10.1071/ CH04290_ AC

Accessory Publication: Aust. J. Chem., 2005, 58(5), 311-314.

Iron(II) Molecular Framework Materials with 4,4′-azopyridine

Gregory J. Halder and Cameron J. Kepert[A]

School of Chemistry, The University of Sydney, NSW 2006, Australia.

[A]Author to whom correspondence should be addressed (e-mail: c.kepert@chem.usyd.edu.au)

Accessory Material

Magnetic Data

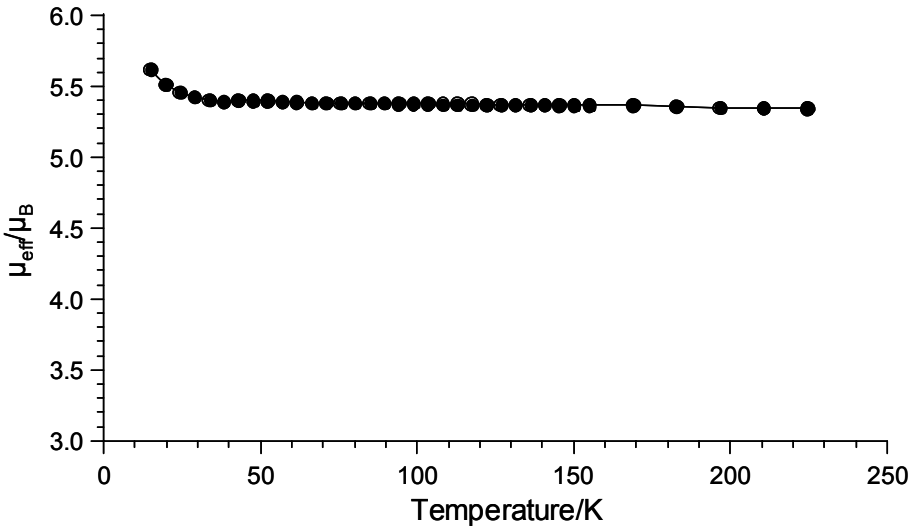

Figure S1. Magnetic susceptibility data for **C**.

The variation of the magnetic moment of **C** with temperature is shown in Figure S1. The magnetic moment remained approximately constant at 5.4 BM on cooling from 225 to 15 K, with a minor increase as the temperature reached a minimum of 15 K. These values are indicative of only high-spin Fe(II) sites (S = 2), with no indication of a spin-transition.

Table A1. Crystal data and structure refinement for $Fe_2(azpy)_4(NCS)_4 \cdot (azpy)$ (A).

Identification code	**A**	
Empirical formula	C54 H40 Fe2 N24 S4	
Formula weight	1265.04 $g.mol^{-1}$	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*m*	
Unit cell dimensions	a = 22.514(5) Å	α= 90°.
	b = 13.402(3) Å	β= 101.613(4)°.
	c = 10.922(2) Å	γ = 90°.
Volume	3228.0(12) $Å^3$	
Z	2	
Density (calculated)	1.301 Mg/m^3	
Absorption coefficient	0.633 mm^{-1}	
F(000)	1296	
Crystal size	0.24 x 0.19 x 0.08 mm^3	
Theta range for data collection	1.78 to 28.10°.	
Index ranges	-29<=h<=29, -17<=k<=17, -14<=l<=14	
Reflections collected	14760	
Independent reflections	4002 [R(int) = 0.0349]	
Completeness to theta = 28.10°	97.3 %	
Absorption correction	Empirical	
Max. and min. transmission	0.951 and 0.856	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4002 / 54 / 231	
Goodness-of-fit on F^2	1.051	
Final R indices [I>2sigma(I)]	R1 = 0.0798, wR2 = 0.2225	
R indices (all data)	R1 = 0.1535, wR2 = 0.3119	
Largest diff. peak and hole	1.189 and -0.987 $e.Å^{-3}$	

