SUPPORTING INFORMATION

Molecular and Electronic Structures of Iron Complexes Containing N,S-Coordinated, Open-Shell *o*-Iminothionebenzosemiquinonate(1-) π Radicals.

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Table S1. Crystal data and structure refinement for 6.

Identification code	6
Empirical formula	C_{56} H_{84} Fe_2 N_4 S_4 * C_6 H_{14}
Formula weight	1139.38
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.539(5) Å alpha = 103.94(2) deg. b = 11.343(5) Å beta = 101.98(2) deg. c = 14.532(6) Å gamma = 99.29(2) deg.
Volume	1607.9(12) Å^3
Z	1
Density (calculated)	1.177 Mg/m^3
Absorption coefficient	0.619 mm^-1
F(000)	614
Crystal size	0.34 x 0.18 x 0.12 mm
Theta range for data collection	1.90 to 23.27 deg.
Index ranges	-11<=h<=10, -12<=k<=12, -16<=l<=12
Reflections collected	6322
Independent reflections	4533 [R(int) = 0.0558]
Absorption correction	Gaussian, face indexed
Max. and min. transmission	0.940 and 0.838
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4519 / 31 / 343
Goodness-of-fit on F^2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0757, wR2 = 0.1897
R indices (all data)	R1 = 0.1272, wR2 = 0.2364
Largest diff. peak and hole	0.880 and -0.378 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 6. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	5187(1)	5797(1)	4409(1)	28(1)
S(1)	5464(2)	6384(2)	6027(1)	29(1)
N(1)	7032(6)	5952(6)	4721(4)	29(2)
C(1)	7233(7)	6783(7)	6418(5)	28(2)
C(2)	7851(7)	6468(7)	5650(5)	30(2)
C(3)	9231(7)	6719(7)	5836(6)	32(2)
C(4)	10038(7)	7278(7)	6765(6)	38(2)
C(5)	9387(7)	7621(7)	7522(6)	39(2)
C(6)	8015(7)	7388(7)	7397(5)	33(2)
C(7)	7437(8)	7837(7)	8263(6)	39(2)
C(8)	6613(9)	6701(8)	8460(6)	52(2)
C(9)	8495(8)	8510(9)	9221(6)	52(2)
C(10)	6557(9)	8745(8)	8072(6)	57(3)
C(11)	11550(7)	7509(7)	6966(5)	47(2)
C(12)	12209(12)	8808(10)	7596(11)	126(9)
C(13)	12004(13)	6587(12)	7517(9)	73(5)
C(14)	12045(11)	7241(13)	6038(8)	63(4)
C(12X)	11951(30)	8355(23)	6352(18)	65(9)
C(13X)	12198(32)	8225(24)	8039(10)	73(12)
C(14X)	12109(36)	6362(21)	6714(22)	106(15)
S(2)	5323(2)	6432(2)	3118(1)	31(1)
N(2)	3498(6)	6113(6)	4169(5)	33(2)
C(21)	3755(7)	6706(6)	2761(5)	28(2)
C(22)	2941(7)	6491(6)	3389(5)	27(2)
C(23)	1627(7)	6675(7)	3221(5)	30(2)
C(24)	1124(7)	7049(7)	2412(6)	37(2)
C(25)	1964(7)	7250(7)	1791(6)	38(2)
C(26)	3229(7)	7095(7)	1926(5)	31(2)
C(27)	4085(7)	7365(7)	1214(5)	35(2)
C(28)	3284(9)	7753(8)	357(6)	49(2)
C(29)	4499(9)	6193(8)	736(6)	49(2)
C(30)	5275(8)	8435(8)	1750(6)	45(2)
C(31)	-298(8)	7276(8)	2159(6)	46(2)
C(32)	-1094(9)	6252(10)	1211(8)	76(3)
C(33)	-990(9)	7192(10)	2980(7)	68(3)
C(34)	-261(9)	8555(9)	2002(7)	64(3)
C(41)	7983(12)	9581(10)	5228(10)	98(4)
C(42)	6720(13)	9690(10)	5561(8)	80(3)
C(43)	5656(10)	9984(9)	4864(8)	70(3)

Table S3. Bond lengths [Å] and angles [deg] for 6.

Fe(1)-N(2)	1.851(6)
Fe(1)-N(1)	1.872(6)
Fe(1)-S(2)	2.187(2)
Fe(1)-S(1)	2.227(2)
Fe(1)-S(1)#1	2.347(2)
Fe(1)-Fe(1)#1	2.816(2)
S(1)-C(1)	1.780(7)
S(1)-Fe(1)#1	2.347(2)
N(1)-C(2)	1.373(9)
C(1)-C(2)	1.408(10)
C(1)-C(6)	1.426(10)
C(2)-C(3)	1.391(10)
C(3)-C(4)	1.372(10)
C(4)-C(5)	1.423(11)
C(4)-C(11)	1.526(10)
C(5)-C(6)	1.392(10)
C(6)-C(7)	1.525(10)
C(7)-C(9)	1.528(10)
C(7)-C(10)	1.529(11)
C(7)-C(8)	1.554(11)
C(11)-C(12)	1.499(9)
C(11)-C(14X)	1.511(10)
C(11)-C(13X)	1.525(10)
C(11)-C(14)	1.527(9)
C(11)-C(12X)	1.529(10)
C(11)-C(13)	1.540(9)
S(2)-C(21)	1.727(7)
N(2)-C(22)	1.360(9)
C(21)-C(22)	1.412(10)
C(21)-C(26)	1.426(10)
C(22)-C(23)	1.414(9)
C(23)-C(24)	1.377(10)
C(24)-C(25)	1.420(10)
C(24)-C(31)	1.546(10)
C(25)-C(26)	1.352(10)
C(26)-C(27)	1.559(10)
C(27)-C(30)	1.517(11)
C(27)-C(29)	1.520(11)
C(27)-C(28)	1.549(10)
C(31)-C(34)	1.517(12)
C(31)-C(33)	1.536(12)
C(31)-C(32)	1.545(12)
C(41)-C(42)	1.52(2)
C(42)-C(43)	1.485(13)
C(43)-C(43)#2	1.52(2)
N(2)-Fe(1)-N(1)	164.2(3)
N(2)-Fe(1)-S(2)	84.4(2)
N(1)-Fe(1)-S(2)	89.0(2)
N(2)-Fe(1)-S(1)	92.5(2)
N(1)-Fe(1)-S(1)	84.7(2)
S(2)-Fe(1)-S(1)	145.26(9)
N(2)-Fe(1)-S(1)#1	97.3(2)
N(1)-Fe(1)-S(1)#1	98.4(2)
S(2)-Fe(1)-S(1)#1	110.66(9)
S(1)-Fe(1)-S(1)#1	104.06(7)
N(2)-Fe(1)-Fe(1)#1	98.1(2)
N(1)-Fe(1)-Fe(1)#1	92.8(2)
S(2)-Fe(1)-Fe(1)#1	160.73(9)

S(1)-Fe(1)-Fe(1)#1	53.96(6)
S(1)#1-Fe(1)-Fe(1)#1	50.10(6)
C(1)-S(1)-Fe(1)	99.7(2)
C(1)-S(1)-Fe(1)#1	107.1(2)
Fe(1)-S(1)-Fe(1)#1	75.94(7)
C(2)-N(1)-Fe(1)	124.0(5)
C(2)-C(1)-C(6)	120.4(7)
C(2)-C(1)-S(1)	113.6(5)
C(6)-C(1)-S(1)	126.0(6)
N(1)-C(2)-C(3)	122.4(7)
N(1)-C(2)-C(1)	116.9(6)
C(3)-C(2)-C(1)	120.6(7)
C(4)-C(3)-C(2)	121.8(7)
C(3)-C(4)-C(5)	116.4(7)
C(3)-C(4)-C(11)	121.3(7)
C(5)-C(4)-C(11)	122.3(7)
C(6)-C(5)-C(4)	125.2(7)
C(5)-C(6)-C(1)	115.6(7)
C(5)-C(6)-C(7)	120.2(7)
C(1)-C(6)-C(7)	124.1(7)
C(6)-C(7)-C(9)	113.4(7)
C(6)-C(7)-C(10)	111.3(7)
C(9)-C(7)-C(10)	106.6(7)
C(6)-C(7)-C(8)	109.6(7)
C(9)-C(7)-C(8)	105.9(7)
C(10)-C(7)-C(8)	109.7(7)
C(14X)-C(11)-C(13X)	108.7(8)
C(12)-C(11)-C(4)	111.7(8)
C(14X)-C(11)-C(4)	116(2)
C(13X)-C(11)-C(4)	110.3(14)
C(12)-C(11)-C(14)	109.6(6)
C(4)-C(11)-C(14)	113.6(7)
C(14X)-C(11)-C(12X)	108.4(8)
C(13X)-C(11)-C(12X)	107.0(8)
C(4)-C(11)-C(12X)	106.3(13)
C(12)-C(11)-C(13)	108.5(6)
C(4)-C(11)-C(13)	107.4(7)
C(14)-C(11)-C(13)	105.7(6)
C(21)-S(2)-Fe(1)	101.4(3)
C(22)-N(2)-Fe(1)	124.3(5)
C(22)-C(21)-C(26)	119.1(6)
C(22)-C(21)-S(2)	113.3(5)
C(26)-C(21)-S(2)	127.5(6)
N(2)-C(22)-C(21)	116.3(6)
N(2)-C(22)-C(23)	122.1(7)
C(21)-C(22)-C(23)	121.6(7)
C(24)-C(23)-C(22)	118.9(7)
C(23)-C(24)-C(25)	118.1(7)
C(23)-C(24)-C(31)	123.2(7)
C(25)-C(24)-C(31)	118.7(7)
C(26)-C(25)-C(24)	125.1(7)
C(25)-C(26)-C(21)	117.1(7)
C(25)-C(26)-C(27)	121.3(7)
C(21)-C(26)-C(27)	121.5(6)
C(30)-C(27)-C(29)	111.9(7)
C(30)-C(27)-C(28)	106.8(6)
C(29)-C(27)-C(28)	105.6(6)
C(30)-C(27)-C(26)	110.5(6)
C(29)-C(27)-C(26)	110.2(6)
C(28)-C(27)-C(26)	111.7(6)
C(34)-C(31)-C(33)	108.4(7)
C(34)-C(31)-C(32)	110.2(8)
C(33)-C(31)-C(32)	108.9(8)

C(34)-C(31)-C(24)	110.6(7)
C(33)-C(31)-C(24)	111.5(7)
C(32)-C(31)-C(24)	107.3(7)
C(43)-C(42)-C(41)	115.2(10)
C(42)-C(43)-C(43)#2	117.0(11)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+1 #2 -x+1,-y+2,-z+1

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 6. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	19(1)	31(1)	33(1)	10(1)	5(1)	6(1)
S(1)	20(1)	32(1)	32(1)	9(1)	3(1)	6(1)
N(1)	25(4)	37(4)	28(4)	9(3)	6(3)	12(3)
C(1)	26(4)	28(4)	32(4)	12(4)	6(4)	7(3)
C(2)	29(4)	23(4)	37(5)	11(4)	0(4)	4(3)
C(3)	27(4)	40(5)	38(5)	18(4)	16(4)	16(4)
C(4)	29(4)	37(5)	46(5)	16(4)	4(4)	4(4)
C(5)	24(4)	49(5)	41(5)	19(4)	-1(4)	3(4)
C(6)	30(4)	32(5)	32(5)	6(4)	4(4)	7(4)
C(7)	34(5)	42(5)	32(5)	3(4)	6(4)	2(4)
C(8)	57(6)	50(6)	50(6)	11(5)	22(5)	7(5)
C(9)	45(5)	66(7)	33(5)	4(5)	4(4)	3(5)
C(10)	65(6)	52(6)	52(6)	3(5)	17(5)	20(5)
C(11)	22(4)	55(6)	53(6)	16(5)	-5(4)	0(4)
C(12)	18(8)	53(11)	256(26)	-23(14)	18(11)	-13(7)
C(13)	39(8)	104(13)	74(11)	19(9)	3(8)	32(8)
C(14)	22(7)	99(12)	71(10)	33(9)	15(7)	5(7)
S(2)	23(1)	38(1)	34(1)	13(1)	9(1)	8(1)
N(2)	29(4)	42(4)	32(4)	17(3)	10(3)	9(3)
C(21)	23(4)	18(4)	34(4)	3(3)	0(3)	-1(3)
C(22)	22(4)	23(4)	32(4)	4(3)	6(3)	6(3)
C(23)	20(4)	37(5)	38(5)	15(4)	11(3)	14(3)
C(24)	23(4)	46(5)	36(5)	8(4)	3(4)	7(4)
C(25)	31(5)	45(5)	33(5)	11(4)	-1(4)	11(4)
C(26)	33(5)	25(4)	29(4)	3(3)	3(4)	6(3)
C(27)	35(5)	37(5)	32(5)	10(4)	6(4)	4(4)
C(28)	64(6)	44(6)	38(5)	14(4)	8(4)	15(5)
C(29)	57(6)	56(6)	40(5)	18(5)	17(4)	11(5)
C(30)	40(5)	48(6)	52(5)	25(5)	15(4)	5(4)
C(31)	28(5)	61(6)	60(6)	35(5)	5(4)	19(4)
C(32)	35(6)	86(8)	86(8)	24(7)	-18(5)	2(5)
C(33)	35(5)	92(8)	94(8)	46(7)	16(5)	33(5)
C(34)	51(6)	74(7)	81(7)	29(6)	20(5)	39(5)
C(41)	100(10)	53(7)	127(12)	15(7)	13(9)	11(7)
C(42)	114(10)	47(7)	70(8)	18(6)	9(7)	13(6)
C(43)	97(9)	46(6)	63(7)	13(5)	19(6)	14(6)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 6.

