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SUPPORTING INFORMATION of SYNTHESES and STRUCTURES

C4-Ferrocenylsilyl-bridged and -substituted N-heterocyclic carbenes: complexation of germanium chloride

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SUPPORTING INFORMATIONS of SYNTHESES

Materials and Methods

General.

The syntheses of air-sensitive compounds were performed under purified argon using Schlenk techniques and an inert atmosphere drybox (M-Braun LabMaster SP). Chemicals were purchased from Aldrich and Strem and used as received. The solvents were dried and distilled under argon from Na/benzophenone prior to use. ^{1}H NMR, ^{13}C{^{1}H} NMR and ^{29}Si{^{1}H} NMR spectra were recorded on a Bruker Avance III HD 400 MHz spectrometer or on a Varian Unity Inova 500 MHz spectrometer. The chemical shifts were referenced to an external TMS standard for ^{29}Si{^{1}H} NMR spectra. X-ray intensity data for **4**, **5·THF**, **6**, **7·0.5(dioxane)**, **8·(THF)$_2$** were collected on a Bruker SMART APEX II X-ray diffractometer system with graphite-monochromated Mo K radiation (λ = 0.71073 Å), using the ω-scan technique. Elemental analyses were performed by Complete Analytical Laboratories, Inc. (Highland Park, NJ).

Compound **4**: 40 mL of THF was added to a Schlenk flask containing both **2** (3.00 g, 5.75 mmol) and [(η^5-$C_5H_4Li)_2Fe]_3$[TMEDA]$_2$ (1.74 g, 6.32 mmol), which was then stirred at room temperature for 1h. The volatile materials were removed in vacuo. The residue was extracted using toluene (30 mL)/hexane (30 mL) mixed solvent. Removing the volatile materials from the filtrate in vacuo gave raw compound **4** (2.77 g, 75.9% yield based on the ^{1}H NMR data). Pure orange powder of **4** can be achieved by rinsing the raw material of **4** with hexane. Mp: decomposed (> 211°C) and melt (> 288°C). X-ray quality orange crystals of **4** were obtained by recrystallization of **4** in Et_2O. ^{1}H NMR (400.14 MHz, C_6D_6): δ 1.18 [d, 6H, CH(CH_3)$_2$], 1.28 [d, 6H, CH(CH_3)$_2$], 1.38 [d, 6H, CH(CH_3)$_2$], 1.44 [d, 6H, CH(CH_3)$_2$], 3.06 [m, 4H, CH(CH$_3$)$_2$], 3.96 (t, 2H, C_5H_4), 4.06 (t, 2H, C_5H_4), 4.26 (d, 2H, C_5H_4), 4.31 (d, 2H, C_5H_4), 7.17-7.32 (m, 6H, Ar-*H*), 7.55 (s, 1H, NC*H*). ^{13}C{^{1}H} NMR (100.63 MHz, C_6D_6): δ 22.7, 24.4, 24.9, 26.9 [CH(*C*H$_3$)$_2$], 29.2, 29.9 [*C*H(CH$_3$)$_2$], 31.7 (C_5H_4-*ipso*), 74.7 (C_5H_4), 76.7 (C_5H_4), 79.1 (C_5H_4), 79.6 (C_5H_4), 123.9, 124.3 (N*C*H), 129.7, 130.0, 134.5, 138.6, 139.1, 146.5, 147.1 (Ar-*C*), 226.8 (N*C*N). ^{29}Si{^{1}H} NMR (C_6D_6, 99.30 MHz): δ -15.46. Crystal data for **4**: $C_{37}H_{43}ClFeN_2Si$, fw = 635.12, monoclinic, $P2_1/n$, a = 18.7276(13) Å, b = 18.1214(12) Å, c = 21.7095(15) Å, β = 112.148(2)°, V = 6823.9(8) Å^3, Z = 8, R1 = 0.0766 for 7397 data ($I > 2\sigma(I)$), wR_2 = 0.1667 (all data). Anal. (CALI, Highland Park, NJ) Calcd (found) for **4**·(toluene)$_{0.5}$ (in terms of ^{1}H NMR data): C 71.41 (71.25); H 6.95 (7.09); N 4.11 (3.70).

Compound **5**: $(CH_3)_2SiCl_2$ (2.06 g, 16.0 mmol) was added to a Schlenk flask containing both **1** (6.30 g, 16.0 mmol) and 70 mL of hexane at 0 °C, which was then stirred for 2h at room temperature. After filtration, the volatile materials were removed from the filtrate in vacuo, giving compound **5** as off-white powder (7.06 g, 91.9% yield). Mp: melt (> 86°C). X-ray quality colorless crystals of **5** were obtained by recrystallization of **5** in THF. ^{1}H NMR (400.14 MHz, C_6D_6): δ 0.15 [s, 6H, Si(CH_3)$_2$]1.15 [d, 6H, CH(CH_3)$_2$], 1.25 [d, 6H, CH(CH_3)$_2$], 1.27 [d, 6H, CH(CH_3)$_2$], 1.36 [d, 6H, CH(CH_3)$_2$], 2.85 [m, 2H, CH(CH$_3$)$_2$], 2.96 [m, 2H, CH(CH$_3$)$_2$], 7.11 (s, 1H, NC*H*), 7.16 (d, 2H, Ar-*H*), 7.17 (d, 2H, Ar-*H*), 7.27

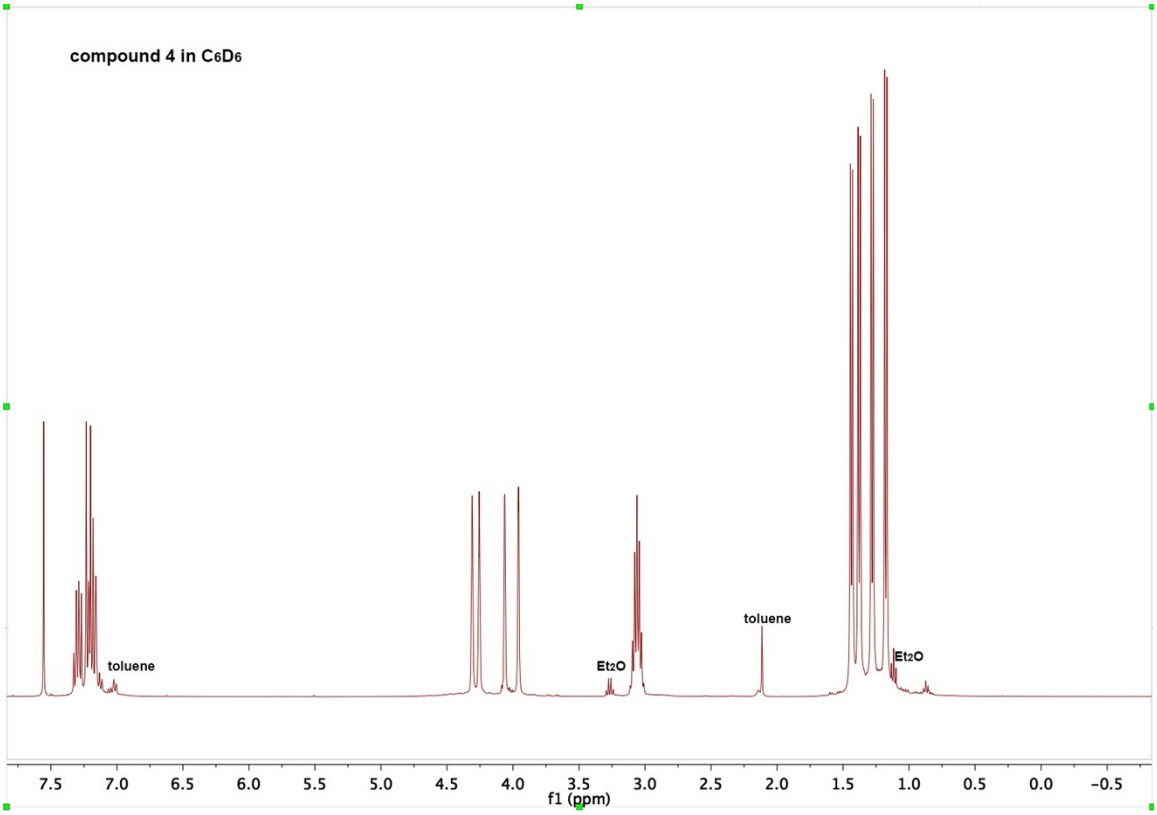
(t, 1H, Ar-*H*), 7.29 (t, 1H, Ar-*H*). $^{13}C\{^1H\}$ NMR (100.63 MHz, C_6D_6): δ 3.0 [Si(*C*H_3)$_2$], 22.3, 24.2, 25.1, 26.7 [CH(*C*H_3)$_2$], 29.1, 29.6 [*C*H(CH$_3$)$_2$], 123.9, 124.2 (N*C*H), 129.5, 129.8, 133.2, 138.7, 139.6, 146.5, 147.1 (Ar-*C*), 224.9 (N*C*N). $^{29}Si\{^1H\}$ NMR (THF-d_8, 99.30 MHz): δ 9.86. Crystal data for **5·THF**: $C_{33}H_{49}ClN_2OSi$, fw = 553.28, triclinic, *P*-1, *a* = 8.935(3) Å, *b* = 12.508(4) Å, *c* = 16.628(5) Å, α = 69.021(10)°, β = 81.901(11)° γ = 81.762(11)°, *V* = 1709.3(10) Å^3, *Z* = 2, R1 = 0.0636 for 4485 data ($I > 2\sigma(I)$), wR_2 = 0.1803 (all data).

