Supporting Information

Quantitative Geometric Descriptions of the Belt Iron Atoms of the Iron-Molybdenum Cofactor of Nitrogenase and Synthetic Iron(II) Model Complexes

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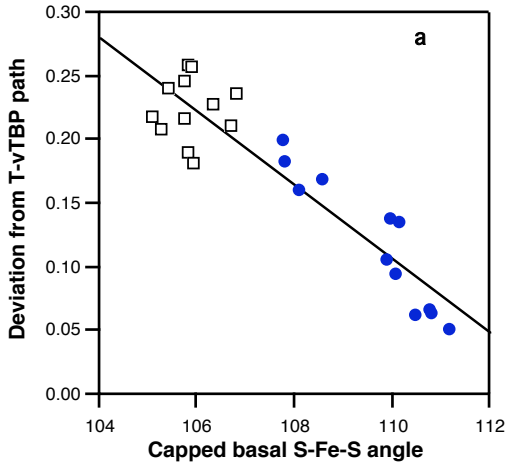

Figure S1. Dependence of the deviation from the T-vTBP path on the S-Fe-S bond angle subtended by the capping Mo (blue circles) or Fe (squares) atoms in the FeMo cofactor.

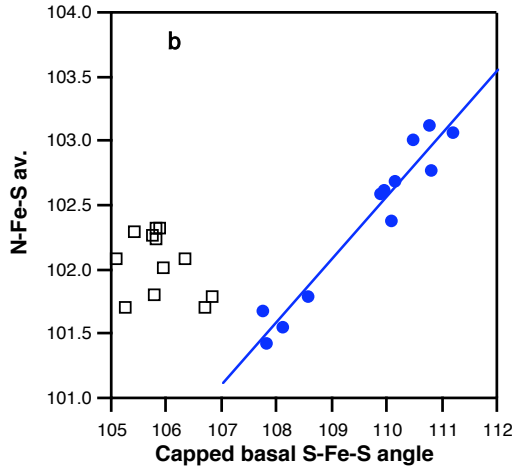

Figure S2. Dependence of the average S-Fe-X bond angle α on the S-Fe-S bond angle subtended by the capping Mo (blue circles) or Fe (squares) atoms in the FeMo cofactor.

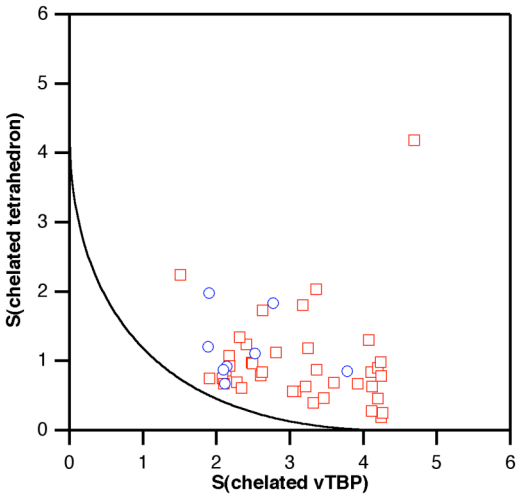

Figure S3. Shape map referred to a chelated tetrahedron and a chelated vTBP, in which one bond angle is constrained to be 95°, showing the position of the Fe atoms in diketiminato complexes. Symbols as in Fig. 11.

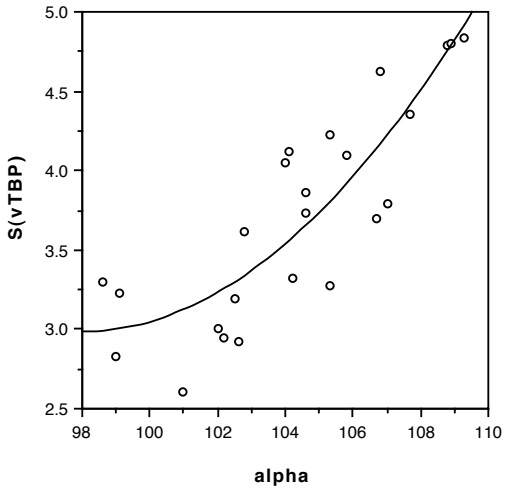

Figure S4. Scatterplot of the vTBP shape measures of Fe(II) diketiminate complexes (Table 2) as a function of the average pyramidality angle α (Scheme 2d).

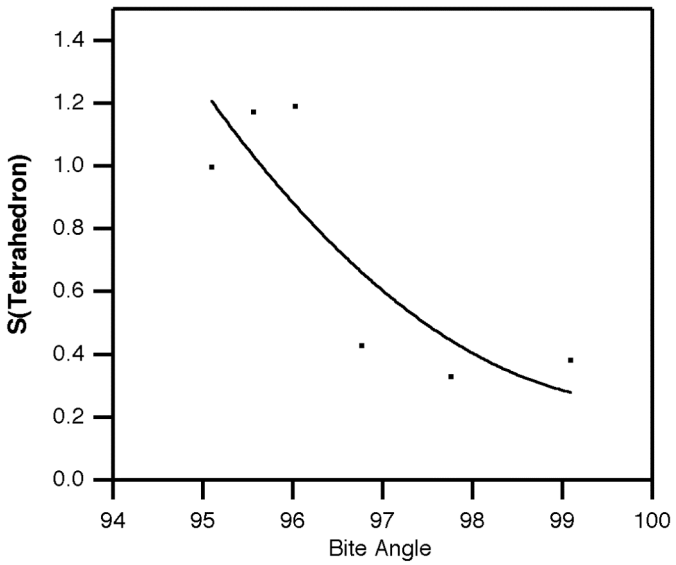

Figure S5. Tetrahedral measures of Fe(III) diketiminate complexes represented as a function of the bite angle.

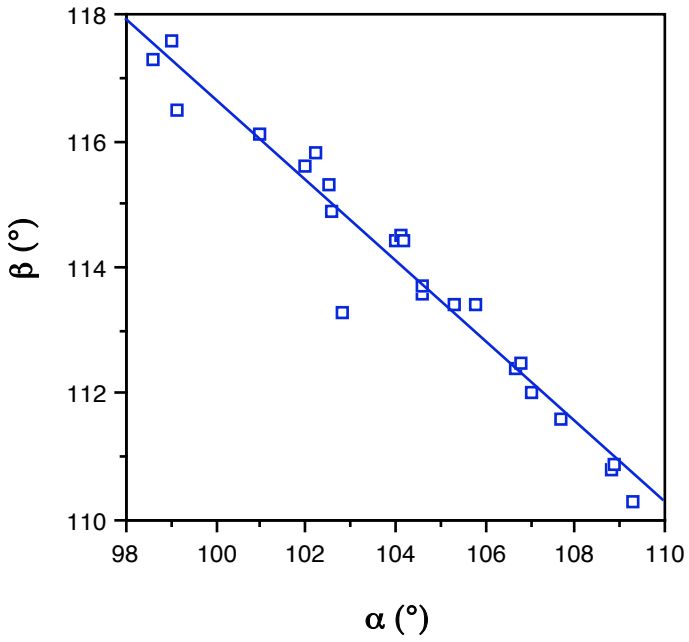

Figure S6. Scatterplot of the basal and axial bond angles (Scheme 2b) of Fe(II) diketiminate complexes (Table 2).

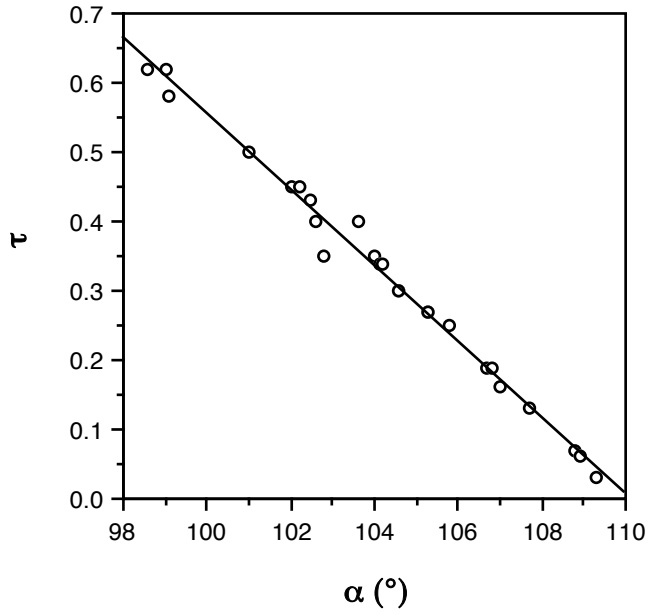

Figure S7. Correlation between the parameter τ defined in eq. 1 and the average axial ligand-metal-basal ligand bond angle α (Scheme 2b) of Fe(II) diketiminate complexes (Table 2).

Table S1. Crystal data and structure refinement for 1.

Identification code	holjv49
Empirical formula	C38 H59 Fe N3
Formula weight	613.73
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 10.0407(10) A alpha = 90 deg. b = 16.3860(16) A beta = 108.979(2) deg. c = 11.8742(12) A gamma = 90 deg.
Volume	1847.4(3) A^3
Z, Calculated density	2, 1.103 Mg/m^3
Absorption coefficient	0.435 mm^-1
F(000)	668
Crystal size	0.50 x 0.50 x 0.45 mm
Theta range for data collection	1.81 to 28.26 deg.
Limiting indices	-13<=h<=13, -21<=k<=21, -15<=l<=15
Reflections collected / unique	22406 / 8838 [R(int) = 0.0188]
Completeness to theta = 28.26	98.8 %
Absorption correction	Empirical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8838 / 1 / 394
Goodness-of-fit on F^2	1.035
Final R indices [I>2sigma(I)]	R1 = 0.0292, wR2 = 0.0699
R indices (all data)	R1 = 0.0339, wR2 = 0.0721
Absolute structure parameter	-0.017(8)
Largest diff. peak and hole	0.214 and -0.196 e.A^-3

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	6460(1)	6269(1)	2390(1)	26(1)
N(11)	6110(1)	5140(1)	1664(1)	26(1)
N(14)	4397(2)	6712(1)	1348(1)	35(1)
N(21)	5781(1)	5949(1)	3759(1)	26(1)
C(11)	4293(2)	5179(1)	4675(2)	38(1)
C(12)	6908(2)	4892(1)	906(1)	29(1)
C(13)	6220(2)	6460(1)	4801(1)	28(1)
C(14)	3214(2)	6594(1)	975(1)	35(1)
C(15)	8022(2)	7013(1)	2236(2)	36(1)
C(21)	4925(2)	5322(1)	3694(1)	27(1)
C(22)	6453(2)	5101(1)	-306(1)	33(1)
C(23)	5341(2)	7087(1)	4967(1)	33(1)
C(24)	1689(2)	6410(1)	488(2)	41(1)
C(25)	7833(2)	7937(1)	2339(2)	36(1)
C(31)	4564(2)	4752(1)	2752(1)	30(1)
C(32)	7292(2)	4874(1)	-988(2)	41(1)
C(33)	5845(2)	7587(1)	5972(2)	41(1)
C(34)	1196(2)	6084(2)	1490(2)	58(1)
C(35)	8077(2)	8188(1)	3621(2)	50(1)
C(41)	5183(2)	4627(1)	1857(1)	28(1)
C(42)	8529(2)	4450(1)	-499(2)	46(1)
C(43)	7165(2)	7476(1)	6782(2)	45(1)
C(44)	891(3)	7195(2)	-20(3)	84(1)
C(45)	8785(2)	8438(1)	1824(2)	52(1)
C(51)	4751(2)	3863(1)	1114(2)	41(1)
C(52)	8970(2)	4259(1)	701(2)	42(1)
C(53)	8032(2)	6870(1)	6598(2)	41(1)
C(54)	1481(3)	5763(2)	-480(2)	77(1)
C(62)	8176(2)	4474(1)	1423(2)	35(1)
C(63)	7598(2)	6362(1)	5608(1)	31(1)
C(72)	5086(2)	5556(1)	-896(2)	39(1)
C(73)	3894(2)	7263(1)	4072(2)	40(1)
C(82)	5355(3)	6431(1)	-1204(2)	67(1)
C(83)	3930(3)	8046(1)	3378(2)	57(1)
C(92)	4142(2)	5107(2)	-1996(2)	60(1)
C(93)	2750(2)	7311(2)	4668(2)	65(1)
C(102)	8715(2)	4250(1)	2746(2)	41(1)
C(103)	8573(2)	5708(1)	5402(2)	36(1)
C(112)	10177(2)	4577(2)	3368(2)	61(1)
C(113)	8352(3)	4890(2)	5912(3)	71(1)
C(122)	8682(3)	3329(2)	2940(2)	65(1)
C(123)	10129(2)	5969(2)	5861(2)	64(1)

Table S3. Bond lengths [A] and angles [deg] for 1.