	x	y	z	U(eq)
H(1)	7525(66)	5911(70)	4361(49)	35
H(3)	9617(7)	6502(7)	5318(6)	38
H(5)	9920(7)	8033(7)	8150(6)	47
H(8A)	6250(9)	6986(8)	9006(6)	79
H(8B)	7178(9)	6152(8)	8608(6)	79
H(8C)	5901(9)	6264(8)	7888(6)	79
H(9A)	8071(8)	8768(9)	9736(6)	78
H(9B)	9034(8)	9228(9)	9142(6)	78
H(9C)	9046(8)	7956(9)	9387(6)	78
H(10A)	6207(9)	9012(8)	8628(6)	86
H(10B)	5835(9)	8338(8)	7500(6)	86
H(10C)	7075(9)	9456(8)	7968(6)	86
H(12A)	13156(12)	8921(10)	7708(11)	189
H(12B)	11979(12)	8940(10)	8213(11)	189
H(12C)	11913(12)	9395(10)	7271(11)	189
H(13A)	11589(13)	5749(12)	7122(9)	110
H(13B)	11752(13)	6736(12)	8126(9)	110
H(13C)	12953(13)	6699(12)	7647(9)	110
H(14A)	11622(11)	6409(13)	5636(8)	94
H(14B)	12992(11)	7322(13)	6214(8)	94
H(14C)	11834(11)	7823(13)	5680(8)	94
H(12D)	11603(30)	9090(23)	6503(18)	97
H(12E)	11598(30)	7919(23)	5667(18)	97
H(12F)	12904(30)	8588(23)	6498(18)	97
H(13D)	11851(32)	8957(24)	8208(10)	109
H(13E)	13143(32)	8463(24)	8136(10)	109
H(13F)	12008(32)	7704(24)	8448(10)	109
H(14D)	11708(36)	5902(21)	6040(22)	159
H(14E)	11919(36)	5847(21)	7127(22)	159
H(14F)	13054(36)	6606(21)	6815(22)	159
H(2)	2986(67)	5933(72)	4485(52)	39
H(23)	1110(7)	6546(7)	3650(5)	35
H(25)	1618(7)	7508(7)	1250(6)	45
H(28A)	2518(9)	7098(8)	-3(6)	73
H(28B)	3836(9)	7900(8)	-71(6)	73
H(28C)	3003(9)	8500(8)	616(6)	73
H(29A)	3721(9)	5539(8)	404(6)	74
H(29B)	5056(9)	5941(8)	1230(6)	74
H(29C)	4980(9)	6358(8)	271(6)	74
H(30A)	4975(8)	9156(8)	2042(6)	67
H(30B)	5764(8)	8621(8)	1295(6)	67
H(30C)	5841(8)	8204(8)	2254(6)	67
H(32A)	-1111(9)	5448(10)	1319(8)	113
H(32B)	-680(9)	6309(10)	690(8)	113
H(32C)	-1988(9)	6362(10)	1035(8)	113
H(33A)	-1022(9)	6387(10)	3089(7)	102
H(33B)	-1879(9)	7309(10)	2792(7)	102
H(33C)	-502(9)	7827(10)	3572(7)	102
H(34A)	169(9)	8624(9)	1490(7)	96
H(34B)	223(9)	9184(9)	2598(7)	96
H(34C)	-1154(9)	8666(9)	1818(7)	96
H(41A)	8612(12)	9391(10)	5721(10)	148
H(41B)	8360(12)	10355(10)	5129(10)	148
H(41C)	7774(12)	8928(10)	4624(10)	148

H(42A)	6367(13)	8911(10)	5678(8)	96
H(42B)	6951(13)	10335(10)	6182(8)	96
H(43A)	5478(10)	9372(9)	4232(8)	84
H(43B)	5998(10)	10789(9)	4784(8)	84

Table S6. Crystal data and structure refinement for 7.

Identification code	7
Empirical formula	C_{56} H_{84} Fe_2 N_4 S_4 * 5 CH_3OH
Formula weight	1213.42
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 10.6112(9) Å alpha = 73.80(2) deg. b = 10.6514(9) Å beta = 76.29(2) deg. c = 16.910 (2) Å gamma = 66.93(2) deg.
Volume	1670.8(3) Å^3
Z	1
Density (calculated)	1.206 Mg/m^3
Absorption coefficient	0.604 mm^-1
F(000)	654
Crystal size	0.20 x 0.12 x 0.05 mm
Theta range for data collection	3.63 to 27.50 deg.
Index ranges	-14<=h<=16, -16<=k<=15, -26<=l<=25
Reflections collected	13640
Independent reflections	7506 [R(int) = 0.0446]
Absorption correction	Gaussian, face indexed
Max. and min. transmission	0.9705 and 0.8997
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7442 / 1 / 378
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0595, wR2 = 0.1405
R indices (all data)	R1 = 0.0936, wR2 = 0.1608
Largest diff. peak and hole	0.921 and -0.385 e.A^-3

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 7. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	4804(1)	4081(1)	4690(1)	20(1)
S(1)	3848(1)	3604(1)	3846(1)	22(1)
S(2)	3266(1)	3500(1)	5709(1)	24(1)
N(1)	6430(3)	3675(3)	3875(2)	25(1)
N(2)	5867(3)	3752(3)	5552(2)	19(1)
C(1)	5158(3)	3372(3)	2997(2)	21(1)
C(2)	6393(3)	3491(3)	3102(2)	22(1)
C(3)	7524(3)	3370(4)	2466(2)	22(1)
C(4)	7470(3)	3134(3)	1718(2)	23(1)
C(5)	6246(3)	2969(3)	1635(2)	23(1)
C(6)	5099(3)	3060(3)	2241(2)	20(1)
C(7)	3858(3)	2777(4)	2104(2)	24(1)
C(8)	4056(4)	2499(4)	1234(2)	30(1)
C(9)	3688(4)	1490(4)	2740(3)	32(1)
C(10)	2507(3)	4042(4)	2173(2)	26(1)
C(11)	8641(3)	3023(4)	987(2)	25(1)
C(12)	9078(4)	1622(4)	732(2)	31(1)
C(13)	9918(4)	3132(4)	1195(2)	34(1)
C(14)	8135(4)	4222(4)	246(2)	34(1)
C(21)	4147(3)	2993(3)	6574(2)	21(1)
C(22)	5441(3)	3149(3)	6385(2)	20(1)
C(23)	6280(3)	2764(3)	6998(2)	21(1)
C(24)	5828(3)	2246(3)	7816(2)	21(1)
C(25)	4529(3)	2107(3)	7995(2)	22(1)
C(26)	3657(3)	2457(4)	7409(2)	21(1)
C(27)	2239(3)	2258(4)	7668(2)	24(1)
C(28)	2187(4)	1197(4)	7234(2)	30(1)
C(29)	1965(4)	1704(4)	8607(2)	33(1)
C(30)	1075(3)	3663(4)	7455(2)	30(1)
C(31)	6640(3)	1910(4)	8532(2)	23(1)
C(32)	8082(3)	2002(4)	8214(2)	27(1)
C(33)	5827(4)	2974(4)	9085(2)	33(1)
C(34)	6819(4)	436(4)	9048(2)	36(1)
O(40)	8892(3)	2722(4)	4939(3)	76(1)
C(41)	9787(7)	3377(8)	5005(7)	140(4)
C(51)	3533(15)	-196(9)	5082(6)	93(5)
C(61)	485(11)	494(10)	3453(6)	65(3)
O(50)	2434(12)	-630(12)	5270(7)	51(3)
O(60)	374(18)	163(17)	4299(11)	111(5)
O(50X)	2625(18)	928(19)	4914(11)	60(5)
O(60X)	406(21)	1696(21)	3772(13)	99(6)
O(60Y)	41(18)	-405(19)	3738(12)	144(6)
C(61Y)	-767(31)	-20(29)	4633(18)	153(10)

Table S8. Bond lengths [Å] and angles [deg] for 7.

Fe(1)-N(1)	1.919(3)
Fe(1)-N(2)	1.924(3)
Fe(1)-N(2)#1	2.080(3)
Fe(1)-S(1)	2.1956(9)
Fe(1)-S(2)	2.2089(11)
Fe(1)-Fe(1)#1	2.6644(10)
S(1)-C(1)	1.742(3)
S(2)-C(21)	1.765(3)
N(1)-C(2)	1.386(4)
N(2)-C(22)	1.422(4)
N(2)-Fe(1)#1	2.080(3)
C(1)-C(2)	1.420(4)
C(1)-C(6)	1.429(5)
C(2)-C(3)	1.400(5)
C(3)-C(4)	1.374(5)
C(4)-C(5)	1.421(4)
C(4)-C(11)	1.525(5)
C(5)-C(6)	1.383(5)
C(6)-C(7)	1.540(4)
C(7)-C(8)	1.530(5)
C(7)-C(9)	1.532(5)
C(7)-C(10)	1.542(5)
C(11)-C(13)	1.531(5)
C(11)-C(12)	1.533(5)
C(11)-C(14)	1.541(5)
C(21)-C(22)	1.398(4)
C(21)-C(26)	1.423(5)
C(22)-C(23)	1.397(4)
C(23)-C(24)	1.384(5)
C(24)-C(25)	1.397(4)
C(24)-C(31)	1.532(4)
C(25)-C(26)	1.391(4)
C(26)-C(27)	1.546(4)
C(27)-C(28)	1.532(5)
C(27)-C(29)	1.532(5)
C(27)-C(30)	1.536(5)
C(31)-C(32)	1.529(5)
C(31)-C(34)	1.531(5)
C(31)-C(33)	1.532(5)
O(40)-C(41)	1.419(7)
C(51)-O(50X)	1.22(2)
C(51)-O(50)	1.36(2)
C(61)-O(60Y)	1.17(2)
C(61)-O(60)	1.36(2)
C(61)-O(60X)	1.49(2)
O(60Y)-C(61Y)	1.63(3)
N(1)-Fe(1)-N(2)	92.39(12)
N(1)-Fe(1)-N(2)#1	100.90(13)
N(2)-Fe(1)-N(2)#1	96.67(11)
N(1)-Fe(1)-S(1)	84.83(9)
N(2)-Fe(1)-S(1)	158.51(9)
N(2)#1-Fe(1)-S(1)	104.79(8)
N(1)-Fe(1)-S(2)	153.61(10)
N(2)-Fe(1)-S(2)	85.74(9)
N(2)#1-Fe(1)-S(2)	105.46(9)
S(1)-Fe(1)-S(2)	87.39(4)
C(1)-S(1)-Fe(1)	101.47(11)
C(21)-S(2)-Fe(1)	101.12(11)
C(2)-N(1)-Fe(1)	121.8(2)

