Figure 8. Cyclic and differential pulse voltammograms recorded at a platinum electrode on a CH_2Cl_2 solution containing **9** (0.8×10^{-3} mol dm^{-3}) and [Nbu4][PF6] (0.2×10^{-3} mol dm^{-3}).

Scan rates: cyclic voltammogram, 0.2 Vs^{-1}; DPV, 0.02 Vs^{-2}.

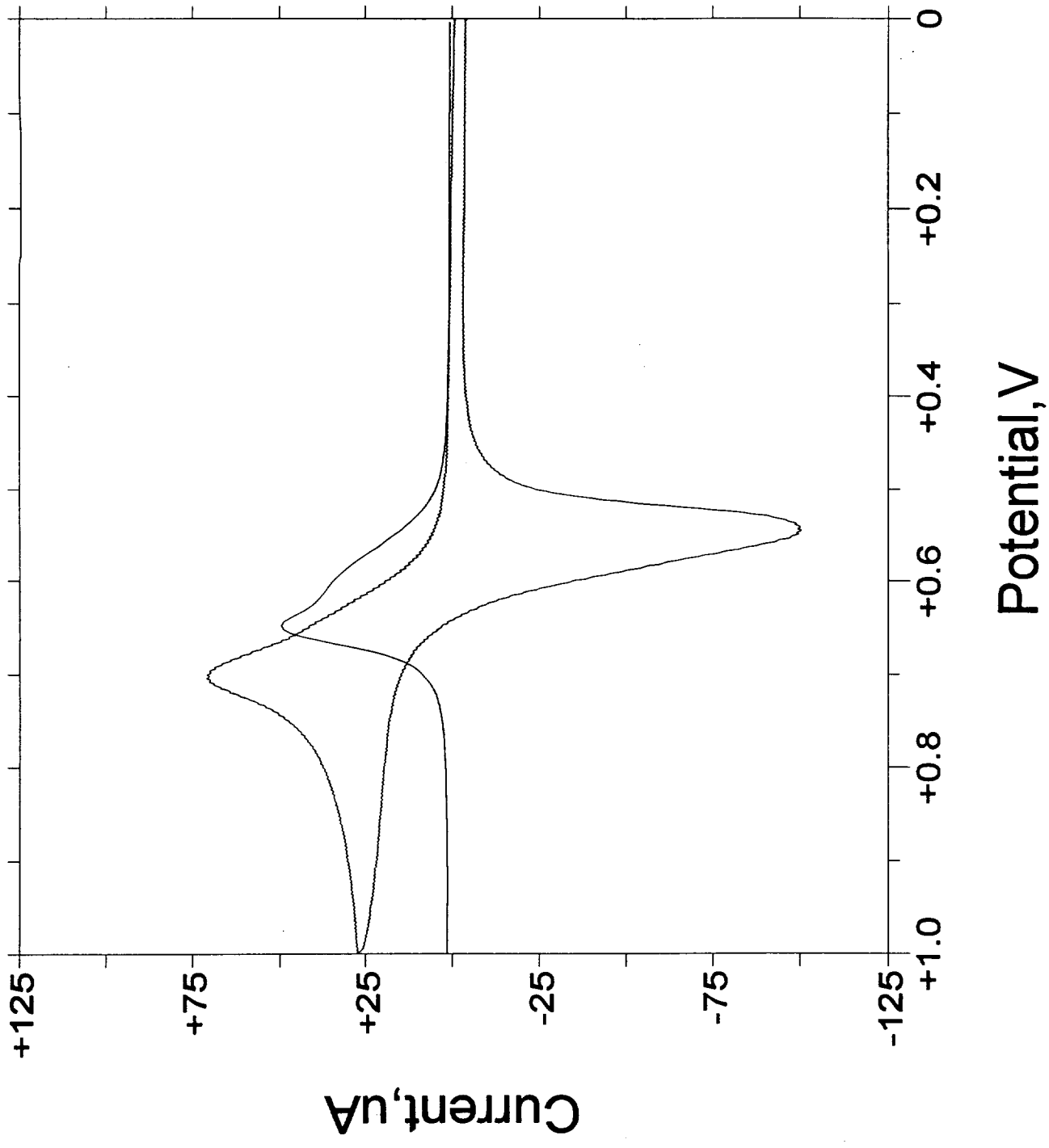

Table 1. Crystal data and structure refinement for 3

Molecular formula	$C_{23}H_{24}Fe_2N_2$
Formula weight	440.14
Crystal system	Orthorhombic
Space group	Pnma (No.62)
Unit cell dimensions	a = 805.4(1) pm $\alpha = 90^\circ$ b = 2291.7(4) pm $\beta = 90^\circ$ c = 999.5(1) pm $\gamma = 90^\circ$
Volume	1.8448(4) nm^3
Z	4
Temperature	218(2) K
Radiation	MoKα (λ =71.073 pm)
Density (calculated)	1.585 Mg/m^3
Absorption coefficient	1.583 mm^{-1}
F(000)	912
Color, Habit	orange platelet
Crystal size	0.45 x 0.45 x 0.06 mm
θ range for data collection	3.25 to 22.99°
Index ranges	$0 \le h \le 8$, $-25 \le k \le 1$, $0 \le \ell \le 11$
Reflections collected	1359
Independent reflections	1315 (R_{int} = 0.0690)
Reflections with I > 2σ(I)	935
Absorption correction	ψ-scan
Max. and min. transmission	0.969 and 0.831
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1177 / 0 / 125
Goodness-of-fit on F^2	1.082
Final R indices [I>2σ(I)]	R1 = 0.0349, wR2 = 0.0712
R indices (all data)	R1 = 0.0685, wR2 = 0.1809
Extinction coefficient	0.0026(3)
Largest diff. peak and hole	287 and −221 $e.nm^{-3}$

Data collection

Diffractometer used	Siemens P4
Monochromator	highly oriented graphite crystal
Scan type	ω
Scan Speed	variable; 4.0 to 35.0°/min in ω
Scan range (ω)	0.75°
Standard reflections	3 measured every 97 reflections

Solution and refinement

System used	SHELXS-86 (Sheldrick, 1990)
	SHELXL-93 (Sheldrick, 1993)
Solution	Direct Methods
Weighting scheme	calc $w=1/[\sigma^2(Fo^2)+(0.0364P)^2+0.0P]$
	where $P = (Fo^2 + 2Fc^2)/3$
Hydrogen Atoms	calculated, with isotropic displacement parameters 1.2 times higher than U_{eq} of the carbon atoms

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^{-1}) for 3. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	1864(1)	6066(1)	9871(1)	27(1)
N(1)	4565(4)	7007(1)	9013(3)	28(1)
C(1)	-224(7)	6517(2)	10308(5)	61(2)
C(2)	-580(6)	5931(2)	10288(4)	53(1)
C(3)	413(6)	5662(2)	11255(5)	50(1)
C(4)	1385(5)	6087(3)	11870(4)	53(1)
C(5)	965(7)	6625(2)	11278(6)	60(2)
C(6)	2601(5)	6293(2)	7976(4)	30(1)
C(7)	2349(5)	5678(2)	8085(4)	34(1)
C(8)	3434(5)	5466(2)	9081(4)	35(1)
C(9)	4355(5)	5949(2)	9592(4)	33(1)
C(10)	3872(5)	6454(2)	8891(4)	26(1)
C(11)	3602(7)	7500	8537(5)	29(1)
C(12)	5284(5)	7170(2)	10317(4)	39(1)

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

Fe(1)-C(1)	202.3(4)	Fe(1)-C(8)	202.8(4)
Fe(1)-C(7)	203.2(4)	Fe(1)-C(3)	203.3(4)
Fe(1)-C(4)	203.6(4)	Fe(1)-C(5)	203.5(4)
Fe(1)-C(2)	203.6(4)	Fe(1)-C(9)	204.3(4)
Fe(1)-C(6)	205.2(4)	Fe(1)-C(10)	208.9(4)
N(1)-C(10)	139.0(5)	N(1)-C(11)	145.0(4)
N(1)-C(12)	147.4(5)	C(1)-C(2)	137.5(7)
C(1)-C(5)	138.5(7)	C(2)-C(3)	139.7(6)
C(3)-C(4)	139.2(6)	C(4)-C(5)	140.8(7)
C(6)-C(10)	142.1(5)	C(6)-C(7)	142.9(5)
C(7)-C(8)	141.1(6)	C(8)-C(9)	142.6(5)
C(9)-C(10)	140.9(5)	C(11)-N(1)#1	145.0(4)
C(12)-C(12)#1	151.2(8)		