Table A2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for A. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5000	5000	5000	18.7(4)
Fe(2)	5000	0	0	18.3(4)
S(21)	6384.8(12)	5000	8970(2)	66.9(11)
S(22)	3628.3(11)	0	-3969(2)	58.5(9)
C(21)	5867(4)	5000	7709(9)	32(2)
C(22)	4166(4)	0	-2740(8)	30(2)
N(21)	5489(3)	5000	6819(6)	25(2)
N(22)	4544(3)	0	-1858(7)	29(2)
N(1)	5903(3)	5000	4382(5)	23(2)
N(2)	7512(3)	5000	3019(8)	39(2)
N(3)	5000	6645(5)	5000	31(2)
N(4)	4815(5)	9758(8)	4606(9)	34(4)
C(1)	5886(3)	5000	3152(7)	31(2)
C(2)	6392(3)	5000	2641(7)	38(2)
C(3)	6948(3)	5000	3423(6)	33(2)
C(4)	6979(3)	5000	4681(7)	45(3)
C(5)	6452(3)	5000	5125(7)	38(2)
C(6)	5484(4)	7156(5)	5511(8)	54(2)
C(7)	5505(5)	8196(6)	5534(10)	77(3)
C(8)	5000	8722(8)	5000	79(5)
N(11)	4100(3)	0	602(6)	22(2)
N(12)	2459(3)	0	1865(7)	34(2)
N(13)	5000	1647(5)	0	31(2)
N(14)	5070(4)	4753(7)	505(8)	28(4)
C(11)	4092(4)	0	1812(8)	33(2)
C(12)	3569(4)	0	2303(9)	34(2)
C(13)	3032(4)	0	1495(8)	29(2)
C(14)	3017(4)	0	225(10)	61(4)
C(15)	3561(4)	0	-167(9)	53(3)
C(16)	4954(4)	2168(5)	1010(8)	52(2)
C(17)	4946(4)	3190(6)	1055(11)	73(3)
C(18)	5000	3715(8)	0	77(5)
N(31)	7188(10)	7554(12)	3896(13)	142(9)

N(32)	7252(6)	7651(18)	102(17)	216(16)
C(31)	7727(8)	7623(14)	3551(15)	128(10)
C(32)	7782(7)	7659(13)	2334(17)	109(8)
C(33)	7274(8)	7625(11)	1415(13)	91(7)
C(34)	6719(7)	7554(12)	1733(15)	95(7)
C(35)	6700(8)	7522(13)	2976(17)	122(9)

Table A3. Bond lengths [Å] and angles [°] for A.

Fe(1)-N(21)#1	2.069(7)
Fe(1)-N(21)	2.069(7)
Fe(1)-N(3)#1	2.204(7)
Fe(1)-N(3)	2.204(7)
Fe(1)-N(1)#1	2.267(6)
Fe(1)-N(1)	2.267(6)
Fe(2)-N(22)	2.081(8)
Fe(2)-N(22)#2	2.081(8)
Fe(2)-N(13)#2	2.207(7)
Fe(2)-N(13)	2.207(7)
Fe(2)-N(11)	2.252(6)
Fe(2)-N(11)#2	2.252(6)
S(21)-C(21)	1.616(10)
S(22)-C(22)	1.616(10)
C(21)-N(21)	1.154(11)
C(22)-N(22)	1.151(11)
N(1)-C(1)	1.336(8)
N(1)-C(5)	1.336(8)
N(2)-N(12)#3	1.242(10)
N(2)-C(3)	1.425(9)
N(3)-C(6)	1.312(8)
N(3)-C(6)#4	1.312(8)
N(4)-N(4)#5	1.25(2)
N(4)-C(8)	1.487(15)
C(1)-C(2)	1.367(7)
C(1)-H(1)	0.9500
C(2)-C(3)	1.365(7)
C(2)-H(2)	0.9500
C(3)-C(4)	1.362(7)
C(4)-C(5)	1.368(7)
C(4)-H(4)	0.9500
C(5)-H(5)	0.9500
C(6)-C(7)	1.396(10)
C(6)-H(6)	0.9500
C(7)-C(8)	1.365(12)
C(7)-H(7)	0.9500

C(8)-C(7)#4	1.365(12)
C(8)-N(4)#4	1.487(15)
N(11)-C(11)	1.326(11)
N(11)-C(15)	1.331(11)
N(12)-N(2)#6	1.242(10)
N(12)-C(13)	1.428(9)
N(13)-C(16)	1.327(8)
N(13)-C(16)#7	1.327(8)
N(14)-N(14)#8	1.272(18)
N(14)-C(18)	1.493(14)
C(11)-C(12)	1.388(11)
C(11)-H(11)	0.9500
C(12)-C(13)	1.345(12)
C(12)-H(12)	0.9500
C(13)-C(14)	1.381(13)
C(14)-C(15)	1.376(12)
C(14)-H(14)	0.9500
C(15)-H(15)	0.9500
C(16)-C(17)	1.371(10)
C(16)-H(16)	0.9500
C(17)-C(18)	1.376(12)
C(17)-H(17)	0.9500
C(18)-C(17)#7	1.376(12)
C(18)-N(14)#7	1.493(14)
N(31)-C(35)	1.331(9)
N(31)-C(31)	1.344(9)
N(32)-N(32)#9	1.249(14)
N(32)-C(33)	1.426(13)
C(31)-C(32)	1.360(8)
C(31)-H(31)	0.9500
C(32)-C(33)	1.361(8)
C(32)-H(32)	0.9500
C(33)-C(34)	1.368(8)
C(34)-C(35)	1.367(8)
C(34)-H(34)	0.9500
C(35)-H(35)	0.9500