C(22)-N(2)-Fe(1)	120.0(2)
C(22)-N(2)-Fe(1)#1	113.5(2)
Fe(1)-N(2)-Fe(1)#1	83.33(11)
C(2)-C(1)-C(6)	119.1(3)
C(2)-C(1)-S(1)	114.6(2)
C(6)-C(1)-S(1)	126.4(2)
N(1)-C(2)-C(3)	122.3(3)
N(1)-C(2)-C(1)	116.4(3)
C(3)-C(2)-C(1)	121.3(3)
C(4)-C(3)-C(2)	120.8(3)
C(3)-C(4)-C(5)	117.1(3)
C(3)-C(4)-C(11)	124.1(3)
C(5)-C(4)-C(11)	118.7(3)
C(6)-C(5)-C(4)	125.0(3)
C(5)-C(6)-C(1)	116.6(3)
C(5)-C(6)-C(7)	120.6(3)
C(1)-C(6)-C(7)	122.7(3)
C(8)-C(7)-C(9)	107.8(3)
C(8)-C(7)-C(6)	111.7(3)
C(9)-C(7)-C(6)	109.9(3)
C(8)-C(7)-C(10)	106.0(3)
C(9)-C(7)-C(10)	109.8(3)
C(6)-C(7)-C(10)	111.6(3)
C(4)-C(11)-C(13)	112.2(3)
C(4)-C(11)-C(12)	110.1(3)
C(13)-C(11)-C(12)	108.1(3)
C(4)-C(11)-C(14)	109.0(3)
C(13)-C(11)-C(14)	108.0(3)
C(12)-C(11)-C(14)	109.4(3)
C(22)-C(21)-C(26)	119.7(3)
C(22)-C(21)-S(2)	114.3(3)
C(26)-C(21)-S(2)	126.0(2)
C(23)-C(22)-C(21)	121.3(3)
C(23)-C(22)-N(2)	120.6(3)
C(21)-C(22)-N(2)	118.1(3)
C(24)-C(23)-C(22)	120.3(3)
C(23)-C(24)-C(25)	117.6(3)
C(23)-C(24)-C(31)	123.2(3)
C(25)-C(24)-C(31)	119.1(3)
C(26)-C(25)-C(24)	124.6(3)
C(25)-C(26)-C(21)	116.5(3)
C(25)-C(26)-C(27)	120.7(3)
C(21)-C(26)-C(27)	122.8(3)
C(28)-C(27)-C(29)	107.1(3)
C(28)-C(27)-C(30)	110.3(3)
C(29)-C(27)-C(30)	107.3(3)
C(28)-C(27)-C(26)	110.6(3)
C(29)-C(27)-C(26)	111.5(3)
C(30)-C(27)-C(26)	109.9(3)
C(32)-C(31)-C(34)	107.8(3)
C(32)-C(31)-C(33)	109.0(3)
C(34)-C(31)-C(33)	109.5(3)
C(32)-C(31)-C(24)	111.7(3)
C(34)-C(31)-C(24)	111.0(3)
C(33)-C(31)-C(24)	107.8(3)
C(61)-O(60Y)-C(61Y)	101(2)

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

Table S9. Anisotropic displacement parameters (A^2 x 10^3) for 7.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	16(1)	29(1)	18(1)	-7(1)	-4(1)	-9(1)
S(1)	17(1)	34(1)	21(1)	-9(1)	-3(1)	-11(1)
S(2)	19(1)	38(1)	21(1)	-6(1)	-5(1)	-13(1)
N(1)	23(2)	34(2)	23(2)	-9(1)	-5(1)	-14(1)
N(2)	17(1)	27(2)	16(1)	-6(1)	-3(1)	-9(1)
C(1)	21(2)	21(2)	22(2)	-2(1)	-6(1)	-8(1)
C(2)	20(2)	23(2)	26(2)	-6(1)	-9(1)	-7(1)
C(3)	16(2)	26(2)	26(2)	-7(2)	-5(1)	-7(1)
C(4)	20(2)	20(2)	28(2)	-8(2)	-3(1)	-6(1)
C(5)	23(2)	24(2)	24(2)	-11(1)	-5(1)	-6(1)
C(6)	16(2)	18(2)	26(2)	-7(1)	-6(1)	-4(1)
C(7)	19(2)	29(2)	28(2)	-12(2)	-6(1)	-8(1)
C(8)	23(2)	40(2)	36(2)	-19(2)	-7(2)	-11(2)
C(9)	28(2)	33(2)	41(2)	-9(2)	-8(2)	-15(2)
C(10)	21(2)	32(2)	30(2)	-12(2)	-8(1)	-8(2)
C(11)	18(2)	32(2)	27(2)	-10(2)	-2(1)	-9(1)
C(12)	24(2)	38(2)	33(2)	-14(2)	2(2)	-11(2)
C(13)	23(2)	50(2)	35(2)	-18(2)	2(2)	-17(2)
C(14)	33(2)	36(2)	31(2)	-2(2)	-2(2)	-15(2)
C(21)	18(2)	24(2)	21(2)	-4(1)	-7(1)	-7(1)
C(22)	15(2)	25(2)	20(2)	-8(1)	-2(1)	-5(1)
C(23)	16(2)	25(2)	22(2)	-6(1)	-2(1)	-8(1)
C(24)	19(2)	22(2)	24(2)	-7(1)	-7(1)	-6(1)
C(25)	22(2)	25(2)	21(2)	-5(1)	-4(1)	-10(1)
C(26)	17(2)	25(2)	23(2)	-7(1)	-1(1)	-9(1)
C(27)	16(2)	32(2)	25(2)	-7(2)	0(1)	-12(1)
C(28)	23(2)	32(2)	37(2)	-8(2)	-4(2)	-14(2)
C(29)	26(2)	50(2)	28(2)	-7(2)	0(2)	-20(2)
C(30)	18(2)	33(2)	38(2)	-10(2)	2(2)	-9(2)
C(31)	22(2)	27(2)	22(2)	-4(1)	-7(1)	-9(1)
C(32)	23(2)	37(2)	26(2)	-6(2)	-8(1)	-13(2)
C(33)	28(2)	47(2)	30(2)	-15(2)	-6(2)	-12(2)
C(34)	38(2)	39(2)	33(2)	4(2)	-16(2)	-18(2)
O(40)	29(2)	64(2)	135(4)	-28(3)	0(2)	-18(2)
C(41)	67(5)	94(6)	269(12)	15(7)	-85(6)	-40(4)
C(51)	138(11)	12(4)	39(6)	19(4)	34(6)	25(5)
C(61)	91(7)	47(5)	58(6)	1(4)	-12(5)	-31(5)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 7.

	x	y	z	U(eq)
H(1)	7004(35)	3865(43)	3888(26)	30
H(2)	6609(29)	3537(39)	5474(24)	23
H(3)	8339(3)	3453(4)	2552(2)	27
H(5)	6212(3)	2782(3)	1124(2)	27
H(8A)	3239(12)	2348(26)	1164(6)	45
H(8B)	4877(15)	1667(15)	1168(6)	45
H(8C)	4179(26)	3304(11)	814(2)	45
H(9A)	2910(17)	1304(17)	2642(11)	47
H(9B)	3508(27)	1661(11)	3303(3)	47
H(9C)	4538(11)	683(7)	2681(11)	47
H(10A)	1727(5)	3799(9)	2133(15)	39
H(10B)	2579(10)	4830(9)	1720(9)	39
H(10C)	2358(13)	4302(16)	2709(7)	39
H(12A)	9828(19)	1561(12)	261(11)	47
H(12B)	8285(8)	1549(12)	570(16)	47
H(12C)	9399(26)	858(4)	1202(6)	47
H(13A)	10652(10)	3028(28)	715(6)	51
H(13B)	10245(17)	2392(17)	1674(10)	51
H(13C)	9674(8)	4044(11)	1329(16)	51
H(14A)	8873(10)	4139(16)	-232(6)	51
H(14B)	7892(26)	5118(4)	401(6)	51
H(14C)	7320(17)	4170(17)	99(11)	51
H(23)	7164(3)	2859(3)	6853(2)	25
H(25)	4219(3)	1748(3)	8556(2)	26
H(28A)	1258(8)	1141(19)	7369(13)	44
H(28B)	2865(18)	279(7)	7425(12)	44
H(28C)	2405(25)	1494(14)	6630(3)	44
H(29A)	1053(12)	1607(27)	8753(3)	50
H(29B)	1990(27)	2358(14)	8907(2)	50
H(29C)	2678(16)	792(13)	8763(3)	50
H(30A)	178(4)	3531(6)	7628(15)	45
H(30B)	1198(15)	4032(13)	6853(3)	45
H(30C)	1105(17)	4323(9)	7748(13)	45
H(32A)	8564(10)	1799(26)	8688(2)	41
H(32B)	7996(4)	2944(8)	7890(13)	41
H(32C)	8610(9)	1323(18)	7861(13)	41
H(33A)	6317(15)	2770(17)	9555(9)	50
H(33B)	4903(10)	2916(19)	9295(13)	50
H(33C)	5739(24)	3915(5)	8760(5)	50
H(34A)	7318(26)	254(11)	9510(10)	53
H(34B)	7347(25)	-245(5)	8695(5)	53
H(34C)	5907(4)	354(10)	9269(14)	53
H(40)	9362(7)	1916(29)	4855(47)	114
H(41A)	10571(43)	3231(70)	4555(29)	210
H(41B)	10129(64)	2973(58)	5543(20)	210
H(41C)	9279(23)	4379(16)	4963(51)	210

Table S11. Crystal data and structure refinement for 8.

Identification code	8
Empirical formula	$C_{28}\ H_{24}\ Fe_2\ N_4\ S_4$ * 5/6 CH_2CL_2
Formula weight	727.22
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 13.9882(8) Å alpha = 70.96(1) deg. b = 16.4986(10) Å beta = 75.89(1) deg. c = 20.688(2) Å gamma = 75.30(1) deg.
Volume	4297.3(5) Å^3
Z	6
Density (calculated)	1.686 Mg/m^3
Absorption coefficient	1.489 mm^-1
F(000)	2226
Crystal size	0.10 x 0.08 x 0.04 mm
Theta range for data collection	3.81 to 22.50 deg.
Index ranges	-19<=h<=19, -17<=k<=22, -27<=l<=28
Reflections collected	24954
Independent reflections	11052 [R(int) = 0.0732]
Absorption correction	Gaussian, face-indexed
Max. and min. transmission	0.9659 and 0.9109
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10969 / 18 / 1097
Goodness-of-fit on F^2	1.027
Final R indices [I>2sigma(I)]	R1 = 0.0671, wR2 = 0.1327
R indices (all data)	R1 = 0.1229, wR2 = 0.1604
Largest diff. peak and hole	0.820 and -0.966 e.A^-3

