Supporting information for

Germanium Hydrides as an Efficient Hydrogen-Storage Material Operated by an Iron Catalyst

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Contents

General. All reactions were carried out under a dry nitrogen atmosphere using either Schlenk-line or glove-box techniques. All solvents used for the reaction were treated with oven-dried molecular sieves before use. ^{1}H and ^{13}C NMR spectra were recorded using a JEOL Lambda 400 spectrometer at ambient temperature. Chemical shifts (δ) are reported in ppm, using the residual protons in the deuterated solvents as internal standards for the ^{1}H NMR and ^{13}C NMR spectra. Elemental analyses (C, H) were carried out on a Thermo Scientific FLASH 2000 Organic Elemental Analyzer or externally at A Rabbit Science Co., Ltd. IR spectra were recorded on a PerkinElmer Spectrum Two spectrometer. FAB-MS spectra were measured on a JEOL SpiralTOF™-plus spectrometer. Starting materials, ^{i}PrIM^{Me},[1] EtIM^{Me},[2] MeIM^{Et},[3] ^{i}PrIM^{H},[4] DippIM^{H},[5] ^{Me}CAAC,[6] Ph_2GeH_2,[7] Et_2GeH_2,[8] Ph_2SnH_2,[9] $^{n}Bu_2SnH_2$,[10] $^{i}Pr_2SiH_2$,[11] [Fe(mesityl)$_2$]$_2$,[12] Fe[Si(SiMe$_3$)$_3$]$_2$(THF)$_2$,[13] Fe[Ge(SiMe$_3$)$_3$]$_2$(THF)$_2$,[14] Fe(OCO^{t}Bu)$_2$,[15] Fe[N(SiMe$_3$)$_2$]$_2$,[16] [Mn(mesityl)$_2$]$_3$,[17] $PhICl_2$[18] were synthesized by the method reported in the literature. ^{i}PrIM^{Ph},[2] ^{i}PrPyC,[19] [Ni(^{i}PrIm^{Me})$_2$(COD)]$_2$[20] were synthesized according to the modified method reported in the literature. Other reagents were purchased from Tokyo Chemical Industries Co., Ltd. or Kanto Chemical Co., Inc. or Sigma Aldrich, and were used without further purification.

General procedure for the dehydrogenative coupling of Ph_2GeH_2 or Et_2GeH_2 catalyzed by [Fe(mesityl)$_2$]$_2$ / NHC. In a 4 mL vial, [Fe(mesityl)$_2$]$_2$ (7 mg, 0.0125 mmol) was dissolved in THF (0.5 mL), then NHC [^{i}PrIM^{Me} (for Ph_2GeH_2, 9 mg, 0.05 mmol) or EtIM^{Me} (for Et_2GeH_2, 7 mg, 0.05 mmol)] was added to this solution under nitrogen atmosphere. The obtained reaction mixture was stirred at room temperature for several minutes, then Ph_2GeH_2 (114 mg, 0.5 mmol) or Et_2GeH_2 (67 mg, 0.5 mmol) was added to this solution. The resulting mixture then stirred room temperature for 40 h, then conversion of Ph_2GeH_2 or Et_2GeH_2 and yield of $(GePh_2)_5$ or $(GeEt_2)_5$ was estimated by ^{1}H NMR spectrum.

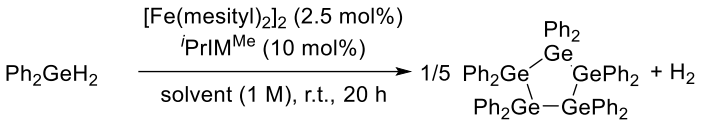
Isolation of $(GePh_2)_5$ by the catalytic dehydrogenative coupling of Ph_2GeH_2 catalyzed by [Fe(mesityl)$_2$]$_2$ / ^{i}PrIM^{Me}. In a 4 mL vial, [Fe(mesityl)$_2$]$_2$ (7.4 mg, 0.0125 mmol) was dissolved in THF (0.5 mL), then ^{i}PrIM^{Me} (9 mg, 0.05 mmol) was added to this solution under nitrogen atmosphere. The mixture was stirred at room temperature for several minutes, then Ph_2GeH_2 (114 mg, 0.5 mmol) was added. The resulting mixture then stirred for 40 h at room temperature, then THF was removed *in vacuo*. The resulting residue was washed by hexane (2 mL) and acetone (2 mL), and the supernatant was cooled to −20 °C. The remaining white powder as well as white powder formed from the cooled supernatant solution was combined, then $(GePh_2)_5$ was obtained as white powder (73 mg, 62%). ^{1}H NMR (400 MHz, r.t., C_6D_6): δ = 7.52-7.51 (m, 10H, *o*-Ph), 6.92-6.90 (m, 5H, *p*-Ph), 6.86-6.84 (m, 10H, *m*-Ph). ^{13}C NMR (100 MHz, r.t., C_6D_6): 138.3 (s, Ph), 137.2 (s, Ph), 128.6 (s, Ph), 128.4 (s, Ph).

Isolation of Ge_5Et_{10} by the catalytic dehydrogenative coupling of Et_2GeH_2 catalyzed by [Fe(mesityl)$_2$]$_2$ / EtIM^{Me}. In a 4 mL vial, [Fe(mesityl)$_2$]$_2$ (15 mg, 0.025 mmol) was dissolved in THF (0.5 mL), then EtIM^{Me} (15 mg, 0.1 mmol) was added to this solution under nitrogen atmosphere. The mixture was stirred at room temperature for several minutes, then Et_2GeH_2 (132 mg, 1mmol) was added. The resulting mixture then stirred for 40 h at room temperature, then THF was removed *in vacuo*. The resulting residue was extracted by acetone (2 mL), then supernatant was cooled to −20 °C to afford $(GeEt_2)_5$ as colorless liquid (68 mg, 52%). ^{1}H NMR (600 MHz, r.t., C_6D_6): δ = 1.23 (t, $J_{H\text{-}H}$ = 6.0

Hz, 6H, -C*H*$_2$-CH$_3$), 1.18 (q, $J_{H\text{-}H}$ = 6.0 Hz, 4H, -CH$_2$-C*H*$_3$), ^{13}C NMR (150 MHz, r.t., C_6D_6): 12.50 (s, -*C*H$_2$-CH$_3$), 6.13 (s, -CH$_2$-*C*H$_3$).

Investigation of the effect of solvent in the dehydrogenative coupling of Ph_2GeH_2 catalyzed by [Fe(mesityl)$_2$]$_2$ / ^{i}PrIM^{Me}. In a 4 mL vial, [Fe(mesityl)$_2$]$_2$ (7.4 mg, 0.0125 mmol) was dissolved in solvent listed in Table S1 (0.5 mL), then ^{i}PrIM^{Me} (9 mg, 0.05 mmol) was added to this solution under nitrogen atmosphere. The obtained reaction mixture was stirred at room temperature for several minutes, then Ph_2GeH_2 (114 mg, 0.5 mmol) was added to this solution. The resulting mixture then stirred room temperature for 20 h, then conversion of Ph_2GeH_2 and yield of $(GePh_2)_5$ was estimated by ^{1}H NMR spectrum.

Table S1. Effect of solvent in the dehydrogenative coupling of Ph_2GeH_2 catalyzed by [Fe(mesityl)$_2$]$_2$ / ^{i}PrIM^{Me}.

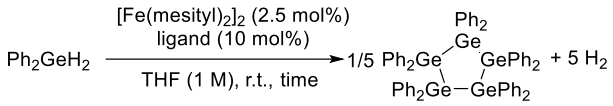


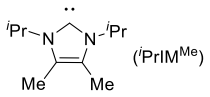
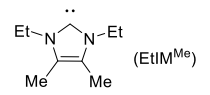
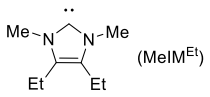
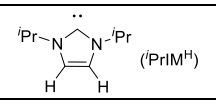
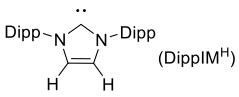
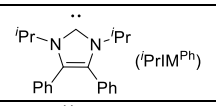
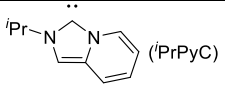
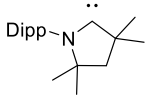
entry	solvent	conv. (%)	yield (%)[a]
1	THF	>99	62
2	toluene	>99	8
3	diethyl ether	>99	36

[a]yield was estimated based on the amount of formed $(GePh_2)_5$. ^{1}H NMR spectrum of the crude reaction mixture suggest the formation of some oligomers as by-product when the reaction was performed in 20 h.

Investigation of the effect of ligand in the catalytic dehydrogenative coupling of Ph_2GeH_2 in the presence of a catalytic amount of $[Fe(mesityl)_2]_2$. In a 4 mL vial, $[Fe(mesityl)_2]_2$ (7.4 mg, 0.0125 mmol) was dissolved in THF (0.5 mL), then ligand shown in Table S2 (0.05 mmol) was added under nitrogen atmosphere. The obtained reaction mixture was stirred at room temperature for several minutes, then Ph_2GeH_2 (114 mg, 0.5 mmol) was added to this solution. The resulting mixture then stirred room temperature for time indicated in Table S2, then conversion of Ph_2GeH_2 and the yield of $(GePh_2)_5$ was estimated by ^1H NMR spectrum.

Table S2. Effect of ligand in the dehydrogenative coupling of Ph_2GeH_2 in the presence of a catalytic amount of $[Fe(mesityl)_2]_2$.



entry	ligand	time (h)	conv. (%)	yield (%)[d]
1	 (^{i}PrIM^{Me})	4	>99	n.d.
2		20	>99	62
3		40	>99	>99 (62)[e]
4[a]		20	<1	n.d.[f]
5[b]		20	70	n.d.[f]
6	 (EtIM^{Me})	20	>99	n.d.[f]
7	 (MeIM^{Et})	20	>99	16
8	 (^{i}PrIM^H)	20	>99	n.d.[f]
9[d]	 (DippIM^H)	4	<1	n.d.[f]
10	 (^{i}PrIM^{Ph})	4	34	n.d.[f]
11	 (^{i}PrPyC)	4	>99	n.d.[f]
12[c]	 (^{Me}CAAC)	4	<1	n.d.[f]
13	without ligand	4	<1	n.d.[f]

[a]20 mol% of ligand was added. [b]5 mol% of ligand was added. [c]Dipp indicates 2,6-diisopropylphenyl. [d]yield was estimated based on the amount of formed $(GePh_2)_5$. [e]value in bracket indicates the isolated yield. [f]n.d. indicates "not detected".

Regeneration of Ph_2GeH_2 from $(GePh_2)_5$ by the reaction with H_2 catalyzed by $[Fe(mesityl)_2]_2$ / NHC. In a 20 mL flask, $[Fe(mesityl)_2]_2$ (2 mg, 0.0025 mmol) was dissolved in THF (0.4 mL), then $^{i}PrIM^{Me}$ (2 mg, 0.01 mmol) was added to this solution under nitrogen atmosphere. The obtained reaction mixture was stirred at room temperature for several minutes, then $(GePh_2)_5$ (23 mg, 0.02 mmol) was added to this solution. The atmosphere of this flask was replaced by 1 atm of hydrogen. The resulting mixture then stirred at 0 °C for 24 h, then conversion of $(GePh_2)_5$ was estimated to be >99%, and the yield of Ph_2GeH_2 and $(Ph_2GeO)_3$ was estimated to be 51 % and 49 %, respectively, by ^1H NMR spectrum.

Reaction of $(GePh_2)_5$ with $PhICl_2$ to afford Ph_2GeCl_2. In a 20 mL schlenk, $(GePh_2)_5$ (57 mg, 0.05 mmol) was dissolved in THF (0.5 mL), then $PhICl_2$ (138 mg, 0.5 mmol) was added to this solution under nitrogen atmosphere. The obtained reaction mixture was stirred at 40 °C for 14 h, then quantitative formation of Ph_2GeCl_2 was confirmed by the ^1H NMR spectrum of the crude product. Then, the reaction mixture was dried *in vacuo*, and the remaining residue was extracted with diethyl ether (10 mL). The filtrate was removed *in vacuo* to afford Ph_2GeCl_2 as pale yellow liquid (47 mg, 64%).

Reaction of Ph_2GeCl_2 with $LiAlH_4$ to afford Ph_2GeH_2. In a 100 mL flask, $LiAlH_4$ (0.38 g, 10 mmol) was suspended in diethyl ether (20 mL), then Ph_2GeCl_2 (3 g, 10 mmol) was added to this solution under nitrogen atmosphere. The obtained reaction mixture was stirred at room temperature for 18 h, then the reaction mixture was quenched by 1M HCl aq. (30 mL). The mixture was extracted by diethyl ether (30 mL×3), then combined organic phases was dried over by $MgSO_4$. The supernatant was collected, and the solvent was removed *in vacuo* to obtain Ph_2GeH_2 as colorless liquid (1.88g, 82%).

Dehydrogenative coupling of Ph_3GeH or $^{t}BuGeH_3$ in the presence of a catalytic amount of $[Fe(mesityl)_2]_2$. In a 4 mL vial, $[Fe(mesityl)_2]_2$ (7.4 mg, 0.0125 mmol) was dissolved in THF (0.5 mL), then ligand shown in Table S3 (0.05 mmol) was added under nitrogen atmosphere. The obtained reaction mixture was stirred at room temperature for several minutes, then hydrogermane (0.5 mmol) was added to this solution. The resulting mixture was then stirred at room temperature for time indicated in Table S3, then conversion of the substrate and yield of the dehydrogenative coupling product was estimated by ^1H NMR spectrum.

Table S3. Dehydrogenative coupling of Ph_3GeH or $^{t}BuGeH_3$ in the presence of a catalytic amount of $[Fe(mesityl)_2]_2$.

entry	substrate	ligand	product	time (h)	conv. (%)
1	Ph_3GeH	$MeIM^{Et}$	$Ph_3Ge\text{-}GePh_3$	66	>99
2	$^{t}BuGeH_3$	$^{i}PrIM^{Me}$	oligomers	20	>99

[a]Formation of oligogermanes was suggested by ^1H NMR and FAB-MS spectrum (see Figures S13 and S14).

Synthesis of *trans*-$Fe(^{i}PrIM^{Me})_2(mesityl)_2$ (1). In 50 mL schlenk tube, $[Fe(mesityl)_2]_2$ (59 mg, 0.1 mmol) was dissolved in diethyl ether (5 mL), then $^{i}PrIM^{Me}$ (72 mg, 0.4 mmol) was added to the solution. The resulting solution

was stirred at room temperature for 16 h. The reaction mixture was dried *in vacuo*, then the remaining residue was extracted by pentane (2 mL). The pentane solution was centrifuged to remove small amount of insoluble materials, then was concentrated to ca. 0.5 mL. The solution was cooled at -20 °C, then *trans*-Fe(^{i}PrIM^{Me})$_2$(mesityl)$_2$ (**1**) was obtained as pale yellow crystals (68 mg, 52%). ^{1}H NMR (400 MHz, r.t., C_6D_6): no signal was observed. Magnetic susceptibility (Evans): μ_{eff} = 3.91 (C_6D_6, 20.1 °C). Anal. Calcd. for $C_{58}H_{70}N_4Ge_3Fe_1$: C, 73.37; H, 9.54; N, 8.56. Found: C, 73.36; H, 9.45, N; 8.83.

Synthesis of *trans*-Fe(^{i}PrIM^{Me})$_2$[Ge(H)Ph$_2$]$_2$ (2) by the reaction of *in situ* generated complex 1 with Ph$_2$GeH$_2$. In a 20 mL vial, [Fe(mesityl)$_2$]$_2$ (59 mg,0.1 mmol) was dissolved in diethyl ether (10 mL), then ^{i}PrIM^{Me} (72 mg, 0.4 mmol) was added to this solution. The resulting solution was stirred at room temperature for 5 min. to generate complex **1**. Then, diethyl ether (5 mL) solution of Ph_2GeH_2 (91 mg, 0.4 mmol) was added to this solution, and the obtained solution was stirred at room temperature for 5 min. The resulting solution was cooled to −20 °C to obtain trace amount of *trans*-Fe(^{i}PrIM^{Me})$_2$[Ge(H)Ph$_2$H]$_2$ (**2**) as red crystals.

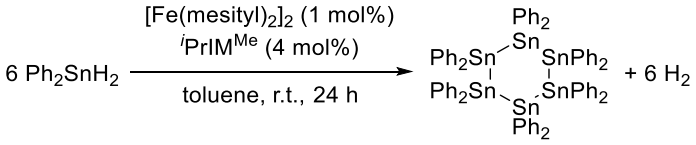
Synthesis of *trans*-Fe(^{i}PrIM^{Me})$_2$[Ge(H)Ph$_2$]$_2$ (2) by the reaction of FeCl$_2$ and *in situ* generated LiGe(H)Ph$_2$. In a 20 mL Schlenk, Ph_2GeH_2 (664 mg, 2.9 mmol) was dissolved in THF (6 mL), then hexane solution of ^{t}BuLi (1.6 M, 2 mL, 3.2 mmol) was added at −78 °C. The resulting solution was warmed to −40 °C, and was stirred for 20 minutes to generate LiGe(H)Ph$_2$ solution. In a 50 mL flask, $FeCl_2$ (152 mg, 1.2 mmol) was dissolved in THF (6 mL), then ^{i}PrIM^{Me} was added to this solution at room temperature. After stirring this solution for overnight, the resulting solution was cooled to −78 °C, and the LiGe(H)Ph$_2$ solution was slowly added. The resulting mixture was stirred for 1 h at −78 °C, and the solvent was removed *in vacuo*. The remaining residue was extracted by toluene (10 mL + 5 mL), and the solution was centrifuged to remove small amount of insoluble materials. The supernatant was concentrated to ca. 5 mL, kept at −20 °C to obtain *trans*-Fe(^{i}PrIM^{Me})$_2$[Ge(H)Ph$_2$H]$_2$ (**2**) as red crystals (445 mg, 43%).^{1}H NMR (400 MHz, r.t., C_6D_6): no signal was observed. Magnetic susceptibility (Evans): μ_{eff} = 3.46 μ_B (in C_6D_6, 21.0 °C). IR (ATR): $\nu_{Ge\text{-}H}$ = 1848 cm^{-1}. Anal. Calcd. for $C_{46}H_{62}N_4Ge_2Fe_1$: C, 63.35; H, 7.17; N, 6.42. Found: C, 63.29; H, 7.56, N; 6.25.

Synthesis of Fe(GePh$_2$)$_4$(^{i}PrIM^{Me})$_2$ (3). In 4 mL vial, Fe(GePh$_2$H)$_2$(^{i}PrIM^{Me})$_2$ (**2**) (44 mg, 0.05 mmol) was dissolved in THF (2 mL), then Ph_2GeH_2 (12 mg, 0.05 mmol) and Et_2GeH_2 (7 mg, 0.05 mmol) were slowly added to this solution. The resulting solution was stirred for 18h at room temperature, then the solvent was removed *in vacuo*. The resulting residue was dissolved in diethyl ether (0.5 mL), then cooled to -20 °C to obtain Fe(GePh$_2$)$_3$(^{i}PrIM^{Me})$_2$ as dark brown crystals (17 mg, 32%). ^{1}H NMR (400 MHz, r.t., C_6D_6): δ = 27.1 (brs, 24H), 21.3 (brs, 10H), 19.8 (brs, 20H), 15.8 (brs, 20H), 14.3 (brs, 10H), 7.5 (brs, 6H), −1.2 (brs, 10H). Magnetic susceptibility (Evans): μ_{eff} = 3.17 μ_B (in C_6D_6, 20.3 °C). Anal. Calcd. for $C_{58}H_{70}N_4Ge_3Fe_1$: C, 63.51; H, 6.43; N, 5.11. Found: C, 63.55; H, 6.28, N; 5.14.

Synthesis of Fe(GePh$_2$)$_4$(^{i}PrIM^{Me})$_2$ (4). In a 20 mL vial, Fe(GePh$_2$H)$_2$(^{i}PrIM^{Me})$_2$ (**2**) (44 mg, 0.5 mmol) was dissolved in diethyl ether (4 mL), then Ph_2GeH_2 (23 mg, 1 mmol) was slowly added to this solution. The resulting solution was stirred at room temperature for 18 h, then solvent was removed *in vacuo*. The remaining residue was

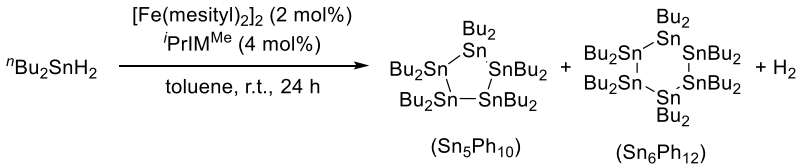
extracted with 1,2-dimethoxyethane (1 mL), and the obtained solution was kept as -20 °C to obtain red crystals. ^{1}H NMR spectrum suggested that the obtained red crystals consists of complex **3** and **4** in ca. 1 : 1 molar ratio, and formation of small amount of $(GePh_2)_5$ was also observed. ^{1}H NMR spectrum data for complex **4** (400 MHz, r.t., C_6D_6): δ = δ = 37.1 (brs, 13H), 35.0 (brs, 14H), 28.9 (brs, 12H), 16.3 (brs, 13H), 13.1 (brs, 24H), 12.1 (brs, 8.5H), 10.1 (brs, 7H), −4.4 (brs, 16.5H), −7.7 (brs, 16.5H), −10.5 (brs, 7H). The actual ^{1}H NMR chart of the mixture of **3** and **4** was shown in Figure S12.

Dehydrogenative coupling of Ph_2SnH_2 catalyzed by $[Fe(mesityl)_2]_2$ / ^{i}PrIM^{Me}. In a 4 mL vial, $[Fe(mesityl)_2]_2$ (6 mg, 0.01 mmol) was dissolved in toluene (3 mL), then ^{i}PrIM^{Me} (7 mg, 0.04 mmol) were added to this solution. The resulting mixture was stirred at room temperature for several minutes, then toluene (2 mL) solution of Ph_2SnH_2 (275 mg, 1 mmol) was added. The resulting mixture was stirred at room temperature for 24 h. Analysis of the crude product by ^{1}H NMR spectrum revealed that Sn_6Ph_{12} was formed in quantitative yield with complete conversion of Ph_2SnH_2. Then, the reaction mixture was dried *in vacuo*, and the remaining residue was washed by pentane (5 mL x 3). The obtained powder was dried under vacuum to afford Sn_6Ph_{12} as white powder (191 mg, 70%).



Dehydrogenative coupling of ^{n}Bu$_2$SnH$_2$ catalyzed by $[Fe(mesityl)_2]_2$ / ^{i}PrIM^{Me}. In a 4 mL vial, $[Fe(mesityl)_2]_2$ (6 mg, 0.01 mmol, 2 mol% for Fe) dissolved in toluene, then ^{i}PrIM^{Me} (7 mg, 0.04 mmol) was added to this solution. The obtained mixture was stirred at room temperature for several minutes, then toluene solution of ^{n}Bu$_2$SnH$_2$ (0.5 mmol) was added to this solution (total concentration of the reaction mixture was listed in Table S4). The resulting mixture was then stirred at room temperature for 24 h, then conversion of ^{n}Bu$_2$SnH$_2$ and the ratio of the formed product were estimated by ^{119}Sn NMR spectrum (see Figures S17 and S18).

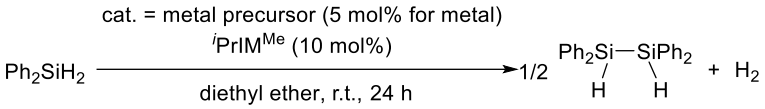
Table S4. Dehydrogenative coupling of Bu_2SnH_2 catalyzed by $[Fe(mesityl)_2]_2$ / ^{i}PrIM^{Me}.



entry	concentration (mol/L)	conversion (%)	ratio of Sn_5Ph_{10} and Sn_6Ph_{12}
1	1	>99	0.7 : 1
2	0.2	>99	2 : 1
3	0.02	>99	3 : 1

General Procedure for the dehydrogenative coupling of Ph_2SiH_2 catalyzed by various transition metal catalyst precursorss in the presence of ^{i}PrIM^{Me}. In a 4 mL vial, transition metal catalyst precursor (5 mol% for metal) was dissolved in diethyl ether (0.25 mL), then ^{i}PrIM^{Me} (10 mg, 0.054 mmol) was added to this solution. The obtained mixture was stirred at room temperature for several minutes, then Ph_2SiH_2 (100 mg, 0.54 mmol) was added to this solution. The resulting mixture was then stirred at room temperature for 24 h, then conversion of Ph_2SiH_2 was estimated by ^{1}H NMR spectrum.

Table S5. Dehydrogenative coupling of Ph_2SiH_2 catalyzed by various metal catalyst precursors.