C(1)-Fe(1)-C(8)	161.7(2)	C(1)-Fe(1)-C(7)	125.0(2)
C(8)-Fe(1)-C(7)	40.7(2)	C(1)-Fe(1)-C(3)	66.9(2)
C(8)-Fe(1)-C(3)	108.3(2)	C(7)-Fe(1)-C(3)	120.6(2)
C(1)-Fe(1)-C(4)	67.6(2)	C(8)-Fe(1)-C(4)	121.1(2)
C(7)-Fe(1)-C(4)	155.4(2)	C(3)-Fe(1)-C(4)	40.0(2)
C(1)-Fe(1)-C(5)	39.9(2)	C(8)-Fe(1)-C(5)	156.5(2)
C(7)-Fe(1)-C(5)	161.9(2)	C(3)-Fe(1)-C(5)	67.2(2)
C(4)-Fe(1)-C(5)	40.5(2)	C(1)-Fe(1)-C(2)	39.6(2)
C(8)-Fe(1)-C(2)	125.4(2)	C(7)-Fe(1)-C(2)	107.4(2)
C(3)-Fe(1)-C(2)	40.2(2)	C(4)-Fe(1)-C(2)	67.6(2)
C(5)-Fe(1)-C(2)	67.1(2)	C(1)-Fe(1)-C(9)	156.0(2)
C(8)-Fe(1)-C(9)	41.0(2)	C(7)-Fe(1)-C(9)	68.5(2)
C(3)-Fe(1)-C(9)	126.7(2)	C(4)-Fe(1)-C(9)	108.8(2)
C(5)-Fe(1)-C(9)	121.8(2)	C(2)-Fe(1)-C(9)	163.2(2)
C(1)-Fe(1)-C(6)	108.1(2)	C(8)-Fe(1)-C(6)	68.4(2)
C(7)-Fe(1)-C(6)	41.0(2)	C(3)-Fe(1)-C(6)	155.5(2)
C(4)-Fe(1)-C(6)	162.7(2)	C(5)-Fe(1)-C(6)	125.5(2)
C(2)-Fe(1)-C(6)	120.5(2)	C(9)-Fe(1)-C(6)	67.9(2)
C(1)-Fe(1)-C(10)	121.8(2)	C(8)-Fe(1)-C(10)	67.9(2)
C(7)-Fe(1)-C(10)	68.0(2)	C(3)-Fe(1)-C(10)	163.2(2)
C(4)-Fe(1)-C(10)	126.6(2)	C(5)-Fe(1)-C(10)	109.4(2)
C(2)-Fe(1)-C(10)	155.4(2)	C(9)-Fe(1)-C(10)	39.84(14)
C(6)-Fe(1)-C(10)	40.1(2)	C(10)-N(1)-C(11)	117.8(3)
C(10)-N(1)-C(12)	117.8(3)	C(11)-N(1)-C(12)	107.6(3)
C(2)-C(1)-C(5)	109.1(4)	C(2)-C(1)-Fe(1)	70.7(3)
C(5)-C(1)-Fe(1)	70.5(3)	C(1)-C(2)-C(3)	107.5(4)
C(1)-C(2)-Fe(1)	69.7(3)	C(3)-C(2)-Fe(1)	69.8(3)
C(4)-C(3)-C(2)	108.6(4)	C(4)-C(3)-Fe(1)	70.1(2)
C(2)-C(3)-Fe(1)	70.0(2)	C(3)-C(4)-C(5)	106.9(4)
C(3)-C(4)-Fe(1)	69.9(2)	C(5)-C(4)-Fe(1)	69.8(3)
C(1)-C(5)-C(4)	107.8(4)	C(1)-C(5)-Fe(1)	69.6(3)
C(4)-C(5)-Fe(1)	69.8(2)	C(10)-C(6)-C(7)	108.0(3)
C(10)-C(6)-Fe(1)	71.3(2)	C(7)-C(6)-Fe(1)	68.8(2)
C(8)-C(7)-C(6)	107.8(3)	C(8)-C(7)-Fe(1)	69.5(2)
C(6)-C(7)-Fe(1)	70.3(2)	C(7)-C(8)-C(9)	108.0(3)
C(7)-C(8)-Fe(1)	69.8(2)	C(9)-C(8)-Fe(1)	70.1(2)
C(10)-C(9)-C(8)	108.4(3)	C(10)-C(9)-Fe(1)	71.9(2)
C(8)-C(9)-Fe(1)	68.9(2)	N(1)-C(10)-C(9)	126.5(3)
N(1)-C(10)-C(6)	125.6(3)	C(9)-C(10)-C(6)	107.8(3)
N(1)-C(10)-Fe(1)	131.1(3)	C(9)-C(10)-Fe(1)	68.3(2)
C(6)-C(10)-Fe(1)	68.5(2)	N(1)#1-C(11)-N(1)	102.4(4)
N(1)-C(12)-C(12)#1	104.7(2)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$pm^2 \times 10^{-1}$] for 3.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	32(1)	28(1)	23(1)	2(1)	3(1)	2(1)
N(1)	29(2)	30(2)	25(2)	1(2)	1(1)	1(2)
C(1)	58(3)	69(4)	57(4)	23(3)	24(3)	30(3)
C(2)	36(2)	86(4)	37(3)	-5(3)	8(2)	-8(3)
C(3)	67(4)	36(2)	46(3)	8(2)	28(3)	-1(3)
C(4)	46(3)	93(4)	18(2)	0(3)	4(2)	2(3)
C(5)	81(4)	37(3)	61(3)	-20(3)	42(3)	-16(3)
C(6)	37(2)	31(2)	22(2)	3(2)	5(2)	2(2)
C(7)	42(3)	33(2)	28(2)	-6(2)	3(2)	-5(2)
C(8)	43(3)	21(2)	40(2)	-1(2)	7(2)	8(2)
C(9)	25(2)	37(3)	38(3)	5(2)	2(2)	6(2)
C(10)	24(2)	27(2)	29(2)	1(2)	7(2)	2(2)
C(11)	35(3)	27(3)	24(3)	0	-1(2)	0
C(12)	38(2)	36(2)	41(3)	5(2)	-12(2)	-1(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2 x 10^{-1}) for 3.

	x	y	z	U(eq)
H(1)	-711	6801	9752	74
H(2)	-1352	5744	9727	63
H(3)	424	5261	11456	60
H(4)	2172	6026	12550	63
H(5)	1411	6991	11502	72
H(6)	2027	6547	7400	36
H(7)	1595	5454	7582	41
H(8)	3532	5076	9359	42
H(9)	5149	5932	10280	40
H(11A)	3520	7500	7559	34
H(11B)	2483	7500	8921	34
H(12A)	6416	7018	10406	46
H(12B)	4606	7018	11053	46

Table 1. Crystal data and structure refinement for 4b

Molecular formula	$C_{23}H_{23}F_6Fe_2N_2P$
Formula weight	584.10
Crystal system	Orthorhombic
Space group	Pnma (No.62)
Unit cell dimensions	a = 959.0(2) pm $\alpha = 90^\circ$ b = 2494.3(9) pm $\beta = 90^\circ$ c = 901.4(1) pm $\gamma = 90^\circ$
Volume	2.1562(9) nm^3
Z	4
Temperature	213(2) K
Radiation	MoKα (λ =71.073 pm)
Density (calculated)	1.799 Mg/m^3
Absorption coefficient	1.487 mm^{-1}
F(000)	1184
Color, Habit	orange plate
Crystal size	0.6 x 0.45 x 0.17 mm
θ range for data collection	3.10 to 23.49°
Index ranges	$0 \le h \le 10$, $-1 \le k \le 27$, $0 \le \ell \le 10$
Reflections collected	1709
Independent reflections	1627 (R_{int} = 0.0164)
Reflections with I > 2σ(I)	1376
Absorption correction	ψ-scan
Max. and min. transmission	1.000 and 0.695
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1535 / 0 / 182
Goodness-of-fit on F^2	1.054
Final R indices [I>2σ(I)]	R1 = 0.0289, wR2 = 0.0702
R indices (all data)	R1 = 0.0415, wR2 = 0.1266
Extinction coefficient	0.0083(6)
Largest diff. peak and hole	386 and -329 $e.nm^{-3}$

Data collection

Diffractometer used	Siemens P4
Monochromator	highly oriented graphite crystal
Scan type	ω
Scan Speed	variable; 5.0 to 35.0°/min in ω
Scan range (ω)	0.8°
Standard reflections	3 measured every 97 reflections

Solution and refinement

System used	SHELXS-86 (Sheldrick, 1990)
	SHELXL-93 (Sheldrick, 1993)
Solution	Direct Methods
Weighting scheme	calc $w=1/[\sigma^2(Fo^2)+(0.0340P)^2+2.9290P]$
	where $P = (Fo^2 + 2Fc^2)/3$
Hydrogen Atoms	calculated, with isotropic displacement parameters 1.2 times higher than U_{eq} of the carbon atoms

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^{-1}) for 4b. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	3155(1)	5901(1)	128(1)	22(1)
N(1)	3361(2)	7062(1)	-1152(2)	23(1)
C(1)	2599(4)	5887(1)	2322(3)	36(1)
C(2)	2686(4)	5360(1)	1749(4)	39(1)
C(3)	1734(4)	5316(1)	573(4)	46(1)
C(4)	1060(4)	5811(2)	408(4)	47(1)
C(5)	1589(3)	6167(1)	1477(4)	37(1)
C(6)	4917(3)	6357(1)	-29(3)	25(1)
C(7)	5214(3)	5812(1)	-388(3)	29(1)
C(8)	4374(3)	5659(1)	-1599(3)	28(1)
C(9)	3544(3)	6106(1)	-2026(3)	26(1)
C(10)	3895(3)	6532(1)	-1053(3)	23(1)
C(11)	4033(4)	7500	-819(4)	23(1)
C(12)	1997(3)	7193(1)	-1820(3)	28(1)
P(1)	8654(1)	7500	977(1)	31(1)
F(1)	7030(3)	7500	657(4)	69(1)
F(2)	10296(3)	7500	1238(4)	67(1)
F(3A)	8281(15)	7500	2597(11)	206(13)
F(4A)	8964(12)	7500	-705(10)	115(8)
F(5A)	8648(13)	6906(3)	893(21)	200(9)
F(3B)	8539(8)	7083(3)	2198(10)	100(4)
F(4B)	8832(8)	7060(4)	-185(10)	143(7)

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

Fe(1)-C(10)	202.9(3)	Fe(1)-C(3)	203.6(3)
Fe(1)-C(4)	203.7(3)	Fe(1)-C(2)	203.9(3)
Fe(1)-C(8)	203.9(3)	Fe(1)-C(7)	204.1(3)
Fe(1)-C(5)	204.3(3)	Fe(1)-C(6)	204.2(3)
Fe(1)-C(9)	204.3(3)	Fe(1)-C(1)	204.8(3)
N(1)-C(11)	130.4(3)	N(1)-C(10)	142.0(4)
N(1)-C(12)	147.6(4)	C(1)-C(2)	141.4(4)
C(1)-C(5)	141.6(5)	C(2)-C(3)	140.4(5)
C(3)-C(4)	140.2(5)	C(4)-C(5)	140.5(5)
C(6)-C(10)	141.6(4)	C(6)-C(7)	142.7(4)
C(7)-C(8)	141.0(4)	C(8)-C(9)	142.3(4)
C(9)-C(10)	142.0(4)	C(11)-N(1)#1	130.4(3)
C(12)-C(12)#1	153.3(6)	P(1)-F(5A)#1	148.4(9)
P(1)-F(5A)	148.4(9)	P(1)-F(3A)	150.3(11)
P(1)-F(3B)#1	151.9(6)	P(1)-F(3B)	151.9(6)
P(1)-F(4B)	152.6(6)	P(1)-F(4B)#1	152.6(6)
P(1)-F(4A)	154.6(9)	P(1)-F(1)	158.3(3)
P(1)-F(2)	159.3(3)	F(3A)-F(3B)#1	112.9(11)
F(3A)-F(3B)	112.9(11)	F(4A)-F(4B)	120.0(13)
F(4A)-F(4B)#1	120.0(13)	F(5A)-F(4B)	106(2)
F(5A)-F(3B)	126(2)		