Fe(1)-N(11)	2.0230(12)
Fe(1)-N(21)	2.0262(12)
Fe(1)-C(15)	2.0400(16)
Fe(1)-N(14)	2.1634(15)
N(11)-C(41)	1.3283(19)
N(11)-C(12)	1.4436(19)
N(14)-C(14)	1.141(2)
N(21)-C(21)	1.3250(19)
N(21)-C(13)	1.4393(19)
C(11)-C(21)	1.516(2)
C(12)-C(62)	1.399(2)
C(12)-C(22)	1.404(2)
C(13)-C(23)	1.409(2)
C(13)-C(63)	1.413(2)
C(14)-C(24)	1.482(2)
C(15)-C(25)	1.536(2)
C(21)-C(31)	1.411(2)
C(22)-C(32)	1.395(2)
C(22)-C(72)	1.518(3)
C(23)-C(33)	1.400(2)
C(23)-C(73)	1.523(2)
C(24)-C(34)	1.526(3)
C(24)-C(54)	1.527(3)
C(24)-C(44)	1.532(3)
C(25)-C(35)	1.518(3)
C(25)-C(45)	1.531(2)
C(31)-C(41)	1.410(2)
C(32)-C(42)	1.375(3)
C(33)-C(43)	1.373(3)
C(41)-C(51)	1.512(2)
C(42)-C(52)	1.383(3)
C(43)-C(53)	1.384(3)
C(52)-C(62)	1.393(2)
C(53)-C(63)	1.391(2)
C(62)-C(102)	1.531(2)
C(63)-C(103)	1.524(2)
C(72)-C(82)	1.526(3)
C(72)-C(92)	1.530(3)
C(73)-C(83)	1.532(3)
C(73)-C(93)	1.535(3)
C(102)-C(112)	1.510(3)
C(102)-C(122)	1.529(3)
C(103)-C(113)	1.517(3)
C(103)-C(123)	1.538(3)
N(11)-Fe(1)-N(21)	92.74(5)
N(11)-Fe(1)-C(15)	122.69(6)
N(21)-Fe(1)-C(15)	134.09(6)
N(11)-Fe(1)-N(14)	93.51(5)
N(21)-Fe(1)-N(14)	92.07(5)
C(15)-Fe(1)-N(14)	111.67(6)
C(41)-N(11)-C(12)	119.47(12)
C(41)-N(11)-Fe(1)	122.64(10)
C(12)-N(11)-Fe(1)	117.90(9)
C(14)-N(14)-Fe(1)	147.96(13)
C(21)-N(21)-C(13)	120.79(12)
C(21)-N(21)-Fe(1)	122.38(10)
C(13)-N(21)-Fe(1)	116.77(9)
C(62)-C(12)-C(22)	120.97(14)
C(62)-C(12)-N(11)	118.37(14)
C(22)-C(12)-N(11)	120.60(14)

C(23)-C(13)-C(63)	120.51(14)
C(23)-C(13)-N(21)	120.93(13)
C(63)-C(13)-N(21)	118.37(13)
N(14)-C(14)-C(24)	177.94(18)
C(25)-C(15)-Fe(1)	117.60(11)
N(21)-C(21)-C(31)	123.58(13)
N(21)-C(21)-C(11)	120.11(13)
C(31)-C(21)-C(11)	116.30(13)
C(32)-C(22)-C(12)	118.28(16)
C(32)-C(22)-C(72)	119.29(15)
C(12)-C(22)-C(72)	122.43(14)
C(33)-C(23)-C(13)	118.50(15)
C(33)-C(23)-C(73)	118.84(15)
C(13)-C(23)-C(73)	122.62(14)
C(14)-C(24)-C(34)	108.87(14)
C(14)-C(24)-C(54)	107.82(15)
C(34)-C(24)-C(54)	110.16(19)
C(14)-C(24)-C(44)	108.89(18)
C(34)-C(24)-C(44)	109.92(19)
C(54)-C(24)-C(44)	111.1(2)
C(35)-C(25)-C(45)	109.69(16)
C(35)-C(25)-C(15)	111.27(15)
C(45)-C(25)-C(15)	112.82(15)
C(41)-C(31)-C(21)	129.18(14)
C(42)-C(32)-C(22)	121.47(17)
C(43)-C(33)-C(23)	121.22(16)
N(11)-C(41)-C(31)	122.94(13)
N(11)-C(41)-C(51)	120.47(14)
C(31)-C(41)-C(51)	116.59(14)
C(32)-C(42)-C(52)	119.50(16)
C(33)-C(43)-C(53)	119.88(16)
C(42)-C(52)-C(62)	121.33(17)
C(43)-C(53)-C(63)	121.53(16)
C(52)-C(62)-C(12)	118.44(16)
C(52)-C(62)-C(102)	119.23(16)
C(12)-C(62)-C(102)	122.33(14)
C(53)-C(63)-C(13)	118.28(15)
C(53)-C(63)-C(103)	121.03(14)
C(13)-C(63)-C(103)	120.68(14)
C(22)-C(72)-C(82)	111.59(17)
C(22)-C(72)-C(92)	111.99(16)
C(82)-C(72)-C(92)	110.83(18)
C(23)-C(73)-C(83)	110.49(16)
C(23)-C(73)-C(93)	112.04(17)
C(83)-C(73)-C(93)	110.95(18)
C(112)-C(102)-C(122)	109.96(18)
C(112)-C(102)-C(62)	112.33(16)
C(122)-C(102)-C(62)	111.95(17)
C(113)-C(103)-C(63)	111.83(15)
C(113)-C(103)-C(123)	111.58(18)
C(63)-C(103)-C(123)	112.33(15)

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 1.
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)	31(1)	23(1)	28(1)	-2(1)	14(1)	-4(1)
N(11)	33(1)	24(1)	26(1)	-2(1)	13(1)	-1(1)
N(14)	42(1)	31(1)	33(1)	2(1)	15(1)	2(1)
N(21)	27(1)	28(1)	23(1)	-1(1)	9(1)	1(1)
C(11)	44(1)	40(1)	37(1)	0(1)	22(1)	-7(1)
C(12)	36(1)	22(1)	33(1)	-4(1)	17(1)	-5(1)
C(13)	32(1)	31(1)	25(1)	-1(1)	14(1)	-4(1)
C(14)	43(1)	33(1)	29(1)	2(1)	13(1)	4(1)
C(15)	35(1)	33(1)	45(1)	-1(1)	20(1)	-5(1)
C(21)	27(1)	29(1)	27(1)	3(1)	11(1)	1(1)
C(22)	43(1)	30(1)	31(1)	-3(1)	17(1)	-6(1)
C(23)	34(1)	35(1)	31(1)	-4(1)	15(1)	-3(1)
C(24)	36(1)	46(1)	37(1)	0(1)	7(1)	4(1)
C(25)	32(1)	33(1)	42(1)	2(1)	12(1)	-4(1)
C(31)	32(1)	27(1)	32(1)	0(1)	14(1)	-5(1)
C(32)	53(1)	47(1)	31(1)	-5(1)	22(1)	-4(1)
C(33)	49(1)	38(1)	41(1)	-12(1)	21(1)	-2(1)
C(34)	41(1)	83(2)	51(1)	3(1)	17(1)	-4(1)
C(35)	61(1)	40(1)	52(1)	-6(1)	20(1)	-10(1)
C(41)	32(1)	24(1)	27(1)	0(1)	9(1)	-1(1)
C(42)	53(1)	49(1)	47(1)	-12(1)	32(1)	-2(1)
C(43)	54(1)	47(1)	34(1)	-16(1)	15(1)	-10(1)
C(44)	54(1)	81(2)	102(2)	35(2)	4(1)	19(1)
C(45)	52(1)	44(1)	65(1)	7(1)	23(1)	-11(1)
C(51)	56(1)	31(1)	43(1)	-10(1)	24(1)	-13(1)
C(52)	43(1)	40(1)	49(1)	-8(1)	22(1)	4(1)
C(53)	41(1)	49(1)	30(1)	-6(1)	7(1)	-6(1)
C(54)	50(1)	113(2)	71(2)	-44(2)	25(1)	-26(1)
C(62)	43(1)	29(1)	37(1)	-3(1)	18(1)	1(1)
C(63)	34(1)	33(1)	26(1)	0(1)	11(1)	-1(1)
C(72)	49(1)	42(1)	30(1)	1(1)	17(1)	2(1)
C(73)	37(1)	40(1)	44(1)	-9(1)	14(1)	7(1)
C(82)	79(2)	49(2)	74(1)	23(1)	27(1)	10(1)
C(83)	64(1)	43(1)	54(1)	-3(1)	6(1)	16(1)
C(92)	54(1)	84(2)	37(1)	-10(1)	9(1)	4(1)
C(93)	44(1)	84(2)	71(2)	-20(1)	26(1)	9(1)
C(102)	45(1)	44(1)	39(1)	3(1)	19(1)	13(1)
C(103)	31(1)	44(1)	30(1)	1(1)	7(1)	4(1)
C(112)	63(1)	71(2)	44(1)	3(1)	11(1)	-2(1)
C(113)	78(2)	52(1)	94(2)	28(1)	46(1)	28(1)
C(122)	79(2)	55(1)	61(1)	18(1)	22(1)	2(1)
C(123)	34(1)	88(2)	67(1)	-22(1)	11(1)	1(1)

Table S5. Crystal data and structure refinement for 2.

Identification code	holjv54
Empirical formula	C39 H61 Fe N3
Formula weight	627.76
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 10.3029(7) A alpha = 90 deg. b = 16.3575(11) A beta = 104.8300(10) deg. c = 11.8844(8) A gamma = 90 deg.
Volume	1936.2(2) A^3
Z, Calculated density	2, 1.077 Mg/m^3
Absorption coefficient	0.417 mm^-1
F(000)	684
Crystal size	0.50 x 0.50 x 0.40 mm
Theta range for data collection	1.77 to 28.29 deg.
Limiting indices	-13<=h<=13, -21<=k<=21, -15<=l<=15
Reflections collected / unique	23593 / 9300 [R(int) = 0.0202]
Completeness to theta = 28.29	98.8 %
Absorption correction	Empirical
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9300 / 1 / 404
Goodness-of-fit on F^2	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0315, wR2 = 0.0758
R indices (all data)	R1 = 0.0349, wR2 = 0.0772
Absolute structure parameter	0.029(8)
Largest diff. peak and hole	0.282 and -0.226 e.A^-3

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	8290(1)	6511(1)	7529(1)	28(1)
N(11)	9098(1)	6190(1)	6204(1)	27(1)
N(15)	10208(2)	6873(1)	8621(1)	41(1)
N(21)	8404(1)	5354(1)	8159(1)	31(1)
C(11)	10575(2)	5358(1)	5308(2)	42(1)
C(12)	8857(1)	6736(1)	5221(1)	29(1)
C(13)	7483(2)	5094(1)	8820(2)	38(1)
C(14)	6658(2)	7238(1)	7500(2)	37(1)
C(15)	11315(2)	6792(1)	9089(2)	42(1)
C(21)	9868(1)	5537(1)	6257(1)	29(1)
C(22)	9822(2)	7316(1)	5102(1)	35(1)
C(23)	6255(2)	4743(1)	8228(2)	44(1)
C(24)	6774(2)	8174(1)	7556(1)	38(1)
C(25)	12746(2)	6659(1)	9696(2)	55(1)
C(31)	10055(2)	4951(1)	7150(1)	32(1)
C(32)	9492(2)	7857(1)	4165(2)	43(1)
C(33)	5361(2)	4488(1)	8865(2)	59(1)
C(34)	7359(2)	8485(1)	6583(2)	58(1)
C(35)	13499(2)	6476(3)	8767(2)	85(1)
C(41)	9311(2)	4824(1)	7971(1)	31(1)
C(42)	8266(2)	7835(1)	3377(2)	46(1)
C(43)	5672(3)	4601(2)	10058(2)	69(1)
C(44)	7663(2)	8434(1)	8737(2)	63(1)
C(45)	12833(3)	5922(2)	10502(3)	85(1)
C(51)	9554(2)	4029(1)	8645(2)	45(1)
C(52)	7313(2)	7271(1)	3503(1)	41(1)
C(53)	6847(3)	4959(2)	10622(2)	68(1)
C(54)	5392(2)	8569(1)	7417(2)	55(1)
C(55)	13257(4)	7437(2)	10369(4)	144(2)
C(62)	7576(2)	6716(1)	4420(1)	32(1)
C(63)	7800(2)	5220(1)	10028(2)	49(1)
C(72)	11196(2)	7378(1)	5969(2)	41(1)
C(73)	5874(2)	4614(1)	6924(2)	45(1)
C(82)	11337(2)	8179(1)	6652(2)	54(1)
C(83)	4493(2)	4970(2)	6344(2)	70(1)
C(92)	12345(2)	7300(2)	5355(2)	61(1)
C(93)	5922(3)	3716(2)	6612(2)	73(1)
C(102)	6528(2)	6096(1)	4551(1)	37(1)
C(103)	9090(2)	5627(1)	10676(2)	59(1)
C(112)	6828(2)	5249(1)	4139(2)	61(1)
C(113)	8841(3)	6517(2)	10958(2)	94(1)
C(122)	5088(2)	6358(2)	3959(2)	67(1)
C(123)	9793(4)	5160(2)	11794(2)	95(1)

Table S7. Bond lengths [A] and angles [deg] for 2.