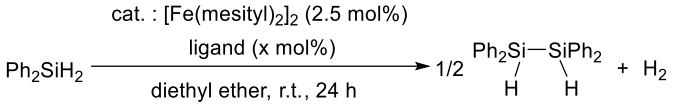


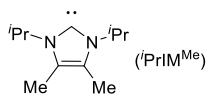
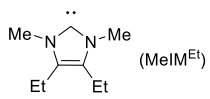
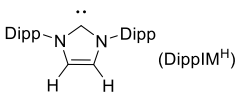
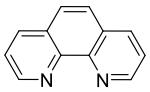
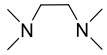
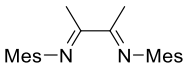
entry	metal precursor	Conversion of Ph_2SiH_2 (%)[a]
1	$[Fe(mesityl)_2]_2$	32
2	$Fe[Si(SiMe_3)_3]_2(THF)_2$	37
3	$Fe[Ge(SiMe_3)_3]_2(THF)_2$	29
4	$Fe(OCO^{t}Bu)_2$	24
5	$FeBr_2$	4
6	$Fe[N(SiMe_3)_2]_2$	<1
8	$[Mn(mesityl)_2]_3$	<1
10	$Co(O^{i}Pr)_2$	37
11[b]	$Ni(COD)_2$	23
12[b]	$[Ni(^{i}PrIM^{Me})_2(COD)]_2$	15
13	without metal precursor	<1

[a]conversion of Ph_2SiH_2 was determined by ^{1}H NMR. [b] ^{i}PrIM^{Me} was not added.

General Procedure for the dehydrogenative coupling of Ph_2SiH_2 catalyzed by $[Fe(mesityl)_2]_2$ in the presence of various auxiliary ligands. In a 4 mL vial, $[Fe(mesityl)_2]_2$ (8 mg, 0.013 mmol) was dissolved in diethyl ether (0.25 mL), then ligand (5 or 10 mol%) was added to this solution. The resulting mixture was stirred at room temperature for several minutes, and the solvent was removed *in vacuo*. Then Ph_2SiH_2 (100 mg, 0.54 mmol) was added to this vial, and the obtained solution was stirred at room temperature for 24 h. Conversion of Ph_2SiH_2 was estimated by ^1H NMR spectrum.

Table S6. Dehydrogenative coupling of Ph_2SiH_2 catalyzed by $[Fe(mesityl)_2]_2$ in the presence of various auxiliary ligands.

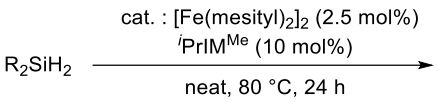


entry	ligand	ligand loading (mol%)	Conversion of Ph_2SiH_2 (%)[a]
1	 ($^iPrIM^{Me}$)	10	32
2	 ($MeIM^{Et}$)	10	<1
3[b]	 ($DippIM^{H}$)	10	<1
4	P(cyclohexyl)$_3$	10	4
5		5	<1
6		5	<1
7[c]		5	3
8	without ligand	−	15

[a]conversion of Ph_2SiH_2 was determined by ^1H NMR. [b]Dipp indicates 2,6-diisopropylphenyl. [c]Mes indicates 2,4,6-trimethylphenyl.

General Procedure for the dehydrogenative coupling of various hydrosilanes catalyzed by [Fe(mesityl)$_2$]$_2$ / ^{i}PrIM^{Me}. In a 4 mL vial, [Fe(mesityl)$_2$]$_2$ (7 mg, 0.0125 mmol) was dissolved in diethyl ether (0.1 mL), then ^{i}PrIM^{Me} (9mg, 0.05 mmol) was added to this solution. The resulting mixture was stirred at room temperature for several minutes, and the solvent was removed *in vacuo*. Then hydrosilane (0.5 mmol) was added to this vial, and the obtained solution was stirred for 24 h at 80 ℃. Conversion of the substrate and the yield and ratio of the dehydrogenative coupling products as well as products due to the redistribution were estimated by ^{1}H NMR spectrum.

Table S7. Dehydrogenative coupling of various hydrosilanes catalyzed by [Fe(mesistyl)$_2$]$_2$ / ^{i}PrIM^{Me}.



entry	substrate	conversion (%)	yield of the products (%)[a]
1	Ph_2SiH_2	82	$Ph_2(H)Si$-$Si(H)Ph_2$: 54%, $Ph_2(H)$-$SiPh_2$-$Si(H)Ph_2$: 8%
2[b]	$MePhSiH_2$	75	Me_2PhSiH: 47%, $MePh_2SiH$: 19%, $PhSiH_3$: 9%
3	$(Et_2N)_2SiH_2$	39	$(Et_2N)_3SiH$: 39%
4	$^iPr_2SiH_2$	~0	<1
6	Bu_2SiH_2	~0	<1

[a]Yield was determined by comparison between product and internal standard 1,4-dioxane. [b]reaction was performed in 1,4-dioxane (0.2 M).

Figure S1. ^{1}H NMR spectrum of isolated $(GePh_2)_5$ in C_6D_6 at room temperature.

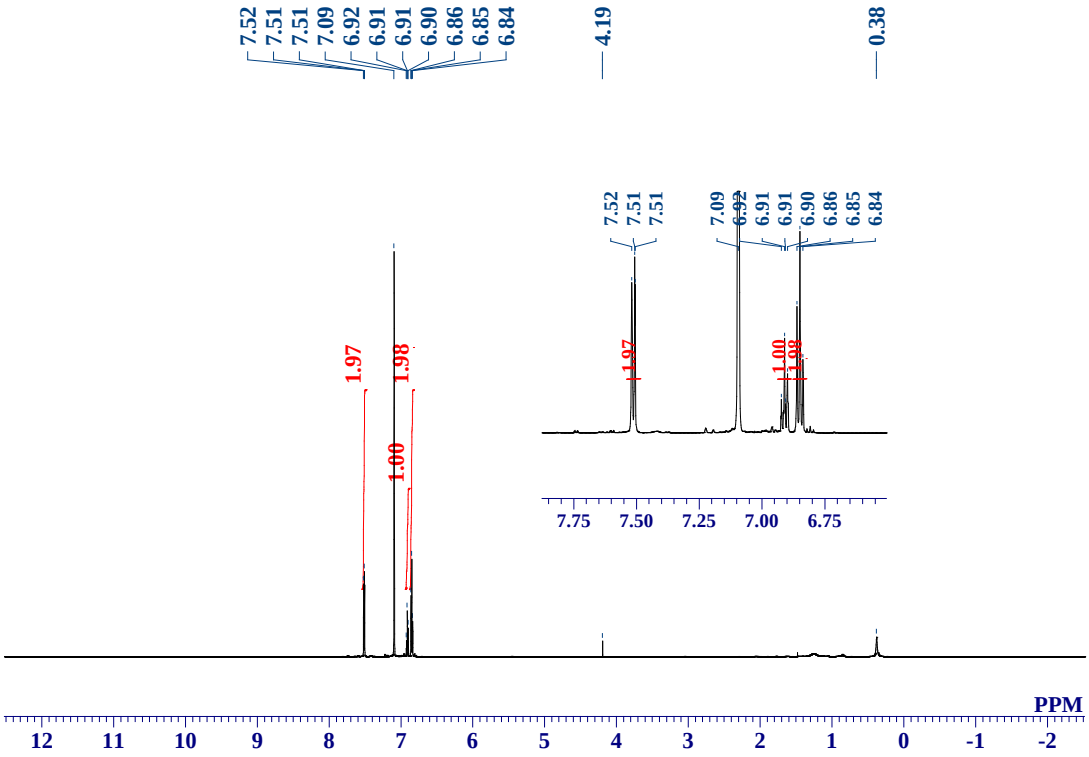


Figure S2. ^{13}C NMR spectrum of isolated $(GePh_2)_5$ in C_6D_6 at room temperature.

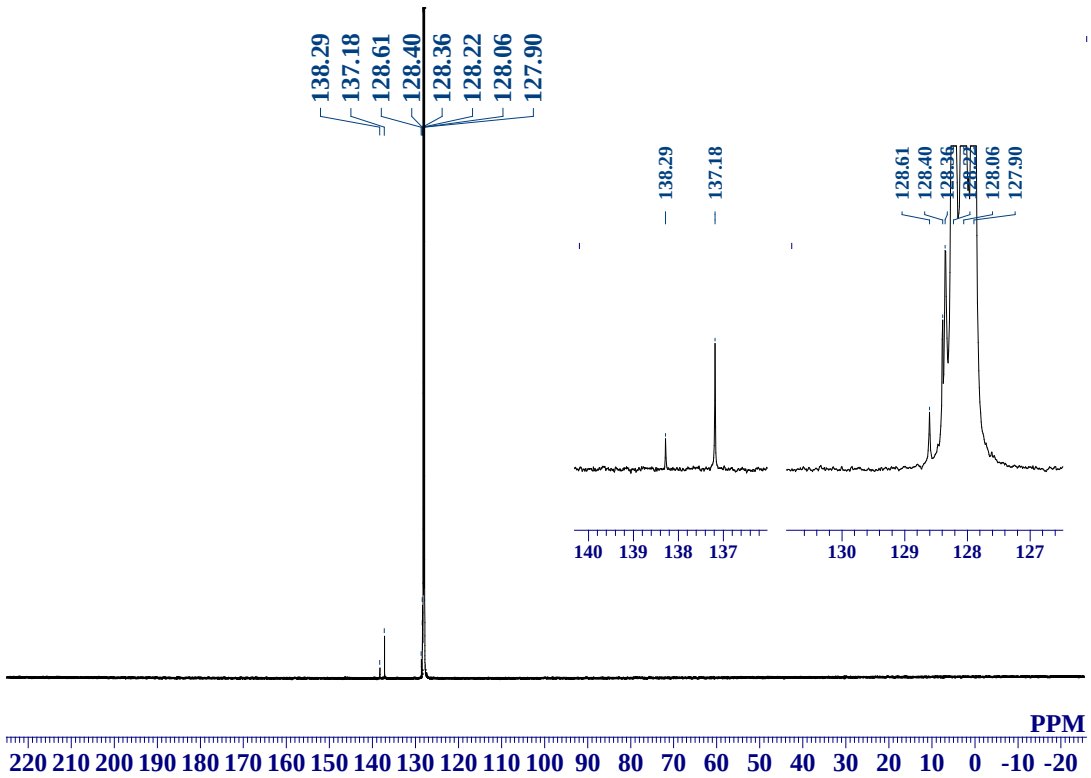


Figure S3. ^{1}H NMR spectrum of isolated Ge_5Et_{10} in C_6D_6 at room temperature.

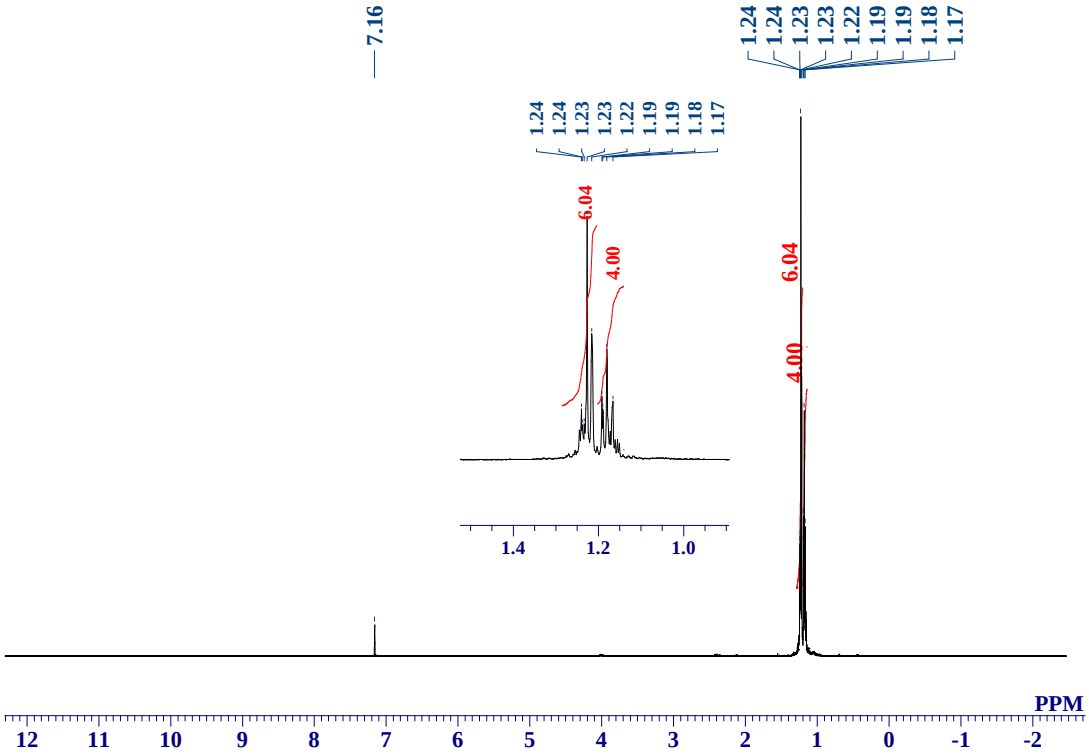


Figure S4. ^{13}C NMR spectrum of isolated Ge_5Et_{10} in C_6D_6 at room temperature.

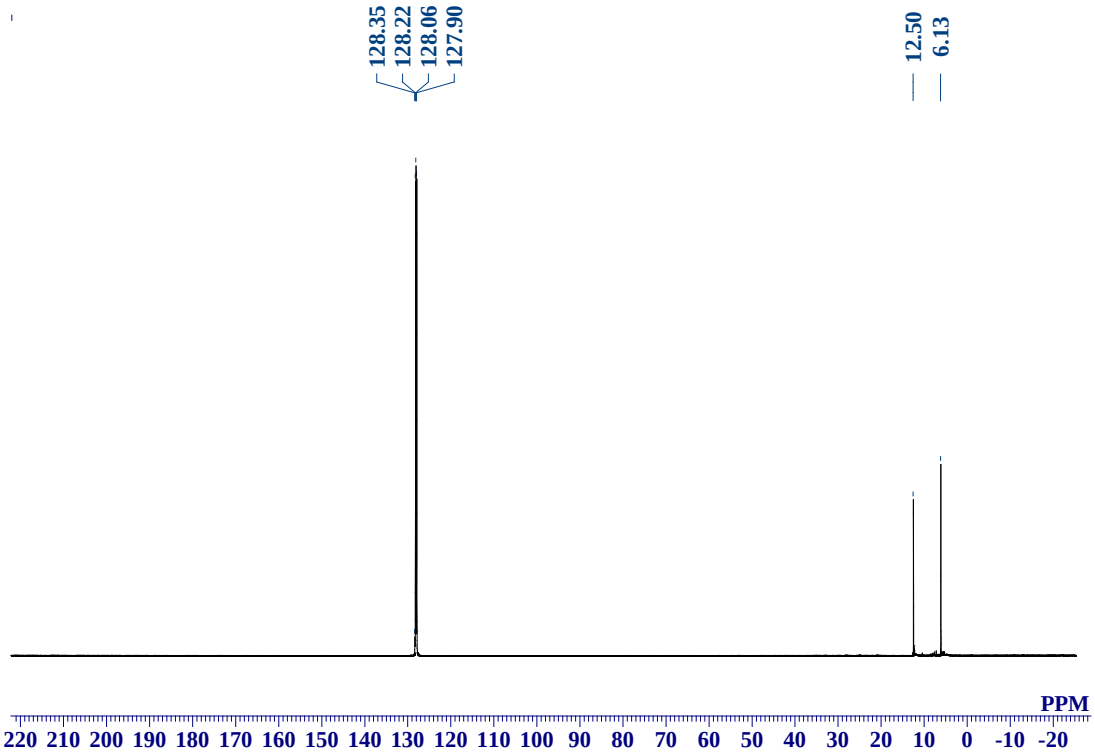


Figure S5. [1]H NMR spectrum of the crude product obtained in the reaction shown in entry 3 in Table S2.

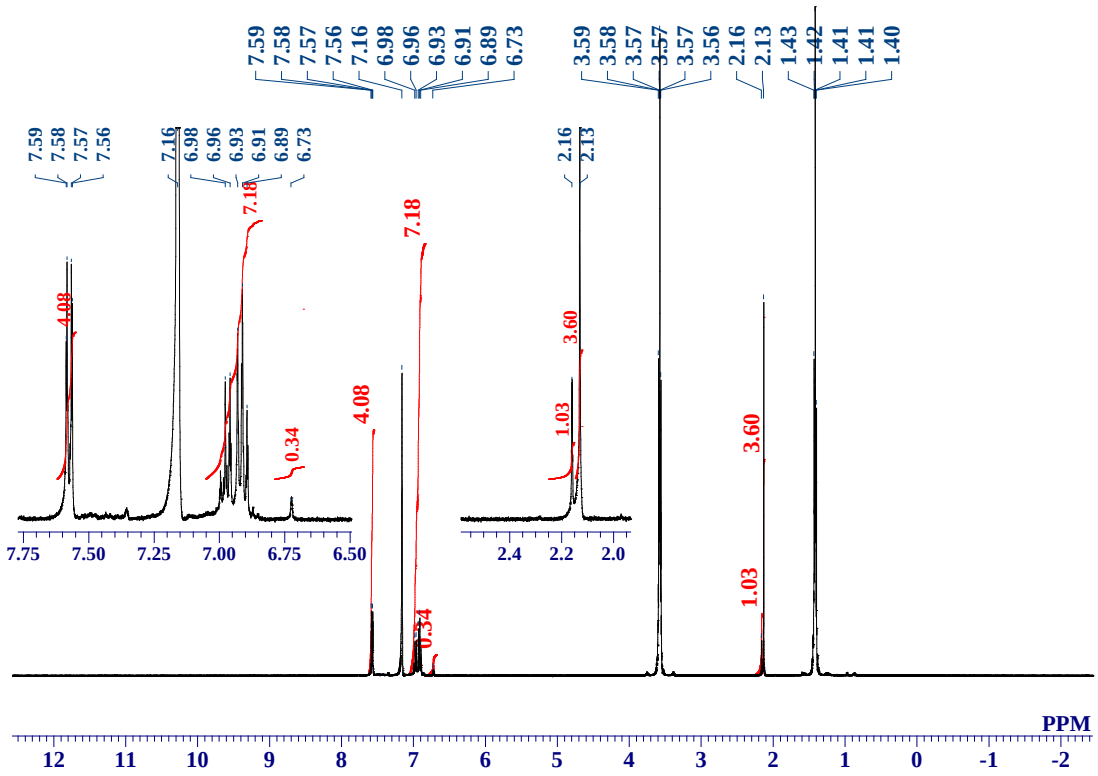


Figure S6. [1]H NMR spectrum of the crude product obtained in the reaction shown in entry 1 in Table S2.

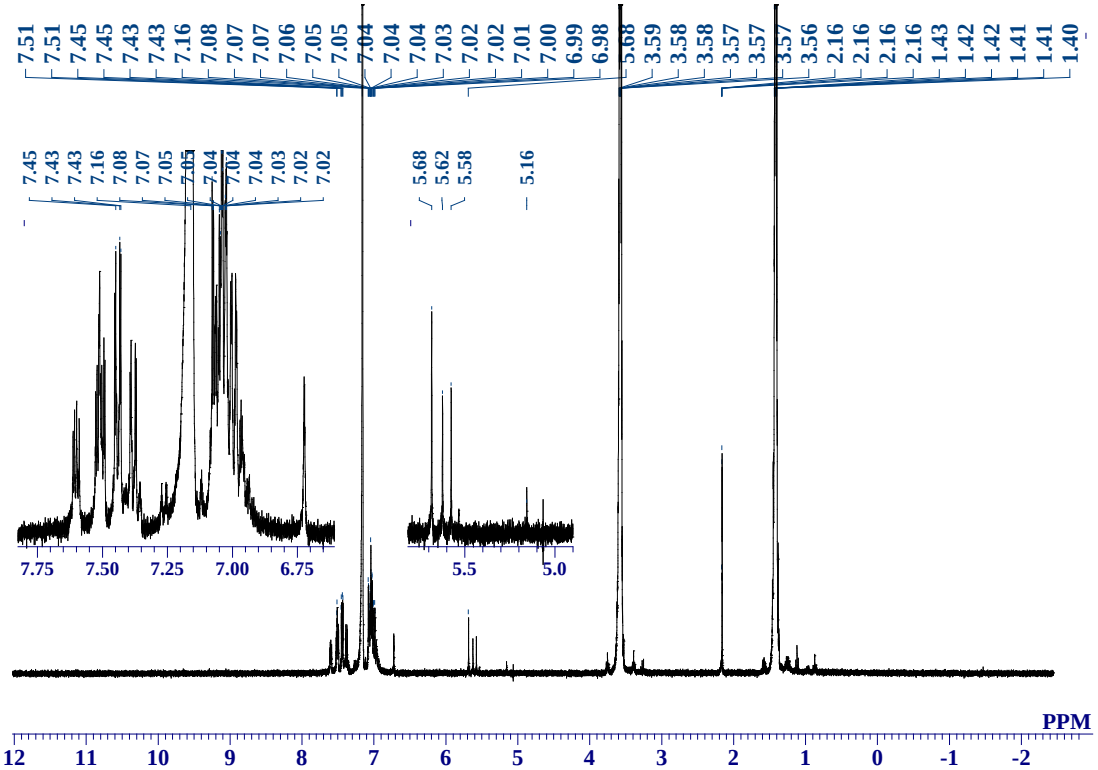


Figure S7. [1]H NMR spectrum of the crude product obtained in the reaction shown in entry 6 in Table S2.

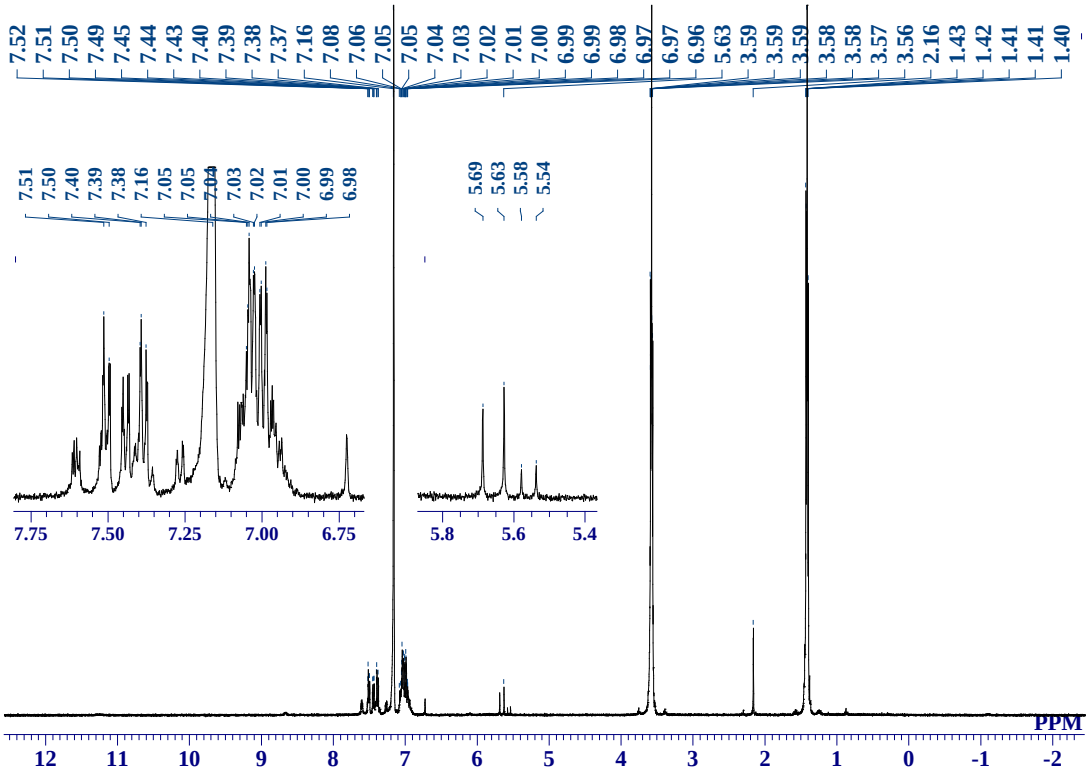


Figure S8. [1]H NMR spectrum of the crude product obtained in the reaction shown in entry 7 in Table S2.