C(10)-Fe(1)-C(3)	153.32(14)	C(10)-Fe(1)-C(4)	119.70(14)
C(3)-Fe(1)-C(4)	40.3(2)	C(10)-Fe(1)-C(2)	165.16(13)
C(3)-Fe(1)-C(2)	40.3(2)	C(4)-Fe(1)-C(2)	67.72(14)
C(10)-Fe(1)-C(8)	68.20(11)	C(3)-Fe(1)-C(8)	108.75(13)
C(4)-Fe(1)-C(8)	128.88(14)	C(2)-Fe(1)-C(8)	118.54(12)
C(10)-Fe(1)-C(7)	68.08(11)	C(3)-Fe(1)-C(7)	127.87(14)
C(4)-Fe(1)-C(7)	166.0(2)	C(2)-Fe(1)-C(7)	107.72(13)
C(8)-Fe(1)-C(7)	40.43(12)	C(10)-Fe(1)-C(5)	108.49(12)
C(3)-Fe(1)-C(5)	67.93(14)	C(4)-Fe(1)-C(5)	40.3(2)
C(2)-Fe(1)-C(5)	68.06(13)	C(8)-Fe(1)-C(5)	166.51(13)
C(7)-Fe(1)-C(5)	151.89(13)	C(10)-Fe(1)-C(6)	40.70(11)
C(3)-Fe(1)-C(6)	165.1(2)	C(4)-Fe(1)-C(6)	152.4(2)
C(2)-Fe(1)-C(6)	126.92(13)	C(8)-Fe(1)-C(6)	68.74(12)
C(7)-Fe(1)-C(6)	40.90(11)	C(5)-Fe(1)-C(6)	117.94(13)
C(10)-Fe(1)-C(9)	40.81(11)	C(3)-Fe(1)-C(9)	119.25(13)
C(4)-Fe(1)-C(9)	109.01(13)	C(2)-Fe(1)-C(9)	152.53(13)
C(8)-Fe(1)-C(9)	40.81(12)	C(7)-Fe(1)-C(9)	68.53(12)
C(5)-Fe(1)-C(9)	128.25(13)	C(6)-Fe(1)-C(9)	69.11(11)
C(10)-Fe(1)-C(1)	127.64(12)	C(3)-Fe(1)-C(1)	67.91(14)
C(4)-Fe(1)-C(1)	67.78(14)	C(2)-Fe(1)-C(1)	40.50(13)
C(8)-Fe(1)-C(1)	151.83(13)	C(7)-Fe(1)-C(1)	118.02(13)
C(5)-Fe(1)-C(1)	40.49(13)	C(6)-Fe(1)-C(1)	106.96(12)
C(9)-Fe(1)-C(1)	165.86(12)	C(11)-N(1)-C(10)	126.0(2)
C(11)-N(1)-C(12)	110.3(2)	C(10)-N(1)-C(12)	123.4(2)
C(2)-C(1)-C(5)	107.6(3)	C(2)-C(1)-Fe(1)	69.4(2)
C(5)-C(1)-Fe(1)	69.5(2)	C(3)-C(2)-C(1)	108.1(3)
C(3)-C(2)-Fe(1)	69.8(2)	C(1)-C(2)-Fe(1)	70.1(2)
C(4)-C(3)-C(2)	108.1(3)	C(4)-C(3)-Fe(1)	69.9(2)
C(2)-C(3)-Fe(1)	69.9(2)	C(3)-C(4)-C(5)	108.5(3)
C(3)-C(4)-Fe(1)	69.8(2)	C(5)-C(4)-Fe(1)	70.0(2)
C(4)-C(5)-C(1)	107.7(3)	C(4)-C(5)-Fe(1)	69.7(2)
C(1)-C(5)-Fe(1)	70.0(2)	C(10)-C(6)-C(7)	106.6(2)
C(10)-C(6)-Fe(1)	69.2(2)	C(7)-C(6)-Fe(1)	69.5(2)
C(8)-C(7)-C(6)	108.6(3)	C(8)-C(7)-Fe(1)	69.7(2)
C(6)-C(7)-Fe(1)	69.6(2)	C(7)-C(8)-C(9)	108.5(2)
C(7)-C(8)-Fe(1)	69.9(2)	C(9)-C(8)-Fe(1)	69.7(2)

C(8)-C(9)-Fe(1)	69.5(2)	C(6)-C(10)-C(9)	109.6(3)
C(6)-C(10)-N(1)	125.3(3)	C(9)-C(10)-N(1)	125.0(2)
C(6)-C(10)-Fe(1)	70.1(2)	C(9)-C(10)-Fe(1)	70.1(2)
N(1)-C(10)-Fe(1)	129.0(2)	N(1)-C(11)-N(1)#1	113.9(3)
N(1)-C(12)-C(12)#1	102.76(14)	F(5A)#1-P(1)-F(5A)	174.1(14)
F(5A)#1-P(1)-F(3A)	92.8(7)	F(5A)-P(1)-F(3A)	92.8(7)
F(5A)#1-P(1)-F(3B)#1	49.6(6)	F(5A)-P(1)-F(3B)#1	136.2(10)
F(3A)-P(1)-F(3B)#1	43.9(4)	F(5A)#1-P(1)-F(3B)	136.2(10)
F(5A)-P(1)-F(3B)	49.6(6)	F(3A)-P(1)-F(3B)	43.9(4)
F(3B)#1-P(1)-F(3B)	86.5(8)	F(5A)#1-P(1)-F(4B)	133.1(10)
F(5A)-P(1)-F(4B)	41.2(7)	F(3A)-P(1)-F(4B)	133.9(5)
F(3B)#1-P(1)-F(4B)	176.3(5)	F(3B)-P(1)-F(4B)	90.7(6)
F(5A)#1-P(1)-F(4B)#1	41.2(7)	F(5A)-P(1)-F(4B)#1	133.1(10)
F(3A)-P(1)-F(4B)#1	133.9(5)	F(3B)#1-P(1)-F(4B)#1	90.7(6)
F(3B)-P(1)-F(4B)#1	176.3(6)	F(4B)-P(1)-F(4B)#1	91.9(10)
F(5A)#1-P(1)-F(4A)	87.2(7)	F(5A)-P(1)-F(4A)	87.2(7)
F(3A)-P(1)-F(4A)	177.3(7)	F(3B)#1-P(1)-F(4A)	136.5(4)
F(3B)-P(1)-F(4A)	136.5(4)	F(4B)-P(1)-F(4A)	46.0(5)
F(4B)#1-P(1)-F(4A)	46.0(5)	F(5A)#1-P(1)-F(1)	89.2(5)
F(5A)-P(1)-F(1)	89.2(5)	F(3A)-P(1)-F(1)	86.7(6)
F(3B)#1-P(1)-F(1)	93.5(3)	F(3B)-P(1)-F(1)	93.5(3)
F(4B)-P(1)-F(1)	89.2(3)	F(4B)#1-P(1)-F(1)	89.2(3)
F(4A)-P(1)-F(1)	90.6(5)	F(5A)#1-P(1)-F(2)	90.7(5)
F(5A)-P(1)-F(2)	90.7(5)	F(3A)-P(1)-F(2)	95.3(6)
F(3B)#1-P(1)-F(2)	88.0(3)	F(3B)-P(1)-F(2)	88.0(3)
F(4B)-P(1)-F(2)	89.5(3)	F(4B)#1-P(1)-F(2)	89.5(3)
F(4A)-P(1)-F(2)	87.4(5)	F(1)-P(1)-F(2)	178.0(2)
F(3B)#1-F(3A)-F(3B)	135(2)	F(3B)#1-F(3A)-P(1)	68.8(7)
F(3B)-F(3A)-P(1)	68.8(7)	F(4B)-F(4A)-F(4B)#1	132.2(12)
F(4B)-F(4A)-P(1)	66.1(6)	F(4B)#1-F(4A)-P(1)	66.1(6)
F(4B)-F(5A)-F(3B)	137.8(11)	F(4B)-F(5A)-P(1)	71.5(6)
F(3B)-F(5A)-P(1)	66.6(6)	F(3A)-F(3B)-F(5A)	129.7(10)
F(3A)-F(3B)-P(1)	67.3(6)	F(5A)-F(3B)-P(1)	63.8(5)
F(5A)-F(4B)-F(4A)	135.2(11)	F(5A)-F(4B)-P(1)	67.3(7)
F(4A)-F(4B)-P(1)	67.9(6)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$pm^2 \times 10^{-1}$] for 4b.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	23(1)	20(1)	23(1)	0(1)	2(1)	-2(1)
N(1)	21(1)	20(1)	27(1)	1(1)	-3(1)	0(1)
C(1)	38(2)	45(2)	24(2)	1(2)	8(1)	-4(2)
C(2)	44(2)	32(2)	40(2)	12(2)	15(2)	1(2)
C(3)	53(2)	40(2)	43(2)	-6(2)	17(2)	-24(2)
C(4)	24(2)	76(3)	41(2)	11(2)	4(2)	-12(2)
C(5)	35(2)	35(2)	40(2)	5(2)	16(2)	7(2)
C(6)	22(1)	23(1)	30(2)	-1(1)	0(1)	-4(1)
C(7)	23(2)	27(2)	36(2)	1(1)	2(1)	4(1)
C(8)	33(2)	22(2)	30(2)	-6(1)	7(1)	1(1)
C(9)	28(2)	27(2)	22(1)	-1(1)	2(1)	-4(1)
C(10)	20(1)	25(2)	23(2)	1(1)	3(1)	-1(1)
C(11)	22(2)	24(2)	24(2)	0	-1(2)	0
C(12)	22(2)	26(2)	37(2)	1(1)	-2(1)	-1(1)
P(1)	26(1)	34(1)	33(1)	0	-2(1)	0
F(1)	23(2)	116(3)	68(2)	0	0(2)	0
F(2)	30(2)	104(3)	66(2)	0	-16(2)	0
F(3A)	85(8)	515(39)	19(4)	0	-5(5)	0
F(4A)	31(4)	284(25)	30(4)	0	1(3)	0
F(5A)	142(9)	28(4)	431(25)	59(12)	-13(17)	-2(4)
F(3B)	67(4)	92(8)	141(8)	98(7)	-19(6)	-27(5)
F(4B)	52(4)	220(16)	159(9)	-178(11)	-18(6)	25(8)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2 x 10^{-1}) for 4b.

	x	y	z	U(eq)
H(1)	3117	6026	3119	43
H(2)	3279	5087	2096	46
H(3)	1577	5008	-4	55
H(4)	369	5891	-298	57
H(5)	1322	6526	1607	44
H(6)	5321	6560	737	30
H(7)	5862	5591	103	35
H(8)	4364	5319	-2049	34
H(9)	2890	6116	-2803	31
H(11)	4921	7500	-380	28
H(12A)	1228	7051	-1221	34
H(12B)	1924	7051	-2830	34

Table 1. Crystal data and structure refinement for 5

Molecular formula	$C_{23}H_{22}Fe_2N_2S$
Formula weight	470.19
Crystal system	Orthorhombic
Space group	Pnma (No.62)
Unit cell dimensions	a = 1075.6(4) pm $\alpha = 90^\circ$ b = 2400.3(4) pm $\beta = 90^\circ$ c = 740.5(1) pm $\gamma = 90^\circ$
Volume	1.9118(8) nm^3
Z	4
Temperature	293(2) K
Radiation	MoKα (λ =71.073 pm)
Density (calculated)	1.634 Mg/m^3
Absorption coefficient	1.638 mm^{-1}
F(000)	968
Color, Habit	red prism
Crystal size	0.4 x 0.35 x 0.20 mm
θ range for data collection	2.88 to 22.49°
Index ranges	$-1 \le h \le 11$, $-1 \le k \le 25$, $-1 \le \ell \le 7$
Reflections collected	1783
Independent reflections	1278 (R_{int} = 0.0428)
Reflections with I > 2σ(I)	942
Absorption correction	ψ-scan
Max. and min. transmission	0.966 and 0.693
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1173 / 0 / 131
Goodness-of-fit on F^2	1.068
Final R indices [I>2σ(I)]	R1 = 0.0410, wR2 = 0.0978
R indices (all data)	R1 = 0.0665, wR2 = 0.1119
Extinction coefficient	0.0042(7)
Largest diff. peak and hole	429 and -404 $e.nm^{-3}$