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 8. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	7240(1)	4388(1)	9358(1)	29(1)
Fe(2)	8602(1)	4304(1)	10230(1)	29(1)
S(1)	6959(2)	4043(2)	10515(1)	30(1)
S(12)	7784(2)	3038(2)	9283(1)	32(1)
C(1)	6221(6)	5055(6)	10611(5)	28(2)
C(2)	5900(7)	5226(7)	11250(5)	38(3)
C(3)	5314(7)	6037(7)	11277(6)	42(3)
C(4)	5038(7)	6655(7)	10685(6)	40(3)
C(5)	5357(7)	6487(6)	10054(6)	38(3)
C(6)	5970(6)	5690(6)	9997(5)	27(2)
N(7)	6349(5)	5454(5)	9390(4)	30(2)
C(8)	5999(7)	5976(6)	8767(5)	38(3)
C(9)	6389(7)	5525(6)	8221(5)	38(3)
N(10)	6856(5)	4654(5)	8491(4)	31(2)
C(11)	7073(7)	4045(6)	8120(5)	34(2)
C(12)	7533(7)	3210(6)	8469(5)	37(3)
C(13)	7764(8)	2540(7)	8140(5)	44(3)
C(14)	7537(9)	2711(7)	7495(6)	52(3)
C(15)	7091(9)	3548(7)	7160(5)	53(3)
C(16)	6844(8)	4210(7)	7457(5)	42(3)
S(21)	8817(2)	4793(2)	9075(1)	30(1)
S(32)	9365(2)	2933(2)	10309(1)	35(1)
C(21)	8459(6)	5933(6)	9004(5)	29(2)
C(22)	8358(7)	6546(6)	8373(5)	39(3)
C(23)	8025(7)	7412(7)	8362(6)	42(3)
C(24)	7814(7)	7647(6)	8970(6)	40(3)
C(25)	7925(6)	7040(6)	9588(5)	33(2)
C(26)	8264(6)	6160(6)	9620(5)	27(2)
N(27)	8385(5)	5486(5)	10215(4)	31(2)
C(28)	8370(7)	5643(6)	10837(5)	38(3)
C(29)	8606(7)	4833(6)	11386(5)	32(2)
N(30)	8869(5)	4105(5)	11118(4)	29(2)
C(31)	9195(6)	3292(6)	11519(5)	29(2)
C(32)	9468(7)	2611(7)	11180(5)	37(3)
C(33)	9771(7)	1755(6)	11552(5)	35(2)
C(34)	9785(7)	1546(7)	12256(6)	43(3)
C(35)	9546(7)	2194(7)	12578(5)	45(3)
C(36)	9257(7)	3060(6)	12231(5)	34(2)
Fe(3)	4874(1)	8203(1)	7318(1)	27(1)
Fe(4)	5776(1)	8881(1)	5923(1)	26(1)
S(41)	6224(2)	7552(1)	6725(1)	29(1)
S(52)	5719(2)	8692(2)	7836(1)	32(1)
C(41)	5659(7)	6848(5)	6530(5)	31(2)
C(42)	6189(8)	6281(6)	6140(5)	39(3)
C(43)	5694(9)	5714(7)	6023(6)	52(3)
C(44)	4699(10)	5716(7)	6309(6)	50(3)
C(45)	4150(8)	6290(6)	6688(5)	42(3)
C(46)	4634(7)	6864(6)	6807(5)	31(2)
N(47)	4188(5)	7451(5)	7181(4)	31(2)
C(48)	3186(7)	7421(6)	7576(5)	37(3)
C(49)	2953(7)	7986(6)	8047(5)	40(3)
N(50)	3854(5)	8229(5)	8083(4)	30(2)
C(51)	3911(7)	8504(6)	8627(5)	29(2)

C(52)	4828(7)	8760(6)	8564(5)	30(2)
C(53)	4970(9)	9047(6)	9098(5)	45(3)
C(54)	4207(9)	9079(7)	9669(6)	53(3)
C(55)	3330(9)	8827(7)	9718(6)	51(3)
C(56)	3158(8)	8535(6)	9219(5)	42(3)
S(61)	4390(2)	9534(1)	6490(1)	28(1)
S(72)	6862(2)	9491(2)	6129(1)	32(1)
C(61)	3506(7)	9269(5)	6156(4)	26(2)
C(62)	2468(7)	9498(6)	6362(5)	36(3)
C(63)	1833(7)	9228(7)	6099(5)	39(3)
C(64)	2192(7)	8727(7)	5650(5)	41(3)
C(65)	3212(7)	8503(6)	5425(5)	36(3)
C(66)	3888(7)	8780(5)	5674(4)	26(2)
N(67)	4913(5)	8607(5)	5488(4)	29(2)
C(68)	5368(7)	8252(6)	4915(5)	33(2)
C(69)	6470(7)	8253(6)	4737(5)	32(2)
N(70)	6746(5)	8663(5)	5167(4)	28(2)
C(71)	7717(7)	8749(6)	5096(5)	29(2)
C(72)	7895(7)	9154(5)	5546(4)	26(2)
C(73)	8872(7)	9279(6)	5499(5)	35(2)
C(74)	9634(7)	9004(6)	5014(5)	39(3)
C(75)	9464(7)	8587(6)	4564(5)	42(3)
C(76)	8523(7)	8463(6)	4597(5)	32(2)
Fe(5)	8095(1)	6254(1)	2671(1)	30(1)
Fe(6)	6427(1)	7299(1)	3255(1)	29(1)
S(81)	6593(2)	6664(2)	2368(1)	38(1)
S(92)	7864(2)	4956(2)	3356(1)	35(1)
C(81)	6876(9)	7510(6)	1593(5)	41(3)
C(82)	6184(10)	7994(7)	1176(7)	64(4)
C(83)	6482(13)	8641(8)	571(7)	74(4)
C(84)	7455(13)	8760(8)	403(7)	70(4)
C(85)	8160(10)	8288(7)	800(6)	57(3)
C(86)	7878(9)	7628(6)	1417(5)	42(3)
N(87)	8513(6)	7083(5)	1852(4)	33(2)
C(88)	9579(8)	7070(6)	1650(5)	45(3)
C(89)	10118(8)	6368(6)	2179(5)	44(3)
N(90)	9463(5)	5782(5)	2596(4)	29(2)
C(91)	9828(7)	4971(7)	2987(5)	32(2)
C(92)	9104(7)	4463(6)	3392(5)	35(2)
C(93)	9417(8)	3599(6)	3780(5)	42(3)
C(94)	10425(10)	3254(8)	3783(6)	58(3)
C(95)	11135(9)	3766(9)	3407(6)	57(3)
C(96)	10877(7)	4598(8)	3009(6)	44(3)
S(101)	7974(2)	7007(2)	3477(1)	30(1)
S(112)	5906(2)	6229(2)	4127(1)	34(1)
C(101)	8337(7)	8002(6)	2951(5)	33(2)
C(102)	9277(8)	8174(7)	2883(5)	46(3)
C(103)	9501(9)	8976(8)	2435(6)	56(3)
C(104)	8800(8)	9579(7)	2073(5)	46(3)
C(105)	7853(8)	9421(6)	2155(5)	41(3)
C(106)	7597(7)	8633(6)	2604(5)	33(2)
N(107)	6676(5)	8414(5)	2735(4)	29(2)
C(108)	5833(7)	9033(6)	2462(5)	42(3)
C(109)	4886(7)	8784(6)	2898(5)	33(2)
N(110)	5100(6)	7885(5)	3336(4)	31(2)
C(111)	4339(7)	7493(6)	3788(5)	30(2)
C(112)	4636(7)	6641(6)	4212(5)	29(2)
C(113)	3921(7)	6194(6)	4677(5)	35(2)
C(114)	2917(8)	6600(7)	4719(5)	44(3)
C(115)	2617(8)	7428(7)	4306(5)	38(3)
C(116)	3304(7)	7892(7)	3847(5)	38(3)
C(200)	8989(9)	4543(5)	15720(6)	75(4)
Cl(1)	9572(3)	3544(2)	15592(2)	98(1)

Cl(2)	8375(3)	5239(2)	15050(2)	99(1)
C(300)	7842(7)	9837(6)	7567(4)	57(3)
Cl(3)	7362(3)	10306(2)	8249(2)	81(1)
Cl(4)	8623(2)	10439(2)	6887(2)	59(1)
C(400)	9424(16)	10472(16)	144(12)	72(8)
Cl(5)	10518(24)	9837(25)	428(13)	134(5)
Cl(6)	9286(24)	10400(26)	-644(13)	134(5)

Table S13. Bond lengths [Å] and angles [deg] for 8.

Fe(1)-N(10)	1.882(7)
Fe(1)-N(7)	1.890(7)
Fe(1)-S(12)	2.207(3)
Fe(1)-S(1)	2.229(3)
Fe(1)-S(21)	2.349(3)
Fe(1)-Fe(2)	2.876(2)
Fe(2)-N(30)	1.872(7)
Fe(2)-N(27)	1.887(7)
Fe(2)-S(32)	2.213(3)
Fe(2)-S(21)	2.228(3)
Fe(2)-S(1)	2.343(3)
S(1)-C(1)	1.771(9)
S(12)-C(12)	1.723(10)
C(1)-C(2)	1.385(12)
C(1)-C(6)	1.413(12)
C(2)-C(3)	1.392(13)
C(3)-C(4)	1.379(13)
C(4)-C(5)	1.367(13)
C(5)-C(6)	1.400(12)
C(6)-N(7)	1.379(11)
N(7)-C(8)	1.417(11)
C(8)-C(9)	1.473(13)
C(9)-N(10)	1.408(11)
N(10)-C(11)	1.388(11)
C(11)-C(12)	1.400(13)
C(11)-C(16)	1.408(13)
C(12)-C(13)	1.411(13)
C(13)-C(14)	1.370(14)
C(14)-C(15)	1.389(14)
C(15)-C(16)	1.353(13)
S(21)-C(21)	1.785(9)
S(32)-C(32)	1.735(10)
C(21)-C(22)	1.379(12)
C(21)-C(26)	1.389(12)
C(22)-C(23)	1.380(13)
C(23)-C(24)	1.378(14)
C(24)-C(25)	1.357(13)
C(25)-C(26)	1.393(12)
C(26)-N(27)	1.375(11)
N(27)-C(28)	1.389(11)
C(28)-C(29)	1.467(12)
C(29)-N(30)	1.411(11)
N(30)-C(31)	1.358(11)
C(31)-C(36)	1.416(12)
C(31)-C(32)	1.436(13)
C(32)-C(33)	1.384(12)
C(33)-C(34)	1.387(13)
C(34)-C(35)	1.369(14)
C(35)-C(36)	1.378(13)
Fe(3)-N(50)	1.859(7)
Fe(3)-N(47)	1.873(7)
Fe(3)-S(52)	2.204(3)
Fe(3)-S(41)	2.220(3)
Fe(3)-S(61)	2.361(3)
Fe(3)-Fe(4)	2.831(2)
Fe(4)-N(70)	1.870(7)
Fe(4)-N(67)	1.882(7)
Fe(4)-S(72)	2.208(3)
Fe(4)-S(61)	2.226(3)

Fe(4)-S(41)	2.322(3)
S(41)-C(41)	1.750(9)
S(52)-C(52)	1.720(10)
C(41)-C(42)	1.387(13)
C(41)-C(46)	1.406(12)
C(42)-C(43)	1.404(13)
C(43)-C(44)	1.373(14)
C(44)-C(45)	1.387(14)
C(45)-C(46)	1.406(13)
C(46)-N(47)	1.368(11)
N(47)-C(48)	1.444(11)
C(48)-C(49)	1.485(13)
C(49)-N(50)	1.442(11)
N(50)-C(51)	1.368(11)
C(51)-C(56)	1.413(13)
C(51)-C(52)	1.414(12)
C(52)-C(53)	1.407(13)
C(53)-C(54)	1.390(14)
C(54)-C(55)	1.365(14)
C(55)-C(56)	1.365(14)
S(61)-C(61)	1.757(9)
S(72)-C(72)	1.740(9)
C(61)-C(62)	1.399(12)
C(61)-C(66)	1.406(12)
C(62)-C(63)	1.369(13)
C(63)-C(64)	1.366(14)
C(64)-C(65)	1.382(13)
C(65)-C(66)	1.406(12)
C(66)-N(67)	1.372(11)
N(67)-C(68)	1.432(11)
C(68)-C(69)	1.496(12)
C(69)-N(70)	1.446(11)
N(70)-C(71)	1.370(11)
C(71)-C(72)	1.406(12)
C(71)-C(76)	1.429(12)
C(72)-C(73)	1.410(12)
C(73)-C(74)	1.370(13)
C(74)-C(75)	1.416(14)
C(75)-C(76)	1.365(12)
Fe(5)-N(90)	1.863(7)
Fe(5)-N(87)	1.869(8)
Fe(5)-S(92)	2.202(3)
Fe(5)-S(81)	2.216(3)
Fe(5)-S(101)	2.336(3)
Fe(5)-Fe(6)	2.796(2)
Fe(6)-N(110)	1.858(7)
Fe(6)-N(107)	1.874(7)
Fe(6)-S(112)	2.199(3)
Fe(6)-S(101)	2.221(3)
Fe(6)-S(81)	2.332(3)
S(81)-C(81)	1.786(10)
S(92)-C(92)	1.728(10)
C(81)-C(82)	1.371(14)
C(81)-C(86)	1.407(14)
C(82)-C(83)	1.41(2)
C(83)-C(84)	1.37(2)
C(84)-C(85)	1.36(2)
C(85)-C(86)	1.425(14)
C(86)-N(87)	1.366(12)
N(87)-C(88)	1.443(12)
C(88)-C(89)	1.496(13)
C(89)-N(90)	1.427(11)
N(90)-C(91)	1.362(11)