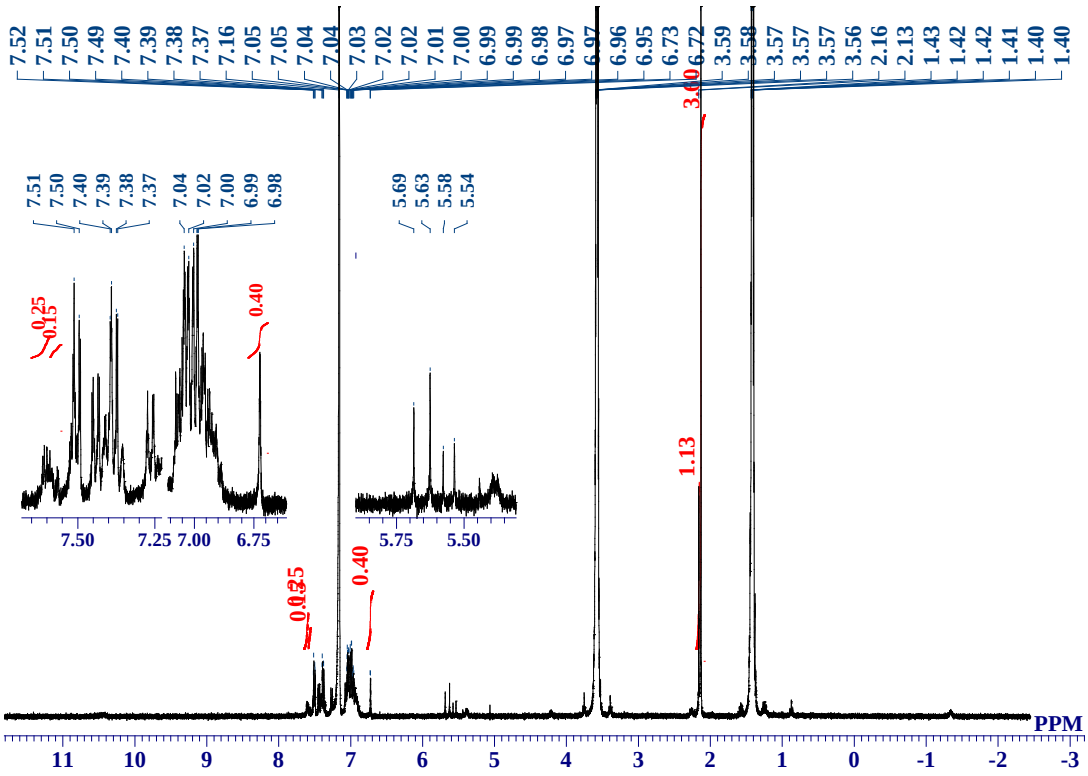


Figure S9. ^{1}H NMR spectrum of the crude product obtained in the reaction shown in entry 8 in Table S2.

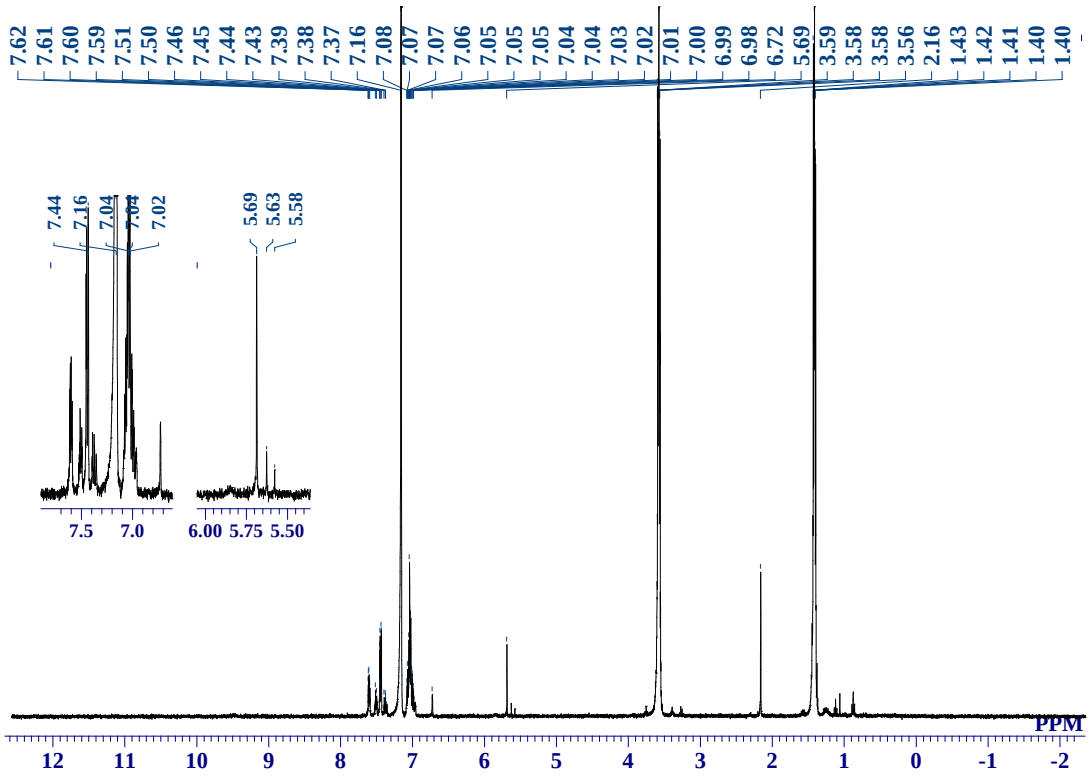


Figure S10. ^{1}H NMR spectrum of the crude product obtained in the reaction shown in entry 11 in Table S2.

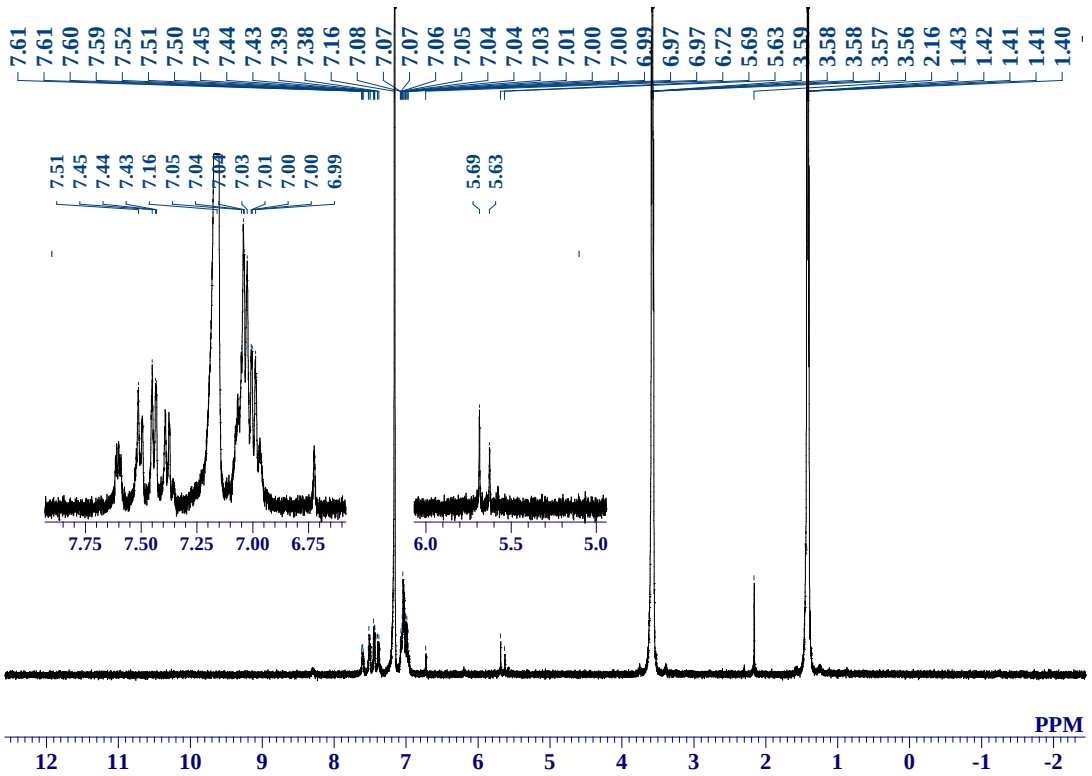


Figure S11. ^{1}H NMR spectrum of Fe(GePh$_2$)$_3$(^{i}PrIM^{Me})$_2$ (**3**) in C_6D_6 at room temperature.

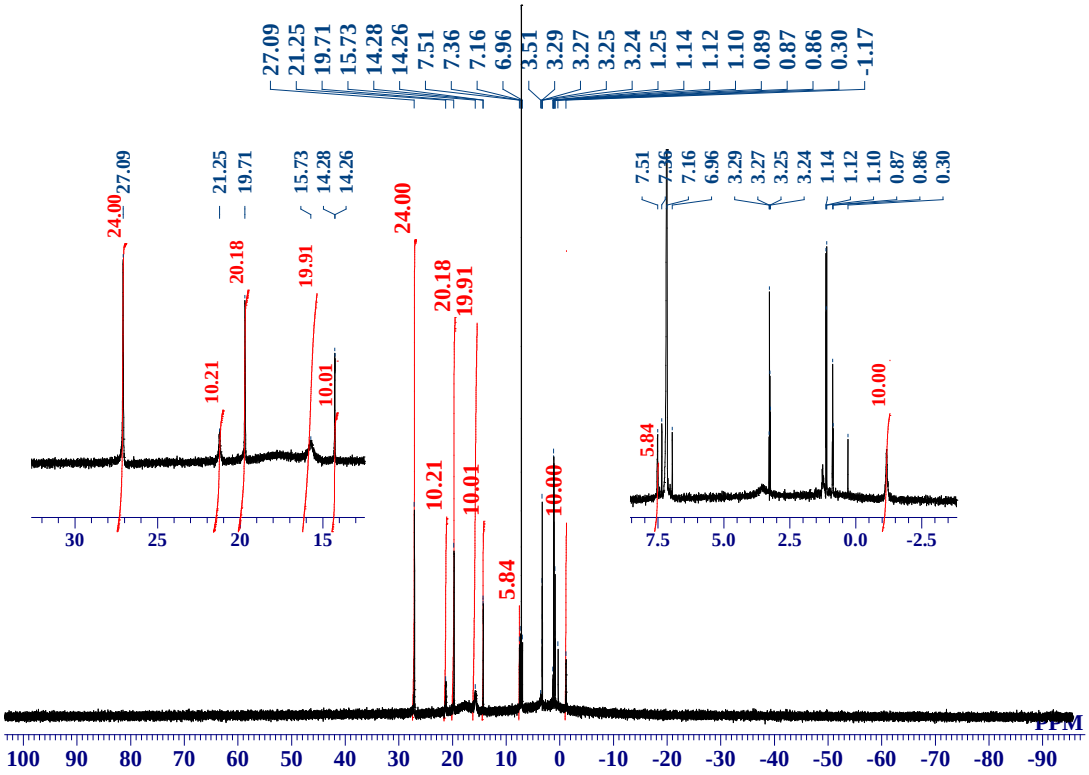


Figure S12. ^{1}H NMR spectrum of the mixture of **3** and **4** obtained by the reaction of **2** with 2 equiv. of Ph$_2$GeH$_2$.

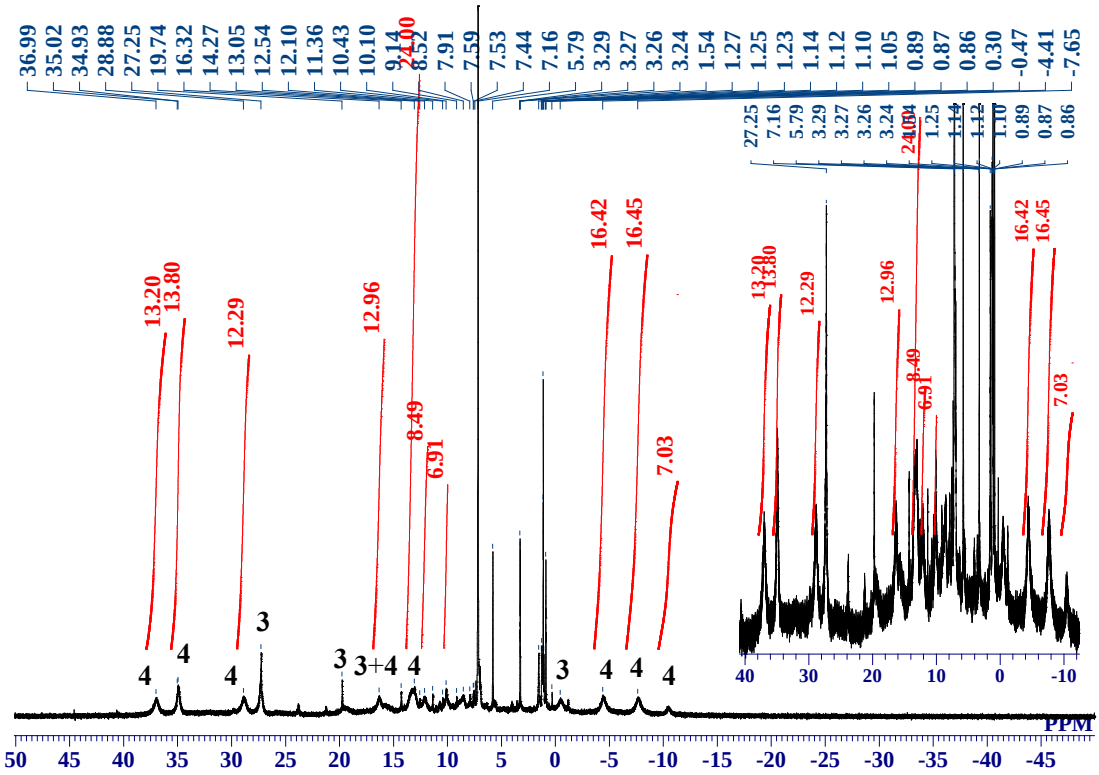


Figure S13. ^{1}H NMR spectrum of crude product obtained in the reaction shown in entry 2 in Table S3.

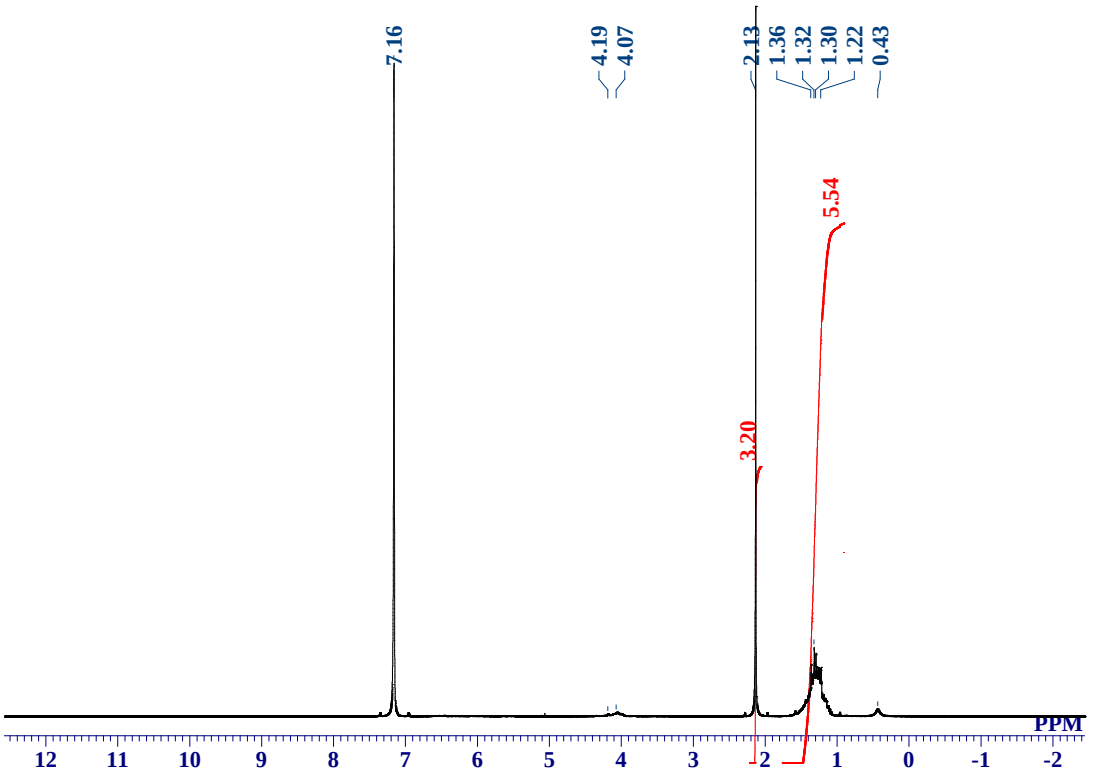


Figure S14. FAB-MS spectrum of the crude product obtained in the reaction shown in entry 2 in Table S3.

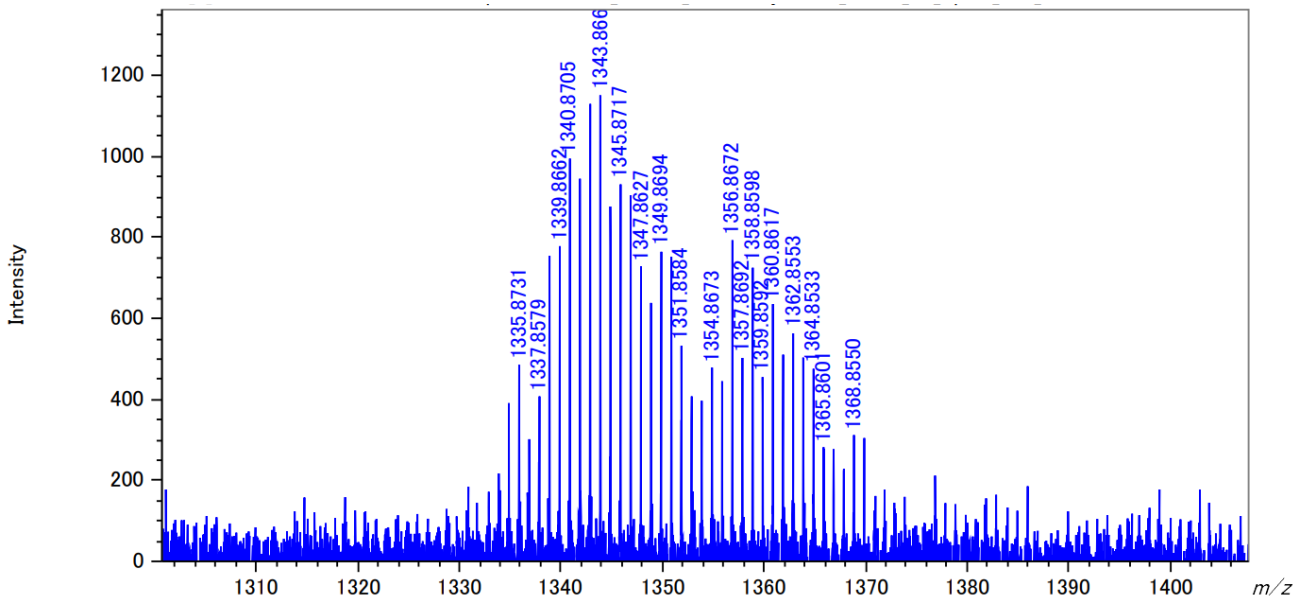


Figure S15. ^{1}H NMR spectrum of isolated $(SnPh_2)_6$ in C_6D_6 at room temperature.

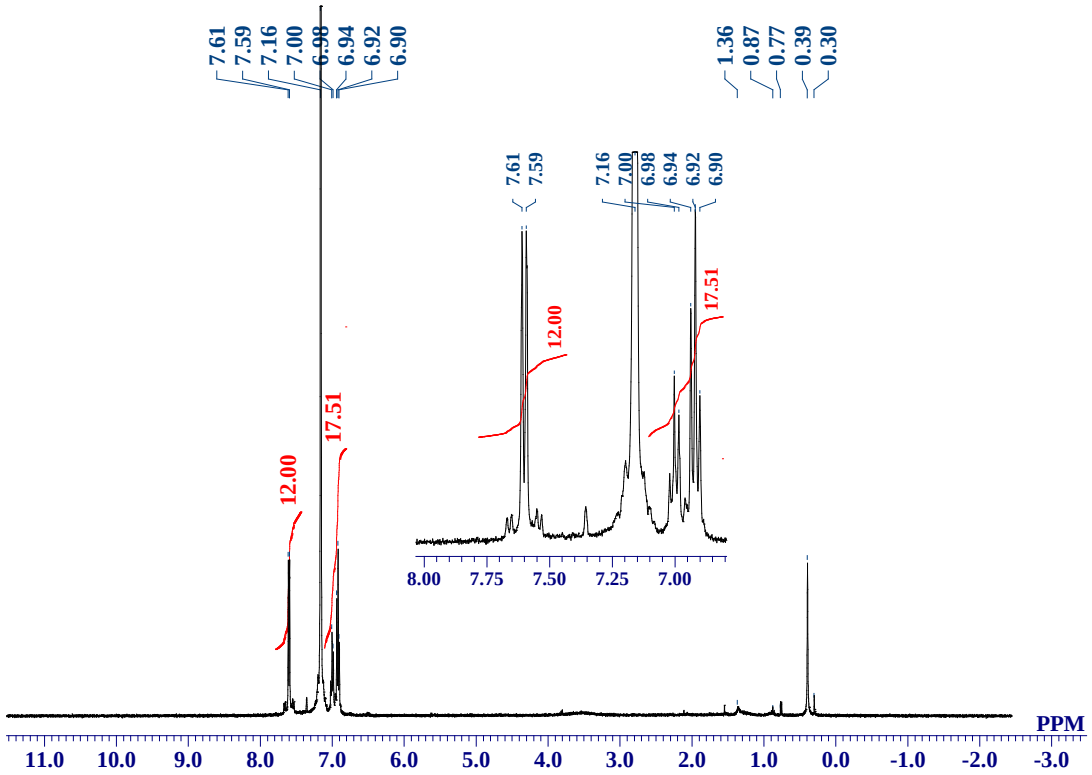


Figure S16. ^{119}Sn NMR spectrum of isolated $(SnPh_2)_6$ in C_6D_6 at room temperature.

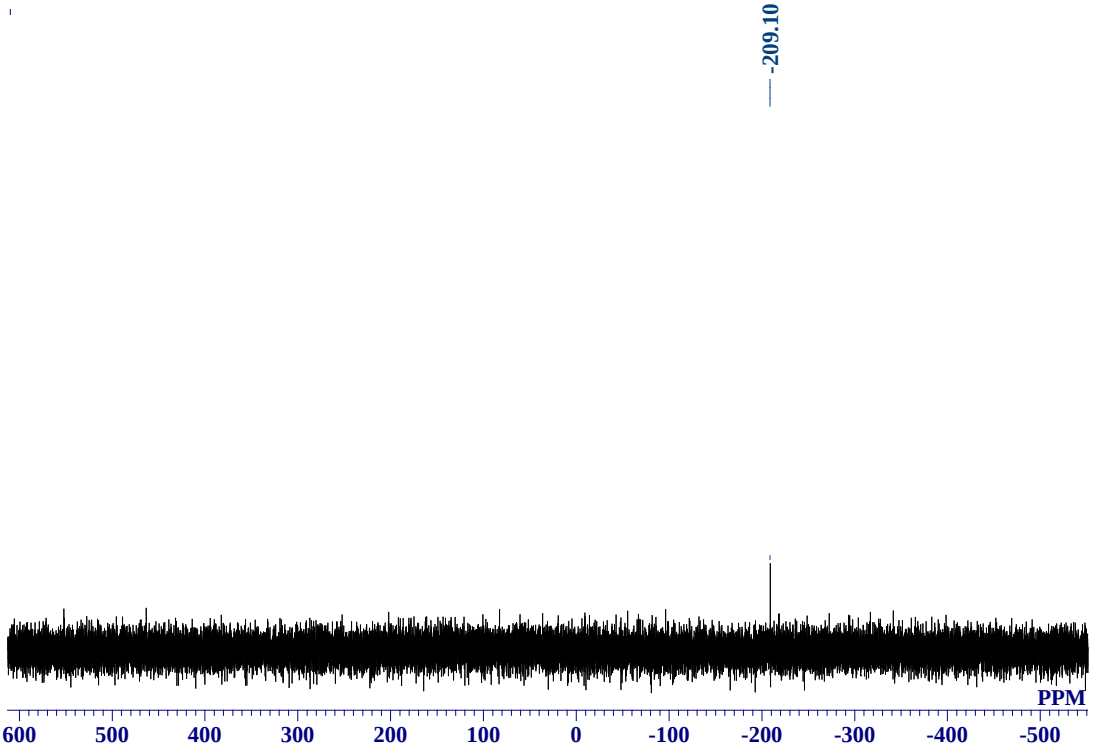


Figure S17. ^{1}H NMR spectrum of the crude product obtained by the reaction shown in entry 3 in Table S4.