Data collection

Diffractometer used	Siemens P4
Monochromator	highly oriented graphite crystal
Scan type	ω
Scan Speed	variable; 5.0 to 35.0°/min in ω
Scan range (ω)	0.8°
Standard reflections	3 measured every 97 reflections

Solution and refinement

System used	SHELXS-86 (Sheldrick, 1990) SHELXL-93 (Sheldrick, 1993)
Solution	Direct Methods
Weighting scheme	calc $w=1/[\sigma^2(Fo^2)+(0.0602P)^2+0.5887P]$ where $P = (Fo^2 + 2Fc^2)/3$
Hydrogen Atoms	calculated, with isotropic displacement parameters 1.2 times higher than U_{eq} of the carbon atoms

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^{-1}) for 5. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	6228(1)	3958(1)	181(1)	24(1)
S(1)	6929(2)	2500	4425(2)	35(1)
N(1)	7850(4)	2957(2)	1367(5)	25(1)
C(1)	4598(5)	3607(3)	-585(8)	45(2)
C(2)	4491(5)	4185(3)	-666(8)	43(2)
C(3)	5393(6)	4379(2)	-1871(8)	46(2)
C(4)	6044(5)	3919(3)	-2531(7)	51(2)
C(5)	5555(6)	3435(2)	-1738(8)	44(2)
C(6)	6556(5)	3732(2)	2796(6)	34(1)
C(7)	6572(6)	4321(2)	2612(7)	40(2)
C(8)	7494(6)	4463(2)	1361(8)	47(2)
C(9)	8095(5)	3970(2)	753(8)	37(1)
C(10)	7505(5)	3519(2)	1676(6)	28(1)
C(11)	7532(6)	2500	2339(9)	23(2)
C(12)	8509(4)	2816(2)	-303(6)	34(1)

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

Fe(1)-C(4)	202.0(5)	Fe(1)-C(8)	202.2(5)
Fe(1)-C(1)	202.6(5)	Fe(1)-C(5)	202.9(5)
Fe(1)-C(3)	203.4(5)	Fe(1)-C(7)	203.4(5)
Fe(1)-C(6)	204.1(5)	Fe(1)-C(2)	204.5(5)
Fe(1)-C(9)	205.3(5)	Fe(1)-C(10)	205.5(5)
S(1)-C(11)	167.5(7)	N(1)-C(11)	135.6(5)
N(1)-C(10)	141.7(6)	N(1)-C(12)	146.5(6)
C(1)-C(2)	139.4(8)	C(1)-C(5)	140.0(8)
C(2)-C(3)	139.8(8)	C(3)-C(4)	139.5(8)
C(4)-C(5)	140.4(8)	C(6)-C(10)	141.1(7)
C(6)-C(7)	142.2(7)	C(7)-C(8)	139.9(8)
C(8)-C(9)	142.3(8)	C(9)-C(10)	142.9(7)
C(11)-N(1)#1	135.6(5)	C(12)-C(12)#1	151.6(11)

C(4)-Fe(1)-C(8)	121.5(3)	C(4)-Fe(1)-C(1)	67.5(2)
C(8)-Fe(1)-C(1)	162.3(3)	C(4)-Fe(1)-C(5)	40.6(2)
C(8)-Fe(1)-C(5)	156.0(3)	C(1)-Fe(1)-C(5)	40.4(2)
C(4)-Fe(1)-C(3)	40.2(2)	C(8)-Fe(1)-C(3)	108.8(2)
C(1)-Fe(1)-C(3)	67.4(2)	C(5)-Fe(1)-C(3)	68.1(2)
C(4)-Fe(1)-C(7)	156.5(3)	C(8)-Fe(1)-C(7)	40.4(2)
C(1)-Fe(1)-C(7)	125.7(3)	C(5)-Fe(1)-C(7)	161.7(3)
C(3)-Fe(1)-C(7)	121.9(2)	C(4)-Fe(1)-C(6)	161.3(3)
C(8)-Fe(1)-C(6)	68.5(2)	C(1)-Fe(1)-C(6)	107.7(2)
C(5)-Fe(1)-C(6)	124.1(2)	C(3)-Fe(1)-C(6)	156.5(2)
C(7)-Fe(1)-C(6)	40.8(2)	C(4)-Fe(1)-C(2)	67.5(2)
C(8)-Fe(1)-C(2)	126.0(2)	C(1)-Fe(1)-C(2)	40.0(2)
C(5)-Fe(1)-C(2)	68.0(2)	C(3)-Fe(1)-C(2)	40.1(2)
C(7)-Fe(1)-C(2)	108.8(2)	C(6)-Fe(1)-C(2)	121.3(2)
C(4)-Fe(1)-C(9)	107.6(2)	C(8)-Fe(1)-C(9)	40.9(2)
C(1)-Fe(1)-C(9)	155.5(2)	C(5)-Fe(1)-C(9)	120.1(2)
C(3)-Fe(1)-C(9)	125.4(2)	C(7)-Fe(1)-C(9)	68.5(2)
C(6)-Fe(1)-C(9)	68.8(2)	C(2)-Fe(1)-C(9)	162.4(2)
C(4)-Fe(1)-C(10)	125.3(2)	C(8)-Fe(1)-C(10)	68.0(2)
C(1)-Fe(1)-C(10)	121.1(2)	C(5)-Fe(1)-C(10)	107.4(2)
C(3)-Fe(1)-C(10)	162.2(2)	C(7)-Fe(1)-C(10)	67.8(2)
C(6)-Fe(1)-C(10)	40.3(2)	C(2)-Fe(1)-C(10)	155.9(2)
C(9)-Fe(1)-C(10)	40.7(2)	C(11)-N(1)-C(10)	128.1(4)
C(11)-N(1)-C(12)	112.6(4)	C(10)-N(1)-C(12)	118.9(4)
C(2)-C(1)-C(5)	109.2(5)	C(2)-C(1)-Fe(1)	70.7(3)
C(5)-C(1)-Fe(1)	70.0(3)	C(1)-C(2)-C(3)	107.5(5)
C(1)-C(2)-Fe(1)	69.2(3)	C(3)-C(2)-Fe(1)	69.5(3)
C(4)-C(3)-C(2)	108.0(5)	C(4)-C(3)-Fe(1)	69.4(3)
C(2)-C(3)-Fe(1)	70.4(3)	C(3)-C(4)-C(5)	108.7(5)
C(3)-C(4)-Fe(1)	70.4(3)	C(5)-C(4)-Fe(1)	70.1(3)
C(1)-C(5)-C(4)	106.6(5)	C(1)-C(5)-Fe(1)	69.7(3)
C(4)-C(5)-Fe(1)	69.4(3)	C(10)-C(6)-C(7)	107.2(5)
C(10)-C(6)-Fe(1)	70.4(3)	C(7)-C(6)-Fe(1)	69.3(3)
C(8)-C(7)-C(6)	108.3(5)	C(8)-C(7)-Fe(1)	69.4(3)
C(6)-C(7)-Fe(1)	69.9(3)	C(7)-C(8)-C(9)	109.2(5)
C(7)-C(8)-Fe(1)	70.3(3)	C(9)-C(8)-Fe(1)	70.7(3)
C(8)-C(9)-C(10)	106.1(5)	C(8)-C(9)-Fe(1)	68.4(3)
C(10)-C(9)-Fe(1)	69.7(3)	C(6)-C(10)-N(1)	129.0(5)
C(6)-C(10)-C(9)	109.2(4)	N(1)-C(10)-C(9)	121.8(5)
C(6)-C(10)-Fe(1)	69.3(3)	N(1)-C(10)-Fe(1)	125.2(3)
C(9)-C(10)-Fe(1)	69.6(3)	N(1)-C(11)-N(1)#1	108.0(6)
N(1)-C(11)-S(1)	126.0(3)	N(1)#1-C(11)-S(1)	126.0(3)
N(1)-C(12)-C(12)#1	103.4(2)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$pm^2 \times 10^{-1}$] for 5.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	26(1)	28(1)	20(1)	0(1)	-4(1)	-4(1)
S(1)	46(1)	33(1)	24(1)	0	10(1)	0
N(1)	29(3)	24(2)	22(2)	2(2)	7(2)	-3(2)
C(1)	33(3)	60(4)	43(3)	6(3)	-7(3)	-21(3)
C(2)	25(3)	66(4)	39(3)	-16(3)	-9(3)	11(3)
C(3)	46(4)	45(3)	47(4)	14(3)	-21(3)	-11(3)
C(4)	27(4)	108(6)	18(3)	-3(3)	1(2)	-5(4)
C(5)	41(4)	44(3)	48(4)	-19(3)	-24(3)	9(3)
C(6)	45(4)	36(3)	21(3)	-2(2)	-2(3)	4(3)
C(7)	59(4)	32(3)	30(3)	-13(3)	-24(3)	14(3)
C(8)	54(4)	32(3)	54(4)	8(3)	-36(3)	-11(3)
C(9)	30(3)	36(3)	44(3)	5(3)	-15(3)	-8(3)
C(10)	32(3)	29(3)	24(3)	2(2)	-9(2)	-3(2)
C(11)	25(4)	29(4)	15(3)	0	-4(3)	0
C(12)	25(3)	44(3)	33(3)	7(2)	7(2)	-2(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2 x 10^{-1}) for 5.

	x	y	z	U(eq)
H(1)	4111	3373	123	54
H(2)	3923	4403	-33	52
H(3)	5535	4749	-2179	55
H(4)	6693	3931	-3359	61
H(5)	5816	3071	-1940	53
H(6)	6020	3525	3518	40
H(7)	6058	4570	3220	48
H(8)	7683	4823	986	56
H(9)	8742	3945	-77	44
H(12A)	9350	2961	-291	41
H(12B)	8075	2961	-1351	41