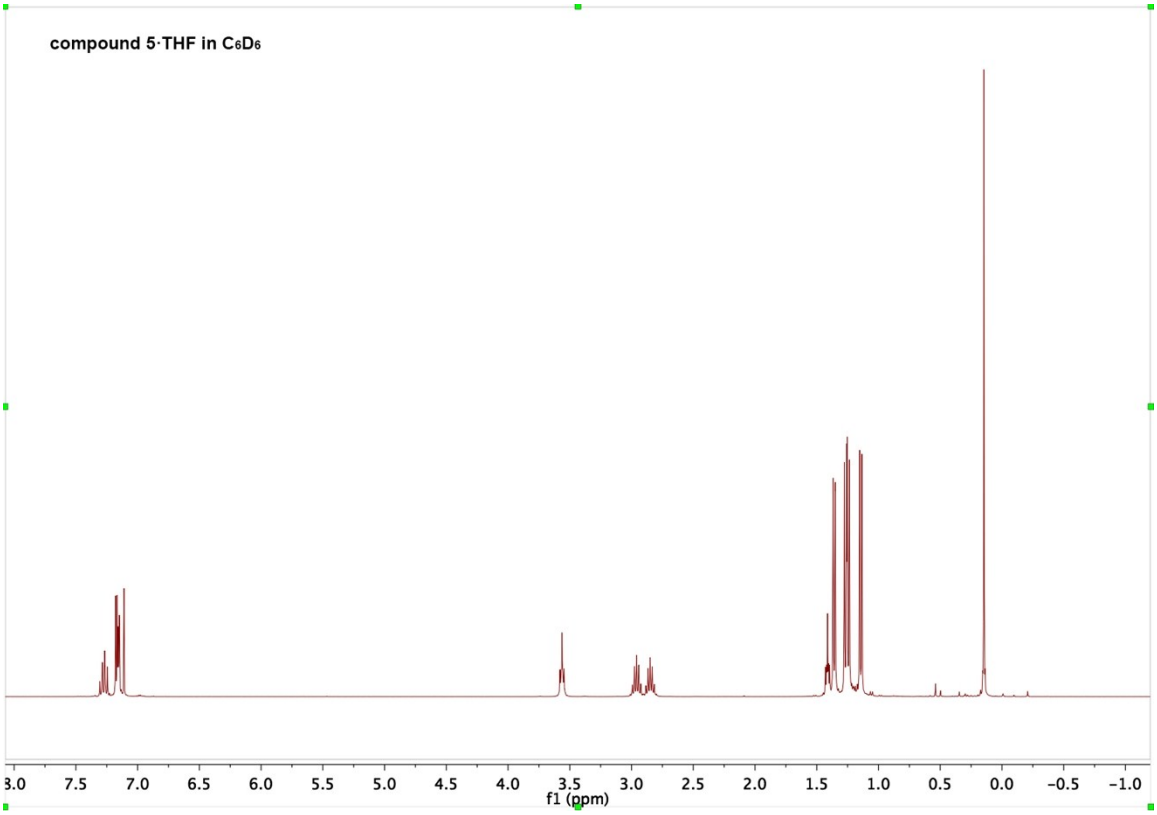
Compound **6**: 20 mL of THF was added to a Schlenk flask containing **5·THF** crystals (1.03 g, 2.0 mmol) and $[(\eta^5\text{-}C_5H_4Li)_2Fe]_3[TMEDA]_2$ (0.27 g, 1.0 mmol), which was then stirred for 1h at room temperature. The volatile materials were removed in vacuo. The residue was extracted using 30 mL of toluene. Removing the volatile materials from the filtrate in vacuo gave raw compound **6** (0.738 g, 70.0% yield based on the ^1H NMR data). Pure yellow powder of **6** can be achieved by rinsing the raw material of **6** with hexane. Mp: gradually decomposed (> 205°C) and melt (> 232°C). X-ray quality yellow crystals of **6** were obtained by recrystallization of **6** in the THF/hexane mixed solvent. ^1H NMR (400.14 MHz, C_6D_6): δ 0.21 [s, 12H, Si(CH_3)$_2$] 1.13 [d, 12H, CH(CH_3)$_2$], 1.25 [d, 12H, CH(CH_3)$_2$], 1.26 [d, 12H, CH(CH_3)$_2$], 1.40 [d, 12H, CH(CH_3)$_2$], 2.81 [m, 4H, C*H*(CH$_3$)$_2$], 2.99 [m, 4H, C*H*(CH$_3$)$_2$], 3.77 (t, 4H, C_5H_4), 4.02 (t, 4H, C_5H_4), 6.91 (s, 2H, NC*H*), 7.16 [d, 4H, Ar-*H*), 7.20 [d, 4H, Ar-*H*), 7.30 (m, 4H, Ar-*H*). $^{13}C\{^1H\}$ NMR (100.63 MHz, C_6D_6): δ -0.65 [Si(CH$_3$)$_2$], 22.3, 24.4, 25.0, 26.9 [CH(*C*H$_3$)$_2$], 29.0, 29.6 [*C*H(CH$_3$)$_2$], 70.2 (*C*$_5$H$_4$-*ipso*), 72.3 (*C*$_5$H$_4$), 74.0 (*C*$_5$H$_4$), 123.7, 124.1 (N*C*H), 129.2, 129.4, 132.14, 132.22, 139.1, 140.5, 146.6, 147.1 (Ar-*C*), 223.9 (N*C*N). $^{29}Si\{^1H\}$ NMR (THF-d_8, 99.30 MHz): δ -15.65. Crystal data for **6**: $C_{68}H_{90}FeN_4Si_2$, fw = 1075.46, monoclinic, *C*2/c, *a* = 28.165(15) Å, *b* = 10.265(5) Å, *c* = 22.785(12) Å, β = 99.308(7)°, *V* = 6500(6) Å^3, *Z* = 4, R1 = 0.0794 for 3388 data ($I > 2\sigma(I)$), wR_2 = 0.1786 (all data). Anal. (CALI, Highland Park, NJ) Calcd (found) for **6**: C 75.94 (76.19); H 8.44 (8.63); N 5.21 (5.08).

Compound **7**: 5 mL of toluene was added to a Schlenk tube containing **4** (0.30 g, 0.47 mmol) and $GeCl_2$·dioxane (0.11 g, 0.47 mmol), which was then sonicated for 30 min. The volatile materials were removed in vacuo, giving compound **7** as orange powder in a quantitative yield. Mp: gradually decomposed (> 240°C) and melt (> 296°C). X-ray quality orange crystals of **7** were obtained by concentrating toluene solution of **7**. ^1H NMR (400.14 MHz, THF-d_8): δ 1.23 [d, 6H, CH(CH_3)$_2$], 1.30 [d, 6H, CH(CH_3)$_2$], 1.36 [d, 6H, CH(CH_3)$_2$], 1.43 [d, 6H, CH(CH_3)$_2$], 2.83 [m, 4H, C*H*(CH$_3$)$_2$], 4.21 (t, 2H, C_5H_4), 4.24 (t, 2H, C_5H_4), 4.68 (m, 4H, C_5H_4), 7.33 (d, 2H, Ar-*H*),), 7.38 (d, 2H, Ar-*H*), 7.49 (t, 1H, Ar-*H*), 7.52 (t, 1H, Ar-*H*), 8.40 (s, 1H, NC*H*). $^{13}C\{^1H\}$ NMR (100.63 MHz, THF-d_8): δ 22.9, 24.9, 25.8, 26.5 [CH(*C*H$_3$)$_2$], 30.0, 30.3 [*C*H(CH$_3$)$_2$], 30.4 (*C*$_5$H$_4$-*ipso*), 74.7 (*C*$_5$H$_4$), 76.3 (*C*$_5$H$_4$), 80.4 (*C*$_5$H$_4$), 80.6 (*C*$_5$H$_4$), 124.9, 125.3 (N*C*H), 129.8, 130.0, 132.0, 134.1, 134.7, 138.3, 146.8, 147.0 (Ar-*C*), 178.9 (N*C*N). $^{29}Si\{^1H\}$ NMR (THF-d_8, 99.30 MHz): δ -15.13. Crystal data for **7·0.5(dioxane)**: $C_{39}H_{47}Cl_3FeGeN_2OSi$, fw = 822.66, triclinic, *P*-1, *a* = 10.5862(5) Å, *b* = 10.6734(5) Å, *c* = 18.5264(10) Å, α = 85.038(2)°, β = 84.783(2)° γ = 74.549(2)°, *V* = 2005.07(17) Å^3, *Z* = 2, R1 = 0.0707 for 6140 data ($I > 2\sigma(I)$), wR_2 = 0.1770 (all data). Anal. (CALI, Highland Park, NJ) Calcd (found) for

7·(dioxane)$_{0.4}$(toluene)$_{0.2}$ (in terms of ^{1}H NMR data): C 57.49 (57.93); H 5.79 (6.01); N 3.35 (3.40).

Compound **8**: 10 mL of THF was added to a Schlenk tube containing **6** (0.46 g, 0.43 mmol) and $GeCl_2$·dioxane (0.20 g, 0.86 mmol), which was then stirred for 30 min at room temperature. The volatile materials were removed in vacuo, giving compound **8** as yellow powder in a quantitative yield. Mp: gradually decomposed (> 159°C) and melt (> 185°C). X-ray quality yellow crystals of **8·(THF)$_2$** were obtained by recrystallization of **8** in the THF/hexane mixed solvent. ^{1}H NMR (400.14 MHz, THF-d_8): δ 0.22 [s, 12H, Si(CH_3)$_2$], 0.97 [d, 12H, CH(CH_3)$_2$], 1.20 [d, 12H, CH(CH_3)$_2$], 1.26 [d, 12H, CH(CH_3)$_2$], 1.31 [d, 12H, CH(CH_3)$_2$], 2.64 [m, 8H, CH(CH$_3$)$_2$], 4.10 (t, 4H, C$_5H_4$), 4.34 (t, 4H, C$_5H_4$), 7.26 [d, 4H, Ar-*H*), 7.30 [d, 4H, Ar-*H*), 7.42 (s, 2H, NC*H*), 7.43 (t, 2H, Ar-*H*), 7.48 (t, 2H, Ar-*H*). ^{13}C{^{1}H} NMR (100.63 MHz, THF-d_8): δ -1.3 [Si(*C*H$_3$)$_2$], 22.8, 24.7, 25.4, 26.6 [CH(*C*H$_3$)$_2$], 29.6, 30.1 [*C*H(CH$_3$)$_2$], 70.3 (*C*$_5$H$_4$-*ipso*), 73.0 (*C*$_5$H$_4$), 74.3 (*C*$_5$H$_4$) 124.7, 125.1 (N*C*H), 131.6, 131.7, 134.2, 135.7, 136.4, 137.2, 146.6, 146.8 (Ar-*C*), 175.5 (N*C*N). ^{29}Si{^{1}H} NMR (THF-d_8, 99.30 MHz): δ -11.85. Crystal data for **8·(THF)$_2$**: $C_{76}H_{106}Cl_4FeGe_2N_4O_2Si_2$, fw = 1506.65, triclinic, *P*-1, *a* = 12.1909(9) Å, *b* = 16.9634(12) Å, *c* = 20.1520(14) Å, α = 80.614(2)°, β = 82.073(2)° γ = 82.496(2)°, *V* = 4047.3(5) Å^3, *Z* = 2, R1 = 0.0653 for 10889 data ($I > 2\sigma(I)$), wR_2 = 0.1898 (all data). Anal. (CALI, Highland Park, NJ) Calcd (found) for **8·(THF)** (in terms of ^{1}H NMR data): C 60.28 (60.10); H 6.89 (6.97); N 3.91 (3.70).


compound 4 in C6D6
toluene
Et2O
toluene
Et2O
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


compound 5·THF in C6D6
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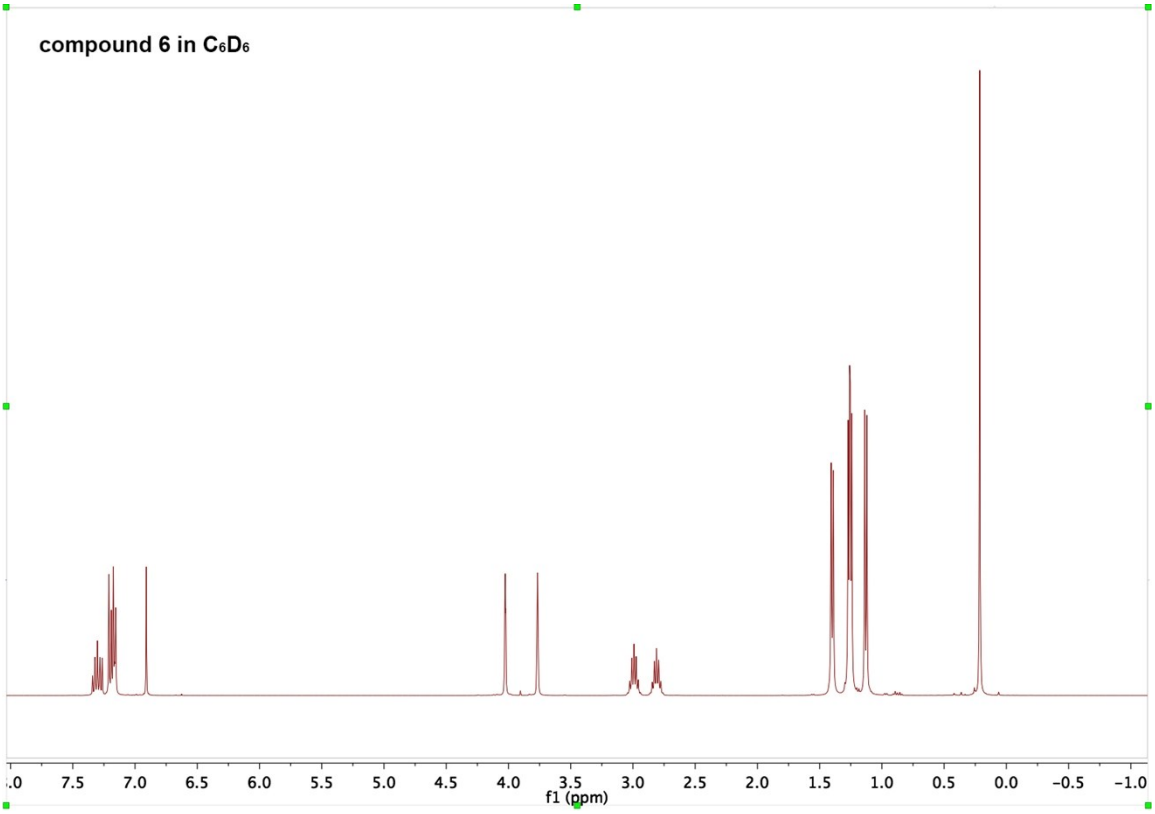
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