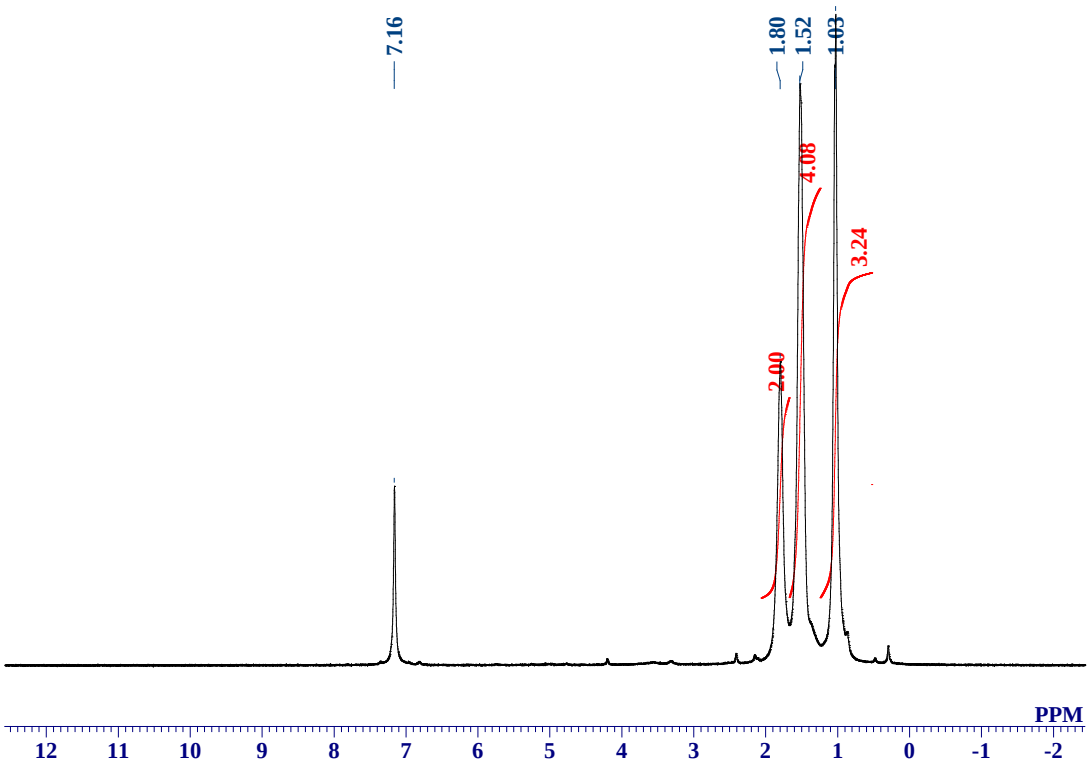


Figure S18. ^{119}Sn NMR spectrum of the crude product obtained by the reaction shown in entry 3 in Table S4.

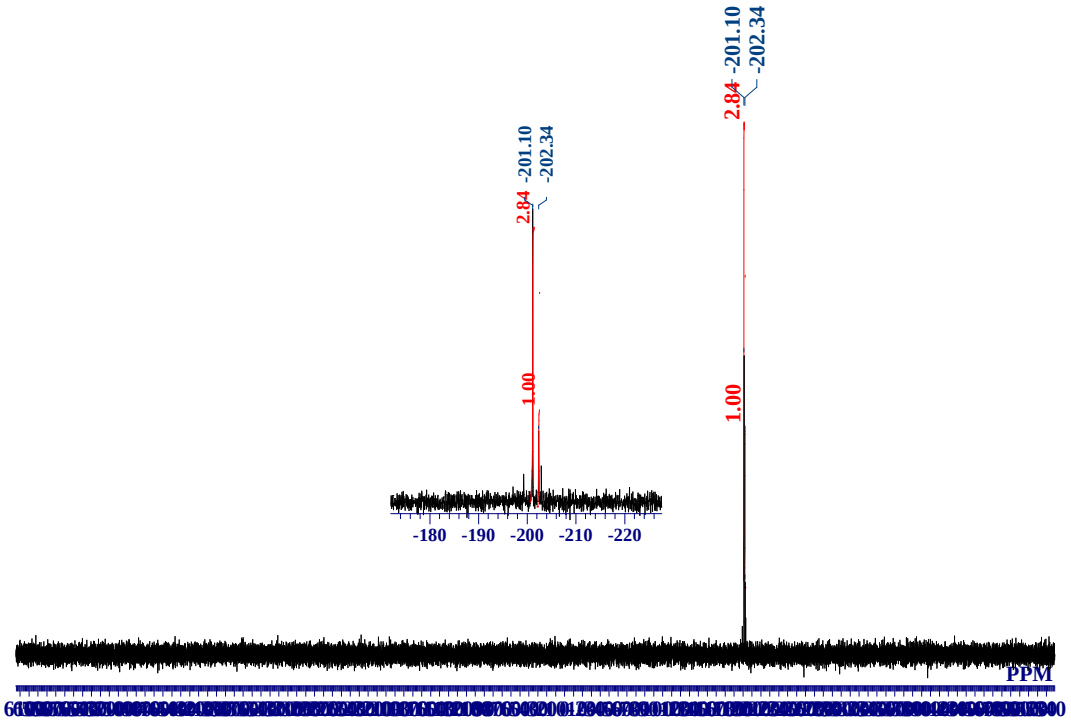
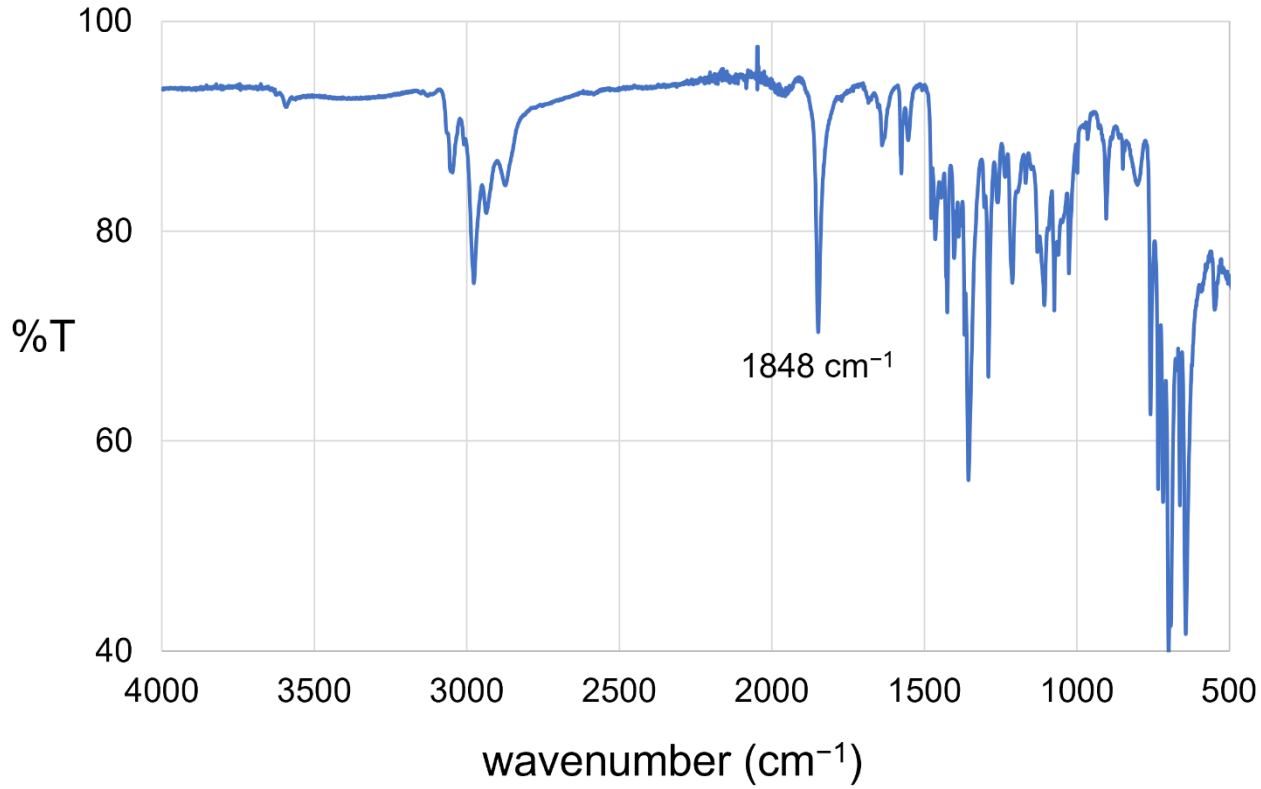


Figure S19. ATR-IR spectrum of **2** in the solid state.



X-ray data collection and reduction

X-ray crystallography for compounds **1**, **2** and **4** was performed on a Rigaku Saturn CCD area detector with graphite monochromated Mo-Kα radiation (λ=0.71075 Å), and single crystals of **3** suitable for X-ray crystallography were analyzed by synchrotron radiation at beam line BL02B1 (λ=0.41220 Å) of Spring-8 (Hyogo, Japan) using PILATUS3 X CdTe 1M detector. The data were collected at 133 K for **1** 203 K for **2** and 100(1) K for **3** and 113 K for **4** using ω scan in the θ range of $1.83 \leq \theta \leq 31.25$ deg (**1**), $3.14 \leq \theta \leq 27.47$ deg (**2**), $1.52 \leq \theta \leq 19.18$ deg (**3**), $1.94 \leq \theta \leq 31.34$ deg (**4**). The data obtained were processed using Crystal-Clear (Rigaku) on a Pentium computer, and were corrected for Lorentz and polarization effects. The structures were solved by direct methods[21], and expanded using Fourier techniques. Hydrogen atoms were refined using the riding model. The final cycle of full-matrix least-squares refinement on F^2 was based on 6,256 observed reflections and 213 variable parameters for **1**, 4,814 observed reflections and 251 variable parameters for **2**, 27,862 observed reflections and 607 variable parameters for **3**, 16,430 observed reflections and 780 variable parameters for **4**. Neutral atom scattering factors were taken from International Tables for Crystallography (IT), Vol. C, Table 6.1.1.4[22]. Anomalous dispersion effects were included in Fcalc[23]; the values for Δf' and Δf'' were those of Creagh and McAuley[24]. The values for the mass attenuation coefficients are those of Creagh and Hubbell[25]. All calculations were performed using the CrystalStructure[26] crystallographic software package except for refinement, which was performed using SHELXL Version 2017/1[27]. Details of final refinement as well as the bond lengths and angle are summarized in Tables S8, S9, S10 and S11, and the numbering scheme employed is also shown in Figures S20 S21, S22 and S23, which were drawn with ORTEP at 50% probability ellipsoids. CCDC 2204746 (**1**), 2204747 (**2**), 2204748 (**3**) and 2204749 (**4**) contain the supplementary crystallographic data for this paper.

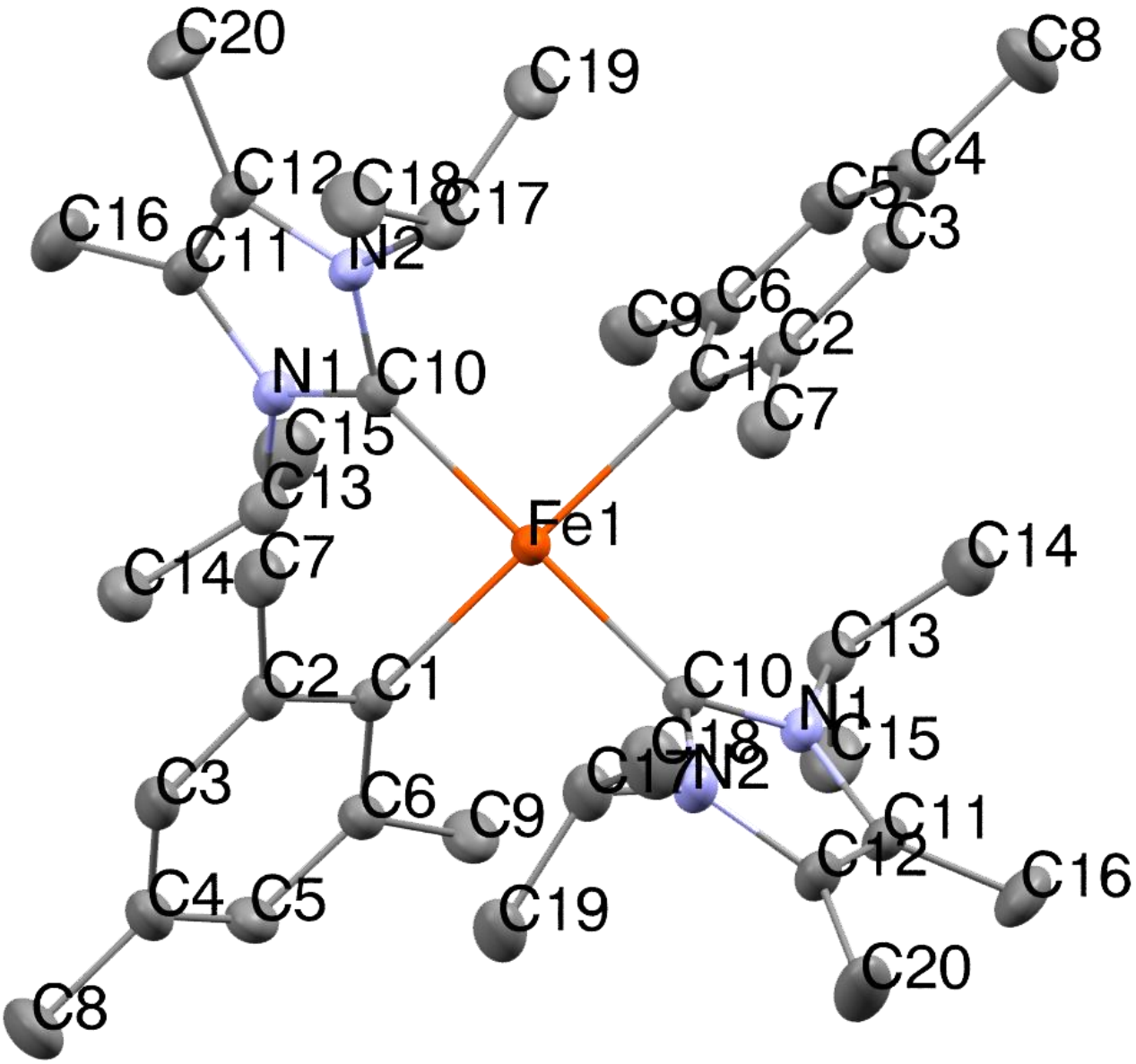


Figure S20. ORTEP drawing of **1** (50% probability of the thermal ellipsoids). Hydrogen atoms were omitted for clarity.

Table S8. Crystal data and structure refinement for **1**.

Empirical Formula	$C_{40}H_{62}FeN_4$
Formula Weight	654.80
Crystal Color, Habit	colorless, platelet
Crystal Dimensions	0.200 X 0.200 X 0.030 mm
Crystal System	monoclinic
Lattice Type	C-centered
Lattice Parameters	a = 20.0556(10) Å
	b = 13.4841(5) Å
	c = 16.4559(7) Å
	β = 107.412(5) º
	V = 4246.3(3) Å^3
Space Group	C2/c (#15)
Z value	4
D_{calc}	1.024 g/cm^3
F_{000}	1424.00
μ(MoKα)	3.828 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å)
	graphite monochromated
Voltage, Current	50kV, 24mA
Temperature	-140.0ºC
Detector Aperture	72.8 x 72.8 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-70.0 - 110.0º
Exposure Rate	10.0 sec./º
Detector Swing Angle	20.00º
ω oscillation Range (χ=45.0, ϕ=90.0)	-70.0 - 110.0º
Exposure Rate	10.0 sec./º
Detector Swing Angle	20.00º
Detector Position	45.00 mm
Pixel Size	0.035 mm
$2\theta_{max}$	62.4º
No. of Reflections Measured	Total: 19705
	Unique: 6256 (R_{int} = 0.0386)
Corrections	Lorentz-polarization
	Absorption

	(trans. factors: 0.581 - 0.989)
Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	$\Sigma\ w\ (Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\ \sigma^2(Fo^2) + (0.0681 \cdot P)^2$ + 2.1911 · P] where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	62.4^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	6256
No. Variables	213
Reflection/Parameter Ratio	29.37
Residuals: R1 (I>2.00σ(I))	0.0497
Residuals: R (All reflections)	0.0743
Residuals: wR2 (All reflections)	0.1327
Goodness of Fit Indicator	1.025
Max Shift/Error in Final Cycle	0.000
Maximum peak in Final Diff. Map	0.35 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.31 $e^-/Å^3$

Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Fe1	0.50000	0.74838(2)	0.25000	1.294(8)	1/2
N1	0.35038(7)	0.81364(10)	0.15767(9)	1.61(2)	1
N2	0.34973(7)	0.68233(11)	0.23013(9)	1.84(2)	1
C1	0.50051(8)	0.74776(12)	0.37524(10)	1.60(2)	1
C2	0.52836(8)	0.66870(13)	0.43121(11)	1.80(3)	1
C3	0.52786(9)	0.66855(15)	0.51590(11)	2.34(3)	1
C4	0.50098(10)	0.74673(15)	0.54968(11)	2.65(3)	1
C5	0.47391(9)	0.82565(15)	0.49690(12)	2.51(3)	1
C6	0.47249(9)	0.82646(13)	0.41146(11)	1.90(3)	1
C7	0.56053(9)	0.57981(13)	0.40190(12)	2.30(3)	1
C8	0.50101(14)	0.7464(2)	0.64124(14)	4.13(5)	1
C9	0.43925(10)	0.91496(14)	0.35905(12)	2.48(3)	1
C10	0.39423(8)	0.74846(11)	0.21087(10)	1.48(2)	1
C11	0.28053(9)	0.78858(14)	0.14392(11)	2.04(3)	1
C12	0.28016(9)	0.70633(15)	0.18934(12)	2.31(3)	1
C13	0.37639(9)	0.90023(12)	0.12146(11)	1.91(3)	1
C14	0.35987(10)	0.89210(15)	0.02553(12)	2.57(3)	1
C15	0.35278(11)	0.99871(13)	0.14840(14)	2.89(4)	1
C16	0.21951(9)	0.84290(16)	0.08683(14)	2.92(4)	1
C17	0.37507(9)	0.59838(13)	0.28828(11)	2.14(3)	1
C18	0.35073(12)	0.49771(15)	0.24723(14)	3.16(4)	1
C19	0.35835(10)	0.61102(15)	0.37151(12)	2.64(3)	1
C20	0.21833(10)	0.64942(19)	0.19711(14)	3.67(5)	1

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe1	0.01486(16)	0.01906(15)	0.01501(15)	0.00000	0.00409(11)	0.00000
N1	0.0172(6)	0.0239(7)	0.0192(7)	0.0016(5)	0.0041(5)	0.0010(5)
N2	0.0172(6)	0.0308(7)	0.0211(7)	-0.0028(6)	0.0046(5)	0.0044(6)
C1	0.0154(7)	0.0262(8)	0.0188(7)	-0.0023(6)	0.0046(6)	-0.0009(6)
C2	0.0171(8)	0.0299(8)	0.0204(8)	-0.0018(6)	0.0038(6)	0.0017(6)
C3	0.0233(9)	0.0437(11)	0.0206(8)	0.0011(8)	0.0048(7)	0.0080(7)
C4	0.0264(9)	0.0548(12)	0.0196(8)	-0.0006(9)	0.0071(7)	0.0004(8)
C5	0.0272(9)	0.0461(11)	0.0238(9)	0.0025(8)	0.0102(7)	-0.0072(8)

C6	0.0204(8)	0.0315(9)	0.0207(8)	-0.0006(7)	0.0067(6)	-0.0022(7)
C7	0.0292(9)	0.0286(9)	0.0277(9)	0.0027(7)	0.0059(7)	0.0058(7)
C8	0.0494(14)	0.0861(19)	0.0234(10)	0.0089(12)	0.0141(9)	0.0021(11)
C9	0.0352(10)	0.0320(9)	0.0280(9)	0.0084(8)	0.0108(8)	-0.0027(7)
C10	0.0178(7)	0.0215(7)	0.0170(7)	0.0008(6)	0.0055(6)	-0.0005(6)
C11	0.0156(8)	0.0378(9)	0.0233(8)	0.0033(7)	0.0045(6)	0.0004(7)
C12	0.0167(8)	0.0447(11)	0.0249(9)	-0.0032(7)	0.0043(7)	0.0024(8)
C13	0.0234(8)	0.0217(8)	0.0260(9)	0.0030(6)	0.0055(7)	0.0038(6)
C14	0.0305(10)	0.0393(10)	0.0272(10)	0.0029(8)	0.0077(8)	0.0090(8)
C15	0.0395(11)	0.0252(9)	0.0427(12)	0.0086(8)	0.0086(9)	0.0017(8)
C16	0.0193(9)	0.0446(11)	0.0430(12)	0.0060(8)	0.0030(8)	0.0028(9)
C17	0.0255(9)	0.0289(9)	0.0255(9)	-0.0050(7)	0.0054(7)	0.0068(7)
C18	0.0461(12)	0.0342(10)	0.0386(11)	-0.0132(9)	0.0109(9)	0.0029(9)
C19	0.0321(10)	0.0403(11)	0.0265(9)	-0.0089(8)	0.0070(8)	0.0077(8)
C20	0.0222(9)	0.0756(16)	0.0394(12)	-0.0128(10)	0.0061(8)	0.0166(11)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Fe1	C1	2.0579(17)	Fe1	$C1^1$	2.0579(17)
Fe1	C10	2.0241(15)	Fe1	$C10^1$	2.0241(15)
N1	C10	1.3607(19)	N1	C11	1.392(2)
N1	C13	1.475(2)	N2	C10	1.364(2)
N2	C12	1.393(2)	N2	C17	1.471(2)
C1	C2	1.410(2)	C1	C6	1.413(3)
C2	C3	1.397(3)	C2	C7	1.507(3)
C3	C4	1.375(3)	C4	C5	1.378(3)
C4	C8	1.507(3)	C5	C6	1.398(3)
C6	C9	1.506(2)	C11	C12	1.339(3)
C11	C16	1.493(2)	C12	C20	1.496(3)
C13	C14	1.517(3)	C13	C15	1.520(3)
C17	C18	1.530(3)	C17	C19	1.514(3)

Symmetry Operators:

(1) -X+1,Y,-Z+1/2

Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
C1	Fe1	C1[1]	179.53(7)	C1	Fe1	C10	90.53(6)
C1	Fe1	C10[1]	89.47(6)	C1[1]	Fe1	C10	89.47(6)
C1[1]	Fe1	C10[1]	90.53(6)	C10	Fe1	C10[1]	179.94(6)
C10	N1	C11	111.90(14)	C10	N1	C13	122.17(13)
C11	N1	C13	125.92(13)	C10	N2	C12	111.51(14)
C10	N2	C17	122.10(13)	C12	N2	C17	126.39(16)
Fe1	C1	C2	122.64(13)	Fe1	C1	C6	122.40(12)
C2	C1	C6	114.95(16)	C1	C2	C3	122.21(17)
C1	C2	C7	121.06(16)	C3	C2	C7	116.73(16)
C2	C3	C4	121.54(17)	C3	C4	C5	117.74(18)
C3	C4	C8	121.29(18)	C5	C4	C8	121.0(2)
C4	C5	C6	121.71(19)	C1	C6	C5	121.82(16)
C1	C6	C9	121.14(16)	C5	C6	C9	117.03(17)
Fe1	C10	N1	128.25(12)	Fe1	C10	N2	128.45(11)
N1	C10	N2	103.29(13)	N1	C11	C12	106.49(14)
N1	C11	C16	125.36(17)	C12	C11	C16	128.12(17)
N2	C12	C11	106.82(16)	N2	C12	C20	125.16(17)
C11	C12	C20	128.02(16)	N1	C13	C14	111.69(14)
N1	C13	C15	113.27(17)	C14	C13	C15	112.13(15)
N2	C17	C18	113.15(14)	N2	C17	C19	112.02(15)
C18	C17	C19	111.81(17)				

Symmetry Operators:

(1) -X+1,Y,-Z+1/2

Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
C1	Fe1	C10	N1	124.94(13)	C1	Fe1	C10	N2	-56.39(13)
C10	Fe1	C1	C2	116.50(11)	C10	Fe1	C1	C6	-63.08(11)
C1	Fe1	C10[1]	N1[1]	-55.52(13)	C1	Fe1	C10[1]	N2[1]	123.15(13)
C10[1]	Fe1	C1	C2	-63.56(11)	C10[1]	Fe1	C1	C6	116.86(11)
C1[1]	Fe1	C10	N1	-55.52(13)	C1[1]	Fe1	C10	N2	123.15(13)
C10	Fe1	C1[1]	C2[1]	-63.56(11)	C10	Fe1	C1[1]	C6[1]	116.86(11)
C1[1]	Fe1	C10[1]	N1[1]	124.94(13)	C1[1]	Fe1	C10[1]	N2[1]	-56.39(13)
C10[1]	Fe1	C1[1]	C2[1]	116.50(11)	C10[1]	Fe1	C1[1]	C6[1]	-63.08(11)
C10	N1	C11	C12	0.16(19)	C10	N1	C11	C16	-178.01(14)

C11	N1	C10	Fe1	178.70(13)	C11	N1	C10	N2	-0.23(18)
C10	N1	C13	C14	114.32(15)	C10	N1	C13	C15	-117.92(16)
C13	N1	C10	Fe1	-2.1(2)	C13	N1	C10	N2	179.00(13)
C11	N1	C13	C14	-66.6(2)	C11	N1	C13	C15	61.2(2)
C13	N1	C11	C12	-179.04(14)	C13	N1	C11	C16	2.8(3)
C10	N2	C12	C11	-0.1(2)	C10	N2	C12	C20	-179.70(15)
C12	N2	C10	Fe1	-178.71(13)	C12	N2	C10	N1	0.22(18)
C10	N2	C17	C18	-122.02(16)	C10	N2	C17	C19	110.48(17)
C17	N2	C10	Fe1	2.2(2)	C17	N2	C10	N1	-178.89(14)
C12	N2	C17	C18	59.0(2)	C12	N2	C17	C19	-68.5(2)
C17	N2	C12	C11	178.93(15)	C17	N2	C12	C20	-0.6(3)
Fe1	C1	C2	C3	-179.38(9)	Fe1	C1	C2	C7	0.8(2)
Fe1	C1	C6	C5	-179.23(10)	Fe1	C1	C6	C9	1.2(2)
C2	C1	C6	C5	1.2(2)	C2	C1	C6	C9	-178.46(13)
C6	C1	C2	C3	0.2(2)	C6	C1	C2	C7	-179.58(13)
C1	C2	C3	C4	-1.0(2)	C7	C2	C3	C4	178.78(13)
C2	C3	C4	C5	0.4(3)	C2	C3	C4	C8	-179.60(14)
C3	C4	C5	C6	1.0(3)	C8	C4	C5	C6	-178.99(17)
C4	C5	C6	C1	-1.8(3)	C4	C5	C6	C9	177.79(15)
N1	C11	C12	N2	-0.0(2)	N1	C11	C12	C20	179.53(16)
C16	C11	C12	N2	178.08(18)	C16	C11	C12	C20	-2.4(3)

