Electronic Supplementary Information for Dalton Transactions

Reactions of 'pincer' pyridine dicarbene complexes of Fe(0) with silanes

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Electronic Supplementary information. List of bond lengths, angles etc. for crystal structures.

Complex 2a

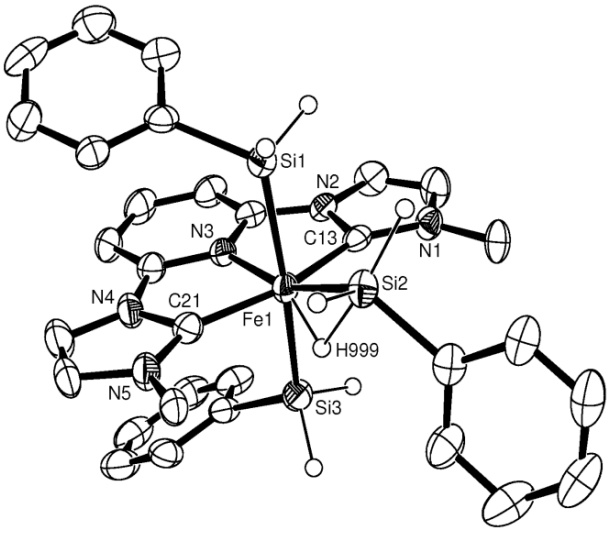

Table 1. Crystal data and structure refinement for **2a**.

Identification code	**2a**	
Empirical formula	C53 H63 Fe N5 Si3	
Formula weight	910.20	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 18.195(19) Å	α= 90°.
	b = 14.27(3) Å	β= 101.44(7)°.
	c = 19.696(9) Å	γ = 90°.
Volume	5013(11) $Å^3$	
Z	4	
Density (calculated)	1.206 Mg/m^3	
Absorption coefficient	0.412 mm^{-1}	
F(000)	1936	
Crystal size	0.10 x 0.02 x 0.01 mm^3	
Theta range for data collection	2.85 to 25.67°.	
Index ranges	-21<=h<=21, -17<=k<=17, -24<=l<=23	
Reflections collected	55154	
Independent reflections	9215 [R(int) = 0.1625]	

Completeness to theta = 25.67°	96.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9959 and 0.9599
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9215 / 730 / 585
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0830, wR2 = 0.1149
R indices (all data)	R1 = 0.1635, wR2 = 0.1345
Largest diff. peak and hole	0.311 and -0.305 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	2289(1)	1639(1)	2371(1)	27(1)
Si(1)	1247(1)	2684(1)	2275(1)	35(1)
Si(2)	2455(1)	2388(1)	3447(1)	33(1)
Si(3)	3259(1)	583(1)	2250(1)	34(1)
C(13)	2804(2)	2587(3)	1913(2)	28(1)
N(1)	3328(2)	3308(3)	1990(2)	32(1)
N(5)	1386(2)	2(2)	2972(2)	35(1)
N(2)	2594(2)	2537(2)	1185(2)	29(1)
N(4)	1281(2)	168(2)	1869(2)	35(1)
N(3)	1880(2)	1336(2)	1425(2)	28(1)
C(15)	2989(3)	3183(3)	853(2)	40(1)
C(21)	1650(3)	574(3)	2497(2)	32(1)
C(29)	2135(3)	-406(3)	4121(2)	35(1)
C(24)	1522(3)	82(3)	3720(2)	34(1)
C(43)	3865(3)	1624(4)	4223(2)	47(1)
C(7)	2723(3)	4970(3)	2582(3)	53(1)
C(6)	4503(3)	3368(4)	2873(2)	41(1)
C(1)	3776(3)	3721(3)	2619(2)	38(1)
C(17)	1791(3)	1643(3)	223(2)	39(1)
C(16)	2076(3)	1843(3)	903(2)	30(1)
C(42)	3377(3)	2399(3)	4110(2)	35(1)
C(22)	825(3)	-594(3)	1961(2)	46(1)
C(25)	995(3)	586(3)	4016(2)	38(1)
C(14)	3443(3)	3657(3)	1355(2)	44(1)
C(2)	3487(3)	4542(3)	2899(2)	42(1)
C(27)	1691(3)	109(4)	5139(3)	50(1)
C(20)	1403(3)	601(3)	1265(2)	34(1)
C(19)	1094(3)	347(3)	590(2)	41(1)
C(28)	2207(3)	-374(3)	4838(2)	42(1)
C(23)	893(3)	-691(3)	2644(2)	42(1)

C(18)	1294(3)	889(3)	67(2)	44(1)
C(33)	2702(3)	-948(3)	3804(2)	42(1)
C(10)	4846(3)	2564(4)	2521(2)	45(1)
C(30)	338(3)	1128(3)	3587(3)	48(1)
C(47)	3576(3)	3185(4)	4537(2)	51(1)
C(36A)	348(10)	2266(14)	1625(11)	33(2)
C(37A)	110(9)	2794(12)	1029(10)	44(2)
C(38A)	-521(8)	2521(13)	549(7)	55(3)
C(39A)	-913(7)	1720(14)	664(7)	53(3)
C(40A)	-674(8)	1192(11)	1260(8)	46(2)
C(41A)	-44(11)	1465(12)	1741(8)	40(2)
C(36B)	344(9)	2395(13)	1600(10)	33(2)
C(37B)	150(8)	3043(12)	1068(9)	44(2)
C(38B)	-482(8)	2897(12)	553(6)	55(3)
C(39B)	-920(6)	2104(13)	570(7)	53(3)
C(40B)	-727(7)	1455(10)	1102(8)	46(2)
C(41B)	-94(10)	1601(11)	1617(8)	40(2)
C(12)	5205(3)	1786(4)	3020(3)	62(2)
C(45)	4685(3)	2413(5)	5156(3)	62(2)
C(11)	5435(3)	2973(4)	2130(2)	60(2)
C(5)	4938(3)	3832(4)	3441(3)	55(2)
C(9)	2298(3)	5395(4)	3116(3)	71(2)
C(26)	1090(3)	589(4)	4735(2)	49(1)
C(34)	2425(3)	-1958(3)	3585(3)	61(2)
C(44)	4516(3)	1624(4)	4745(2)	60(2)
C(4)	4662(3)	4617(4)	3730(3)	62(2)
C(3)	3954(3)	4970(4)	3460(3)	55(2)
C(35)	3488(3)	-1010(4)	4256(3)	60(2)
C(46)	4219(3)	3187(4)	5057(3)	61(2)
C(32)	198(3)	2099(4)	3904(3)	63(2)
C(48A)	3038(6)	-341(5)	1522(4)	33(2)
C(49A)	2749(6)	-1216(5)	1635(3)	42(3)
C(50A)	2638(5)	-1883(4)	1110(4)	58(3)
C(51A)	2815(5)	-1674(5)	472(3)	56(3)
C(52A)	3103(5)	-798(6)	359(3)	57(3)

C(53A)	3214(6)	-132(5)	884(4)	45(2)
C(48B)	2904(10)	-466(8)	1623(7)	33(2)
C(49B)	2517(9)	-1231(9)	1813(5)	42(3)
C(50B)	2335(7)	-1980(7)	1360(6)	58(3)
C(51B)	2540(7)	-1964(7)	716(5)	56(3)
C(52B)	2927(8)	-1199(9)	526(5)	57(3)
C(53B)	3109(8)	-451(8)	980(7)	45(2)
C(31)	-389(3)	543(4)	3462(3)	79(2)
C(8)	2801(3)	5742(4)	2054(3)	71(2)

Table 3. Bond lengths [Å] and angles [°] for **2a**.

Fe(1)-N(3)	1.914(3)	C(15)-C(14)	1.339(6)
Fe(1)-C(21)	1.958(5)	C(15)-H(15)	0.9500
Fe(1)-C(13)	1.965(5)	C(29)-C(28)	1.393(6)
Fe(1)-Si(2)	2.3389(18)	C(29)-C(24)	1.417(6)
Fe(1)-Si(3)	2.369(3)	C(29)-C(33)	1.519(6)
Fe(1)-Si(1)	2.391(3)	C(24)-C(25)	1.414(6)
Fe(1)-H(999)	1.29(5)	C(43)-C(44)	1.407(7)
Si(1)-C(36B)	1.941(7)	C(43)-C(42)	1.407(7)
Si(1)-C(36A)	1.958(7)	C(43)-H(43)	0.9500
Si(1)-H(55)	1.46(3)	C(7)-C(2)	1.534(7)
Si(1)-H(54)	1.38(4)	C(7)-C(8)	1.541(7)
Si(2)-C(42)	1.911(5)	C(7)-C(9)	1.548(7)
Si(2)-H(57)	1.43(3)	C(7)-H(7)	1.0000
Si(2)-H(56)	1.49(4)	C(6)-C(5)	1.401(6)
Si(2)-H(999)	1.92(5)	C(6)-C(1)	1.410(6)
Si(3)-C(48A)	1.930(5)	C(6)-C(10)	1.536(7)
Si(3)-C(48B)	1.966(7)	C(1)-C(2)	1.439(7)
Si(3)-H(58)	1.43(4)	C(17)-C(16)	1.368(6)
Si(3)-H(59)	1.44(4)	C(17)-C(18)	1.400(6)
C(13)-N(1)	1.391(5)	C(17)-H(17)	0.9500
C(13)-N(2)	1.410(5)	C(42)-C(47)	1.406(6)
N(1)-C(14)	1.400(5)	C(22)-C(23)	1.332(6)
N(1)-C(1)	1.465(5)	C(22)-H(22)	0.9500
N(5)-C(21)	1.397(5)	C(25)-C(26)	1.393(6)
N(5)-C(23)	1.404(5)	C(25)-C(30)	1.529(6)
N(5)-C(24)	1.448(5)	C(14)-H(14)	0.9500
N(2)-C(16)	1.403(5)	C(2)-C(3)	1.394(6)
N(2)-C(15)	1.407(5)	C(27)-C(28)	1.389(7)
N(4)-C(20)	1.397(5)	C(27)-C(26)	1.397(7)
N(4)-C(22)	1.402(6)	C(27)-H(27)	0.9500
N(4)-C(21)	1.409(5)	C(20)-C(19)	1.386(5)
N(3)-C(20)	1.358(5)	C(19)-C(18)	1.391(6)
N(3)-C(16)	1.360(5)	C(19)-H(19)	0.9500

C(28)-H(28)	0.9500	C(41B)-H(41B)	0.9500
C(23)-H(23)	0.9500	C(12)-H(12A)	0.9800
C(18)-H(18)	0.9500	C(12)-H(12B)	0.9800
C(33)-C(35)	1.530(7)	C(12)-H(12C)	0.9800
C(33)-C(34)	1.560(7)	C(45)-C(46)	1.384(7)
C(33)-H(33)	1.0000	C(45)-C(44)	1.385(7)
C(10)-C(12)	1.541(7)	C(45)-H(45)	0.9500
C(10)-C(11)	1.553(6)	C(11)-H(11A)	0.9800
C(10)-H(10)	1.0000	C(11)-H(11B)	0.9800
C(30)-C(31)	1.543(7)	C(11)-H(11C)	0.9800
C(30)-C(32)	1.562(7)	C(5)-C(4)	1.396(7)
C(30)-H(30)	1.0000	C(5)-H(5)	0.9500
C(47)-C(46)	1.393(7)	C(9)-H(9A)	0.9800
C(47)-H(47)	0.9500	C(9)-H(9B)	0.9800
C(36A)-C(37A)	1.3900	C(9)-H(9C)	0.9800
C(36A)-C(41A)	1.3900	C(26)-H(26)	0.9500
C(37A)-C(38A)	1.3900	C(34)-H(34A)	0.9800
C(37A)-H(37A)	0.9500	C(34)-H(34B)	0.9800
C(38A)-C(39A)	1.3900	C(34)-H(34C)	0.9800
C(38A)-H(38A)	0.9500	C(44)-H(44)	0.9500
C(39A)-C(40A)	1.3900	C(4)-C(3)	1.387(7)
C(39A)-H(39A)	0.9500	C(4)-H(4)	0.9500
C(40A)-C(41A)	1.3900	C(3)-H(3)	0.9500
C(40A)-H(40A)	0.9500	C(35)-H(35A)	0.9800
C(41A)-H(41A)	0.9500	C(35)-H(35B)	0.9800
C(36B)-C(37B)	1.3900	C(35)-H(35C)	0.9800
C(36B)-C(41B)	1.3900	C(46)-H(46)	0.9500
C(37B)-C(38B)	1.3900	C(32)-H(32A)	0.9800
C(37B)-H(37B)	0.9500	C(32)-H(32B)	0.9800
C(38B)-C(39B)	1.3900	C(32)-H(32C)	0.9800
C(38B)-H(38B)	0.9500	C(48A)-C(49A)	1.3900
C(39B)-C(40B)	1.3900	C(48A)-C(53A)	1.3900
C(39B)-H(39B)	0.9500	C(49A)-C(50A)	1.3900
C(40B)-C(41B)	1.3900	C(49A)-H(49A)	0.9500
C(40B)-H(40B)	0.9500	C(50A)-C(51A)	1.3900

C(50A)-H(50A)	0.9500	C(51B)-C(52B)	1.3900
C(51A)-C(52A)	1.3900	C(51B)-H(51B)	0.9500
C(51A)-H(51A)	0.9500	C(52B)-C(53B)	1.3900
C(52A)-C(53A)	1.3900	C(52B)-H(52B)	0.9500
C(52A)-H(52A)	0.9500	C(53B)-H(53B)	0.9500
C(53A)-H(53A)	0.9500	C(31)-H(31A)	0.9800
C(48B)-C(49B)	1.3900	C(31)-H(31B)	0.9800
C(48B)-C(53B)	1.3900	C(31)-H(31C)	0.9800
C(49B)-C(50B)	1.3900	C(8)-H(8A)	0.9800
C(49B)-H(49B)	0.9500	C(8)-H(8B)	0.9800
C(50B)-C(51B)	1.3900	C(8)-H(8C)	0.9800
C(50B)-H(50B)	0.9500		

N(3)-Fe(1)-C(21)	79.79(17)	C(36B)-Si(1)-Fe(1)	118.1(7)
N(3)-Fe(1)-C(13)	80.60(17)	C(36A)-Si(1)-Fe(1)	114.0(8)
C(21)-Fe(1)-C(13)	160.36(17)	C(36B)-Si(1)-H(55)	102.4(16)
N(3)-Fe(1)-Si(2)	160.20(11)	C(36A)-Si(1)-H(55)	102.3(16)
C(21)-Fe(1)-Si(2)	102.28(14)	Fe(1)-Si(1)-H(55)	119.7(13)
C(13)-Fe(1)-Si(2)	96.56(15)	C(36B)-Si(1)-H(54)	95.2(18)
N(3)-Fe(1)-Si(3)	84.91(12)	C(36A)-Si(1)-H(54)	100.5(18)
C(21)-Fe(1)-Si(3)	89.51(18)	Fe(1)-Si(1)-H(54)	111.4(18)
C(13)-Fe(1)-Si(3)	87.63(17)	H(55)-Si(1)-H(54)	107(2)
Si(2)-Fe(1)-Si(3)	114.67(8)	C(42)-Si(2)-Fe(1)	124.07(16)
N(3)-Fe(1)-Si(1)	85.14(13)	C(42)-Si(2)-H(57)	100.8(13)
C(21)-Fe(1)-Si(1)	90.75(18)	Fe(1)-Si(2)-H(57)	111.6(12)
C(13)-Fe(1)-Si(1)	88.72(17)	C(42)-Si(2)-H(56)	100.2(14)
Si(2)-Fe(1)-Si(1)	75.18(9)	Fe(1)-Si(2)-H(56)	113.5(12)
Si(3)-Fe(1)-Si(1)	169.83(5)	H(57)-Si(2)-H(56)	104.4(18)
N(3)-Fe(1)-H(999)	144(2)	C(42)-Si(2)-H(999)	93.0(15)
C(21)-Fe(1)-H(999)	93(2)	Fe(1)-Si(2)-H(999)	33.4(15)
C(13)-Fe(1)-H(999)	103(2)	H(57)-Si(2)-H(999)	111.3(18)
Si(2)-Fe(1)-H(999)	55(2)	H(56)-Si(2)-H(999)	138.8(19)
Si(3)-Fe(1)-H(999)	60(2)	C(48A)-Si(3)-C(48B)	11.3(6)
Si(1)-Fe(1)-H(999)	130(2)	C(48A)-Si(3)-Fe(1)	117.3(4)
C(36B)-Si(1)-C(36A)	5.6(10)	C(48B)-Si(3)-Fe(1)	112.9(5)