N(21)#1-Fe(1)-N(21)	180.000(1)

N(21)#1-Fe(1)-N(3)#1	90.000(1)
N(21)-Fe(1)-N(3)#1	90.000(1)
N(21)#1-Fe(1)-N(3)	90.000(1)
N(21)-Fe(1)-N(3)	90.000(1)
N(3)#1-Fe(1)-N(3)	180.000(1)
N(21)#1-Fe(1)-N(1)#1	87.1(2)
N(21)-Fe(1)-N(1)#1	92.9(2)
N(3)#1-Fe(1)-N(1)#1	90.000(1)
N(3)-Fe(1)-N(1)#1	90.000(1)
N(21)#1-Fe(1)-N(1)	92.9(2)
N(21)-Fe(1)-N(1)	87.1(2)
N(3)#1-Fe(1)-N(1)	90.000(1)
N(3)-Fe(1)-N(1)	90.000(1)
N(1)#1-Fe(1)-N(1)	180.0
N(22)-Fe(2)-N(22)#2	180.0(5)
N(22)-Fe(2)-N(13)#2	90.0
N(22)#2-Fe(2)-N(13)#2	90.0
N(22)-Fe(2)-N(13)	90.0
N(22)#2-Fe(2)-N(13)	90.0
N(13)#2-Fe(2)-N(13)	180.0
N(22)-Fe(2)-N(11)	89.4(3)
N(22)#2-Fe(2)-N(11)	90.6(3)
N(13)#2-Fe(2)-N(11)	90.0
N(13)-Fe(2)-N(11)	90.0
N(22)-Fe(2)-N(11)#2	90.6(3)
N(22)#2-Fe(2)-N(11)#2	89.4(3)
N(13)#2-Fe(2)-N(11)#2	90.0
N(13)-Fe(2)-N(11)#2	90.0
N(11)-Fe(2)-N(11)#2	180.00(9)
N(21)-C(21)-S(21)	178.8(7)
N(22)-C(22)-S(22)	179.4(8)
C(21)-N(21)-Fe(1)	165.3(6)
C(22)-N(22)-Fe(2)	162.3(7)
C(1)-N(1)-C(5)	116.5(7)
C(1)-N(1)-Fe(1)	117.0(5)
C(5)-N(1)-Fe(1)	126.5(5)
N(12)#3-N(2)-C(3)	113.8(7)
C(6)-N(3)-C(6)#4	117.1(9)

C(6)-N(3)-Fe(1)	121.5(5)
C(6)#4-N(3)-Fe(1)	121.5(5)
N(4)#5-N(4)-C(8)	100.2(11)
N(1)-C(1)-C(2)	123.6(7)
N(1)-C(1)-H(1)	118.2
C(2)-C(1)-H(1)	118.2
C(3)-C(2)-C(1)	118.6(7)
C(3)-C(2)-H(2)	120.7
C(1)-C(2)-H(2)	120.7
C(4)-C(3)-C(2)	119.1(7)
C(4)-C(3)-N(2)	116.3(6)
C(2)-C(3)-N(2)	124.6(7)
C(3)-C(4)-C(5)	119.0(7)
C(3)-C(4)-H(4)	120.5
C(5)-C(4)-H(4)	120.5
N(1)-C(5)-C(4)	123.2(7)
N(1)-C(5)-H(5)	118.4
C(4)-C(5)-H(5)	118.4
N(3)-C(6)-C(7)	123.5(9)
N(3)-C(6)-H(6)	118.2
C(7)-C(6)-H(6)	118.2
C(8)-C(7)-C(6)	119.0(10)
C(8)-C(7)-H(7)	120.5
C(6)-C(7)-H(7)	120.5
C(7)#4-C(8)-C(7)	117.9(11)
C(7)#4-C(8)-N(4)#4	139.9(7)
C(7)-C(8)-N(4)#4	101.4(6)
C(7)#4-C(8)-N(4)	101.4(6)
C(7)-C(8)-N(4)	139.9(7)
N(4)#4-C(8)-N(4)	42.1(8)
C(11)-N(11)-C(15)	115.7(7)
C(11)-N(11)-Fe(2)	119.1(6)
C(15)-N(11)-Fe(2)	125.2(6)
N(2)#6-N(12)-C(13)	112.3(7)
C(16)-N(13)-C(16)#7	116.5(8)
C(16)-N(13)-Fe(2)	121.8(4)
C(16)#7-N(13)-Fe(2)	121.8(4)
N(14)#8-N(14)-C(18)	100.1(9)