Fe(1)-N(21)	2.0269(13)
Fe(1)-N(11)	2.0294(12)
Fe(1)-C(14)	2.0526(16)
Fe(1)-N(15)	2.1513(15)
N(11)-C(21)	1.3227(19)
N(11)-C(12)	1.4407(19)
N(15)-C(15)	1.142(2)
N(21)-C(41)	1.3360(19)
N(21)-C(13)	1.443(2)
C(11)-C(21)	1.519(2)
C(12)-C(22)	1.406(2)
C(12)-C(62)	1.416(2)
C(13)-C(23)	1.403(3)
C(13)-C(63)	1.404(2)
C(14)-C(24)	1.536(2)
C(15)-C(25)	1.482(3)
C(21)-C(31)	1.406(2)
C(22)-C(32)	1.395(2)
C(22)-C(72)	1.526(2)
C(23)-C(33)	1.398(2)
C(23)-C(73)	1.513(3)
C(24)-C(34)	1.521(3)
C(24)-C(44)	1.527(2)
C(24)-C(54)	1.533(2)
C(25)-C(55)	1.524(4)
C(25)-C(45)	1.528(4)
C(25)-C(35)	1.533(3)
C(31)-C(41)	1.402(2)
C(32)-C(42)	1.367(3)
C(33)-C(43)	1.384(4)
C(41)-C(51)	1.513(2)
C(42)-C(52)	1.383(3)
C(43)-C(53)	1.357(4)
C(52)-C(62)	1.391(2)
C(53)-C(63)	1.414(3)
C(62)-C(102)	1.519(2)
C(63)-C(103)	1.509(3)
C(72)-C(82)	1.529(3)
C(72)-C(92)	1.546(3)
C(73)-C(93)	1.519(3)
C(73)-C(83)	1.528(3)
C(102)-C(112)	1.527(3)
C(102)-C(122)	1.532(3)
C(103)-C(113)	1.530(4)
C(103)-C(123)	1.543(3)
N(21)-Fe(1)-N(11)	92.81(5)
N(21)-Fe(1)-C(14)	121.14(6)
N(11)-Fe(1)-C(14)	129.30(6)
N(21)-Fe(1)-N(15)	94.39(6)
N(11)-Fe(1)-N(15)	92.48(5)
C(14)-Fe(1)-N(15)	118.21(6)
C(21)-N(11)-C(12)	121.03(12)
C(21)-N(11)-Fe(1)	122.16(10)
C(12)-N(11)-Fe(1)	116.71(9)
C(15)-N(15)-Fe(1)	155.62(14)
C(41)-N(21)-C(13)	119.01(13)
C(41)-N(21)-Fe(1)	121.45(10)
C(13)-N(21)-Fe(1)	119.54(10)
C(22)-C(12)-C(62)	120.60(13)
C(22)-C(12)-N(11)	121.31(13)

C(62)-C(12)-N(11)	117.92(12)
C(23)-C(13)-C(63)	121.21(17)
C(23)-C(13)-N(21)	118.76(15)
C(63)-C(13)-N(21)	119.99(17)
C(24)-C(14)-Fe(1)	121.49(11)
N(15)-C(15)-C(25)	178.2(2)
N(11)-C(21)-C(31)	123.40(13)
N(11)-C(21)-C(11)	121.15(14)
C(31)-C(21)-C(11)	115.41(14)
C(32)-C(22)-C(12)	118.31(15)
C(32)-C(22)-C(72)	119.36(15)
C(12)-C(22)-C(72)	122.32(14)
C(33)-C(23)-C(13)	118.98(19)
C(33)-C(23)-C(73)	118.58(19)
C(13)-C(23)-C(73)	122.42(15)
C(34)-C(24)-C(44)	110.18(18)
C(34)-C(24)-C(54)	108.38(16)
C(44)-C(24)-C(54)	107.66(16)
C(34)-C(24)-C(14)	109.99(15)
C(44)-C(24)-C(14)	109.80(15)
C(54)-C(24)-C(14)	110.79(15)
C(15)-C(25)-C(55)	107.4(2)
C(15)-C(25)-C(45)	108.19(19)
C(55)-C(25)-C(45)	111.9(3)
C(15)-C(25)-C(35)	107.56(17)
C(55)-C(25)-C(35)	111.7(3)
C(45)-C(25)-C(35)	109.8(2)
C(41)-C(31)-C(21)	129.32(14)
C(42)-C(32)-C(22)	121.55(16)
C(43)-C(33)-C(23)	120.2(2)
N(21)-C(41)-C(31)	123.36(14)
N(21)-C(41)-C(51)	119.81(14)
C(31)-C(41)-C(51)	116.82(14)
C(32)-C(42)-C(52)	120.06(16)
C(53)-C(43)-C(33)	120.50(19)
C(42)-C(52)-C(62)	121.23(16)
C(43)-C(53)-C(63)	122.0(2)
C(52)-C(62)-C(12)	118.23(14)
C(52)-C(62)-C(102)	121.03(14)
C(12)-C(62)-C(102)	120.73(13)
C(13)-C(63)-C(53)	117.1(2)
C(13)-C(63)-C(103)	122.09(17)
C(53)-C(63)-C(103)	120.81(18)
C(22)-C(72)-C(82)	111.15(15)
C(22)-C(72)-C(92)	111.46(16)
C(82)-C(72)-C(92)	109.96(16)
C(23)-C(73)-C(93)	111.64(17)
C(23)-C(73)-C(83)	112.09(17)
C(93)-C(73)-C(83)	110.1(2)
C(62)-C(102)-C(112)	111.39(14)
C(62)-C(102)-C(122)	113.32(15)
C(112)-C(102)-C(122)	111.04(18)
C(63)-C(103)-C(113)	110.9(2)
C(63)-C(103)-C(123)	112.2(2)
C(113)-C(103)-C(123)	110.5(2)

Table S8. Anisotropic displacement parameters (A^2 x 10^3) for 2.
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)	33(1)	25(1)	27(1)	-1(1)	11(1)	4(1)
N(11)	30(1)	27(1)	26(1)	-1(1)	10(1)	-1(1)
N(15)	45(1)	39(1)	40(1)	-6(1)	9(1)	2(1)
N(21)	40(1)	28(1)	28(1)	4(1)	14(1)	5(1)
C(11)	50(1)	39(1)	44(1)	0(1)	27(1)	6(1)
C(12)	34(1)	29(1)	27(1)	0(1)	13(1)	1(1)
C(13)	51(1)	32(1)	38(1)	10(1)	23(1)	13(1)
C(14)	35(1)	34(1)	43(1)	-6(1)	12(1)	3(1)
C(15)	46(1)	39(1)	38(1)	-8(1)	6(1)	0(1)
C(21)	29(1)	29(1)	32(1)	-4(1)	12(1)	-2(1)
C(22)	36(1)	34(1)	38(1)	2(1)	15(1)	0(1)
C(23)	48(1)	34(1)	57(1)	14(1)	28(1)	8(1)
C(24)	37(1)	32(1)	40(1)	-8(1)	5(1)	6(1)
C(25)	44(1)	52(1)	61(1)	-2(1)	-5(1)	2(1)
C(31)	33(1)	29(1)	35(1)	0(1)	11(1)	9(1)
C(32)	49(1)	37(1)	50(1)	9(1)	23(1)	-5(1)
C(33)	59(1)	55(1)	74(1)	26(1)	40(1)	10(1)
C(34)	70(1)	41(1)	67(1)	4(1)	24(1)	5(1)
C(35)	50(1)	112(2)	95(2)	29(2)	21(1)	22(2)
C(41)	36(1)	29(1)	29(1)	2(1)	8(1)	5(1)
C(42)	57(1)	44(1)	40(1)	15(1)	17(1)	1(1)
C(43)	77(2)	72(2)	79(2)	34(1)	56(1)	24(1)
C(44)	68(1)	48(1)	57(1)	-20(1)	-11(1)	13(1)
C(45)	64(2)	107(2)	77(2)	31(2)	7(1)	24(2)
C(51)	56(1)	37(1)	46(1)	12(1)	21(1)	15(1)
C(52)	47(1)	44(1)	30(1)	5(1)	7(1)	1(1)
C(53)	95(2)	77(2)	45(1)	23(1)	45(1)	34(1)
C(54)	47(1)	47(1)	68(1)	-8(1)	8(1)	18(1)
C(55)	81(2)	100(3)	201(5)	-72(3)	-56(3)	5(2)
C(62)	37(1)	33(1)	26(1)	-1(1)	11(1)	-1(1)
C(63)	70(1)	49(1)	35(1)	11(1)	26(1)	20(1)
C(72)	34(1)	39(1)	52(1)	3(1)	16(1)	-6(1)
C(73)	41(1)	44(1)	55(1)	6(1)	19(1)	-6(1)
C(82)	46(1)	44(1)	68(1)	-6(1)	8(1)	-10(1)
C(83)	60(1)	77(2)	72(2)	14(1)	15(1)	10(1)
C(92)	41(1)	69(1)	79(2)	2(1)	28(1)	-6(1)
C(93)	84(2)	57(1)	74(2)	-6(1)	16(1)	6(1)
C(102)	37(1)	43(1)	30(1)	-1(1)	8(1)	-7(1)
C(103)	84(2)	64(1)	32(1)	3(1)	21(1)	16(1)
C(112)	73(1)	51(1)	66(1)	-26(1)	31(1)	-26(1)
C(113)	137(2)	76(2)	72(2)	-24(2)	34(2)	10(2)
C(122)	39(1)	88(2)	66(1)	27(1)	1(1)	-14(1)
C(123)	109(2)	124(3)	47(1)	25(2)	8(1)	14(2)

Table S9. Crystal data and structure refinement for 3.

Identification code	holjs104
Empirical formula	C79 H108 Cl2 Fe2 N6
Formula weight	1324.31
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.7967(17)A alpha = 88.453(2) deg. b = 17.485(2) A beta = 76.926(2) deg. c = 17.643(2) A gamma = 89.798(2) deg.
Volume	3843.9(9) A^3
Z, Calculated density	2, 1.144 Mg/m^3
Absorption coefficient	0.491 mm^-1
F(000)	1420
Crystal size	0.40 x 0.10 x 0.10 mm
Theta range for data collection	1.63 to 28.37 deg.
Limiting indices	-17<=h<=17, -23<=k<=23, -23<=l<=23
Reflections collected / unique	34674 / 17992 [R(int) = 0.0458]
Completeness to theta = 28.37	93.5 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17992 / 0 / 813
Goodness-of-fit on F^2	0.964
Final R indices [I>2sigma(I)]	R1 = 0.0579, wR2 = 0.1254
R indices (all data)	R1 = 0.1427, wR2 = 0.1523
Largest diff. peak and hole	0.580 and -0.345 e.A^-3

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 3.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(2)	7218(1)	4422(1)	7571(1)	34(1)
Fe(1)	9275(1)	9530(1)	7905(1)	41(1)
Cl(2)	6780(1)	3271(1)	8137(1)	55(1)
Cl(1)	9221(1)	8473(1)	8657(1)	70(1)
N(22)	8751(2)	4657(1)	7055(1)	31(1)
N(21)	10461(2)	9863(1)	7012(1)	34(1)
N(18)	6862(2)	5161(1)	8518(1)	37(1)
N(14)	9081(2)	10426(2)	8702(1)	41(1)
N(11)	8129(2)	9718(2)	7309(1)	43(1)
N(12)	6624(2)	4915(1)	6720(1)	35(1)
C(35)	8306(3)	5500(2)	6082(2)	40(1)
C(67)	9792(2)	3488(2)	7055(2)	39(1)
C(17)	9551(2)	4223(2)	7335(2)	33(1)
C(45)	9036(2)	5149(2)	6456(2)	35(1)
C(31)	9278(2)	10409(2)	6256(2)	36(1)
C(25)	7202(3)	5363(2)	6162(2)	42(1)
C(13)	11543(3)	9629(2)	7036(2)	40(1)
C(14)	8964(2)	11141(2)	8437(2)	39(1)
C(27)	10022(2)	4510(2)	7914(2)	40(1)
C(58)	6485(2)	4952(2)	9261(2)	42(1)
C(28)	7009(2)	6435(2)	8946(2)	41(1)
C(18)	7105(2)	5902(2)	8377(2)	39(1)
C(55)	10213(2)	5332(2)	6128(2)	47(1)
C(51)	11237(3)	10564(2)	5778(2)	50(1)
C(34)	8568(2)	11664(2)	9714(2)	40(1)
C(107)	9330(3)	3178(2)	6400(2)	50(1)
C(16)	5528(3)	4721(2)	6695(2)	41(1)
C(26)	4685(3)	5210(2)	7006(2)	46(1)
C(44)	8727(3)	10935(2)	9983(2)	50(1)
C(24)	8713(2)	11758(2)	8907(2)	41(1)
C(21)	8279(2)	10128(2)	6650(2)	38(1)
C(63)	11865(3)	8883(2)	6813(2)	48(1)
C(41)	10292(2)	10255(2)	6389(2)	36(1)
C(37)	10740(3)	4043(2)	8193(2)	54(1)
C(68)	6576(3)	6792(2)	10371(2)	49(1)
C(72)	6358(3)	10476(4)	8400(3)	110(2)
C(57)	10512(3)	3047(2)	7355(2)	50(1)
C(33)	13256(3)	9854(2)	7329(2)	66(1)
C(76)	4839(3)	5964(2)	7367(2)	49(1)
C(64)	8242(3)	12347(2)	10243(2)	51(1)
C(48)	6367(2)	5450(2)	9868(2)	44(1)
C(23)	12234(3)	10117(2)	7310(2)	49(1)
C(54)	8965(3)	10340(2)	9477(2)	51(1)
C(62)	7065(3)	8563(2)	7360(3)	69(1)
C(103)	11119(3)	8343(2)	6533(2)	55(1)
C(11)	7338(3)	10311(2)	6286(2)	56(1)
C(73)	11913(3)	10918(2)	7586(2)	56(1)
C(38)	6637(2)	6217(2)	9730(2)	40(1)
C(47)	10984(3)	3314(2)	7923(2)	59(1)
C(77)	9794(3)	5296(2)	8239(2)	48(1)
C(53)	12899(3)	8661(2)	6840(2)	65(1)
C(15)	6688(3)	5747(2)	5556(2)	65(1)
C(98)	6222(3)	6421(2)	11188(2)	71(1)
C(12)	7145(3)	9311(2)	7601(2)	57(1)

