

## Supplementary Information

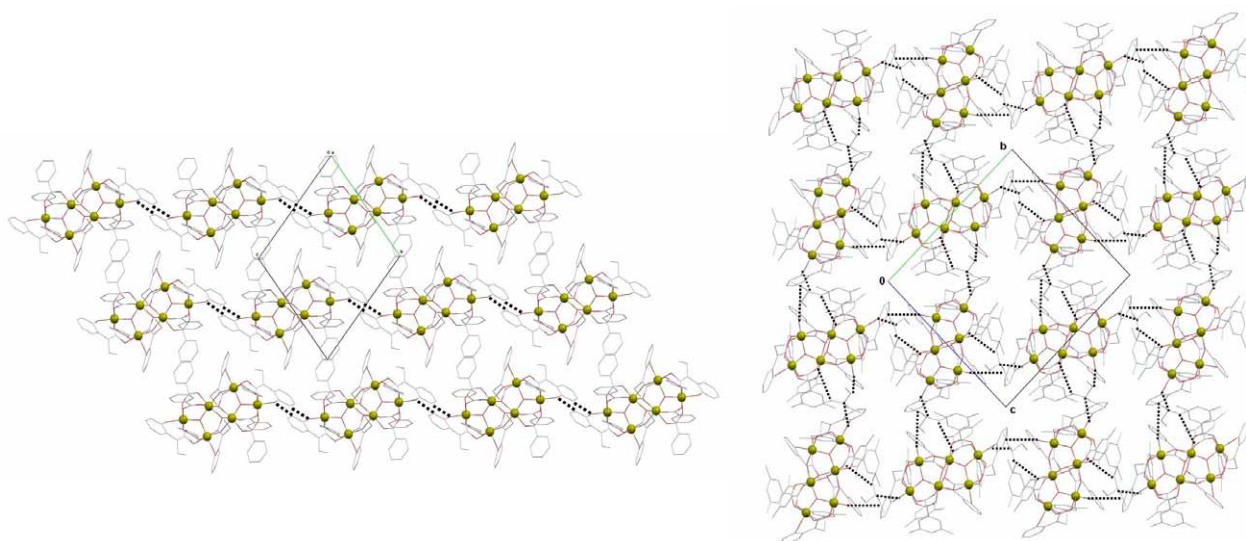


Fig S11. Packing of **4** (left) and **5** (right) as viewed down the a-axis.

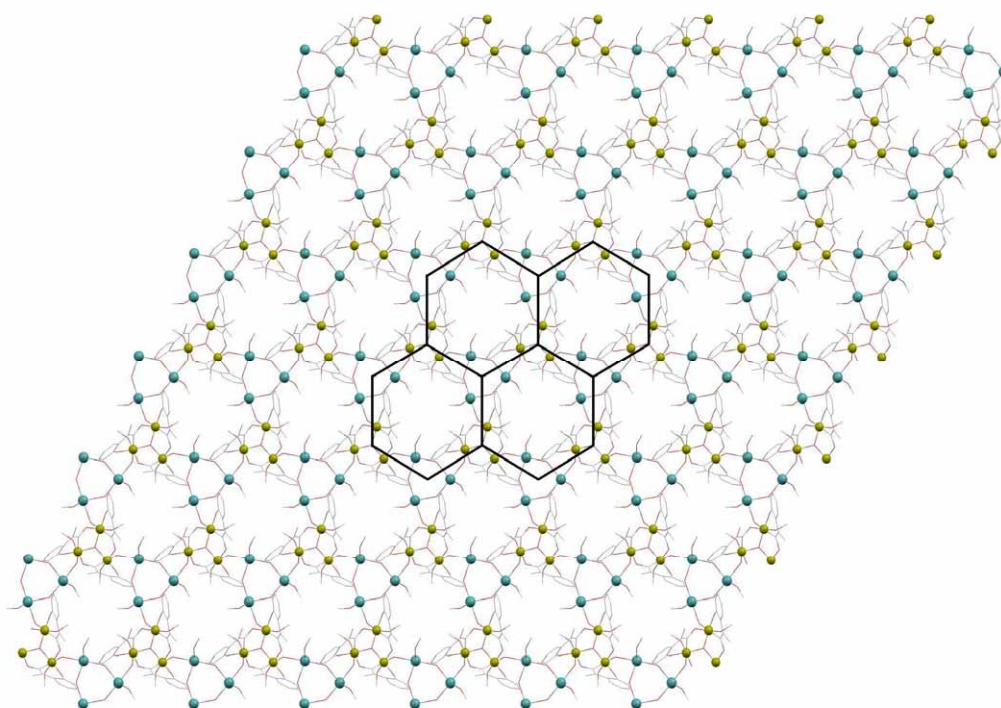


Fig S12. The packing of **8** as viewed through c with the black lines highlighting the (6,3) 2D net.

