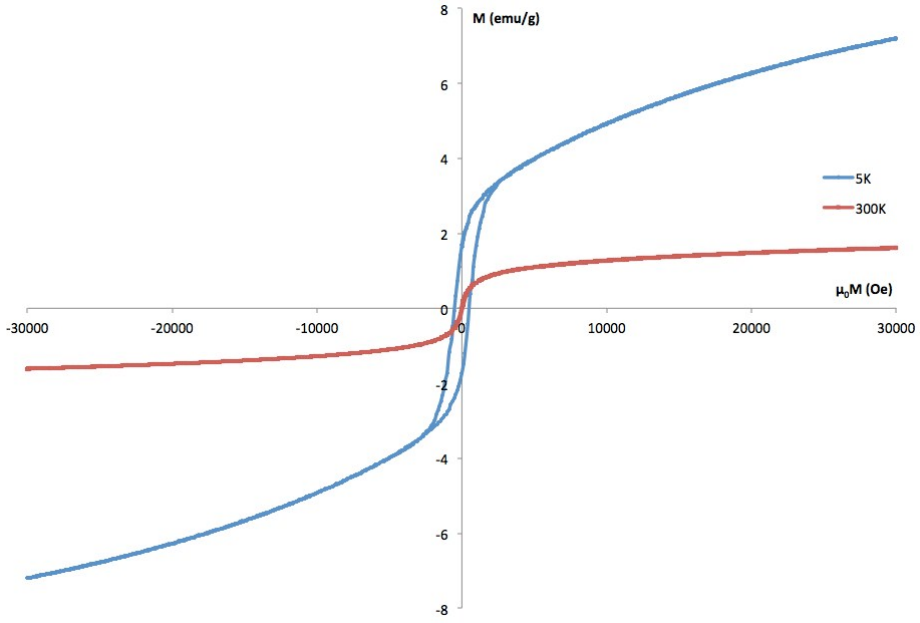


Figure S12. Plot of M vs H measurements at 5K and 300K of the NPs prepared from **2a**.

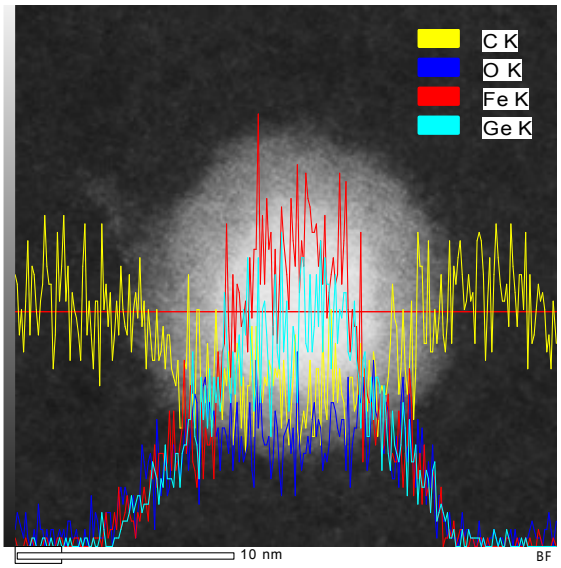


Figure S13. STEM-HAADF image and EDS elemental analysis of NPs prepared from **2a**.

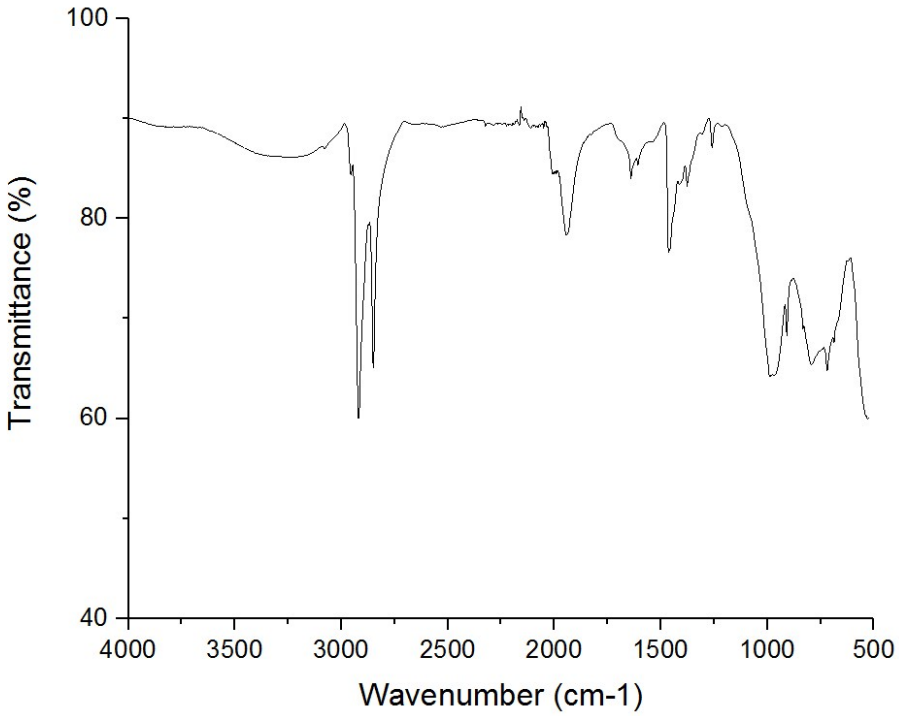


Figure S14. IR spectrum of the NPs prepared from **2a**.