C(86)	4311(3)	6629(2)	7004(3)	79(1)
C(056)	5339(3)	4015(2)	6387(2)	56(1)
C(117)	10169(4)	3187(3)	5645(2)	108(2)
C(94)	7212(4)	12686(3)	10089(2)	101(2)
C(127)	8881(3)	2379(2)	6565(2)	66(1)
C(43)	13584(3)	9137(3)	7093(2)	74(1)
C(36)	3652(3)	4973(2)	6991(2)	62(1)
C(22)	6322(3)	9646(3)	8163(2)	76(1)
C(87)	10800(3)	5809(2)	8076(2)	71(1)
C(42)	5376(4)	8446(4)	8271(3)	105(2)
C(46)	3458(3)	4291(3)	6684(2)	71(1)
C(116)	6010(5)	2646(3)	6277(4)	124(2)
C(74)	8025(3)	12112(2)	11104(2)	73(1)
C(78)	5779(4)	7412(3)	10268(2)	94(2)
C(102)	7912(4)	8216(2)	6715(3)	88(2)
C(84)	9147(4)	12923(3)	10083(3)	108(2)
C(97)	9316(3)	5256(2)	9110(2)	70(1)
C(106)	6251(4)	3479(2)	6038(3)	79(1)
C(32)	5428(4)	9198(4)	8490(3)	104(2)
C(93)	12729(3)	11524(2)	7169(3)	84(1)
C(88)	7690(3)	7141(2)	10301(2)	67(1)
C(96)	4415(3)	5929(2)	8244(2)	67(1)
C(82)	5500(4)	10975(3)	8132(4)	138(3)
C(83)	11762(3)	10952(2)	8468(2)	75(1)
C(123)	11207(4)	8435(2)	5660(2)	80(1)
C(112)	7485(6)	8144(3)	5963(3)	147(3)
C(56)	4296(4)	3821(2)	6387(2)	72(1)
C(122)	8312(5)	7442(2)	6943(3)	118(2)
C(113)	11284(4)	7499(2)	6748(3)	97(2)
C(52)	6155(4)	8136(3)	7710(3)	95(2)
C(92)	6264(4)	10544(5)	9270(3)	205(4)
C(126)	6561(5)	3585(4)	5165(3)	148(3)
C(1S)	5311(4)	9690(3)	5085(3)	81(1)
C(2S)	4838(5)	9063(4)	4820(4)	143(2)
C(3S)	5383(10)	8433(8)	5113(7)	303(6)

Table S11. Bond lengths [A] and angles [deg] for 3.

Fe(2)-N(12)	2.004(2)
Fe(2)-N(22)	2.007(2)
Fe(2)-N(18)	2.106(2)
Fe(2)-Cl(2)	2.2372(9)
Fe(1)-N(21)	1.999(2)
Fe(1)-N(11)	2.010(3)
Fe(1)-N(14)	2.110(3)
Fe(1)-Cl(1)	2.2376(10)
N(22)-C(45)	1.331(4)
N(22)-C(17)	1.438(4)
N(21)-C(41)	1.338(3)
N(21)-C(13)	1.452(4)
N(18)-C(58)	1.332(4)
N(18)-C(18)	1.338(4)
N(14)-C(14)	1.344(4)
N(14)-C(54)	1.346(4)
N(11)-C(21)	1.325(4)
N(11)-C(12)	1.433(4)
N(12)-C(25)	1.328(4)
N(12)-C(16)	1.454(4)
C(35)-C(45)	1.393(4)
C(35)-C(25)	1.408(4)
C(67)-C(57)	1.384(4)
C(67)-C(17)	1.398(4)
C(67)-C(107)	1.524(4)
C(17)-C(27)	1.403(4)
C(45)-C(55)	1.518(4)
C(31)-C(21)	1.393(4)
C(31)-C(41)	1.394(4)
C(25)-C(15)	1.518(4)
C(13)-C(23)	1.401(4)
C(13)-C(63)	1.407(4)
C(14)-C(24)	1.372(4)
C(27)-C(37)	1.389(4)
C(27)-C(77)	1.506(4)
C(58)-C(48)	1.380(4)
C(28)-C(18)	1.374(4)
C(28)-C(38)	1.399(4)
C(51)-C(41)	1.517(4)
C(34)-C(44)	1.379(4)
C(34)-C(24)	1.398(4)
C(34)-C(64)	1.534(4)
C(107)-C(127)	1.508(4)
C(107)-C(117)	1.510(5)
C(16)-C(26)	1.395(4)
C(16)-C(056)	1.405(4)
C(26)-C(36)	1.392(5)
C(26)-C(76)	1.513(5)
C(44)-C(54)	1.377(4)
C(21)-C(11)	1.518(4)
C(63)-C(53)	1.388(5)
C(63)-C(103)	1.514(5)
C(37)-C(47)	1.383(5)
C(68)-C(78)	1.521(5)
C(68)-C(38)	1.523(4)
C(68)-C(88)	1.529(5)
C(68)-C(98)	1.535(5)
C(72)-C(92)	1.520(6)
C(72)-C(22)	1.525(7)
C(72)-C(82)	1.549(8)
C(57)-C(47)	1.374(5)

C(33)-C(43)	1.365(5)
C(33)-C(23)	1.393(5)
C(76)-C(96)	1.519(5)
C(76)-C(86)	1.539(5)
C(64)-C(84)	1.510(5)
C(64)-C(94)	1.520(5)
C(64)-C(74)	1.527(5)
C(48)-C(38)	1.387(4)
C(23)-C(73)	1.519(4)
C(62)-C(52)	1.396(6)
C(62)-C(12)	1.398(5)
C(62)-C(102)	1.520(6)
C(103)-C(123)	1.523(5)
C(103)-C(113)	1.538(5)
C(73)-C(83)	1.527(5)
C(73)-C(93)	1.541(5)
C(77)-C(97)	1.521(5)
C(77)-C(87)	1.540(5)
C(53)-C(43)	1.365(5)
C(12)-C(22)	1.410(5)
C(056)-C(56)	1.379(5)
C(056)-C(106)	1.522(5)
C(36)-C(46)	1.370(5)
C(22)-C(32)	1.393(6)
C(42)-C(52)	1.359(7)
C(42)-C(32)	1.386(7)
C(46)-C(56)	1.364(5)
C(116)-C(106)	1.518(6)
C(102)-C(122)	1.522(6)
C(102)-C(112)	1.553(7)
C(106)-C(126)	1.508(7)
C(1S)-C(2S)	1.397(7)
C(1S)-C(1S)#1	1.407(8)
C(2S)-C(3S)	1.448(13)

N(12)-Fe(2)-N(22)	94.47(10)
N(12)-Fe(2)-N(18)	106.53(10)
N(22)-Fe(2)-N(18)	104.41(9)
N(12)-Fe(2)-Cl(2)	126.73(8)
N(22)-Fe(2)-Cl(2)	119.77(7)
N(18)-Fe(2)-Cl(2)	102.83(7)
N(21)-Fe(1)-N(11)	93.51(10)
N(21)-Fe(1)-N(14)	105.75(10)
N(11)-Fe(1)-N(14)	104.32(10)
N(21)-Fe(1)-Cl(1)	127.15(7)
N(11)-Fe(1)-Cl(1)	120.06(8)
N(14)-Fe(1)-Cl(1)	103.71(7)
C(45)-N(22)-C(17)	120.5(2)
C(45)-N(22)-Fe(2)	123.1(2)
C(17)-N(22)-Fe(2)	116.25(17)
C(41)-N(21)-C(13)	119.5(2)
C(41)-N(21)-Fe(1)	123.1(2)
C(13)-N(21)-Fe(1)	117.41(18)
C(58)-N(18)-C(18)	116.1(3)
C(58)-N(18)-Fe(2)	126.0(2)
C(18)-N(18)-Fe(2)	117.7(2)
C(14)-N(14)-C(54)	115.9(3)
C(14)-N(14)-Fe(1)	118.3(2)
C(54)-N(14)-Fe(1)	125.6(2)
C(21)-N(11)-C(12)	120.7(3)
C(21)-N(11)-Fe(1)	123.8(2)
C(12)-N(11)-Fe(1)	115.2(2)
C(25)-N(12)-C(16)	119.5(2)
C(25)-N(12)-Fe(2)	123.2(2)
C(16)-N(12)-Fe(2)	117.18(18)

C(45)-C(35)-C(25)	130.1(3)
C(57)-C(67)-C(17)	118.9(3)
C(57)-C(67)-C(107)	119.4(3)
C(17)-C(67)-C(107)	121.7(3)
C(67)-C(17)-C(27)	120.8(3)
C(67)-C(17)-N(22)	118.4(3)
C(27)-C(17)-N(22)	120.7(3)
N(22)-C(45)-C(35)	123.4(3)
N(22)-C(45)-C(55)	120.0(3)
C(35)-C(45)-C(55)	116.5(3)
C(21)-C(31)-C(41)	129.5(3)
N(12)-C(25)-C(35)	123.4(3)
N(12)-C(25)-C(15)	120.4(3)
C(35)-C(25)-C(15)	116.2(3)
C(23)-C(13)-C(63)	120.6(3)
C(23)-C(13)-N(21)	121.3(3)
C(63)-C(13)-N(21)	118.1(3)
N(14)-C(14)-C(24)	123.9(3)
C(37)-C(27)-C(17)	117.9(3)
C(37)-C(27)-C(77)	118.9(3)
C(17)-C(27)-C(77)	123.2(3)
N(18)-C(58)-C(48)	123.5(3)
C(18)-C(28)-C(38)	120.2(3)
N(18)-C(18)-C(28)	124.0(3)
C(44)-C(34)-C(24)	116.0(3)
C(44)-C(34)-C(64)	123.9(3)
C(24)-C(34)-C(64)	120.1(3)
C(127)-C(107)-C(117)	108.9(3)
C(127)-C(107)-C(67)	113.5(3)
C(117)-C(107)-C(67)	110.6(3)
C(26)-C(16)-C(056)	121.2(3)
C(26)-C(16)-N(12)	120.4(3)
C(056)-C(16)-N(12)	118.3(3)
C(36)-C(26)-C(16)	117.3(3)
C(36)-C(26)-C(76)	119.2(3)
C(16)-C(26)-C(76)	123.4(3)
C(54)-C(44)-C(34)	120.7(3)
C(14)-C(24)-C(34)	120.1(3)
N(11)-C(21)-C(31)	123.3(3)
N(11)-C(21)-C(11)	120.1(3)
C(31)-C(21)-C(11)	116.6(3)
C(53)-C(63)-C(13)	117.9(3)
C(53)-C(63)-C(103)	120.9(3)
C(13)-C(63)-C(103)	121.2(3)
N(21)-C(41)-C(31)	123.9(3)
N(21)-C(41)-C(51)	120.0(3)
C(31)-C(41)-C(51)	116.1(3)
C(47)-C(37)-C(27)	122.0(3)
C(78)-C(68)-C(38)	108.4(3)
C(78)-C(68)-C(88)	110.3(3)
C(38)-C(68)-C(88)	108.7(3)
C(78)-C(68)-C(98)	109.2(3)
C(38)-C(68)-C(98)	112.3(3)
C(88)-C(68)-C(98)	107.9(3)
C(92)-C(72)-C(22)	112.1(6)
C(92)-C(72)-C(82)	110.6(5)
C(22)-C(72)-C(82)	112.3(3)
C(47)-C(57)-C(67)	121.5(3)
C(43)-C(33)-C(23)	121.4(4)
C(26)-C(76)-C(96)	111.5(3)
C(26)-C(76)-C(86)	111.7(3)
C(96)-C(76)-C(86)	110.1(3)
C(84)-C(64)-C(94)	111.8(4)
C(84)-C(64)-C(74)	107.8(3)
C(94)-C(64)-C(74)	107.5(3)

C(84)-C(64)-C(34)	108.8(3)
C(94)-C(64)-C(34)	108.8(3)
C(74)-C(64)-C(34)	112.1(3)
C(58)-C(48)-C(38)	120.8(3)
C(33)-C(23)-C(13)	118.3(3)
C(33)-C(23)-C(73)	118.9(3)
C(13)-C(23)-C(73)	122.8(3)
N(14)-C(54)-C(44)	123.4(3)
C(52)-C(62)-C(12)	118.2(5)
C(52)-C(62)-C(102)	119.6(5)
C(12)-C(62)-C(102)	122.2(3)
C(63)-C(103)-C(123)	111.8(3)
C(63)-C(103)-C(113)	113.1(3)
C(123)-C(103)-C(113)	109.9(3)
C(23)-C(73)-C(83)	110.6(3)
C(23)-C(73)-C(93)	111.8(3)
C(83)-C(73)-C(93)	110.9(3)
C(48)-C(38)-C(28)	115.3(3)
C(48)-C(38)-C(68)	123.8(3)
C(28)-C(38)-C(68)	120.9(3)
C(57)-C(47)-C(37)	119.0(3)
C(27)-C(77)-C(97)	111.4(3)
C(27)-C(77)-C(87)	112.5(3)
C(97)-C(77)-C(87)	109.2(3)
C(43)-C(53)-C(63)	121.9(3)
C(62)-C(12)-C(22)	121.8(4)
C(62)-C(12)-N(11)	118.1(4)
C(22)-C(12)-N(11)	119.9(4)
C(56)-C(056)-C(16)	118.2(3)
C(56)-C(056)-C(106)	119.9(4)
C(16)-C(056)-C(106)	121.9(3)
C(53)-C(43)-C(33)	119.9(4)
C(46)-C(36)-C(26)	122.0(4)
C(32)-C(22)-C(12)	117.7(5)
C(32)-C(22)-C(72)	119.4(5)
C(12)-C(22)-C(72)	122.9(4)
C(52)-C(42)-C(32)	121.8(5)
C(56)-C(46)-C(36)	119.6(4)
C(122)-C(102)-C(62)	113.3(4)
C(122)-C(102)-C(112)	109.7(4)
C(62)-C(102)-C(112)	110.8(5)
C(126)-C(106)-C(116)	111.5(4)
C(126)-C(106)-C(056)	110.7(4)
C(116)-C(106)-C(056)	113.2(4)
C(42)-C(32)-C(22)	120.0(5)
C(46)-C(56)-C(056)	121.7(4)
C(42)-C(52)-C(62)	120.4(5)
C(2S)-C(1S)-C(1S)#1	103.1(6)
C(1S)-C(2S)-C(3S)	101.3(7)