compound 6 in C6D6
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7.0
6.5
6.0
5.5
5.0
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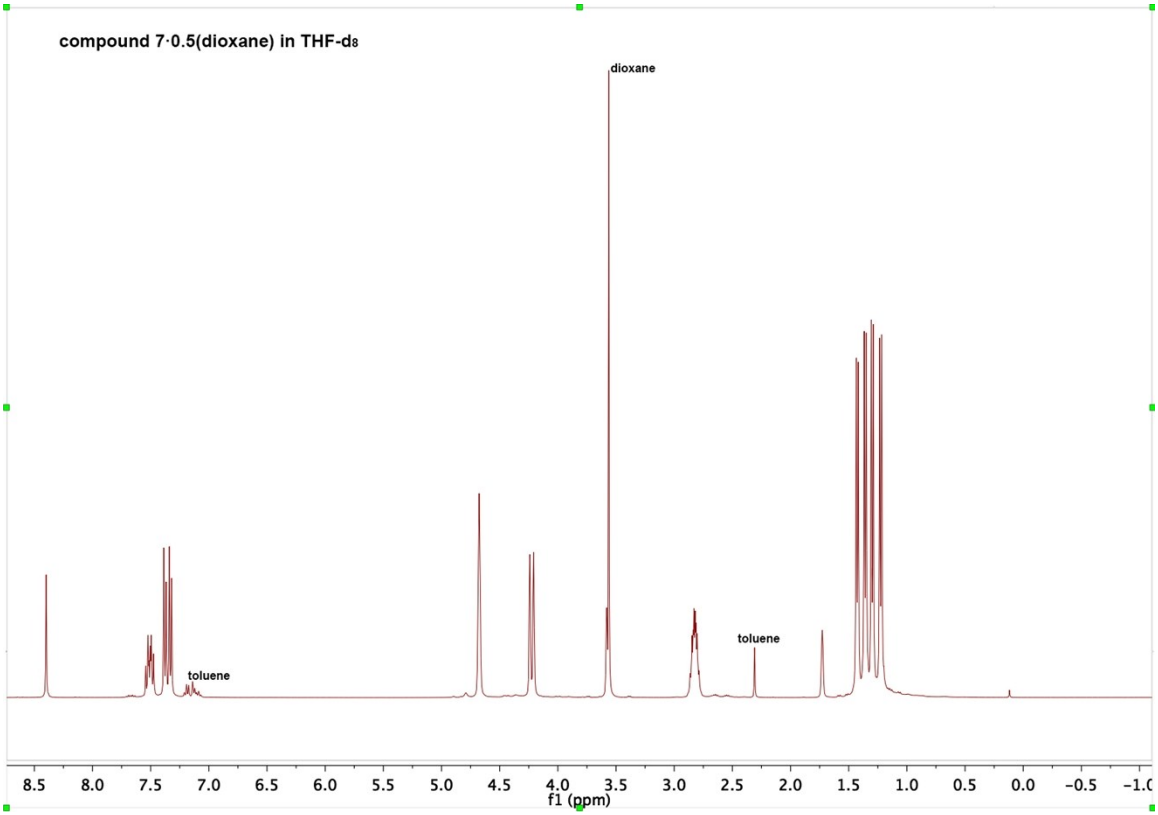
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


compound 7·0.5(dioxane) in THF-d8
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toluene
toluene
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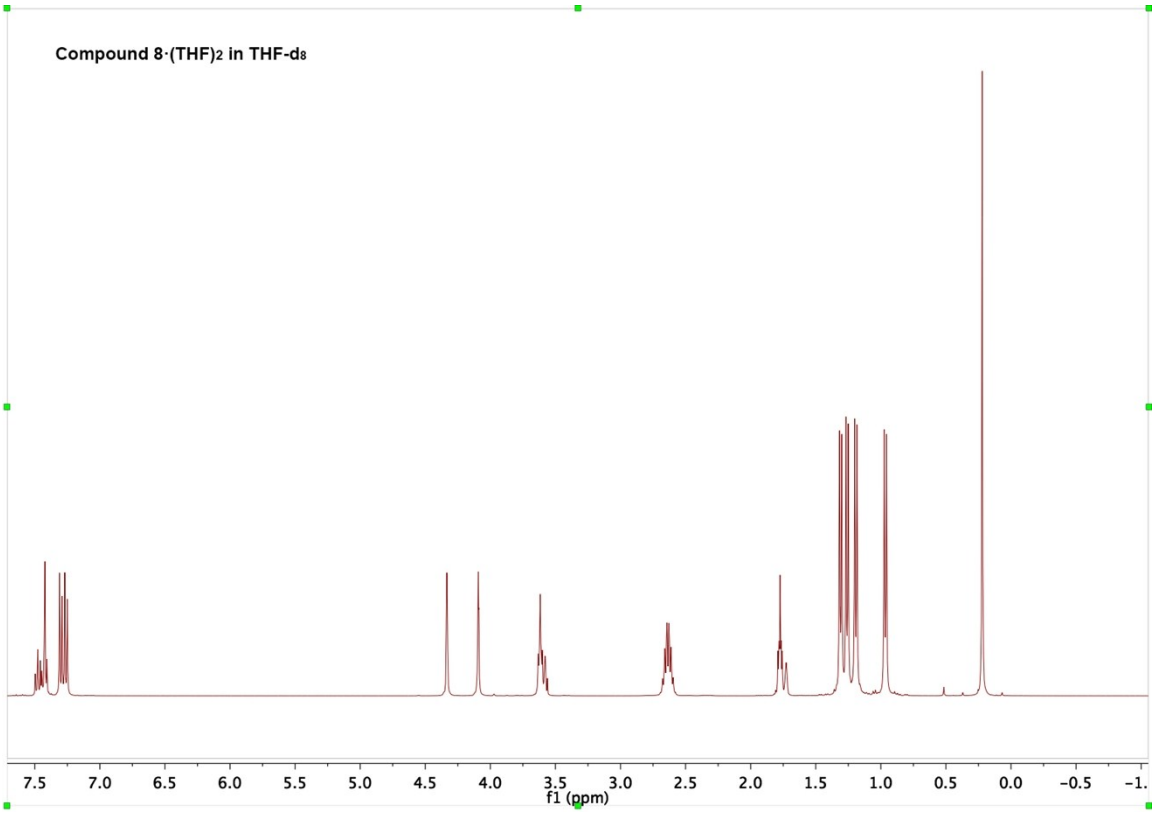
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)


Compound 8·(THF)2 in THF-d8
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6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
f1 (ppm)

SUPPORTING INFORMATIONS of X-RAY

Compound 4

Table S1. Sample and crystal data for **4**.

Identification code	**4**
Chemical formula	$C_{37}H_{43}ClFeN_2Si$
Formula weight	635.12 g/mol
Temperature	297(2) K
Wavelength	0.71073 Å
Crystal size	0.060 x 0.260 x 0.300 mm
Crystal system	monoclinic
Space group	P21/n (No. 14)
Unit cell dimensions	a = 18.7276(13) Å α = 90°
	b = 18.1214(12) Å β = 112.148(2)°
	c = 21.7095(15) Å γ = 90°
Volume	6823.9(8) Å3
Z	8
Density (calculated)	1.236 g/cm3
Absorption coefficient	0.583 mm-1
F(000)	2688

Table S2. Data collection and structure refinement for **4**.

Theta range for data collection	2.03 to 26.02°	
Index ranges	-22<=h<=23, -22<=k<=22, -26<=l<=26	
Reflections collected	224402	
Independent reflections	13426 [R(int) = 0.2246]	
Coverage of independent reflections	99.9%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.7454 and 0.6347	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	Σ w(Fo2 - Fc2)2	
Data / restraints / parameters	13426 / 165 / 813	
Goodness-of-fit on F2	1.049	
Δ/σmax	0.001	
Final R indices	7397 data; I>2σ(I)	R1 = 0.0766, wR2 = 0.1372
	all data	R1 = 0.1661, wR2 = 0.1667
Weighting scheme	w=1/[σ2(Fo2)+(0.0536P)2+9.1638P] where P=(Fo2+2Fc2)/3	
Largest diff. peak and hole	0.469 and -0.462 eÅ-3	
R.M.S. deviation from mean	0.063 eÅ-3	

Table S3. Bond lengths (Å) for **4**.

Si1-C3	1.842(4)	Si1-C28	1.862(4)
Si1-C33	1.866(4)	Si1-Cl1	2.0524(16)
Si1-Fe1	2.6154(13)	Si2-C40	1.849(4)
Si2-C70	1.854(5)	Si2-C65	1.859(5)
Si2-Cl2	2.052(2)	Si2-Fe2	2.6181(14)
Fe1-C28	1.991(4)	Fe1-C33	2.008(4)
Fe1-C37	2.014(5)	Fe1-C29	2.008(4)
Fe1-C32	2.012(4)	Fe1-C34	2.027(4)
Fe1-C35	2.070(5)	Fe1-C36	2.072(5)
Fe1-C30	2.083(5)	Fe1-C31	2.079(5)
Fe2-C65	1.992(5)	Fe2-C69	2.007(5)
Fe2-C70	2.014(5)	Fe2-C74	2.004(5)
Fe2-C66	2.005(5)	Fe2-C73	2.062(6)
Fe2-C71	2.017(6)	Fe2-C68	2.070(5)
Fe2-C72	2.063(6)	Fe2-C67	2.085(6)
N1-C1	1.360(5)	N1-C2	1.372(5)
N1-C16	1.445(5)	N2-C1	1.358(5)
N2-C3	1.401(5)	N2-C4	1.445(5)
N3-C38	1.374(5)	N3-C39	1.370(5)
N3-C53	1.432(5)	N4-C38	1.358(5)
N4-C40	1.405(5)	N4-C41	1.441(5)
C2-C3	1.343(5)	C4-C9	1.396(6)
C4-C5	1.386(6)	C5-C6	1.396(6)
C5-C13	1.509(6)	C6-C7	1.361(7)
C7-C8	1.346(7)	C8-C9	1.394(6)
C9-C10	1.508(7)	C10-C12	1.525(8)
C10-C11	1.516(7)	C13-C15	1.511(7)
C13-C14	1.536(7)	C16-C17	1.403(7)
C16-C21	1.398(7)	C17-C18	1.382(7)
C17-C25	1.499(7)	C18-C19	1.375(10)
C19-C20	1.360(11)	C20-C21	1.389(8)
C21-C22'	1.485(16)	C21-C22	1.526(16)
C22-C23	1.523(14)	C22-C24	1.565(18)
C22'-C23'	1.531(12)	C22'-C24'	1.557(13)
C25-C26	1.502(7)	C25-C27	1.505(8)
C28-C29	1.417(6)	C28-C32	1.428(6)
C29-C30	1.407(6)	C30-C31	1.398(6)
C31-C32	1.411(6)	C33-C37	1.426(6)
C33-C34	1.435(6)	C34-C35	1.414(6)
C35-C36	1.408(7)	C36-C37	1.419(7)

C39-C40	1.346(6)	C41-C42	1.386(6)
C41-C46	1.394(6)	C42-C43	1.394(6)
C42-C50	1.516(7)	C43-C44	1.352(7)
C44-C45	1.367(7)	C45-C46	1.386(6)
C46-C47	1.525(6)	C47-C49	1.520(8)
C47-C48	1.543(7)	C50-C52	1.519(8)
C50-C51	1.539(8)	C53-C58	1.386(6)
C53-C54	1.407(6)	C54-C55	1.382(7)
C54-C62'	1.51(2)	C54-C62	1.518(9)
C55-C56	1.379(8)	C56-C57	1.366(7)
C57-C58	1.384(6)	C58-C59	1.511(7)
C59-C61	1.509(8)	C59-C60	1.507(8)
C62-C63	1.514(10)	C62-C64	1.515(11)
C62'-C64'	1.527(14)	C62'-C63'	1.525(15)
C65-C66	1.415(7)	C65-C69	1.454(7)
C66-C67	1.419(7)	C67-C68	1.402(8)
C68-C69	1.412(7)	C70-C74	1.421(8)
C70-C71	1.439(7)	C71-C72	1.399(8)
C72-C73	1.390(9)	C73-C74	1.433(8)

Table S4. Bond angles (°) for **4**.