C(48A)-Si(3)-H(58)	107.0(14)	C(25)-C(24)-N(5)	117.9(4)
C(48B)-Si(3)-H(58)	102.0(15)	C(29)-C(24)-N(5)	119.0(4)
Fe(1)-Si(3)-H(58)	117.7(14)	C(44)-C(43)-C(42)	122.0(5)
C(48A)-Si(3)-H(59)	95.6(16)	C(44)-C(43)-H(43)	119.0
C(48B)-Si(3)-H(59)	106.7(16)	C(42)-C(43)-H(43)	119.0
Fe(1)-Si(3)-H(59)	113.4(16)	C(2)-C(7)-C(8)	111.2(4)
H(58)-Si(3)-H(59)	103(2)	C(2)-C(7)-C(9)	114.5(4)
N(1)-C(13)-N(2)	101.0(3)	C(8)-C(7)-C(9)	107.7(4)
N(1)-C(13)-Fe(1)	147.0(3)	C(2)-C(7)-H(7)	107.7
N(2)-C(13)-Fe(1)	112.0(3)	C(8)-C(7)-H(7)	107.7
C(13)-N(1)-C(14)	112.7(4)	C(9)-C(7)-H(7)	107.7
C(13)-N(1)-C(1)	130.1(3)	C(5)-C(6)-C(1)	117.1(5)
C(14)-N(1)-C(1)	117.2(4)	C(5)-C(6)-C(10)	119.8(5)
C(21)-N(5)-C(23)	112.1(3)	C(1)-C(6)-C(10)	122.9(4)
C(21)-N(5)-C(24)	128.5(4)	C(6)-C(1)-C(2)	122.9(4)
C(23)-N(5)-C(24)	119.2(4)	C(6)-C(1)-N(1)	118.8(4)
C(16)-N(2)-C(15)	130.1(4)	C(2)-C(1)-N(1)	117.9(4)
C(16)-N(2)-C(13)	117.6(3)	C(16)-C(17)-C(18)	118.5(4)
C(15)-N(2)-C(13)	112.2(4)	C(16)-C(17)-H(17)	120.7
C(20)-N(4)-C(22)	130.6(4)	C(18)-C(17)-H(17)	120.7
C(20)-N(4)-C(21)	115.9(4)	N(3)-C(16)-C(17)	121.6(4)
C(22)-N(4)-C(21)	113.4(4)	N(3)-C(16)-N(2)	109.5(4)
C(20)-N(3)-C(16)	119.2(4)	C(17)-C(16)-N(2)	129.0(4)
C(20)-N(3)-Fe(1)	120.4(3)	C(47)-C(42)-C(43)	116.9(5)
C(16)-N(3)-Fe(1)	120.4(3)	C(47)-C(42)-Si(2)	120.2(4)
C(14)-C(15)-N(2)	106.6(4)	C(43)-C(42)-Si(2)	122.9(4)
C(14)-C(15)-H(15)	126.7	C(23)-C(22)-N(4)	105.8(4)
N(2)-C(15)-H(15)	126.7	C(23)-C(22)-H(22)	127.1
N(5)-C(21)-N(4)	100.3(4)	N(4)-C(22)-H(22)	127.1
N(5)-C(21)-Fe(1)	146.1(3)	C(26)-C(25)-C(24)	117.6(4)
N(4)-C(21)-Fe(1)	113.5(3)	C(26)-C(25)-C(30)	119.1(5)
C(28)-C(29)-C(24)	117.1(4)	C(24)-C(25)-C(30)	123.2(4)
C(28)-C(29)-C(33)	119.9(4)	C(15)-C(14)-N(1)	107.5(4)
C(24)-C(29)-C(33)	123.0(4)	C(15)-C(14)-H(14)	126.3
C(25)-C(24)-C(29)	122.9(4)	N(1)-C(14)-H(14)	126.3

C(3)-C(2)-C(1)	116.7(5)	C(31)-C(30)-C(32)	109.9(5)
C(3)-C(2)-C(7)	120.6(5)	C(25)-C(30)-H(30)	107.2
C(1)-C(2)-C(7)	122.6(4)	C(31)-C(30)-H(30)	107.2
C(28)-C(27)-C(26)	121.4(5)	C(32)-C(30)-H(30)	107.2
C(28)-C(27)-H(27)	119.3	C(46)-C(47)-C(42)	121.4(5)
C(26)-C(27)-H(27)	119.3	C(46)-C(47)-H(47)	119.3
N(3)-C(20)-C(19)	122.8(4)	C(42)-C(47)-H(47)	119.3
N(3)-C(20)-N(4)	110.3(4)	C(37A)-C(36A)-C(41A)	120.0
C(19)-C(20)-N(4)	126.9(4)	C(37A)-C(36A)-Si(1)	117.8(9)
C(20)-C(19)-C(18)	116.7(4)	C(41A)-C(36A)-Si(1)	122.2(9)
C(20)-C(19)-H(19)	121.7	C(38A)-C(37A)-C(36A)	120.0
C(18)-C(19)-H(19)	121.7	C(38A)-C(37A)-H(37A)	120.0
C(27)-C(28)-C(29)	120.8(5)	C(36A)-C(37A)-H(37A)	120.0
C(27)-C(28)-H(28)	119.6	C(37A)-C(38A)-C(39A)	120.0
C(29)-C(28)-H(28)	119.6	C(37A)-C(38A)-H(38A)	120.0
C(22)-C(23)-N(5)	108.3(4)	C(39A)-C(38A)-H(38A)	120.0
C(22)-C(23)-H(23)	125.8	C(40A)-C(39A)-C(38A)	120.0
N(5)-C(23)-H(23)	125.8	C(40A)-C(39A)-H(39A)	120.0
C(19)-C(18)-C(17)	121.2(4)	C(38A)-C(39A)-H(39A)	120.0
C(19)-C(18)-H(18)	119.4	C(41A)-C(40A)-C(39A)	120.0
C(17)-C(18)-H(18)	119.4	C(41A)-C(40A)-H(40A)	120.0
C(29)-C(33)-C(35)	115.0(4)	C(39A)-C(40A)-H(40A)	120.0
C(29)-C(33)-C(34)	112.1(4)	C(40A)-C(41A)-C(36A)	120.0
C(35)-C(33)-C(34)	108.8(4)	C(40A)-C(41A)-H(41A)	120.0
C(29)-C(33)-H(33)	106.8	C(36A)-C(41A)-H(41A)	120.0
C(35)-C(33)-H(33)	106.8	C(37B)-C(36B)-C(41B)	120.0
C(34)-C(33)-H(33)	106.8	C(37B)-C(36B)-Si(1)	115.3(8)
C(6)-C(10)-C(12)	114.2(4)	C(41B)-C(36B)-Si(1)	124.6(8)
C(6)-C(10)-C(11)	109.0(4)	C(38B)-C(37B)-C(36B)	120.0
C(12)-C(10)-C(11)	109.9(4)	C(38B)-C(37B)-H(37B)	120.0
C(6)-C(10)-H(10)	107.9	C(36B)-C(37B)-H(37B)	120.0
C(12)-C(10)-H(10)	107.9	C(39B)-C(38B)-C(37B)	120.0
C(11)-C(10)-H(10)	107.9	C(39B)-C(38B)-H(38B)	120.0
C(25)-C(30)-C(31)	111.5(4)	C(37B)-C(38B)-H(38B)	120.0
C(25)-C(30)-C(32)	113.5(4)	C(38B)-C(39B)-C(40B)	120.0

C(38B)-C(39B)-H(39B)	120.0	C(33)-C(34)-H(34A)	109.5
C(40B)-C(39B)-H(39B)	120.0	C(33)-C(34)-H(34B)	109.5
C(41B)-C(40B)-C(39B)	120.0	H(34A)-C(34)-H(34B)	109.5
C(41B)-C(40B)-H(40B)	120.0	C(33)-C(34)-H(34C)	109.5
C(39B)-C(40B)-H(40B)	120.0	H(34A)-C(34)-H(34C)	109.5
C(40B)-C(41B)-C(36B)	120.0	H(34B)-C(34)-H(34C)	109.5
C(40B)-C(41B)-H(41B)	120.0	C(45)-C(44)-C(43)	119.0(5)
C(36B)-C(41B)-H(41B)	120.0	C(45)-C(44)-H(44)	120.5
C(10)-C(12)-H(12A)	109.5	C(43)-C(44)-H(44)	120.5
C(10)-C(12)-H(12B)	109.5	C(3)-C(4)-C(5)	121.1(5)
H(12A)-C(12)-H(12B)	109.5	C(3)-C(4)-H(4)	119.5
C(10)-C(12)-H(12C)	109.5	C(5)-C(4)-H(4)	119.5
H(12A)-C(12)-H(12C)	109.5	C(4)-C(3)-C(2)	121.3(5)
H(12B)-C(12)-H(12C)	109.5	C(4)-C(3)-H(3)	119.4
C(46)-C(45)-C(44)	120.5(5)	C(2)-C(3)-H(3)	119.4
C(46)-C(45)-H(45)	119.7	C(33)-C(35)-H(35A)	109.5
C(44)-C(45)-H(45)	119.7	C(33)-C(35)-H(35B)	109.5
C(10)-C(11)-H(11A)	109.5	H(35A)-C(35)-H(35B)	109.5
C(10)-C(11)-H(11B)	109.5	C(33)-C(35)-H(35C)	109.5
H(11A)-C(11)-H(11B)	109.5	H(35A)-C(35)-H(35C)	109.5
C(10)-C(11)-H(11C)	109.5	H(35B)-C(35)-H(35C)	109.5
H(11A)-C(11)-H(11C)	109.5	C(45)-C(46)-C(47)	120.2(5)
H(11B)-C(11)-H(11C)	109.5	C(45)-C(46)-H(46)	119.9
C(4)-C(5)-C(6)	120.9(5)	C(47)-C(46)-H(46)	119.9
C(4)-C(5)-H(5)	119.6	C(30)-C(32)-H(32A)	109.5
C(6)-C(5)-H(5)	119.6	C(30)-C(32)-H(32B)	109.5
C(7)-C(9)-H(9A)	109.5	H(32A)-C(32)-H(32B)	109.5
C(7)-C(9)-H(9B)	109.5	C(30)-C(32)-H(32C)	109.5
H(9A)-C(9)-H(9B)	109.5	H(32A)-C(32)-H(32C)	109.5
C(7)-C(9)-H(9C)	109.5	H(32B)-C(32)-H(32C)	109.5
H(9A)-C(9)-H(9C)	109.5	C(49A)-C(48A)-C(53A)	120.0
H(9B)-C(9)-H(9C)	109.5	C(49A)-C(48A)-Si(3)	121.6(4)
C(25)-C(26)-C(27)	120.2(5)	C(53A)-C(48A)-Si(3)	118.3(4)
C(25)-C(26)-H(26)	119.9	C(48A)-C(49A)-C(50A)	120.0
C(27)-C(26)-H(26)	119.9	C(48A)-C(49A)-H(49A)	120.0

C(50A)-C(49A)-H(49A)	120.0	H(31A)-C(31)-H(31C)	109.5
C(51A)-C(50A)-C(49A)	120.0	H(31B)-C(31)-H(31C)	109.5
C(51A)-C(50A)-H(50A)	120.0	C(7)-C(8)-H(8A)	109.5
C(49A)-C(50A)-H(50A)	120.0	C(7)-C(8)-H(8B)	109.5
C(52A)-C(51A)-C(50A)	120.0	H(8A)-C(8)-H(8B)	109.5
C(52A)-C(51A)-H(51A)	120.0	C(7)-C(8)-H(8C)	109.5
C(50A)-C(51A)-H(51A)	120.0	H(8A)-C(8)-H(8C)	109.5
C(51A)-C(52A)-C(53A)	120.0	H(8B)-C(8)-H(8C)	109.5
C(51A)-C(52A)-H(52A)	120.0		
C(53A)-C(52A)-H(52A)	120.0		
C(52A)-C(53A)-C(48A)	120.0		
C(52A)-C(53A)-H(53A)	120.0		
C(48A)-C(53A)-H(53A)	120.0		
C(49B)-C(48B)-C(53B)	120.0		
C(49B)-C(48B)-Si(3)	123.3(7)		
C(53B)-C(48B)-Si(3)	116.5(7)		
C(48B)-C(49B)-C(50B)	120.0		
C(48B)-C(49B)-H(49B)	120.0		
C(50B)-C(49B)-H(49B)	120.0		
C(49B)-C(50B)-C(51B)	120.0		
C(49B)-C(50B)-H(50B)	120.0		
C(51B)-C(50B)-H(50B)	120.0		
C(52B)-C(51B)-C(50B)	120.0		
C(52B)-C(51B)-H(51B)	120.0		
C(50B)-C(51B)-H(51B)	120.0		
C(51B)-C(52B)-C(53B)	120.0		
C(51B)-C(52B)-H(52B)	120.0		
C(53B)-C(52B)-H(52B)	120.0		
C(52B)-C(53B)-C(48B)	120.0		
C(52B)-C(53B)-H(53B)	120.0		
C(48B)-C(53B)-H(53B)	120.0		
C(30)-C(31)-H(31A)	109.5		
C(30)-C(31)-H(31B)	109.5		
H(31A)-C(31)-H(31B)	109.5		
C(30)-C(31)-H(31C)	109.5		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	26(1)	27(1)	28(1)	-3(1)	2(1)	-2(1)
Si(1)	26(1)	30(1)	47(1)	-2(1)	3(1)	-1(1)
Si(2)	30(1)	36(1)	32(1)	-6(1)	7(1)	-4(1)
Si(3)	32(1)	32(1)	35(1)	-6(1)	4(1)	2(1)
C(13)	21(3)	31(3)	30(2)	-1(2)	3(2)	6(2)
N(1)	24(2)	36(2)	36(2)	2(2)	9(2)	-7(2)
N(5)	35(3)	35(2)	32(2)	0(2)	1(2)	-11(2)
N(2)	23(2)	34(2)	29(2)	2(2)	2(2)	1(2)
N(4)	36(3)	31(2)	36(2)	1(2)	0(2)	-11(2)
N(3)	27(2)	25(2)	29(2)	-4(2)	1(2)	1(2)
C(15)	40(3)	50(3)	34(3)	11(2)	14(2)	-3(3)
C(21)	33(3)	31(3)	29(2)	-2(2)	-1(2)	0(2)
C(29)	38(3)	31(3)	38(3)	5(2)	11(2)	-5(2)
C(24)	29(3)	32(3)	38(3)	3(2)	4(2)	-10(2)
C(43)	42(4)	62(4)	35(3)	-12(3)	1(2)	1(3)
C(7)	53(4)	32(3)	74(4)	-6(3)	15(3)	-16(3)
C(6)	23(3)	56(3)	44(3)	0(3)	8(2)	-19(3)
C(1)	29(3)	47(3)	39(3)	-6(2)	12(2)	-19(3)
C(17)	40(3)	49(3)	24(2)	-1(2)	-1(2)	4(3)
C(16)	28(3)	32(3)	30(3)	1(2)	4(2)	6(2)
C(42)	38(3)	45(3)	24(2)	-2(2)	10(2)	-8(3)
C(22)	52(4)	36(3)	47(3)	-1(2)	0(3)	-17(3)
C(25)	33(3)	37(3)	43(3)	2(2)	3(2)	-2(3)
C(14)	43(4)	51(3)	38(3)	6(2)	11(3)	-18(3)
C(2)	35(3)	42(3)	49(3)	-2(3)	10(3)	-16(3)
C(27)	46(4)	64(4)	42(3)	1(3)	13(3)	-11(3)
C(20)	34(3)	31(3)	34(3)	-5(2)	-3(2)	0(2)
C(19)	42(3)	39(3)	35(3)	-6(2)	-11(2)	-8(3)
C(28)	31(3)	52(3)	44(3)	12(2)	5(2)	-1(3)
C(23)	42(3)	33(3)	51(3)	3(2)	4(3)	-18(3)

C(18)	43(4)	55(4)	30(3)	-8(2)	-7(2)	-1(3)
C(33)	39(4)	41(3)	47(3)	15(2)	10(3)	10(3)
C(10)	23(3)	61(4)	49(3)	-1(3)	1(2)	-2(3)
C(30)	38(4)	46(3)	57(3)	1(3)	7(3)	4(3)
C(47)	41(4)	62(4)	45(3)	-9(3)	0(3)	-11(3)
C(36A)	33(3)	28(5)	37(3)	-1(3)	6(2)	9(3)
C(37A)	42(3)	45(6)	46(3)	3(4)	7(3)	7(4)
C(38A)	54(4)	59(6)	49(3)	12(5)	5(3)	8(5)
C(39A)	31(4)	80(9)	43(5)	-10(6)	-5(3)	18(6)
C(40A)	34(4)	56(5)	45(5)	3(4)	4(3)	-4(4)
C(41A)	37(3)	40(4)	38(4)	9(3)	-6(3)	-2(3)
C(36B)	33(3)	28(5)	37(3)	-1(3)	6(2)	9(3)
C(37B)	42(3)	45(6)	46(3)	3(4)	7(3)	7(4)
C(38B)	54(4)	59(6)	49(3)	12(5)	5(3)	8(5)
C(39B)	31(4)	80(9)	43(5)	-10(6)	-5(3)	18(6)
C(40B)	34(4)	56(5)	45(5)	3(4)	4(3)	-4(4)
C(41B)	37(3)	40(4)	38(4)	9(3)	-6(3)	-2(3)
C(12)	46(4)	77(4)	63(4)	15(3)	13(3)	17(3)
C(45)	40(4)	101(5)	40(3)	-7(3)	-6(3)	-3(4)
C(11)	41(4)	87(5)	53(3)	-4(3)	15(3)	-11(3)
C(5)	32(3)	76(4)	55(3)	-8(3)	5(3)	-23(3)
C(9)	78(5)	36(3)	107(5)	-11(3)	37(4)	8(3)
C(26)	40(4)	56(4)	52(3)	-7(3)	16(3)	-1(3)
C(34)	71(5)	45(4)	71(4)	4(3)	24(3)	13(3)
C(44)	47(4)	89(5)	42(3)	-5(3)	2(3)	24(4)
C(4)	52(4)	72(4)	62(4)	-24(3)	8(3)	-28(4)
C(3)	50(4)	54(4)	63(4)	-20(3)	17(3)	-20(3)
C(35)	48(4)	65(4)	69(4)	17(3)	19(3)	13(3)
C(46)	56(4)	72(4)	50(3)	-15(3)	-1(3)	-24(4)
C(32)	63(4)	61(4)	67(4)	5(3)	16(3)	12(3)
C(48A)	32(4)	32(3)	32(3)	4(3)	2(3)	7(3)
C(49A)	52(7)	30(3)	39(4)	-3(3)	-5(4)	7(4)
C(50A)	61(5)	43(4)	61(5)	-3(4)	-13(4)	14(4)
C(51A)	50(5)	60(5)	50(4)	-23(4)	-11(4)	21(4)
C(52A)	56(4)	68(5)	42(4)	-7(4)	-3(3)	16(4)

C(53A)	41(4)	54(5)	38(3)	-2(4)	4(3)	17(4)
C(48B)	32(4)	32(3)	32(3)	4(3)	2(3)	7(3)
C(49B)	52(7)	30(3)	39(4)	-3(3)	-5(4)	7(4)
C(50B)	61(5)	43(4)	61(5)	-3(4)	-13(4)	14(4)
C(51B)	50(5)	60(5)	50(4)	-23(4)	-11(4)	21(4)
C(52B)	56(4)	68(5)	42(4)	-7(4)	-3(3)	16(4)
C(53B)	41(4)	54(5)	38(3)	-2(4)	4(3)	17(4)
C(31)	38(4)	74(5)	117(5)	6(4)	-4(4)	4(4)
C(8)	46(4)	75(5)	88(4)	12(4)	6(3)	-8(3)

Complex 2b

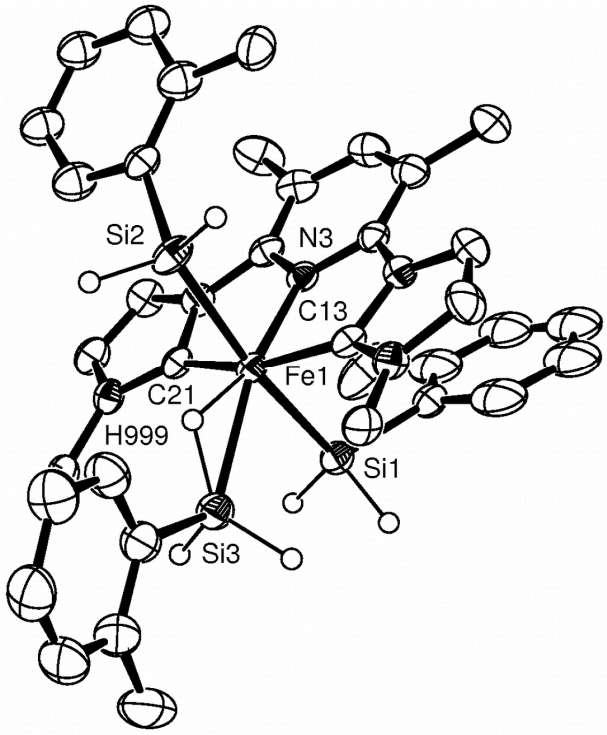

Table 1. Crystal data and structure refinement for **2b**.