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

Table S12. Anisotropic displacement parameters (A^2 x 10^3) for 3. 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(2)	40(1)	33(1)	28(1)	3(1)	-7(1)	0(1)
Fe(1)	52(1)	38(1)	31(1)	4(1)	-9(1)	-2(1)
Cl(2)	65(1)	41(1)	53(1)	11(1)	-5(1)	-7(1)
Cl(1)	92(1)	54(1)	60(1)	22(1)	-13(1)	2(1)
N(22)	39(1)	28(1)	27(1)	-1(1)	-7(1)	1(1)
N(21)	43(2)	26(1)	33(1)	-2(1)	-7(1)	5(1)
N(18)	38(2)	42(2)	31(1)	1(1)	-6(1)	-4(1)
N(14)	47(2)	47(2)	29(1)	2(1)	-12(1)	-2(1)
N(11)	44(2)	52(2)	32(2)	-1(1)	-7(1)	-10(1)
N(12)	43(2)	35(1)	28(1)	-1(1)	-7(1)	6(1)
C(35)	54(2)	28(2)	34(2)	9(1)	-4(2)	3(2)
C(67)	46(2)	32(2)	35(2)	5(1)	-2(2)	1(2)
C(17)	34(2)	31(2)	32(2)	3(1)	-3(1)	1(1)
C(45)	44(2)	29(2)	30(2)	-2(1)	-4(1)	2(1)
C(31)	46(2)	27(2)	33(2)	3(1)	-7(2)	5(1)
C(25)	54(2)	43(2)	29(2)	0(2)	-10(2)	12(2)
C(13)	47(2)	35(2)	37(2)	1(1)	-9(2)	10(2)
C(14)	39(2)	51(2)	28(2)	3(2)	-7(1)	-1(2)
C(27)	36(2)	43(2)	39(2)	-2(2)	-7(2)	2(2)
C(58)	44(2)	46(2)	32(2)	4(2)	-2(2)	-9(2)
C(28)	40(2)	42(2)	41(2)	-3(2)	-8(2)	2(2)
C(18)	46(2)	43(2)	28(2)	0(2)	-7(1)	3(2)
C(55)	48(2)	47(2)	42(2)	6(2)	0(2)	-3(2)
C(51)	50(2)	51(2)	45(2)	9(2)	-2(2)	1(2)
C(34)	33(2)	53(2)	38(2)	-6(2)	-14(2)	1(2)
C(107)	77(3)	31(2)	46(2)	-4(2)	-20(2)	11(2)
C(16)	48(2)	45(2)	35(2)	2(2)	-17(2)	2(2)
C(26)	42(2)	54(2)	42(2)	4(2)	-12(2)	3(2)
C(44)	64(2)	57(2)	32(2)	-1(2)	-18(2)	6(2)
C(24)	44(2)	41(2)	35(2)	1(2)	-5(2)	2(2)
C(21)	43(2)	38(2)	36(2)	-8(2)	-14(2)	4(2)
C(63)	63(2)	43(2)	39(2)	-3(2)	-13(2)	19(2)
C(41)	48(2)	27(2)	30(2)	-2(1)	-6(1)	4(1)
C(37)	52(2)	62(3)	53(2)	-2(2)	-24(2)	6(2)
C(68)	48(2)	59(2)	41(2)	-16(2)	-9(2)	11(2)
C(72)	44(3)	194(6)	87(4)	-82(4)	6(2)	-34(3)
C(57)	55(2)	37(2)	56(2)	1(2)	-11(2)	10(2)
C(33)	54(2)	72(3)	79(3)	-19(2)	-28(2)	18(2)
C(76)	43(2)	53(2)	52(2)	-4(2)	-12(2)	15(2)
C(64)	57(2)	59(2)	38(2)	-13(2)	-12(2)	11(2)
C(48)	40(2)	62(2)	28(2)	0(2)	-1(1)	-7(2)
C(23)	44(2)	49(2)	54(2)	-10(2)	-11(2)	13(2)
C(54)	71(3)	50(2)	36(2)	1(2)	-22(2)	4(2)
C(62)	71(3)	68(3)	73(3)	32(2)	-32(2)	-32(2)
C(103)	87(3)	33(2)	48(2)	-6(2)	-18(2)	15(2)
C(11)	55(2)	68(3)	50(2)	-4(2)	-22(2)	2(2)
C(73)	43(2)	49(2)	80(3)	-19(2)	-20(2)	5(2)
C(38)	26(2)	55(2)	38(2)	-7(2)	-4(1)	3(2)
C(47)	57(2)	54(2)	69(3)	8(2)	-23(2)	13(2)
C(77)	46(2)	58(2)	46(2)	-15(2)	-20(2)	10(2)
C(53)	88(3)	51(2)	61(3)	-10(2)	-24(2)	33(2)
C(15)	67(3)	82(3)	44(2)	22(2)	-9(2)	17(2)
C(98)	73(3)	96(3)	42(2)	-23(2)	-4(2)	0(2)
C(12)	53(2)	83(3)	38(2)	8(2)	-18(2)	-27(2)
C(86)	80(3)	65(3)	101(3)	0(2)	-42(3)	25(2)

C(056)	62(3)	57(2)	54(2)	-14(2)	-24(2)	3(2)
C(117)	174(5)	96(4)	42(3)	-7(2)	1(3)	-59(4)
C(94)	111(4)	140(5)	59(3)	-37(3)	-30(3)	82(3)
C(127)	89(3)	47(2)	61(2)	-11(2)	-16(2)	-8(2)
C(43)	68(3)	83(3)	77(3)	-13(2)	-30(2)	40(3)
C(36)	47(2)	77(3)	62(3)	-4(2)	-9(2)	5(2)
C(22)	43(2)	140(4)	46(2)	-8(3)	-10(2)	-33(3)
C(87)	74(3)	59(3)	83(3)	-24(2)	-25(2)	-2(2)
C(42)	57(3)	159(6)	104(4)	77(4)	-36(3)	-51(4)
C(46)	53(3)	87(3)	77(3)	1(3)	-25(2)	-12(2)
C(116)	150(5)	64(3)	184(6)	-40(4)	-90(5)	26(3)
C(74)	89(3)	94(3)	41(2)	-22(2)	-22(2)	23(3)
C(78)	113(4)	102(4)	74(3)	-37(3)	-31(3)	59(3)
C(102)	122(4)	37(2)	98(4)	3(2)	-10(3)	-29(2)
C(84)	139(5)	85(4)	84(3)	-40(3)	13(3)	-42(3)
C(97)	60(3)	100(3)	55(2)	-28(2)	-21(2)	25(2)
C(106)	83(3)	68(3)	99(4)	-41(3)	-42(3)	13(2)
C(32)	58(3)	191(6)	65(3)	16(4)	-17(2)	-42(4)
C(93)	52(3)	59(3)	137(4)	-16(3)	-10(3)	0(2)
C(88)	71(3)	75(3)	57(2)	-19(2)	-17(2)	-13(2)
C(96)	54(2)	87(3)	57(2)	-16(2)	-7(2)	16(2)
C(82)	55(3)	165(6)	189(6)	-115(5)	-3(4)	-5(3)
C(83)	64(3)	79(3)	89(3)	-39(2)	-29(2)	9(2)
C(123)	131(4)	63(3)	53(2)	-7(2)	-33(3)	-4(3)
C(112)	252(8)	98(4)	83(4)	13(3)	-25(5)	-35(5)
C(56)	75(3)	72(3)	78(3)	-18(2)	-38(3)	-6(2)
C(122)	169(6)	54(3)	129(5)	-6(3)	-31(4)	-14(3)
C(113)	177(5)	37(2)	89(3)	2(2)	-54(3)	13(3)
C(52)	86(4)	98(4)	111(4)	56(3)	-51(3)	-39(3)
C(92)	96(4)	423(13)	82(4)	-118(6)	22(3)	-107(6)
C(126)	175(6)	150(6)	103(5)	-58(4)	8(4)	51(5)

Table S13. Crystal data and structure refinement for 4.

Identification code	holjs18
Empirical formula	C84 H136 Cl2 Fe2 N6
Formula weight	1412.59
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 12.8392(7) A alpha=113.493(1) deg. b = 18.2881(10) A beta = 97.623(1) deg. c = 19.5619(11) A gamma= 92.430(1) deg.
Volume	4152.3(4) A^3
Z, Calculated density	2, 1.130 Mg/m^3
Absorption coefficient	0.458 mm^-1
F(000)	1536
Crystal size	0.14 x 0.25 x 0.44 mm
Theta range for data collection	1.15 to 23.29 deg.
Limiting indices	-14<=h<=13, -16<=k<=20, -21<=l<=21
Reflections collected / unique	19223 / 11947 [R(int) = 0.0517]
Completeness to theta = 23.29	99.6 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11947 / 0 / 831
Goodness-of-fit on F^2	1.018
Final R indices [I>2sigma(I)]	R1 = 0.0757, wR2 = 0.1589
R indices (all data)	R1 = 0.1447, wR2 = 0.1822
Largest diff. peak and hole	0.751 and -0.407 e.A^-3

Table S14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 4.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	3521(1)	933(1)	7307(1)	30(1)
Fe(2)	9974(1)	3935(1)	2972(1)	31(1)
Cl(1)	3097(1)	1422(1)	6445(1)	53(1)
Cl(2)	10041(1)	3111(1)	3572(1)	49(1)
C(12)	2766(5)	2180(4)	8582(3)	33(2)
N(21)	4910(3)	513(3)	7448(3)	26(1)
C(65)	8620(5)	3463(4)	611(3)	39(2)
C(105)	9284(5)	3155(5)	-38(4)	62(2)
C(25)	12015(5)	4932(4)	1804(4)	42(2)
N(11)	3393(3)	1507(3)	8395(3)	29(1)
C(16)	12050(4)	4760(4)	3333(3)	31(2)
C(23)	5217(5)	-468(4)	6206(3)	33(2)
C(102)	4466(5)	3143(4)	9123(4)	42(2)
C(31)	3911(5)	1259(3)	8898(3)	30(2)
C(66)	12127(5)	5551(4)	3904(4)	39(2)
C(13)	5440(4)	298(4)	6800(3)	30(2)
N(12)	11161(3)	4487(3)	2732(3)	27(1)
C(55)	9328(4)	3695(3)	1391(3)	28(1)
C(106)	11316(5)	6131(4)	3929(4)	42(2)
C(111)	6960(5)	611(4)	8997(4)	54(2)
C(22)	1661(5)	2032(4)	8376(4)	39(2)
N(22)	9137(3)	3455(3)	1927(3)	30(1)
C(26)	12778(5)	4227(4)	3384(3)	36(2)
C(61)	6257(5)	39(3)	8245(3)	34(2)
N(14)	2509(4)	-111(3)	7001(3)	42(1)
C(62)	3277(5)	2961(4)	8912(3)	36(2)
C(56)	13005(6)	5806(4)	4472(4)	56(2)
C(85)	11592(6)	5614(5)	1616(5)	70(2)
C(51)	5259(4)	452(3)	8091(3)	28(1)
C(35)	11123(4)	4545(3)	2063(4)	31(2)
C(63)	6100(5)	894(4)	6731(4)	35(2)
C(116)	11714(6)	6834(4)	3759(4)	66(2)
C(42)	1586(6)	3468(4)	8866(4)	56(2)
C(71)	6985(5)	-205(4)	7658(4)	45(2)
C(52)	2657(6)	3596(4)	9050(4)	47(2)
C(72)	1063(5)	1207(4)	8013(4)	41(2)
C(75)	7690(5)	2822(4)	394(4)	47(2)
C(14)	1977(5)	-675(5)	6861(4)	46(2)
C(32)	1082(5)	2696(5)	8525(4)	49(2)
N(18)	9247(4)	4813(3)	3753(3)	43(1)
C(93)	3504(5)	-1329(4)	5569(4)	56(2)
C(91)	4676(5)	1771(4)	10306(3)	47(2)
C(53)	6577(5)	678(4)	6099(4)	48(2)
C(67)	7471(5)	2869(4)	2090(3)	37(2)
C(117)	6163(5)	3856(4)	2004(4)	59(2)
C(73)	4448(5)	-1116(4)	6213(3)	37(2)
C(97)	10560(5)	1544(4)	1725(4)	59(2)
C(103)	6283(5)	1746(4)	7315(4)	44(2)
C(17)	8431(5)	2762(3)	1804(3)	31(2)
C(77)	9835(5)	1846(4)	1230(4)	41(2)
C(37)	8104(5)	1347(4)	1414(4)	45(2)
C(76)	12672(5)	3358(4)	2840(4)	44(2)
C(21)	3663(5)	1464(3)	9713(3)	34(2)
C(41)	4705(5)	749(3)	8711(3)	31(2)