C3-Si1-C28	110.79(18)	C3-Si1-C33	117.06(19)
C28-Si1-C33	99.22(18)	C3-Si1-Cl1	111.21(13)
C28-Si1-Cl1	109.15(14)	C33-Si1-Cl1	108.64(15)
C3-Si1-Fe1	129.61(13)	C28-Si1-Fe1	49.35(13)
C33-Si1-Fe1	49.88(13)	Cl1-Si1-Fe1	119.03(6)
C40-Si2-C70	115.6(2)	C40-Si2-C65	112.5(2)
C70-Si2-C65	99.3(2)	C40-Si2-Cl2	111.50(15)
C70-Si2-Cl2	108.76(19)	C65-Si2-Cl2	108.28(17)
C40-Si2-Fe2	130.57(15)	C70-Si2-Fe2	50.04(15)
C65-Si2-Fe2	49.33(14)	Cl2-Si2-Fe2	117.86(7)
C28-Fe1-C33	90.48(17)	C28-Fe1-C37	110.05(18)
C33-Fe1-C37	41.53(17)	C28-Fe1-C29	41.51(16)
C33-Fe1-C29	112.26(17)	C37-Fe1-C29	102.79(19)
C28-Fe1-C32	41.80(17)	C33-Fe1-C32	109.99(18)
C37-Fe1-C32	146.60(18)	C29-Fe1-C32	68.44(19)
C28-Fe1-C34	111.71(18)	C33-Fe1-C34	41.67(18)
C37-Fe1-C34	68.7(2)	C29-Fe1-C34	149.23(18)
C32-Fe1-C34	101.8(2)	C28-Fe1-C35	151.89(19)
C33-Fe1-C35	69.21(19)	C37-Fe1-C35	67.7(2)
C29-Fe1-C35	164.7(2)	C32-Fe1-C35	126.2(2)
C34-Fe1-C35	40.37(18)	C28-Fe1-C36	150.1(2)
C33-Fe1-C36	69.55(19)	C37-Fe1-C36	40.62(19)
C29-Fe1-C36	125.4(2)	C32-Fe1-C36	165.8(2)
C34-Fe1-C36	68.0(2)	C35-Fe1-C36	39.7(2)
C28-Fe1-C30	69.22(17)	C33-Fe1-C30	152.29(18)
C37-Fe1-C30	127.1(2)	C29-Fe1-C30	40.20(17)
C32-Fe1-C30	67.51(19)	C34-Fe1-C30	163.7(2)
C35-Fe1-C30	135.89(19)	C36-Fe1-C30	119.9(2)
C28-Fe1-C31	69.20(17)	C33-Fe1-C31	149.85(19)
C37-Fe1-C31	166.3(2)	C29-Fe1-C31	67.15(19)
C32-Fe1-C31	40.31(17)	C34-Fe1-C31	124.8(2)
C35-Fe1-C31	119.8(2)	C36-Fe1-C31	137.2(2)
C30-Fe1-C31	39.26(18)	C28-Fe1-Si1	45.20(12)
C33-Fe1-Si1	45.29(12)	C37-Fe1-Si1	73.78(13)
C29-Fe1-Si1	75.20(12)	C32-Fe1-Si1	72.82(13)
C34-Fe1-Si1	74.03(13)	C35-Fe1-Si1	111.73(14)
C36-Fe1-Si1	111.94(15)	C30-Fe1-Si1	112.37(13)
C31-Fe1-Si1	110.86(13)	C65-Fe2-C69	42.6(2)
C65-Fe2-C70	89.90(19)	C69-Fe2-C70	110.7(2)

C65-Fe2-C74	109.5(2)	C69-Fe2-C74	147.3(2)
C70-Fe2-C74	41.4(2)	C65-Fe2-C66	41.46(19)
C69-Fe2-C66	68.8(2)	C70-Fe2-C66	111.3(2)
C74-Fe2-C66	102.0(2)	C65-Fe2-C73	150.5(3)
C69-Fe2-C73	164.6(3)	C70-Fe2-C73	69.5(2)
C74-Fe2-C73	41.2(2)	C66-Fe2-C73	126.1(3)
C65-Fe2-C71	111.3(2)	C69-Fe2-C71	102.1(3)
C70-Fe2-C71	41.8(2)	C74-Fe2-C71	68.8(3)
C66-Fe2-C71	148.5(2)	C73-Fe2-C71	67.4(3)
C65-Fe2-C68	70.3(2)	C69-Fe2-C68	40.5(2)
C70-Fe2-C68	150.8(2)	C74-Fe2-C68	165.5(3)
C66-Fe2-C68	67.8(2)	C73-Fe2-C68	136.2(2)
C71-Fe2-C68	125.4(3)	C65-Fe2-C72	151.1(3)
C69-Fe2-C72	125.5(3)	C70-Fe2-C72	69.4(2)
C74-Fe2-C72	68.2(3)	C66-Fe2-C72	165.2(3)
C73-Fe2-C72	39.4(3)	C71-Fe2-C72	40.1(2)
C68-Fe2-C72	119.3(3)	C65-Fe2-C67	69.7(2)
C69-Fe2-C67	67.6(2)	C70-Fe2-C67	151.5(2)
C74-Fe2-C67	126.2(3)	C66-Fe2-C67	40.5(2)
C73-Fe2-C67	119.9(3)	C71-Fe2-C67	164.5(3)
C68-Fe2-C67	39.4(2)	C72-Fe2-C67	136.2(3)
C65-Fe2-Si2	45.07(13)	C69-Fe2-Si2	73.68(15)
C70-Fe2-Si2	44.86(15)	C74-Fe2-Si2	73.63(17)
C66-Fe2-Si2	74.97(15)	C73-Fe2-Si2	111.94(19)
C71-Fe2-Si2	73.50(16)	C68-Fe2-Si2	111.84(16)
C72-Fe2-Si2	111.2(2)	C67-Fe2-Si2	112.62(16)
C1-N1-C2	112.3(3)	C1-N1-C16	125.1(3)
C2-N1-C16	122.5(3)	C1-N2-C3	113.5(3)
C1-N2-C4	122.6(3)	C3-N2-C4	123.9(3)
C38-N3-C39	112.4(4)	C38-N3-C53	124.7(4)
C39-N3-C53	122.9(3)	C38-N4-C40	113.6(3)
C38-N4-C41	120.8(3)	C40-N4-C41	125.5(4)
N2-C1-N1	101.9(3)	C3-C2-N1	108.2(3)
C2-C3-N2	104.0(3)	C2-C3-Si1	124.0(3)
N2-C3-Si1	132.0(3)	C9-C4-C5	122.7(4)
C9-C4-N2	118.2(4)	C5-C4-N2	119.1(4)
C4-C5-C6	117.0(4)	C4-C5-C13	121.9(4)
C6-C5-C13	121.1(4)	C7-C6-C5	121.1(5)
C6-C7-C8	121.0(5)	C7-C8-C9	121.5(5)
C4-C9-C8	116.8(4)	C4-C9-C10	122.8(4)
C8-C9-C10	120.4(4)	C9-C10-C12	109.8(5)
C9-C10-C11	114.1(5)	C12-C10-C11	111.1(5)

C15-C13-C5	111.9(4)	C15-C13-C14	110.6(4)
C5-C13-C14	113.2(5)	C17-C16-C21	124.1(5)
C17-C16-N1	118.1(4)	C21-C16-N1	117.7(5)
C16-C17-C18	116.7(6)	C16-C17-C25	122.3(4)
C18-C17-C25	121.0(6)	C19-C18-C17	120.3(7)
C20-C19-C18	121.8(6)	C19-C20-C21	121.3(7)
C16-C21-C20	115.7(6)	C16-C21-C22'	126.8(16)
C20-C21-C22'	117.4(17)	C16-C21-C22	120.5(13)
C20-C21-C22	123.8(14)	C21-C22-C23	103(2)
C21-C22-C24	106(3)	C23-C22-C24	107.7(17)
C21-C22'-C23'	125(3)	C21-C22'-C24'	116(2)
C23'-C22'-C24'	107.3(15)	C17-C25-C26	110.3(5)
C17-C25-C27	113.5(5)	C26-C25-C27	109.6(6)
C29-C28-C32	105.2(4)	C29-C28-Si1	121.0(3)
C32-C28-Si1	115.3(3)	C29-C28-Fe1	69.9(2)
C32-C28-Fe1	69.9(2)	Si1-C28-Fe1	85.45(16)
C30-C29-C28	110.1(4)	C30-C29-Fe1	72.8(3)
C28-C29-Fe1	68.6(2)	C29-C30-C31	107.4(4)
C29-C30-Fe1	67.0(2)	C31-C30-Fe1	70.2(3)
C30-C31-C32	108.2(4)	C30-C31-Fe1	70.5(3)
C32-C31-Fe1	67.3(2)	C28-C32-C31	109.0(4)
C28-C32-Fe1	68.3(2)	C31-C32-Fe1	72.4(3)
C37-C33-C34	105.6(4)	C37-C33-Si1	117.3(3)
C34-C33-Si1	117.7(3)	C37-C33-Fe1	69.4(2)
C34-C33-Fe1	69.9(2)	Si1-C33-Fe1	84.83(17)
C33-C34-C35	108.8(4)	C33-C34-Fe1	68.5(2)
C35-C34-Fe1	71.5(3)	C36-C35-C34	108.7(5)
C36-C35-Fe1	70.2(3)	C34-C35-Fe1	68.2(3)
C35-C36-C37	107.1(4)	C35-C36-Fe1	70.1(3)
C37-C36-Fe1	67.5(3)	C33-C37-C36	109.8(4)
C33-C37-Fe1	69.0(2)	C36-C37-Fe1	71.9(3)
N4-C38-N3	101.6(3)	C40-C39-N3	108.1(4)
C39-C40-N4	104.2(4)	C39-C40-Si2	124.9(3)
N4-C40-Si2	130.9(3)	C42-C41-C46	122.8(4)
C42-C41-N4	118.2(4)	C46-C41-N4	119.0(4)
C41-C42-C43	117.2(5)	C41-C42-C50	122.4(4)
C43-C42-C50	120.4(4)	C44-C43-C42	121.1(5)
C45-C44-C43	120.9(5)	C44-C45-C46	121.2(5)
C41-C46-C45	116.9(4)	C41-C46-C47	121.5(4)
C45-C46-C47	121.4(4)	C46-C47-C49	109.2(5)
C46-C47-C48	113.2(5)	C49-C47-C48	110.9(5)