Identification code	2b	
Empirical formula	C58 H73 Fe N5 Si3	
Formula weight	980.33	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 14.6347(5) Å	α= 90°.
	b = 17.4275(7) Å	β= 90.266(2)°.
	c = 20.4980(7) Å	γ = 90°.
Volume	5227.9(3) Å^3	
Z	4	
Density (calculated)	1.246 Mg/m^3	
Absorption coefficient	0.400 mm^{-1}	
F(000)	2096	

Crystal size	0.40 x 0.36 x 0.36 mm^3
Theta range for data collection	3.02 to 27.59°.
Index ranges	-18<=h<=18, -22<=k<=22, -26<=l<=25
Reflections collected	60685
Independent reflections	11952 [R(int) = 0.0959]
Completeness to theta = 27.59°	98.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8693 and 0.8563
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11952 / 2 / 625
Goodness-of-fit on F^2	1.017
Final R indices [I>2sigma(I)]	R1 = 0.0684, wR2 = 0.1279
R indices (all data)	R1 = 0.1251, wR2 = 0.1468
Largest diff. peak and hole	0.485 and -0.485 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 2b. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3475(2)	4584(2)	1882(2)	31(1)
C(2)	3660(2)	5262(2)	2230(2)	33(1)
C(3)	2972(3)	5558(2)	2611(2)	40(1)
C(4)	2125(3)	5218(2)	2635(2)	44(1)
C(5)	1936(2)	4591(2)	2249(2)	40(1)
C(6)	2600(2)	4260(2)	1857(2)	32(1)
C(7)	4556(3)	5689(2)	2145(2)	42(1)
C(8)	4800(3)	6231(2)	2701(2)	56(1)
C(9)	4545(3)	6156(2)	1516(2)	66(1)
C(10)	2340(2)	3614(2)	1399(2)	37(1)
C(11)	1794(3)	2976(2)	1728(2)	45(1)
C(12)	1784(3)	3937(2)	821(2)	45(1)
C(13)	4839(2)	3726(2)	1670(2)	26(1)
C(14)	4202(3)	4373(2)	815(2)	39(1)
C(15)	4859(2)	3955(2)	559(2)	37(1)
C(16)	5947(2)	3011(2)	1085(2)	26(1)
C(17)	6459(2)	2739(2)	564(2)	33(1)
C(18)	7068(2)	2159(2)	711(2)	36(1)
C(19)	7193(2)	1850(2)	1327(2)	34(1)
C(20)	6670(2)	2182(2)	1815(2)	27(1)
C(21)	6051(2)	2420(2)	2867(2)	25(1)
C(22)	7170(2)	1481(2)	2836(2)	34(1)
C(23)	6894(2)	1549(2)	3446(2)	35(1)
C(24)	5875(2)	2372(2)	4101(2)	30(1)
C(25)	6443(2)	2813(2)	4500(2)	35(1)
C(26)	6090(3)	3064(2)	5088(2)	44(1)
C(27)	5219(3)	2886(2)	5274(2)	50(1)
C(28)	4684(3)	2421(2)	4886(2)	46(1)
C(29)	5003(2)	2138(2)	4298(2)	36(1)
C(30)	7420(2)	3002(2)	4325(2)	40(1)

C(31)	7655(3)	3842(2)	4469(2)	59(1)
C(32)	8084(3)	2471(2)	4688(2)	52(1)
C(33)	4468(3)	1547(2)	3917(2)	44(1)
C(34)	3445(3)	1560(3)	4032(2)	61(1)
C(35)	4843(3)	748(2)	4085(2)	62(1)
C(36)	6352(3)	3014(2)	-127(2)	43(1)
C(37)	7842(3)	1192(2)	1422(2)	51(1)
C(38A)	7265(3)	4173(3)	1819(2)	29(1)
C(39A)	8099(3)	3833(3)	1674(2)	69(1)
C(40A)	8539(3)	4010(3)	1094(3)	69(1)
C(41A)	8146(4)	4526(3)	658(2)	69(1)
C(42A)	7312(4)	4866(3)	803(2)	69(1)
C(43A)	6871(3)	4689(3)	1383(3)	69(1)
C(44A)	8504(6)	3285(5)	2140(6)	88(3)
C(38B)	7536(4)	3903(4)	2063(3)	29(1)
C(39B)	8160(5)	3420(4)	2370(3)	69(1)
C(40B)	8970(4)	3226(4)	2060(4)	69(1)
C(41B)	9157(4)	3515(4)	1443(4)	69(1)
C(42B)	8534(5)	3998(5)	1135(3)	69(1)
C(43B)	7723(5)	4192(4)	1445(3)	69(1)
C(44B)	7067(7)	4707(6)	1176(5)	53(3)
C(45A)	4887(5)	1225(4)	1813(3)	29(1)
C(46A)	5022(4)	939(3)	1183(3)	42(1)
C(47A)	5446(5)	225(4)	1086(4)	42(1)
C(48A)	5716(4)	-203(4)	1627(3)	42(1)
C(49A)	5599(4)	57(4)	2246(3)	42(1)
C(50A)	5194(6)	775(4)	2320(4)	42(1)
C(51A)	4711(5)	1362(4)	584(4)	44(2)
C(45B)	4771(8)	1372(7)	1586(5)	29(1)
C(46B)	5201(7)	704(5)	1780(5)	42(1)
C(47B)	5567(8)	216(7)	1314(5)	42(1)
C(48B)	5473(7)	391(5)	650(5)	42(1)
C(49B)	5016(7)	1013(6)	462(6)	42(1)
C(50B)	4683(8)	1495(6)	926(6)	42(1)
C(51B)	5294(7)	497(6)	2479(6)	41(3)

C(52)	3602(3)	3845(2)	3621(2)	39(1)
C(53)	3347(3)	4293(2)	4166(2)	49(1)
C(54)	2451(3)	4293(2)	4379(2)	57(1)
C(55)	1786(3)	3863(2)	4077(2)	55(1)
C(56)	2011(3)	3407(2)	3552(2)	51(1)
C(57)	2914(3)	3404(2)	3335(2)	43(1)
C(58)	4051(3)	4772(3)	4522(2)	69(1)
N(1)	4181(2)	4247(2)	1487(1)	29(1)
N(2)	5259(2)	3557(1)	1077(1)	28(1)
N(3)	6060(2)	2745(1)	1696(1)	24(1)
N(4)	6663(2)	2009(1)	2477(1)	28(1)
N(5)	6222(2)	2115(1)	3474(1)	28(1)
Si(1)	6494(1)	4041(1)	2564(1)	30(1)
Si(2)	4313(1)	2165(1)	2079(1)	32(1)
Si(3)	4794(1)	3893(1)	3271(1)	33(1)
Fe(1)	5326(1)	3141(1)	2385(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for 2b.

C(1)-C(6)	1.401(5)	C(14)-C(15)	1.316(5)
C(1)-C(2)	1.407(4)	C(14)-N(1)	1.395(4)
C(1)-N(1)	1.440(4)	C(14)-H(14)	0.9500
C(2)-C(3)	1.376(5)	C(15)-N(2)	1.395(4)
C(2)-C(7)	1.519(5)	C(15)-H(15)	0.9500
C(3)-C(4)	1.376(5)	C(16)-N(3)	1.345(4)
C(3)-H(3)	0.9500	C(16)-N(2)	1.386(4)
C(4)-C(5)	1.377(5)	C(16)-C(17)	1.389(4)
C(4)-H(4)	0.9500	C(17)-C(18)	1.380(5)
C(5)-C(6)	1.390(5)	C(17)-C(36)	1.502(5)
C(5)-H(5)	0.9500	C(18)-C(19)	1.384(5)
C(6)-C(10)	1.513(5)	C(18)-H(18)	0.9500
C(7)-C(8)	1.522(5)	C(19)-C(20)	1.388(4)
C(7)-C(9)	1.526(5)	C(19)-C(37)	1.501(5)
C(7)-H(7)	1.0000	C(20)-N(3)	1.349(4)
C(8)-H(8A)	0.9800	C(20)-N(4)	1.392(4)
C(8)-H(8B)	0.9800	C(21)-N(5)	1.373(4)
C(8)-H(8C)	0.9800	C(21)-N(4)	1.400(4)
C(9)-H(9A)	0.9800	C(21)-Fe(1)	1.916(3)
C(9)-H(9B)	0.9800	C(22)-C(23)	1.320(5)
C(9)-H(9C)	0.9800	C(22)-N(4)	1.390(4)
C(10)-C(11)	1.528(5)	C(22)-H(22)	0.9500
C(10)-C(12)	1.542(5)	C(23)-N(5)	1.395(4)
C(10)-H(10)	1.0000	C(23)-H(23)	0.9500
C(11)-H(11A)	0.9800	C(24)-C(25)	1.394(5)
C(11)-H(11B)	0.9800	C(24)-C(29)	1.402(5)
C(11)-H(11C)	0.9800	C(24)-N(5)	1.456(4)
C(12)-H(12A)	0.9800	C(25)-C(26)	1.386(5)
C(12)-H(12B)	0.9800	C(25)-C(30)	1.512(5)
C(12)-H(12C)	0.9800	C(26)-C(27)	1.366(6)
C(13)-N(1)	1.375(4)	C(26)-H(26)	0.9500
C(13)-N(2)	1.396(4)	C(27)-C(28)	1.377(6)
C(13)-Fe(1)	1.921(3)	C(27)-H(27)	0.9500

C(28)-C(29)	1.385(5)	C(41A)-H(41A)	0.9500
C(28)-H(28)	0.9500	C(42A)-C(43A)	1.3900
C(29)-C(33)	1.510(5)	C(42A)-H(42A)	0.9500
C(30)-C(31)	1.532(5)	C(43A)-H(43A)	0.9500
C(30)-C(32)	1.532(5)	C(44A)-H(44A)	0.9800
C(30)-H(30)	1.0000	C(44A)-H(44B)	0.9800
C(31)-H(31A)	0.9800	C(44A)-H(44C)	0.9800
C(31)-H(31B)	0.9800	C(38B)-C(39B)	1.3900
C(31)-H(31C)	0.9800	C(38B)-C(43B)	1.3900
C(32)-H(32A)	0.9800	C(38B)-Si(1)	1.859(5)
C(32)-H(32B)	0.9800	C(39B)-C(40B)	1.3900
C(32)-H(32C)	0.9800	C(39B)-H(39B)	0.9500
C(33)-C(34)	1.517(5)	C(40B)-C(41B)	1.3900
C(33)-C(35)	1.534(5)	C(40B)-H(40B)	0.9500
C(33)-H(33)	1.0000	C(41B)-C(42B)	1.3900
C(34)-H(34A)	0.9800	C(41B)-H(41B)	0.9500
C(34)-H(34B)	0.9800	C(42B)-C(43B)	1.3900
C(34)-H(34C)	0.9800	C(42B)-H(42B)	0.9500
C(35)-H(35A)	0.9800	C(43B)-C(44B)	1.423(12)
C(35)-H(35B)	0.9800	C(44B)-H(44D)	0.9800
C(35)-H(35C)	0.9800	C(44B)-H(44E)	0.9800
C(36)-H(36A)	0.9800	C(44B)-H(44F)	0.9800
C(36)-H(36B)	0.9800	C(45A)-C(50A)	1.376(10)
C(36)-H(36C)	0.9800	C(45A)-C(46A)	1.399(9)
C(37)-H(37A)	0.9800	C(45A)-Si(2)	1.921(7)
C(37)-H(37B)	0.9800	C(46A)-C(47A)	1.404(9)
C(37)-H(37C)	0.9800	C(46A)-C(51A)	1.501(9)
C(38A)-C(39A)	1.3900	C(47A)-C(48A)	1.393(9)
C(38A)-C(43A)	1.3900	C(47A)-H(47A)	0.9500
C(38A)-Si(1)	1.917(4)	C(48A)-C(49A)	1.358(9)
C(39A)-C(40A)	1.3900	C(48A)-H(48A)	0.9500
C(39A)-C(44A)	1.475(10)	C(49A)-C(50A)	1.394(9)
C(40A)-C(41A)	1.3900	C(49A)-H(49A)	0.9500
C(40A)-H(40A)	0.9500	C(50A)-H(50A)	0.9500
C(41A)-C(42A)	1.3900	C(51A)-H(51A)	0.9800

C(51A)-H(51B)	0.9800	C(54)-C(55)	1.373(6)
C(51A)-H(51C)	0.9800	C(54)-H(54)	0.9500
C(45B)-C(50B)	1.376(15)	C(55)-C(56)	1.379(6)
C(45B)-C(46B)	1.382(14)	C(55)-H(55)	0.9500
C(45B)-Si(2)	1.839(12)	C(56)-C(57)	1.395(5)
C(46B)-C(47B)	1.388(15)	C(56)-H(56)	0.9500
C(46B)-C(51B)	1.483(15)	C(57)-H(57)	0.9500
C(47B)-C(48B)	1.402(14)	C(58)-H(58A)	0.9800
C(47B)-H(47B)	0.9500	C(58)-H(58B)	0.9800
C(48B)-C(49B)	1.329(14)	C(58)-H(58C)	0.9800
C(48B)-H(48B)	0.9500	N(3)-Fe(1)	1.908(2)
C(49B)-C(50B)	1.361(15)	Si(1)-Fe(1)	2.3475(10)
C(49B)-H(49B)	0.9500	Si(1)-H(1B)	1.38(4)
C(50B)-H(50B)	0.9500	Si(1)-H(1A)	1.44(4)
C(51B)-H(51D)	0.9800	Si(2)-Fe(1)	2.3412(10)
C(51B)-H(51E)	0.9800	Si(2)-H(2A)	1.38(4)
C(51B)-H(51F)	0.9800	Si(2)-H(2B)	1.39(4)
C(52)-C(57)	1.394(5)	Si(3)-Fe(1)	2.3727(11)
C(52)-C(53)	1.414(5)	Si(3)-H(3B)	1.396(10)
C(52)-Si(3)	1.892(4)	Si(3)-H(3A)	1.388(10)
C(53)-C(54)	1.385(6)	Si(3)-H(999)	1.45(3)
C(53)-C(58)	1.511(6)	Fe(1)-H(999)	1.58(3)

C(6)-C(1)-C(2)	122.1(3)	C(4)-C(5)-C(6)	121.6(3)
C(6)-C(1)-N(1)	118.3(3)	C(4)-C(5)-H(5)	119.2
C(2)-C(1)-N(1)	119.4(3)	C(6)-C(5)-H(5)	119.2
C(3)-C(2)-C(1)	117.6(3)	C(5)-C(6)-C(1)	116.9(3)
C(3)-C(2)-C(7)	121.1(3)	C(5)-C(6)-C(10)	119.6(3)
C(1)-C(2)-C(7)	121.1(3)	C(1)-C(6)-C(10)	123.4(3)
C(4)-C(3)-C(2)	121.4(3)	C(2)-C(7)-C(8)	114.6(3)
C(4)-C(3)-H(3)	119.3	C(2)-C(7)-C(9)	110.6(3)
C(2)-C(3)-H(3)	119.3	C(8)-C(7)-C(9)	107.7(3)
C(3)-C(4)-C(5)	119.9(4)	C(2)-C(7)-H(7)	107.9
C(3)-C(4)-H(4)	120.0	C(8)-C(7)-H(7)	107.9
C(5)-C(4)-H(4)	120.0	C(9)-C(7)-H(7)	107.9