C(15)	13062(5)	5278(4)	2351(4)	47(2)
C(33)	5710(5)	-643(4)	5573(4)	45(2)
C(27)	8770(5)	2000(4)	1489(3)	37(2)
C(18)	8788(5)	5197(4)	4196(4)	41(2)
C(45)	10221(5)	4227(3)	1500(3)	33(2)
C(101)	5847(5)	-731(4)	8319(4)	50(2)
C(82)	253(6)	1090(4)	8480(5)	66(2)
C(107)	7099(5)	3688(4)	2485(4)	42(2)
C(11)	2870(5)	2082(4)	10002(4)	48(2)
C(57)	6845(5)	2192(4)	1995(4)	49(2)
C(43)	6384(6)	-77(5)	5517(4)	55(2)
C(81)	3154(6)	680(4)	9698(4)	54(2)
C(96)	12728(6)	2814(4)	3263(4)	62(2)
C(123)	6025(5)	2334(4)	6953(4)	57(2)
C(28)	8197(5)	5690(4)	4760(4)	57(2)
C(46)	13750(6)	5297(5)	4497(4)	63(2)
C(92)	538(5)	1030(4)	7210(4)	58(2)
C(112)	4838(6)	3761(4)	9930(4)	61(2)
C(95)	12304(5)	4280(5)	1081(4)	71(2)
C(47)	7141(5)	1437(4)	1654(4)	53(2)
C(115)	8151(6)	4224(4)	615(4)	62(2)
C(36)	13636(5)	4516(4)	3956(4)	55(2)
C(127)	6812(5)	3796(4)	3256(4)	60(2)
C(126)	10947(6)	6463(4)	4696(4)	59(2)
C(24)	1279(6)	-1405(4)	6683(4)	70(2)
C(83)	4948(5)	-1885(4)	6139(4)	57(2)
C(122)	4903(6)	3442(5)	8579(4)	67(2)
C(87)	9749(6)	1258(4)	402(4)	65(2)
C(113)	7437(6)	1980(5)	7732(5)	87(3)
C(86)	13534(7)	3173(5)	2334(5)	87(3)
C(8S)	7070(5)	6091(4)	3338(4)	39(2)
C(3S)	9573(5)	8654(4)	5283(4)	41(2)
C(4S)	9750(7)	8708(6)	4643(6)	98(3)
C(5S)	10870(7)	9040(5)	4707(5)	91(3)
C(10S)	8592(8)	6164(6)	2864(6)	126(4)
C(2S)	8510(9)	8344(7)	5249(7)	139(4)
C(1S)	8313(9)	8592(7)	5990(7)	138(4)
C(9S)	7519(9)	6245(7)	2845(7)	132(4)
C(7S)	6081(10)	6306(8)	3346(8)	153(5)
C(6S)	5684(9)	6474(7)	4010(7)	139(4)

Table S15. Bond lengths [A] and angles [deg] for 4.

Fe(1)-N(11)	1.996(5)
Fe(1)-N(21)	2.001(4)
Fe(1)-N(14)	2.090(6)
Fe(1)-Cl(1)	2.2224(18)
Fe(2)-N(12)	2.000(4)
Fe(2)-N(22)	2.002(5)
Fe(2)-N(18)	2.081(6)
Fe(2)-Cl(2)	2.2471(17)
C(12)-C(62)	1.400(8)
C(12)-C(22)	1.407(8)
C(12)-N(11)	1.450(7)
N(21)-C(51)	1.326(7)
N(21)-C(13)	1.443(7)
C(65)-C(75)	1.525(8)
C(65)-C(115)	1.538(8)
C(65)-C(105)	1.553(9)
C(65)-C(55)	1.555(8)
C(25)-C(15)	1.535(8)
C(25)-C(85)	1.536(9)
C(25)-C(95)	1.545(9)
C(25)-C(35)	1.563(8)
N(11)-C(31)	1.351(7)
C(16)-C(26)	1.402(8)
C(16)-C(66)	1.422(8)
C(16)-N(12)	1.436(7)
C(23)-C(33)	1.396(8)
C(23)-C(13)	1.404(8)
C(23)-C(73)	1.517(8)
C(102)-C(62)	1.514(8)
C(102)-C(112)	1.526(9)
C(102)-C(122)	1.532(9)
C(31)-C(41)	1.397(7)
C(31)-C(21)	1.566(8)
C(66)-C(56)	1.391(9)
C(66)-C(106)	1.508(8)
C(13)-C(63)	1.413(8)
N(12)-C(35)	1.348(7)
C(55)-N(22)	1.334(7)
C(55)-C(45)	1.408(8)
C(106)-C(126)	1.526(9)
C(106)-C(116)	1.534(8)
C(111)-C(61)	1.554(8)
C(22)-C(32)	1.401(8)
C(22)-C(72)	1.509(9)
N(22)-C(17)	1.444(7)
C(26)-C(36)	1.377(8)
C(26)-C(76)	1.506(9)
C(61)-C(71)	1.518(8)
C(61)-C(101)	1.548(8)
C(61)-C(51)	1.570(8)
N(14)-C(14)	1.127(8)
C(62)-C(52)	1.394(8)
C(56)-C(46)	1.372(9)
C(51)-C(41)	1.419(8)
C(35)-C(45)	1.410(8)
C(63)-C(53)	1.376(8)
C(63)-C(103)	1.507(9)
C(42)-C(52)	1.360(9)
C(42)-C(32)	1.383(9)
C(72)-C(92)	1.522(9)
C(72)-C(82)	1.533(9)

C(14)-C(24)	1.468(10)
N(18)-C(18)	1.130(8)
C(93)-C(73)	1.541(8)
C(91)-C(21)	1.539(8)
C(53)-C(43)	1.381(9)
C(67)-C(57)	1.380(8)
C(67)-C(17)	1.409(8)
C(67)-C(107)	1.518(8)
C(117)-C(107)	1.544(8)
C(73)-C(83)	1.532(8)
C(97)-C(77)	1.529(8)
C(103)-C(123)	1.531(8)
C(103)-C(113)	1.546(9)
C(17)-C(27)	1.395(8)
C(77)-C(27)	1.521(8)
C(77)-C(87)	1.531(9)
C(37)-C(47)	1.373(9)
C(37)-C(27)	1.386(8)
C(76)-C(96)	1.525(8)
C(76)-C(86)	1.541(9)
C(21)-C(81)	1.537(8)
C(21)-C(11)	1.542(8)
C(33)-C(43)	1.367(9)
C(18)-C(28)	1.447(10)
C(107)-C(127)	1.538(9)
C(57)-C(47)	1.370(9)
C(46)-C(36)	1.386(10)
C(8S)-C(9S)	1.300(11)
C(8S)-C(7S)	1.345(12)
C(3S)-C(4S)	1.342(10)
C(3S)-C(2S)	1.439(12)
C(4S)-C(5S)	1.506(11)
C(10S)-C(9S)	1.390(12)
C(2S)-C(1S)	1.397(14)
C(7S)-C(6S)	1.384(14)

N(11)-Fe(1)-N(21)	98.01(18)
N(11)-Fe(1)-N(14)	101.0(2)
N(21)-Fe(1)-N(14)	99.56(19)
N(11)-Fe(1)-Cl(1)	123.80(14)
N(21)-Fe(1)-Cl(1)	122.81(14)
N(14)-Fe(1)-Cl(1)	107.39(16)
N(12)-Fe(2)-N(22)	96.54(19)
N(12)-Fe(2)-N(18)	107.66(19)
N(22)-Fe(2)-N(18)	113.8(2)
N(12)-Fe(2)-Cl(2)	129.08(14)
N(22)-Fe(2)-Cl(2)	114.46(14)
N(18)-Fe(2)-Cl(2)	95.85(16)
C(62)-C(12)-C(22)	121.5(6)
C(62)-C(12)-N(11)	119.3(5)
C(22)-C(12)-N(11)	119.0(6)
C(51)-N(21)-C(13)	126.3(5)
C(51)-N(21)-Fe(1)	120.3(4)
C(13)-N(21)-Fe(1)	113.4(3)
C(75)-C(65)-C(115)	106.5(5)
C(75)-C(65)-C(105)	105.8(5)
C(115)-C(65)-C(105)	108.8(6)
C(75)-C(65)-C(55)	117.3(5)
C(115)-C(65)-C(55)	107.3(5)
C(105)-C(65)-C(55)	110.7(5)
C(15)-C(25)-C(85)	107.0(5)
C(15)-C(25)-C(95)	105.8(5)
C(85)-C(25)-C(95)	108.9(6)
C(15)-C(25)-C(35)	118.0(5)
C(85)-C(25)-C(35)	108.9(5)

C(95)-C(25)-C(35)	107.9(5)
C(31)-N(11)-C(12)	125.1(5)
C(31)-N(11)-Fe(1)	118.5(4)
C(12)-N(11)-Fe(1)	116.4(3)
C(26)-C(16)-C(66)	120.9(6)
C(26)-C(16)-N(12)	119.8(5)
C(66)-C(16)-N(12)	119.1(5)
C(33)-C(23)-C(13)	119.0(6)
C(33)-C(23)-C(73)	117.9(6)
C(13)-C(23)-C(73)	123.0(5)
C(62)-C(102)-C(112)	113.9(5)
C(62)-C(102)-C(122)	109.9(5)
C(112)-C(102)-C(122)	108.6(6)
N(11)-C(31)-C(41)	121.5(5)
N(11)-C(31)-C(21)	125.0(5)
C(41)-C(31)-C(21)	113.4(5)
C(56)-C(66)-C(16)	117.9(6)
C(56)-C(66)-C(106)	118.1(6)
C(16)-C(66)-C(106)	124.0(6)
C(23)-C(13)-C(63)	120.0(6)
C(23)-C(13)-N(21)	120.6(5)
C(63)-C(13)-N(21)	119.0(5)
C(35)-N(12)-C(16)	125.6(5)
C(35)-N(12)-Fe(2)	122.5(4)
C(16)-N(12)-Fe(2)	111.8(3)
N(22)-C(55)-C(45)	121.3(5)
N(22)-C(55)-C(65)	126.2(5)
C(45)-C(55)-C(65)	112.5(5)
C(66)-C(106)-C(126)	111.0(6)
C(66)-C(106)-C(116)	113.2(5)
C(126)-C(106)-C(116)	108.9(5)
C(32)-C(22)-C(12)	117.6(6)
C(32)-C(22)-C(72)	118.2(6)
C(12)-C(22)-C(72)	124.1(6)
C(55)-N(22)-C(17)	124.9(5)
C(55)-N(22)-Fe(2)	122.4(4)
C(17)-N(22)-Fe(2)	112.1(4)
C(36)-C(26)-C(16)	118.2(6)
C(36)-C(26)-C(76)	118.6(6)
C(16)-C(26)-C(76)	123.1(5)
C(71)-C(61)-C(101)	107.4(5)
C(71)-C(61)-C(111)	105.8(5)
C(101)-C(61)-C(111)	109.6(5)
C(71)-C(61)-C(51)	117.7(5)
C(101)-C(61)-C(51)	106.8(5)
C(111)-C(61)-C(51)	109.5(5)
C(14)-N(14)-Fe(1)	177.4(6)
C(52)-C(62)-C(12)	118.1(6)
C(52)-C(62)-C(102)	119.0(6)
C(12)-C(62)-C(102)	123.0(5)
C(46)-C(56)-C(66)	121.0(7)
N(21)-C(51)-C(41)	120.7(5)
N(21)-C(51)-C(61)	125.9(5)
C(41)-C(51)-C(61)	113.4(5)
N(12)-C(35)-C(45)	120.9(5)
N(12)-C(35)-C(25)	126.9(5)
C(45)-C(35)-C(25)	112.2(5)
C(53)-C(63)-C(13)	117.9(6)
C(53)-C(63)-C(103)	119.7(6)
C(13)-C(63)-C(103)	122.4(5)
C(52)-C(42)-C(32)	120.4(7)
C(42)-C(52)-C(62)	121.5(7)
C(22)-C(72)-C(92)	110.6(6)
C(22)-C(72)-C(82)	112.4(5)
C(92)-C(72)-C(82)	111.0(6)