C42-C50-C52	112.8(5)	C42-C50-C51	109.8(5)
C52-C50-C51	111.0(5)	C58-C53-C54	122.9(4)
C58-C53-N3	118.2(4)	C54-C53-N3	118.9(4)
C55-C54-C53	116.2(5)	C55-C54-C62'	123.1(15)
C53-C54-C62'	120.3(15)	C55-C54-C62	121.6(6)
C53-C54-C62	122.0(6)	C54-C55-C56	121.8(5)
C57-C56-C55	120.3(5)	C56-C57-C58	120.8(5)
C53-C58-C57	117.8(5)	C53-C58-C59	121.1(4)
C57-C58-C59	120.9(4)	C58-C59-C61	113.1(5)
C58-C59-C60	110.2(5)	C61-C59-C60	111.7(6)
C54-C62-C63	111.3(7)	C54-C62-C64	114.9(9)
C63-C62-C64	109.1(8)	C64'-C62'-C54	104(2)
C64'-C62'-C63'	108(2)	C54-C62'-C63'	112(3)
C66-C65-C69	104.4(4)	C66-C65-Si2	120.8(4)
C69-C65-Si2	115.9(4)	C66-C65-Fe2	69.8(3)
C69-C65-Fe2	69.2(3)	Si2-C65-Fe2	85.60(19)
C65-C66-C67	110.7(5)	C65-C66-Fe2	68.8(3)
C67-C66-Fe2	72.8(3)	C68-C67-C66	107.4(5)
C68-C67-Fe2	69.7(3)	C66-C67-Fe2	66.7(3)
C69-C68-C67	108.1(5)	C69-C68-Fe2	67.3(3)
C67-C68-Fe2	70.9(3)	C68-C69-C65	109.4(5)
C68-C69-Fe2	72.2(3)	C65-C69-Fe2	68.1(3)
C74-C70-C71	105.1(5)	C74-C70-Si2	117.8(4)
C71-C70-Si2	116.9(4)	C74-C70-Fe2	68.9(3)
C71-C70-Fe2	69.2(3)	Si2-C70-Fe2	85.1(2)
C72-C71-C70	109.7(6)	C72-C71-Fe2	71.7(4)
C70-C71-Fe2	69.0(3)	C73-C72-C71	108.4(6)
C73-C72-Fe2	70.2(4)	C71-C72-Fe2	68.2(3)
C72-C73-C74	107.8(6)	C72-C73-Fe2	70.4(4)
C74-C73-Fe2	67.2(3)	C70-C74-C73	109.0(6)
C70-C74-Fe2	69.7(3)	C73-C74-Fe2	71.5(3)

Compound 5·THF

Table S5. Sample and crystal data for **5·THF**

Identification code	**5·THF**	
Chemical formula	$C_{33}H_{49}ClN_2OSi$	
Formula weight	553.28 g/mol	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.120 x 0.250 x 0.350 mm	
Crystal system	triclinic	
Space group	P-1 (No. 2)	
Unit cell dimensions	a = 8.935(3) Å	α = 69.021(10)°
	b = 12.508(4) Å	β = 81.901(11)°
	c = 16.628(5) Å	γ = 81.762(11)°
Volume	1709.3(10) $Å^3$	
Z	2	
Density (calculated)	1.075 g/cm^3	
Absorption coefficient	0.172 mm^{-1}	
F(000)	600	

Table S6. Data collection and structure refinement for **5·THF**

Theta range for data collection	2.61 to 26.02°	
Index ranges	-10<=h<=11, -15<=k<=15, -20<=l<=20	
Reflections collected	50407	
Independent reflections	6716 [R(int) = 0.0789]	
Coverage of independent reflections	99.9%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.7454 and 0.6370	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6716 / 316 / 424	
Goodness-of-fit on F^2	1.052	
Final R indices	4485 data; I>2σ(I)	R1 = 0.0636, wR2 = 0.1594
	all data	R1 = 0.1017, wR2 = 0.1803
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0839P)^2+0.6074P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.361 and -0.507 eÅ^{-3}	
R.M.S. deviation from mean	0.041 eÅ^{-3}	

Table S7. Bond lengths (Å) for **5·THF**

Si1-C33	1.891(8)	Si1-C3	1.859(2)
Si1-C28	1.877(3)	Si1-C33'	1.886(8)
Si1-Cl1'	2.042(3)	Si1-Cl1	2.046(4)
N1-C1	1.370(3)	N1-C2	1.372(3)
N1-C16	1.445(3)	N2-C1	1.358(3)
N2-C3	1.410(3)	N2-C4	1.451(3)
C2-C3	1.344(3)	C4-C9	1.395(3)
C4-C5	1.402(3)	C5-C6	1.394(4)
C5-C13	1.508(4)	C6-C7	1.358(4)
C7-C8	1.372(5)	C8-C9	1.395(4)
C9-C10	1.515(4)	C10-C12	1.520(5)
C10-C11	1.542(4)	C13-C15	1.524(4)
C13-C14	1.539(4)	C16-C21	1.390(3)
C16-C17	1.403(4)	C17-C18	1.395(3)
C17-C25	1.516(3)	C18-C19	1.361(4)
C19-C20	1.367(5)	C20-C21	1.399(4)
C21-C22	1.522(7)	C21-C22'	1.519(19)
C22-C24	1.557(12)	C22-C23	1.516(9)
C22'-C24'	1.54(2)	C22'-C23'	1.545(19)
C25-C27	1.514(4)	C25-C26	1.515(4)
O1-C29	1.470(11)	O1-C32	1.513(11)
C29-C30	1.326(14)	C30-C31	1.583(17)
C31-C32	1.261(14)	O1'-C29'	1.467(15)
O1'-C32'	1.580(14)	C29'-C30'	1.318(14)
C30'-C31'	1.564(16)	C31'-C32'	1.322(15)

Table S8. Bond angles (°) for **5·THF**

C33-Si1-C3	114.3(3)	C33-Si1-C28	114.0(3)
C3-Si1-C28	106.94(12)	C3-Si1-C33'	116.9(2)
C28-Si1-C33'	114.2(3)	C3-Si1-Cl1'	108.17(10)
C28-Si1-Cl1'	109.25(16)	C3-Si1-Cl1	109.19(11)
C28-Si1-Cl1	105.87(16)	C1-N1-C2	112.51(17)
C1-N1-C16	123.93(17)	C2-N1-C16	123.50(17)
C1-N2-C3	113.94(17)	C1-N2-C4	122.84(17)
C3-N2-C4	123.21(17)	N2-C1-N1	101.46(17)
C3-C2-N1	108.41(18)	C2-C3-N2	103.68(18)
C2-C3-Si1	125.04(16)	N2-C3-Si1	131.28(16)
C9-C4-C5	122.9(2)	C9-C4-N2	118.91(19)
C5-C4-N2	118.2(2)	C6-C5-C4	116.5(2)
C6-C5-C13	121.3(2)	C4-C5-C13	122.0(2)
C7-C6-C5	121.5(3)	C8-C7-C6	121.1(3)
C7-C8-C9	120.6(3)	C8-C9-C4	117.2(2)
C8-C9-C10	120.7(2)	C4-C9-C10	121.9(2)
C9-C10-C12	109.7(3)	C9-C10-C11	112.8(3)
C12-C10-C11	110.8(3)	C5-C13-C15	109.4(2)
C5-C13-C14	113.4(2)	C15-C13-C14	110.6(2)
C21-C16-C17	123.2(2)	C21-C16-N1	118.2(2)
C17-C16-N1	118.6(2)	C18-C17-C16	116.6(2)
C18-C17-C25	121.2(2)	C16-C17-C25	122.1(2)
C19-C18-C17	121.4(3)	C18-C19-C20	120.8(3)
C19-C20-C21	121.3(3)	C16-C21-C20	116.7(3)
C16-C21-C22	120.4(6)	C20-C21-C22	122.8(6)
C16-C21-C22'	128(2)	C20-C21-C22'	115(2)
C21-C22-C24	109.5(10)	C21-C22-C23	107.8(7)
C24-C22-C23	109.0(8)	C24'-C22'-C21	118(3)
C24'-C22'-C23'	109(3)	C21-C22'-C23'	126(3)
C27-C25-C17	113.4(2)	C27-C25-C26	112.0(3)
C17-C25-C26	109.5(2)	C29-O1-C32	94.0(11)
C30-C29-O1	106.1(13)	C29-C30-C31	97.6(9)
C32-C31-C30	102.7(9)	C31-C32-O1	113.8(12)
C29'-O1'-C32'	88.3(13)	C30'-C29'-O1'	107.5(14)
C29'-C30'-C31'	102.7(9)	C32'-C31'-C30'	101.5(9)
C31'-C32'-O1'	101.9(14)		

Compound 6

Table S9. Sample and crystal data for **6**.

Identification code	**6**
Chemical formula	$C_{68}H_{90}FeN_4Si_2$
Formula weight	1075.46 g/mol
Temperature	297(2) K
Wavelength	0.71073 Å
Crystal size	0.050 x 0.180 x 0.240 mm
Crystal system	monoclinic
Space group	C2/c (No. 15)
Unit cell dimensions	a = 28.165(15) Å α = 90°
	b = 10.265(5) Å β = 99.308(7)°
	c = 22.785(12) Å γ = 90°
Volume	6500(6) $Å^3$
Z	4
Density (calculated)	1.099 g/cm^3
Absorption coefficient	0.309 mm^{-1}
F(000)	2320

Table S10. Data collection and structure refinement for **6**.

Theta range for data collection	2.51 to 25.99°	
Index ranges	-34<=h<=34, -12<=k<=12, -28<=l<=28	
Reflections collected	99660	
Independent reflections	6375 [R(int) = 0.1769]	
Coverage of independent reflections	99.8%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.7454 and 0.6168	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	6375 / 254 / 464	
Goodness-of-fit on F^2	1.047	
Δ/σ_{max}	0.001	
Final R indices	3388 data; I>2σ(I)	R1 = 0.0794, wR2 = 0.1474
	all data	R1 = 0.1693, wR2 = 0.1786
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0616P)^2+8.7337P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.349 and -0.389 eÅ^{-3}	
R.M.S. deviation from mean	0.042 eÅ^{-3}	

Table S11. Bond lengths (Å) for **6**.

Si1-C28'	1.822(8)	Si1-C33'	1.816(11)
Si1-C3	1.879(3)	Si1-C34	1.866(6)
Si1-C34'	1.919(9)	Si1-C28	1.869(10)
Si1-C33	1.916(7)	Fe1-C29	1.869(9)
Fe1-C29	1.869(9)	Fe1-C30	1.948(17)
Fe1-C30	1.948(17)	Fe1-C28	2.062(13)
Fe1-C28	2.062(13)	Fe1-C32	2.276(11)
Fe1-C32	2.276(11)	Fe1-C31	2.358(10)
Fe1-C31	2.358(10)	C28-C32	1.440(12)
C28-C29	1.490(12)	C29-C30	1.361(18)
C30-C31	1.45(2)	C31-C32	1.405(13)
Fe1'-C31'	1.94(2)	Fe1'-C29'	1.959(10)
Fe1'-C30'	2.003(13)	Fe1'-C28'	2.074(11)
Fe1'-C28'	2.184(15)	Fe1'-C32'	2.200(12)
Fe1'-C31'	2.303(15)	Fe1'-C30'	2.438(15)
C28'-C32'	1.379(11)	C28'-C29'	1.398(11)
C28'-Fe1'	2.184(15)	C29'-C30'	1.377(14)
C30'-C31'	1.48(2)	C30'-Fe1'	2.438(15)
C31'-C32'	1.423(16)	C31'-Fe1'	1.94(2)
N1-C1	1.361(4)	N1-C2	1.371(4)
N1-C16	1.445(4)	N2-C1	1.366(4)
N2-C3	1.400(4)	N2-C4	1.448(4)
C2-C3	1.349(4)	C4-C9	1.389(4)
C4-C5	1.396(4)	C5-C6	1.394(4)
C5-C13	1.516(5)	C6-C7	1.370(5)
C7-C8	1.367(5)	C8-C9	1.388(5)
C9-C10	1.517(5)	C10-C11	1.523(6)
C10-C12	1.542(6)	C13-C15	1.526(5)
C13-C14	1.521(5)	C16-C17	1.389(5)
C16-C21	1.392(5)	C17-C18	1.391(5)
C17-C25	1.519(12)	C17-C25'	1.518(17)
C18-C19	1.364(6)	C19-C20	1.369(6)
C20-C21	1.400(5)	C21-C22	1.511(5)
C21-C22'	1.53(2)	C22-C23	1.516(7)
C22-C24	1.522(8)	C22'-C24'	1.52(2)
C22'-C23'	1.51(2)	C25-C27	1.529(11)
C25-C26	1.539(10)	C25'-C27'	1.514(14)
C25'-C26'	1.526(16)		

Table S12. Bond angles (°) for **6**.