N(11)-C(11)-C(12)	124.7(8)
N(11)-C(11)-H(11)	117.7
C(12)-C(11)-H(11)	117.7
C(13)-C(12)-C(11)	117.8(8)
C(13)-C(12)-H(12)	121.1
C(11)-C(12)-H(12)	121.1
C(12)-C(13)-C(14)	119.8(8)
C(12)-C(13)-N(12)	123.9(8)
C(14)-C(13)-N(12)	116.3(8)
C(15)-C(14)-C(13)	117.9(9)
C(15)-C(14)-H(14)	121.0
C(13)-C(14)-H(14)	121.0
N(11)-C(15)-C(14)	124.1(9)
N(11)-C(15)-H(15)	117.9
C(14)-C(15)-H(15)	117.9
N(13)-C(16)-C(17)	124.0(9)
N(13)-C(16)-H(16)	118.0
C(17)-C(16)-H(16)	118.0
C(16)-C(17)-C(18)	118.4(9)
C(16)-C(17)-H(17)	120.8
C(18)-C(17)-H(17)	120.8
C(17)#7-C(18)-C(17)	118.5(10)
C(17)#7-C(18)-N(14)	139.9(7)
C(17)-C(18)-N(14)	100.8(5)
C(17)#7-C(18)-N(14)#7	100.8(5)
C(17)-C(18)-N(14)#7	139.9(7)
N(14)-C(18)-N(14)#7	42.6(8)
C(35)-N(31)-C(31)	116.4(10)
N(32)#9-N(32)-C(33)	109(2)
N(31)-C(31)-C(32)	122.8(8)
N(31)-C(31)-H(31)	118.6
C(32)-C(31)-H(31)	118.6
C(31)-C(32)-C(33)	119.4(8)
C(31)-C(32)-H(32)	120.3
C(33)-C(32)-H(32)	120.3
C(32)-C(33)-C(34)	119.4(9)
C(32)-C(33)-N(32)	126.5(15)
C(34)-C(33)-N(32)	114.1(14)

C(35)-C(34)-C(33)	117.8(8)
C(35)-C(34)-H(34)	121.1
C(33)-C(34)-H(34)	121.1
N(31)-C(35)-C(34)	124.2(8)
N(31)-C(35)-H(35)	117.9
C(34)-C(35)-H(35)	117.9

Symmetry transformations used to generate equivalent atoms:

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

#4 -x+1,y,-z+1 #5 -x+1,-y+2,-z+1 #6 x-1/2,y-1/2,z

#7 -x+1,y,-z #8 -x+1,-y+1,-z #9 -x+3/2,-y+3/2,-z

Table A4. Anisotropic displacement parameters ($Å^2 x 10^3$) for A. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	13.3(8)	25.3(9)	19.4(9)	0	8.2(7)	0
Fe(2)	12.5(8)	24.2(9)	20.6(9)	0	9.0(7)	0
S(22)	21.1(13)	152(3)	26.0(15)	0	1.6(11)	0
S(21)	20.9(13)	125(3)	28.3(15)	0	1.4(1)	0
C(21)	24(5)	51(6)	27(5)	0	19(4)	0
C(22)	23(5)	52(6)	20(5)	0	12(4)	0
N(21)	16(3)	43(4)	17(4)	0	6(3)	0
N(22)	17(4)	44(4)	28(4)	0	10(3)	0
N(1)	16(3)	32(4)	23(4)	0	10(3)	0
N(2)	20(4)	72(6)	31(4)	0	18(3)	0
N(3)	38(4)	21(4)	40(5)	0	21(4)	0
N(4)	38(6)	44(13)	21(5)	-1(4)	8(4)	-5(4)
C(1)	14(4)	57(6)	26(5)	0	12(4)	0
C(2)	30(5)	64(6)	23(5)	0	16(4)	0
C(3)	10(4)	62(6)	33(5)	0	14(4)	0
C(4)	17(5)	88(8)	32(6)	0	10(4)	0
C(5)	21(5)	75(7)	22(5)	0	14(4)	0
C(6)	60(5)	36(4)	74(6)	-12(4)	33(4)	-16(4)
C(7)	109(9)	39(5)	104(8)	-26(5)	74(7)	-32(5)
C(8)	127(13)	20(6)	125(13)	0	109(11)	0
N(11)	15(3)	31(4)	24(4)	0	12(3)	0
N(12)	14(4)	58(5)	36(5)	0	17(3)	0
N(13)	30(4)	19(4)	50(5)	0	22(4)	0
N(14)	25(5)	32(10)	26(5)	0(3)	1(4)	-1(4)
C(11)	21(5)	58(6)	22(5)	0	8(4)	0
C(12)	23(4)	54(6)	25(5)	0	10(4)	0
C(13)	16(4)	43(5)	31(5)	0	15(4)	0
C(14)	15(5)	138(12)	35(6)	0	12(4)	0
C(15)	20(5)	118(10)	21(5)	0	7(4)	0
C(16)	51(5)	33(4)	81(6)	-8(4)	34(4)	-3(3)
C(17)	50(5)	45(5)	136(10)	-38(5)	47(6)	-10(4)
C(18)	41(6)	24(6)	184(16)	0	66(9)	0