C(91)-C(92)	1.411(13)
C(91)-C(96)	1.445(13)
C(92)-C(93)	1.405(13)
C(93)-C(94)	1.380(14)
C(94)-C(95)	1.39(2)
C(95)-C(96)	1.359(15)
S(101)-C(101)	1.767(9)
S(112)-C(112)	1.721(9)
C(101)-C(102)	1.380(12)
C(101)-C(106)	1.413(13)
C(102)-C(103)	1.406(14)
C(103)-C(104)	1.374(15)
C(104)-C(105)	1.374(13)
C(105)-C(106)	1.402(12)
C(106)-N(107)	1.367(11)
N(107)-C(108)	1.445(11)
C(108)-C(109)	1.479(12)
C(109)-N(110)	1.463(11)
N(110)-C(111)	1.377(11)
C(111)-C(112)	1.412(12)
C(111)-C(116)	1.423(12)
C(112)-C(113)	1.384(12)
C(113)-C(114)	1.389(13)
C(114)-C(115)	1.376(13)
C(115)-C(116)	1.366(13)
C(200)-Cl(1)	1.717(7)
C(200)-Cl(2)	1.736(7)
C(300)-Cl(3)	1.740(7)
C(300)-Cl(4)	1.746(7)
C(400)-Cl(6)	1.733(9)
C(400)-Cl(5)	1.735(9)
Cl(5)-Cl(6)#1	0.56(3)
Cl(5)-C(400)#1	1.41(5)
Cl(5)-Cl(5)#1	2.40(4)
Cl(6)-Cl(5)#1	0.56(3)
Cl(6)-C(400)#1	2.24(3)

N(10)-Fe(1)-N(7)	82.5(3)
N(10)-Fe(1)-S(12)	86.5(2)
N(7)-Fe(1)-S(12)	159.5(2)
N(10)-Fe(1)-S(1)	153.8(2)
N(7)-Fe(1)-S(1)	86.3(2)
S(12)-Fe(1)-S(1)	96.31(10)
N(10)-Fe(1)-S(21)	103.7(2)
N(7)-Fe(1)-S(21)	102.4(2)
S(12)-Fe(1)-S(21)	97.04(10)
S(1)-Fe(1)-S(21)	101.72(10)
N(10)-Fe(1)-Fe(2)	152.9(2)
N(7)-Fe(1)-Fe(2)	101.6(2)
S(12)-Fe(1)-Fe(2)	96.01(8)
S(1)-Fe(1)-Fe(2)	52.81(7)
S(21)-Fe(1)-Fe(2)	49.22(7)
N(30)-Fe(2)-N(27)	82.9(3)
N(30)-Fe(2)-S(32)	86.4(2)
N(27)-Fe(2)-S(32)	160.2(2)
N(30)-Fe(2)-S(21)	156.8(2)
N(27)-Fe(2)-S(21)	86.0(2)
S(32)-Fe(2)-S(21)	97.62(10)
N(30)-Fe(2)-S(1)	100.2(2)
N(27)-Fe(2)-S(1)	101.9(2)
S(32)-Fe(2)-S(1)	96.38(10)
S(21)-Fe(2)-S(1)	101.94(10)
N(30)-Fe(2)-Fe(1)	149.5(2)

N(27)-Fe(2)-Fe(1)	101.1(2)
S(32)-Fe(2)-Fe(1)	96.50(8)
S(21)-Fe(2)-Fe(1)	52.97(7)
S(1)-Fe(2)-Fe(1)	49.27(7)
C(1)-S(1)-Fe(1)	98.1(3)
C(1)-S(1)-Fe(2)	103.1(3)
Fe(1)-S(1)-Fe(2)	77.92(9)
C(12)-S(12)-Fe(1)	98.0(3)
C(2)-C(1)-C(6)	121.1(9)
C(2)-C(1)-S(1)	122.5(7)
C(6)-C(1)-S(1)	116.4(7)
C(1)-C(2)-C(3)	118.5(9)
C(4)-C(3)-C(2)	121.2(10)
C(5)-C(4)-C(3)	120.3(9)
C(4)-C(5)-C(6)	120.7(10)
N(7)-C(6)-C(5)	125.8(9)
N(7)-C(6)-C(1)	116.0(8)
C(5)-C(6)-C(1)	118.2(9)
C(6)-N(7)-C(8)	120.1(8)
C(6)-N(7)-Fe(1)	122.6(6)
C(8)-N(7)-Fe(1)	117.0(6)
N(7)-C(8)-C(9)	110.1(8)
N(10)-C(9)-C(8)	111.6(8)
C(11)-N(10)-C(9)	122.0(8)
C(11)-N(10)-Fe(1)	122.2(6)
C(9)-N(10)-Fe(1)	115.8(6)
N(10)-C(11)-C(12)	114.2(8)
N(10)-C(11)-C(16)	125.1(9)
C(12)-C(11)-C(16)	120.7(9)
C(11)-C(12)-C(13)	118.5(9)
C(11)-C(12)-S(12)	118.9(7)
C(13)-C(12)-S(12)	122.6(8)
C(14)-C(13)-C(12)	120.2(10)
C(13)-C(14)-C(15)	119.9(10)
C(16)-C(15)-C(14)	122.1(10)
C(15)-C(16)-C(11)	118.7(10)
C(21)-S(21)-Fe(2)	97.7(3)
C(21)-S(21)-Fe(1)	101.1(3)
Fe(2)-S(21)-Fe(1)	77.81(8)
C(32)-S(32)-Fe(2)	98.1(4)
C(22)-C(21)-C(26)	122.4(9)
C(22)-C(21)-S(21)	121.4(8)
C(26)-C(21)-S(21)	116.2(7)
C(21)-C(22)-C(23)	118.3(10)
C(24)-C(23)-C(22)	120.0(10)
C(25)-C(24)-C(23)	121.3(9)
C(24)-C(25)-C(26)	120.5(9)
N(27)-C(26)-C(21)	116.6(8)
N(27)-C(26)-C(25)	125.8(9)
C(21)-C(26)-C(25)	117.6(9)
C(26)-N(27)-C(28)	121.3(8)
C(26)-N(27)-Fe(2)	122.3(6)
C(28)-N(27)-Fe(2)	116.4(6)
N(27)-C(28)-C(29)	112.2(8)
N(30)-C(29)-C(28)	110.6(8)
C(31)-N(30)-C(29)	121.0(8)
C(31)-N(30)-Fe(2)	122.2(6)
C(29)-N(30)-Fe(2)	116.5(6)
N(30)-C(31)-C(36)	126.1(9)
N(30)-C(31)-C(32)	115.6(8)
C(36)-C(31)-C(32)	118.2(9)
C(33)-C(32)-C(31)	119.9(9)
C(33)-C(32)-S(32)	123.9(8)

C(31)-C(32)-S(32)	116.2(7)
C(32)-C(33)-C(34)	120.4(10)
C(35)-C(34)-C(33)	119.9(9)
C(34)-C(35)-C(36)	122.3(10)
C(35)-C(36)-C(31)	119.2(10)
N(50)-Fe(3)-N(47)	83.6(3)
N(50)-Fe(3)-S(52)	86.1(2)
N(47)-Fe(3)-S(52)	158.7(2)
N(50)-Fe(3)-S(41)	153.4(2)
N(47)-Fe(3)-S(41)	86.0(2)
S(52)-Fe(3)-S(41)	95.21(10)
N(50)-Fe(3)-S(61)	103.3(2)
N(47)-Fe(3)-S(61)	102.7(2)
S(52)-Fe(3)-S(61)	97.73(9)
S(41)-Fe(3)-S(61)	102.81(10)
N(50)-Fe(3)-Fe(4)	152.9(2)
N(47)-Fe(3)-Fe(4)	98.6(2)
S(52)-Fe(3)-Fe(4)	99.03(8)
S(41)-Fe(3)-Fe(4)	53.08(7)
S(61)-Fe(3)-Fe(4)	49.77(7)
N(70)-Fe(4)-N(67)	83.7(3)
N(70)-Fe(4)-S(72)	86.7(2)
N(67)-Fe(4)-S(72)	162.9(2)
N(70)-Fe(4)-S(61)	158.2(2)
N(67)-Fe(4)-S(61)	86.2(2)
S(72)-Fe(4)-S(61)	97.87(10)
N(70)-Fe(4)-S(41)	97.1(2)
N(67)-Fe(4)-S(41)	101.7(2)
S(72)-Fe(4)-S(41)	93.48(10)
S(61)-Fe(4)-S(41)	103.90(10)
N(70)-Fe(4)-Fe(3)	146.7(2)
N(67)-Fe(4)-Fe(3)	98.1(2)
S(72)-Fe(4)-Fe(3)	97.67(8)
S(61)-Fe(4)-Fe(3)	54.08(7)
S(41)-Fe(4)-Fe(3)	49.85(7)
C(41)-S(41)-Fe(3)	98.4(3)
C(41)-S(41)-Fe(4)	103.0(3)
Fe(3)-S(41)-Fe(4)	77.08(8)
C(52)-S(52)-Fe(3)	98.4(3)
C(42)-C(41)-C(46)	120.9(9)
C(42)-C(41)-S(41)	122.6(7)
C(46)-C(41)-S(41)	116.5(7)
C(41)-C(42)-C(43)	119.5(10)
C(44)-C(43)-C(42)	119.5(10)
C(43)-C(44)-C(45)	121.9(10)
C(44)-C(45)-C(46)	119.2(10)
N(47)-C(46)-C(41)	115.8(8)
N(47)-C(46)-C(45)	125.2(9)
C(41)-C(46)-C(45)	119.0(9)
C(46)-N(47)-C(48)	119.7(8)
C(46)-N(47)-Fe(3)	123.2(6)
C(48)-N(47)-Fe(3)	116.5(6)
N(47)-C(48)-C(49)	109.5(8)
N(50)-C(49)-C(48)	110.4(8)
C(51)-N(50)-C(49)	121.4(8)
C(51)-N(50)-Fe(3)	123.7(6)
C(49)-N(50)-Fe(3)	114.8(6)
N(50)-C(51)-C(56)	125.8(9)
N(50)-C(51)-C(52)	114.1(8)
C(56)-C(51)-C(52)	120.1(9)
C(53)-C(52)-C(51)	118.8(9)
C(53)-C(52)-S(52)	123.6(8)
C(51)-C(52)-S(52)	117.6(7)

C(54)-C(53)-C(52)	119.6(10)
C(55)-C(54)-C(53)	120.6(11)
C(54)-C(55)-C(56)	122.2(11)
C(55)-C(56)-C(51)	118.8(10)
C(61)-S(61)-Fe(4)	98.2(3)
C(61)-S(61)-Fe(3)	101.5(3)
Fe(4)-S(61)-Fe(3)	76.15(8)
C(72)-S(72)-Fe(4)	97.6(3)
C(62)-C(61)-C(66)	120.0(8)
C(62)-C(61)-S(61)	123.3(7)
C(66)-C(61)-S(61)	116.7(7)
C(63)-C(62)-C(61)	119.4(9)
C(64)-C(63)-C(62)	121.4(9)
C(63)-C(64)-C(65)	120.7(10)
C(64)-C(65)-C(66)	119.6(9)
N(67)-C(66)-C(65)	125.1(9)
N(67)-C(66)-C(61)	116.0(8)
C(65)-C(66)-C(61)	118.9(8)
C(66)-N(67)-C(68)	120.2(7)
C(66)-N(67)-Fe(4)	122.6(6)
C(68)-N(67)-Fe(4)	117.1(6)
N(67)-C(68)-C(69)	110.6(7)
N(70)-C(69)-C(68)	110.4(7)
C(71)-N(70)-C(69)	121.2(7)
C(71)-N(70)-Fe(4)	121.1(6)
C(69)-N(70)-Fe(4)	116.7(6)
N(70)-C(71)-C(72)	116.0(8)
N(70)-C(71)-C(76)	123.7(8)
C(72)-C(71)-C(76)	120.3(8)
C(71)-C(72)-C(73)	119.5(8)
C(71)-C(72)-S(72)	116.8(7)
C(73)-C(72)-S(72)	123.7(7)
C(74)-C(73)-C(72)	119.4(9)
C(73)-C(74)-C(75)	121.4(9)
C(76)-C(75)-C(74)	120.3(9)
C(75)-C(76)-C(71)	119.1(9)
N(90)-Fe(5)-N(87)	83.2(3)
N(90)-Fe(5)-S(92)	86.2(2)
N(87)-Fe(5)-S(92)	157.4(2)
N(90)-Fe(5)-S(81)	156.8(2)
N(87)-Fe(5)-S(81)	86.5(3)
S(92)-Fe(5)-S(81)	95.83(11)
N(90)-Fe(5)-S(101)	98.2(2)
N(87)-Fe(5)-S(101)	99.7(2)
S(92)-Fe(5)-S(101)	101.59(10)
S(81)-Fe(5)-S(101)	104.01(10)
N(90)-Fe(5)-Fe(6)	148.5(2)
N(87)-Fe(5)-Fe(6)	99.7(2)
S(92)-Fe(5)-Fe(6)	99.79(8)
S(81)-Fe(5)-Fe(6)	53.97(8)
S(101)-Fe(5)-Fe(6)	50.32(7)
N(110)-Fe(6)-N(107)	82.9(3)
N(110)-Fe(6)-S(112)	86.8(2)
N(107)-Fe(6)-S(112)	160.8(2)
N(110)-Fe(6)-S(101)	152.2(2)
N(107)-Fe(6)-S(101)	86.5(2)
S(112)-Fe(6)-S(101)	95.35(10)
N(110)-Fe(6)-S(81)	103.3(2)
N(107)-Fe(6)-S(81)	100.6(2)
S(112)-Fe(6)-S(81)	97.49(10)
S(101)-Fe(6)-S(81)	103.96(10)
N(110)-Fe(6)-Fe(5)	153.5(2)
N(107)-Fe(6)-Fe(5)	100.5(2)