C28'-Si1-C33'	124.6(6)	C28'-Si1-C3	112.4(4)
C33'-Si1-C3	113.1(5)	C3-Si1-C34	105.9(3)
C28'-Si1-C34'	84.5(6)	C33'-Si1-C34'	114.2(7)
C3-Si1-C34'	102.2(4)	C3-Si1-C28	111.9(5)
C34-Si1-C28	127.2(6)	C3-Si1-C33	107.9(3)
C34-Si1-C33	106.0(5)	C28-Si1-C33	96.0(5)
C29-Fe1-C30	138.3(6)	C29-Fe1-C30	41.7(6)
C29-Fe1-C30	41.7(6)	C29-Fe1-C30	138.3(6)
C29-Fe1-C28	135.8(4)	C29-Fe1-C28	44.2(4)
C30-Fe1-C28	72.2(6)	C30-Fe1-C28	107.8(6)
C29-Fe1-C28	44.2(4)	C29-Fe1-C28	135.8(4)
C30-Fe1-C28	107.8(6)	C30-Fe1-C28	72.2(6)
C29-Fe1-C32	64.9(4)	C29-Fe1-C32	115.1(4)
C30-Fe1-C32	115.4(6)	C30-Fe1-C32	64.6(6)
C28-Fe1-C32	141.6(3)	C28-Fe1-C32	38.4(3)
C29-Fe1-C32	115.1(4)	C29-Fe1-C32	64.9(4)
C30-Fe1-C32	64.6(6)	C30-Fe1-C32	115.4(6)
C28-Fe1-C32	38.4(3)	C28-Fe1-C32	141.6(3)
C32-Fe1-C32	180.0(3)	C29-Fe1-C31	116.4(5)
C29-Fe1-C31	63.6(5)	C30-Fe1-C31	37.9(7)
C30-Fe1-C31	142.0(7)	C28-Fe1-C31	64.5(4)
C28-Fe1-C31	115.5(4)	C32-Fe1-C31	144.8(3)
C32-Fe1-C31	35.2(3)	C29-Fe1-C31	63.6(5)
C29-Fe1-C31	116.4(5)	C30-Fe1-C31	142.1(7)
C30-Fe1-C31	38.0(7)	C28-Fe1-C31	115.5(4)
C28-Fe1-C31	64.5(4)	C32-Fe1-C31	35.2(3)
C32-Fe1-C31	144.8(3)	C32-C28-C29	100.4(9)
C32-C28-Si1	125.1(8)	C29-C28-Si1	134.3(9)
C32-C28-Fe1	78.9(7)	C29-C28-Fe1	61.0(5)
Si1-C28-Fe1	120.1(8)	C30-C29-C28	112.1(12)
C30-C29-Fe1	72.3(9)	C28-C29-Fe1	74.8(7)
C29-C30-C31	107.2(14)	C29-C30-Fe1	66.0(7)
C31-C30-Fe1	86.5(10)	C32-C31-C30	105.5(10)
C32-C31-Fe1	69.2(6)	C30-C31-Fe1	55.6(8)
C31-C32-C28	113.0(10)	C31-C32-Fe1	75.6(6)
C28-C32-Fe1	62.7(6)	C32'-Fe1'-C31'	46.1(7)
C32'-Fe1'-C29'	143.8(7)	C31'-Fe1'-C29'	134.2(8)
Fe1'-Fe1'-C30'	96.8(10)	C32'-Fe1'-C30'	131.3(8)

C31'-Fe1'-C30'	171.1(9)	C29'-Fe1'-C30'	40.7(4)
Fe1'-Fe1'-C28'	79.3(9)	C32'-Fe1'-C28'	161.8(8)
C31'-Fe1'-C28'	116.3(8)	C29'-Fe1'-C28'	40.5(4)
C30'-Fe1'-C28'	65.1(5)	C32'-Fe1'-C28'	39.1(5)
C31'-Fe1'-C28'	66.3(7)	C29'-Fe1'-C28'	157.8(7)
C30'-Fe1'-C28'	117.6(6)	C28'-Fe1'-C28'	148.2(4)
C32'-Fe1'-C32'	148.8(5)	C31'-Fe1'-C32'	121.7(8)
C29'-Fe1'-C32'	67.2(5)	C30'-Fe1'-C32'	65.2(5)
C28'-Fe1'-C32'	37.5(3)	C28'-Fe1'-C32'	112.1(5)
C32'-Fe1'-C31'	134.7(8)	C31'-Fe1'-C31'	149.4(5)
C29'-Fe1'-C31'	66.7(7)	C30'-Fe1'-C31'	39.5(7)
C28'-Fe1'-C31'	62.1(5)	C28'-Fe1'-C31'	98.9(7)
C32'-Fe1'-C31'	36.7(5)	C32'-Fe1'-C30'	64.5(6)
C31'-Fe1'-C30'	37.4(8)	C29'-Fe1'-C30'	143.6(6)
C30'-Fe1'-C30'	151.5(4)	C28'-Fe1'-C30'	104.9(6)
C28'-Fe1'-C30'	56.3(4)	C32'-Fe1'-C30'	90.4(5)
C31'-Fe1'-C30'	112.0(6)	C32'-C28'-C29'	112.5(9)
C32'-C28'-Si1	127.2(8)	C29'-C28'-Si1	120.1(8)
C32'-C28'-Fe1'	76.2(6)	C29'-C28'-Fe1'	65.4(5)
Si1-C28'-Fe1'	120.9(7)	C32'-C28'-Fe1'	47.3(6)
C29'-C28'-Fe1'	92.1(7)	Si1-C28'-Fe1'	122.8(7)
C30'-C29'-C28'	104.4(10)	C30'-C29'-Fe1'	71.4(6)
C28'-C29'-Fe1'	74.2(6)	C29'-C30'-C31'	111.4(11)
C29'-C30'-Fe1'	68.0(5)	C31'-C30'-Fe1'	81.3(8)
C29'-C30'-Fe1'	82.4(6)	C31'-C30'-Fe1'	52.7(8)
C32'-C31'-C30'	102.8(12)	C32'-C31'-Fe1'	54.5(8)
C30'-C31'-Fe1'	89.8(10)	C32'-C31'-Fe1'	67.7(7)
C30'-C31'-Fe1'	59.3(8)	C28'-C32'-C31'	107.9(13)
C28'-C32'-Fe1'	93.7(9)	C31'-C32'-Fe1'	79.4(11)
C28'-C32'-Fe1'	66.3(6)	C31'-C32'-Fe1'	75.6(8)
C1-N1-C2	112.4(2)	C1-N1-C16	122.9(3)
C2-N1-C16	124.6(3)	C1-N2-C3	114.0(2)
C1-N2-C4	122.5(2)	C3-N2-C4	123.4(2)
N1-C1-N2	101.5(2)	C3-C2-N1	108.7(3)
C2-C3-N2	103.4(3)	C2-C3-Si1	126.9(3)
N2-C3-Si1	129.5(2)	C9-C4-C5	123.0(3)
C9-C4-N2	119.2(3)	C5-C4-N2	117.9(3)
C4-C5-C6	116.7(3)	C4-C5-C13	122.1(3)
C6-C5-C13	121.2(3)	C7-C6-C5	121.3(3)
C6-C7-C8	120.6(3)	C7-C8-C9	121.1(4)
C4-C9-C8	117.4(3)	C4-C9-C10	121.8(3)

C8-C9-C10	120.7(3)	C9-C10-C11	109.7(4)
C9-C10-C12	113.9(4)	C11-C10-C12	109.5(4)
C5-C13-C15	110.8(3)	C5-C13-C14	114.5(3)
C15-C13-C14	109.8(3)	C17-C16-C21	123.3(3)
C17-C16-N1	118.6(3)	C21-C16-N1	118.0(3)
C16-C17-C18	117.0(4)	C16-C17-C25	123.2(7)
C18-C17-C25	119.8(7)	C16-C17-C25'	123.5(10)
C18-C17-C25'	119.5(10)	C19-C18-C17	121.0(4)
C18-C19-C20	121.3(4)	C19-C20-C21	120.5(4)
C16-C21-C20	116.9(4)	C16-C21-C22	122.4(3)
C20-C21-C22	120.7(4)	C16-C21-C22'	121.(8)
C20-C21-C22'	117.(7)	C21-C22-C23	112.8(4)
C21-C22-C24	110.9(4)	C23-C22-C24	110.6(5)
C24'-C22'-C23'	111.(3)	C24'-C22'-C21	118.(10)
C23'-C22'-C21	124.(10)	C17-C25-C27	112.8(15)
C17-C25-C26	112.3(12)	C27-C25-C26	109.0(10)
C27'-C25'-C17	109.3(18)	C27'-C25'-C26'	114.3(16)
C17-C25'-C26'	110.8(19)		

Compound 7·0.5(dioxane)

Table S13. Sample and crystal data for **7·0.5(dioxane)**.

Identification code	**7·0.5(dioxane)**
Chemical formula	$C_{39}H_{47}Cl_3FeGeN_2OSi$
Formula weight	822.66 g/mol
Temperature	296(2) K
Wavelength	0.71073 Å
Crystal size	0.050 x 0.260 x 0.280 mm
Crystal system	triclinic
Space group	P-1(No. 2)
Unit cell dimensions	a = 10.5862(5) Å α = 85.038(2)°
	b = 10.6734(5) Å β = 84.783(2)°
	c = 18.5264(10) Å γ = 74.549(2)°
Volume	2005.07(17) $Å^3$
Z	2
Density (calculated)	1.363 g/cm^3
Absorption coefficient	1.373 mm^{-1}
F(000)	852

Table S14. Data collection and structure refinement for **7·0.5(dioxane)**.

Theta range for data collection	2.21 to 26.48°	
Reflections collected	8265	
Coverage of independent reflections	99.6%	
Max. and min. transmission	0.7454 and 0.4354	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	8265 / 2 / 434	
Goodness-of-fit on F^2	1.073	
Δ/σ_{max}	0.001	
Final R indices	6140 data; I>2σ(I)	R1 = 0.0707, wR2 = 0.1598
	all data	R1 = 0.1034, wR2 = 0.1770
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0858P)^2+1.9342P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.748 and -0.503 eÅ^{-3}	
R.M.S. deviation from mean	0.094 eÅ^{-3}	

Table S15. Bond lengths (Å) for **7·0.5(dioxane)**.

Si1-C33	1.854(6)	Si1-C28	1.858(6)
Si1-C3	1.867(4)	Si1-Cl1	2.039(2)
Si1-Fe1	2.6035(15)	Ge1-C1	2.132(5)
Ge1-Cl2	2.2618(19)	Ge1-Cl3	2.267(2)
Fe1-C28	1.999(6)	Fe1-C33	2.007(6)
Fe1-C37	2.009(6)	Fe1-C34	2.016(6)
Fe1-C29	2.022(6)	Fe1-C32	2.027(6)
Fe1-C35	2.046(6)	Fe1-C31	2.057(7)
Fe1-C30	2.060(6)	Fe1-C36	2.066(7)
N1-C1	1.339(6)	N1-C2	1.366(6)
N1-C16	1.465(6)	N2-C1	1.347(6)
N2-C3	1.412(6)	N2-C4	1.453(6)
C2-C3	1.342(7)	C4-C9	1.380(8)
C4-C5	1.400(8)	C5-C6	1.390(8)
C5-C13	1.500(9)	C6-C7	1.341(10)
C7-C8	1.366(10)	C8-C9	1.399(9)
C9-C10	1.506(9)	C10-C11	1.536(11)
C10-C12	1.526(10)	C13-C15	1.537(10)
C13-C14	1.510(11)	C16-C21	1.396(10)
C16-C17	1.390(10)	C17-C18	1.404(10)
C17-C25	1.507(11)	C18-C19	1.364(13)
C19-C20	1.373(13)	C20-C21	1.387(9)
C21-C22	1.527(10)	C22-C23	1.498(13)
C22-C24	1.547(12)	C25-C26	1.552(12)
C25-C27	1.526(11)	C28-C32	1.447(8)
C28-C29	1.441(9)	C29-C30	1.405(9)
C30-C31	1.394(10)	C31-C32	1.422(9)
C33-C37	1.447(9)	C33-C34	1.460(8)
C34-C35	1.414(10)	C35-C36	1.395(10)
C36-C37	1.410(9)	O1-C38	1.415(10)
O1-C39	1.469(13)	C38-C39	1.471(15)
C39-O1	1.469(13)		

Table S16. Bond angles (°) for **7·0.5(dioxane)**.