Table A5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for A.

	x	y	z	U(eq)
H(1)	5501	5000	2603	38
H(2)	6358	5000	1760	45
H(4)	7361	5000	5243	54
H(5)	6479	5000	6004	45
H(6)	5838	6798	5887	65
H(7)	5866	8534	5914	92
H(11)	4470	0	2385	40
H(12)	3589	0	3180	40
H(14)	2642	0	-361	74
H(15)	3550	0	-1041	63
H(16)	4924	1811	1746	63
H(17)	4905	3528	1798	87
H(31)	8084	7648	4183	153
H(32)	8171	7707	2128	131
H(34)	6357	7527	1111	115
H(35)	6314	7475	3198	146

Table B1. Crystal data and structure refinement for $Fe(azpy)(NCSe)_2(EtOH)_2 \cdot (azpy)$ (B).

Identification code	**B**	
Empirical formula	C26 H28 Fe N10 O2 Se2	
Formula weight	726.35 $g.mol^{-1}$	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 7.2556(19) Å	α= 90°.
	b = 17.061(4) Å	β= 96.843(4)°.
	c = 12.298(3) Å	γ = 90°.
Volume	1511.5(7) $Å^3$	
Z	2	
Density (calculated)	1.596 Mg/m^3	
Absorption coefficient	2.949 mm^{-1}	
F(000)	728	
Crystal size	0.48 x 0.19 x 0.07 mm^3	
Theta range for data collection	2.05 to 28.00°.	
Index ranges	-9<=h<=9, -22<=k<=22, -16<=l<=16	
Reflections collected	14731	
Independent reflections	3573 [R(int) = 0.0261]	
Completeness to theta = 28.00°	97.6 %	
Absorption correction	Empirical	
Max. and min. transmission	0.813 and 0.661	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3573 / 0 / 191	
Goodness-of-fit on F^2	1.098	
Final R indices [I>2sigma(I)]	R1 = 0.0344, wR2 = 0.0857	
R indices (all data)	R1 = 0.0426, wR2 = 0.0915	
Largest diff. peak and hole	0.992 and -0.538 $e.Å^{-3}$	

Table B2. Atomic coordinates (x 10^5) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for B. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	50000	50000	50000	213.7(11)
N(11)	33380(30)	40810(12)	55072(16)	291(4)
C(11)	25550(30)	35339(13)	57466(19)	274(5)
Se(11)	13301(4)	26829(2)	61322(3)	478.1(12)
N(1)	31840(30)	50787(11)	33917(15)	247(4)
N(2)	-480(30)	52791(12)	3204(15)	278(4)
C(1)	21910(40)	57170(14)	30874(19)	327(5)
C(2)	11080(40)	57931(14)	20853(19)	333(5)
C(3)	10540(30)	51712(13)	13512(17)	242(4)
C(4)	20590(30)	44958(13)	16608(18)	260(5)
C(5)	30830(30)	44790(13)	26764(18)	270(5)
N(3)	43120(30)	74037(12)	54990(20)	422(6)
N(4)	53650(30)	98239(12)	54135(19)	346(5)
C(6)	36160(40)	78277(16)	46370(30)	471(7)
C(7)	39020(40)	86241(16)	45420(30)	432(6)
C(8)	49750(40)	89976(14)	53910(20)	341(5)
C(9)	53400(50)	77701(17)	62960(30)	483(7)
C(10)	57240(40)	85714(16)	62790(30)	438(6)
O(12)	33920(20)	58785(10)	56511(13)	263(3)
C(12)	17850(50)	57827(17)	62060(30)	504(8)
C(13)	11810(50)	65239(19)	67050(30)	542(8)

Table B3. Bond lengths [Å] and angles [°] for B.

Fe(1)-O(12)#1	2.1148(17)
Fe(1)-O(12)	2.1148(17)
Fe(1)-N(11)	2.117(2)
Fe(1)-N(11)#1	2.117(2)
Fe(1)-N(1)#1	2.2462(19)
Fe(1)-N(1)	2.2462(19)
N(11)-C(11)	1.149(3)
C(11)-Se(11)	1.795(2)
N(1)-C(1)	1.334(3)
N(1)-C(5)	1.346(3)
N(2)-N(2)#2	1.243(4)
N(2)-C(3)	1.428(3)
C(1)-C(2)	1.386(3)
C(1)-H(1)	0.9500
C(2)-C(3)	1.391(3)
C(2)-H(2)	0.9500
C(3)-C(4)	1.392(3)
C(4)-C(5)	1.375(3)
C(4)-H(4)	0.9500
C(5)-H(5)	0.9500
N(3)-C(9)	1.316(4)
N(3)-C(6)	1.332(4)
N(4)-N(4)#3	1.244(5)
N(4)-C(8)	1.437(3)
C(6)-C(7)	1.382(4)
C(6)-H(6)	0.9500
C(7)-C(8)	1.381(4)
C(7)-H(7)	0.9500
C(8)-C(10)	1.369(4)
C(9)-C(10)	1.396(4)
C(9)-H(9)	0.9500
C(10)-H(10)	0.9500
O(12)-C(12)	1.428(3)
O(12)-H(12)	0.76(4)
C(12)-C(13)	1.494(4)
C(12)-H(12A)	0.9900