Table 1. Crystal data and structure refinement for 7

Molecular formula	$C_{47}H_{41}BFe_2N_2$
Formula weight	756.33
Crystal system	Orthorhombic (No.19)
Space group	$P2_12_12_1$
Unit cell dimensions	a = 1009.2(2) pm $\alpha = 90^o$ b = 1868.9(2) pm $\beta = 90^o$ c = 1932.9(2) pm $\gamma = 90^o$
Volume	3.6456(9) nm^3
Z	4
Temperature	213(2) K
Radiation	MoKα (λ =71.073 pm)
Density (calculated)	1.378 Mg/m^3
Absorption coefficient	0.833 mm^{-1}
F(000)	1576
Color, Habit	yellow prism
Crystal size	0.9 x 0.3 x 0.25 mm
θ range for data collection	2.52 to 23.00^o
Index ranges	$-1 \le h \le 11$, $-1 \le k \le 20$, $-1 \le \ell \le 21$
Reflections collected	3649
Independent reflections	3450 (R_{int} = 0.0136)
Reflections with I > 2σ(I)	3017
Absorption correction	ψ-scan
Max. and min. transmission	0.942 and 0.898
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3350 / 0 / 470
Goodness-of-fit on F^2	1.061
Final R indices [I>2σ(I)]	R1 = 0.0306, wR2 = 0.0565
R indices (all data)	R1 = 0.0424, wR2 = 0.0621
Absolute structure parameter	-0.02(2)
Extinction coefficient	0.0029(2)
Largest diff. peak and hole	220 and -234 $e.nm^{-3}$

Data collection

Diffractometer used	Siemens P4
Monochromator	highly oriented graphite crystal
Scan type	ω
Scan Speed	4.5°/min in ω
Scan range (ω)	0.7°
Standard reflections	3 measured every 97 reflections

Solution and refinement

System used	SHELXS-86 (Sheldrick, 1990)
	SHELXL-93 (Sheldrick, 1993)
Solution	Direct Methods
Weighting scheme	calc $w=1/[\sigma^2(Fo^2)+(0.0237P)^2+1.3402P]$
	where $P = (Fo^2 + 2Fc^2)/3$
Hydrogen Atoms	calculated, with isotropic displacement parameters 1.2 times higher than U_{eq} of the carbon atoms

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^{-1}) for 7. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	8813(1)	6722(1)	9221(1)	36(1)
Fe(2)	9381(1)	6553(1)	5183(1)	35(1)
N(1)	8811(4)	6056(2)	7758(2)	32(1)
N(2)	8922(3)	5974(2)	6647(2)	31(1)
B(1)	10806(5)	5205(2)	12033(2)	28(1)
C(1)	9115(10)	7781(3)	9139(7)	132(4)
C(2)	8968(9)	7571(6)	9843(6)	137(5)
C(3)	9999(9)	7118(4)	9966(3)	93(2)
C(4)	10693(6)	7040(3)	9375(5)	79(2)
C(5)	10170(10)	7428(4)	8890(3)	96(3)
C(6)	7159(4)	6453(3)	8667(2)	44(1)
C(7)	6992(5)	6277(3)	9377(2)	51(1)
C(8)	7999(6)	5800(3)	9573(2)	51(1)
C(9)	8817(5)	5661(2)	8997(2)	46(1)
C(10)	8287(4)	6072(2)	8442(2)	34(1)
C(11)	8098(4)	6031(2)	7178(2)	32(1)
C(12)	10129(5)	5997(2)	7584(2)	40(1)
C(13)	10201(4)	5943(3)	6898(2)	42(1)
C(14)	8546(4)	5957(2)	5930(2)	30(1)
C(15)	9133(5)	5503(2)	5433(2)	41(1)
C(16)	8520(5)	5655(2)	4798(2)	42(1)
C(17)	7555(5)	6186(2)	4905(2)	41(1)
C(18)	7562(4)	6383(2)	5616(2)	32(1)
C(19)	10693(5)	7247(2)	5608(2)	50(1)
C(20)	11365(4)	6767(3)	5187(3)	59(1)
C(21)	10831(6)	6826(3)	4516(3)	71(2)
C(22)	9840(6)	7358(3)	4525(3)	66(2)
C(23)	9760(5)	7616(2)	5213(3)	53(1)
C(24)	11637(4)	5847(2)	12422(2)	28(1)
C(25)	11187(4)	6555(2)	12420(2)	36(1)
C(26)	11877(5)	7109(2)	12728(2)	42(1)
C(27)	13063(5)	6987(2)	13050(2)	39(1)
C(28)	13550(4)	6301(2)	13071(2)	42(1)
C(29)	12847(4)	5751(2)	12753(2)	37(1)
C(30)	11284(4)	5137(2)	11218(2)	28(1)
C(31)	12411(4)	5465(2)	10954(2)	32(1)
C(32)	12795(4)	5408(2)	10266(2)	38(1)
C(33)	12061(5)	4995(2)	9811(2)	42(1)
C(34)	10943(5)	4653(2)	10052(2)	37(1)
C(35)	10577(4)	4728(2)	10737(2)	32(1)
C(36)	9235(4)	5435(2)	12054(2)	26(1)
C(37)	8455(5)	5393(2)	12652(2)	37(1)
C(38)	7181(5)	5657(2)	12695(2)	48(1)
C(39)	6592(5)	5967(3)	12133(3)	49(1)
C(40)	7305(5)	6027(3)	11530(2)	47(1)
C(41)	8593(4)	5766(2)	11501(2)	38(1)
C(42)	11032(4)	4425(2)	12425(2)	29(1)
C(43)	11055(4)	4372(2)	13150(2)	35(1)
C(44)	11236(5)	3730(2)	13493(2)	39(1)
C(45)	11396(4)	3102(2)	13133(2)	41(1)
C(46)	11388(5)	3123(2)	12418(2)	45(1)

Table 3. Bond lengths [pm] and angles [°] for 7.

Fe(1)-C(2)	199.8(6)	Fe(1)-C(10)	200.5(4)
Fe(1)-C(5)	200.7(6)	Fe(1)-C(1)	200.9(6)
Fe(1)-C(4)	201.0(5)	Fe(1)-C(3)	201.4(5)
Fe(1)-C(8)	202.6(5)	Fe(1)-C(9)	203.0(4)
Fe(1)-C(7)	203.9(4)	Fe(1)-C(6)	204.4(4)
Fe(2)-C(14)	200.8(4)	Fe(2)-C(21)	201.7(5)
Fe(2)-C(23)	202.5(4)	Fe(2)-C(22)	202.5(5)
Fe(2)-C(19)	202.7(4)	Fe(2)-C(16)	203.0(4)
Fe(2)-C(15)	203.5(4)	Fe(2)-C(17)	203.8(4)
Fe(2)-C(20)	204.2(5)	Fe(2)-C(18)	204.2(4)
N(1)-C(11)	133.4(5)	N(1)-C(12)	137.6(5)
N(1)-C(10)	142.4(5)	N(2)-C(11)	132.5(5)
N(2)-C(13)	138.0(5)	N(2)-C(14)	143.8(5)
B(1)-C(36)	164.4(6)	B(1)-C(24)	164.6(6)
B(1)-C(30)	165.2(5)	B(1)-C(42)	165.8(5)
C(1)-C(5)	134.2(10)	C(1)-C(2)	142.5(12)
C(2)-C(3)	136.1(11)	C(3)-C(4)	134.7(9)
C(4)-C(5)	129.9(9)	C(6)-C(10)	141.1(6)
C(6)-C(7)	142.0(6)	C(7)-C(8)	140.3(7)
C(8)-C(9)	141.0(6)	C(9)-C(10)	142.3(6)
C(12)-C(13)	133.1(6)	C(14)-C(18)	140.9(5)
C(14)-C(15)	141.2(5)	C(15)-C(16)	140.4(6)
C(16)-C(17)	140.5(6)	C(17)-C(18)	142.1(6)
C(19)-C(20)	138.8(6)	C(19)-C(23)	139.5(6)
C(20)-C(21)	140.9(7)	C(21)-C(22)	141.0(7)
C(22)-C(23)	141.7(7)	C(24)-C(29)	139.1(6)
C(24)-C(25)	139.9(5)	C(25)-C(26)	138.3(6)
C(26)-C(27)	136.9(6)	C(27)-C(28)	137.4(6)
C(28)-C(29)	139.2(6)	C(30)-C(31)	139.0(5)
C(30)-C(35)	139.8(5)	C(31)-C(32)	138.9(6)
C(32)-C(33)	138.5(6)	C(33)-C(34)	137.9(6)
C(34)-C(35)	138.2(5)	C(36)-C(41)	139.6(5)
C(36)-C(37)	140.0(6)	C(37)-C(38)	138.0(6)
C(38)-C(39)	136.7(6)	C(39)-C(40)	137.4(6)
C(40)-C(41)	139.0(6)	C(42)-C(47)	138.9(5)
C(42)-C(43)	140.6(5)	C(43)-C(44)	138.2(5)
C(44)-C(45)	137.3(6)	C(45)-C(46)	138.2(6)
C(46)-C(47)	139.8(5)		

C(2)-Fe(1)-C(10)	162.6(5)	C(2)-Fe(1)-C(5)	67.4(3)
C(10)-Fe(1)-C(5)	109.9(2)	C(2)-Fe(1)-C(1)	41.7(4)
C(10)-Fe(1)-C(1)	125.4(4)	C(5)-Fe(1)-C(1)	39.0(3)
C(2)-Fe(1)-C(4)	66.5(3)	C(10)-Fe(1)-C(4)	122.7(2)
C(5)-Fe(1)-C(4)	37.7(3)	C(1)-Fe(1)-C(4)	65.0(3)
C(2)-Fe(1)-C(3)	39.7(3)	C(10)-Fe(1)-C(3)	156.4(3)
C(5)-Fe(1)-C(3)	65.2(3)	C(1)-Fe(1)-C(3)	66.6(3)
C(4)-Fe(1)-C(3)	39.1(3)	C(2)-Fe(1)-C(8)	120.3(4)
C(10)-Fe(1)-C(8)	68.3(2)	C(5)-Fe(1)-C(8)	160.5(4)
C(1)-Fe(1)-C(8)	157.8(5)	C(4)-Fe(1)-C(8)	125.7(3)
C(3)-Fe(1)-C(8)	108.2(2)	C(2)-Fe(1)-C(9)	154.7(5)
C(10)-Fe(1)-C(9)	41.3(2)	C(5)-Fe(1)-C(9)	125.0(3)
C(1)-Fe(1)-C(9)	161.0(5)	C(4)-Fe(1)-C(9)	108.5(2)
C(3)-Fe(1)-C(9)	120.7(3)	C(8)-Fe(1)-C(9)	40.7(2)
C(2)-Fe(1)-C(7)	107.8(2)	C(10)-Fe(1)-C(7)	68.0(2)
C(5)-Fe(1)-C(7)	158.5(4)	C(1)-Fe(1)-C(7)	123.4(4)
C(4)-Fe(1)-C(7)	161.6(3)	C(3)-Fe(1)-C(7)	125.4(3)
C(8)-Fe(1)-C(7)	40.4(2)	C(9)-Fe(1)-C(7)	68.6(2)
C(2)-Fe(1)-C(6)	125.1(4)	C(10)-Fe(1)-C(6)	40.8(2)