S(112)-Fe(6)-Fe(5)	95.95(8)
S(101)-Fe(6)-Fe(5)	54.03(7)
S(81)-Fe(6)-Fe(5)	50.21(7)
C(81)-S(81)-Fe(5)	98.2(4)
C(81)-S(81)-Fe(6)	103.8(3)
Fe(5)-S(81)-Fe(6)	75.82(9)
C(92)-S(92)-Fe(5)	98.7(3)
C(82)-C(81)-C(86)	121.6(11)
C(82)-C(81)-S(81)	123.0(10)
C(86)-C(81)-S(81)	115.3(8)
C(81)-C(82)-C(83)	118.9(12)
C(84)-C(83)-C(82)	119.5(12)
C(85)-C(84)-C(83)	123.1(13)
C(84)-C(85)-C(86)	118.6(13)
N(87)-C(86)-C(81)	116.6(9)
N(87)-C(86)-C(85)	125.0(11)
C(81)-C(86)-C(85)	118.4(10)
C(86)-N(87)-C(88)	119.6(8)
C(86)-N(87)-Fe(5)	123.3(7)
C(88)-N(87)-Fe(5)	116.8(6)
N(87)-C(88)-C(89)	109.4(8)
N(90)-C(89)-C(88)	109.2(8)
C(91)-N(90)-C(89)	121.1(8)
C(91)-N(90)-Fe(5)	122.5(6)
C(89)-N(90)-Fe(5)	115.7(6)
N(90)-C(91)-C(92)	115.8(8)
N(90)-C(91)-C(96)	125.6(9)
C(92)-C(91)-C(96)	118.7(9)
C(93)-C(92)-C(91)	119.6(9)
C(93)-C(92)-S(92)	124.1(8)
C(91)-C(92)-S(92)	116.3(7)
C(94)-C(93)-C(92)	120.5(10)
C(93)-C(94)-C(95)	119.9(11)
C(96)-C(95)-C(94)	122.1(11)
C(95)-C(96)-C(91)	119.2(10)
C(101)-S(101)-Fe(6)	98.0(3)
C(101)-S(101)-Fe(5)	103.1(3)
Fe(6)-S(101)-Fe(5)	75.65(8)
C(112)-S(112)-Fe(6)	98.7(3)
C(102)-C(101)-C(106)	120.8(9)
C(102)-C(101)-S(101)	123.0(8)
C(106)-C(101)-S(101)	116.1(7)
C(101)-C(102)-C(103)	118.6(10)
C(104)-C(103)-C(102)	120.9(10)
C(105)-C(104)-C(103)	120.7(10)
C(104)-C(105)-C(106)	120.0(10)
N(107)-C(106)-C(105)	125.1(9)
N(107)-C(106)-C(101)	116.1(8)
C(105)-C(106)-C(101)	118.8(9)
C(106)-N(107)-C(108)	121.4(8)
C(106)-N(107)-Fe(6)	122.8(6)
C(108)-N(107)-Fe(6)	115.8(6)
N(107)-C(108)-C(109)	109.5(8)
N(110)-C(109)-C(108)	109.2(7)
C(111)-N(110)-C(109)	120.7(7)
C(111)-N(110)-Fe(6)	121.8(6)
C(109)-N(110)-Fe(6)	117.6(6)
N(110)-C(111)-C(112)	115.9(8)
N(110)-C(111)-C(116)	124.3(9)
C(112)-C(111)-C(116)	119.8(9)
C(113)-C(112)-C(111)	119.9(9)
C(113)-C(112)-S(112)	123.6(7)
C(111)-C(112)-S(112)	116.5(7)

C(112)-C(113)-C(114)	118.8(9)
C(115)-C(114)-C(113)	121.8(10)
C(116)-C(115)-C(114)	120.9(9)
C(115)-C(116)-C(111)	118.8(9)
Cl(1)-C(200)-Cl(2)	113.9(6)
Cl(3)-C(300)-Cl(4)	113.2(5)
Cl(6)-C(400)-Cl(5)	114.1(9)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+2,-z

Table S14. Anisotropic displacement parameters (A^2 x 10^3) for 8. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	34(1)	24(1)	28(1)	-5(1)	-6(1)	-10(1)
Fe(2)	32(1)	25(1)	30(1)	-9(1)	-6(1)	-5(1)
S(1)	34(1)	28(1)	28(1)	-5(1)	-6(1)	-9(1)
S(12)	46(2)	26(1)	28(1)	-8(1)	-7(1)	-10(1)
C(1)	20(5)	33(6)	38(6)	-15(5)	-8(5)	-7(4)
C(2)	35(6)	48(7)	36(6)	-17(5)	-11(5)	-6(5)
C(3)	30(6)	50(7)	53(7)	-31(6)	2(6)	-5(5)
C(4)	29(6)	38(7)	54(7)	-23(6)	-12(6)	10(5)
C(5)	25(6)	37(6)	51(7)	-12(5)	-5(5)	-7(5)
C(6)	19(5)	18(5)	41(6)	-4(5)	-1(5)	-7(4)
N(7)	27(4)	32(5)	29(5)	-5(4)	-6(4)	-10(4)
C(8)	34(6)	40(6)	38(6)	1(5)	-13(5)	-11(5)
C(9)	43(6)	37(7)	33(6)	-3(5)	-6(5)	-12(5)
N(10)	32(5)	33(5)	27(5)	-3(4)	-2(4)	-17(4)
C(11)	40(6)	26(6)	35(6)	-4(5)	-1(5)	-15(5)
C(12)	38(6)	37(7)	44(6)	-18(5)	-5(5)	-14(5)
C(13)	57(7)	44(7)	34(6)	-13(5)	-7(6)	-14(5)
C(14)	80(9)	43(8)	44(7)	-21(6)	-7(7)	-23(6)
C(15)	94(9)	52(8)	25(6)	-12(6)	-6(6)	-35(7)
C(16)	64(8)	40(7)	23(6)	-4(5)	-9(5)	-15(5)
S(21)	33(1)	26(1)	30(1)	-9(1)	-1(1)	-7(1)
S(32)	39(2)	27(1)	37(2)	-10(1)	-8(1)	-1(1)
C(21)	20(5)	25(5)	40(6)	-6(5)	-1(5)	-10(4)
C(22)	49(7)	36(7)	36(6)	-12(5)	-3(5)	-13(5)
C(23)	34(6)	31(7)	54(7)	4(5)	-15(6)	-8(5)
C(24)	35(6)	27(6)	55(7)	-11(6)	-5(6)	-2(5)
C(25)	30(6)	28(6)	40(6)	-8(5)	0(5)	-11(5)
C(26)	25(5)	22(6)	34(6)	-9(5)	-1(5)	-6(4)
N(27)	33(5)	34(5)	26(5)	-13(4)	2(4)	-10(4)
C(28)	25(6)	49(7)	38(6)	-21(6)	10(5)	-11(5)
C(29)	31(6)	25(6)	40(6)	-5(5)	-10(5)	-10(4)
N(30)	24(4)	24(5)	38(5)	-8(4)	-7(4)	-1(4)
C(31)	14(5)	37(6)	36(6)	-9(5)	-6(5)	-5(4)
C(32)	29(6)	43(7)	38(6)	-4(5)	-5(5)	-17(5)
C(33)	32(6)	23(6)	40(7)	2(5)	-5(5)	-6(4)
C(34)	34(6)	34(7)	45(7)	14(6)	-12(5)	-8(5)
C(35)	41(7)	57(8)	30(6)	-2(6)	0(5)	-19(6)
C(36)	31(6)	36(7)	31(6)	-3(5)	-2(5)	-11(5)
Fe(3)	26(1)	24(1)	29(1)	-5(1)	-7(1)	-5(1)
Fe(4)	27(1)	24(1)	27(1)	-8(1)	-3(1)	-8(1)
S(41)	30(1)	23(1)	36(1)	-9(1)	-11(1)	-5(1)
S(52)	34(1)	30(1)	34(1)	-10(1)	-10(1)	-3(1)
C(41)	37(6)	13(5)	42(6)	-6(5)	-18(5)	6(4)
C(42)	51(7)	19(6)	49(7)	-2(5)	-26(6)	-8(5)
C(43)	68(9)	32(7)	64(8)	-19(6)	-27(7)	-2(6)
C(44)	76(9)	26(6)	57(8)	-1(6)	-35(7)	-17(6)
C(45)	49(7)	30(6)	50(7)	1(5)	-22(6)	-17(5)
C(46)	37(6)	27(6)	31(6)	1(5)	-19(5)	-8(5)
N(47)	28(5)	30(5)	34(5)	-7(4)	-13(4)	1(4)
C(48)	21(6)	37(6)	41(6)	7(5)	-4(5)	-8(5)
C(49)	37(6)	30(6)	41(6)	7(5)	-7(5)	-8(5)
N(50)	28(5)	27(5)	30(5)	3(4)	-12(4)	-5(4)
C(51)	40(6)	23(5)	18(5)	4(4)	-7(5)	-4(4)