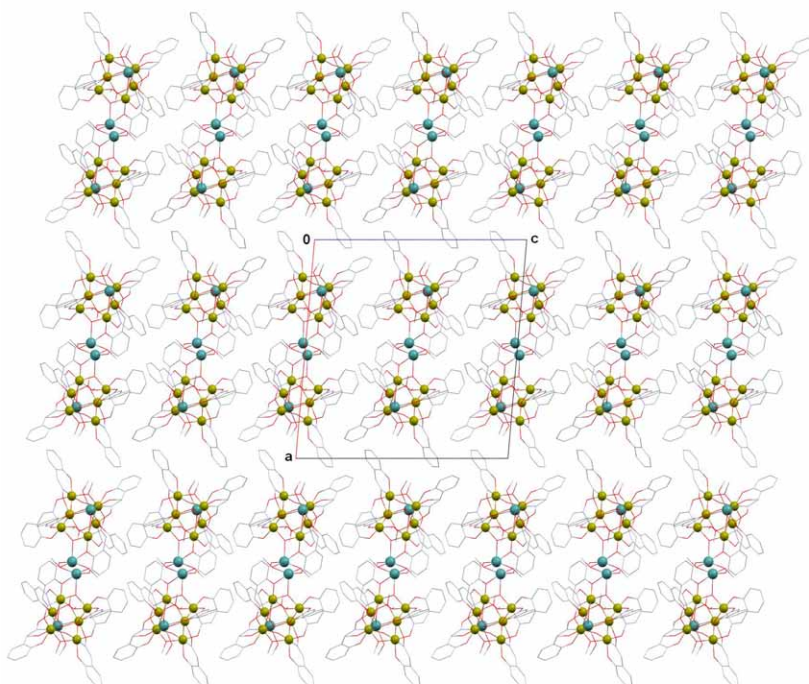


Fig SI3. The packing of **9** as viewed down the b-axis.

### Selected Bond Lengths and Angles

**Table SII.** Selected bond lengths (Å) and bond angles (°) for complex 1·2MeOH

Fe(1)-O(123)	1.863(3)	O(1F)-Fe(2)-N(22B)	150.84(13)
Fe(1)-O(2A)	1.962(3)	O(1B)-Fe(2)-Cl(2)	109.03(10)
Fe(1)-O(2B)	1.969(3)	O(123)-Fe(2)-Cl(2)	111.40(10)
Fe(1)-N(1E)	2.173(3)	O(1F)-Fe(2)-Cl(2)	106.82(10)
Fe(1)-N(1D)	2.199(4)	N(22B)-Fe(2)-Cl(2)	100.62(10)
Fe(1)-N(1C)	2.202(3)	O(1A)-Fe(3)-O(123)	138.65(13)
Fe(2)-O(1B)	1.864(3)	O(1A)-Fe(3)-O(1F)	95.70(13)
Fe(2)-O(123)	1.892(3)	O(123)-Fe(3)-O(1F)	77.90(12)
Fe(2)-O(1F)	1.986(3)	O(1A)-Fe(3)-N(22A)	86.16(12)
Fe(2)-N(22B)	2.133(3)	O(123)-Fe(3)-N(22A)	82.08(12)
Fe(2)-Cl(2)	2.2478(12)	O(1F)-Fe(3)-N(22A)	151.60(13)
Fe(3)-O(1A)	1.870(3)	O(1A)-Fe(3)-Cl(1)	107.28(10)
Fe(3)-O(123)	1.899(3)	O(123)-Fe(3)-Cl(1)	113.53(10)
Fe(3)-O(1F)	1.982(3)	O(1F)-Fe(3)-Cl(1)	108.49(10)
Fe(3)-N(22A)	2.127(3)	N(22A)-Fe(3)-Cl(1)	97.86(9)
Fe(3)-Cl(1)	2.2470(12)	Fe(1)-O(123)-Fe(2)	126.58(15)
O(123)-Fe(1)-O(2A)	87.11(12)	Fe(1)-O(123)-Fe(3)	128.14(15)

O(123)-Fe(1)-O(2B)	88.51(12)	Fe(2)-O(123)-Fe(3)	105.28(14)
O(2A)-Fe(1)-O(2B)	175.61(12)	C(2F)-O(1F)-Fe(3)	134.5(3)
O(123)-Fe(1)-N(1E)	176.64(13)	C(2F)-O(1F)-Fe(2)	126.6(3)
O(2A)-Fe(1)-N(1E)	89.68(12)	Fe(3)-O(1F)-Fe(2)	98.84(13)
O(2B)-Fe(1)-N(1E)	94.70(12)	C(1A)-O(1A)-Fe(3)	131.6(3)
O(123)-Fe(1)-N(1D)	97.40(13)	C(21A)-N(22A)-Fe(3)	128.2(3)
O(2A)-Fe(1)-N(1D)	91.06(12)	O(2A)-N(22A)-Fe(3)	116.7(2)
O(2B)-Fe(1)-N(1D)	89.22(12)	N(22A)-O(2A)-Fe(1)	120.1(2)
N(1E)-Fe(1)-N(1D)	81.66(13)	C(1B)-O(1B)-Fe(2)	132.9(3)
O(123)-Fe(1)-N(1C)	96.11(13)	C(21B)-N(22B)-Fe(2)	127.9(3)
O(2A)-Fe(1)-N(1C)	90.05(12)	O(2B)-N(22B)-Fe(2)	116.6(2)
O(2B)-Fe(1)-N(1C)	90.70(12)	N(22B)-O(2B)-Fe(1)	119.1(2)
N(1E)-Fe(1)-N(1C)	84.88(12)	C(2C)-N(1C)-Fe(1)	120.3(3)
N(1D)-Fe(1)-N(1C)	166.48(13)	C(6C)-N(1C)-Fe(1)	122.6(3)
O(1B)-Fe(2)-O(123)	139.43(13)	C(6D)-N(1D)-Fe(1)	123.2(3)
O(1B)-Fe(2)-O(1F)	93.69(13)	C(2D)-N(1D)-Fe(1)	119.9(3)
O(123)-Fe(2)-O(1F)	77.96(12)	C(2E)-N(1E)-Fe(1)	120.4(3)
O(1B)-Fe(2)-N(22B)	86.43(13)	C(6E)-N(1E)-Fe(1)	120.7(3)
O(123)-Fe(2)-N(22B)	83.09(12)		