C(12)-H(12B)	0.9900
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800

O(12)#1-Fe(1)-O(12)	180.00(8)
O(12)#1-Fe(1)-N(11)	86.91(7)
O(12)-Fe(1)-N(11)	93.09(7)
O(12)#1-Fe(1)-N(11)#1	93.09(7)
O(12)-Fe(1)-N(11)#1	86.91(7)
N(11)-Fe(1)-N(11)#1	180.00(7)
O(12)#1-Fe(1)-N(1)#1	89.92(7)
O(12)-Fe(1)-N(1)#1	90.08(7)
N(11)-Fe(1)-N(1)#1	89.50(7)
N(11)#1-Fe(1)-N(1)#1	90.50(7)
O(12)#1-Fe(1)-N(1)	90.08(7)
O(12)-Fe(1)-N(1)	89.92(7)
N(11)-Fe(1)-N(1)	90.50(7)
N(11)#1-Fe(1)-N(1)	89.50(7)
N(1)#1-Fe(1)-N(1)	180.0
C(11)-N(11)-Fe(1)	173.5(2)
N(11)-C(11)-Se(11)	179.5(2)
C(1)-N(1)-C(5)	116.9(2)
C(1)-N(1)-Fe(1)	122.43(15)
C(5)-N(1)-Fe(1)	120.70(15)
N(2)#2-N(2)-C(3)	113.3(2)
N(1)-C(1)-C(2)	123.8(2)
N(1)-C(1)-H(1)	118.1
C(2)-C(1)-H(1)	118.1
C(1)-C(2)-C(3)	118.3(2)
C(1)-C(2)-H(2)	120.8
C(3)-C(2)-H(2)	120.8
C(2)-C(3)-C(4)	118.7(2)
C(2)-C(3)-N(2)	116.6(2)
C(4)-C(3)-N(2)	124.7(2)
C(5)-C(4)-C(3)	118.3(2)
C(5)-C(4)-H(4)	120.9
C(3)-C(4)-H(4)	120.9

N(1)-C(5)-C(4)	124.0(2)
N(1)-C(5)-H(5)	118.0
C(4)-C(5)-H(5)	118.0
C(9)-N(3)-C(6)	117.5(2)
N(4)#3-N(4)-C(8)	113.2(3)
N(3)-C(6)-C(7)	123.7(3)
N(3)-C(6)-H(6)	118.1
C(7)-C(6)-H(6)	118.1
C(8)-C(7)-C(6)	117.8(3)
C(8)-C(7)-H(7)	121.1
C(6)-C(7)-H(7)	121.1
C(10)-C(8)-C(7)	119.5(2)
C(10)-C(8)-N(4)	116.6(2)
C(7)-C(8)-N(4)	124.0(3)
N(3)-C(9)-C(10)	123.4(3)
N(3)-C(9)-H(9)	118.3
C(10)-C(9)-H(9)	118.3
C(8)-C(10)-C(9)	118.1(3)
C(8)-C(10)-H(10)	120.9
C(9)-C(10)-H(10)	120.9
C(12)-O(12)-Fe(1)	128.19(16)
C(12)-O(12)-H(12)	111(2)
Fe(1)-O(12)-H(12)	121(2)
O(12)-C(12)-C(13)	113.3(2)
O(12)-C(12)-H(12A)	108.9
C(13)-C(12)-H(12A)	108.9
O(12)-C(12)-H(12B)	108.9
C(13)-C(12)-H(12B)	108.9
H(12A)-C(12)-H(12B)	107.7
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5

Symmetry transformations used to generate equivalent atoms:

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

Table B4. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for B. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	294(2)	139(2)	204(2)	16(2)	15(2)	-32(2)
N(11)	364(11)	208(9)	299(10)	18(8)	37(8)	-48(8)
C(11)	313(12)	184(10)	328(12)	25(9)	59(9)	-3(9)
Se(11)	473(2)	220(2)	775(2)	102.9(12)	216(2)	-65.6(11)
N(1)	324(10)	196(9)	216(8)	10(7)	18(7)	-36(7)
N(2)	346(10)	250(10)	231(9)	-15(7)	5(8)	9(8)
C(1)	462(14)	231(11)	271(11)	-47(9)	-22(10)	34(10)
C(2)	463(15)	230(11)	285(12)	-28(9)	-35(10)	83(10)
C(3)	288(11)	221(11)	215(10)	6(8)	24(8)	-22(9)
C(4)	332(12)	192(10)	255(11)	-11(8)	31(9)	-7(9)
C(5)	352(12)	185(11)	265(11)	0(8)	2(9)	5(9)
N(3)	411(13)	190(10)	696(16)	-14(10)	199(12)	-26(9)
N(4)	375(11)	194(10)	492(12)	-38(8)	152(10)	-33(8)
C(6)	490(17)	229(13)	690(20)	-56(13)	59(15)	-81(12)
C(7)	497(16)	231(13)	567(17)	-6(12)	56(13)	-65(11)
C(8)	354(13)	191(11)	509(15)	-56(10)	177(11)	-46(9)
C(9)	548(18)	258(14)	643(19)	41(13)	75(15)	-28(12)
C(10)	493(16)	254(13)	566(17)	-17(12)	59(13)	-62(12)
O(12)	337(9)	159(8)	297(8)	10(6)	59(7)	-31(6)
C(12)	519(17)	304(15)	750(20)	-55(14)	332(16)	-78(13)
C(13)	670(20)	434(17)	584(19)	32(14)	352(16)	39(15)

Table B5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2$x 10^3) for B.

	x	y	z	U(eq)
H(1)	223	614	359	39
H(2)	42	626	191	40
H(4)	204	406	118	31
H(5)	376	402	289	32
H(6)	288	757	406	56
H(7)	338	891	391	52
H(9)	585	747	692	58
H(10)	648	881	687	53
H(12)	364(4)	631(2)	560(3)	45(9)
H(12A)	205	539	679	60
H(12B)	75	558	568	60
H(13A)	8	642	707	81
H(13B)	88	692	613	81
H(13C)	219	672	724	81

Table B6. Hydrogen bonds for B [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(12)-H(12)...N(3)	0.76(4)	1.94(4)	2.698(3)	179(4)

Symmetry transformations used to generate equivalent atoms:

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

Table C1. Crystal data and structure refinement for $Fe(azpy)_2(NCSe)_2 \cdot 2(MeCN)$ (C).

Identification code	**C**	
Empirical formula	C26 H22 Fe N12 Se2	
Formula weight	716.33 $g.mol^{-1}$	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*C*2/*m*	
Unit cell dimensions	a = 9.2518(16) Å	α= 90°.
	b = 20.446(4) Å	β= 103.215(3)°.
	c = 8.5790(15) Å	γ = 90°.
Volume	1579.9(5) $Å^3$	
Z	2	
Density (calculated)	1.506 Mg/m^3	
Absorption coefficient	2.818 mm^{-1}	
F(000)	712	
Crystal size	0.27 x 0.19 x 0.08 mm^3	
Theta range for data collection	1.99 to 28.01°.	
Index ranges	-12<=h<=12, -27<=k<=27, -11<=l<=11	
Reflections collected	15813	
Independent reflections	1940 [R(int) = 0.0186]	
Completeness to theta = 28.01°	98.4 %	
Absorption correction	Empirical	
Max. and min. transmission	0.798 and 0.586	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1940 / 0 / 108	
Goodness-of-fit on F^2	1.092	
Final R indices [I>2sigma(I)]	R1 = 0.0344, wR2 = 0.0775	
R indices (all data)	R1 = 0.0435, wR2 = 0.0847	
Largest diff. peak and hole	0.789 and -0.766 $e.Å^{-3}$	

TableC2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^4) for C. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0	5000	5000	148.6(14)
N(11)	1905(3)	5000	4026(3)	225(5)
C(11)	2643(4)	5000	3113(4)	224(6)
Se(11)	3769.6(5)	5000	1673.0(16)	459.1(16)
N(1)	988(2)	4205.7(9)	6679(2)	207(4)
C(2)	665(3)	3243.1(13)	8170(3)	324(6)
C(1)	117(3)	3754.7(12)	7151(3)	299(5)
N(2)	2925(2)	2696.0(10)	9802(3)	310(5)
C(3)	2190(3)	3196.6(11)	8736(3)	246(5)
C(5)	2454(3)	4141.8(11)	7220(3)	255(5)
C(4)	3098(3)	3649.7(12)	8257(3)	287(5)
C(21)	5000	3440(4)	5000	831(19)
C(22)	3763(9)	2988(4)	4862(9)	595(18)
N(21)	2798(10)	2640(4)	4761(10)	810(20)

Table C3. Bond lengths [Å] and angles [°] for C.