C33-Si1-C28	100.0(2)	C33-Si1-C3	111.6(3)
C28-Si1-C3	113.3(2)	C33-Si1-Cl1	110.1(2)
C28-Si1-Cl1	107.9(2)	C3-Si1-Cl1	113.12(17)
C33-Si1-Fe1	50.13(18)	C28-Si1-Fe1	49.88(17)
C3-Si1-Fe1	126.33(16)	Cl1-Si1-Fe1	120.55(7)
C1-Ge1-Cl2	92.88(14)	C1-Ge1-Cl3	96.49(15)
Cl2-Ge1-Cl3	97.85(8)	C28-Fe1-C33	90.5(2)
C28-Fe1-C37	111.5(2)	C33-Fe1-C37	42.3(3)
C28-Fe1-C34	111.4(3)	C33-Fe1-C34	42.6(2)
C37-Fe1-C34	69.6(3)	C28-Fe1-C29	42.0(3)
C33-Fe1-C29	112.6(2)	C37-Fe1-C29	103.8(3)
C34-Fe1-C29	149.9(3)	C28-Fe1-C32	42.1(2)
C33-Fe1-C32	109.9(3)	C37-Fe1-C32	148.0(3)
C34-Fe1-C32	100.5(3)	C29-Fe1-C32	69.1(3)
C28-Fe1-C35	151.8(3)	C33-Fe1-C35	70.2(2)
C37-Fe1-C35	67.9(3)	C34-Fe1-C35	40.7(3)
C29-Fe1-C35	165.1(3)	C32-Fe1-C35	124.7(3)
C28-Fe1-C31	70.2(2)	C33-Fe1-C31	150.0(3)
C37-Fe1-C31	166.7(3)	C34-Fe1-C31	122.8(3)
C29-Fe1-C31	68.2(3)	C32-Fe1-C31	40.7(3)
C35-Fe1-C31	117.3(2)	C28-Fe1-C30	69.4(3)
C33-Fe1-C30	152.7(2)	C37-Fe1-C30	127.6(3)
C34-Fe1-C30	162.1(3)	C29-Fe1-C30	40.2(3)
C32-Fe1-C30	67.5(3)	C35-Fe1-C30	134.9(3)
C31-Fe1-C30	39.6(3)	C28-Fe1-C36	151.5(3)
C33-Fe1-C36	70.2(3)	C37-Fe1-C36	40.5(3)
C34-Fe1-C36	68.4(3)	C29-Fe1-C36	126.2(3)
C32-Fe1-C36	164.2(3)	C35-Fe1-C36	39.7(3)
C31-Fe1-C36	135.4(3)	C30-Fe1-C36	120.0(3)
C28-Fe1-Si1	45.29(17)	C33-Fe1-Si1	45.17(18)
C37-Fe1-Si1	74.5(2)	C34-Fe1-Si1	74.70(19)
C29-Fe1-Si1	75.21(18)	C32-Fe1-Si1	73.57(19)
C35-Fe1-Si1	112.6(2)	C31-Fe1-Si1	112.09(19)
C30-Fe1-Si1	112.43(19)	C36-Fe1-Si1	112.4(2)
C1-N1-C2	110.6(4)	C1-N1-C16	128.6(4)
C2-N1-C16	120.8(4)	C1-N2-C3	111.7(4)
C1-N2-C4	123.6(4)	C3-N2-C4	124.7(3)
N1-C1-N2	104.8(4)	N1-C1-Ge1	138.0(3)

N2-C1-Ge1	117.1(3)	C3-C2-N1	109.4(4)
C2-C3-N2	103.5(4)	C2-C3-Si1	125.9(4)
N2-C3-Si1	130.5(3)	C9-C4-C5	124.2(4)
C9-C4-N2	118.3(5)	C5-C4-N2	117.5(4)
C4-C5-C6	115.9(5)	C4-C5-C13	122.9(5)
C6-C5-C13	121.2(6)	C7-C6-C5	121.3(6)
C6-C7-C8	121.9(5)	C7-C8-C9	120.5(6)
C4-C9-C8	116.2(6)	C4-C9-C10	122.1(5)
C8-C9-C10	121.7(5)	C9-C10-C11	110.2(6)
C9-C10-C12	114.2(7)	C11-C10-C12	110.3(7)
C5-C13-C15	114.0(7)	C5-C13-C14	111.5(6)
C15-C13-C14	110.1(7)	C21-C16-C17	124.8(5)
C21-C16-N1	117.6(6)	C17-C16-N1	117.4(6)
C16-C17-C18	115.2(7)	C16-C17-C25	123.7(5)
C18-C17-C25	120.9(7)	C19-C18-C17	121.5(8)
C18-C19-C20	121.3(6)	C19-C20-C21	120.5(8)
C16-C21-C20	116.6(7)	C16-C21-C22	123.5(5)
C20-C21-C22	119.9(7)	C21-C22-C23	114.8(7)
C21-C22-C24	110.2(8)	C23-C22-C24	109.2(7)
C17-C25-C26	112.3(6)	C17-C25-C27	111.8(8)
C26-C25-C27	110.3(7)	C32-C28-C29	105.3(5)
C32-C28-Si1	116.0(4)	C29-C28-Si1	119.7(5)
C32-C28-Fe1	70.0(3)	C29-C28-Fe1	69.9(3)
Si1-C28-Fe1	84.8(2)	C30-C29-C28	108.6(6)
C30-C29-Fe1	71.3(3)	C28-C29-Fe1	68.1(3)
C29-C30-C31	109.6(6)	C29-C30-Fe1	68.4(3)
C31-C30-Fe1	70.1(4)	C30-C31-C32	107.6(6)
C30-C31-Fe1	70.4(4)	C32-C31-Fe1	68.5(3)
C31-C32-C28	108.8(6)	C31-C32-Fe1	70.7(4)
C28-C32-Fe1	67.9(3)	C37-C33-C34	104.4(6)
C37-C33-Si1	117.5(4)	C34-C33-Si1	117.5(5)
C37-C33-Fe1	69.0(3)	C34-C33-Fe1	69.1(3)
Si1-C33-Fe1	84.7(2)	C35-C34-C33	108.3(6)
C35-C34-Fe1	70.8(4)	C33-C34-Fe1	68.4(3)
C36-C35-C34	109.6(6)	C36-C35-Fe1	70.9(4)
C34-C35-Fe1	68.5(3)	C35-C36-C37	107.6(6)
C35-C36-Fe1	69.4(4)	C37-C36-Fe1	67.6(4)
C36-C37-C33	110.1(6)	C36-C37-Fe1	71.9(4)
C33-C37-Fe1	68.8(3)	C38-O1-C39	102.7(9)
C39-C38-O1	103.4(10)	C38-C39-O1	104.8(12)

Compound 8·(THF)$_2$

Table S17. Sample and crystal data for **8·(THF)$_2$**.

Identification code	**8·(THF)$_2$**
Chemical formula	$C_{76}H_{106}Cl_4FeGe_2N_4O_2Si_2$
Formula weight	1506.65 g/mol
Temperature	298(2) K
Wavelength	0.71073 Å
Crystal size	0.150 x 0.280 x 0.320 mm
Crystal system	triclinic
Space group	P-1(No. 2)
Unit cell dimensions	a = 12.1909(9) Å α = 80.614(2)°
	b = 16.9634(12) Å β = 82.073(2)°
	c = 20.1520(14) Å γ = 82.496(2)°
Volume	4047.3(5) Å^3
Z	2
Density (calculated)	1.236 g/cm^3
Absorption coefficient	1.120 mm^{-1}
F(000)	1584

Table S18. Data collection and structure refinement for **8·(THF)$_2$**.

Theta range for data collection	2.42 to 26.52°	
Reflections collected	16757	
Coverage of independent reflections	99.2%	
Max. and min. transmission	0.7454 and 0.5332	
Structure solution technique	direct methods	
Structure solution program	SHELXS-97 (Sheldrick 2008)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	16757 / 392 / 916	
Goodness-of-fit on F^2	1.033	
Δ/σ_{max}	0.002	
Final R indices	10889 data; I>2σ(I)	R1 = 0.0653, wR2 = 0.1599
	all data	R1 = 0.1155, wR2 = 0.1898
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0992P)^2+1.8101P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.568 and -0.559 eÅ^{-3}	
R.M.S. deviation from mean	0.073 eÅ^{-3}	

Table S19. Bond lengths (Å) for **8·(THF)$_2$**.

Ge1-C1	2.107(4)	Ge1-Cl1	2.242(2)
Ge1-Cl2	2.2861(16)	Ge2-C35	2.117(3)
Ge2-Cl4	2.2373(18)	Ge2-Cl3	2.2726(17)
Si1-C28'	1.855(12)	Si1-C33	1.853(5)
Si1-C34	1.854(5)	Si1-C28	1.81(2)
Si1-C3	1.895(4)	Si2-C62	1.806(13)
Si2-C62'	1.845(14)	Si2-C68	1.837(5)
Si2-C67	1.852(6)	Si2-C37	1.894(4)
Fe1-C29	2.014(18)	Fe1-C29	2.014(18)
Fe1-C28	2.08(7)	Fe1-C28	2.08(7)
Fe1-C32'	2.02(2)	Fe1-C32'	2.02(2)
Fe1-C30	2.00(3)	Fe1-C30	2.00(3)
Fe1-C31'	2.072(13)	Fe1-C31'	2.072(13)
Fe1-C31	2.05(2)	Fe1-C31	2.05(2)
Fe2-C64	1.94(3)	Fe2-C64	1.94(3)
Fe2-C62'	2.06(3)	Fe2-C62'	2.06(3)
Fe2-C63	2.022(12)	Fe2-C63	2.022(12)
Fe2-C66'	1.992(18)	Fe2-C66'	1.992(18)
Fe2-C63'	2.021(14)	Fe2-C63'	2.021(14)
Fe2-C64'	2.044(15)	Fe2-C64'	2.044(15)
N1-C1	1.348(5)	N1-C2	1.379(5)
N1-C16	1.447(5)	N2-C1	1.354(5)
N2-C3	1.395(5)	N2-C4	1.463(5)
N3-C35	1.344(5)	N3-C36	1.365(5)
N3-C50	1.459(6)	N4-C35	1.352(5)
N4-C37	1.392(4)	N4-C38	1.445(5)
C2-C3	1.350(6)	C4-C5	1.388(7)
C4-C9	1.401(6)	C5-C6	1.408(7)
C5-C13	1.495(8)	C6-C7	1.373(9)
C7-C8	1.359(9)	C8-C9	1.386(7)
C9-C10	1.499(7)	C10-C12	1.513(8)
C10-C11	1.525(8)	C13-C15	1.528(9)
C13-C14	1.560(8)	C16-C21	1.394(6)
C16-C17	1.397(6)	C17-C18	1.391(7)
C17-C25	1.506(7)	C18-C19	1.356(8)
C19-C20	1.385(8)	C20-C21	1.377(7)
C21-C22	1.512(7)	C22-C24	1.492(10)
C22-C23	1.542(9)	C25-C26	1.519(8)
C25-C27	1.543(7)	C28-C29	1.437(15)

C28-C32	1.442(15)	C29-C30	1.422(16)
C30-C31	1.388(17)	C31-C32	1.409(16)
C28'-C29'	1.433(10)	C28'-C32'	1.440(11)
C29'-C30'	1.417(12)	C30'-C31'	1.397(12)
C31'-C32'	1.410(11)	C36-C37	1.346(6)
C38-C39	1.392(6)	C38-C43	1.398(6)
C39-C40	1.385(7)	C39-C47	1.503(8)
C40-C41	1.330(9)	C41-C42	1.386(10)
C42-C43	1.388(7)	C43-C44	1.509(8)
C44-C45	1.514(8)	C44-C46	1.517(9)
C47-C49	1.527(9)	C47-C48	1.543(9)
C50-C55	1.367(8)	C50-C51	1.379(8)
C51-C52	1.407(11)	C51-C59	1.476(10)
C52-C53	1.344(15)	C53-C54	1.314(15)
C54-C55	1.405(9)	C55-C56	1.523(10)
C56-C57	1.509(11)	C56-C58	1.567(10)
C59-C61	1.544(9)	C59-C60	1.538(10)
C62-C63	1.402(16)	C62-C66	1.416(15)
C63-C64	1.43(2)	C64-C65	1.30(3)
C65-C66	1.410(19)	C62'-C63'	1.407(17)
C62'-C66'	1.403(17)	C63'-C64'	1.433(18)
C64'-C65'	1.28(3)	C65'-C66'	1.41(2)
O1-C72	1.374(13)	O1-C69	1.440(16)
C69-C70	1.384(16)	C71-C70	1.489(15)
C71-C72	1.450(15)	O2-C76	1.415(16)
O2-C73	1.448(16)	C73-C74	1.480(16)
C74-C75	1.473(16)	C75-C76	1.457(16)

Table S20. Bond angles (°) for **8·(THF)$_2$**.