C(7)-C(8)-H(8A)	109.5	N(1)-C(14)-H(14)	125.5
C(7)-C(8)-H(8B)	109.5	C(14)-C(15)-N(2)	106.1(3)
H(8A)-C(8)-H(8B)	109.5	C(14)-C(15)-H(15)	127.0
C(7)-C(8)-H(8C)	109.5	N(2)-C(15)-H(15)	127.0
H(8A)-C(8)-H(8C)	109.5	N(3)-C(16)-N(2)	109.4(3)
H(8B)-C(8)-H(8C)	109.5	N(3)-C(16)-C(17)	122.3(3)
C(7)-C(9)-H(9A)	109.5	N(2)-C(16)-C(17)	128.3(3)
C(7)-C(9)-H(9B)	109.5	C(18)-C(17)-C(16)	115.6(3)
H(9A)-C(9)-H(9B)	109.5	C(18)-C(17)-C(36)	120.2(3)
C(7)-C(9)-H(9C)	109.5	C(16)-C(17)-C(36)	124.1(3)
H(9A)-C(9)-H(9C)	109.5	C(17)-C(18)-C(19)	124.5(3)
H(9B)-C(9)-H(9C)	109.5	C(17)-C(18)-H(18)	117.8
C(6)-C(10)-C(11)	113.4(3)	C(19)-C(18)-H(18)	117.8
C(6)-C(10)-C(12)	109.6(3)	C(18)-C(19)-C(20)	115.1(3)
C(11)-C(10)-C(12)	109.3(3)	C(18)-C(19)-C(37)	119.7(3)
C(6)-C(10)-H(10)	108.1	C(20)-C(19)-C(37)	125.1(3)
C(11)-C(10)-H(10)	108.1	N(3)-C(20)-C(19)	122.7(3)
C(12)-C(10)-H(10)	108.1	N(3)-C(20)-N(4)	109.0(3)
C(10)-C(11)-H(11A)	109.5	C(19)-C(20)-N(4)	128.3(3)
C(10)-C(11)-H(11B)	109.5	N(5)-C(21)-N(4)	101.8(2)
H(11A)-C(11)-H(11B)	109.5	N(5)-C(21)-Fe(1)	144.9(2)
C(10)-C(11)-H(11C)	109.5	N(4)-C(21)-Fe(1)	113.3(2)
H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-N(4)	106.0(3)
H(11B)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	127.0
C(10)-C(12)-H(12A)	109.5	N(4)-C(22)-H(22)	127.0
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-N(5)	108.7(3)
H(12A)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	125.6
C(10)-C(12)-H(12C)	109.5	N(5)-C(23)-H(23)	125.6
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-C(29)	122.2(3)
H(12B)-C(12)-H(12C)	109.5	C(25)-C(24)-N(5)	118.6(3)
N(1)-C(13)-N(2)	102.2(3)	C(29)-C(24)-N(5)	119.1(3)
N(1)-C(13)-Fe(1)	144.8(3)	C(26)-C(25)-C(24)	117.4(3)
N(2)-C(13)-Fe(1)	112.9(2)	C(26)-C(25)-C(30)	119.7(3)
C(15)-C(14)-N(1)	109.0(3)	C(24)-C(25)-C(30)	122.9(3)
C(15)-C(14)-H(14)	125.5	C(27)-C(26)-C(25)	121.5(4)

C(27)-C(26)-H(26)	119.2	C(33)-C(34)-H(34A)	109.5
C(25)-C(26)-H(26)	119.2	C(33)-C(34)-H(34B)	109.5
C(26)-C(27)-C(28)	120.1(4)	H(34A)-C(34)-H(34B)	109.5
C(26)-C(27)-H(27)	119.9	C(33)-C(34)-H(34C)	109.5
C(28)-C(27)-H(27)	119.9	H(34A)-C(34)-H(34C)	109.5
C(27)-C(28)-C(29)	121.2(4)	H(34B)-C(34)-H(34C)	109.5
C(27)-C(28)-H(28)	119.4	C(33)-C(35)-H(35A)	109.5
C(29)-C(28)-H(28)	119.4	C(33)-C(35)-H(35B)	109.5
C(28)-C(29)-C(24)	117.3(3)	H(35A)-C(35)-H(35B)	109.5
C(28)-C(29)-C(33)	121.2(3)	C(33)-C(35)-H(35C)	109.5
C(24)-C(29)-C(33)	121.3(3)	H(35A)-C(35)-H(35C)	109.5
C(25)-C(30)-C(31)	111.9(3)	H(35B)-C(35)-H(35C)	109.5
C(25)-C(30)-C(32)	110.6(3)	C(17)-C(36)-H(36A)	109.5
C(31)-C(30)-C(32)	110.0(3)	C(17)-C(36)-H(36B)	109.5
C(25)-C(30)-H(30)	108.1	H(36A)-C(36)-H(36B)	109.5
C(31)-C(30)-H(30)	108.1	C(17)-C(36)-H(36C)	109.5
C(32)-C(30)-H(30)	108.1	H(36A)-C(36)-H(36C)	109.5
C(30)-C(31)-H(31A)	109.5	H(36B)-C(36)-H(36C)	109.5
C(30)-C(31)-H(31B)	109.5	C(19)-C(37)-H(37A)	109.5
H(31A)-C(31)-H(31B)	109.5	C(19)-C(37)-H(37B)	109.5
C(30)-C(31)-H(31C)	109.5	H(37A)-C(37)-H(37B)	109.5
H(31A)-C(31)-H(31C)	109.5	C(19)-C(37)-H(37C)	109.5
H(31B)-C(31)-H(31C)	109.5	H(37A)-C(37)-H(37C)	109.5
C(30)-C(32)-H(32A)	109.5	H(37B)-C(37)-H(37C)	109.5
C(30)-C(32)-H(32B)	109.5	C(39A)-C(38A)-C(43A)	120.0
H(32A)-C(32)-H(32B)	109.5	C(39A)-C(38A)-Si(1)	129.8(3)
C(30)-C(32)-H(32C)	109.5	C(43A)-C(38A)-Si(1)	110.2(3)
H(32A)-C(32)-H(32C)	109.5	C(38A)-C(39A)-C(40A)	120.0
H(32B)-C(32)-H(32C)	109.5	C(38A)-C(39A)-C(44A)	119.2(5)
C(29)-C(33)-C(34)	114.7(3)	C(40A)-C(39A)-C(44A)	120.8(5)
C(29)-C(33)-C(35)	108.6(3)	C(41A)-C(40A)-C(39A)	120.0
C(34)-C(33)-C(35)	109.3(3)	C(41A)-C(40A)-H(40A)	120.0
C(29)-C(33)-H(33)	108.0	C(39A)-C(40A)-H(40A)	120.0
C(34)-C(33)-H(33)	108.0	C(40A)-C(41A)-C(42A)	120.0
C(35)-C(33)-H(33)	108.0	C(40A)-C(41A)-H(41A)	120.0

C(42A)-C(41A)-H(41A)	120.0	C(45A)-C(46A)-C(51A)	122.5(6)
C(43A)-C(42A)-C(41A)	120.0	C(47A)-C(46A)-C(51A)	116.8(6)
C(43A)-C(42A)-H(42A)	120.0	C(48A)-C(47A)-C(46A)	119.1(7)
C(41A)-C(42A)-H(42A)	120.0	C(48A)-C(47A)-H(47A)	120.5
C(42A)-C(43A)-C(38A)	120.0	C(46A)-C(47A)-H(47A)	120.5
C(42A)-C(43A)-H(43A)	120.0	C(49A)-C(48A)-C(47A)	121.9(6)
C(38A)-C(43A)-H(43A)	120.0	C(49A)-C(48A)-H(48A)	119.0
C(39B)-C(38B)-C(43B)	120.0	C(47A)-C(48A)-H(48A)	119.0
C(39B)-C(38B)-Si(1)	111.5(4)	C(48A)-C(49A)-C(50A)	117.2(7)
C(43B)-C(38B)-Si(1)	128.4(4)	C(48A)-C(49A)-H(49A)	121.4
C(40B)-C(39B)-C(38B)	120.0	C(50A)-C(49A)-H(49A)	121.4
C(40B)-C(39B)-H(39B)	120.0	C(45A)-C(50A)-C(49A)	124.5(8)
C(38B)-C(39B)-H(39B)	120.0	C(45A)-C(50A)-H(50A)	117.8
C(39B)-C(40B)-C(41B)	120.0	C(49A)-C(50A)-H(50A)	117.8
C(39B)-C(40B)-H(40B)	120.0	C(50B)-C(45B)-C(46B)	117.0(11)
C(41B)-C(40B)-H(40B)	120.0	C(50B)-C(45B)-Si(2)	113.0(8)
C(40B)-C(41B)-C(42B)	120.0	C(46B)-C(45B)-Si(2)	130.0(8)
C(40B)-C(41B)-H(41B)	120.0	C(45B)-C(46B)-C(47B)	119.7(10)
C(42B)-C(41B)-H(41B)	120.0	C(45B)-C(46B)-C(51B)	121.5(10)
C(43B)-C(42B)-C(41B)	120.0	C(47B)-C(46B)-C(51B)	118.8(9)
C(43B)-C(42B)-H(42B)	120.0	C(46B)-C(47B)-C(48B)	119.9(11)
C(41B)-C(42B)-H(42B)	120.0	C(46B)-C(47B)-H(47B)	120.1
C(42B)-C(43B)-C(38B)	120.0	C(48B)-C(47B)-H(47B)	120.1
C(42B)-C(43B)-C(44B)	123.5(6)	C(49B)-C(48B)-C(47B)	120.4(10)
C(38B)-C(43B)-C(44B)	116.5(6)	C(49B)-C(48B)-H(48B)	119.8
C(43B)-C(44B)-H(44D)	109.5	C(47B)-C(48B)-H(48B)	119.8
C(43B)-C(44B)-H(44E)	109.5	C(48B)-C(49B)-C(50B)	118.9(10)
H(44D)-C(44B)-H(44E)	109.5	C(48B)-C(49B)-H(49B)	120.6
C(43B)-C(44B)-H(44F)	109.5	C(50B)-C(49B)-H(49B)	120.6
H(44D)-C(44B)-H(44F)	109.5	C(49B)-C(50B)-C(45B)	124.0(10)
H(44E)-C(44B)-H(44F)	109.5	C(49B)-C(50B)-H(50B)	118.0
C(50A)-C(45A)-C(46A)	116.6(7)	C(45B)-C(50B)-H(50B)	118.0
C(50A)-C(45A)-Si(2)	114.4(6)	C(57)-C(52)-C(53)	116.3(4)
C(46A)-C(45A)-Si(2)	129.0(5)	C(57)-C(52)-Si(3)	122.1(3)
C(45A)-C(46A)-C(47A)	120.7(6)	C(53)-C(52)-Si(3)	121.5(3)

C(54)-C(53)-C(52)	120.2(4)	C(23)-N(5)-C(24)	120.1(3)
C(54)-C(53)-C(58)	119.5(4)	C(38B)-Si(1)-Fe(1)	115.2(2)
C(52)-C(53)-C(58)	120.3(4)	C(38A)-Si(1)-Fe(1)	112.73(15)
C(55)-C(54)-C(53)	121.8(4)	C(38B)-Si(1)-H(1B)	91.4(18)
C(55)-C(54)-H(54)	119.1	C(38A)-Si(1)-H(1B)	112.6(18)
C(53)-C(54)-H(54)	119.1	Fe(1)-Si(1)-H(1B)	114.6(18)
C(54)-C(55)-C(56)	119.7(4)	C(38B)-Si(1)-H(1A)	110.8(17)
C(54)-C(55)-H(55)	120.2	C(38A)-Si(1)-H(1A)	94.1(17)
C(56)-C(55)-H(55)	120.2	Fe(1)-Si(1)-H(1A)	118.8(17)
C(55)-C(56)-C(57)	118.7(4)	H(1B)-Si(1)-H(1A)	102(2)
C(55)-C(56)-H(56)	120.6	C(45B)-Si(2)-Fe(1)	117.4(4)
C(57)-C(56)-H(56)	120.6	C(45A)-Si(2)-Fe(1)	114.7(2)
C(52)-C(57)-C(56)	123.2(4)	C(45B)-Si(2)-H(2A)	113.5(17)
C(52)-C(57)-H(57)	118.4	C(45A)-Si(2)-H(2A)	102.3(16)
C(56)-C(57)-H(57)	118.4	Fe(1)-Si(2)-H(2A)	113.2(16)
C(53)-C(58)-H(58A)	109.5	C(45B)-Si(2)-H(2B)	92.5(16)
C(53)-C(58)-H(58B)	109.5	C(45A)-Si(2)-H(2B)	108.0(16)
H(58A)-C(58)-H(58B)	109.5	Fe(1)-Si(2)-H(2B)	112.9(16)
C(53)-C(58)-H(58C)	109.5	H(2A)-Si(2)-H(2B)	105(2)
H(58A)-C(58)-H(58C)	109.5	C(52)-Si(3)-Fe(1)	124.94(12)
H(58B)-C(58)-H(58C)	109.5	C(52)-Si(3)-H(3B)	106.0(14)
C(13)-N(1)-C(14)	110.8(3)	Fe(1)-Si(3)-H(3B)	108.7(13)
C(13)-N(1)-C(1)	128.2(3)	C(52)-Si(3)-H(3A)	100.0(12)
C(14)-N(1)-C(1)	120.7(3)	Fe(1)-Si(3)-H(3A)	110.3(12)
C(16)-N(2)-C(15)	130.7(3)	H(3B)-Si(3)-H(3A)	105.1(18)
C(16)-N(2)-C(13)	117.3(3)	C(52)-Si(3)-H(999)	84.7(11)
C(15)-N(2)-C(13)	111.9(3)	Fe(1)-Si(3)-H(999)	40.5(11)
C(16)-N(3)-C(20)	119.8(3)	H(3B)-Si(3)-H(999)	122.7(17)
C(16)-N(3)-Fe(1)	119.9(2)	H(3A)-Si(3)-H(999)	128.8(16)
C(20)-N(3)-Fe(1)	120.3(2)	N(3)-Fe(1)-C(21)	80.38(12)
C(22)-N(4)-C(20)	130.8(3)	N(3)-Fe(1)-C(13)	80.48(12)
C(22)-N(4)-C(21)	112.2(3)	C(21)-Fe(1)-C(13)	160.86(14)
C(20)-N(4)-C(21)	117.0(2)	N(3)-Fe(1)-Si(2)	84.07(8)
C(21)-N(5)-C(23)	111.2(3)	C(21)-Fe(1)-Si(2)	90.62(9)
C(21)-N(5)-C(24)	128.2(3)	C(13)-Fe(1)-Si(2)	87.02(9)

N(3)-Fe(1)-Si(1)	86.87(8)
C(21)-Fe(1)-Si(1)	87.53(9)
C(13)-Fe(1)-Si(1)	91.82(9)
Si(2)-Fe(1)-Si(1)	170.94(4)
N(3)-Fe(1)-Si(3)	162.55(8)
C(21)-Fe(1)-Si(3)	98.66(10)
C(13)-Fe(1)-Si(3)	99.70(10)
Si(2)-Fe(1)-Si(3)	113.37(4)
Si(1)-Fe(1)-Si(3)	75.68(4)
N(3)-Fe(1)-H(999)	160.9(10)
C(21)-Fe(1)-H(999)	100.9(10)
C(13)-Fe(1)-H(999)	97.0(10)
Si(2)-Fe(1)-H(999)	76.8(10)
Si(1)-Fe(1)-H(999)	112.2(10)
Si(3)-Fe(1)-H(999)	36.6(10)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 2b. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(2)	26(2)	35(2)	2(1)	-5(2)	10(1)
C(2)	39(2)	27(2)	34(2)	3(1)	-13(2)	8(2)
C(3)	50(2)	26(2)	45(2)	-9(2)	-11(2)	11(2)
C(4)	46(2)	34(2)	51(2)	-6(2)	2(2)	18(2)
C(5)	33(2)	31(2)	57(2)	-2(2)	-1(2)	7(2)
C(6)	34(2)	24(2)	39(2)	0(2)	-6(2)	7(1)
C(7)	46(2)	30(2)	50(2)	0(2)	-8(2)	0(2)
C(8)	58(3)	34(2)	74(3)	-4(2)	-20(2)	-3(2)
C(9)	82(3)	46(3)	69(3)	17(2)	-11(3)	-16(2)
C(10)	37(2)	29(2)	44(2)	-2(2)	-8(2)	4(2)
C(11)	46(2)	33(2)	55(2)	-3(2)	-7(2)	-1(2)
C(12)	48(2)	38(2)	48(2)	-3(2)	-13(2)	6(2)
C(13)	26(2)	21(2)	32(2)	-3(1)	-3(1)	-3(1)
C(14)	46(2)	43(2)	29(2)	7(2)	-7(2)	6(2)
C(15)	45(2)	40(2)	25(2)	2(2)	-2(2)	0(2)
C(16)	26(2)	23(2)	29(2)	-3(1)	4(1)	-6(1)
C(17)	30(2)	37(2)	33(2)	-6(2)	2(2)	-6(2)
C(18)	24(2)	45(2)	38(2)	-11(2)	8(2)	-3(2)
C(19)	22(2)	37(2)	43(2)	-10(2)	-2(2)	1(2)
C(20)	20(2)	24(2)	37(2)	-4(1)	1(1)	-3(1)
C(21)	21(2)	22(2)	32(2)	1(1)	-1(1)	-4(1)
C(22)	26(2)	33(2)	43(2)	1(2)	0(2)	7(2)
C(23)	34(2)	24(2)	45(2)	5(2)	-2(2)	7(2)
C(24)	37(2)	23(2)	30(2)	6(1)	-1(2)	6(1)
C(25)	45(2)	26(2)	32(2)	12(2)	-6(2)	3(2)
C(26)	67(3)	36(2)	30(2)	5(2)	-7(2)	5(2)
C(27)	71(3)	47(2)	33(2)	3(2)	8(2)	16(2)
C(28)	46(2)	51(2)	40(2)	13(2)	11(2)	12(2)
C(29)	38(2)	30(2)	40(2)	11(2)	7(2)	7(2)
C(30)	46(2)	38(2)	37(2)	4(2)	-5(2)	-8(2)

C(31)	76(3)	50(3)	50(3)	4(2)	-11(2)	-20(2)
C(32)	45(2)	54(3)	58(3)	3(2)	-13(2)	-6(2)
C(33)	40(2)	46(2)	47(2)	5(2)	11(2)	-8(2)
C(34)	43(2)	74(3)	65(3)	15(2)	9(2)	-11(2)
C(35)	61(3)	36(2)	90(3)	6(2)	18(3)	-13(2)
C(36)	51(2)	47(2)	31(2)	-4(2)	10(2)	-2(2)
C(37)	42(2)	62(3)	48(2)	-13(2)	0(2)	25(2)
C(38A)	23(2)	27(2)	36(3)	-1(2)	-4(2)	-5(2)
C(39A)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(40A)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(41A)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(42A)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(43A)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(44A)	61(6)	54(6)	147(10)	-2(6)	-6(6)	-22(5)
C(38B)	23(2)	27(2)	36(3)	-1(2)	-4(2)	-5(2)
C(39B)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(40B)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(41B)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(42B)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(43B)	66(2)	69(2)	71(2)	-33(2)	18(2)	-39(2)
C(44B)	55(7)	49(6)	54(7)	0(5)	11(5)	-39(5)
C(45A)	23(2)	27(2)	36(3)	-1(2)	-4(2)	-5(2)
C(46A)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(47A)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(48A)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(49A)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(50A)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(51A)	47(4)	39(4)	45(4)	8(4)	-11(4)	-8(3)
C(45B)	23(2)	27(2)	36(3)	-1(2)	-4(2)	-5(2)
C(46B)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(47B)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(48B)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(49B)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(50B)	43(1)	34(1)	47(2)	-4(1)	-4(1)	6(1)
C(51B)	30(5)	27(6)	65(8)	-8(5)	-16(5)	-3(5)