N(14)-C(14)-C(24)	179.5(9)
C(42)-C(32)-C(22)	120.9(6)
C(18)-N(18)-Fe(2)	169.7(5)
C(63)-C(53)-C(43)	122.6(6)
C(57)-C(67)-C(17)	117.9(6)
C(57)-C(67)-C(107)	119.2(6)
C(17)-C(67)-C(107)	122.9(5)
C(23)-C(73)-C(83)	113.4(5)
C(23)-C(73)-C(93)	110.2(5)
C(83)-C(73)-C(93)	108.6(5)
C(63)-C(103)-C(123)	110.8(6)
C(63)-C(103)-C(113)	112.5(6)
C(123)-C(103)-C(113)	107.8(5)
C(27)-C(17)-C(67)	120.6(5)
C(27)-C(17)-N(22)	119.3(5)
C(67)-C(17)-N(22)	119.6(5)
C(27)-C(77)-C(97)	111.9(5)
C(27)-C(77)-C(87)	113.3(5)
C(97)-C(77)-C(87)	109.1(6)
C(47)-C(37)-C(27)	121.6(6)
C(26)-C(76)-C(96)	110.8(6)
C(26)-C(76)-C(86)	112.3(6)
C(96)-C(76)-C(86)	108.5(6)
C(81)-C(21)-C(91)	110.3(5)
C(81)-C(21)-C(11)	105.2(5)
C(91)-C(21)-C(11)	106.2(5)
C(81)-C(21)-C(31)	106.0(5)
C(91)-C(21)-C(31)	111.3(5)
C(11)-C(21)-C(31)	117.5(5)
C(31)-C(41)-C(51)	134.8(5)
C(43)-C(33)-C(23)	121.0(7)
C(37)-C(27)-C(17)	118.4(6)
C(37)-C(27)-C(77)	117.9(6)
C(17)-C(27)-C(77)	123.6(5)
N(18)-C(18)-C(28)	179.7(9)
C(55)-C(45)-C(35)	133.9(5)
C(67)-C(107)-C(127)	111.1(5)
C(67)-C(107)-C(117)	113.1(6)
C(127)-C(107)-C(117)	110.1(5)
C(47)-C(57)-C(67)	122.2(6)
C(33)-C(43)-C(53)	119.3(6)
C(56)-C(46)-C(36)	120.3(7)
C(57)-C(47)-C(37)	119.2(6)
C(26)-C(36)-C(46)	121.4(7)
C(9S)-C(8S)-C(7S)	111.6(9)
C(4S)-C(3S)-C(2S)	113.8(8)
C(3S)-C(4S)-C(5S)	111.8(8)
C(1S)-C(2S)-C(3S)	107.7(10)
C(8S)-C(9S)-C(10S)	116.8(10)
C(8S)-C(7S)-C(6S)	116.4(11)

Table S16. Anisotropic displacement parameters (A^2 x 10^3) for 4. 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)	32(1)	31(1)	26(1)	12(1)	4(1)	5(1)
Fe(2)	32(1)	32(1)	28(1)	10(1)	5(1)	-6(1)
Cl(1)	55(1)	70(1)	47(1)	36(1)	6(1)	10(1)
Cl(2)	64(1)	44(1)	42(1)	22(1)	5(1)	-5(1)
C(12)	41(4)	41(4)	18(4)	9(3)	14(3)	15(3)
N(21)	28(3)	24(3)	22(3)	7(2)	0(2)	0(2)
C(65)	36(4)	40(4)	31(4)	12(3)	-8(3)	-6(3)
C(105)	51(5)	94(6)	30(5)	15(4)	2(4)	-8(4)
C(25)	44(4)	41(4)	35(4)	11(3)	9(3)	-13(3)
N(11)	29(3)	29(3)	30(3)	15(3)	4(2)	5(2)
C(16)	26(3)	38(4)	24(4)	10(3)	2(3)	-8(3)
C(23)	39(4)	34(4)	25(4)	7(3)	7(3)	12(3)
C(102)	52(4)	26(4)	49(5)	14(3)	12(4)	7(3)
C(31)	33(4)	28(4)	26(4)	9(3)	5(3)	-2(3)
C(66)	33(4)	39(4)	37(4)	8(3)	6(3)	-11(3)
C(13)	26(3)	34(4)	29(4)	13(3)	-1(3)	7(3)
N(12)	24(3)	25(3)	25(3)	3(2)	6(2)	-4(2)
C(55)	28(3)	25(3)	23(4)	2(3)	2(3)	2(3)
C(106)	43(4)	33(4)	38(4)	3(3)	12(3)	-7(3)
C(111)	46(4)	58(5)	44(5)	11(4)	-7(4)	5(4)
C(22)	40(4)	46(4)	37(4)	20(4)	14(3)	19(4)
N(22)	31(3)	22(3)	32(3)	8(2)	4(2)	-4(2)
C(26)	28(4)	46(4)	30(4)	13(3)	1(3)	-3(3)
C(61)	35(4)	30(4)	35(4)	15(3)	1(3)	8(3)
N(14)	36(3)	37(4)	45(4)	9(3)	6(3)	-4(3)
C(62)	44(4)	35(4)	32(4)	14(3)	13(3)	7(3)
C(56)	57(5)	49(5)	37(5)	-3(4)	-1(4)	-23(4)
C(85)	67(5)	71(6)	91(7)	59(5)	-1(5)	-20(4)
C(51)	33(4)	23(3)	25(4)	10(3)	2(3)	-3(3)
C(35)	31(4)	20(3)	36(4)	4(3)	9(3)	-1(3)
C(63)	31(4)	43(4)	35(4)	19(3)	12(3)	6(3)
C(116)	88(6)	43(5)	71(6)	19(4)	34(5)	9(4)
C(42)	66(6)	47(5)	61(5)	25(4)	22(4)	24(4)
C(71)	41(4)	46(4)	51(5)	25(4)	3(4)	16(3)
C(52)	57(5)	36(4)	51(5)	18(4)	15(4)	10(4)
C(72)	37(4)	38(4)	41(4)	7(3)	13(3)	7(3)
C(75)	38(4)	60(5)	33(4)	16(4)	-8(3)	-3(4)
C(14)	41(4)	56(5)	40(5)	18(4)	7(4)	14(4)
C(32)	36(4)	69(6)	46(5)	24(4)	15(4)	17(4)
N(18)	46(4)	34(3)	41(4)	5(3)	15(3)	-3(3)
C(93)	49(5)	50(5)	51(5)	4(4)	8(4)	0(4)
C(91)	67(5)	49(4)	19(4)	7(3)	8(4)	7(4)
C(53)	51(5)	49(5)	55(5)	26(4)	24(4)	9(4)
C(67)	30(4)	37(4)	32(4)	6(3)	2(3)	-12(3)
C(117)	47(5)	63(5)	59(5)	15(4)	9(4)	16(4)
C(73)	42(4)	33(4)	26(4)	1(3)	3(3)	2(3)
C(97)	60(5)	58(5)	50(5)	14(4)	5(4)	7(4)
C(103)	49(4)	41(4)	47(5)	25(4)	11(4)	-3(3)
C(17)	33(4)	26(4)	25(4)	5(3)	-2(3)	-6(3)
C(77)	43(4)	33(4)	40(4)	7(3)	9(3)	-1(3)
C(37)	49(5)	26(4)	42(4)	-4(3)	4(4)	-6(3)
C(76)	33(4)	44(4)	55(5)	22(4)	4(3)	6(3)
C(21)	48(4)	29(4)	22(4)	7(3)	9(3)	2(3)
C(41)	41(4)	31(4)	27(4)	19(3)	1(3)	4(3)
C(15)	41(4)	45(4)	45(5)	8(4)	15(3)	-15(3)

C(33)	51(5)	47(5)	31(4)	9(4)	7(4)	13(4)
C(27)	42(4)	33(4)	30(4)	9(3)	-1(3)	-5(3)
C(18)	44(4)	38(4)	37(5)	14(4)	-1(4)	-5(4)
C(45)	39(4)	34(4)	27(4)	15(3)	1(3)	-4(3)
C(101)	54(5)	49(5)	55(5)	29(4)	12(4)	18(4)
C(82)	55(5)	62(5)	78(6)	23(5)	22(4)	-7(4)
C(107)	32(4)	44(4)	40(4)	9(3)	8(3)	-4(3)
C(11)	68(5)	44(4)	32(4)	12(3)	20(4)	10(4)
C(57)	36(4)	53(5)	55(5)	20(4)	6(4)	-13(4)
C(43)	67(5)	68(6)	42(5)	27(4)	32(4)	29(5)
C(81)	80(5)	45(5)	42(5)	20(4)	23(4)	-2(4)
C(96)	65(5)	44(5)	79(6)	27(4)	8(4)	21(4)
C(123)	56(5)	48(5)	77(6)	30(4)	31(4)	12(4)
C(28)	49(5)	61(5)	47(5)	5(4)	10(4)	6(4)
C(46)	44(5)	74(6)	54(6)	17(5)	-18(4)	-6(4)
C(92)	43(4)	71(5)	49(5)	15(4)	6(4)	6(4)
C(112)	61(5)	55(5)	59(6)	17(4)	2(4)	-10(4)
C(95)	46(5)	90(6)	51(5)	1(5)	22(4)	-21(4)
C(47)	46(5)	37(5)	64(5)	12(4)	3(4)	-21(4)
C(115)	61(5)	58(5)	67(6)	35(4)	-18(4)	-8(4)
C(36)	40(4)	55(5)	57(5)	15(4)	-6(4)	6(4)
C(127)	54(5)	59(5)	50(5)	2(4)	14(4)	-7(4)
C(126)	58(5)	48(5)	53(5)	0(4)	18(4)	-10(4)
C(24)	74(6)	58(5)	70(6)	25(5)	1(5)	-30(4)
C(83)	63(5)	36(4)	67(6)	16(4)	10(4)	4(4)
C(122)	54(5)	84(6)	66(6)	30(5)	24(4)	0(4)
C(87)	62(5)	74(6)	52(5)	14(4)	15(4)	17(4)
C(113)	87(7)	50(5)	105(8)	28(5)	-30(6)	-14(5)
C(86)	113(8)	66(6)	93(7)	25(5)	71(6)	30(5)

Table S17. Crystal data and structure refinement for 5.
*Note: 30s/Frame data to 56.5 deg.

Identification code	holjs46
Empirical formula	C36 H53 F3 Fe N2 O3 S
Formula weight	706.71
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P2(1)/n
Unit cell dimensions	a = 9.7581(12) A alpha = 90 deg. b = 17.336(2) A beta = 95.194(2) deg. c = 21.989(3) A gamma = 90 deg.
Volume, Z	3704.4(8) A^3, 4
Density (calculated)	1.267 Mg/m^3
Absorption coefficient	0.514 mm^-1
F(000)	1504
Crystal size	0.14 x 0.18 x 0.18 mm
Theta range for data collection	1.50 to 28.25 deg.
Limiting indices	-12<=h<=11, -18<=k<=23, -29<=l<=28
Reflections collected	21706
Independent reflections	8649 [R(int) = 0.0488]
Reflections >2Sig(I)	5578
Absorption correction	Empirical; SADABS
Max. and min. transmission	0.928 and 0.839
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8649 / 0 / 415
Goodness-of-fit on F^2	1.143
Final R indices [I>2sigma(I)]	R1 = 0.0984, wR2 = 0.1662
R indices (all data)	R1 = 0.1635, wR2 = 0.1892
Largest diff. peak and hole	0.433 and -0.492 e.A^-3

Table S18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	9159(1)	2485(1)	6303(1)	31(1)
N(11)	7882(3)	2583(2)	5566(1)	23(1)
N(21)	9116(3)	3579(2)	6527(1)	26(1)
C(11)	6205(4)	3306(2)	4794(2)	28(1)
C(21)	7251(4)	3230(2)	5365(2)	24(1)
C(31)	7531(4)	3933(2)	5679(2)	27(1)
C(41)	8384(4)	4118(2)	6202(2)	26(1)
C(51)	8369(4)	5009(2)	6359(2)	35(1)
C(61)	5855(4)	2568(2)	4424(2)	41(1)
C(71)	4833(4)	3601(3)	5002(2)	42(1)
C(81)	6758(5)	3891(3)	4354(2)	44(1)
C(91)	6891(5)	5232(3)	6491(2)	50(1)
C(101)	8738(5)	5467(2)	5789(2)	47(1)
C(111)	9339(5)	5300(2)	6891(2)	42(1)
C(12)	7827(4)	1824(2)	5290(2)	25(1)
C(22)	6932(4)	1263(2)	5501(2)	30(1)
C(32)	7062(5)	511(2)	5296(2)	39(1)
C(42)	8027(5)	319(2)	4899(2)	42(1)
C(52)	8870(4)	876(2)	4692(2)	40(1)
C(62)	8794(4)	1640(2)	4876(2)	29(1)
C(72)	5805(4)	1467(3)	5906(2)	40(1)
C(82)	4388(5)	1263(4)	5633(3)	78(2)
C(92)	5980(6)	1098(5)	6533(3)	102(3)
C(102)	9726(4)	2244(3)	4622(2)	36(1)
C(112)	9516(5)	2284(3)	3919(2)	51(1)
C(122)	11254(5)	2090(3)	4812(2)	57(1)
C(13)	9885(4)	3695(2)	7112(2)	27(1)
C(23)	9184(4)	3702(2)	7643(2)	33(1)
C(33)	9953(5)	3830(3)	8195(2)	46(1)
C(43)	11350(5)	3943(3)	8228(2)	46(1)
C(53)	12033(5)	3873(3)	7714(2)	41(1)
C(63)	11340(4)	3725(2)	7143(2)	31(1)
C(73)	7635(5)	3551(3)	7624(2)	44(1)
C(83)	7381(6)	2722(3)	7809(3)	67(2)
C(93)	6885(5)	4114(3)	8022(2)	58(1)
C(103)	12127(4)	3602(3)	6583(2)	39(1)
C(113)	12247(6)	4318(3)	6201(2)	61(2)
C(123)	13546(5)	3236(4)	6736(3)	73(2)
S(14)	10524(1)	1173(1)	6692(1)	39(1)
O(14)	9168(3)	1453(2)	6830(2)	52(1)
O(24)	11060(3)	1786(2)	6322(1)	51(1)
O(34)	10621(4)	405(2)	6494(2)	73(1)
C(14)	11549(6)	1215(3)	7419(2)	61(2)
F(14)	12836(4)	1065(3)	7352(2)	111(2)
F(24)	11463(4)	1897(2)	7671(2)	101(1)
F(34)	11091(4)	693(2)	7792(2)	94(1)

Table S19. Bond lengths [A] and angles [deg] for 5.