C(52)	38(6)	19(5)	33(6)	-5(4)	-15(5)	2(4)
C(53)	63(8)	32(6)	35(7)	3(5)	-21(6)	-7(5)
C(54)	77(9)	46(7)	36(7)	-13(6)	-5(7)	-14(6)
C(55)	58(8)	46(7)	40(7)	-9(6)	8(6)	-13(6)
C(56)	45(7)	31(6)	36(6)	0(5)	1(6)	-5(5)
S(61)	30(1)	23(1)	29(1)	-7(1)	-4(1)	-3(1)
S(72)	31(1)	35(2)	35(1)	-15(1)	-1(1)	-13(1)
C(61)	32(6)	18(5)	25(5)	-1(4)	-3(5)	-7(4)
C(62)	38(7)	37(6)	21(5)	-2(5)	-1(5)	1(5)
C(63)	24(6)	47(7)	29(6)	9(5)	-10(5)	3(5)
C(64)	31(7)	42(7)	46(7)	0(6)	-12(6)	-13(5)
C(65)	37(6)	37(6)	33(6)	-5(5)	-10(5)	-7(5)
C(66)	25(6)	24(5)	26(5)	3(4)	-12(5)	-6(4)
N(67)	30(5)	31(5)	30(5)	-15(4)	-3(4)	-5(4)
C(68)	30(6)	41(6)	28(6)	-8(5)	-3(5)	-8(5)
C(69)	36(6)	31(6)	29(6)	-11(5)	-8(5)	1(5)
N(70)	30(5)	29(5)	21(4)	-6(4)	-1(4)	-5(4)
C(71)	31(6)	23(5)	26(5)	3(4)	-5(5)	-8(4)
C(72)	30(6)	23(5)	27(5)	-3(4)	-12(5)	-6(4)
C(73)	29(6)	36(6)	47(7)	-17(5)	-11(5)	-6(5)
C(74)	23(6)	35(6)	54(7)	-5(5)	-6(6)	-6(5)
C(75)	33(7)	41(7)	40(7)	-6(5)	7(5)	-6(5)
C(76)	31(6)	35(6)	27(6)	-9(5)	7(5)	-14(5)
Fe(5)	33(1)	26(1)	30(1)	-11(1)	-6(1)	-2(1)
Fe(6)	29(1)	23(1)	35(1)	-11(1)	-7(1)	-2(1)
S(81)	42(2)	31(2)	50(2)	-19(1)	-22(1)	3(1)
S(92)	34(2)	28(1)	41(2)	-9(1)	-4(1)	-4(1)
C(81)	73(8)	21(6)	39(6)	-15(5)	-31(6)	1(5)
C(82)	87(9)	44(8)	78(9)	-22(7)	-56(8)	4(7)
C(83)	124(14)	40(8)	61(9)	-8(7)	-61(10)	15(8)
C(84)	111(12)	43(8)	64(9)	-21(7)	-31(10)	-6(8)
C(85)	102(10)	32(7)	38(7)	-8(6)	-13(7)	-17(7)
C(86)	69(8)	27(6)	36(7)	-21(5)	-17(6)	2(6)
N(87)	40(5)	27(5)	33(5)	-12(4)	-7(4)	-2(4)
C(88)	72(8)	34(6)	32(6)	-12(5)	-4(6)	-15(6)
C(89)	46(7)	32(6)	48(7)	-13(5)	9(6)	-8(5)
N(90)	28(4)	32(5)	29(5)	-14(4)	-4(4)	1(4)
C(91)	24(6)	50(7)	30(6)	-22(5)	-8(5)	-1(5)
C(92)	42(6)	31(6)	26(6)	-15(5)	4(5)	4(5)
C(93)	57(8)	30(6)	29(6)	-7(5)	-13(6)	10(5)
C(94)	75(10)	53(8)	36(7)	-9(6)	-20(7)	12(7)
C(95)	48(8)	64(9)	57(8)	-33(7)	-21(7)	25(7)
C(96)	30(6)	61(8)	49(7)	-36(6)	0(5)	-1(6)
S(101)	30(1)	35(1)	29(1)	-14(1)	-3(1)	-6(1)
S(112)	30(1)	24(1)	45(2)	-7(1)	-4(1)	-3(1)
C(101)	39(6)	33(6)	34(6)	-13(5)	-2(5)	-18(5)
C(102)	36(7)	58(8)	52(7)	-21(6)	-11(6)	-16(6)
C(103)	51(8)	62(8)	61(8)	-14(7)	5(7)	-41(7)
C(104)	50(7)	47(7)	42(7)	-13(6)	4(6)	-24(6)
C(105)	56(8)	33(6)	40(6)	-21(5)	2(6)	-16(5)
C(106)	39(6)	32(6)	31(6)	-19(5)	6(5)	-12(5)
N(107)	32(5)	27(5)	33(5)	-12(4)	-10(4)	-5(4)
C(108)	48(7)	28(6)	53(7)	-20(5)	-12(6)	3(5)
C(109)	41(6)	29(6)	31(6)	-10(5)	-14(5)	0(5)
N(110)	36(5)	31(5)	30(5)	-11(4)	-8(4)	-7(4)
C(111)	21(5)	46(7)	34(6)	-30(5)	-4(5)	-4(5)
C(112)	43(6)	18(5)	31(6)	-8(4)	-8(5)	-8(5)
C(113)	38(6)	33(6)	39(6)	-19(5)	-6(5)	-6(5)
C(114)	45(7)	61(8)	40(7)	-30(6)	3(6)	-25(6)
C(115)	34(6)	46(7)	41(6)	-23(6)	-12(6)	-1(5)
C(116)	40(7)	42(7)	41(6)	-15(5)	-21(6)	-6(5)
C(200)	76(9)	92(11)	65(9)	-25(8)	-12(8)	-27(8)
Cl(1)	93(3)	82(3)	121(3)	-15(2)	-45(3)	-15(2)

Cl(2)	104(3)	79(3)	111(3)	-26(2)	-27(3)	-7(2)
C(300)	52(7)	43(7)	82(9)	-14(6)	-29(7)	-7(6)
Cl(3)	120(3)	55(2)	79(2)	-17(2)	-25(2)	-33(2)
Cl(4)	58(2)	42(2)	78(2)	-5(2)	-29(2)	-11(1)
Cl(5)	111(11)	162(18)	83(14)	-28(14)	22(7)	9(8)
Cl(6)	111(11)	162(18)	83(14)	-28(14)	22(7)	9(8)

Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 8.

	x	y	z	U(eq)
H(2)	6076(7)	4799(7)	11661(5)	45
H(3)	5099(7)	6168(7)	11710(6)	50
H(4)	4625(7)	7200(7)	10716(6)	48
H(5)	5161(7)	6916(6)	9650(6)	45
H(8A)	6223(7)	6543(6)	8614(5)	46
H(8B)	5256(7)	6093(6)	8852(5)	46
H(9A)	5829(7)	5535(6)	8003(5)	46
H(9B)	6879(7)	5840(6)	7858(5)	46
H(13)	8079(8)	1969(7)	8367(5)	53
H(14)	7684(9)	2256(7)	7278(6)	63
H(15)	6956(9)	3661(7)	6707(5)	64
H(16)	6523(8)	4774(7)	7224(5)	51
H(22)	8514(7)	6376(6)	7957(5)	47
H(23)	7940(7)	7846(7)	7935(6)	51
H(24)	7588(7)	8245(6)	8957(6)	48
H(25)	7771(6)	7217(6)	10001(5)	39
H(28A)	7697(7)	5966(6)	10990(5)	45
H(28B)	8865(7)	6015(6)	10763(5)	45
H(29A)	9171(7)	4862(6)	11582(5)	38
H(29B)	8016(7)	4766(6)	11764(5)	38
H(33)	9971(7)	1308(6)	11325(5)	42
H(34)	9960(7)	953(7)	12515(6)	51
H(35)	9582(7)	2042(7)	13057(5)	54
H(36)	9101(7)	3496(6)	12468(5)	41
H(42)	6881(8)	6277(6)	5954(5)	46
H(43)	6045(9)	5332(7)	5748(6)	62
H(44)	4377(10)	5312(7)	6245(6)	60
H(45)	3455(8)	6295(6)	6865(5)	50
H(48A)	3138(7)	6812(6)	7852(5)	45
H(48B)	2695(7)	7626(6)	7257(5)	45
H(49A)	2461(7)	8518(6)	7873(5)	48
H(49B)	2648(7)	7669(6)	8517(5)	48
H(53)	5582(9)	9218(6)	9069(5)	54
H(54)	4299(9)	9278(7)	10028(6)	64
H(55)	2821(9)	8855(7)	10114(6)	62
H(56)	2544(8)	8356(6)	9268(5)	50
H(62)	2206(7)	9838(6)	6680(5)	43
H(63)	1128(7)	9392(7)	6233(5)	47
H(64)	1736(7)	8529(7)	5489(5)	49
H(65)	3455(7)	8165(6)	5105(5)	44
H(68A)	5050(7)	8603(6)	4506(5)	40
H(68B)	5257(7)	7647(6)	5036(5)	40
H(69A)	6848(7)	7645(6)	4808(5)	39
H(69B)	6647(7)	8574(6)	4241(5)	39
H(73)	9001(7)	9553(6)	5799(5)	42
H(74)	10291(7)	9094(6)	4980(5)	47
H(75)	10008(7)	8392(6)	4239(5)	51
H(76)	8405(7)	8190(6)	4291(5)	38
H(82)	5516(10)	7894(7)	1295(7)	77
H(83)	6011(13)	8993(8)	281(7)	89
H(84)	7647(13)	9192(8)	-12(7)	84
H(85)	8826(10)	8395(7)	671(6)	68
H(88A)	9718(8)	7644(6)	1614(5)	54
H(88B)	9819(8)	6960(6)	1189(5)	54

H(89A)	10726(8)	6047(6)	1943(5)	53
H(89B)	10329(8)	6631(6)	2476(5)	53
H(93)	8932(8)	3250(6)	4043(5)	50
H(94)	10632(10)	2668(8)	4041(6)	70
H(95)	11824(9)	3528(9)	3428(6)	68
H(96)	11379(7)	4930(8)	2749(6)	53
H(102)	9762(8)	7760(7)	3134(5)	55
H(103)	10147(9)	9102(8)	2381(6)	67
H(104)	8972(8)	10110(7)	1763(5)	55
H(105)	7371(8)	9847(6)	1908(5)	49
H(10A)	5860(7)	9039(6)	1978(5)	50
H(10B)	5863(7)	9626(6)	2461(5)	50
H(10C)	4576(7)	9182(6)	3193(5)	40
H(10D)	4408(7)	8832(6)	2598(5)	40
H(113)	4113(7)	5620(6)	4963(5)	42
H(114)	2423(8)	6298(7)	5041(5)	53
H(115)	1922(8)	7680(7)	4340(5)	45
H(116)	3096(7)	8470(7)	3573(5)	46
H(20A)	9497(9)	4828(5)	15773(6)	90
H(20B)	8496(9)	4452(5)	16158(6)	90
H(30A)	7276(7)	9781(6)	7386(4)	68
H(30B)	8225(7)	9243(6)	7746(4)	68
H(40A)	8842(16)	10292(16)	500(12)	87
H(40B)	9414(16)	11089(16)	101(12)	87

Table S16. Crystal data and structure refinement for 9.

Identification code	9
Empirical formula	C_{46} H_{57} Fe N_2 O_3 P S_2 * C_7 H_8
Formula weight	929.01
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Aba2 , No. 41
Unit cell dimensions	a = 28.436(2) Å alpha = 90 deg. b = 17.4172(9) Å beta = 90 deg. c = 9.9671(6) Å gamma = 90 deg.
Volume	4936.5(5) Å^3
Z	4
Density (calculated)	1.250 Mg/m^3
Absorption coefficient	0.466 mm^-1
F(000)	1976
Crystal size	0.12 x 0.11 x 0.06 mm
Theta range for data collection	2.45 to 27.50 deg.
Index ranges	-41<=h<=18, -25<=k<=25, -14<=l<=14
Reflections collected	15790
Independent reflections	5204 [R(int) = 0.0584]
Absorption correction	Gaussian, face-indexed
Max. and min. transmission	0.9734 and 0.9440
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5187 / 1 / 257
Goodness-of-fit on F^2	1.048
Final R indices [I>2sigma(I)]	R1 = 0.0516, wR2 = 0.0936
R indices (all data)	R1 = 0.0751, wR2 = 0.1030
Absolute structure parameter	0.05(2)
Largest diff. peak and hole	0.464 and -0.439 e.A^-3

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for 9. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	0	0	3762(1)	14(1)
S(1)	698(1)	-485(1)	4146(1)	21(1)
N(2)	297(1)	938(1)	3944(3)	15(1)
C(1)	1042(1)	337(2)	4142(4)	14(1)
C(2)	768(1)	1024(2)	4041(3)	15(1)
C(3)	989(1)	1753(2)	4024(3)	16(1)
C(4)	1468(1)	1804(2)	4111(3)	15(1)
C(5)	1731(1)	1112(2)	4213(4)	17(1)
C(6)	1539(1)	386(2)	4225(4)	15(1)
C(7)	1859(1)	-329(2)	4307(4)	22(1)
C(8)	1747(2)	-801(2)	5569(4)	29(1)
C(9)	1796(1)	-827(2)	3041(4)	27(1)
C(10)	2382(1)	-112(2)	4388(4)	31(1)
C(11)	1733(1)	2572(2)	4088(4)	21(1)
C(12)	1401(1)	3255(2)	3871(5)	30(1)
C(13)	2090(2)	2560(2)	2929(4)	30(1)
C(14)	1993(2)	2677(2)	5427(4)	37(1)
P(1)	146(1)	53(1)	1647(2)	17(1)
O(30)	24(1)	-673(1)	722(2)	41(1)
C(31)	39(2)	-1457(2)	1072(4)	33(1)
C(32)	433(2)	-1758(2)	1648(4)	38(1)
C(33)	435(2)	-2533(3)	1984(4)	46(1)
C(34)	56(2)	-3000(3)	1706(5)	51(1)
C(35)	-331(2)	-2679(2)	1084(5)	45(1)
C(36)	-346(2)	-1907(2)	751(5)	40(1)
O(20)	696(2)	123(3)	1346(4)	20(1)
C(21)	916(2)	340(3)	183(4)	23(2)
C(22)	1319(2)	780(3)	370(4)	29(2)
C(23)	1566(2)	1054(3)	-733(5)	39(2)
C(24)	1411(2)	889(3)	-2024(5)	46(3)
C(25)	1008(2)	449(3)	-2211(4)	37(2)
C(26)	761(2)	175(3)	-1108(5)	35(2)
C(41)	-1058(2)	-375(3)	-1409(5)	32(2)
C(42)	-1174(2)	-323(2)	-57(4)	27(2)
C(43)	-1505(2)	-821(3)	490(4)	31(2)
C(44)	-1719(2)	-1372(3)	-315(5)	32(2)
C(45)	-1602(2)	-1424(3)	-1667(5)	40(2)
C(46)	-1272(2)	-925(3)	-2214(4)	30(2)
C(47)	-690(3)	118(5)	-2078(8)	39(2)

Table S18. Bond lengths [Å] and angles [deg] for 9.