C(52)	49(2)	33(2)	36(2)	2(2)	1(2)	7(2)
C(53)	59(3)	40(2)	48(2)	-5(2)	12(2)	5(2)
C(54)	66(3)	50(3)	54(3)	-4(2)	23(2)	12(2)
C(55)	48(3)	53(3)	64(3)	5(2)	19(2)	6(2)
C(56)	42(2)	57(3)	56(3)	3(2)	5(2)	5(2)
C(57)	41(2)	47(2)	42(2)	0(2)	7(2)	5(2)
C(58)	83(4)	63(3)	61(3)	-26(2)	18(3)	-4(3)
N(1)	30(2)	26(1)	32(2)	3(1)	-2(1)	5(1)
N(2)	33(2)	24(1)	25(1)	0(1)	-1(1)	0(1)
N(3)	21(1)	21(1)	28(1)	-3(1)	3(1)	-3(1)
N(4)	23(1)	27(2)	33(2)	-1(1)	1(1)	2(1)
N(5)	29(2)	23(1)	32(2)	5(1)	0(1)	2(1)
Si(1)	32(1)	29(1)	30(1)	-1(1)	-1(1)	-8(1)
Si(2)	24(1)	21(1)	51(1)	-2(1)	-5(1)	1(1)
Si(3)	39(1)	28(1)	34(1)	1(1)	-1(1)	5(1)
Fe(1)	22(1)	19(1)	28(1)	0(1)	1(1)	0(1)

Complex 3

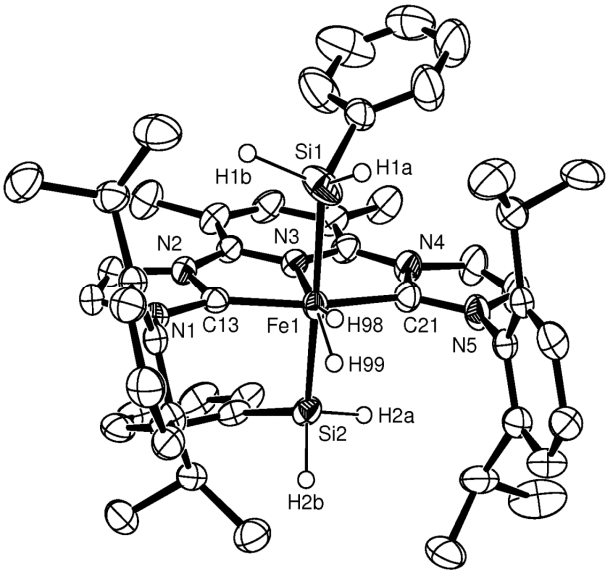

Table 1. Crystal data and structure refinement for **3**

Identification code	3	
Empirical formula	C49 H61 Fe N5 Si2	
Formula weight	832.06	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 12.2235(4) Å	α= 90°.
	b = 19.7035(8) Å	β= 90°.
	c = 37.4328(13) Å	γ = 90°.
Volume	9015.5(6) $Å^3$	
Z	8	
Density (calculated)	1.226 Mg/m^3	
Absorption coefficient	0.427 mm^{-1}	
F(000)	3552	
Crystal size	0.36 x 0.28 x 0.08 mm^3	
Theta range for data collection	2.55 to 27.54°.	
Index ranges	-15<=h<=15, -25<=k<=25, -48<=l<=48	
Reflections collected	99536	
Independent reflections	10340 [R(int) = 0.1130]	

Completeness to theta = 27.54°	99.5 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9667 and 0.8615
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10340 / 2 / 607
Goodness-of-fit on F^2	1.016
Final R indices [I>2sigma(I)]	R1 = 0.0553, wR2 = 0.1102
R indices (all data)	R1 = 0.1162, wR2 = 0.1303
Largest diff. peak and hole	0.428 and -0.587 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for 3 U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	8971(2)	2579(1)	1791(1)	27(1)
C(2)	8652(2)	2055(1)	2024(1)	29(1)
C(3)	9370(2)	1519(2)	2074(1)	35(1)
C(4)	10370(2)	1502(2)	1905(1)	39(1)
C(5)	10672(2)	2021(2)	1677(1)	35(1)
C(6)	9983(2)	2571(1)	1617(1)	30(1)
C(7)	7578(2)	2078(1)	2226(1)	31(1)
C(8)	7741(3)	2414(2)	2591(1)	43(1)
C(9)	7044(2)	1380(2)	2262(1)	41(1)
C(10)	10381(2)	3135(2)	1372(1)	37(1)
C(11)	11325(2)	3523(2)	1547(1)	48(1)
C(12)	10737(3)	2864(2)	1009(1)	54(1)
C(13)	7364(2)	3202(1)	1529(1)	26(1)
C(14)	8563(2)	3803(1)	1876(1)	33(1)
C(15)	7869(2)	4260(1)	1740(1)	32(1)
C(16)	6245(2)	4104(1)	1318(1)	28(1)
C(17)	5859(2)	4754(1)	1252(1)	37(1)
C(18)	4925(2)	4794(2)	1043(1)	42(1)
C(19)	4397(2)	4233(2)	896(1)	39(1)
C(20)	4865(2)	3606(2)	966(1)	34(1)
C(21)	5191(2)	2416(1)	967(1)	31(1)
C(22)	3666(3)	2735(2)	643(1)	47(1)
C(23)	3740(3)	2066(2)	631(1)	50(1)
C(24A)	5100(5)	1177(3)	865(2)	27(1)
C(25A)	4601(6)	790(4)	1129(2)	34(1)
C(26A)	4932(8)	124(4)	1186(2)	42(1)
C(27A)	5762(7)	-155(3)	979(2)	38(2)
C(28A)	6260(5)	232(2)	715(2)	41(2)
C(29A)	5929(4)	898(2)	658(1)	36(2)
C(30A)	4031(8)	1027(5)	1473(2)	43(2)

C(31A)	2823(8)	873(5)	1395(3)	70(3)
C(32A)	4342(10)	735(5)	1839(2)	66(3)
C(33A)	6489(6)	1289(3)	350(2)	45(2)
C(34A)	7675(7)	1100(4)	295(2)	68(3)
C(35A)	5875(9)	1180(6)	7(3)	66(3)
C(24B)	4886(4)	1159(3)	858(2)	27(1)
C(25B)	4718(7)	776(4)	1165(2)	34(1)
C(26B)	5057(9)	103(4)	1177(2)	42(1)
C(27B)	5565(7)	-187(2)	881(2)	51(3)
C(28B)	5733(5)	197(2)	575(2)	45(2)
C(29B)	5394(4)	870(2)	563(1)	31(2)
C(30B)	3596(7)	1064(5)	1339(2)	38(2)
C(31B)	2555(6)	762(4)	1173(2)	48(2)
C(32B)	3664(7)	893(4)	1736(2)	47(2)
C(33B)	5458(6)	1246(3)	204(2)	41(2)
C(34B)	4516(6)	1048(4)	-38(2)	60(2)
C(35B)	6564(8)	1119(6)	10(3)	66(3)
C(36)	6398(3)	5392(1)	1392(1)	48(1)
C(37)	3393(3)	4320(2)	664(1)	54(1)
C(38)	6863(2)	3301(2)	383(1)	38(1)
C(39)	6444(4)	3012(2)	83(1)	72(1)
C(40)	5919(4)	3374(3)	-183(1)	91(2)
C(41)	5809(3)	4050(3)	-162(1)	72(1)
C(42)	6198(4)	4371(2)	131(1)	91(2)
C(43)	6730(4)	4002(2)	397(1)	77(1)
C(44)	5014(2)	3513(1)	1996(1)	33(1)
C(45)	4146(3)	3962(2)	1938(1)	44(1)
C(46)	4043(3)	4567(2)	2123(1)	53(1)
C(47)	4807(3)	4751(2)	2370(1)	50(1)
C(48)	5681(3)	4326(2)	2435(1)	46(1)
C(49)	5775(3)	3718(2)	2251(1)	39(1)
N(1)	8276(2)	3163(1)	1744(1)	27(1)
N(2)	7145(2)	3901(1)	1523(1)	27(1)
N(3)	5774(2)	3545(1)	1174(1)	27(1)
N(4)	4549(2)	2962(1)	849(1)	35(1)
N(5)	4666(2)	1866(1)	825(1)	37(1)
Si(1)	7498(1)	2817(1)	770(1)	48(1)

Si(2)	5115(1)	2685(1)	1733(1)	31(1)
Fe(1)	6365(1)	2679(1)	1263(1)	27(1)

Table 3. Bond lengths [Å] and angles [°] for 3

C(1)-C(6)	1.399(4)	C(13)-Fe(1)	1.883(3)
C(1)-C(2)	1.406(4)	C(14)-C(15)	1.336(4)
C(1)-N(1)	1.441(3)	C(14)-N(1)	1.399(3)
C(2)-C(3)	1.385(4)	C(14)-H(14)	0.9500
C(2)-C(7)	1.517(4)	C(15)-N(2)	1.394(3)
C(3)-C(4)	1.377(4)	C(15)-H(15)	0.9500
C(3)-H(3)	0.9500	C(16)-N(3)	1.355(3)
C(4)-C(5)	1.381(4)	C(16)-C(17)	1.386(4)
C(4)-H(4)	0.9500	C(16)-N(2)	1.400(3)
C(5)-C(6)	1.391(4)	C(17)-C(18)	1.387(4)
C(5)-H(5)	0.9500	C(17)-C(36)	1.512(4)
C(6)-C(10)	1.521(4)	C(18)-C(19)	1.393(4)
C(7)-C(8)	1.529(4)	C(18)-H(18)	0.9500
C(7)-C(9)	1.529(4)	C(19)-C(20)	1.386(4)
C(7)-H(7)	1.0000	C(19)-C(37)	1.512(4)
C(8)-H(8A)	0.9800	C(20)-N(3)	1.364(3)
C(8)-H(8B)	0.9800	C(20)-N(4)	1.398(4)
C(8)-H(8C)	0.9800	C(21)-N(5)	1.367(3)
C(9)-H(9A)	0.9800	C(21)-N(4)	1.403(3)
C(9)-H(9B)	0.9800	C(21)-Fe(1)	1.887(3)
C(9)-H(9C)	0.9800	C(22)-C(23)	1.324(4)
C(10)-C(12)	1.525(4)	C(22)-N(4)	1.398(3)
C(10)-C(11)	1.530(4)	C(22)-H(22)	0.9500
C(10)-H(10)	1.0000	C(23)-N(5)	1.400(4)
C(11)-H(11A)	0.9800	C(23)-H(23)	0.9500
C(11)-H(11B)	0.9800	C(24A)-C(25A)	1.3900
C(11)-H(11C)	0.9800	C(24A)-C(29A)	1.3900
C(12)-H(12A)	0.9800	C(24A)-N(5)	1.465(5)
C(12)-H(12B)	0.9800	C(25A)-C(26A)	1.3900
C(12)-H(12C)	0.9800	C(25A)-C(30A)	1.535(10)
C(13)-N(1)	1.376(3)	C(26A)-C(27A)	1.3900
C(13)-N(2)	1.403(3)	C(26A)-H(26A)	0.9500

C(27A)-C(28A)	1.3900	C(30B)-C(32B)	1.526(11)
C(27A)-H(27A)	0.9500	C(30B)-C(31B)	1.536(11)
C(28A)-C(29A)	1.3900	C(30B)-H(30B)	1.0000
C(28A)-H(28A)	0.9500	C(31B)-H(31D)	0.9800
C(29A)-C(33A)	1.545(7)	C(31B)-H(31E)	0.9800
C(30A)-C(32A)	1.533(11)	C(31B)-H(31F)	0.9800
C(30A)-C(31A)	1.535(13)	C(32B)-H(32D)	0.9800
C(30A)-H(30A)	1.0000	C(32B)-H(32E)	0.9800
C(31A)-H(31A)	0.9800	C(32B)-H(32F)	0.9800
C(31A)-H(31B)	0.9800	C(33B)-C(34B)	1.516(10)
C(31A)-H(31C)	0.9800	C(33B)-C(35B)	1.553(10)
C(32A)-H(32A)	0.9800	C(33B)-H(33B)	1.0000
C(32A)-H(32B)	0.9800	C(34B)-H(34D)	0.9800
C(32A)-H(32C)	0.9800	C(34B)-H(34E)	0.9800
C(33A)-C(35A)	1.503(14)	C(34B)-H(34F)	0.9800
C(33A)-C(34A)	1.511(10)	C(35B)-H(35D)	0.9800
C(33A)-H(33A)	1.0000	C(35B)-H(35E)	0.9800
C(34A)-H(34A)	0.9800	C(35B)-H(35F)	0.9800
C(34A)-H(34B)	0.9800	C(36)-H(36A)	0.9800
C(34A)-H(34C)	0.9800	C(36)-H(36B)	0.9800
C(35A)-H(35A)	0.9800	C(36)-H(36C)	0.9800
C(35A)-H(35B)	0.9800	C(37)-H(37A)	0.9800
C(35A)-H(35C)	0.9800	C(37)-H(37B)	0.9800
C(24B)-C(25B)	1.3900	C(37)-H(37C)	0.9800
C(24B)-C(29B)	1.3900	C(38)-C(39)	1.359(4)
C(24B)-N(5)	1.424(5)	C(38)-C(43)	1.393(5)
C(25B)-C(26B)	1.3900	C(38)-Si(1)	1.901(3)
C(25B)-C(30B)	1.620(11)	C(39)-C(40)	1.382(5)
C(26B)-C(27B)	1.3900	C(39)-H(39)	0.9500
C(26B)-H(26B)	0.9500	C(40)-C(41)	1.341(6)
C(27B)-C(28B)	1.3900	C(40)-H(40)	0.9500
C(27B)-H(27B)	0.9500	C(41)-C(42)	1.352(6)
C(28B)-C(29B)	1.3900	C(41)-H(41)	0.9500
C(28B)-H(28B)	0.9500	C(42)-C(43)	1.394(6)
C(29B)-C(33B)	1.538(8)	C(42)-H(42)	0.9500

C(43)-H(43)	0.9500	C(48)-H(48)	0.9500
C(44)-C(49)	1.392(4)	C(49)-H(49)	0.9500
C(44)-C(45)	1.399(4)	N(3)-Fe(1)	1.882(2)
C(44)-Si(2)	1.909(3)	Si(1)-Fe(1)	2.3228(10)
C(45)-C(46)	1.385(5)	Si(1)-H(1A)	1.37(4)
C(45)-H(45)	0.9500	Si(1)-H(1B)	1.50(4)
C(46)-C(47)	1.364(5)	Si(2)-Fe(1)	2.3299(9)
C(46)-H(46)	0.9500	Si(2)-H(2A)	1.42(3)
C(47)-C(48)	1.378(5)	Si(2)-H(2B)	1.39(3)
C(47)-H(47)	0.9500	Fe(1)-H(98)	1.53(4)
C(48)-C(49)	1.386(4)	Fe(1)-H(99)	1.57(3)

C(6)-C(1)-C(2)	121.7(2)	C(9)-C(7)-H(7)	107.4
C(6)-C(1)-N(1)	118.3(2)	C(7)-C(8)-H(8A)	109.5
C(2)-C(1)-N(1)	120.0(2)	C(7)-C(8)-H(8B)	109.5
C(3)-C(2)-C(1)	117.9(3)	H(8A)-C(8)-H(8B)	109.5
C(3)-C(2)-C(7)	120.3(2)	C(7)-C(8)-H(8C)	109.5
C(1)-C(2)-C(7)	121.8(2)	H(8A)-C(8)-H(8C)	109.5
C(4)-C(3)-C(2)	121.2(3)	H(8B)-C(8)-H(8C)	109.5
C(4)-C(3)-H(3)	119.4	C(7)-C(9)-H(9A)	109.5
C(2)-C(3)-H(3)	119.4	C(7)-C(9)-H(9B)	109.5
C(3)-C(4)-C(5)	120.2(3)	H(9A)-C(9)-H(9B)	109.5
C(3)-C(4)-H(4)	119.9	C(7)-C(9)-H(9C)	109.5
C(5)-C(4)-H(4)	119.9	H(9A)-C(9)-H(9C)	109.5
C(4)-C(5)-C(6)	121.0(3)	H(9B)-C(9)-H(9C)	109.5
C(4)-C(5)-H(5)	119.5	C(6)-C(10)-C(12)	111.9(3)
C(6)-C(5)-H(5)	119.5	C(6)-C(10)-C(11)	110.4(2)
C(5)-C(6)-C(1)	117.9(2)	C(12)-C(10)-C(11)	110.0(3)
C(5)-C(6)-C(10)	118.3(2)	C(6)-C(10)-H(10)	108.2
C(1)-C(6)-C(10)	123.8(2)	C(12)-C(10)-H(10)	108.2
C(2)-C(7)-C(8)	110.2(2)	C(11)-C(10)-H(10)	108.2
C(2)-C(7)-C(9)	112.7(2)	C(10)-C(11)-H(11A)	109.5
C(8)-C(7)-C(9)	111.5(2)	C(10)-C(11)-H(11B)	109.5
C(2)-C(7)-H(7)	107.4	H(11A)-C(11)-H(11B)	109.5
C(8)-C(7)-H(7)	107.4	C(10)-C(11)-H(11C)	109.5