Fe(1)-N(11)	1.959(3)
Fe(1)-N(21)	1.961(3)
Fe(1)-O(14)	2.131(3)
Fe(1)-O(24)	2.213(3)
Fe(1)-S(14)	2.7338(12)
N(11)-C(21)	1.335(5)
N(11)-C(12)	1.448(4)
N(21)-C(41)	1.341(5)
N(21)-C(13)	1.444(5)
C(11)-C(81)	1.534(6)
C(11)-C(61)	1.538(5)
C(11)-C(71)	1.541(6)
C(11)-C(21)	1.551(5)
C(21)-C(31)	1.416(5)
C(31)-C(41)	1.394(5)
C(41)-C(51)	1.584(5)
C(51)-C(111)	1.523(6)
C(51)-C(91)	1.545(6)
C(51)-C(101)	1.552(6)
C(12)-C(62)	1.406(5)
C(12)-C(22)	1.413(5)
C(22)-C(32)	1.389(6)
C(22)-C(72)	1.517(6)
C(32)-C(42)	1.382(6)
C(42)-C(52)	1.374(6)
C(52)-C(62)	1.388(6)
C(62)-C(102)	1.526(6)
C(72)-C(82)	1.499(7)
C(72)-C(92)	1.516(7)
C(102)-C(122)	1.536(6)
C(102)-C(112)	1.543(6)
C(13)-C(23)	1.407(5)
C(13)-C(63)	1.415(5)
C(23)-C(33)	1.384(6)
C(23)-C(73)	1.531(6)
C(33)-C(43)	1.372(6)
C(43)-C(53)	1.369(6)
C(53)-C(63)	1.395(6)
C(63)-C(103)	1.525(6)
C(73)-C(83)	1.521(7)
C(73)-C(93)	1.540(6)
C(103)-C(113)	1.510(6)
C(103)-C(123)	1.532(6)
S(14)-O(34)	1.406(3)
S(14)-O(24)	1.463(3)
S(14)-O(14)	1.467(3)
S(14)-C(14)	1.809(6)
C(14)-F(14)	1.303(6)
C(14)-F(24)	1.312(6)
C(14)-F(34)	1.326(6)
N(11)-Fe(1)-N(21)	95.56(12)
N(11)-Fe(1)-O(14)	119.57(13)
N(21)-Fe(1)-O(14)	132.41(14)
N(11)-Fe(1)-O(24)	122.21(12)
N(21)-Fe(1)-O(24)	124.18(13)
O(14)-Fe(1)-O(24)	64.40(12)
N(11)-Fe(1)-S(14)	125.90(9)
N(21)-Fe(1)-S(14)	138.34(9)
O(14)-Fe(1)-S(14)	32.17(9)
O(24)-Fe(1)-S(14)	32.28(8)

C(21)-N(11)-C(12)	128.7(3)
C(21)-N(11)-Fe(1)	125.9(2)
C(12)-N(11)-Fe(1)	105.3(2)
C(41)-N(21)-C(13)	125.9(3)
C(41)-N(21)-Fe(1)	124.2(3)
C(13)-N(21)-Fe(1)	109.7(2)
C(81)-C(11)-C(61)	106.9(3)
C(81)-C(11)-C(71)	109.4(3)
C(61)-C(11)-C(71)	106.0(3)
C(81)-C(11)-C(21)	108.9(3)
C(61)-C(11)-C(21)	117.2(3)
C(71)-C(11)-C(21)	108.3(3)
N(11)-C(21)-C(31)	120.0(3)
N(11)-C(21)-C(11)	126.1(3)
C(31)-C(21)-C(11)	113.9(3)
C(41)-C(31)-C(21)	132.4(3)
N(21)-C(41)-C(31)	121.9(3)
N(21)-C(41)-C(51)	125.3(3)
C(31)-C(41)-C(51)	112.8(3)
C(111)-C(51)-C(91)	107.3(4)
C(111)-C(51)-C(101)	106.2(4)
C(91)-C(51)-C(101)	108.2(4)
C(111)-C(51)-C(41)	118.2(3)
C(91)-C(51)-C(41)	108.2(3)
C(101)-C(51)-C(41)	108.4(3)
C(62)-C(12)-C(22)	121.8(4)
C(62)-C(12)-N(11)	118.4(3)
C(22)-C(12)-N(11)	119.2(3)
C(32)-C(22)-C(12)	117.5(4)
C(32)-C(22)-C(72)	120.1(4)
C(12)-C(22)-C(72)	122.3(4)
C(42)-C(32)-C(22)	121.3(4)
C(52)-C(42)-C(32)	120.1(4)
C(42)-C(52)-C(62)	121.7(4)
C(52)-C(62)-C(12)	117.5(4)
C(52)-C(62)-C(102)	119.9(4)
C(12)-C(62)-C(102)	122.5(3)
C(82)-C(72)-C(92)	106.8(4)
C(82)-C(72)-C(22)	113.6(4)
C(92)-C(72)-C(22)	114.1(4)
C(62)-C(102)-C(122)	112.2(4)
C(62)-C(102)-C(112)	111.6(4)
C(122)-C(102)-C(112)	108.5(4)
C(23)-C(13)-C(63)	121.3(3)
C(23)-C(13)-N(21)	119.3(3)
C(63)-C(13)-N(21)	119.1(3)
C(33)-C(23)-C(13)	117.6(4)
C(33)-C(23)-C(73)	120.5(4)
C(13)-C(23)-C(73)	121.9(4)
C(43)-C(33)-C(23)	121.8(4)
C(33)-C(43)-C(53)	119.9(4)
C(43)-C(53)-C(63)	121.8(4)
C(53)-C(63)-C(13)	116.9(4)
C(53)-C(63)-C(103)	120.9(4)
C(13)-C(63)-C(103)	122.1(4)
C(83)-C(73)-C(93)	110.4(4)
C(83)-C(73)-C(23)	109.8(4)
C(93)-C(73)-C(23)	113.2(4)
C(113)-C(103)-C(63)	113.8(4)
C(113)-C(103)-C(123)	110.4(4)
C(63)-C(103)-C(123)	113.1(4)
O(34)-S(14)-O(24)	118.6(2)
O(34)-S(14)-O(14)	117.7(2)
O(24)-S(14)-O(14)	104.42(19)
O(34)-S(14)-C(14)	105.3(2)

O(24)-S(14)-C(14)	105.4(2)
O(14)-S(14)-C(14)	103.9(2)
O(34)-S(14)-Fe(1)	137.34(17)
O(24)-S(14)-Fe(1)	53.86(13)
O(14)-S(14)-Fe(1)	50.68(13)
C(14)-S(14)-Fe(1)	117.24(18)
S(14)-O(14)-Fe(1)	97.15(17)
S(14)-O(24)-Fe(1)	93.86(16)
F(14)-C(14)-F(24)	109.1(5)
F(14)-C(14)-F(34)	108.4(5)
F(24)-C(14)-F(34)	108.4(5)
F(14)-C(14)-S(14)	110.7(4)
F(24)-C(14)-S(14)	111.0(4)
F(34)-C(14)-S(14)	109.2(4)

Table S20. Anisotropic displacement parameters (A^2 x 10^3) for 5. 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)	37(1)	24(1)	31(1)	3(1)	-8(1)	6(1)
N(11)	24(2)	22(2)	24(2)	0(1)	0(1)	2(1)
N(21)	28(2)	24(2)	24(2)	1(1)	-3(1)	1(1)
C(11)	29(2)	27(2)	26(2)	2(2)	-3(2)	2(2)
C(21)	18(2)	27(2)	26(2)	0(2)	4(2)	1(2)
C(31)	31(2)	17(2)	30(2)	3(2)	-6(2)	8(2)
C(41)	29(2)	24(2)	27(2)	0(2)	4(2)	1(2)
C(51)	47(3)	21(2)	34(2)	1(2)	-5(2)	0(2)
C(61)	42(3)	38(3)	40(2)	-5(2)	-11(2)	3(2)
C(71)	35(3)	45(3)	43(3)	-4(2)	-7(2)	6(2)
C(81)	53(3)	46(3)	33(2)	8(2)	-4(2)	-3(2)
C(91)	58(3)	38(3)	52(3)	-7(2)	-3(2)	17(2)
C(101)	66(3)	26(2)	48(3)	3(2)	-8(2)	-5(2)
C(111)	58(3)	23(2)	42(3)	-4(2)	-11(2)	-1(2)
C(12)	22(2)	26(2)	26(2)	-1(2)	-4(2)	1(2)
C(22)	27(2)	28(2)	33(2)	5(2)	-3(2)	2(2)
C(32)	36(3)	25(2)	54(3)	2(2)	-4(2)	-4(2)
C(42)	43(3)	22(2)	59(3)	-8(2)	-5(2)	5(2)
C(52)	34(3)	38(3)	47(3)	-14(2)	2(2)	7(2)
C(62)	26(2)	30(2)	31(2)	-1(2)	-3(2)	1(2)
C(72)	42(3)	32(2)	46(3)	-2(2)	13(2)	-9(2)
C(82)	33(3)	135(6)	67(4)	4(4)	6(3)	9(3)
C(92)	49(4)	200(9)	60(4)	36(5)	12(3)	1(4)
C(102)	33(2)	40(2)	37(2)	-8(2)	11(2)	-3(2)
C(112)	50(3)	61(3)	43(3)	3(2)	7(2)	0(2)
C(122)	32(3)	87(4)	51(3)	9(3)	3(2)	-14(3)
C(13)	32(2)	23(2)	26(2)	5(2)	-5(2)	2(2)
C(23)	37(2)	32(2)	31(2)	3(2)	2(2)	4(2)
C(33)	60(3)	54(3)	23(2)	2(2)	3(2)	3(3)
C(43)	49(3)	53(3)	31(2)	2(2)	-13(2)	0(2)
C(53)	32(2)	44(3)	45(3)	6(2)	-7(2)	-1(2)
C(63)	32(2)	25(2)	35(2)	7(2)	-2(2)	-5(2)
C(73)	38(3)	55(3)	40(3)	2(2)	10(2)	-1(2)
C(83)	64(4)	59(4)	85(4)	-9(3)	36(3)	-13(3)
C(93)	52(3)	61(3)	64(4)	-1(3)	20(3)	1(3)
C(103)	35(3)	37(2)	44(3)	0(2)	5(2)	-3(2)
C(113)	78(4)	52(3)	60(3)	12(3)	31(3)	3(3)
C(123)	51(3)	102(5)	69(4)	23(4)	22(3)	26(3)
S(14)	48(1)	30(1)	38(1)	6(1)	1(1)	9(1)
O(14)	45(2)	49(2)	61(2)	17(2)	6(2)	12(2)
O(24)	54(2)	51(2)	49(2)	15(2)	10(2)	8(2)
O(34)	116(3)	29(2)	71(3)	-3(2)	-2(2)	24(2)
C(14)	76(4)	51(3)	52(3)	14(3)	-9(3)	14(3)
F(14)	52(2)	141(4)	132(3)	33(3)	-29(2)	22(2)
F(24)	152(4)	71(2)	69(2)	-9(2)	-46(2)	12(2)
F(34)	137(3)	90(3)	53(2)	36(2)	-1(2)	12(2)

Table S21. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 5.

	x	y	z	U(eq)
H(31A)	7053	4353	5503	32
H(61A)	6679	2359	4281	61
H(61B)	5210	2688	4081	61
H(61C)	5456	2195	4679	61
H(71A)	4993	4066	5235	62
H(71B)	4448	3216	5250	62
H(71C)	4203	3705	4650	62
H(81A)	7612	3707	4223	67
H(81B)	6908	4377	4557	67
H(81C)	6102	3955	4005	67
H(91A)	6861	5771	6588	75
H(91B)	6626	4935	6830	75
H(91C)	6269	5128	6137	75
H(10A)	8735	6009	5877	71
H(10B)	8071	5358	5452	71
H(10C)	9635	5316	5687	71
H(11A)	9222	5847	6936	63
H(11B)	10272	5192	6815	63
H(11C)	9133	5045	7260	63
H(32A)	6488	130	5428	47
H(42A)	8107	-190	4772	50
H(52A)	9507	739	4421	48
H(72A)	5831	2027	5965	48
H(82A)	4229	1495	5236	117
H(82B)	3721	1452	5891	117
H(82C)	4307	713	5596	117
H(92A)	6874	1221	6727	154
H(92B)	5891	548	6493	154
H(92C)	5285	1290	6776	154
H(10D)	9489	2749	4785	43
H(11D)	8567	2391	3794	76
H(11E)	9769	1799	3750	76
H(11F)	10082	2686	3776	76
H(12A)	11404	2074	5249	85
H(12B)	11800	2495	4659	85
H(12C)	11515	1605	4646	85
H(33A)	9510	3840	8552	55
H(43A)	11831	4067	8600	55
H(53A)	12985	3925	7746	49
H(73A)	7246	3616	7200	52
H(83A)	7839	2378	7552	101
H(83B)	6411	2618	7766	101
H(83C)	7733	2646	8227	101
H(93A)	5921	3993	7990	87
H(93B)	7011	4633	7885	87
H(93C)	7256	4067	8440	87
H(10E)	11591	3230	6323	47
H(11G)	11349	4536	6103	92
H(11H)	12644	4187	5831	92
H(11I)	12823	4688	6426	92
H(12D)	13452	2775	6970	109
H(12E)	14132	3594	6969	109
H(12F)	13944	3111	6365	109