C(4)-Fe(1)-C(6)	157.0(3)	C(3)-Fe(1)-C(6)	161.7(3)
C(8)-Fe(1)-C(6)	68.6(2)	C(9)-Fe(1)-C(6)	69.5(2)
C(7)-Fe(1)-C(6)	40.7(2)	C(14)-Fe(2)-C(21)	154.8(2)
C(14)-Fe(2)-C(23)	127.1(2)	C(21)-Fe(2)-C(23)	68.4(2)
C(14)-Fe(2)-C(22)	163.7(2)	C(21)-Fe(2)-C(22)	40.8(2)
C(23)-Fe(2)-C(22)	41.0(2)	C(14)-Fe(2)-C(19)	109.7(2)
C(21)-Fe(2)-C(19)	67.9(2)	C(23)-Fe(2)-C(19)	40.3(2)
C(22)-Fe(2)-C(19)	68.3(2)	C(14)-Fe(2)-C(16)	68.1(2)
C(21)-Fe(2)-C(16)	106.6(2)	C(23)-Fe(2)-C(16)	154.4(2)
C(22)-Fe(2)-C(16)	118.8(2)	C(19)-Fe(2)-C(16)	163.0(2)
C(14)-Fe(2)-C(15)	40.9(2)	C(21)-Fe(2)-C(15)	119.0(2)
C(23)-Fe(2)-C(15)	164.2(2)	C(22)-Fe(2)-C(15)	153.3(2)
C(19)-Fe(2)-C(15)	126.9(2)	C(16)-Fe(2)-C(15)	40.4(2)
C(14)-Fe(2)-C(17)	67.9(2)	C(21)-Fe(2)-C(17)	125.0(2)
C(23)-Fe(2)-C(17)	120.6(2)	C(22)-Fe(2)-C(17)	107.0(2)
C(19)-Fe(2)-C(17)	155.8(2)	C(16)-Fe(2)-C(17)	40.4(2)
C(15)-Fe(2)-C(17)	68.1(2)	C(14)-Fe(2)-C(20)	121.2(2)
C(21)-Fe(2)-C(20)	40.6(2)	C(23)-Fe(2)-C(20)	67.8(2)
C(22)-Fe(2)-C(20)	68.4(2)	C(19)-Fe(2)-C(20)	39.9(2)
C(16)-Fe(2)-C(20)	125.7(2)	C(15)-Fe(2)-C(20)	108.0(2)
C(17)-Fe(2)-C(20)	162.5(2)	C(14)-Fe(2)-C(18)	40.7(2)
C(21)-Fe(2)-C(18)	162.5(2)	C(23)-Fe(2)-C(18)	108.1(2)
C(22)-Fe(2)-C(18)	125.4(2)	C(19)-Fe(2)-C(18)	121.4(2)
C(16)-Fe(2)-C(18)	68.7(2)	C(15)-Fe(2)-C(18)	69.1(2)
C(17)-Fe(2)-C(18)	40.8(2)	C(20)-Fe(2)-C(18)	155.6(2)
C(11)-N(1)-C(12)	108.2(4)	C(11)-N(1)-C(10)	125.5(4)
C(12)-N(1)-C(10)	126.0(4)	C(11)-N(2)-C(13)	108.5(3)
C(11)-N(2)-C(14)	125.6(4)	C(13)-N(2)-C(14)	125.8(4)
C(36)-B(1)-C(24)	106.8(3)	C(36)-B(1)-C(30)	109.0(3)
C(24)-B(1)-C(30)	110.1(3)	C(36)-B(1)-C(42)	110.5(3)
C(24)-B(1)-C(42)	111.2(3)	C(30)-B(1)-C(42)	109.1(3)
C(5)-C(1)-C(2)	106.9(8)	C(5)-C(1)-Fe(1)	70.4(3)
C(2)-C(1)-Fe(1)	68.7(4)	C(3)-C(2)-C(1)	105.0(6)
C(3)-C(2)-Fe(1)	70.8(4)	C(1)-C(2)-Fe(1)	69.6(4)
C(4)-C(3)-C(2)	108.5(7)	C(4)-C(3)-Fe(1)	70.3(3)
C(2)-C(3)-Fe(1)	69.5(4)	C(5)-C(4)-C(3)	109.9(7)
C(5)-C(4)-Fe(1)	71.0(4)	C(3)-C(4)-Fe(1)	70.6(3)
C(4)-C(5)-C(1)	109.7(8)	C(4)-C(5)-Fe(1)	71.3(4)
C(1)-C(5)-Fe(1)	70.6(4)	C(10)-C(6)-C(7)	106.1(4)
C(10)-C(6)-Fe(1)	68.1(2)	C(7)-C(6)-Fe(1)	69.5(3)
C(8)-C(7)-C(6)	108.8(4)	C(8)-C(7)-Fe(1)	69.3(3)
C(6)-C(7)-Fe(1)	69.9(3)	C(7)-C(8)-C(9)	109.2(4)
C(7)-C(8)-Fe(1)	70.3(3)	C(9)-C(8)-Fe(1)	69.8(3)
C(8)-C(9)-C(10)	106.0(4)	C(8)-C(9)-Fe(1)	69.5(3)
C(10)-C(9)-Fe(1)	68.4(2)	C(6)-C(10)-C(9)	110.0(4)
C(6)-C(10)-N(1)	126.6(4)	C(9)-C(10)-N(1)	123.3(4)
C(6)-C(10)-Fe(1)	71.1(2)	C(9)-C(10)-Fe(1)	70.3(2)
N(1)-C(10)-Fe(1)	127.6(3)	N(2)-C(11)-N(1)	108.4(4)
C(13)-C(12)-N(1)	107.6(4)	C(12)-C(13)-N(2)	107.3(4)
C(18)-C(14)-C(15)	110.0(4)	C(18)-C(14)-N(2)	126.1(4)
C(15)-C(14)-N(2)	123.9(4)	C(18)-C(14)-Fe(2)	70.9(2)
C(15)-C(14)-Fe(2)	70.6(2)	N(2)-C(14)-Fe(2)	124.8(3)
C(16)-C(15)-C(14)	106.7(4)	C(16)-C(15)-Fe(2)	69.6(2)
C(14)-C(15)-Fe(2)	68.5(2)	C(15)-C(16)-C(17)	108.6(4)
C(15)-C(16)-Fe(2)	70.0(2)	C(17)-C(16)-Fe(2)	70.1(2)
C(16)-C(17)-C(18)	108.8(4)	C(16)-C(17)-Fe(2)	69.5(2)
C(18)-C(17)-Fe(2)	69.8(3)	C(14)-C(18)-C(17)	105.8(4)
C(14)-C(18)-Fe(2)	68.3(2)	C(17)-C(18)-Fe(2)	69.4(3)
C(20)-C(19)-C(23)	109.1(5)	C(20)-C(19)-Fe(2)	70.6(3)
C(23)-C(19)-Fe(2)	69.8(3)	C(19)-C(20)-C(21)	107.7(5)
C(19)-C(20)-Fe(2)	69.5(3)	C(21)-C(20)-Fe(2)	68.7(3)
C(20)-C(21)-C(22)	108.3(5)	C(20)-C(21)-Fe(2)	70.7(3)
C(22)-C(21)-Fe(2)	69.9(3)	C(21)-C(22)-C(23)	107.0(5)

C(21)-C(22)-Fe(2)	69.3(3)	C(23)-C(22)-Fe(2)	69.5(2)
C(19)-C(23)-C(22)	107.9(4)	C(19)-C(23)-Fe(2)	70.0(2)
C(22)-C(23)-Fe(2)	69.5(3)	C(29)-C(24)-C(25)	114.1(4)
C(29)-C(24)-B(1)	124.3(4)	C(25)-C(24)-B(1)	121.5(4)
C(26)-C(25)-C(24)	122.9(4)	C(27)-C(26)-C(25)	120.8(4)
C(26)-C(27)-C(28)	118.8(4)	C(27)-C(28)-C(29)	119.6(4)
C(24)-C(29)-C(28)	123.8(4)	C(31)-C(30)-C(35)	114.5(3)
C(31)-C(30)-B(1)	123.7(4)	C(35)-C(30)-B(1)	121.8(4)
C(32)-C(31)-C(30)	123.1(4)	C(33)-C(32)-C(31)	120.1(4)
C(34)-C(33)-C(32)	118.8(4)	C(33)-C(34)-C(35)	119.7(4)
C(34)-C(35)-C(30)	123.8(4)	C(41)-C(36)-C(37)	113.4(4)
C(41)-C(36)-B(1)	123.0(4)	C(37)-C(36)-B(1)	123.3(4)
C(38)-C(37)-C(36)	123.6(4)	C(39)-C(38)-C(37)	120.6(4)
C(38)-C(39)-C(40)	118.7(4)	C(39)-C(40)-C(41)	119.7(4)
C(40)-C(41)-C(36)	123.9(4)	C(47)-C(42)-C(43)	114.2(4)
C(47)-C(42)-B(1)	124.4(3)	C(43)-C(42)-B(1)	121.4(3)
C(44)-C(43)-C(42)	122.8(4)	C(45)-C(44)-C(43)	120.9(4)
C(44)-C(45)-C(46)	118.8(4)	C(45)-C(46)-C(47)	119.2(4)
C(42)-C(47)-C(46)	124.0(4)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$pm^2 \times 10^{-1}$] for 7.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	35(1)	33(1)	40(1)	-5(1)	-2(1)	-4(1)
Fe(2)	34(1)	32(1)	38(1)	2(1)	6(1)	-3(1)
N(1)	32(2)	30(2)	34(2)	5(2)	-8(2)	1(2)
N(2)	32(2)	28(2)	34(2)	5(2)	-5(2)	0(2)
B(1)	32(3)	26(2)	25(3)	4(2)	3(2)	4(2)
C(1)	106(7)	18(3)	272(13)	-17(6)	-68(9)	8(4)
C(2)	74(6)	142(8)	194(10)	-139(8)	72(7)	-52(6)
C(3)	97(6)	126(6)	55(4)	-8(4)	-15(4)	-66(5)
C(4)	41(3)	71(4)	127(6)	-45(4)	8(4)	-27(3)
C(5)	145(8)	62(4)	82(5)	6(4)	1(5)	-68(5)
C(6)	30(3)	56(3)	44(3)	11(3)	-5(2)	-4(3)
C(7)	38(3)	73(4)	41(3)	-4(3)	6(2)	-21(3)
C(8)	68(4)	50(3)	36(3)	8(2)	-11(3)	-24(3)
C(9)	66(3)	33(2)	38(3)	-3(2)	-21(3)	-5(3)
C(10)	37(3)	34(3)	30(3)	8(2)	-8(2)	-6(2)
C(11)	35(3)	25(2)	36(3)	4(2)	-6(2)	-1(2)
C(12)	29(3)	45(3)	45(3)	1(2)	-13(2)	6(2)
C(13)	28(3)	55(3)	43(3)	-3(2)	-8(2)	11(2)
C(14)	27(2)	29(2)	35(2)	1(2)	5(2)	-3(2)
C(15)	44(3)	23(2)	56(3)	-2(2)	8(3)	3(2)
C(16)	60(3)	34(2)	33(2)	-5(2)	7(3)	-12(3)
C(17)	42(3)	46(3)	36(3)	2(2)	-9(2)	-7(3)
C(18)	30(2)	32(2)	34(2)	5(2)	1(2)	-2(2)
C(19)	36(3)	45(3)	70(3)	1(3)	-2(3)	-10(3)
C(20)	33(3)	52(3)	91(4)	5(4)	16(3)	-7(3)
C(21)	73(4)	68(4)	72(4)	-4(3)	46(3)	-14(4)
C(22)	67(4)	65(4)	65(4)	29(3)	4(3)	-27(3)
C(23)	51(3)	28(2)	82(4)	8(3)	6(3)	-9(2)
C(24)	31(3)	33(2)	21(2)	-3(2)	10(2)	-4(2)
C(25)	42(3)	29(2)	37(2)	5(2)	-5(2)	1(3)
C(26)	54(3)	28(2)	45(3)	-1(2)	2(3)	-4(2)
C(27)	39(3)	40(3)	38(3)	-5(2)	2(2)	-9(2)
C(28)	26(3)	54(3)	45(3)	-11(2)	-3(2)	-6(2)
C(29)	27(3)	34(2)	49(3)	-3(2)	6(2)	4(2)
C(30)	31(2)	22(2)	32(2)	2(2)	2(2)	4(2)
C(31)	30(2)	28(2)	39(3)	6(2)	2(2)	0(2)
C(32)	32(2)	39(2)	44(3)	17(2)	13(3)	7(2)
C(33)	57(3)	43(3)	26(2)	8(2)	13(3)	24(3)
C(34)	55(3)	31(2)	25(2)	1(2)	-4(2)	10(2)
C(35)	33(2)	30(2)	34(2)	9(2)	1(3)	3(2)
C(36)	32(3)	21(2)	25(2)	-2(2)	2(2)	-3(2)
C(37)	40(3)	31(2)	39(3)	9(2)	3(2)	6(2)
C(38)	48(3)	47(3)	49(3)	12(3)	27(3)	7(3)
C(39)	37(3)	47(3)	63(3)	5(3)	11(3)	11(3)
C(40)	42(3)	54(3)	45(3)	2(3)	-8(3)	17(3)
C(41)	40(3)	44(3)	28(2)	-3(2)	5(2)	8(3)
C(42)	23(2)	30(2)	33(2)	-1(2)	-2(2)	-3(2)
C(43)	34(3)	37(2)	33(2)	0(2)	-4(2)	6(2)
C(44)	44(3)	44(3)	28(2)	10(2)	-5(2)	5(3)
C(45)	38(3)	35(3)	51(3)	17(2)	-9(3)	-4(2)
C(46)	61(3)	29(2)	44(3)	2(2)	-8(3)	2(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2 x 10^{-1}) for 7.