Symmetry Operators:

(1) -X+1,Y,-Z+1/2

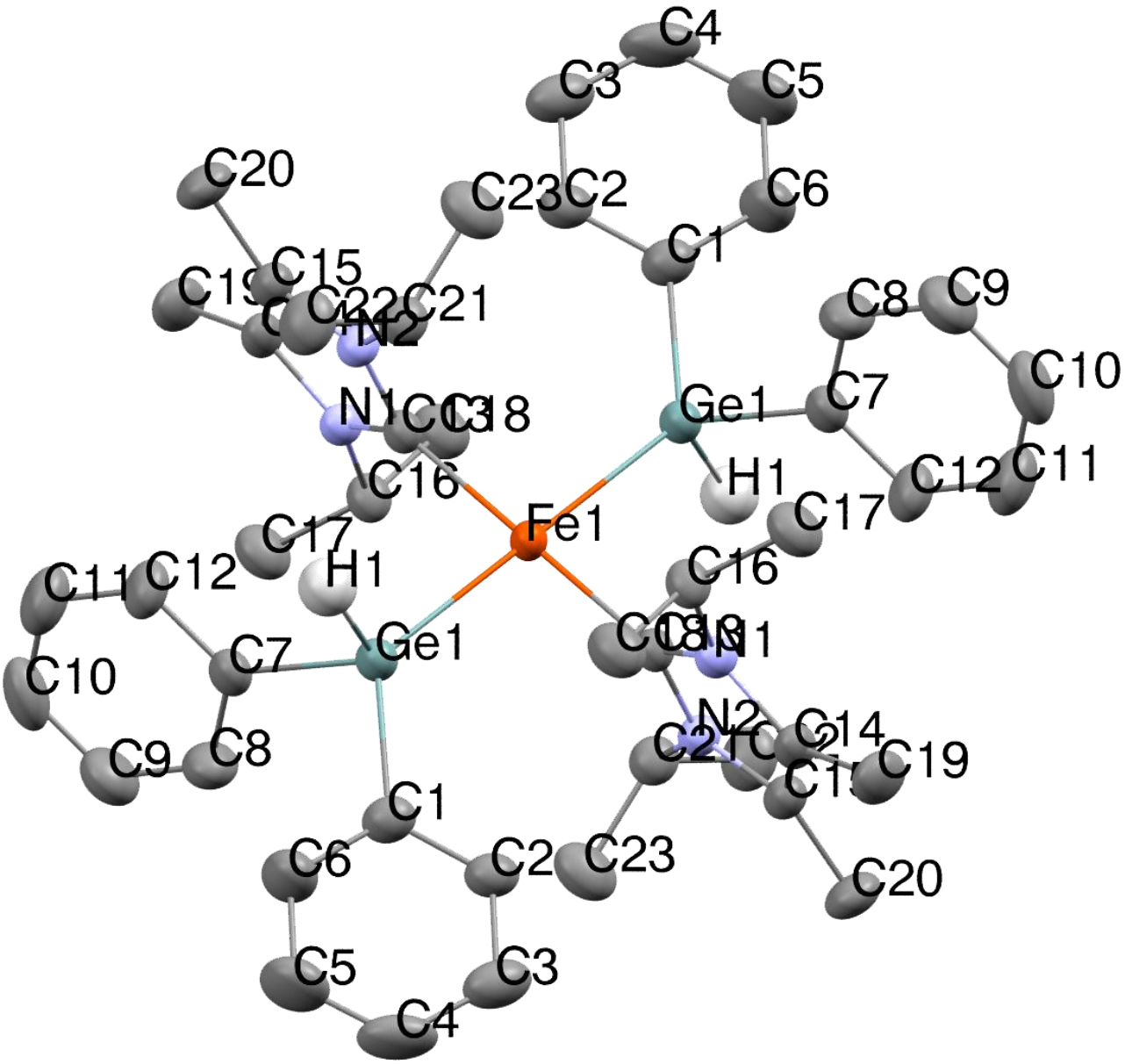


Figure S21. ORTEP drawing of **2** (50% probability of the thermal ellipsoids). Hydrogen atoms were omitted for clarity.

Table S9. Crystal data and structure refinement for **2**.

Empirical Formula	$C_{46}H_{62}FeGe_2N_4$
Formula Weight	872.05
Crystal Color, Habit	red, block
Crystal Dimensions	0.100 X 0.100 X 0.050 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 12.836(4) Å b = 12.928(4) Å c = 13.403(4) Å β = 104.798(4) º V = 2150.4(11) Å^3
Space Group	$P2_1/n$ (#14)
Z value	2
D_{calc}	1.347 g/cm^3
F_{000}	912.00
μ(MoKα)	17.564 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å) multi-layer mirror monochromated
Voltage, Current	50kV, 24mA
Temperature	-69.8ºC
Detector Aperture	72.8 x 72.8 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-70.0 - 110.0º
Exposure Rate	16.0 sec./º
Detector Swing Angle	19.96º
ω oscillation Range (χ=45.0, ϕ=90.0)	-70.0 - 110.0º
Exposure Rate	16.0 sec./º
Detector Swing Angle	19.96º
Detector Position	44.81 mm
Pixel Size	0.141 mm
$2\theta_{max}$	55.0º
No. of Reflections Measured	Total: 17535 Unique: 4814 (R_{int} = 0.1537)
Corrections	Lorentz-polarization Absorption

	(trans. factors: 0.728 - 0.916)
Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + (0.0394 · P)^2 + 0.8991 · P] where P = (Max(Fo^2,0) + 2Fc^2)/3
$2\theta_{max}$ cutoff	55.0^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	4814
No. Variables	251
Reflection/Parameter Ratio	19.18
Residuals: R1 (I>2.00σ(I))	0.0607
Residuals: R (All reflections)	0.0878
Residuals: wR2 (All reflections)	0.1470
Goodness of Fit Indicator	1.083
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.00 e^-/Å^3
Minimum peak in Final Diff. Map	-0.82 e^-/Å^3

Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Ge1	0.49474(3)	0.50917(3)	0.68114(3)	2.379(12)	1
Fe1	0.50000	0.50000	0.50000	1.903(14)	1/2
N1	0.2726(2)	0.5896(2)	0.4459(2)	2.08(5)	1
N2	0.3923(2)	0.7097(2)	0.4813(2)	2.09(5)	1
C1	0.5728(3)	0.4202(3)	0.7991(3)	2.86(7)	1
C2	0.6509(3)	0.3502(3)	0.7918(3)	2.88(7)	1
C3	0.7085(4)	0.2944(4)	0.8778(4)	3.84(9)	1
C4	0.6864(4)	0.3093(4)	0.9721(4)	4.56(11)	1
C5	0.6086(5)	0.3770(5)	0.9807(4)	4.93(12)	1
C6	0.5511(4)	0.4323(4)	0.8947(3)	4.26(10)	1
C7	0.3505(3)	0.5168(3)	0.7097(3)	2.64(7)	1
C8	0.3017(4)	0.4290(4)	0.7345(3)	3.79(9)	1
C9	0.2001(4)	0.4310(5)	0.7534(4)	4.52(10)	1
C10	0.1465(4)	0.5230(5)	0.7491(4)	4.33(11)	1
C11	0.1926(4)	0.6107(4)	0.7239(4)	4.29(10)	1
C12	0.2945(4)	0.6084(4)	0.7043(3)	3.37(8)	1
C13	0.3823(3)	0.6051(3)	0.4745(3)	2.05(6)	1
C14	0.2173(3)	0.6828(3)	0.4338(3)	2.48(7)	1
C15	0.2909(3)	0.7590(3)	0.4549(3)	2.50(7)	1
C16	0.2265(3)	0.4852(3)	0.4221(3)	2.39(6)	1
C17	0.1345(3)	0.4629(4)	0.4725(3)	3.42(8)	1
C18	0.1924(4)	0.4678(4)	0.3059(3)	3.43(8)	1
C19	0.0965(3)	0.6948(4)	0.4051(3)	3.44(8)	1
C20	0.2717(4)	0.8727(3)	0.4545(3)	3.35(8)	1
C21	0.4987(3)	0.7603(3)	0.5072(3)	2.66(7)	1
C22	0.5117(4)	0.8331(4)	0.5996(3)	3.68(9)	1
C23	0.5209(4)	0.8128(4)	0.4134(3)	3.84(9)	1

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ge1	0.0349(2)	0.0311(2)	0.0248(2)	0.00495(17)	0.00843(17)	0.00073(16)
Fe1	0.0254(4)	0.0259(4)	0.0214(4)	0.0044(3)	0.0066(3)	0.0001(3)
N1	0.0220(15)	0.0291(16)	0.0269(16)	0.0010(13)	0.0041(13)	0.0016(13)
N2	0.0274(15)	0.0238(15)	0.0271(16)	-0.0002(13)	0.0052(13)	-0.0014(12)

C1	0.038(2)	0.033(2)	0.034(2)	0.0012(18)	0.0016(18)	0.0001(17)
C2	0.037(2)	0.034(2)	0.035(2)	-0.0008(18)	0.0041(18)	0.0052(17)
C3	0.039(2)	0.040(3)	0.058(3)	-0.000(2)	-0.003(2)	0.011(2)
C4	0.060(3)	0.052(3)	0.047(3)	-0.004(3)	-0.012(2)	0.020(2)
C5	0.081(4)	0.070(4)	0.032(3)	0.006(3)	0.007(3)	0.010(2)
C6	0.069(3)	0.059(3)	0.035(3)	0.016(3)	0.015(2)	0.007(2)
C7	0.038(2)	0.038(2)	0.026(2)	0.0040(18)	0.0108(17)	-0.0003(16)
C8	0.056(3)	0.036(2)	0.056(3)	0.003(2)	0.023(2)	0.010(2)
C9	0.058(3)	0.063(4)	0.058(3)	-0.004(3)	0.029(3)	0.011(3)
C10	0.043(3)	0.084(4)	0.044(3)	-0.002(3)	0.022(2)	-0.012(3)
C11	0.048(3)	0.052(3)	0.064(3)	0.013(2)	0.016(2)	-0.014(2)
C12	0.044(2)	0.037(2)	0.048(3)	0.0054(19)	0.015(2)	-0.0112(19)
C13	0.0276(18)	0.0277(19)	0.0228(18)	0.0003(15)	0.0072(15)	-0.0029(14)
C14	0.0276(19)	0.038(2)	0.029(2)	0.0091(16)	0.0071(16)	0.0040(16)
C15	0.035(2)	0.031(2)	0.028(2)	0.0071(17)	0.0070(17)	0.0000(16)
C16	0.0279(18)	0.032(2)	0.031(2)	-0.0059(16)	0.0073(16)	-0.0052(16)
C17	0.040(2)	0.050(3)	0.042(3)	-0.010(2)	0.014(2)	0.002(2)
C18	0.050(3)	0.043(2)	0.037(2)	-0.012(2)	0.010(2)	-0.0050(19)
C19	0.027(2)	0.050(3)	0.051(3)	0.0113(19)	0.0047(19)	0.007(2)
C20	0.048(3)	0.027(2)	0.049(3)	0.0098(19)	0.007(2)	0.0026(18)
C21	0.0319(19)	0.032(2)	0.036(2)	-0.0030(16)	0.0053(17)	-0.0033(16)
C22	0.042(3)	0.046(3)	0.047(3)	-0.005(2)	0.003(2)	-0.016(2)
C23	0.043(3)	0.060(3)	0.043(3)	-0.016(2)	0.011(2)	0.003(2)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ge1	Fe1	2.4488(8)	Ge1	C1	2.004(4)
Ge1	C7	1.986(4)	Fe1	C13	1.995(4)
Fe1	C13[1]	1.995(4)	N1	C13	1.376(5)
N1	C14	1.387(5)	N1	C16	1.475(5)
N2	C13	1.359(5)	N2	C15	1.411(5)
N2	C21	1.473(5)	C1	C2	1.372(6)
C1	C6	1.388(6)	C2	C3	1.400(6)
C3	C4	1.377(8)	C4	C5	1.354(8)
C5	C6	1.397(6)	C7	C8	1.378(7)
C7	C12	1.378(6)	C8	C9	1.391(8)

C9	C10	1.367(8)	C10	C11	1.360(8)
C11	C12	1.399(7)	C14	C15	1.344(6)
C14	C19	1.508(5)	C15	C20	1.491(6)
C16	C17	1.531(6)	C16	C18	1.523(5)
C21	C22	1.531(6)	C21	C23	1.519(6)
Ge1	H1	1.76(4)			

Symmetry Operators:

(1) -X+1,-Y+1,-Z+1

Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Fe1	Ge1	C1	128.28(13)	Fe1	Ge1	C7	117.17(10)
C1	Ge1	C7	100.33(17)	Ge1	Fe1	Ge1[1]	180.000(18)
Ge1	Fe1	C13	85.74(10)	Ge1	Fe1	C13[1]	94.26(10)
Ge1[1]	Fe1	C13	94.26(10)	Ge1[1]	Fe1	C13[1]	85.74(10)
C13	Fe1	C13[1]	180.0(2)	C13	N1	C14	111.2(3)
C13	N1	C16	121.3(3)	C14	N1	C16	127.2(3)
C13	N2	C15	111.5(3)	C13	N2	C21	121.5(3)
C15	N2	C21	126.8(3)	Ge1	C1	C2	123.3(3)
Ge1	C1	C6	119.1(3)	C2	C1	C6	117.5(4)
C1	C2	C3	121.6(4)	C2	C3	C4	119.6(4)
C3	C4	C5	119.8(4)	C4	C5	C6	120.4(5)
C1	C6	C5	121.1(5)	Ge1	C7	C8	120.6(3)
Ge1	C7	C12	122.2(3)	C8	C7	C12	117.2(4)
C7	C8	C9	122.3(5)	C8	C9	C10	119.6(5)
C9	C10	C11	119.3(5)	C10	C11	C12	121.1(5)
C7	C12	C11	120.6(4)	Fe1	C13	N1	128.6(3)
Fe1	C13	N2	127.7(3)	N1	C13	N2	103.6(3)
N1	C14	C15	107.5(3)	N1	C14	C19	125.6(4)
C15	C14	C19	126.9(4)	N2	C15	C14	106.0(3)
N2	C15	C20	126.0(3)	C14	C15	C20	128.0(4)
N1	C16	C17	112.9(3)	N1	C16	C18	110.6(3)
C17	C16	C18	111.8(3)	N2	C21	C22	111.5(3)
N2	C21	C23	111.2(3)	C22	C21	C23	112.9(4)

Symmetry Operators:

(1) -X+1,-Y+1,-Z+1

Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Fe1	Ge1	C1	C2	8.7(4)	Fe1	Ge1	C1	C6	-174.25(17)
C1	Ge1	Fe1	C13	172.50(15)	C1	Ge1	Fe1	C13[1]	-7.50(15)
Fe1	Ge1	C7	C8	97.2(2)	Fe1	Ge1	C7	C12	-81.8(3)
C7	Ge1	Fe1	C13	41.07(14)	C7	Ge1	Fe1	C13[1]	-138.93(14)
C1	Ge1	C7	C8	-46.1(3)	C1	Ge1	C7	C12	135.0(3)
C7	Ge1	C1	C2	146.0(3)	C7	Ge1	C1	C6	-36.9(3)
Ge1	Fe1	C13	N1	-93.2(3)	Ge1	Fe1	C13	N2	86.8(3)
Ge1	Fe1	C13[1]	N1[1]	-86.8(3)	Ge1	Fe1	C13[1]	N2[1]	93.2(3)
Ge1[1]	Fe1	C13	N1	86.8(3)	Ge1[1]	Fe1	C13	N2	-93.2(3)
Ge1[1]	Fe1	C13[1]	N1[1]	93.2(3)	Ge1[1]	Fe1	C13[1]	N2[1]	-86.8(3)
C13	N1	C14	C15	-0.3(4)	C13	N1	C14	C19	-178.6(3)
C14	N1	C13	Fe1	-178.8(3)	C14	N1	C13	N2	1.1(4)
C13	N1	C16	C17	134.6(3)	C13	N1	C16	C18	-99.4(3)
C16	N1	C13	Fe1	-4.7(5)	C16	N1	C13	N2	175.3(3)
C14	N1	C16	C17	-52.3(4)	C14	N1	C16	C18	73.8(4)
C16	N1	C14	C15	-174.0(3)	C16	N1	C14	C19	7.7(6)
C13	N2	C15	C14	1.4(4)	C13	N2	C15	C20	179.6(3)
C15	N2	C13	Fe1	178.4(3)	C15	N2	C13	N1	-1.6(4)
C13	N2	C21	C22	-125.8(3)	C13	N2	C21	C23	107.1(3)
C21	N2	C13	Fe1	2.0(5)	C21	N2	C13	N1	-178.0(3)
C15	N2	C21	C22	58.3(4)	C15	N2	C21	C23	-68.7(4)
C21	N2	C15	C14	177.6(3)	C21	N2	C15	C20	-4.2(6)
Ge1	C1	C2	C3	175.7(2)	Ge1	C1	C6	C5	-175.7(3)
C2	C1	C6	C5	1.5(7)	C6	C1	C2	C3	-1.4(6)
C1	C2	C3	C4	0.3(6)	C2	C3	C4	C5	0.6(7)
C3	C4	C5	C6	-0.5(8)	C4	C5	C6	C1	-0.6(8)
Ge1	C7	C8	C9	-178.9(2)	Ge1	C7	C12	C11	179.4(2)
C8	C7	C12	C11	0.3(5)	C12	C7	C8	C9	0.1(6)
C7	C8	C9	C10	-1.1(6)	C8	C9	C10	C11	1.6(6)
C9	C10	C11	C12	-1.2(7)	C10	C11	C12	C7	0.2(6)
N1	C14	C15	N2	-0.6(4)	N1	C14	C15	C20	-178.8(3)
C19	C14	C15	N2	177.6(3)	C19	C14	C15	C20	-0.5(6)

Symmetry Operators:

(1) -X+1,-Y+1,-Z+1

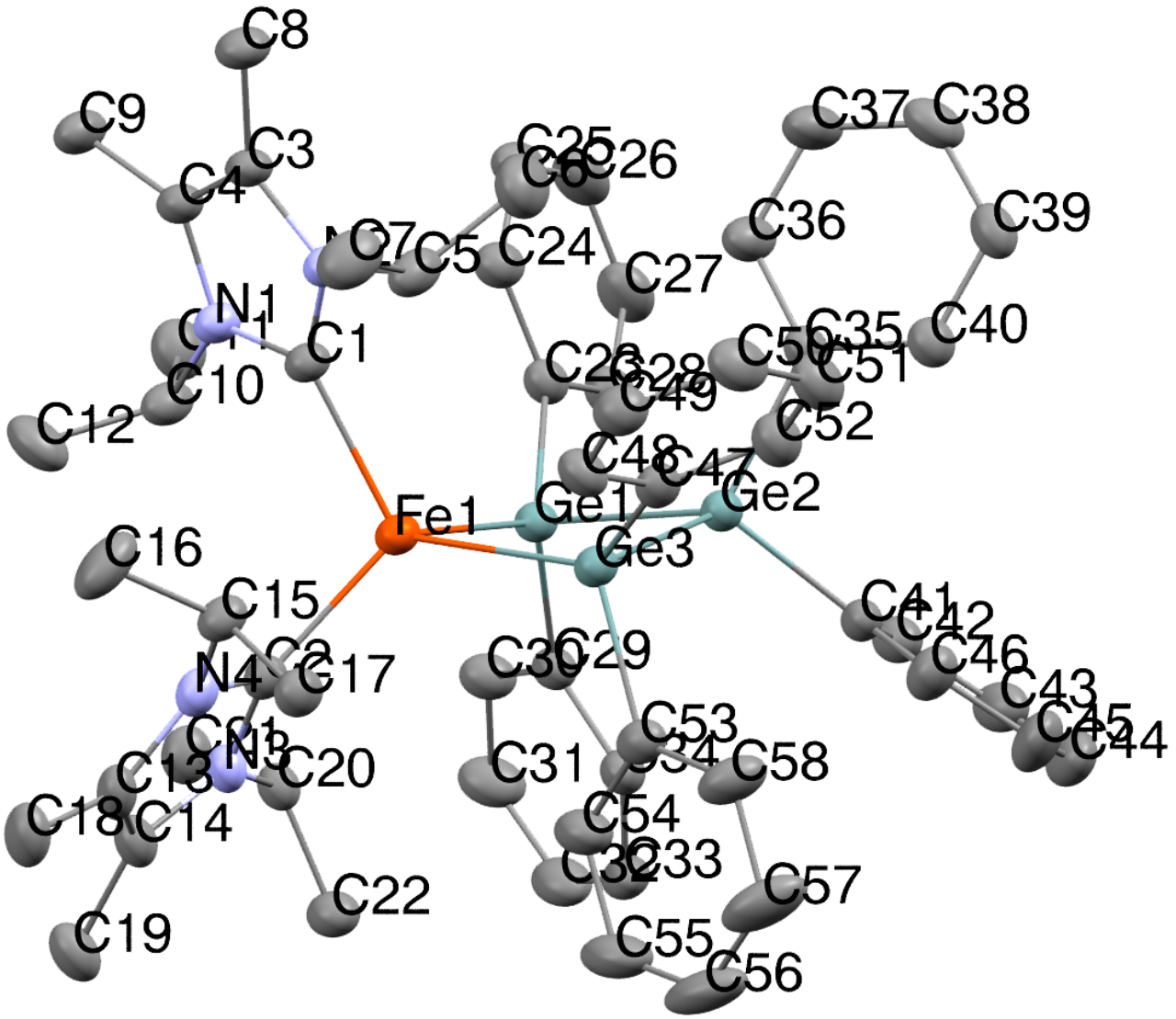


Figure S22. ORTEP drawing of **3** (50% probability of the thermal ellipsoids). Hydrogen atoms were omitted for clarity.

Table S10. Crystal data and structure refinement for **3**.