C1-Ge1-Cl1	96.86(12)	C1-Ge1-Cl2	91.34(11)
Cl1-Ge1-Cl2	96.08(8)	C35-Ge2-Cl4	95.78(12)
C35-Ge2-Cl3	93.87(11)	Cl4-Ge2-Cl3	97.49(9)
C28'-Si1-C33	110.8(9)	C28'-Si1-C34	109.5(7)
C33-Si1-C34	112.8(3)	C33-Si1-C28	111.9(18)
C34-Si1-C28	109.2(14)	C28'-Si1-C3	104.5(11)
C33-Si1-C3	105.0(2)	C34-Si1-C3	113.9(2)
C28-Si1-C3	104(2)	C62-Si2-C68	105.0(7)
C62'-Si2-C68	116.6(7)	C62-Si2-C67	114.1(6)
C62'-Si2-C67	105.9(9)	C68-Si2-C67	113.1(4)
C62-Si2-C37	106.3(9)	C62'-Si2-C37	101.6(12)
C68-Si2-C37	113.7(2)	C67-Si2-C37	104.7(2)
C29-Fe1-C28	139.0(9)	C29-Fe1-C28	41.0(9)
C29-Fe1-C28	41.0(9)	C29-Fe1-C28	139.0(9)
C29-Fe1-C30	138.5(6)	C29-Fe1-C30	41.5(6)
C28-Fe1-C30	69.2(15)	C28-Fe1-C30	110.8(15)
C29-Fe1-C30	41.5(6)	C29-Fe1-C30	138.5(6)
C28-Fe1-C30	110.8(15)	C28-Fe1-C30	69.2(15)
C32'-Fe1-C31'	139.7(4)	C32'-Fe1-C31'	40.3(4)
C32'-Fe1-C31'	40.3(4)	C32'-Fe1-C31'	139.7(4)
C29-Fe1-C31	112.0(8)	C29-Fe1-C31	68.0(8)
C28-Fe1-C31	67.8(13)	C28-Fe1-C31	112.2(13)
C30-Fe1-C31	40.1(6)	C30-Fe1-C31	139.9(6)
C29-Fe1-C31	68.0(8)	C29-Fe1-C31	112.0(8)
C28-Fe1-C31	112.2(13)	C28-Fe1-C31	67.8(13)
C30-Fe1-C31	139.9(6)	C30-Fe1-C31	40.1(6)
C64-Fe2-C63	137.8(8)	C64-Fe2-C63	42.2(8)
C64-Fe2-C63	42.2(8)	C64-Fe2-C63	137.8(8)
C62'-Fe2-C66'	40.5(7)	C62'-Fe2-C66'	139.5(7)
C62'-Fe2-C66'	139.5(7)	C62'-Fe2-C66'	40.5(7)
C62'-Fe2-C63'	139.7(5)	C62'-Fe2-C63'	40.3(5)
C66'-Fe2-C63'	113.4(7)	C66'-Fe2-C63'	66.6(7)
C62'-Fe2-C63'	40.3(5)	C62'-Fe2-C63'	139.7(5)
C66'-Fe2-C63'	66.6(7)	C66'-Fe2-C63'	113.4(7)
C62'-Fe2-C64'	68.4(8)	C62'-Fe2-C64'	111.6(8)
C66'-Fe2-C64'	65.5(7)	C66'-Fe2-C64'	114.5(7)
C63'-Fe2-C64'	138.7(6)	C63'-Fe2-C64'	41.3(6)
C62'-Fe2-C64'	111.6(8)	C62'-Fe2-C64'	68.4(8)

C66'-Fe2-C64'	114.5(7)	C66'-Fe2-C64'	65.5(7)
C63'-Fe2-C64'	41.3(6)	C63'-Fe2-C64'	138.7(6)
C1-N1-C2	109.7(3)	C1-N1-C16	128.7(3)
C2-N1-C16	121.3(3)	C1-N2-C3	112.4(3)
C1-N2-C4	124.1(3)	C3-N2-C4	122.5(3)
C35-N3-C36	109.7(3)	C35-N3-C50	128.8(3)
C36-N3-C50	121.1(3)	C35-N4-C37	112.1(3)
C35-N4-C38	123.6(3)	C37-N4-C38	124.1(3)
N1-C1-N2	104.8(3)	N1-C1-Ge1	136.8(3)
N2-C1-Ge1	118.1(3)	C3-C2-N1	109.5(3)
C2-C3-N2	103.7(3)	C2-C3-Si1	123.2(3)
N2-C3-Si1	133.2(3)	C5-C4-C9	124.0(4)
C5-C4-N2	119.4(4)	C9-C4-N2	116.5(4)
C4-C5-C6	116.3(5)	C4-C5-C13	123.8(4)
C6-C5-C13	119.9(5)	C7-C6-C5	120.7(6)
C8-C7-C6	120.7(5)	C7-C8-C9	122.1(6)
C8-C9-C4	116.0(5)	C8-C9-C10	120.8(5)
C4-C9-C10	123.2(4)	C9-C10-C12	111.6(5)
C9-C10-C11	113.0(5)	C12-C10-C11	110.1(5)
C5-C13-C15	112.4(5)	C5-C13-C14	111.1(5)
C15-C13-C14	108.4(6)	C21-C16-C17	123.2(4)
C21-C16-N1	118.3(4)	C17-C16-N1	118.3(4)
C18-C17-C16	116.5(4)	C18-C17-C25	120.5(4)
C16-C17-C25	122.9(4)	C19-C18-C17	121.8(5)
C18-C19-C20	120.0(5)	C19-C20-C21	121.5(5)
C16-C21-C20	116.9(5)	C16-C21-C22	122.2(4)
C20-C21-C22	120.9(5)	C24-C22-C21	113.0(6)
C24-C22-C23	110.8(6)	C21-C22-C23	112.4(6)
C26-C25-C17	110.8(5)	C26-C25-C27	111.0(5)
C17-C25-C27	111.9(4)	C29-C28-C32	106.0(13)
C29-C28-Si1	135(2)	C32-C28-Si1	119(2)
C29-C28-Fe1	67(2)	C32-C28-Fe1	70(3)
Si1-C28-Fe1	127(4)	C28-C29-C30	108.5(13)
C28-C29-Fe1	72(3)	C30-C29-Fe1	68.7(14)
C31-C30-C29	107.9(13)	C31-C30-Fe1	71.9(14)
C29-C30-Fe1	69.8(12)	C30-C31-C32	109.6(13)
C30-C31-Fe1	68.0(14)	C32-C31-Fe1	71.6(16)
C31-C32-C28	108.0(13)	C31-C32-Fe1	68.6(13)
C28-C32-Fe1	70(3)	C29'-C28'-C32'	106.1(8)
C29'-C28'-Si1	123.0(13)	C32'-C28'-Si1	130.9(13)
C29'-C28'-Fe1	70.1(11)	C32'-C28'-Fe1	68.8(13)

Si1-C28'-Fe1	127.5(18)	C28'-C29'-C30'	108.7(8)
C28'-C29'-Fe1	68.8(13)	C30'-C29'-Fe1	72.8(7)
C31'-C30'-C29'	107.9(8)	C31'-C30'-Fe1	68.7(7)
C29'-C30'-Fe1	67.5(6)	C30'-C31'-C32'	109.2(8)
C30'-C31'-Fe1	72.3(8)	C32'-C31'-Fe1	67.9(10)
C31'-C32'-C28'	108.1(8)	C31'-C32'-Fe1	71.8(10)
C28'-C32'-Fe1	69.6(15)	N3-C35-N4	104.8(3)
N3-C35-Ge2	137.6(3)	N4-C35-Ge2	117.6(2)
C37-C36-N3	109.9(3)	C36-C37-N4	103.5(3)
C36-C37-Si2	123.7(3)	N4-C37-Si2	132.8(3)
C39-C38-C43	123.5(4)	C39-C38-N4	119.5(4)
C43-C38-N4	117.0(4)	C40-C39-C38	116.9(5)
C40-C39-C47	119.8(5)	C38-C39-C47	123.3(4)
C41-C40-C39	121.1(6)	C40-C41-C42	122.2(5)
C41-C42-C43	120.0(6)	C42-C43-C38	116.3(5)
C42-C43-C44	120.9(5)	C38-C43-C44	122.8(4)
C43-C44-C45	112.8(5)	C43-C44-C46	112.3(5)
C45-C44-C46	110.5(5)	C39-C47-C49	112.1(6)
C39-C47-C48	112.1(6)	C49-C47-C48	108.9(5)
C55-C50-C51	124.3(5)	C55-C50-N3	117.2(5)
C51-C50-N3	118.2(5)	C50-C51-C52	115.6(8)
C50-C51-C59	123.0(6)	C52-C51-C59	121.3(7)
C53-C52-C51	120.7(9)	C54-C53-C52	121.9(9)
C53-C54-C55	121.5(10)	C50-C55-C54	115.9(8)
C50-C55-C56	122.6(5)	C54-C55-C56	121.5(7)
C57-C56-C55	112.1(6)	C57-C56-C58	109.9(7)
C55-C56-C58	112.7(7)	C51-C59-C61	114.6(8)
C51-C59-C60	110.7(6)	C61-C59-C60	109.7(6)
C63-C62-C66	103.6(11)	C63-C62-Si2	130.2(13)
C66-C62-Si2	125.5(11)	C63-C62-Fe2	69.1(9)
C66-C62-Fe2	70.4(10)	Si2-C62-Fe2	130.6(14)
C62-C63-C64	109.2(17)	C62-C63-Fe2	70.5(12)
C64-C63-Fe2	65.8(15)	C65-C64-C63	107.6(17)
C65-C64-Fe2	75.8(17)	C63-C64-Fe2	72.0(11)
C64-C65-C66	109.6(14)	C64-C65-Fe2	66.4(14)
C66-C65-Fe2	70.1(7)	C65-C66-C62	108.8(14)
C65-C66-Fe2	69.8(6)	C62-C66-Fe2	69.2(10)
C63'-C62'-C66'	103.2(12)	C63'-C62'-Si2	125.4(13)
C66'-C62'-Si2	131.3(14)	C63'-C62'-Fe2	68.3(13)
C66'-C62'-Fe2	67.1(12)	Si2-C62'-Fe2	127.0(19)
C62'-C63'-C64'	108.6(15)	C62'-C63'-Fe2	71.4(14)

C64'-C63'-Fe2	70.2(8)	C65'-C64'-C63'	109.0(16)
C65'-C64'-Fe2	76.(2)	C63'-C64'-Fe2	68.5(8)
C64'-C65'-C66'	108.3(19)	C64'-C65'-Fe2	68.5(18)
C66'-C65'-Fe2	64.8(16)	C65'-C66'-C62'	109.9(18)
C65'-C66'-Fe2	75.3(19)	C62'-C66'-Fe2	72.4(17)
C72-O1-C69	104.5(12)	C70-C69-O1	101.4(15)
C70-C71-C72	95.4(12)	O1-C72-C71	108.1(13)
C69-C70-C71	99.2(13)	C76-O2-C73	112.9(17)
O2-C73-C74	88.3(14)	C73-C74-C75	96.0(13)
C76-C75-C74	91.3(17)	O2-C76-C75	97.8(14)