	x	y	z	U(eq)
H(1)	8577	8105	8896	158
H(2)	8304	7713	10155	164
H(3)	10193	6898	10391	111
H(4)	11443	6747	9323	95
H(5)	10484	7458	8432	116
H(6)	6627	6760	8402	52
H(7)	6318	6451	9667	61
H(8)	8111	5606	10017	62
H(9)	9560	5358	8983	55
H(11)	7169	6050	7150	38
H(12)	10848	5995	7893	48
H(13)	10978	5893	6635	51
H(15)	9805	5165	5512	49
H(16)	8721	5438	4372	51
H(17)	6997	6379	4564	49
H(18)	7021	6726	5832	39
H(19)	10842	7312	6084	60
H(20)	12052	6459	5325	71
H(21)	11091	6557	4128	85
H(22)	9330	7512	4146	79
H(23)	9181	7973	5374	64
H(25)	10380	6659	12198	43
H(26)	11527	7575	12717	51
H(27)	13537	7366	13253	47
H(28)	14353	6204	13299	50
H(29)	13211	5288	12763	44
H(31)	12940	5737	11255	39
H(32)	13554	5651	10110	46
H(33)	12321	4950	9346	50
H(34)	10432	4369	9752	45
H(35)	9808	4492	10888	39
H(37)	8820	5174	13046	44
H(38)	6714	5623	13114	58
H(39)	5715	6135	12158	59
H(40)	6924	6245	11140	57
H(41)	9060	5815	11082	45
H(43)	10943	4790	13413	42
H(44)	11251	3723	13979	46
H(45)	11508	2666	13368	50
H(46)	11501	2701	12160	54
H(47)	11206	3782	11597	45

Table 1. Crystal data and structure refinement for 8

Molecular formula	$C_{23}H_{20}Fe_2N_2S$
Formula weight	468.17
Crystal system	Monoclinic
Space group	C2/c (No.15)
Unit cell dimensions	a = 2674.0(5) pm $\alpha = 90^{\circ}$ b = 739.0(2) pm $\beta = 112.59(2)^{\circ}$ c = 1050.3(3) pm $\gamma = 90^{\circ}$
Volume	1.9162(8) nm^3
Z	4
Temperature	213(2) K
Radiation	MoKα (λ =71.073 pm)
Density (calculated)	1.623 Mg/m^3
Absorption coefficient	1.634 mm^{-1}
F(000)	960
Color, Habit	yellow prism
Crystal size	0.35 x 0.3 x 0.05 mm
θ range for data collection	2.88 to 22.00°
Index ranges	$-1 \le h \le 28$, $-1 \le k \le 7$, $-11 \le \ell \le 11$
Reflections collected	1400
Independent reflections	1141 (R_{int} = 0.0542)
Reflections with I > 2σ(I)	864
Absorption correction	ψ-scan
Max. and min. transmission	1.000 and 0.741
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	918 / 0 / 128
Goodness-of-fit on F^2	1.083
Final R indices [I>2σ(I)]	R1 = 0.0588, wR2 = 0.1460
R indices (all data)	R1 = 0.1319, wR2 = 0.5098
Largest diff. peak and hole	723 and -420 $e.nm^{-3}$

Data collection

Diffractometer used	Siemens P4
Monochromator	highly oriented graphite crystal
Scan type	ω
Scan Speed	3.0^{o}/min in ω
Scan range (ω)	0.75^{o}
Standard reflections	3 measured every 97 reflections

Solution and refinement

System used	SHELXS-86 (Sheldrick, 1990)
	SHELXL-93 (Sheldrick, 1993)
Solution	Direct Methods
Weighting scheme	calc $w=1/[\sigma^2(Fo^2)+(0.0811P)^2+27.5307P]$
	where $P = (Fo^2 + 2Fc^2)/3$
Hydrogen Atoms	calculated, with isotropic displacement parameters 1.2 times higher than U_{eq} of the carbon atoms

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^{-1}) for 8. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	-1466(1)	-2392(1)	4202(1)	20(1)
S(1)	0	1668(4)	7500	44(1)
N(1)	-423(2)	-1735(8)	6787(7)	22(2)
C(1)	-1411(4)	-5117(10)	4067(9)	35(2)
C(2)	-1922(3)	-4545(12)	3187(9)	35(2)
C(3)	-1879(3)	-3303(11)	2230(9)	33(2)
C(4)	-1319(4)	-3097(13)	2503(9)	35(2)
C(5)	-1017(3)	-4250(12)	3633(9)	33(2)
C(6)	-1435(3)	-1748(10)	6125(8)	24(2)
C(7)	-1877(3)	-871(10)	5092(9)	28(2)
C(8)	-1671(3)	253(10)	4298(8)	26(2)
C(9)	-1096(3)	55(10)	4841(8)	24(2)
C(10)	-955(3)	-1164(10)	5961(8)	24(2)
C(11)	0	-593(15)	7500	29(3)
C(12)	-260(3)	-3542(10)	7079(9)	27(2)

Table 3. Bond lengths [pm] and angles [°] for 8.

Fe(1)-C(1)	202.8(8)	Fe(1)-C(7)	203.4(8)
Fe(1)-C(4)	203.7(8)	Fe(1)-C(2)	204.0(8)
Fe(1)-C(10)	204.1(8)	Fe(1)-C(8)	204.3(8)
Fe(1)-C(9)	204.6(8)	Fe(1)-C(6)	204.6(8)
Fe(1)-C(3)	205.1(8)	Fe(1)-C(5)	205.6(8)
S(1)-C(11)	167.1(11)	N(1)-C(11)	137.9(9)
N(1)-C(12)	140.2(10)	N(1)-C(10)	141.5(10)
C(1)-C(2)	138.9(12)	C(1)-C(5)	144.8(13)
C(2)-C(3)	139.8(13)	C(3)-C(4)	142.1(12)
C(4)-C(5)	143.1(13)	C(6)-C(7)	141.7(12)
C(6)-C(10)	142.8(11)	C(7)-C(8)	142.8(12)
C(8)-C(9)	142.8(10)	C(9)-C(10)	141.4(11)
C(11)-N(1)#1	137.9(9)	C(12)-C(12)#1	133(2)