Fe(1)-N(2)	1.848(2)
Fe(1)-N(2)#1	1.848(2)
Fe(1)-P(1)#1	2.149(2)
Fe(1)-P(1)	2.149(2)
Fe(1)-S(1)#1	2.1905(8)
Fe(1)-S(1)	2.1906(8)
S(1)-C(1)	1.733(3)
N(2)-C(2)	1.352(3)
C(1)-C(6)	1.420(4)
C(1)-C(2)	1.430(4)
C(2)-C(3)	1.416(4)
C(3)-C(4)	1.366(4)
C(4)-C(5)	1.423(4)
C(4)-C(11)	1.537(4)
C(5)-C(6)	1.378(4)
C(6)-C(7)	1.544(4)
C(7)-C(10)	1.536(4)
C(7)-C(8)	1.537(5)
C(7)-C(9)	1.542(5)
C(11)-C(12)	1.534(4)
C(11)-C(14)	1.536(5)
C(11)-C(13)	1.537(5)
P(1)-P(1)#1	0.848(3)
P(1)-O(30)#1	1.499(3)
P(1)-O(20)	1.600(5)
P(1)-O(30)	1.604(3)
O(30)-C(31)	1.410(4)
O(30)-P(1)#1	1.499(3)
C(31)-C(32)	1.364(6)
C(31)-C(36)	1.383(6)
C(32)-C(33)	1.391(6)
C(33)-C(34)	1.377(7)
C(34)-C(35)	1.383(7)
C(35)-C(36)	1.386(6)
O(20)-C(21)	1.370(6)
C(21)-C(22)	1.39
C(21)-C(26)	1.39
C(22)-C(23)	1.39
C(23)-C(24)	1.39
C(24)-C(25)	1.39
C(25)-C(26)	1.39
C(41)-C(42)	1.39
C(41)-C(46)	1.39
C(41)-C(47)	1.510(9)
C(42)-C(43)	1.39
C(43)-C(44)	1.39
C(44)-C(45)	1.39
C(45)-C(46)	1.39

N(2)-Fe(1)-N(2)#1	168.7(2)
N(2)-Fe(1)-P(1)#1	102.87(11)
N(2)#1-Fe(1)-P(1)#1	88.30(10)
N(2)-Fe(1)-P(1)	88.30(10)
N(2)#1-Fe(1)-P(1)	102.87(11)
P(1)#1-Fe(1)-P(1)	22.75(9)
N(2)-Fe(1)-S(1)#1	93.21(8)
N(2)#1-Fe(1)-S(1)#1	84.81(8)
P(1)#1-Fe(1)-S(1)#1	90.79(6)
P(1)-Fe(1)-S(1)#1	109.22(6)

N(2)-Fe(1)-S(1)	84.82(8)
N(2)#1-Fe(1)-S(1)	93.21(8)
P(1)#1-Fe(1)-S(1)	109.22(6)
P(1)-Fe(1)-S(1)	90.79(6)
S(1)#1-Fe(1)-S(1)	159.85(6)
C(1)-S(1)-Fe(1)	101.05(10)
C(2)-N(2)-Fe(1)	123.9(2)
C(6)-C(1)-C(2)	119.7(3)
C(6)-C(1)-S(1)	127.6(2)
C(2)-C(1)-S(1)	112.6(2)
N(2)-C(2)-C(3)	122.5(3)
N(2)-C(2)-C(1)	116.8(2)
C(3)-C(2)-C(1)	120.7(3)
C(4)-C(3)-C(2)	119.9(3)
C(3)-C(4)-C(5)	118.3(3)
C(3)-C(4)-C(11)	123.1(3)
C(5)-C(4)-C(11)	118.6(3)
C(6)-C(5)-C(4)	124.7(3)
C(5)-C(6)-C(1)	116.7(3)
C(5)-C(6)-C(7)	120.5(3)
C(1)-C(6)-C(7)	122.9(3)
C(10)-C(7)-C(8)	106.9(3)
C(10)-C(7)-C(9)	107.1(3)
C(8)-C(7)-C(9)	110.1(3)
C(10)-C(7)-C(6)	112.0(3)
C(8)-C(7)-C(6)	110.6(3)
C(9)-C(7)-C(6)	110.0(3)
C(12)-C(11)-C(14)	109.0(3)
C(12)-C(11)-C(4)	112.0(3)
C(14)-C(11)-C(4)	109.1(3)
C(12)-C(11)-C(13)	108.1(3)
C(14)-C(11)-C(13)	109.7(3)
C(4)-C(11)-C(13)	108.9(3)
P(1)#1-P(1)-O(30)#1	81.1(3)
P(1)#1-P(1)-O(20)	166.4(3)
O(30)#1-P(1)-O(20)	98.3(2)
P(1)#1-P(1)-O(30)	67.4(2)
O(30)#1-P(1)-O(30)	98.3(2)
O(20)-P(1)-O(30)	99.4(2)
P(1)#1-P(1)-Fe(1)	78.62(4)
O(30)#1-P(1)-Fe(1)	124.9(2)
O(20)-P(1)-Fe(1)	112.1(2)
O(30)-P(1)-Fe(1)	119.22(13)
C(31)-O(30)-P(1)#1	123.7(2)
C(31)-O(30)-P(1)	128.0(3)
P(1)#1-O(30)-P(1)	31.49(13)
C(32)-C(31)-C(36)	122.0(4)
C(32)-C(31)-O(30)	120.1(4)
C(36)-C(31)-O(30)	117.9(4)
C(31)-C(32)-C(33)	118.6(4)
C(34)-C(33)-C(32)	121.3(5)
C(33)-C(34)-C(35)	118.4(4)
C(34)-C(35)-C(36)	121.6(4)
C(31)-C(36)-C(35)	118.1(5)
C(21)-O(20)-P(1)	128.8(4)
O(20)-C(21)-C(22)	114.4(4)
O(20)-C(21)-C(26)	125.5(4)
C(22)-C(21)-C(26)	120.0
C(23)-C(22)-C(21)	120.0
C(22)-C(23)-C(24)	120.0
C(25)-C(24)-C(23)	120.0
C(24)-C(25)-C(26)	120.0
C(25)-C(26)-C(21)	120.0

C(42)-C(41)-C(46)	120.0
C(42)-C(41)-C(47)	123.8(4)
C(46)-C(41)-C(47)	116.2(4)
C(43)-C(42)-C(41)	120.0
C(42)-C(43)-C(44)	120.0
C(45)-C(44)-C(43)	120.0
C(44)-C(45)-C(46)	120.0
C(45)-C(46)-C(41)	120.0

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

Table S19. Anisotropic displacement parameters (A^2 x 10^3) for 9. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Fe(1)	14(1)	12(1)	17(1)	0	0	-2(1)
S(1)	13(1)	11(1)	40(1)	1(1)	2(1)	-1(1)
N(2)	12(1)	8(1)	25(2)	-4(1)	1(1)	0(1)
C(1)	13(1)	10(1)	20(2)	-2(1)	2(2)	-2(1)
C(2)	16(1)	15(1)	14(2)	0(1)	3(1)	-3(1)
C(3)	17(1)	12(1)	19(2)	1(1)	2(2)	1(1)
C(4)	17(1)	15(1)	11(2)	2(1)	1(1)	-5(1)
C(5)	13(1)	22(2)	15(2)	3(1)	-1(2)	-2(1)
C(6)	13(1)	17(1)	15(2)	2(1)	3(2)	3(1)
C(7)	17(2)	17(2)	31(2)	4(2)	-3(2)	3(1)
C(8)	25(2)	24(2)	36(2)	13(2)	-7(2)	0(2)
C(9)	18(2)	25(2)	38(2)	-1(2)	4(2)	7(2)
C(10)	15(2)	24(2)	54(2)	6(2)	-3(2)	4(2)
C(11)	18(1)	17(1)	26(2)	4(2)	0(2)	-7(1)
C(12)	29(2)	15(1)	47(2)	1(2)	8(2)	-6(1)
C(13)	28(2)	22(2)	39(2)	6(2)	3(2)	-8(2)
C(14)	45(3)	30(2)	36(2)	-3(2)	-15(2)	-18(2)
P(1)	17(1)	18(1)	16(1)	-1(1)	-4(1)	-2(1)
O(30)	71(2)	27(1)	26(1)	-4(1)	6(2)	-21(2)
C(31)	45(3)	26(2)	28(2)	-9(2)	18(2)	-13(2)
C(32)	45(3)	36(2)	32(2)	-15(2)	5(2)	-7(2)
C(33)	59(3)	43(3)	36(2)	-17(2)	7(3)	11(3)
C(34)	73(4)	24(2)	57(3)	-14(2)	27(3)	-1(3)
C(35)	43(3)	29(2)	62(3)	-26(2)	28(3)	-13(2)
C(36)	48(3)	26(2)	45(3)	-16(2)	14(2)	-16(2)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for 9.

	x	y	z	U(eq)
H(2)	141(11)	1374(18)	4074(38)	18
H(3)	804(1)	2206(2)	3953(3)	19
H(5)	2063(1)	1154(2)	4278(4)	20
H(8A)	1415(2)	-952(2)	5555(4)	43
H(8B)	1809(2)	-490(2)	6369(4)	43
H(8C)	1944(2)	-1262(2)	5586(4)	43
H(9A)	1465(1)	-977(2)	2956(4)	40
H(9B)	1992(1)	-1288(2)	3115(4)	40
H(9C)	1891(1)	-532(2)	2248(4)	40
H(10A)	2469(1)	192(2)	3598(4)	46
H(10B)	2573(1)	-580(2)	4418(4)	46
H(10C)	2438(1)	192(2)	5201(4)	46
H(12A)	1234(1)	3192(2)	3019(5)	45
H(12B)	1584(1)	3732(2)	3849(5)	45
H(12C)	1173(1)	3278(2)	4608(5)	45
H(13A)	2306(2)	2127(2)	3048(4)	45
H(13B)	2268(2)	3041(2)	2925(4)	45
H(13C)	1922(2)	2504(2)	2075(4)	45
H(14A)	2206(2)	2243(2)	5572(4)	55
H(14B)	1764(2)	2702(2)	6161(4)	55
H(14C)	2175(2)	3155(2)	5402(4)	55
H(32)	700(2)	-1445(2)	1815(4)	45
H(33)	704(2)	-2745(3)	2414(4)	55
H(34)	61(2)	-3529(3)	1937(5)	61
H(35)	-594(2)	-2995(2)	881(5)	54
H(36)	-612(2)	-1693(2)	313(5)	48
H(22)	1425(3)	892(4)	1252(5)	35
H(23)	1841(2)	1355(4)	-605(7)	47
H(24)	1580(3)	1077(5)	-2777(6)	55
H(25)	902(3)	337(5)	-3093(4)	45
H(26)	486(2)	-126(4)	-1236(7)	41
H(42)	-1028(2)	53(3)	493(6)	32
H(43)	-1584(3)	-786(4)	1413(4)	37
H(44)	-1944(2)	-1712(4)	59(7)	38
H(45)	-1749(3)	-1800(3)	-2217(6)	48
H(46)	-1193(3)	-961(4)	-3137(4)	36
H(47A)	-668(3)	-18(5)	-3030(8)	59
H(47B)	-385(3)	33(5)	-1645(8)	59
H(47C)	-777(3)	660(5)	-1993(8)	59