H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-N(4)	106.5(3)
H(11B)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	126.7
C(10)-C(12)-H(12A)	109.5	N(4)-C(22)-H(22)	126.7
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-N(5)	108.5(3)
H(12A)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	125.7
C(10)-C(12)-H(12C)	109.5	N(5)-C(23)-H(23)	125.7
H(12A)-C(12)-H(12C)	109.5	C(25A)-C(24A)-C(29A)	120.0
H(12B)-C(12)-H(12C)	109.5	C(25A)-C(24A)-N(5)	115.0(4)
N(1)-C(13)-N(2)	102.7(2)	C(29A)-C(24A)-N(5)	125.0(5)
N(1)-C(13)-Fe(1)	143.4(2)	C(26A)-C(25A)-C(24A)	120.0
N(2)-C(13)-Fe(1)	113.89(18)	C(26A)-C(25A)-C(30A)	106.8(6)
C(15)-C(14)-N(1)	108.3(2)	C(24A)-C(25A)-C(30A)	129.0(6)
C(15)-C(14)-H(14)	125.8	C(27A)-C(26A)-C(25A)	120.0
N(1)-C(14)-H(14)	125.8	C(27A)-C(26A)-H(26A)	120.0
C(14)-C(15)-N(2)	106.4(2)	C(25A)-C(26A)-H(26A)	120.0
C(14)-C(15)-H(15)	126.8	C(26A)-C(27A)-C(28A)	120.0
N(2)-C(15)-H(15)	126.8	C(26A)-C(27A)-H(27A)	120.0
N(3)-C(16)-C(17)	122.4(2)	C(28A)-C(27A)-H(27A)	120.0
N(3)-C(16)-N(2)	108.6(2)	C(29A)-C(28A)-C(27A)	120.0
C(17)-C(16)-N(2)	128.9(2)	C(29A)-C(28A)-H(28A)	120.0
C(16)-C(17)-C(18)	115.6(3)	C(27A)-C(28A)-H(28A)	120.0
C(16)-C(17)-C(36)	123.9(3)	C(28A)-C(29A)-C(24A)	120.0
C(18)-C(17)-C(36)	120.5(3)	C(28A)-C(29A)-C(33A)	117.2(4)
C(17)-C(18)-C(19)	124.1(3)	C(24A)-C(29A)-C(33A)	122.8(4)
C(17)-C(18)-H(18)	118.0	C(32A)-C(30A)-C(25A)	121.5(8)
C(19)-C(18)-H(18)	118.0	C(32A)-C(30A)-C(31A)	109.5(8)
C(20)-C(19)-C(18)	116.1(3)	C(25A)-C(30A)-C(31A)	102.6(8)
C(20)-C(19)-C(37)	123.0(3)	C(32A)-C(30A)-H(30A)	107.5
C(18)-C(19)-C(37)	120.9(3)	C(25A)-C(30A)-H(30A)	107.5
N(3)-C(20)-C(19)	121.6(3)	C(31A)-C(30A)-H(30A)	107.5
N(3)-C(20)-N(4)	108.9(2)	C(35A)-C(33A)-C(34A)	109.0(6)
C(19)-C(20)-N(4)	129.5(3)	C(35A)-C(33A)-C(29A)	110.1(6)
N(5)-C(21)-N(4)	102.8(2)	C(34A)-C(33A)-C(29A)	113.8(6)
N(5)-C(21)-Fe(1)	143.5(2)	C(35A)-C(33A)-H(33A)	107.9
N(4)-C(21)-Fe(1)	113.56(19)	C(34A)-C(33A)-H(33A)	107.9

C(29A)-C(33A)-H(33A)	107.9	H(32D)-C(32B)-H(32F)	109.5
C(25B)-C(24B)-C(29B)	120.0	H(32E)-C(32B)-H(32F)	109.5
C(25B)-C(24B)-N(5)	125.2(4)	C(34B)-C(33B)-C(29B)	111.0(5)
C(29B)-C(24B)-N(5)	114.6(4)	C(34B)-C(33B)-C(35B)	109.9(6)
C(24B)-C(25B)-C(26B)	120.0	C(29B)-C(33B)-C(35B)	112.0(6)
C(24B)-C(25B)-C(30B)	105.5(6)	C(34B)-C(33B)-H(33B)	107.9
C(26B)-C(25B)-C(30B)	125.0(6)	C(29B)-C(33B)-H(33B)	107.9
C(27B)-C(26B)-C(25B)	120.0	C(35B)-C(33B)-H(33B)	107.9
C(27B)-C(26B)-H(26B)	120.0	C(33B)-C(34B)-H(34D)	109.5
C(25B)-C(26B)-H(26B)	120.0	C(33B)-C(34B)-H(34E)	109.5
C(26B)-C(27B)-C(28B)	120.0	H(34D)-C(34B)-H(34E)	109.5
C(26B)-C(27B)-H(27B)	120.0	C(33B)-C(34B)-H(34F)	109.5
C(28B)-C(27B)-H(27B)	120.0	H(34D)-C(34B)-H(34F)	109.5
C(29B)-C(28B)-C(27B)	120.0	H(34E)-C(34B)-H(34F)	109.5
C(29B)-C(28B)-H(28B)	120.0	C(33B)-C(35B)-H(35D)	109.5
C(27B)-C(28B)-H(28B)	120.0	C(33B)-C(35B)-H(35E)	109.5
C(28B)-C(29B)-C(24B)	120.0	H(35D)-C(35B)-H(35E)	109.5
C(28B)-C(29B)-C(33B)	118.2(4)	C(33B)-C(35B)-H(35F)	109.5
C(24B)-C(29B)-C(33B)	121.3(4)	H(35D)-C(35B)-H(35F)	109.5
C(32B)-C(30B)-C(31B)	110.6(7)	H(35E)-C(35B)-H(35F)	109.5
C(32B)-C(30B)-C(25B)	105.6(7)	C(17)-C(36)-H(36A)	109.5
C(31B)-C(30B)-C(25B)	113.8(7)	C(17)-C(36)-H(36B)	109.5
C(32B)-C(30B)-H(30B)	108.9	H(36A)-C(36)-H(36B)	109.5
C(31B)-C(30B)-H(30B)	108.9	C(17)-C(36)-H(36C)	109.5
C(25B)-C(30B)-H(30B)	108.9	H(36A)-C(36)-H(36C)	109.5
C(30B)-C(31B)-H(31D)	109.5	H(36B)-C(36)-H(36C)	109.5
C(30B)-C(31B)-H(31E)	109.5	C(19)-C(37)-H(37A)	109.5
H(31D)-C(31B)-H(31E)	109.5	C(19)-C(37)-H(37B)	109.5
C(30B)-C(31B)-H(31F)	109.5	H(37A)-C(37)-H(37B)	109.5
H(31D)-C(31B)-H(31F)	109.5	C(19)-C(37)-H(37C)	109.5
H(31E)-C(31B)-H(31F)	109.5	H(37A)-C(37)-H(37C)	109.5
C(30B)-C(32B)-H(32D)	109.5	H(37B)-C(37)-H(37C)	109.5
C(30B)-C(32B)-H(32E)	109.5	C(39)-C(38)-C(43)	113.8(3)
H(32D)-C(32B)-H(32E)	109.5	C(39)-C(38)-Si(1)	125.0(3)
C(30B)-C(32B)-H(32F)	109.5	C(43)-C(38)-Si(1)	121.1(2)

C(38)-C(39)-C(40)	123.5(4)	C(14)-N(1)-C(1)	121.9(2)
C(38)-C(39)-H(39)	118.2	C(15)-N(2)-C(16)	132.4(2)
C(40)-C(39)-H(39)	118.2	C(15)-N(2)-C(13)	111.5(2)
C(41)-C(40)-C(39)	121.2(4)	C(16)-N(2)-C(13)	116.1(2)
C(41)-C(40)-H(40)	119.4	C(16)-N(3)-C(20)	120.1(2)
C(39)-C(40)-H(40)	119.4	C(16)-N(3)-Fe(1)	120.27(17)
C(40)-C(41)-C(42)	118.5(4)	C(20)-N(3)-Fe(1)	119.66(18)
C(40)-C(41)-H(41)	120.8	C(20)-N(4)-C(22)	132.5(2)
C(42)-C(41)-H(41)	120.8	C(20)-N(4)-C(21)	116.3(2)
C(41)-C(42)-C(43)	120.0(4)	C(22)-N(4)-C(21)	111.1(2)
C(41)-C(42)-H(42)	120.0	C(21)-N(5)-C(23)	111.0(2)
C(43)-C(42)-H(42)	120.0	C(21)-N(5)-C(24B)	130.6(3)
C(38)-C(43)-C(42)	123.0(4)	C(23)-N(5)-C(24B)	118.3(3)
C(38)-C(43)-H(43)	118.5	C(21)-N(5)-C(24A)	121.6(3)
C(42)-C(43)-H(43)	118.5	C(23)-N(5)-C(24A)	127.3(3)
C(49)-C(44)-C(45)	115.5(3)	C(38)-Si(1)-Fe(1)	114.92(9)
C(49)-C(44)-Si(2)	123.9(2)	C(38)-Si(1)-H(1A)	103.5(16)
C(45)-C(44)-Si(2)	120.5(2)	Fe(1)-Si(1)-H(1A)	118.6(16)
C(46)-C(45)-C(44)	122.3(3)	C(38)-Si(1)-H(1B)	102.4(14)
C(46)-C(45)-H(45)	118.8	Fe(1)-Si(1)-H(1B)	111.9(14)
C(44)-C(45)-H(45)	118.8	H(1A)-Si(1)-H(1B)	104(2)
C(47)-C(46)-C(45)	120.4(3)	C(44)-Si(2)-Fe(1)	115.87(9)
C(47)-C(46)-H(46)	119.8	C(44)-Si(2)-H(2A)	101.6(10)
C(45)-C(46)-H(46)	119.8	Fe(1)-Si(2)-H(2A)	110.0(10)
C(46)-C(47)-C(48)	119.2(3)	C(44)-Si(2)-H(2B)	104.6(11)
C(46)-C(47)-H(47)	120.4	Fe(1)-Si(2)-H(2B)	119.4(10)
C(48)-C(47)-H(47)	120.4	H(2A)-Si(2)-H(2B)	103.2(14)
C(47)-C(48)-C(49)	120.1(3)	N(3)-Fe(1)-C(13)	81.16(10)
C(47)-C(48)-H(48)	119.9	N(3)-Fe(1)-C(21)	81.56(11)
C(49)-C(48)-H(48)	119.9	C(13)-Fe(1)-C(21)	162.71(12)
C(48)-C(49)-C(44)	122.4(3)	N(3)-Fe(1)-Si(1)	88.96(7)
C(48)-C(49)-H(49)	118.8	C(13)-Fe(1)-Si(1)	88.24(8)
C(44)-C(49)-H(49)	118.8	C(21)-Fe(1)-Si(1)	91.02(9)
C(13)-N(1)-C(14)	111.0(2)	N(3)-Fe(1)-Si(2)	82.95(7)
C(13)-N(1)-C(1)	126.4(2)	C(13)-Fe(1)-Si(2)	91.34(8)

C(21)-Fe(1)-Si(2)	86.97(9)
Si(1)-Fe(1)-Si(2)	171.86(4)
N(3)-Fe(1)-H(98)	163.6(14)
C(13)-Fe(1)-H(98)	98.4(13)
C(21)-Fe(1)-H(98)	98.1(13)
Si(1)-Fe(1)-H(98)	74.7(14)
Si(2)-Fe(1)-H(98)	113.4(14)
N(3)-Fe(1)-H(99)	164.6(11)
C(13)-Fe(1)-H(99)	100.5(10)
C(21)-Fe(1)-H(99)	96.2(10)
Si(1)-Fe(1)-H(99)	106.4(11)
Si(2)-Fe(1)-H(99)	81.7(11)
H(98)-Fe(1)-H(99)	31.7(14)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 3 The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	24(1)	33(1)	25(1)	-1(1)	-7(1)	-4(1)
C(2)	29(1)	35(2)	23(1)	-1(1)	-6(1)	-3(1)
C(3)	35(2)	35(2)	35(2)	5(1)	-6(1)	-4(1)
C(4)	30(2)	45(2)	41(2)	5(2)	-7(1)	7(1)
C(5)	23(1)	47(2)	36(2)	5(1)	-1(1)	1(1)
C(6)	24(1)	39(2)	28(1)	3(1)	-5(1)	-5(1)
C(7)	31(2)	35(2)	26(1)	5(1)	0(1)	-4(1)
C(8)	45(2)	54(2)	29(2)	1(1)	-4(1)	-4(2)
C(9)	36(2)	43(2)	43(2)	6(2)	4(1)	-5(1)
C(10)	26(2)	48(2)	36(2)	11(1)	-1(1)	-2(1)
C(11)	32(2)	52(2)	61(2)	15(2)	-6(2)	-7(2)
C(12)	36(2)	80(3)	45(2)	14(2)	8(2)	5(2)
C(13)	24(1)	30(1)	24(1)	1(1)	3(1)	1(1)
C(14)	34(2)	38(2)	28(2)	-3(1)	-5(1)	-11(1)
C(15)	36(2)	29(2)	32(2)	-3(1)	-1(1)	-8(1)
C(16)	26(1)	27(1)	30(2)	2(1)	0(1)	-3(1)
C(17)	33(2)	29(2)	48(2)	2(1)	3(1)	-3(1)
C(18)	36(2)	29(2)	62(2)	14(2)	-2(2)	0(1)
C(19)	30(2)	39(2)	48(2)	14(2)	-5(1)	1(1)
C(20)	28(2)	34(2)	39(2)	6(1)	-2(1)	-2(1)
C(21)	29(2)	31(2)	33(2)	1(1)	-7(1)	-3(1)
C(22)	38(2)	43(2)	60(2)	8(2)	-28(2)	-5(2)
C(23)	49(2)	48(2)	55(2)	2(2)	-31(2)	-8(2)
C(24A)	24(1)	33(1)	25(1)	-1(1)	-7(1)	-4(1)
C(25A)	32(2)	39(2)	30(2)	0(2)	-1(2)	-5(2)
C(26A)	48(3)	43(2)	35(2)	11(2)	6(2)	-2(2)
C(27A)	41(5)	40(5)	33(4)	5(3)	-6(4)	-7(4)
C(28A)	49(5)	44(4)	31(4)	-10(3)	0(3)	-5(4)
C(29A)	41(4)	43(4)	23(4)	-3(3)	-6(3)	-19(3)
C(30A)	62(7)	33(4)	35(6)	7(4)	14(4)	3(5)

C(31A)	48(6)	74(7)	87(8)	24(6)	35(6)	29(5)
C(32A)	111(8)	58(6)	28(4)	-3(4)	14(5)	-16(6)
C(33A)	62(5)	43(4)	32(4)	-12(3)	14(3)	-15(3)
C(34A)	81(6)	54(5)	68(5)	-22(4)	47(5)	-15(4)
C(35A)	107(8)	50(3)	39(3)	-6(2)	36(7)	-16(6)
C(24B)	24(1)	33(1)	25(1)	-1(1)	-7(1)	-4(1)
C(25B)	32(2)	39(2)	30(2)	0(2)	-1(2)	-5(2)
C(26B)	48(3)	43(2)	35(2)	11(2)	6(2)	-2(2)
C(27B)	57(6)	40(5)	55(6)	12(4)	10(5)	25(4)
C(28B)	58(5)	40(4)	36(4)	9(3)	19(4)	10(4)
C(29B)	42(4)	32(3)	18(3)	-5(3)	1(3)	3(3)
C(30B)	32(5)	32(4)	51(6)	-1(4)	4(4)	-3(4)
C(31B)	38(4)	48(4)	56(5)	-9(4)	9(4)	-11(3)
C(32B)	58(5)	45(4)	37(5)	-4(3)	13(4)	-17(4)
C(33B)	61(5)	26(3)	35(4)	1(3)	20(4)	10(3)
C(34B)	79(5)	70(5)	31(4)	8(3)	-2(4)	22(4)
C(35B)	107(8)	50(3)	39(3)	-6(2)	36(7)	-16(6)
C(36)	46(2)	27(2)	72(2)	3(2)	-5(2)	1(2)
C(37)	39(2)	47(2)	76(2)	21(2)	-17(2)	1(2)
C(38)	33(2)	48(2)	31(2)	-7(1)	5(1)	-3(1)
C(39)	119(4)	49(2)	50(2)	8(2)	-33(2)	-24(2)
C(40)	121(4)	88(4)	63(3)	26(3)	-49(3)	-46(3)
C(41)	66(3)	97(4)	54(3)	28(3)	4(2)	5(2)
C(42)	155(5)	55(3)	62(3)	12(2)	30(3)	39(3)
C(43)	133(4)	54(2)	44(2)	-11(2)	-7(2)	3(3)
C(44)	29(2)	32(2)	38(2)	8(1)	10(1)	-1(1)
C(45)	33(2)	36(2)	64(2)	10(2)	6(2)	-1(1)
C(46)	47(2)	33(2)	79(3)	8(2)	14(2)	7(2)
C(47)	63(2)	34(2)	52(2)	5(2)	28(2)	1(2)
C(48)	62(2)	45(2)	30(2)	-3(2)	13(2)	-5(2)
C(49)	43(2)	40(2)	34(2)	-1(1)	7(1)	5(1)
N(1)	24(1)	33(1)	25(1)	2(1)	-2(1)	-4(1)
N(2)	28(1)	26(1)	29(1)	0(1)	-1(1)	-3(1)
N(3)	24(1)	27(1)	31(1)	2(1)	-2(1)	1(1)
N(4)	32(1)	34(1)	39(1)	6(1)	-13(1)	-2(1)

N(5)	45(2)	32(1)	35(1)	0(1)	-16(1)	-4(1)
Si(1)	36(1)	80(1)	29(1)	-6(1)	-1(1)	19(1)
Si(2)	24(1)	31(1)	38(1)	5(1)	-1(1)	-2(1)
Fe(1)	25(1)	27(1)	27(1)	-1(1)	-5(1)	1(1)

Complex 4

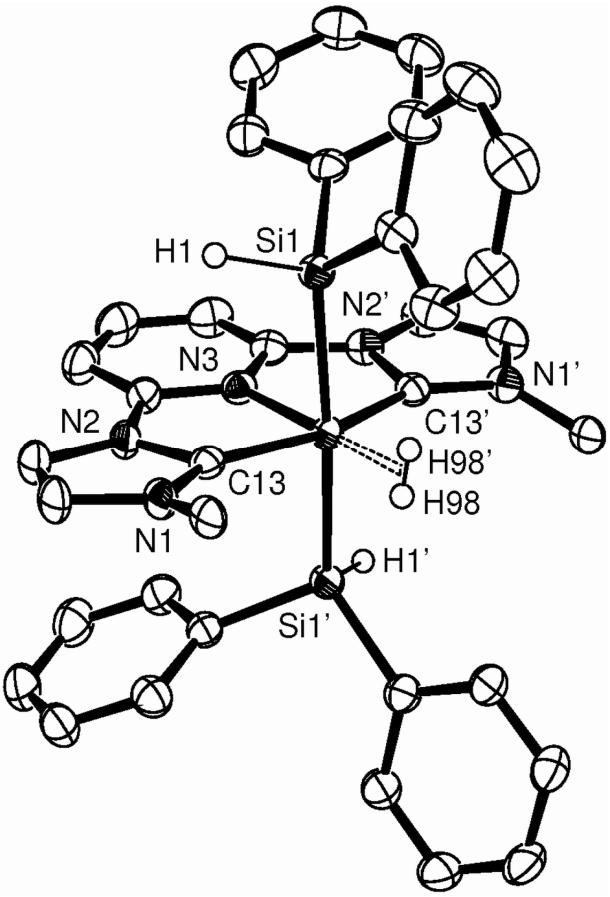

Table 1. Crystal data and structure refinement for 4.