Fe(1)-N(11)#1	2.116(3)
Fe(1)-N(11)	2.116(3)
Fe(1)-N(1)#2	2.2238(18)
Fe(1)-N(1)#1	2.2238(18)
Fe(1)-N(1)	2.2238(18)
Fe(1)-N(1)#3	2.2238(18)
N(11)-C(11)	1.151(4)
C(11)-Se(11)	1.789(3)
N(1)-C(5)	1.336(3)
N(1)-C(1)	1.347(3)
C(2)-C(1)	1.383(3)
C(2)-C(3)	1.386(3)
C(2)-H(2)	0.90(3)
C(1)-H(1)	0.94(3)
N(2)-N(2)#4	1.223(4)
N(2)-C(3)	1.436(3)
C(3)-C(4)	1.376(3)
C(5)-C(4)	1.384(3)
C(5)-H(5)	0.93(3)
C(4)-H(4)	0.96(3)
C(21)-C(22)	1.454(9)
C(21)-H(21A)	0.9800
C(21)-H(21B)	0.9800
C(21)-H(21C)	0.9800
C(22)-N(21)	1.129(10)

N(11)#1-Fe(1)-N(11)	180.0
N(11)#1-Fe(1)-N(1)#2	90.04(7)
N(11)-Fe(1)-N(1)#2	89.96(7)
N(11)#1-Fe(1)-N(1)#1	89.96(7)
N(11)-Fe(1)-N(1)#1	90.04(7)
N(1)#2-Fe(1)-N(1)#1	86.18(10)
N(11)#1-Fe(1)-N(1)	90.04(7)
N(11)-Fe(1)-N(1)	89.96(7)
N(1)#2-Fe(1)-N(1)	93.82(10)
N(1)#1-Fe(1)-N(1)	180.00(6)

N(11)#1-Fe(1)-N(1)#3	89.96(7)
N(11)-Fe(1)-N(1)#3	90.04(7)
N(1)#2-Fe(1)-N(1)#3	180.00(6)
N(1)#1-Fe(1)-N(1)#3	93.82(10)
N(1)-Fe(1)-N(1)#3	86.18(10)
C(11)-N(11)-Fe(1)	161.1(3)
N(11)-C(11)-Se(11)	179.3(3)
C(5)-N(1)-C(1)	117.28(19)
C(5)-N(1)-Fe(1)	122.07(15)
C(1)-N(1)-Fe(1)	120.61(15)
C(1)-C(2)-C(3)	118.0(2)
C(1)-C(2)-H(2)	118(2)
C(3)-C(2)-H(2)	124(2)
N(1)-C(1)-C(2)	123.4(2)
N(1)-C(1)-H(1)	116.5(19)
C(2)-C(1)-H(1)	120.1(19)
N(2)#4-N(2)-C(3)	113.8(3)
C(4)-C(3)-C(2)	119.4(2)
C(4)-C(3)-N(2)	116.0(2)
C(2)-C(3)-N(2)	124.6(2)
N(1)-C(5)-C(4)	123.2(2)
N(1)-C(5)-H(5)	116.0(17)
C(4)-C(5)-H(5)	120.8(18)
C(3)-C(4)-C(5)	118.6(2)
C(3)-C(4)-H(4)	120.3(18)
C(5)-C(4)-H(4)	121.0(18)
C(22)-C(21)-H(21A)	109.5
C(22)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(22)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
N(21)-C(22)-C(21)	179.5(10)

Symmetry transformations used to generate equivalent atoms:

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

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

Table C4. Anisotropic displacement parameters ($Å^2 x 10^4$) for C. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	174(3)	109(3)	152(3)	0	14(2)	0
N(11)	234(13)	194(13)	246(13)	0	51(11)	0
C(11)	207(15)	195(14)	253(16)	0	15(12)	0
Se(11)	366(2)	694(3)	374(2)	0	202.3(18)	0
N(1)	223(9)	166(8)	217(9)	29(7)	21(7)	8(7)
C(2)	274(12)	274(12)	420(15)	178(11)	70(11)	2(10)
C(1)	224(12)	273(12)	381(14)	148(10)	31(10)	17(9)
N(2)	274(11)	286(11)	361(12)	141(9)	55(9)	48(8)
C(3)	267(11)	217(11)	241(11)	74(9)	30(9)	52(9)
C(5)	251(11)	206(11)	281(12)	63(9)	3(9)	-24(9)
C(4)	220(11)	286(12)	323(13)	90(10)	-6(10)	21(9)

Table C5. Hydrogen coordinates (x 10^3) and isotropic displacement parameters ($Å^2 x 10^3$) for C.

	x	y	z	U(eq)
H(2)	2(3)	296(2)	843(4)	39
H(1)	-91(3)	379(2)	673(4)	36
H(5)	304(3)	445(2)	685(3)	31
H(4)	416(3)	361.2(14)	860(3)	34
H(21A)	479	375	410	125
H(21B)	591	320	498	125
H(21C)	514	368	601	125