C(1)-Fe(1)-C(7)	130.3(3)	C(1)-Fe(1)-C(4)	69.0(4)
C(7)-Fe(1)-C(4)	149.8(4)	C(1)-Fe(1)-C(2)	39.9(4)
C(7)-Fe(1)-C(2)	110.5(3)	C(4)-Fe(1)-C(2)	67.7(4)
C(1)-Fe(1)-C(10)	117.6(3)	C(7)-Fe(1)-C(10)	68.3(3)
C(4)-Fe(1)-C(10)	128.3(3)	C(2)-Fe(1)-C(10)	151.4(3)
C(1)-Fe(1)-C(8)	168.8(3)	C(7)-Fe(1)-C(8)	41.0(3)
C(4)-Fe(1)-C(8)	115.7(4)	C(2)-Fe(1)-C(8)	130.8(3)
C(10)-Fe(1)-C(8)	68.3(3)	C(1)-Fe(1)-C(9)	149.6(3)
C(7)-Fe(1)-C(9)	68.9(3)	C(4)-Fe(1)-C(9)	106.4(4)
C(2)-Fe(1)-C(9)	167.8(3)	C(10)-Fe(1)-C(9)	40.5(3)
C(8)-Fe(1)-C(9)	40.9(3)	C(1)-Fe(1)-C(6)	108.9(3)
C(7)-Fe(1)-C(6)	40.6(3)	C(4)-Fe(1)-C(6)	167.6(3)
C(2)-Fe(1)-C(6)	119.1(3)	C(10)-Fe(1)-C(6)	40.9(3)
C(8)-Fe(1)-C(6)	68.8(3)	C(9)-Fe(1)-C(6)	68.9(3)
C(1)-Fe(1)-C(3)	68.2(3)	C(7)-Fe(1)-C(3)	117.9(3)
C(4)-Fe(1)-C(3)	40.7(4)	C(2)-Fe(1)-C(3)	40.0(4)
C(10)-Fe(1)-C(3)	166.9(3)	C(8)-Fe(1)-C(3)	108.2(3)
C(9)-Fe(1)-C(3)	128.8(3)	C(6)-Fe(1)-C(3)	151.0(3)
C(1)-Fe(1)-C(5)	41.5(4)	C(7)-Fe(1)-C(5)	168.8(4)
C(4)-Fe(1)-C(5)	40.9(4)	C(2)-Fe(1)-C(5)	68.0(3)
C(10)-Fe(1)-C(5)	107.3(3)	C(8)-Fe(1)-C(5)	148.3(4)
C(9)-Fe(1)-C(5)	115.1(3)	C(6)-Fe(1)-C(5)	129.5(3)
C(3)-Fe(1)-C(5)	68.6(3)	C(11)-N(1)-C(12)	110.1(6)
C(11)-N(1)-C(10)	124.9(7)	C(12)-N(1)-C(10)	124.9(6)
C(2)-C(1)-C(5)	107.7(7)	C(2)-C(1)-Fe(1)	70.5(5)
C(5)-C(1)-Fe(1)	70.3(4)	C(1)-C(2)-C(3)	110.3(7)
C(1)-C(2)-Fe(1)	69.6(4)	C(3)-C(2)-Fe(1)	70.5(5)
C(2)-C(3)-C(4)	107.3(7)	C(2)-C(3)-Fe(1)	69.6(5)
C(4)-C(3)-Fe(1)	69.1(5)	C(3)-C(4)-C(5)	108.5(7)
C(3)-C(4)-Fe(1)	70.2(5)	C(5)-C(4)-Fe(1)	70.3(5)
C(4)-C(5)-C(1)	106.2(7)	C(4)-C(5)-Fe(1)	68.8(5)
C(1)-C(5)-Fe(1)	68.2(5)	C(7)-C(6)-C(10)	107.1(7)
C(7)-C(6)-Fe(1)	69.2(5)	C(10)-C(6)-Fe(1)	69.3(4)
C(6)-C(7)-C(8)	108.6(7)	C(6)-C(7)-Fe(1)	70.1(4)
C(8)-C(7)-Fe(1)	69.9(5)	C(9)-C(8)-C(7)	107.7(7)
C(9)-C(8)-Fe(1)	69.7(4)	C(7)-C(8)-Fe(1)	69.1(4)
C(10)-C(9)-C(8)	107.5(7)	C(10)-C(9)-Fe(1)	69.6(4)
C(8)-C(9)-Fe(1)	69.5(4)	C(9)-C(10)-N(1)	125.8(7)
C(9)-C(10)-C(6)	109.1(6)	N(1)-C(10)-C(6)	125.1(7)
C(9)-C(10)-Fe(1)	70.0(4)	N(1)-C(10)-Fe(1)	126.0(5)
C(6)-C(10)-Fe(1)	69.8(4)	N(1)-C(11)-N(1)#1	104.6(9)
N(1)-C(11)-S(1)	127.7(5)	N(1)#1-C(11)-S(1)	127.7(5)
C(12)#1-C(12)-N(1)	107.6(4)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$pm^2 \times 10^{-1}$] for 8.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	16(1)	16(1)	25(1)	-1(1)	5(1)	-1(1)
S(1)	23(2)	15(2)	75(2)	0	-1(2)	0
N(1)	20(3)	13(3)	29(4)	1(3)	5(3)	0(3)
C(1)	59(6)	11(4)	38(5)	2(4)	22(5)	-3(4)
C(2)	25(4)	34(5)	35(5)	-5(4)	1(4)	-13(4)
C(3)	32(5)	29(5)	29(5)	-6(4)	1(4)	-7(4)
C(4)	39(5)	41(5)	32(5)	-2(4)	22(4)	0(4)
C(5)	24(4)	36(5)	33(5)	-13(4)	5(4)	8(4)
C(6)	29(4)	20(4)	26(4)	3(3)	14(3)	-3(3)
C(7)	18(4)	24(4)	40(5)	-3(4)	10(4)	5(3)
C(8)	21(4)	13(4)	36(5)	-5(3)	2(3)	0(3)
C(9)	22(4)	13(4)	30(4)	10(3)	2(3)	-1(3)
C(10)	20(4)	25(4)	24(4)	-3(3)	4(3)	1(3)
C(11)	28(6)	22(6)	30(6)	0	4(5)	0
C(12)	30(4)	13(4)	33(4)	5(3)	7(3)	3(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (pm^2 x 10^{-1}) for 8.

	x	y	z	U(eq)
H(1)	-1335	-5923	4811	42
H(2)	-2250	-4937	3229	42
H(3)	-2167	-2715	1535	40
H(4)	-1171	-2332	2023	41
H(5)	-640	-4411	4016	39
H(6)	-1455	-2560	6793	29
H(7)	-2244	-1007	4952	33
H(8)	-1878	991	3552	31
H(9)	-856	630	4513	29
H(12)	-479	-4568	6741	32

Table 1. Crystal data and structure refinement for 9

Molecular formula	$C_{70}H_{60}AgBFe_4N_4 x0.5\ CHCl_3 x1.5\ MeOH$
Formula weight	1407.05
Crystal system	Triclinic
Space group	$P\bar{1}$ (No.2)
Unit cell dimensions	a = 1385.4(2) pm α = 92.23(1)°
	b = 1464.6(2) pm β = 110.54(1)°
	c = 1756.3(1) pm γ = 104.350(10)°
Volume	3.2017(7) nm^3
Z	2
Temperature	213(2) K
Radiation	MoKα (λ =71.073 pm)
Density (calculated)	1.460 Mg/m^3
Absorption coefficient	1.296 mm^{-1}
F(000)	1440
Color, Habit	yellow prism
Crystal size	0.7 x 0.3 x 0.22 mm
θ range for data collection	2.50 to 23.50°
Index ranges	$0 \le h \le 14$, $-16 \le k \le 15$, $-19 \le \ell \le 18$
Reflections collected	9667
Independent reflections	9232 (R_{int} = 0.0133)
Reflections with I > 2σ(I)	7717
Absorption correction	ψ-scan
Max. and min. transmission	0.942 and 0.898
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8763 / 1 / 782
Goodness-of-fit on F^2	1.039
Final R indices [I>2σ(I)]	R1 = 0.0393, wR2 = 0.1028
R indices (all data)	R1 = 0.0516, wR2 = 0.1237
Extinction coefficient	0.0011(2)
Largest diff. peak and hole	881 and -399 $e.nm^{-3}$

Data collection

Diffractometer used	Siemens P4
Monochromator	highly oriented graphite crystal
Scan type	ω
Scan Speed	4.0^{o}/min in ω
Scan range (ω)	0.7^{o}
Standard reflections	3 measured every 97 reflections

Solution and refinement

System used	SHELXS-86 (Sheldrick, 1990)
	SHELXL-93 (Sheldrick, 1993)
Solution	Direct Methods
Weighting scheme	calc $w=1/[\sigma^2(Fo^2)+(0.0619P)^2+5.0958P]$
	where $P = (Fo^2 + 2Fc^2)/3$
Hydrogen Atoms	calculated, with isotropic displacement parameters 1.2 times higher than U_{eq} of the carbon atoms, omitted at MeOH

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (pm^2 x 10^{-1}) for 9. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ag(1)	38(1)	950(1)	2489(1)	29(1)
Fe(1)	1278(1)	-1322(1)	4618(1)	36(1)
Fe(2)	1719(1)	3657(1)	2814(1)	38(1)
Fe(3)	-3398(1)	2124(1)	1490(1)	40(1)
Fe(4)	-1203(1)	-2167(1)	656(1)	39(1)
N(1)	1797(3)	676(2)	4063(2)	30(1)
N(2)	1945(3)	2162(2)	4028(2)	29(1)
N(3)	-1969(3)	1044(2)	1022(2)	31(1)
N(4)	-1396(3)	-91(2)	704(2)	31(1)
C(1)	1318(3)	1294(3)	3616(2)	28(1)
C(2)	2711(3)	1168(3)	4726(3)	40(1)
C(3)	2809(3)	2087(3)	4705(2)	38(1)
C(4)	-1189(3)	589(3)	1326(2)	30(1)
C(5)	-2625(4)	647(4)	213(3)	42(1)
C(6)	-2270(4)	-57(3)	20(3)	43(1)
C(10)	1425(3)	-330(3)	3858(2)	31(1)
C(11)	349(3)	-877(3)	3614(3)	39(1)
C(12)	327(4)	-1844(3)	3431(3)	46(1)
C(13)	1376(5)	-1864(3)	3572(3)	52(1)
C(14)	2069(4)	-937(3)	3834(3)	42(1)
C(15)	1806(15)	-715(5)	5797(5)	137(6)
C(16)	701(10)	-1248(12)	5510(6)	122(4)
C(17)	682(9)	-2159(7)	5322(4)	102(3)
C(18)	1644(12)	-2203(8)	5456(6)	113(3)
C(19)	2322(6)	-1362(12)	5743(5)	121(4)
C(20)	1743(3)	3047(3)	3829(2)	31(1)
C(21)	725(4)	3194(3)	3433(3)	40(1)
C(22)	906(4)	4185(3)	3398(3)	48(1)
C(23)	2011(4)	4638(3)	3768(3)	46(1)
C(24)	2538(4)	3936(3)	4048(3)	39(1)
C(25)	1991(6)	2781(4)	2044(4)	69(2)
C(26)	994(6)	2958(4)	1650(3)	68(2)
C(27)	1189(5)	3941(4)	1636(3)	66(2)
C(28)	2298(5)	4374(4)	2023(3)	62(2)
C(29)	2792(5)	3649(5)	2275(3)	65(2)
C(30)	-2055(3)	1824(3)	1473(2)	32(1)
C(31)	-2049(3)	1856(3)	2280(3)	38(1)
C(32)	-2086(4)	2784(4)	2510(3)	50(1)
C(33)	-2113(4)	3297(3)	1848(4)	59(2)
C(34)	-2083(4)	2711(3)	1200(3)	48(1)
C(35)	-4708(4)	1006(4)	885(3)	57(1)
C(36)	-4695(4)	1264(5)	1668(4)	64(2)
C(37)	-4722(5)	2223(5)	1709(5)	79(2)
C(38)	-4745(5)	2541(5)	954(5)	82(2)
C(39)	-4743(4)	1779(5)	443(4)	69(2)
C(40)	-758(3)	-732(3)	739(3)	35(1)
C(41)	-610(4)	-1143(3)	55(3)	43(1)
C(42)	119(4)	-1680(4)	358(3)	51(1)
C(43)	415(4)	-1606(4)	1220(3)	50(1)
C(44)	-130(3)	-1016(3)	1461(3)	39(1)
C(45)	-2767(4)	-2612(4)	556(3)	52(1)