Identification code	4	
Empirical formula	C59 H65 Fe N5 Si2	
Formula weight	956.19	
Temperature	120(2) K	
Wavelength	0.8462 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 23.466(5) Å	α= 90°.
	b = 10.382(2) Å	β= 111.47(3)°.
	c = 22.594(4) Å	γ = 90°.
Volume	5123(2) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	

Absorption coefficient	0.385 mm^{-1}
F(000)	2032
Crystal size	0.20 x 0.14 x 0.03 mm^3
Theta range for data collection	3.13 to 27.23°.
Index ranges	-29<=h<=29, -13<=k<=13, -28<=l<=28
Reflections collected	17951
Independent reflections	5426 [R(int) = 0.0398]
Completeness to theta = 27.23°	94.7 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.993 and 0.918
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5426 / 0 / 316
Goodness-of-fit on F^2	1.030
Final R indices [I>2sigma(I)]	R1 = 0.0407, wR2 = 0.0985
R indices (all data)	R1 = 0.0572, wR2 = 0.1065
Largest diff. peak and hole	0.572 and -0.532 e.$Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1007(1)	2413(2)	1671(1)	25(1)
C(2)	1312(1)	1444(2)	2107(1)	26(1)
C(3)	1304(1)	203(2)	1874(1)	31(1)
C(4)	1010(1)	-79(2)	1236(1)	35(1)
C(5)	734(1)	896(2)	814(1)	34(1)
C(6)	729(1)	2165(2)	1014(1)	29(1)
C(7)	1690(1)	1763(2)	2795(1)	30(1)
C(8)	2307(1)	2325(3)	2831(1)	42(1)
C(9)	1795(1)	615(3)	3240(1)	46(1)
C(10)	482(1)	3220(2)	519(1)	36(1)
C(11)	967(1)	3563(3)	234(1)	44(1)
C(12)	-110(1)	2847(3)	-28(1)	46(1)
C(13)	622(1)	4271(2)	2155(1)	22(1)
C(14)	1372(1)	4671(2)	1748(1)	33(1)
C(15)	1209(1)	5819(2)	1890(1)	32(1)
C(16)	395(1)	6451(2)	2307(1)	26(1)
C(17)	405(1)	7780(2)	2292(1)	35(1)
C(18)	0	8438(3)	2500	39(1)
C(36)	-1000(1)	2555(2)	981(1)	28(1)
C(37)	-695(1)	1376(2)	1123(1)	32(1)
C(38)	-909(1)	290(2)	746(1)	38(1)
C(39)	-1442(1)	362(2)	216(1)	41(1)
C(40)	-1755(1)	1514(3)	61(1)	41(1)
C(41)	-1537(1)	2600(2)	432(1)	35(1)
C(42)	-1346(1)	5225(2)	1320(1)	26(1)
C(43)	-1902(1)	4861(2)	1360(1)	32(1)
C(44)	-2367(1)	5744(2)	1299(1)	39(1)
C(45)	-2287(1)	7021(2)	1189(1)	43(1)
C(46)	-1741(1)	7419(2)	1147(1)	41(1)
C(47)	-1281(1)	6529(2)	1214(1)	33(1)

Fe(1)	0	3969(1)	2500	19(1)
N(1)	1017(1)	3723(2)	1893(1)	25(1)
N(2)	752(1)	5587(2)	2131(1)	25(1)
N(3)	0	5781(2)	2500	23(1)
Si(1)	-678(1)	4079(1)	1453(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for 4.

C(1)-C(2)	1.406(3)	C(14)-C(15)	1.325(3)
C(1)-C(6)	1.411(3)	C(14)-N(1)	1.403(3)
C(1)-N(1)	1.447(3)	C(14)-H(14)	0.9500
C(2)-C(3)	1.389(3)	C(15)-N(2)	1.391(2)
C(2)-C(7)	1.519(3)	C(15)-H(15)	0.9500
C(3)-C(4)	1.384(3)	C(16)-N(3)	1.352(2)
C(3)-H(3)	0.9500	C(16)-C(17)	1.381(3)
C(4)-C(5)	1.378(3)	C(16)-N(2)	1.382(3)
C(4)-H(4)	0.9500	C(17)-C(18)	1.385(3)
C(5)-C(6)	1.394(3)	C(17)-H(17)	0.9500
C(5)-H(5)	0.9500	C(18)-C(17)#1	1.385(3)
C(6)-C(10)	1.520(3)	C(18)-H(18)	0.9500
C(7)-C(9)	1.521(3)	C(36)-C(37)	1.396(3)
C(7)-C(8)	1.536(3)	C(36)-C(41)	1.407(3)
C(7)-H(7)	1.0000	C(36)-Si(1)	1.903(2)
C(8)-H(8A)	0.9800	C(37)-C(38)	1.391(3)
C(8)-H(8B)	0.9800	C(37)-H(37)	0.9500
C(8)-H(8C)	0.9800	C(38)-C(39)	1.382(3)
C(9)-H(9A)	0.9800	C(38)-H(38)	0.9500
C(9)-H(9B)	0.9800	C(39)-C(40)	1.379(4)
C(9)-H(9C)	0.9800	C(39)-H(39)	0.9500
C(10)-C(12)	1.533(3)	C(40)-C(41)	1.387(3)
C(10)-C(11)	1.541(3)	C(40)-H(40)	0.9500
C(10)-H(10)	1.0000	C(41)-H(41)	0.9500
C(11)-H(11A)	0.9800	C(42)-C(43)	1.391(3)
C(11)-H(11B)	0.9800	C(42)-C(47)	1.393(3)
C(11)-H(11C)	0.9800	C(42)-Si(1)	1.903(2)
C(12)-H(12A)	0.9800	C(43)-C(44)	1.394(3)
C(12)-H(12B)	0.9800	C(43)-H(43)	0.9500
C(12)-H(12C)	0.9800	C(44)-C(45)	1.374(3)
C(13)-N(1)	1.390(2)	C(44)-H(44)	0.9500
C(13)-N(2)	1.406(3)	C(45)-C(46)	1.382(3)
C(13)-Fe(1)	1.9160(19)	C(45)-H(45)	0.9500

C(46)-C(47)	1.386(3)	Fe(1)-Si(1)#1	2.3210(10)
C(46)-H(46)	0.9500	Fe(1)-Si(1)	2.3210(10)
C(47)-H(47)	0.9500	Fe(1)-H(98)	1.616(15)
Fe(1)-N(3)	1.882(2)	N(3)-C(16)#1	1.352(2)
Fe(1)-C(13)#1	1.9160(19)	Si(1)-H(1)	1.45(2)

C(2)-C(1)-C(6)	121.81(19)	H(8B)-C(8)-H(8C)	109.5
C(2)-C(1)-N(1)	119.42(17)	C(7)-C(9)-H(9A)	109.5
C(6)-C(1)-N(1)	118.59(18)	C(7)-C(9)-H(9B)	109.5
C(3)-C(2)-C(1)	117.81(19)	H(9A)-C(9)-H(9B)	109.5
C(3)-C(2)-C(7)	120.75(19)	C(7)-C(9)-H(9C)	109.5
C(1)-C(2)-C(7)	121.19(19)	H(9A)-C(9)-H(9C)	109.5
C(4)-C(3)-C(2)	121.5(2)	H(9B)-C(9)-H(9C)	109.5
C(4)-C(3)-H(3)	119.2	C(6)-C(10)-C(12)	113.5(2)
C(2)-C(3)-H(3)	119.2	C(6)-C(10)-C(11)	109.42(18)
C(5)-C(4)-C(3)	119.6(2)	C(12)-C(10)-C(11)	108.23(19)
C(5)-C(4)-H(4)	120.2	C(6)-C(10)-H(10)	108.5
C(3)-C(4)-H(4)	120.2	C(12)-C(10)-H(10)	108.5
C(4)-C(5)-C(6)	121.9(2)	C(11)-C(10)-H(10)	108.5
C(4)-C(5)-H(5)	119.0	C(10)-C(11)-H(11A)	109.5
C(6)-C(5)-H(5)	119.0	C(10)-C(11)-H(11B)	109.5
C(5)-C(6)-C(1)	117.2(2)	H(11A)-C(11)-H(11B)	109.5
C(5)-C(6)-C(10)	119.31(19)	C(10)-C(11)-H(11C)	109.5
C(1)-C(6)-C(10)	123.2(2)	H(11A)-C(11)-H(11C)	109.5
C(2)-C(7)-C(9)	113.54(19)	H(11B)-C(11)-H(11C)	109.5
C(2)-C(7)-C(8)	108.80(17)	C(10)-C(12)-H(12A)	109.5
C(9)-C(7)-C(8)	109.97(19)	C(10)-C(12)-H(12B)	109.5
C(2)-C(7)-H(7)	108.1	H(12A)-C(12)-H(12B)	109.5
C(9)-C(7)-H(7)	108.1	C(10)-C(12)-H(12C)	109.5
C(8)-C(7)-H(7)	108.1	H(12A)-C(12)-H(12C)	109.5
C(7)-C(8)-H(8A)	109.5	H(12B)-C(12)-H(12C)	109.5
C(7)-C(8)-H(8B)	109.5	N(1)-C(13)-N(2)	101.14(15)
H(8A)-C(8)-H(8B)	109.5	N(1)-C(13)-Fe(1)	146.30(15)
C(7)-C(8)-H(8C)	109.5	N(2)-C(13)-Fe(1)	112.54(13)
H(8A)-C(8)-H(8C)	109.5	C(15)-C(14)-N(1)	109.05(18)

C(15)-C(14)-H(14)	125.5	C(42)-C(43)-C(44)	122.2(2)
N(1)-C(14)-H(14)	125.5	C(42)-C(43)-H(43)	118.9
C(14)-C(15)-N(2)	105.67(18)	C(44)-C(43)-H(43)	118.9
C(14)-C(15)-H(15)	127.2	C(45)-C(44)-C(43)	120.0(2)
N(2)-C(15)-H(15)	127.2	C(45)-C(44)-H(44)	120.0
N(3)-C(16)-C(17)	122.9(2)	C(43)-C(44)-H(44)	120.0
N(3)-C(16)-N(2)	108.59(18)	C(44)-C(45)-C(46)	119.4(2)
C(17)-C(16)-N(2)	128.54(19)	C(44)-C(45)-H(45)	120.3
C(16)-C(17)-C(18)	117.6(2)	C(46)-C(45)-H(45)	120.3
C(16)-C(17)-H(17)	121.2	C(45)-C(46)-C(47)	119.8(2)
C(18)-C(17)-H(17)	121.2	C(45)-C(46)-H(46)	120.1
C(17)#1-C(18)-C(17)	120.9(3)	C(47)-C(46)-H(46)	120.1
C(17)#1-C(18)-H(18)	119.5	C(46)-C(47)-C(42)	122.5(2)
C(17)-C(18)-H(18)	119.5	C(46)-C(47)-H(47)	118.8
C(37)-C(36)-C(41)	116.8(2)	C(42)-C(47)-H(47)	118.8
C(37)-C(36)-Si(1)	122.29(16)	N(3)-Fe(1)-C(13)	80.59(6)
C(41)-C(36)-Si(1)	120.67(17)	N(3)-Fe(1)-C(13)#1	80.59(6)
C(38)-C(37)-C(36)	122.0(2)	C(13)-Fe(1)-C(13)#1	161.17(12)
C(38)-C(37)-H(37)	119.0	N(3)-Fe(1)-Si(1)#1	87.183(16)
C(36)-C(37)-H(37)	119.0	C(13)-Fe(1)-Si(1)#1	93.81(6)
C(39)-C(38)-C(37)	119.7(2)	C(13)#1-Fe(1)-Si(1)#1	85.26(6)
C(39)-C(38)-H(38)	120.1	N(3)-Fe(1)-Si(1)	87.183(16)
C(37)-C(38)-H(38)	120.1	C(13)-Fe(1)-Si(1)	85.26(6)
C(40)-C(39)-C(38)	119.8(2)	C(13)#1-Fe(1)-Si(1)	93.81(6)
C(40)-C(39)-H(39)	120.1	Si(1)#1-Fe(1)-Si(1)	174.37(3)
C(38)-C(39)-H(39)	120.1	N(3)-Fe(1)-H(98)	168.4(6)
C(39)-C(40)-C(41)	120.5(2)	C(13)-Fe(1)-H(98)	97.4(8)
C(39)-C(40)-H(40)	119.8	C(13)#1-Fe(1)-H(98)	101.0(8)
C(41)-C(40)-H(40)	119.8	Si(1)#1-Fe(1)-H(98)	81.6(6)
C(40)-C(41)-C(36)	121.2(2)	Si(1)-Fe(1)-H(98)	104.1(6)
C(40)-C(41)-H(41)	119.4	C(13)-N(1)-C(14)	110.95(17)
C(36)-C(41)-H(41)	119.4	C(13)-N(1)-C(1)	127.09(16)
C(43)-C(42)-C(47)	116.09(19)	C(14)-N(1)-C(1)	120.96(16)
C(43)-C(42)-Si(1)	123.86(16)	C(16)-N(2)-C(15)	129.55(18)
C(47)-C(42)-Si(1)	119.93(16)	C(16)-N(2)-C(13)	117.16(16)

C(15)-N(2)-C(13)	113.15(17)
C(16)-N(3)-C(16)#1	118.1(2)
C(16)-N(3)-Fe(1)	120.95(12)
C(16)#1-N(3)-Fe(1)	120.95(12)
C(36)-Si(1)-C(42)	107.20(9)
C(36)-Si(1)-Fe(1)	120.95(7)
C(42)-Si(1)-Fe(1)	114.14(6)
C(36)-Si(1)-H(1)	102.1(9)
C(42)-Si(1)-H(1)	101.3(9)
Fe(1)-Si(1)-H(1)	108.7(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 4. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	23(1)	35(1)	23(1)	-1(1)	14(1)	0(1)
C(2)	23(1)	35(1)	25(1)	2(1)	15(1)	-1(1)
C(3)	33(1)	33(1)	33(1)	2(1)	19(1)	-2(1)
C(4)	38(1)	37(1)	36(1)	-9(1)	20(1)	-7(1)
C(5)	32(1)	49(1)	25(1)	-7(1)	15(1)	-4(1)
C(6)	25(1)	43(1)	25(1)	-1(1)	15(1)	2(1)
C(7)	31(1)	39(1)	22(1)	1(1)	10(1)	6(1)
C(8)	28(1)	60(2)	37(1)	-9(1)	10(1)	4(1)
C(9)	58(2)	51(2)	29(1)	9(1)	17(1)	19(1)
C(10)	36(1)	49(1)	25(1)	3(1)	15(1)	9(1)
C(11)	48(2)	60(2)	30(1)	12(1)	22(1)	9(1)
C(12)	41(1)	70(2)	26(1)	1(1)	11(1)	9(1)
C(13)	22(1)	27(1)	17(1)	2(1)	6(1)	1(1)
C(14)	29(1)	44(1)	32(1)	4(1)	19(1)	-5(1)
C(15)	30(1)	37(1)	31(1)	6(1)	15(1)	-6(1)
C(16)	25(1)	29(1)	23(1)	2(1)	8(1)	-2(1)
C(17)	40(1)	28(1)	35(1)	3(1)	11(1)	-7(1)
C(18)	48(2)	24(2)	41(2)	0	12(2)	0
C(36)	27(1)	37(1)	23(1)	-5(1)	11(1)	-1(1)
C(37)	31(1)	39(1)	26(1)	-7(1)	11(1)	2(1)
C(38)	40(1)	38(1)	39(1)	-12(1)	18(1)	0(1)
C(39)	42(1)	47(1)	37(1)	-21(1)	18(1)	-9(1)
C(40)	31(1)	57(2)	31(1)	-15(1)	8(1)	-4(1)
C(41)	31(1)	45(1)	27(1)	-6(1)	8(1)	3(1)
C(42)	26(1)	33(1)	17(1)	0(1)	6(1)	2(1)
C(43)	30(1)	38(1)	29(1)	2(1)	11(1)	1(1)
C(44)	27(1)	52(2)	38(1)	-4(1)	12(1)	5(1)
C(45)	37(1)	46(2)	43(1)	-5(1)	11(1)	14(1)
C(46)	49(2)	32(1)	42(1)	1(1)	16(1)	7(1)
C(47)	34(1)	34(1)	31(1)	-1(1)	12(1)	-1(1)

Fe(1)	21(1)	22(1)	17(1)	0	9(1)	0
N(1)	24(1)	33(1)	22(1)	1(1)	12(1)	-2(1)
N(2)	25(1)	27(1)	24(1)	2(1)	11(1)	-4(1)
N(3)	24(1)	25(1)	19(1)	0	6(1)	0
Si(1)	22(1)	29(1)	18(1)	0(1)	8(1)	1(1)

Complex 5

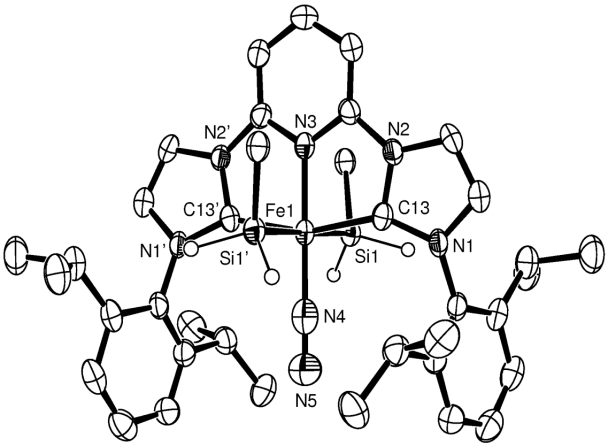

Table 1. Crystal data and structure refinement for 5.