Empirical Formula	$C_{58}H_{70}FeGe_3N_4$
Formula Weight	1096.83
Crystal Color, Habit	paleyellow, plate
Crystal Dimensions	0.050 X 0.020 X 0.020 mm
Crystal System	monoclinic
Lattice Type	Primitive
Lattice Parameters	a = 12.2039(2) Å b = 20.0943(3) Å c = 22.0081(4) Å β = 98.0205(16) ° V = 5344.23(15) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.363 g/cm^3
F_{000}	2272.00
μ(synchrotron radiation, λ = 0.41220Å)	0.000 cm^{-1}
Diffractometer	R-AXIS IV
Radiation (λ = 0.41220Å)	
Voltage, Current	8kV, 100mA
Temperature	-173.0°C
Detector Aperture	300.0 x 300.0 mm
Data Images	1080 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	0.0 - 180.0°
Exposure Rate	10.0 sec./°
ω oscillation Range (χ=45.0, ϕ=-90.0)	0.0 - 180.0°
Exposure Rate	10.0 sec./°
ω oscillation Range (χ=45.0, ϕ=-180.0)	0.0 - 180.0°
Exposure Rate	600.0 sec./°
Detector Position	130.00 mm
Pixel Size	0.172 mm
$2\theta_{max}$	43.6°
No. of Reflections Measured	Total: 204926 Unique: 27862 (R_{int} = 0.1399)
Corrections	Lorentz-polarization Absorption (trans. factors: 0.349 - 1.000)

Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w $(Fo^2 - Fc^2)^2$
Least Squares Weights	$w = 1/ [\sigma^2(Fo^2) + (0.0492 \cdot P)^2 + 6.4759 \cdot P]$ where $P = (Max(Fo^2,0) + 2Fc^2)/3$
$2\theta_{max}$ cutoff	43.6^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	27862
No. Variables	607
Reflection/Parameter Ratio	45.90
Residuals: R1 (I>2.00σ(I))	0.0750
Residuals: R (All reflections)	0.1582
Residuals: wR2 (All reflections)	0.1567
Goodness of Fit Indicator	1.032
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	1.85 $e^-/Å^3$
Minimum peak in Final Diff. Map	-0.93 $e^-/Å^3$

Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}
Ge1	0.74795(2)	0.26880(2)	0.46608(2)	1.840(5)
Ge2	0.54800(2)	0.24203(2)	0.44546(2)	1.930(5)
Ge3	0.55670(2)	0.24276(2)	0.33371(2)	1.946(5)
Fe1	0.75035(3)	0.29377(2)	0.35169(2)	1.904(6)
N1	0.8559(2)	0.43343(11)	0.36329(11)	2.07(4)
N2	0.6876(2)	0.44494(11)	0.32185(11)	2.03(4)
N3	0.95137(19)	0.20761(12)	0.31643(11)	2.01(3)
N4	0.8621(2)	0.25635(12)	0.23821(11)	2.12(4)
C1	0.7633(2)	0.39816(13)	0.34325(13)	1.96(4)
C2	0.8643(2)	0.24799(13)	0.29976(12)	1.92(4)
C3	0.7325(3)	0.50842(13)	0.32891(14)	2.16(4)
C4	0.8388(3)	0.50130(13)	0.35477(13)	2.14(4)
C5	0.5750(3)	0.42722(15)	0.29358(16)	2.76(5)
C6	0.4875(3)	0.4495(2)	0.3306(2)	4.20(8)
C7	0.5543(3)	0.44926(19)	0.22675(17)	3.59(7)
C8	0.6734(3)	0.57154(14)	0.30962(16)	2.71(5)
C9	0.9230(3)	0.55490(15)	0.36956(17)	2.80(5)
C10	0.9597(3)	0.40011(14)	0.38849(15)	2.45(5)
C11	1.0036(3)	0.42196(19)	0.45285(16)	3.15(6)
C12	1.0450(3)	0.4057(2)	0.34566(18)	3.59(7)
C13	0.9476(3)	0.22115(16)	0.21688(14)	2.41(5)
C14	1.0034(2)	0.19008(16)	0.26590(14)	2.36(5)
C15	0.7702(3)	0.29134(14)	0.20114(14)	2.29(4)
C16	0.8100(4)	0.34159(19)	0.15735(19)	3.90(8)
C17	0.6885(3)	0.24162(15)	0.16849(15)	2.44(5)
C18	0.9714(3)	0.21925(19)	0.15203(15)	3.07(6)
C19	1.1014(3)	0.14458(19)	0.26787(16)	3.13(6)
C20	0.9820(2)	0.18557(14)	0.38011(13)	2.07(4)
C21	1.0901(3)	0.21676(17)	0.40969(15)	2.76(5)
C22	0.9835(3)	0.11047(15)	0.38634(16)	2.77(5)
C23	0.7662(2)	0.33465(14)	0.53367(13)	2.09(4)
C24	0.7557(3)	0.40303(15)	0.52240(15)	2.50(5)
C25	0.7575(3)	0.44830(16)	0.56988(18)	3.02(6)
C26	0.7719(3)	0.42658(19)	0.62991(18)	3.37(6)
C27	0.7851(3)	0.3595(2)	0.64242(16)	3.38(6)
C28	0.7804(3)	0.31458(17)	0.59471(14)	2.68(5)

C29	0.8257(3)	0.18887(14)	0.50373(13)	2.18(4)
C30	0.9303(3)	0.19486(16)	0.53875(14)	2.56(5)
C31	0.9899(3)	0.13932(18)	0.56165(16)	3.24(6)
C32	0.9475(3)	0.07648(17)	0.55029(16)	3.28(6)
C33	0.8460(3)	0.06907(16)	0.51492(18)	3.20(6)
C34	0.7858(3)	0.12449(15)	0.49213(16)	2.58(5)
C35	0.4489(2)	0.30733(14)	0.47714(13)	2.05(4)
C36	0.4779(3)	0.37289(16)	0.49029(18)	3.05(6)
C37	0.4074(3)	0.41662(17)	0.51467(19)	3.47(7)
C38	0.3054(3)	0.39627(18)	0.52501(16)	3.03(6)
C39	0.2733(3)	0.33133(17)	0.51255(14)	2.63(5)
C40	0.3445(2)	0.28728(16)	0.48947(14)	2.34(4)
C41	0.4968(3)	0.15914(14)	0.48011(14)	2.30(5)
C42	0.5385(3)	0.13953(15)	0.53988(15)	2.68(5)
C43	0.4966(4)	0.08490(17)	0.56649(17)	3.45(7)
C44	0.4127(4)	0.04795(19)	0.5342(2)	4.15(8)
C45	0.3708(4)	0.06614(19)	0.4751(2)	4.13(8)
C46	0.4137(3)	0.12139(17)	0.44844(17)	3.08(6)
C47	0.4167(2)	0.27522(14)	0.28641(13)	2.13(4)
C48	0.4141(3)	0.29869(16)	0.22706(14)	2.51(5)
C49	0.3191(3)	0.32526(16)	0.19382(15)	2.72(5)
C50	0.2233(3)	0.32593(18)	0.21945(17)	3.08(6)
C51	0.2219(3)	0.29955(19)	0.27739(17)	3.21(6)
C52	0.3183(3)	0.27564(17)	0.31078(16)	2.83(5)
C53	0.5547(3)	0.14646(14)	0.31457(13)	2.29(4)
C54	0.6525(3)	0.11038(17)	0.32527(17)	3.27(6)
C55	0.6535(4)	0.04188(18)	0.3147(2)	4.24(8)
C56	0.5579(5)	0.00928(17)	0.29283(17)	4.46(9)
C57	0.4602(4)	0.04383(18)	0.28175(19)	4.62(10)
C58	0.4592(3)	0.11182(16)	0.29297(16)	3.34(6)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ge1	0.02443(13)	0.02132(12)	0.02406(13)	0.00047(10)	0.00303(10)	-0.00006(10)
Ge2	0.02458(13)	0.02243(13)	0.02674(14)	-0.00079(10)	0.00502(10)	-0.00115(11)
Ge3	0.02570(14)	0.02183(12)	0.02626(14)	-0.00135(10)	0.00305(11)	-0.00082(10)

Fe1	0.02592(19)	0.01989(16)	0.02611(19)	-0.00065(14)	0.00220(15)	0.00033(14)
N1	0.0274(12)	0.0204(10)	0.0300(12)	-0.0008(8)	0.0013(9)	-0.0008(9)
N2	0.0261(11)	0.0207(10)	0.0296(12)	-0.0004(8)	0.0014(9)	0.0004(9)
N3	0.0241(11)	0.0295(11)	0.0235(11)	-0.0021(9)	0.0057(9)	0.0002(9)
N4	0.0273(11)	0.0277(11)	0.0251(11)	-0.0051(9)	0.0017(9)	0.0024(9)
C1	0.0272(13)	0.0194(11)	0.0275(13)	-0.0002(9)	0.0021(10)	0.0004(9)
C2	0.0254(12)	0.0225(11)	0.0244(12)	-0.0037(9)	0.0015(9)	-0.0001(9)
C3	0.0312(14)	0.0190(11)	0.0322(14)	0.0014(10)	0.0059(11)	-0.0018(10)
C4	0.0313(14)	0.0207(11)	0.0300(14)	0.0009(10)	0.0061(11)	-0.0012(10)
C5	0.0293(15)	0.0258(13)	0.0473(19)	-0.0024(11)	-0.0037(13)	0.0040(12)
C6	0.0351(19)	0.054(2)	0.072(3)	-0.0027(16)	0.0129(18)	-0.000(2)
C7	0.045(2)	0.0394(18)	0.047(2)	-0.0031(15)	-0.0117(16)	0.0067(15)
C8	0.0378(16)	0.0223(12)	0.0422(17)	0.0027(11)	0.0027(13)	0.0005(12)
C9	0.0308(15)	0.0225(12)	0.052(2)	-0.0028(11)	0.0022(14)	-0.0027(12)
C10	0.0271(14)	0.0233(12)	0.0405(17)	0.0005(10)	-0.0030(12)	0.0003(11)
C11	0.0297(16)	0.0503(19)	0.0378(18)	-0.0003(14)	-0.0015(13)	-0.0001(14)
C12	0.0364(18)	0.054(2)	0.047(2)	0.0174(16)	0.0098(15)	-0.0019(17)
C13	0.0286(14)	0.0374(15)	0.0268(14)	-0.0085(11)	0.0084(11)	-0.0021(11)
C14	0.0244(13)	0.0379(15)	0.0283(14)	-0.0012(11)	0.0064(11)	-0.0020(11)
C15	0.0325(14)	0.0236(12)	0.0295(14)	-0.0024(11)	-0.0005(11)	0.0035(10)
C16	0.055(2)	0.0378(18)	0.051(2)	-0.0170(16)	-0.0094(18)	0.0159(16)
C17	0.0282(14)	0.0298(13)	0.0340(15)	-0.0036(11)	0.0017(11)	-0.0026(12)
C18	0.0386(17)	0.051(2)	0.0287(15)	-0.0092(14)	0.0100(13)	-0.0002(13)
C19	0.0303(16)	0.052(2)	0.0376(17)	0.0041(14)	0.0092(13)	-0.0043(15)
C20	0.0241(13)	0.0312(13)	0.0235(12)	0.0018(10)	0.0045(10)	0.0010(10)
C21	0.0311(15)	0.0420(17)	0.0302(15)	-0.0054(12)	-0.0010(12)	0.0002(12)
C22	0.0417(17)	0.0279(14)	0.0364(16)	0.0040(12)	0.0088(14)	0.0024(12)
C23	0.0235(13)	0.0288(13)	0.0268(13)	0.0001(10)	0.0029(10)	-0.0029(10)
C24	0.0290(14)	0.0294(13)	0.0360(16)	0.0019(11)	0.0029(12)	-0.0025(11)
C25	0.0292(15)	0.0295(14)	0.056(2)	-0.0011(12)	0.0077(14)	-0.0105(14)
C26	0.0352(17)	0.049(2)	0.044(2)	-0.0031(14)	0.0076(14)	-0.0210(16)
C27	0.0443(19)	0.053(2)	0.0317(16)	-0.0015(16)	0.0092(14)	-0.0118(15)
C28	0.0347(16)	0.0371(16)	0.0308(15)	0.0016(12)	0.0073(12)	-0.0030(12)
C29	0.0311(14)	0.0254(12)	0.0276(13)	0.0037(10)	0.0090(11)	0.0019(10)
C30	0.0343(15)	0.0312(14)	0.0302(14)	0.0058(11)	-0.0012(12)	-0.0027(11)
C31	0.0435(19)	0.0419(18)	0.0350(17)	0.0154(14)	-0.0042(14)	-0.0011(14)
C32	0.052(2)	0.0340(16)	0.0397(18)	0.0141(15)	0.0113(16)	0.0096(14)
C33	0.048(2)	0.0237(13)	0.055(2)	0.0021(13)	0.0245(17)	0.0057(13)

C34	0.0291(14)	0.0277(13)	0.0434(17)	0.0018(11)	0.0122(13)	-0.0002(12)
C35	0.0205(12)	0.0295(13)	0.0271(13)	0.0008(10)	0.0009(10)	-0.0020(10)
C36	0.0295(15)	0.0283(14)	0.058(2)	0.0008(12)	0.0058(14)	-0.0058(14)
C37	0.0394(18)	0.0300(15)	0.063(2)	0.0013(13)	0.0076(17)	-0.0126(15)
C38	0.0334(16)	0.0448(18)	0.0364(17)	0.0137(13)	0.0026(13)	-0.0062(14)
C39	0.0273(14)	0.0431(17)	0.0304(15)	0.0041(12)	0.0064(12)	0.0036(13)
C40	0.0265(13)	0.0340(14)	0.0280(14)	0.0009(11)	0.0024(11)	-0.0007(11)
C41	0.0323(14)	0.0232(12)	0.0344(15)	-0.0014(10)	0.0142(12)	-0.0008(11)
C42	0.0422(17)	0.0296(14)	0.0322(15)	0.0028(12)	0.0124(13)	0.0012(12)
C43	0.063(2)	0.0326(16)	0.0398(18)	0.0050(15)	0.0230(17)	0.0045(14)
C44	0.070(3)	0.0349(17)	0.060(3)	-0.0074(17)	0.035(2)	0.0036(17)
C45	0.062(3)	0.0382(18)	0.061(3)	-0.0214(17)	0.024(2)	-0.0049(17)
C46	0.0450(19)	0.0334(15)	0.0395(18)	-0.0109(14)	0.0086(14)	-0.0018(13)
C47	0.0272(13)	0.0256(12)	0.0279(13)	-0.0041(10)	0.0029(11)	-0.0042(10)
C48	0.0275(14)	0.0356(15)	0.0325(15)	0.0050(11)	0.0052(11)	-0.0028(12)
C49	0.0390(17)	0.0325(14)	0.0306(15)	0.0001(12)	0.0006(13)	0.0003(12)
C50	0.0286(15)	0.0422(17)	0.0434(19)	0.0042(13)	-0.0045(13)	-0.0069(14)
C51	0.0289(16)	0.0476(19)	0.046(2)	0.0006(14)	0.0067(14)	-0.0071(15)
C52	0.0312(15)	0.0398(16)	0.0368(16)	-0.0016(12)	0.0059(13)	-0.0037(13)
C53	0.0389(16)	0.0247(12)	0.0234(13)	-0.0012(11)	0.0049(11)	-0.0001(10)
C54	0.050(2)	0.0303(15)	0.047(2)	0.0088(14)	0.0141(16)	0.0012(14)
C55	0.080(3)	0.0313(17)	0.052(2)	0.0175(18)	0.020(2)	0.0024(16)
C56	0.109(4)	0.0217(14)	0.0364(19)	0.0016(19)	0.004(2)	-0.0012(13)
C57	0.095(3)	0.0281(16)	0.045(2)	-0.0118(19)	-0.017(2)	-0.0038(15)
C58	0.059(2)	0.0252(14)	0.0385(18)	-0.0038(14)	-0.0067(16)	-0.0024(12)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ge1	Ge2	2.4780(4)	Ge1	Fe1	2.5712(6)
Ge1	C23	1.980(3)	Ge1	C29	1.987(3)
Ge2	Ge3	2.4765(6)	Ge2	C35	1.976(3)
Ge2	C41	1.970(3)	Ge3	Fe1	2.5557(5)
Ge3	C47	1.983(3)	Ge3	C53	1.980(3)
Fe1	C1	2.114(3)	Fe1	C2	2.128(3)
N1	C1	1.354(4)	N1	C4	1.388(3)
N1	C10	1.471(4)	N2	C1	1.356(3)

N2	C3	1.389(3)	N2	C5	1.470(4)
N3	C2	1.347(4)	N3	C14	1.400(4)
N3	C20	1.468(4)	N4	C2	1.362(4)
N4	C13	1.395(4)	N4	C15	1.471(4)
C3	C4	1.349(4)	C3	C8	1.491(4)
C4	C9	1.493(4)	C5	C6	1.499(6)
C5	C7	1.523(5)	C10	C11	1.508(5)
C10	C12	1.503(5)	C13	C14	1.346(4)
C13	C18	1.496(5)	C14	C19	1.501(5)
C15	C16	1.521(5)	C15	C17	1.520(4)
C20	C21	1.522(4)	C20	C22	1.515(4)
C23	C24	1.399(4)	C23	C28	1.390(4)
C24	C25	1.383(5)	C25	C26	1.379(5)
C26	C27	1.381(6)	C27	C28	1.380(5)
C29	C30	1.401(4)	C29	C34	1.393(4)
C30	C31	1.388(5)	C31	C32	1.374(5)
C32	C33	1.376(5)	C33	C34	1.389(5)
C35	C36	1.384(4)	C35	C40	1.399(4)
C36	C37	1.389(5)	C37	C38	1.359(5)
C38	C39	1.379(5)	C39	C40	1.385(5)
C41	C42	1.399(4)	C41	C46	1.376(4)
C42	C43	1.376(5)	C43	C44	1.379(6)
C44	C45	1.378(6)	C45	C46	1.392(6)
C47	C48	1.385(4)	C47	C52	1.382(5)
C48	C49	1.389(4)	C49	C50	1.366(5)
C50	C51	1.383(5)	C51	C52	1.383(5)
C53	C54	1.388(5)	C53	C58	1.384(5)
C54	C55	1.396(5)	C55	C56	1.365(7)
C56	C57	1.373(7)	C57	C58	1.389(5)

Bond angles (^{o})

atom	atom	atom	angle	atom	atom	atom	angle
Ge2	Ge1	Fe1	90.487(17)	Ge2	Ge1	C23	106.68(8)
Ge2	Ge1	C29	107.57(9)	Fe1	Ge1	C23	126.14(9)
Fe1	Ge1	C29	119.74(9)	C23	Ge1	C29	103.29(11)
Ge1	Ge2	Ge3	90.173(17)	Ge1	Ge2	C35	115.26(8)
Ge1	Ge2	C41	118.05(9)	Ge3	Ge2	C35	117.36(8)
Ge3	Ge2	C41	116.71(9)	C35	Ge2	C41	100.49(12)

Ge2	Ge3	Fe1	90.886(17)	Ge2	Ge3	C47	111.72(9)
Ge2	Ge3	C53	101.80(9)	Fe1	Ge3	C47	131.29(9)
Fe1	Ge3	C53	114.12(9)	C47	Ge3	C53	103.04(12)
Ge1	Fe1	Ge3	86.372(17)	Ge1	Fe1	C1	106.91(8)
Ge1	Fe1	C2	122.62(7)	Ge3	Fe1	C1	117.60(8)
Ge3	Fe1	C2	113.76(7)	C1	Fe1	C2	108.62(11)
C1	N1	C4	111.5(2)	C1	N1	C10	121.3(2)
C4	N1	C10	127.1(2)	C1	N2	C3	111.0(2)
C1	N2	C5	122.0(2)	C3	N2	C5	126.9(2)
C2	N3	C14	111.3(2)	C2	N3	C20	121.9(2)
C14	N3	C20	126.8(2)	C2	N4	C13	111.1(2)
C2	N4	C15	121.2(2)	C13	N4	C15	127.2(2)
Fe1	C1	N1	124.05(19)	Fe1	C1	N2	131.5(2)
N1	C1	N2	104.3(2)	Fe1	C2	N3	131.6(2)
Fe1	C2	N4	123.88(19)	N3	C2	N4	104.5(2)
N2	C3	C4	106.9(2)	N2	C3	C8	125.6(3)
C4	C3	C8	127.5(3)	N1	C4	C3	106.2(2)
N1	C4	C9	126.4(3)	C3	C4	C9	127.4(3)
N2	C5	C6	113.1(3)	N2	C5	C7	111.0(3)
C6	C5	C7	113.7(3)	N1	C10	C11	113.3(3)
N1	C10	C12	111.4(3)	C11	C10	C12	112.4(3)
N4	C13	C14	106.5(3)	N4	C13	C18	126.0(3)
C14	C13	C18	127.5(3)	N3	C14	C13	106.6(3)
N3	C14	C19	125.3(3)	C13	C14	C19	128.1(3)
N4	C15	C16	112.5(3)	N4	C15	C17	110.3(2)
C16	C15	C17	112.5(3)	N3	C20	C21	112.0(2)
N3	C20	C22	112.7(2)	C21	C20	C22	111.9(2)
Ge1	C23	C24	121.7(2)	Ge1	C23	C28	121.2(2)
C24	C23	C28	116.9(3)	C23	C24	C25	121.4(3)
C24	C25	C26	120.1(3)	C25	C26	C27	119.7(3)
C26	C27	C28	119.7(3)	C23	C28	C27	122.1(3)
Ge1	C29	C30	120.4(2)	Ge1	C29	C34	122.6(2)
C30	C29	C34	116.7(3)	C29	C30	C31	121.4(3)
C30	C31	C32	120.5(3)	C31	C32	C33	119.3(3)
C32	C33	C34	120.4(3)	C29	C34	C33	121.6(3)
Ge2	C35	C36	123.7(2)	Ge2	C35	C40	119.7(2)
C36	C35	C40	116.5(3)	C35	C36	C37	121.9(3)
C36	C37	C38	120.4(3)	C37	C38	C39	119.5(3)

C38	C39	C40	120.2(3)	C35	C40	C39	121.5(3)
Ge2	C41	C42	120.6(2)	Ge2	C41	C46	121.4(2)
C42	C41	C46	117.8(3)	C41	C42	C43	121.1(3)
C42	C43	C44	120.2(3)	C43	C44	C45	119.7(4)
C44	C45	C46	119.8(4)	C41	C46	C45	121.3(3)
Ge3	C47	C48	120.8(2)	Ge3	C47	C52	122.0(2)
C48	C47	C52	117.2(3)	C47	C48	C49	122.3(3)
C48	C49	C50	119.1(3)	C49	C50	C51	119.9(3)
C50	C51	C52	120.3(3)	C47	C52	C51	121.1(3)
Ge3	C53	C54	119.3(2)	Ge3	C53	C58	123.3(2)
C54	C53	C58	117.3(3)	C53	C54	C55	120.9(4)
C54	C55	C56	120.3(4)	C55	C56	C57	119.9(3)
C56	C57	C58	119.7(4)	C53	C58	C57	121.9(4)

Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Ge2	Ge1	Fe1	Ge3	-10.711(15)	Ge2	Ge1	Fe1	C1	107.058(18)
Ge2	Ge1	Fe1	C2	-126.73(2)	Fe1	Ge1	Ge2	Ge3	11.036(16)
Fe1	Ge1	Ge2	C35	-109.60(2)	Fe1	Ge1	Ge2	C41	131.75(2)
Ge2	Ge1	C23	C24	-87.67(19)	Ge2	Ge1	C23	C28	86.70(19)
C23	Ge1	Ge2	Ge3	139.22(9)	C23	Ge1	Ge2	C35	18.59(9)
C23	Ge1	Ge2	C41	-100.06(9)	Ge2	Ge1	C29	C30	-158.44(17)
Ge2	Ge1	C29	C34	28.1(2)	C29	Ge1	Ge2	Ge3	-110.50(9)
C29	Ge1	Ge2	C35	128.87(9)	C29	Ge1	Ge2	C41	10.22(9)
Fe1	Ge1	C23	C24	15.6(2)	Fe1	Ge1	C23	C28	-170.02(13)
C23	Ge1	Fe1	Ge3	-121.91(10)	C23	Ge1	Fe1	C1	-4.14(10)
C23	Ge1	Fe1	C2	122.07(10)	Fe1	Ge1	C29	C30	100.54(19)
Fe1	Ge1	C29	C34	-73.0(2)	C29	Ge1	Fe1	Ge3	99.93(10)
C29	Ge1	Fe1	C1	-142.30(10)	C29	Ge1	Fe1	C2	-16.09(10)
C23	Ge1	C29	C30	-45.9(2)	C23	Ge1	C29	C34	140.7(2)
C29	Ge1	C23	C24	159.10(19)	C29	Ge1	C23	C28	-26.5(2)
Ge1	Ge2	Ge3	Fe1	-11.104(16)	Ge1	Ge2	Ge3	C47	-146.869(19)
Ge1	Ge2	Ge3	C53	103.777(15)	Ge1	Ge2	C35	C36	22.0(2)
Ge1	Ge2	C35	C40	-155.73(14)	Ge1	Ge2	C41	C42	41.4(2)
Ge1	Ge2	C41	C46	-143.42(17)	Ge3	Ge2	C35	C36	-82.38(19)
Ge3	Ge2	C35	C40	99.92(18)	C35	Ge2	Ge3	Fe1	107.71(9)
C35	Ge2	Ge3	C47	-28.05(9)	C35	Ge2	Ge3	C53	-137.41(9)