Identification code	5	
Empirical formula	C53 H67 Fe N7 Si2	
Formula weight	914.17	
Temperature	120(2) K	
Wavelength	0.7977 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 19.556(5) Å	α= 90°.
	b = 17.102(5) Å	β= 107.316(3)°.
	c = 15.405(4) Å	γ = 90°.
Volume	4919(2) $Å^3$	
Z	4	
Density (calculated)	1.234 Mg/m^3	
Absorption coefficient	0.398 mm^{-1}	
F(000)	1952	
Crystal size	0.08 x 0.08 x 0.04 mm^3	
Theta range for data collection	4.60 to 30.03°.	
Index ranges	-23<=h<=24, -21<=k<=21, -19<=l<=19	
Reflections collected	17290	
Independent reflections	5048 [R(int) = 0.0627]	
Completeness to theta = 30.03°	99.0 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9842 and 0.9688
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5048 / 0 / 302
Goodness-of-fit on F^2	1.046
Final R indices [I>2sigma(I)]	R1 = 0.0693, wR2 = 0.1901
R indices (all data)	R1 = 0.1131, wR2 = 0.2172
Largest diff. peak and hole	2.157 and -0.474 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3873(2)	1408(3)	8876(3)	32(1)
C(2)	4158(2)	1294(3)	9824(3)	37(1)
C(3)	4228(2)	532(3)	10144(3)	43(1)
C(4)	4037(3)	-107(3)	9565(4)	47(1)
C(5)	3733(2)	24(3)	8640(3)	42(1)
C(6)	3637(2)	775(3)	8285(3)	35(1)
C(7)	4341(3)	1956(3)	10520(3)	42(1)
C(8)	5051(3)	1827(4)	11269(3)	53(1)
C(9)	3730(3)	2059(4)	10957(4)	58(1)
C(10)	3222(3)	910(3)	7285(3)	41(1)
C(11)	2434(3)	1077(3)	7202(3)	51(1)
C(12)	3260(3)	223(3)	6676(4)	62(2)
C(13)	4260(2)	2534(2)	8061(3)	29(1)
C(14)	3375(2)	2761(3)	8728(3)	36(1)
C(15)	3530(2)	3469(3)	8448(3)	34(1)
C(16)	4503(2)	3852(2)	7765(3)	30(1)
C(17)	4479(3)	4653(3)	7776(3)	41(1)
C(18)	5000	5076(4)	7500	47(2)
C(19)	6280(2)	3328(3)	9320(3)	30(1)
C(20)	5973(2)	3937(3)	9713(3)	33(1)
C(21)	6245(2)	4695(3)	9799(3)	36(1)
C(22)	6829(2)	4895(3)	9510(3)	37(1)
C(23)	7161(2)	4295(3)	9162(3)	37(1)
C(24)	6906(2)	3529(3)	9075(3)	34(1)
C(25)	5363(2)	3770(3)	10108(3)	40(1)
C(26)	7107(3)	5718(3)	9571(4)	48(1)
C(27)	7330(2)	2921(3)	8743(3)	37(1)
N(1)	3816(2)	2199(2)	8519(2)	30(1)
N(2)	4073(2)	3328(2)	8051(2)	29(1)
N(3)	5000	3443(3)	7500	28(1)

N(4)	5000	1275(4)	7500	51(2)
N(5)	5000	604(4)	7500	64(2)
Si(1)	5823(1)	2347(1)	8991(1)	29(1)
Fe(1)	5000	2343(1)	7500	26(1)

Table 3. Bond lengths [Å] and angles [°] for 5.

C(1)-C(6)	1.402(6)	C(14)-C(15)	1.350(6)
C(1)-C(2)	1.412(6)	C(14)-N(1)	1.391(5)
C(1)-N(1)	1.452(5)	C(14)-H(14)	0.9500
C(2)-C(3)	1.387(7)	C(15)-N(2)	1.393(5)
C(2)-C(7)	1.527(6)	C(15)-H(15)	0.9500
C(3)-C(4)	1.389(7)	C(16)-N(3)	1.355(5)
C(3)-H(3)	0.9500	C(16)-C(17)	1.370(6)
C(4)-C(5)	1.389(7)	C(16)-N(2)	1.388(5)
C(4)-H(4)	0.9500	C(17)-C(18)	1.414(6)
C(5)-C(6)	1.387(6)	C(17)-H(17)	0.9500
C(5)-H(5)	0.9500	C(18)-C(17)#1	1.414(6)
C(6)-C(10)	1.530(6)	C(18)-H(18)	0.9500
C(7)-C(8)	1.533(7)	C(19)-C(20)	1.424(6)
C(7)-C(9)	1.547(6)	C(19)-C(24)	1.426(6)
C(7)-H(7)	1.0000	C(19)-Si(1)	1.898(4)
C(8)-H(8A)	0.9800	C(20)-C(21)	1.393(6)
C(8)-H(8B)	0.9800	C(20)-C(25)	1.519(6)
C(8)-H(8C)	0.9800	C(21)-C(22)	1.385(6)
C(9)-H(9A)	0.9800	C(21)-H(21)	0.9500
C(9)-H(9B)	0.9800	C(22)-C(23)	1.402(6)
C(9)-H(9C)	0.9800	C(22)-C(26)	1.503(6)
C(10)-C(12)	1.519(7)	C(23)-C(24)	1.395(6)
C(10)-C(11)	1.536(7)	C(23)-H(23)	0.9500
C(10)-H(10)	1.0000	C(24)-C(27)	1.511(6)
C(11)-H(11A)	0.9800	C(25)-H(25A)	0.9800
C(11)-H(11B)	0.9800	C(25)-H(25B)	0.9800
C(11)-H(11C)	0.9800	C(25)-H(25C)	0.9800
C(12)-H(12A)	0.9800	C(26)-H(26A)	0.9800
C(12)-H(12B)	0.9800	C(26)-H(26B)	0.9800
C(12)-H(12C)	0.9800	C(26)-H(26C)	0.9800
C(13)-N(1)	1.394(5)	C(27)-H(27A)	0.9800
C(13)-N(2)	1.405(5)	C(27)-H(27B)	0.9800
C(13)-Fe(1)	1.922(4)	C(27)-H(27C)	0.9800

N(3)-C(16)#1	1.355(5)	Si(1)-H(2)	1.35(4)
N(3)-Fe(1)	1.882(5)	Si(1)-H(1)	1.41(5)
N(4)-N(5)	1.147(9)	Fe(1)-C(13)#1	1.922(4)
N(4)-Fe(1)	1.827(7)	Fe(1)-Si(1)#1	2.3805(12)
Si(1)-Fe(1)	2.3805(12)		

C(6)-C(1)-C(2)	121.2(4)	H(8B)-C(8)-H(8C)	109.5
C(6)-C(1)-N(1)	120.0(4)	C(7)-C(9)-H(9A)	109.5
C(2)-C(1)-N(1)	118.8(4)	C(7)-C(9)-H(9B)	109.5
C(3)-C(2)-C(1)	117.6(4)	H(9A)-C(9)-H(9B)	109.5
C(3)-C(2)-C(7)	118.0(4)	C(7)-C(9)-H(9C)	109.5
C(1)-C(2)-C(7)	124.2(4)	H(9A)-C(9)-H(9C)	109.5
C(2)-C(3)-C(4)	122.1(4)	H(9B)-C(9)-H(9C)	109.5
C(2)-C(3)-H(3)	118.9	C(12)-C(10)-C(6)	113.3(4)
C(4)-C(3)-H(3)	118.9	C(12)-C(10)-C(11)	108.9(4)
C(3)-C(4)-C(5)	118.9(5)	C(6)-C(10)-C(11)	109.3(4)
C(3)-C(4)-H(4)	120.6	C(12)-C(10)-H(10)	108.4
C(5)-C(4)-H(4)	120.6	C(6)-C(10)-H(10)	108.4
C(6)-C(5)-C(4)	121.4(5)	C(11)-C(10)-H(10)	108.4
C(6)-C(5)-H(5)	119.3	C(10)-C(11)-H(11A)	109.5
C(4)-C(5)-H(5)	119.3	C(10)-C(11)-H(11B)	109.5
C(5)-C(6)-C(1)	118.6(4)	H(11A)-C(11)-H(11B)	109.5
C(5)-C(6)-C(10)	120.4(4)	C(10)-C(11)-H(11C)	109.5
C(1)-C(6)-C(10)	120.7(4)	H(11A)-C(11)-H(11C)	109.5
C(2)-C(7)-C(8)	113.2(4)	H(11B)-C(11)-H(11C)	109.5
C(2)-C(7)-C(9)	109.8(4)	C(10)-C(12)-H(12A)	109.5
C(8)-C(7)-C(9)	109.4(4)	C(10)-C(12)-H(12B)	109.5
C(2)-C(7)-H(7)	108.1	H(12A)-C(12)-H(12B)	109.5
C(8)-C(7)-H(7)	108.1	C(10)-C(12)-H(12C)	109.5
C(9)-C(7)-H(7)	108.1	H(12A)-C(12)-H(12C)	109.5
C(7)-C(8)-H(8A)	109.5	H(12B)-C(12)-H(12C)	109.5
C(7)-C(8)-H(8B)	109.5	N(1)-C(13)-N(2)	101.7(3)
H(8A)-C(8)-H(8B)	109.5	N(1)-C(13)-Fe(1)	145.4(3)
C(7)-C(8)-H(8C)	109.5	N(2)-C(13)-Fe(1)	112.9(3)
H(8A)-C(8)-H(8C)	109.5	C(15)-C(14)-N(1)	109.4(4)

C(15)-C(14)-H(14)	125.3	C(20)-C(25)-H(25C)	109.5
N(1)-C(14)-H(14)	125.3	H(25A)-C(25)-H(25C)	109.5
C(14)-C(15)-N(2)	105.0(4)	H(25B)-C(25)-H(25C)	109.5
C(14)-C(15)-H(15)	127.5	C(22)-C(26)-H(26A)	109.5
N(2)-C(15)-H(15)	127.5	C(22)-C(26)-H(26B)	109.5
N(3)-C(16)-C(17)	123.3(4)	H(26A)-C(26)-H(26B)	109.5
N(3)-C(16)-N(2)	108.7(4)	C(22)-C(26)-H(26C)	109.5
C(17)-C(16)-N(2)	128.0(4)	H(26A)-C(26)-H(26C)	109.5
C(16)-C(17)-C(18)	118.5(4)	H(26B)-C(26)-H(26C)	109.5
C(16)-C(17)-H(17)	120.7	C(24)-C(27)-H(27A)	109.5
C(18)-C(17)-H(17)	120.7	C(24)-C(27)-H(27B)	109.5
C(17)-C(18)-C(17)#1	118.5(6)	H(27A)-C(27)-H(27B)	109.5
C(17)-C(18)-H(18)	120.8	C(24)-C(27)-H(27C)	109.5
C(17)#1-C(18)-H(18)	120.8	H(27A)-C(27)-H(27C)	109.5
C(20)-C(19)-C(24)	116.2(4)	H(27B)-C(27)-H(27C)	109.5
C(20)-C(19)-Si(1)	122.4(3)	C(14)-N(1)-C(13)	110.8(3)
C(24)-C(19)-Si(1)	121.0(3)	C(14)-N(1)-C(1)	122.6(3)
C(21)-C(20)-C(19)	121.5(4)	C(13)-N(1)-C(1)	125.9(3)
C(21)-C(20)-C(25)	117.5(4)	C(16)-N(2)-C(15)	129.8(4)
C(19)-C(20)-C(25)	120.9(4)	C(16)-N(2)-C(13)	116.5(3)
C(22)-C(21)-C(20)	121.9(4)	C(15)-N(2)-C(13)	113.1(3)
C(22)-C(21)-H(21)	119.1	C(16)#1-N(3)-C(16)	117.9(5)
C(20)-C(21)-H(21)	119.1	C(16)#1-N(3)-Fe(1)	121.0(3)
C(21)-C(22)-C(23)	117.5(4)	C(16)-N(3)-Fe(1)	121.0(3)
C(21)-C(22)-C(26)	122.0(4)	N(5)-N(4)-Fe(1)	180.000(1)
C(23)-C(22)-C(26)	120.6(4)	C(19)-Si(1)-Fe(1)	112.93(13)
C(24)-C(23)-C(22)	122.1(4)	C(19)-Si(1)-H(2)	107.5(17)
C(24)-C(23)-H(23)	119.0	Fe(1)-Si(1)-H(2)	116.6(17)
C(22)-C(23)-H(23)	119.0	C(19)-Si(1)-H(1)	107.0(19)
C(23)-C(24)-C(19)	120.7(4)	Fe(1)-Si(1)-H(1)	115.2(19)
C(23)-C(24)-C(27)	117.6(4)	H(2)-Si(1)-H(1)	96(3)
C(19)-C(24)-C(27)	121.7(4)	N(4)-Fe(1)-N(3)	180.000(1)
C(20)-C(25)-H(25A)	109.5	N(4)-Fe(1)-C(13)#1	99.79(13)
C(20)-C(25)-H(25B)	109.5	N(3)-Fe(1)-C(13)#1	80.21(13)
H(25A)-C(25)-H(25B)	109.5	N(4)-Fe(1)-C(13)	99.79(13)

N(3)-Fe(1)-C(13)	80.21(13)
C(13)#1-Fe(1)-C(13)	160.4(3)
N(4)-Fe(1)-Si(1)	90.17(3)
N(3)-Fe(1)-Si(1)	89.83(3)
C(13)#1-Fe(1)-Si(1)	92.86(12)
C(13)-Fe(1)-Si(1)	87.09(12)
N(4)-Fe(1)-Si(1)#1	90.17(3)
N(3)-Fe(1)-Si(1)#1	89.83(3)
C(13)#1-Fe(1)-Si(1)#1	87.09(12)
C(13)-Fe(1)-Si(1)#1	92.86(12)
Si(1)-Fe(1)-Si(1)#1	179.67(7)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+3/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for 5. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	35(2)	37(2)	31(2)	5(2)	20(2)	3(2)
C(2)	32(2)	51(3)	32(2)	7(2)	16(2)	-1(2)
C(3)	38(3)	59(3)	34(3)	15(2)	15(2)	2(2)
C(4)	39(3)	50(3)	55(3)	15(2)	21(2)	3(2)
C(5)	45(3)	39(3)	47(3)	2(2)	22(2)	0(2)
C(6)	36(2)	39(2)	34(2)	0(2)	16(2)	-1(2)
C(7)	46(3)	55(3)	29(2)	1(2)	16(2)	-1(2)
C(8)	57(3)	74(4)	29(3)	5(2)	13(2)	-1(3)
C(9)	68(4)	72(4)	42(3)	3(3)	31(3)	4(3)
C(10)	49(3)	42(3)	33(2)	0(2)	15(2)	-4(2)
C(11)	49(3)	59(3)	40(3)	4(2)	4(2)	-12(2)
C(12)	94(5)	59(4)	40(3)	-12(3)	30(3)	2(3)
C(13)	31(2)	36(2)	21(2)	2(2)	9(2)	-1(2)
C(14)	36(2)	46(3)	29(2)	-3(2)	16(2)	0(2)
C(15)	37(2)	41(3)	30(2)	-7(2)	16(2)	5(2)
C(16)	35(2)	32(2)	24(2)	-2(2)	11(2)	2(2)
C(17)	53(3)	39(3)	38(3)	1(2)	26(2)	5(2)
C(18)	72(5)	28(3)	50(4)	0	30(4)	0
C(19)	30(2)	41(2)	19(2)	-1(2)	5(2)	0(2)
C(20)	30(2)	40(2)	26(2)	-3(2)	7(2)	-4(2)
C(21)	37(2)	42(3)	29(2)	-7(2)	11(2)	0(2)
C(22)	36(2)	41(3)	33(2)	-5(2)	9(2)	-5(2)
C(23)	31(2)	47(3)	33(2)	-1(2)	12(2)	-7(2)
C(24)	31(2)	44(3)	25(2)	-2(2)	6(2)	-1(2)
C(25)	37(2)	49(3)	36(2)	-8(2)	15(2)	-1(2)
C(26)	50(3)	45(3)	54(3)	-7(2)	21(2)	-9(2)
C(27)	33(2)	43(2)	36(2)	-3(2)	13(2)	-2(2)
N(1)	34(2)	37(2)	24(2)	-2(1)	16(2)	-1(2)
N(2)	32(2)	33(2)	26(2)	0(1)	15(1)	3(2)
N(3)	31(3)	35(3)	20(2)	0	9(2)	0
N(4)	50(4)	62(4)	47(4)	0	24(3)	0
N(5)	75(5)	50(4)	76(5)	0	36(4)	0
Si(1)	32(1)	34(1)	22(1)	0(1)	10(1)	-1(1)

Fe(1)	28(1)	32(1)	21(1)	0	10(1)	0