Ge3	Ge2	C41	C42	147.19(17)	Ge3	Ge2	C41	C46	-37.6(2)
C41	Ge2	Ge3	Fe1	-132.97(10)	C41	Ge2	Ge3	C47	91.27(10)
C41	Ge2	Ge3	C53	-18.09(10)	C35	Ge2	C41	C42	-84.8(2)
C35	Ge2	C41	C46	90.4(2)	C41	Ge2	C35	C36	150.0(2)
C41	Ge2	C35	C40	-27.7(2)	Ge2	Ge3	Fe1	Ge1	10.719(15)
Ge2	Ge3	Fe1	C1	-96.48(2)	Ge2	Ge3	Fe1	C2	134.93(2)
Ge2	Ge3	C47	C48	160.16(15)	Ge2	Ge3	C47	C52	-19.7(2)
Ge2	Ge3	C53	C54	-82.1(2)	Ge2	Ge3	C53	C58	95.3(2)
Fe1	Ge3	C47	C48	48.3(2)	Fe1	Ge3	C47	C52	-131.55(15)
C47	Ge3	Fe1	Ge1	131.13(12)	C47	Ge3	Fe1	C1	23.92(12)
C47	Ge3	Fe1	C2	-104.67(12)	Fe1	Ge3	C53	C54	14.2(2)
Fe1	Ge3	C53	C58	-168.38(17)	C53	Ge3	Fe1	Ge1	-92.64(9)
C53	Ge3	Fe1	C1	160.16(9)	C53	Ge3	Fe1	C2	31.57(10)
C47	Ge3	C53	C54	161.98(19)	C47	Ge3	C53	C58	-20.6(2)
C53	Ge3	C47	C48	-91.3(2)	C53	Ge3	C47	C52	88.8(2)
Ge1	Fe1	C1	N1	71.1(2)	Ge1	Fe1	C1	N2	-104.7(2)
Ge1	Fe1	C2	N3	-6.4(3)	Ge1	Fe1	C2	N4	174.82(14)
Ge3	Fe1	C1	N1	165.95(17)	Ge3	Fe1	C1	N2	-9.9(3)
Ge3	Fe1	C2	N3	-107.9(2)	Ge3	Fe1	C2	N4	73.3(2)
C1	Fe1	C2	N3	119.0(2)	C1	Fe1	C2	N4	-59.7(2)
C2	Fe1	C1	N1	-63.1(2)	C2	Fe1	C1	N2	121.1(2)
C1	N1	C4	C3	0.2(3)	C1	N1	C4	C9	-177.9(2)
C4	N1	C1	Fe1	-176.7(2)	C4	N1	C1	N2	0.1(3)
C1	N1	C10	C11	-122.7(3)	C1	N1	C10	C12	109.4(3)
C10	N1	C1	Fe1	5.2(4)	C10	N1	C1	N2	-178.0(2)
C4	N1	C10	C11	59.5(4)	C4	N1	C10	C12	-68.4(3)
C10	N1	C4	C3	178.2(3)	C10	N1	C4	C9	0.0(5)
C1	N2	C3	C4	0.5(3)	C1	N2	C3	C8	179.1(3)
C3	N2	C1	Fe1	176.1(2)	C3	N2	C1	N1	-0.4(3)
C1	N2	C5	C6	113.6(3)	C1	N2	C5	C7	-117.1(3)
C5	N2	C1	Fe1	-5.7(4)	C5	N2	C1	N1	177.8(2)
C3	N2	C5	C6	-68.4(4)	C3	N2	C5	C7	60.8(4)
C5	N2	C3	C4	-177.6(3)	C5	N2	C3	C8	1.0(5)
C2	N3	C14	C13	0.7(3)	C2	N3	C14	C19	-178.6(2)
C14	N3	C2	Fe1	-179.4(2)	C14	N3	C2	N4	-0.5(3)
C2	N3	C20	C21	-110.4(3)	C2	N3	C20	C22	122.4(3)
C20	N3	C2	Fe1	1.7(4)	C20	N3	C2	N4	-179.4(2)
C14	N3	C20	C21	70.9(3)	C14	N3	C20	C22	-56.3(3)

C20	N3	C14	C13	179.5(2)	C20	N3	C14	C19	0.2(4)
C2	N4	C13	C14	0.4(3)	C2	N4	C13	C18	-179.4(2)
C13	N4	C2	Fe1	179.1(2)	C13	N4	C2	N3	0.1(3)
C2	N4	C15	C16	134.1(2)	C2	N4	C15	C17	-99.3(3)
C15	N4	C2	Fe1	-8.2(4)	C15	N4	C2	N3	172.7(2)
C13	N4	C15	C16	-54.5(4)	C13	N4	C15	C17	72.1(3)
C15	N4	C13	C14	-171.7(2)	C15	N4	C13	C18	8.5(5)
N2	C3	C4	N1	-0.4(3)	N2	C3	C4	C9	177.7(2)
C8	C3	C4	N1	-178.9(3)	C8	C3	C4	C9	-0.8(5)
N4	C13	C14	N3	-0.6(3)	N4	C13	C14	C19	178.6(2)
C18	C13	C14	N3	179.1(3)	C18	C13	C14	C19	-1.6(5)
Ge1	C23	C24	C25	173.46(18)	Ge1	C23	C28	C27	-175.15(19)
C24	C23	C28	C27	-0.5(4)	C28	C23	C24	C25	-1.1(4)
C23	C24	C25	C26	1.2(5)	C24	C25	C26	C27	0.4(5)
C25	C26	C27	C28	-2.0(5)	C26	C27	C28	C23	2.1(5)
Ge1	C29	C30	C31	-175.09(19)	Ge1	C29	C34	C33	174.6(2)
C30	C29	C34	C33	0.9(5)	C34	C29	C30	C31	-1.2(5)
C29	C30	C31	C32	0.2(5)	C30	C31	C32	C33	1.2(5)
C31	C32	C33	C34	-1.5(6)	C32	C33	C34	C29	0.4(6)
Ge2	C35	C36	C37	-177.5(2)	Ge2	C35	C40	C39	179.04(17)
C36	C35	C40	C39	1.2(4)	C40	C35	C36	C37	0.2(5)
C35	C36	C37	C38	-1.6(5)	C36	C37	C38	C39	1.6(5)
C37	C38	C39	C40	-0.2(5)	C38	C39	C40	C35	-1.2(4)
Ge2	C41	C42	C43	174.3(2)	Ge2	C41	C46	C45	-174.2(2)
C42	C41	C46	C45	1.1(5)	C46	C41	C42	C43	-1.0(5)
C41	C42	C43	C44	0.5(5)	C42	C43	C44	C45	-0.2(6)
C43	C44	C45	C46	0.4(6)	C44	C45	C46	C41	-0.8(6)
Ge3	C47	C48	C49	-176.30(18)	Ge3	C47	C52	C51	178.88(19)
C48	C47	C52	C51	-1.0(4)	C52	C47	C48	C49	3.6(4)
C47	C48	C49	C50	-2.7(5)	C48	C49	C50	C51	-0.9(5)
C49	C50	C51	C52	3.4(5)	C50	C51	C52	C47	-2.4(5)
Ge3	C53	C54	C55	177.4(2)	Ge3	C53	C58	C57	-178.0(2)
C54	C53	C58	C57	-0.6(5)	C58	C53	C54	C55	-0.1(5)
C53	C54	C55	C56	0.7(6)	C54	C55	C56	C57	-0.6(6)
C55	C56	C57	C58	-0.1(6)	C56	C57	C58	C53	0.7(6)

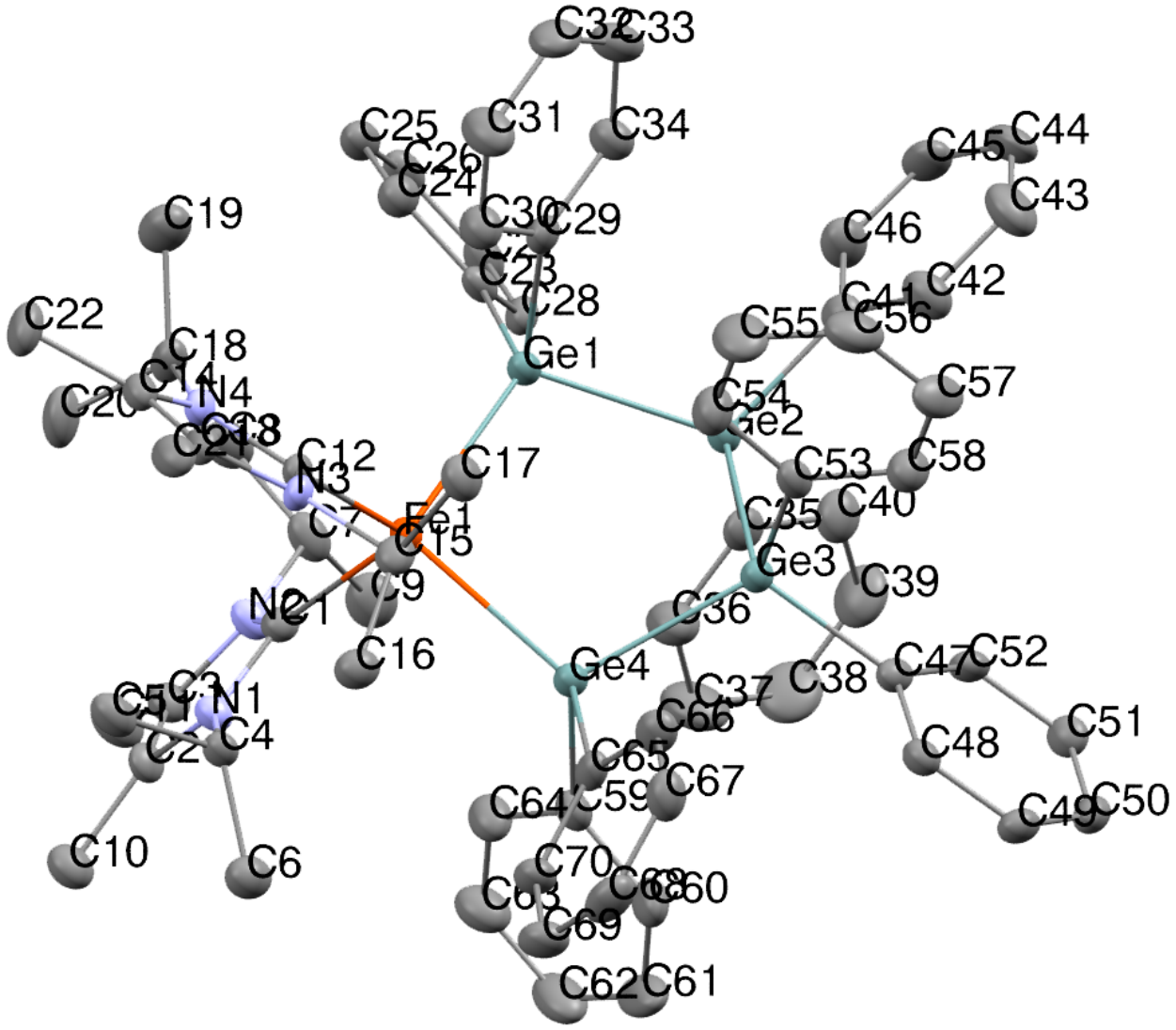


Figure S23. ORTEP drawing of **4** (50% probability of the thermal ellipsoids). Hydrogen atoms and solvated 1,2-dimethoxyethane molecule were omitted for clarity

Table S11. Crystal data and structure refinement for **4**.

Empirical Formula	$C_{74}H_{90}FeGe_4N_4O_2$
Formula Weight	1413.76
Crystal Color, Habit	red, plate
Crystal Dimensions	0.100 X 0.100 X 0.020 mm
Crystal System	monoclinic
Lattice Type	C-centered
Lattice Parameters	a = 14.0493(6) Å
	b = 24.0246(9) Å
	c = 19.8466(7) Å
	β = 92.615(4) º
	V = 6691.8(4) Å^3
Space Group	Cc (#9)
Z value	4
D_{calc}	1.403 g/cm^3
F_{000}	2928.00
μ(MoKα)	20.348 cm^{-1}
Diffractometer	Saturn724
Radiation	MoKα (λ = 0.71075 Å)
	graphite monochromated
Voltage, Current	50kV, 24mA
Temperature	-160.0ºC
Detector Aperture	72.8 x 72.8 mm
Data Images	720 exposures
ω oscillation Range (χ=45.0, ϕ=0.0)	-70.0 - 110.0º
Exposure Rate	32.0 sec./º
Detector Swing Angle	20.00º
ω oscillation Range (χ=45.0, ϕ=90.0)	-70.0 - 110.0º
Exposure Rate	32.0 sec./º
Detector Swing Angle	20.00º
Detector Position	45.00 mm
Pixel Size	0.035 mm
$2\theta_{max}$	62.4º
No. of Reflections Measured	Total: 32128
	Unique: 16430 (R_{int} = 0.0461)
	Parsons quotients (Flack x parameter): 4190
Corrections	Lorentz-polarization

	Absorption (trans. factors: 0.895 - 0.960)
Structure Solution	Direct Methods (SHELXT Version 2014/5)
Refinement	Full-matrix least-squares on F^2
Function Minimized	Σ w (Fo^2 - Fc^2)^2
Least Squares Weights	w = 1/ [$\sigma^2(Fo^2)$ + (0.0401 · P)^2 + 0.0000 · P] where P = (Max(Fo^2,0) + 2Fc^2)/3
$2\theta_{max}$ cutoff	62.4^o
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (All reflections)	16430
No. Variables	780
Reflection/Parameter Ratio	21.06
Residuals: R1 (I>2.00σ(I))	0.0505
Residuals: R (All reflections)	0.0749
Residuals: wR2 (All reflections)	0.0996
Goodness of Fit Indicator	1.015
Flack parameter (Parsons' quotients = 4190)	-0.010(6)
Max Shift/Error in Final Cycle	0.001
Maximum peak in Final Diff. Map	0.82 e^-/Å^3
Minimum peak in Final Diff. Map	-0.71 e^-/Å^3

Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}
Ge1	0.49738(4)	0.30083(2)	0.36211(3)	1.445(11)
Ge2	0.52922(4)	0.40196(2)	0.35782(3)	1.484(11)
Ge3	0.54345(4)	0.42699(2)	0.47649(3)	1.409(10)
Ge4	0.62965(4)	0.34871(2)	0.53249(3)	1.445(11)
Fe1	0.58069(6)	0.25881(3)	0.46838(4)	1.277(14)
O1	0.0880(4)	0.4817(3)	0.6586(3)	4.70(13)
O2	0.0794(4)	0.5231(2)	0.8030(3)	3.90(11)
N1	0.7545(3)	0.1864(2)	0.5145(2)	1.49(8)
N2	0.7607(4)	0.1986(2)	0.4079(2)	1.68(9)
N3	0.4520(3)	0.19854(19)	0.5744(2)	1.40(8)
N4	0.4735(4)	0.14734(18)	0.4877(3)	1.55(8)
C1	0.7059(4)	0.2104(2)	0.4607(3)	1.50(10)
C2	0.8379(4)	0.1614(2)	0.4954(3)	1.67(10)
C3	0.8413(4)	0.1686(3)	0.4282(3)	1.84(11)
C4	0.7191(4)	0.1903(2)	0.5833(3)	1.54(10)
C5	0.6814(5)	0.1351(3)	0.6068(3)	2.25(12)
C6	0.7930(5)	0.2150(3)	0.6325(3)	2.39(12)
C7	0.7356(5)	0.2202(3)	0.3394(3)	2.12(11)
C8	0.7089(5)	0.1746(3)	0.2898(3)	2.74(13)
C9	0.8130(5)	0.2576(3)	0.3143(4)	2.88(14)
C10	0.9109(5)	0.1352(3)	0.5422(3)	2.34(12)
C11	0.9174(5)	0.1489(3)	0.3829(4)	2.82(14)
C12	0.4922(4)	0.1988(2)	0.5133(3)	1.33(9)
C13	0.4103(5)	0.1474(2)	0.5870(3)	1.66(10)
C14	0.4241(4)	0.1154(2)	0.5326(3)	1.71(10)
C15	0.4516(4)	0.2486(3)	0.6173(3)	1.72(10)
C16	0.5060(5)	0.2401(3)	0.6841(3)	2.11(11)
C17	0.3519(5)	0.2708(3)	0.6246(3)	2.20(11)
C18	0.5019(5)	0.1311(3)	0.4199(3)	1.99(11)
C19	0.4163(6)	0.1167(3)	0.3733(4)	3.24(15)
C20	0.5780(6)	0.0868(3)	0.4229(4)	2.87(14)
C21	0.3622(5)	0.1325(3)	0.6495(3)	2.16(11)
C22	0.3948(5)	0.0554(3)	0.5213(4)	2.60(13)
C23	0.5183(4)	0.2754(3)	0.2676(3)	1.66(10)
C24	0.4703(5)	0.2289(3)	0.2427(3)	2.09(11)
C25	0.4868(5)	0.2080(3)	0.1791(3)	2.30(12)

C26	0.5515(5)	0.2340(3)	0.1394(3)	2.41(12)
C27	0.5982(5)	0.2797(3)	0.1632(3)	2.02(11)
C28	0.5826(4)	0.3006(3)	0.2271(3)	1.79(10)
C29	0.3561(5)	0.2947(2)	0.3631(3)	1.82(11)
C30	0.3126(5)	0.2626(3)	0.4107(3)	2.21(12)
C31	0.2147(5)	0.2553(3)	0.4104(4)	2.94(14)
C32	0.1575(5)	0.2787(3)	0.3605(4)	2.72(13)
C33	0.1984(5)	0.3105(3)	0.3122(4)	2.73(13)
C34	0.2958(5)	0.3187(3)	0.3143(3)	2.14(11)
C35	0.6543(5)	0.4231(3)	0.3249(3)	1.94(11)
C36	0.7353(5)	0.3991(3)	0.3533(4)	3.11(14)
C37	0.8255(6)	0.4192(4)	0.3432(4)	4.15(18)
C38	0.8360(6)	0.4640(4)	0.3007(4)	3.87(18)
C39	0.7561(6)	0.4883(3)	0.2692(4)	3.45(16)
C40	0.6667(5)	0.4680(3)	0.2814(4)	2.56(13)
C41	0.4380(5)	0.4462(3)	0.3033(3)	1.95(11)
C42	0.3754(5)	0.4827(3)	0.3290(4)	2.68(13)
C43	0.3141(6)	0.5145(3)	0.2877(4)	3.47(15)
C44	0.3168(5)	0.5108(3)	0.2197(4)	3.30(15)
C45	0.3799(6)	0.4746(3)	0.1912(4)	2.92(14)
C46	0.4375(6)	0.4427(3)	0.2329(4)	2.90(14)
C47	0.5966(4)	0.5014(2)	0.4961(3)	1.62(10)
C48	0.6066(4)	0.5198(3)	0.5625(3)	1.76(10)
C49	0.6402(4)	0.5721(3)	0.5784(3)	1.94(11)
C50	0.6661(5)	0.6075(3)	0.5277(3)	2.09(11)
C51	0.6590(4)	0.5909(3)	0.4617(3)	1.97(11)
C52	0.6239(4)	0.5379(2)	0.4459(3)	1.81(11)
C53	0.4099(5)	0.4324(3)	0.5033(3)	1.70(11)
C54	0.3523(5)	0.3864(3)	0.5081(4)	2.56(13)
C55	0.2577(5)	0.3907(3)	0.5226(4)	3.32(15)
C56	0.2188(5)	0.4425(3)	0.5327(4)	2.97(14)
C57	0.2729(5)	0.4890(3)	0.5270(3)	2.67(13)
C58	0.3681(5)	0.4841(3)	0.5134(3)	2.39(12)
C59	0.7683(5)	0.3650(3)	0.5263(3)	2.05(11)
C60	0.8124(5)	0.4094(3)	0.5591(4)	3.01(14)
C61	0.9105(6)	0.4165(3)	0.5575(5)	4.07(18)
C62	0.9658(5)	0.3796(3)	0.5226(5)	3.76(17)
C63	0.9231(5)	0.3352(3)	0.4909(4)	2.98(14)

C64	0.8257(5)	0.3284(3)	0.4941(4)	2.46(12)
C65	0.6168(5)	0.3638(2)	0.6307(3)	1.69(10)
C66	0.5371(5)	0.3884(3)	0.6567(3)	2.09(11)
C67	0.5293(5)	0.3966(3)	0.7257(3)	2.32(12)
C68	0.6011(6)	0.3794(3)	0.7693(3)	2.71(13)
C69	0.6800(5)	0.3543(3)	0.7457(3)	2.53(13)
C70	0.6879(5)	0.3467(3)	0.6771(3)	2.11(11)
C71	0.0790(9)	0.4311(4)	0.6970(6)	6.8(3)
C72	0.0351(8)	0.5234(4)	0.6843(4)	5.3(2)
C73	0.0862(6)	0.5547(3)	0.7430(4)	3.37(15)
C74	0.1136(7)	0.5560(3)	0.8600(4)	4.36(19)

$B_{eq} = 8/3\ \pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos\gamma + 2U_{13}(aa^*cc^*)\cos\beta + 2U_{23}(bb^*cc^*)\cos\alpha)$

Anisotropic displacement parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ge1	0.0224(3)	0.0178(3)	0.0145(3)	0.0016(3)	-0.0015(3)	-0.0012(3)
Ge2	0.0238(3)	0.0174(3)	0.0150(3)	0.0013(3)	-0.0009(3)	0.0001(3)
Ge3	0.0210(3)	0.0165(3)	0.0158(3)	0.0005(3)	-0.0007(3)	-0.0014(3)
Ge4	0.0214(3)	0.0178(3)	0.0155(3)	0.0001(3)	-0.0013(3)	-0.0009(3)
Fe1	0.0179(4)	0.0157(4)	0.0149(4)	0.0018(3)	0.0003(3)	0.0002(3)
O1	0.058(4)	0.062(4)	0.059(4)	-0.006(3)	0.000(3)	0.009(3)
O2	0.066(4)	0.049(3)	0.034(3)	-0.016(3)	-0.001(3)	0.006(3)
N1	0.018(3)	0.023(3)	0.016(2)	0.002(2)	0.001(2)	0.002(2)
N2	0.021(3)	0.027(3)	0.016(3)	0.006(2)	0.004(2)	0.003(2)
N3	0.022(3)	0.013(2)	0.018(3)	-0.0001(19)	0.000(2)	-0.003(2)
N4	0.022(3)	0.015(2)	0.022(3)	0.003(2)	-0.000(2)	-0.003(2)
C1	0.018(3)	0.021(3)	0.018(3)	-0.001(2)	0.002(2)	-0.001(2)
C2	0.020(3)	0.021(3)	0.023(3)	0.007(2)	0.003(3)	-0.003(2)
C3	0.019(3)	0.028(3)	0.024(3)	0.003(3)	0.003(3)	-0.001(3)
C4	0.023(3)	0.020(3)	0.014(3)	0.001(2)	-0.001(2)	0.001(2)
C5	0.029(4)	0.034(4)	0.022(3)	0.008(3)	0.000(3)	0.002(3)
C6	0.031(4)	0.033(4)	0.027(4)	0.003(3)	-0.001(3)	-0.005(3)
C7	0.031(4)	0.032(4)	0.018(3)	0.010(3)	0.008(3)	0.004(3)
C8	0.042(4)	0.041(4)	0.021(4)	0.008(3)	-0.002(3)	-0.000(3)
C9	0.046(5)	0.041(4)	0.023(4)	0.003(3)	0.009(3)	0.001(3)
C10	0.025(4)	0.035(4)	0.029(4)	0.006(3)	0.002(3)	0.002(3)
C11	0.033(4)	0.047(5)	0.028(4)	0.015(3)	0.006(3)	-0.002(3)

C12	0.019(3)	0.014(3)	0.017(3)	0.002(2)	0.001(2)	-0.003(2)
C13	0.023(3)	0.017(3)	0.023(3)	-0.004(2)	0.001(3)	0.004(2)
C14	0.020(3)	0.018(3)	0.026(3)	-0.000(2)	-0.001(3)	0.003(3)
C15	0.018(3)	0.023(3)	0.025(3)	-0.002(2)	0.005(3)	-0.001(3)
C16	0.027(3)	0.030(4)	0.023(3)	-0.001(3)	0.001(3)	-0.004(3)
C17	0.031(4)	0.027(3)	0.026(3)	0.006(3)	0.004(3)	-0.002(3)
C18	0.040(4)	0.019(3)	0.017(3)	-0.001(3)	-0.000(3)	-0.001(2)
C19	0.057(5)	0.038(4)	0.027(4)	-0.007(4)	-0.007(4)	-0.001(3)
C20	0.056(5)	0.021(3)	0.034(4)	0.006(3)	0.012(4)	-0.002(3)
C21	0.025(3)	0.028(4)	0.029(4)	-0.006(3)	0.002(3)	0.008(3)
C22	0.040(4)	0.018(3)	0.041(4)	-0.002(3)	0.008(3)	-0.001(3)
C23	0.025(3)	0.022(3)	0.016(3)	0.009(3)	-0.004(3)	-0.003(2)
C24	0.030(4)	0.026(3)	0.024(3)	0.002(3)	-0.000(3)	-0.002(3)
C25	0.035(4)	0.025(4)	0.027(4)	0.006(3)	-0.008(3)	-0.007(3)
C26	0.042(4)	0.030(4)	0.019(3)	0.013(3)	-0.005(3)	-0.003(3)
C27	0.034(4)	0.028(3)	0.015(3)	0.008(3)	0.006(3)	0.005(3)
C28	0.024(3)	0.016(3)	0.028(3)	-0.001(2)	-0.001(3)	-0.000(3)
C29	0.028(3)	0.016(3)	0.025(3)	-0.000(3)	-0.003(3)	-0.004(2)
C30	0.028(4)	0.028(4)	0.028(4)	-0.000(3)	0.002(3)	0.003(3)
C31	0.028(4)	0.043(4)	0.041(4)	-0.003(3)	0.003(3)	0.013(4)
C32	0.020(3)	0.039(4)	0.043(4)	-0.006(3)	-0.003(3)	-0.002(3)
C33	0.030(4)	0.044(4)	0.029(4)	0.003(3)	-0.007(3)	-0.002(3)
C34	0.029(4)	0.031(4)	0.021(3)	0.002(3)	-0.001(3)	0.003(3)
C35	0.031(4)	0.024(3)	0.020(3)	0.002(3)	0.004(3)	-0.008(3)
C36	0.032(4)	0.042(4)	0.044(5)	-0.005(3)	-0.005(4)	0.006(4)
C37	0.024(4)	0.073(6)	0.060(6)	-0.004(4)	-0.002(4)	0.012(5)
C38	0.032(5)	0.062(6)	0.055(6)	-0.010(4)	0.022(4)	0.000(4)
C39	0.049(5)	0.039(4)	0.044(5)	-0.012(4)	0.017(4)	0.006(4)
C40	0.039(4)	0.029(4)	0.030(4)	0.003(3)	0.010(3)	-0.003(3)
C41	0.029(3)	0.024(3)	0.021(3)	-0.005(3)	-0.000(3)	0.003(3)
C42	0.035(4)	0.040(4)	0.027(4)	0.004(3)	0.001(3)	0.010(3)
C43	0.034(4)	0.046(5)	0.052(5)	0.012(3)	-0.003(4)	0.009(4)
C44	0.039(4)	0.042(5)	0.043(5)	-0.003(3)	-0.021(4)	0.015(4)
C45	0.053(5)	0.035(4)	0.022(4)	-0.007(4)	-0.014(3)	0.001(3)
C46	0.051(5)	0.033(4)	0.026(4)	0.006(3)	-0.003(3)	-0.005(3)
C47	0.019(3)	0.021(3)	0.021(3)	0.003(2)	-0.001(3)	-0.005(2)
C48	0.022(3)	0.023(3)	0.021(3)	0.001(2)	-0.002(3)	0.003(3)
C49	0.025(3)	0.026(3)	0.022(3)	-0.002(3)	-0.003(3)	-0.006(3)

C50	0.027(3)	0.020(3)	0.032(4)	-0.002(3)	-0.005(3)	-0.003(3)
C51	0.027(3)	0.025(3)	0.023(3)	-0.004(3)	0.002(3)	0.005(3)
C52	0.024(3)	0.025(3)	0.019(3)	-0.002(3)	-0.006(3)	-0.002(3)
C53	0.026(3)	0.021(3)	0.017(3)	0.006(3)	0.000(3)	-0.003(2)
C54	0.035(4)	0.025(4)	0.037(4)	-0.000(3)	0.003(3)	-0.001(3)
C55	0.022(4)	0.046(5)	0.058(5)	-0.007(3)	0.004(4)	0.003(4)
C56	0.023(4)	0.055(5)	0.034(4)	0.005(3)	-0.001(3)	-0.005(4)
C57	0.025(4)	0.041(4)	0.035(4)	0.012(3)	0.001(3)	-0.018(3)
C58	0.029(4)	0.027(4)	0.034(4)	0.002(3)	-0.000(3)	-0.005(3)
C59	0.028(4)	0.022(3)	0.027(4)	0.003(3)	-0.004(3)	0.005(3)
C60	0.038(4)	0.021(4)	0.054(5)	-0.001(3)	-0.007(4)	0.008(3)
C61	0.044(5)	0.034(4)	0.075(6)	-0.020(4)	-0.025(4)	0.017(4)
C62	0.023(4)	0.047(5)	0.072(6)	-0.005(4)	-0.004(4)	0.019(4)
C63	0.025(4)	0.050(5)	0.039(4)	0.002(3)	0.002(3)	0.008(4)
C64	0.025(4)	0.029(4)	0.040(4)	-0.002(3)	0.004(3)	0.006(3)
C65	0.034(4)	0.015(3)	0.016(3)	-0.003(3)	-0.001(3)	0.002(2)
C66	0.037(4)	0.026(3)	0.016(3)	-0.002(3)	0.001(3)	0.003(3)
C67	0.040(4)	0.024(3)	0.025(4)	0.003(3)	0.007(3)	0.000(3)
C68	0.053(5)	0.031(4)	0.019(3)	-0.011(3)	-0.001(3)	-0.004(3)
C69	0.033(4)	0.038(4)	0.024(4)	-0.004(3)	-0.008(3)	-0.000(3)
C70	0.032(4)	0.027(3)	0.021(3)	-0.001(3)	-0.007(3)	0.000(3)
C71	0.130(11)	0.047(6)	0.078(8)	-0.022(6)	-0.031(7)	0.012(6)
C72	0.089(8)	0.085(7)	0.030(5)	0.040(6)	0.010(5)	0.007(5)
C73	0.052(5)	0.049(5)	0.028(4)	-0.007(4)	0.001(4)	0.002(3)
C74	0.086(7)	0.044(5)	0.035(5)	-0.020(5)	-0.004(5)	0.001(4)

The general temperature factor expression: $\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

Bond lengths (Å)

atom	atom	distance	atom	atom	distance
Ge1	Ge2	2.4726(7)	Ge1	Fe1	2.5714(10)
Ge1	C23	2.007(6)	Ge1	C29	1.991(6)
Ge2	Ge3	2.4301(8)	Ge2	C35	1.969(7)
Ge2	C41	1.954(6)	Ge3	Ge4	2.4730(7)
Ge3	C47	1.970(6)	Ge3	C53	1.979(6)
Ge4	Fe1	2.5840(9)	Ge4	C59	1.996(7)
Ge4	C65	1.998(6)	Fe1	C1	2.121(6)
Fe1	C12	2.126(6)	O1	C71	1.443(12)

O1	C72	1.361(12)	O2	C73	1.420(9)
O2	C74	1.445(10)	N1	C1	1.368(7)
N1	C2	1.386(8)	N1	C4	1.476(7)
N2	C1	1.357(8)	N2	C3	1.387(8)
N2	C7	1.482(8)	N3	C12	1.359(7)
N3	C13	1.388(7)	N3	C15	1.474(8)
N4	C12	1.358(7)	N4	C14	1.387(8)
N4	C18	1.474(8)	C2	C3	1.348(9)
C2	C10	1.491(9)	C3	C11	1.504(10)
C4	C5	1.511(9)	C4	C6	1.513(9)
C7	C8	1.508(9)	C7	C9	1.514(10)
C13	C14	1.347(9)	C13	C21	1.484(9)
C14	C22	1.511(9)	C15	C16	1.514(9)
C15	C17	1.511(9)	C18	C19	1.521(10)
C18	C20	1.508(10)	C23	C24	1.383(9)
C23	C28	1.377(9)	C24	C25	1.387(9)
C25	C26	1.379(10)	C26	C27	1.354(9)
C27	C28	1.390(9)	C29	C30	1.383(9)
C29	C34	1.383(9)	C30	C31	1.387(10)
C31	C32	1.368(10)	C32	C33	1.372(10)
C33	C34	1.382(10)	C35	C36	1.374(10)
C35	C40	1.398(9)	C36	C37	1.379(11)
C37	C38	1.379(12)	C38	C39	1.389(11)
C39	C40	1.377(11)	C41	C42	1.358(10)
C41	C46	1.399(9)	C42	C43	1.390(10)
C43	C44	1.356(11)	C44	C45	1.380(11)
C45	C46	1.365(10)	C47	C48	1.392(8)
C47	C52	1.393(8)	C48	C49	1.373(9)
C49	C50	1.380(9)	C50	C51	1.368(9)
C51	C52	1.397(8)	C53	C54	1.376(9)
C53	C58	1.392(9)	C54	C55	1.377(10)
C55	C56	1.377(11)	C56	C57	1.358(10)
C57	C58	1.381(10)	C59	C60	1.383(10)
C59	C64	1.371(10)	C60	C61	1.391(11)
C61	C62	1.384(12)	C62	C63	1.363(11)
C63	C64	1.383(10)	C65	C66	1.387(9)
C65	C70	1.390(9)	C66	C67	1.393(9)
C67	C68	1.363(10)	C68	C69	1.364(10)

C69	C70	1.383(9)		C72	C73	1.537(12)	

Bond angles (°)

atom	atom	atom	angle	atom	atom	atom	angle
Ge2	Ge1	Fe1	109.74(3)	Ge2	Ge1	C23	103.46(17)
Ge2	Ge1	C29	104.74(17)	Fe1	Ge1	C23	124.48(17)
Fe1	Ge1	C29	112.33(18)	C23	Ge1	C29	100.1(3)
Ge1	Ge2	Ge3	102.52(3)	Ge1	Ge2	C35	115.51(18)
Ge1	Ge2	C41	115.99(19)	Ge3	Ge2	C35	102.86(18)
Ge3	Ge2	C41	115.18(19)	C35	Ge2	C41	104.4(3)
Ge2	Ge3	Ge4	105.33(3)	Ge2	Ge3	C47	115.46(17)
Ge2	Ge3	C53	103.90(17)	Ge4	Ge3	C47	115.36(17)
Ge4	Ge3	C53	112.33(18)	C47	Ge3	C53	104.0(2)
Ge3	Ge4	Fe1	107.48(3)	Ge3	Ge4	C59	106.43(19)
Ge3	Ge4	C65	103.67(17)	Fe1	Ge4	C59	111.82(19)
Fe1	Ge4	C65	126.70(17)	C59	Ge4	C65	99.0(3)
Ge1	Fe1	Ge4	100.18(3)	Ge1	Fe1	C1	120.30(16)
Ge1	Fe1	C12	110.92(15)	Ge4	Fe1	C1	106.91(16)
Ge4	Fe1	C12	120.51(15)	C1	Fe1	C12	99.3(2)
C71	O1	C72	111.1(7)	C73	O2	C74	109.3(6)
C1	N1	C2	111.4(5)	C1	N1	C4	121.2(5)
C2	N1	C4	127.3(5)	C1	N2	C3	111.7(5)
C1	N2	C7	121.0(5)	C3	N2	C7	127.2(5)
C12	N3	C13	111.2(5)	C12	N3	C15	121.6(5)
C13	N3	C15	127.2(5)	C12	N4	C14	110.9(5)
C12	N4	C18	121.8(5)	C14	N4	C18	127.2(5)
Fe1	C1	N1	124.1(4)	Fe1	C1	N2	132.1(4)
N1	C1	N2	103.6(5)	N1	C2	C3	106.5(5)
N1	C2	C10	125.3(5)	C3	C2	C10	128.1(6)
N2	C3	C2	106.7(5)	N2	C3	C11	125.8(5)
C2	C3	C11	127.5(6)	N1	C4	C5	111.5(5)
N1	C4	C6	111.8(5)	C5	C4	C6	112.6(5)
N2	C7	C8	112.8(5)	N2	C7	C9	111.4(5)
C8	C7	C9	112.2(5)	Fe1	C12	N3	130.7(4)
Fe1	C12	N4	124.5(4)	N3	C12	N4	104.4(5)
N3	C13	C14	106.5(5)	N3	C13	C21	125.3(5)
C14	C13	C21	128.2(5)	N4	C14	C13	107.0(5)
N4	C14	C22	124.9(5)	C13	C14	C22	128.0(6)

N3	C15	C16	112.3(5)	N3	C15	C17	111.8(5)
C16	C15	C17	113.3(5)	N4	C18	C19	112.0(6)
N4	C18	C20	111.8(5)	C19	C18	C20	113.8(6)
Ge1	C23	C24	119.3(5)	Ge1	C23	C28	122.7(4)
C24	C23	C28	117.9(6)	C23	C24	C25	121.3(6)
C24	C25	C26	119.8(6)	C25	C26	C27	119.3(6)
C26	C27	C28	121.1(6)	C23	C28	C27	120.6(6)
Ge1	C29	C30	121.2(5)	Ge1	C29	C34	122.8(5)
C30	C29	C34	115.8(6)	C29	C30	C31	122.4(6)
C30	C31	C32	120.1(7)	C31	C32	C33	118.9(6)
C32	C33	C34	120.3(6)	C29	C34	C33	122.4(6)
Ge2	C35	C36	119.4(5)	Ge2	C35	C40	122.9(5)
C36	C35	C40	116.9(6)	C35	C36	C37	122.8(7)
C36	C37	C38	119.2(7)	C37	C38	C39	119.7(8)
C38	C39	C40	119.9(7)	C35	C40	C39	121.4(7)
Ge2	C41	C42	124.3(5)	Ge2	C41	C46	119.6(5)
C42	C41	C46	116.1(6)	C41	C42	C43	121.9(7)
C42	C43	C44	120.3(7)	C43	C44	C45	119.8(7)
C44	C45	C46	118.7(7)	C41	C46	C45	123.1(7)
Ge3	C47	C48	119.8(4)	Ge3	C47	C52	122.9(4)
C48	C47	C52	117.3(5)	C47	C48	C49	121.8(6)
C48	C49	C50	119.8(6)	C49	C50	C51	120.5(6)
C50	C51	C52	119.4(6)	C47	C52	C51	121.3(6)
Ge3	C53	C54	122.2(5)	Ge3	C53	C58	120.6(5)
C54	C53	C58	117.0(6)	C53	C54	C55	122.0(6)
C54	C55	C56	119.5(7)	C55	C56	C57	120.2(7)
C56	C57	C58	119.8(7)	C53	C58	C57	121.5(6)
Ge4	C59	C60	122.6(5)	Ge4	C59	C64	120.0(5)
C60	C59	C64	117.1(6)	C59	C60	C61	120.4(7)
C60	C61	C62	120.9(7)	C61	C62	C63	119.1(7)
C62	C63	C64	119.2(7)	C59	C64	C63	123.3(7)
Ge4	C65	C66	123.4(4)	Ge4	C65	C70	119.9(5)
C66	C65	C70	116.6(5)	C65	C66	C67	121.8(6)
C66	C67	C68	119.5(6)	C67	C68	C69	120.4(6)
C68	C69	C70	120.0(6)	C65	C70	C69	121.7(6)
O1	C72	C73	113.7(8)	O2	C73	C72	109.0(7)

Torsion Angles(°)

(Those having bond angles > 160 or < 20 degrees are excluded.)

atom1	atom2	atom3	atom4	angle	atom1	atom2	atom3	atom4	angle
Ge2	Ge1	Fe1	Ge4	11.28(4)	Ge2	Ge1	Fe1	C1	-105.29(4)
Ge2	Ge1	Fe1	C12	139.66(3)	Fe1	Ge1	Ge2	Ge3	-31.29(4)
Fe1	Ge1	Ge2	C35	79.72(4)	Fe1	Ge1	Ge2	C41	-157.66(3)
Ge2	Ge1	C23	C24	-152.5(3)	Ge2	Ge1	C23	C28	30.8(4)
C23	Ge1	Ge2	Ge3	-166.06(18)	C23	Ge1	Ge2	C35	-55.05(18)
C23	Ge1	Ge2	C41	67.57(18)	Ge2	Ge1	C29	C30	-129.5(4)
Ge2	Ge1	C29	C34	55.0(4)	C29	Ge1	Ge2	Ge3	89.50(19)
C29	Ge1	Ge2	C35	-159.49(19)	C29	Ge1	Ge2	C41	-36.87(19)
Fe1	Ge1	C23	C24	81.7(4)	Fe1	Ge1	C23	C28	-95.0(4)
C23	Ge1	Fe1	Ge4	134.4(2)	C23	Ge1	Fe1	C1	17.8(2)
C23	Ge1	Fe1	C12	-97.2(2)	Fe1	Ge1	C29	C30	-10.4(5)
Fe1	Ge1	C29	C34	174.1(3)	C29	Ge1	Fe1	Ge4	-104.81(19)
C29	Ge1	Fe1	C1	138.63(19)	C29	Ge1	Fe1	C12	23.58(19)
C23	Ge1	C29	C30	123.6(4)	C23	Ge1	C29	C34	-51.9(5)
C29	Ge1	C23	C24	-44.5(4)	C29	Ge1	C23	C28	138.8(4)
Ge1	Ge2	Ge3	Ge4	38.74(3)	Ge1	Ge2	Ge3	C47	167.23(3)
Ge1	Ge2	Ge3	C53	-79.53(3)	Ge1	Ge2	C35	C36	-51.4(5)
Ge1	Ge2	C35	C40	139.2(4)	Ge1	Ge2	C41	C42	110.0(4)
Ge1	Ge2	C41	C46	-72.6(4)	Ge3	Ge2	C35	C36	59.4(4)
Ge3	Ge2	C35	C40	-110.0(4)	C35	Ge2	Ge3	Ge4	-81.47(19)
C35	Ge2	Ge3	C47	47.02(19)	C35	Ge2	Ge3	C53	160.26(19)
Ge3	Ge2	C41	C42	-9.7(5)	Ge3	Ge2	C41	C46	167.7(3)
C41	Ge2	Ge3	Ge4	165.6(2)	C41	Ge2	Ge3	C47	-65.9(2)
C41	Ge2	Ge3	C53	47.4(2)	C35	Ge2	C41	C42	-121.7(5)
C35	Ge2	C41	C46	55.7(5)	C41	Ge2	C35	C36	-180.0(4)
C41	Ge2	C35	C40	10.6(5)	Ge2	Ge3	Ge4	Fe1	-32.97(3)
Ge2	Ge3	Ge4	C59	86.98(3)	Ge2	Ge3	Ge4	C65	-169.14(2)
Ge2	Ge3	C47	C48	179.3(3)	Ge2	Ge3	C47	C52	0.4(5)
Ge2	Ge3	C53	C54	69.8(4)	Ge2	Ge3	C53	C58	-105.3(4)
Ge4	Ge3	C47	C48	-57.3(4)	Ge4	Ge3	C47	C52	123.7(4)
C47	Ge3	Ge4	Fe1	-161.52(19)	C47	Ge3	Ge4	C59	-41.57(19)
C47	Ge3	Ge4	C65	62.31(19)	Ge4	Ge3	C53	C54	-43.6(5)
Ge4	Ge3	C53	C58	141.3(3)	C53	Ge3	Ge4	Fe1	79.48(19)
C53	Ge3	Ge4	C59	-160.57(19)	C53	Ge3	Ge4	C65	-56.69(19)
C47	Ge3	C53	C54	-169.0(4)	C47	Ge3	C53	C58	15.9(5)

C53	Ge3	C47	C48	66.2(4)	C53	Ge3	C47	C52	-112.8(4)
Ge3	Ge4	Fe1	Ge1	12.79(4)	Ge3	Ge4	Fe1	C1	138.97(3)
Ge3	Ge4	Fe1	C12	-109.01(4)	Ge3	Ge4	C59	C60	66.0(5)
Ge3	Ge4	C59	C64	-120.6(4)	Ge3	Ge4	C65	C66	33.7(4)
Ge3	Ge4	C65	C70	-149.7(3)	Fe1	Ge4	C59	C60	-176.9(4)
Fe1	Ge4	C59	C64	-3.5(5)	C59	Ge4	Fe1	Ge1	-103.7(2)
C59	Ge4	Fe1	C1	22.5(2)	C59	Ge4	Fe1	C12	134.5(2)
Fe1	Ge4	C65	C66	-90.9(4)	Fe1	Ge4	C65	C70	85.8(4)
C65	Ge4	Fe1	Ge1	135.7(2)	C65	Ge4	Fe1	C1	-98.1(2)
C65	Ge4	Fe1	C12	13.9(2)	C59	Ge4	C65	C66	143.1(4)
C59	Ge4	C65	C70	-40.2(4)	C65	Ge4	C59	C60	-41.2(5)
C65	Ge4	C59	C64	132.2(4)	Ge1	Fe1	C1	N1	-179.8(3)
Ge1	Fe1	C1	N2	5.7(6)	Ge1	Fe1	C12	N3	-115.8(4)
Ge1	Fe1	C12	N4	73.0(4)	Ge4	Fe1	C1	N1	67.2(4)
Ge4	Fe1	C1	N2	-107.3(5)	Ge4	Fe1	C12	N3	0.6(5)
Ge4	Fe1	C12	N4	-170.6(3)	C1	Fe1	C12	N3	116.6(4)
C1	Fe1	C12	N4	-54.6(4)	C12	Fe1	C1	N1	-58.8(4)
C12	Fe1	C1	N2	126.7(5)	C71	O1	C72	C73	84.4(9)
C74	O2	C73	C72	-170.9(6)	C1	N1	C2	C3	-1.3(6)
C1	N1	C2	C10	175.2(5)	C2	N1	C1	Fe1	-174.8(4)
C2	N1	C1	N2	1.0(6)	C1	N1	C4	C5	108.4(5)
C1	N1	C4	C6	-124.5(5)	C4	N1	C1	Fe1	3.3(7)
C4	N1	C1	N2	179.0(4)	C2	N1	C4	C5	-73.9(7)
C2	N1	C4	C6	53.2(7)	C4	N1	C2	C3	-179.1(5)
C4	N1	C2	C10	-2.7(9)	C1	N2	C3	C2	-0.4(6)
C1	N2	C3	C11	-179.7(5)	C3	N2	C1	Fe1	174.9(4)
C3	N2	C1	N1	-0.4(6)	C1	N2	C7	C8	-114.1(6)
C1	N2	C7	C9	118.7(5)	C7	N2	C1	Fe1	-1.3(8)
C7	N2	C1	N1	-176.6(4)	C3	N2	C7	C8	70.3(7)
C3	N2	C7	C9	-56.9(7)	C7	N2	C3	C2	175.6(5)
C7	N2	C3	C11	-3.7(9)	C12	N3	C13	C14	-0.5(6)
C12	N3	C13	C21	178.5(5)	C13	N3	C12	Fe1	-171.6(4)
C13	N3	C12	N4	0.9(6)	C12	N3	C15	C16	-117.9(5)
C12	N3	C15	C17	113.3(5)	C15	N3	C12	Fe1	11.1(8)
C15	N3	C12	N4	-176.3(4)	C13	N3	C15	C16	65.3(7)
C13	N3	C15	C17	-63.4(7)	C15	N3	C13	C14	176.6(5)
C15	N3	C13	C21	-4.4(9)	C12	N4	C14	C13	0.8(6)
C12	N4	C14	C22	-177.8(5)	C14	N4	C12	Fe1	172.1(4)

C14	N4	C12	N3	-1.1(6)	C12	N4	C18	C19	-118.0(5)
C12	N4	C18	C20	112.9(5)	C18	N4	C12	Fe1	-9.5(7)
C18	N4	C12	N3	177.4(4)	C14	N4	C18	C19	60.2(7)
C14	N4	C18	C20	-68.9(7)	C18	N4	C14	C13	-177.5(5)
C18	N4	C14	C22	3.8(9)	N1	C2	C3	N2	1.0(6)
N1	C2	C3	C11	-179.7(5)	C10	C2	C3	N2	-175.4(5)
C10	C2	C3	C11	3.9(10)	N3	C13	C14	N4	-0.2(6)
N3	C13	C14	C22	178.3(5)	C21	C13	C14	N4	-179.2(5)
C21	C13	C14	C22	-0.6(10)	Ge1	C23	C24	C25	-176.2(4)
Ge1	C23	C28	C27	176.7(4)	C24	C23	C28	C27	-0.1(8)
C28	C23	C24	C25	0.6(9)	C23	C24	C25	C26	-0.6(9)
C24	C25	C26	C27	0.0(9)	C25	C26	C27	C28	0.5(10)
C26	C27	C28	C23	-0.5(9)	Ge1	C29	C30	C31	-176.6(4)
Ge1	C29	C34	C33	174.5(4)	C30	C29	C34	C33	-1.2(9)
C34	C29	C30	C31	-0.8(9)	C29	C30	C31	C32	2.3(10)
C30	C31	C32	C33	-1.8(10)	C31	C32	C33	C34	-0.1(10)
C32	C33	C34	C29	1.7(10)	Ge2	C35	C36	C37	-166.6(5)
Ge2	C35	C40	C39	167.7(4)	C36	C35	C40	C39	-1.9(9)
C40	C35	C36	C37	3.4(10)	C35	C36	C37	C38	-2.7(12)
C36	C37	C38	C39	0.4(12)	C37	C38	C39	C40	1.0(12)
C38	C39	C40	C35	-0.2(11)	Ge2	C41	C42	C43	177.8(4)
Ge2	C41	C46	C45	-176.0(4)	C42	C41	C46	C45	1.6(10)
C46	C41	C42	C43	0.3(10)	C41	C42	C43	C44	-1.5(11)
C42	C43	C44	C45	0.9(11)	C43	C44	C45	C46	0.9(11)
C44	C45	C46	C41	-2.2(11)	Ge3	C47	C48	C49	-177.7(4)
Ge3	C47	C52	C51	178.3(3)	C48	C47	C52	C51	-0.6(8)
C52	C47	C48	C49	1.3(8)	C47	C48	C49	C50	-0.9(9)
C48	C49	C50	C51	-0.3(9)	C49	C50	C51	C52	0.9(9)
C50	C51	C52	C47	-0.4(9)	Ge3	C53	C54	C55	-175.8(4)
Ge3	C53	C58	C57	174.8(4)	C54	C53	C58	C57	-0.5(9)
C58	C53	C54	C55	-0.5(9)	C53	C54	C55	C56	0.1(11)
C54	C55	C56	C57	1.3(11)	C55	C56	C57	C58	-2.4(10)
C56	C57	C58	C53	2.0(10)	Ge4	C59	C60	C61	175.0(4)
Ge4	C59	C64	C63	-176.4(4)	C60	C59	C64	C63	-2.7(10)
C64	C59	C60	C61	1.4(10)	C59	C60	C61	C62	0.6(12)
C60	C61	C62	C63	-1.6(12)	C61	C62	C63	C64	0.4(12)
C62	C63	C64	C59	1.8(11)	Ge4	C65	C66	C67	177.8(4)
Ge4	C65	C70	C69	-177.3(4)	C66	C65	C70	C69	-0.4(9)

C70	C65	C66	C67	1.0(9)	C65	C66	C67	C68	-0.8(9)
C66	C67	C68	C69	-0.2(10)	C67	C68	C69	C70	0.7(10)
C68	C69	C70	C65	-0.5(10)	O1	C72	C73	O2	-79.9(9)

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