**Table S12.** Selected bond lengths (Å) and bond angles (°) for complex **2**·2Et<sub>2</sub>O

Fe(1)-O(1A)	1.872(2)	O(123)-Fe(3)-O(23A)	88.73(9)
Fe(1)-O(123)	1.890(2)	O(23B)-Fe(3)-O(23A)	176.07(9)
Fe(1)-O(1C)	1.974(2)	O(123)-Fe(3)-N(1E)	176.32(9)
Fe(1)-N(22A)	2.135(3)	O(23B)-Fe(3)-N(1E)	88.99(9)
Fe(1)-Br(1)	2.3716(6)	O(23A)-Fe(3)-N(1E)	94.92(9)
Fe(2)-O(1B)	1.873(2)	O(123)-Fe(3)-N(1F)	96.91(9)
Fe(2)-O(123)	1.908(2)	O(23B)-Fe(3)-N(1F)	90.99(9)
Fe(2)-O(1C)	1.974(2)	O(23A)-Fe(3)-N(1F)	89.21(9)
Fe(2)-N(22B)	2.125(2)	N(1E)-Fe(3)-N(1F)	82.65(9)
Fe(2)-Br(2)	2.3739(6)	O(123)-Fe(3)-N(1D)	96.15(9)
Fe(3)-O(123)	1.858(2)	O(23B)-Fe(3)-N(1D)	91.04(9)
Fe(3)-O(23B)	1.9687(19)	O(23A)-Fe(3)-N(1D)	89.65(9)
Fe(3)-O(23A)	1.971(2)	N(1E)-Fe(3)-N(1D)	84.41(9)
Fe(3)-N(1E)	2.169(3)	N(1F)-Fe(3)-N(1D)	166.87(10)
Fe(3)-N(1F)	2.206(3)	Fe(3)-O(123)-Fe(1)	127.58(11)
Fe(3)-N(1D)	2.207(2)	Fe(3)-O(123)-Fe(2)	127.46(11)

O(1A)-Fe(1)-O(123)	137.15(9)	Fe(1)-O(123)-Fe(2)	104.80(10)
O(1A)-Fe(1)-O(1C)	93.50(9)	C(1A)-O(1A)-Fe(1)	128.6(2)
O(123)-Fe(1)-O(1C)	78.16(9)	C(21A)-N(22A)-Fe(1)	126.6(2)
O(1A)-Fe(1)-N(22A)	86.38(10)	O(23A)-N(22A)-Fe(1)	117.37(17)
O(123)-Fe(1)-N(22A)	83.38(9)	N(22A)-O(23A)-Fe(3)	119.08(17)
O(1C)-Fe(1)-N(22A)	152.60(9)	C(1B)-O(1B)-Fe(2)	129.7(2)
O(1A)-Fe(1)-Br(1)	109.59(7)	C(21B)-N(22B)-Fe(2)	127.4(2)
O(123)-Fe(1)-Br(1)	113.10(6)	O(23B)-N(22B)-Fe(2)	116.70(17)
O(1C)-Fe(1)-Br(1)	106.42(7)	N(22B)-O(23B)-Fe(3)	120.11(16)
N(22A)-Fe(1)-Br(1)	99.36(7)	C(2C)-O(1C)-Fe(1)	129.0(2)
O(1B)-Fe(2)-O(123)	136.52(9)	C(2C)-O(1C)-Fe(2)	131.4(2)
O(1B)-Fe(2)-O(1C)	95.98(9)	Fe(1)-O(1C)-Fe(2)	99.29(10)
O(123)-Fe(2)-O(1C)	77.76(9)	C(6D)-N(1D)-Fe(3)	122.7(2)
O(1B)-Fe(2)-N(22B)	86.50(9)	C(2D)-N(1D)-Fe(3)	120.3(2)
O(123)-Fe(2)-N(22B)	82.30(9)	C(2E)-N(1E)-Fe(3)	121.1(2)
O(1C)-Fe(2)-N(22B)	153.42(9)	C(6E)-N(1E)-Fe(3)	121.3(2)
O(1B)-Fe(2)-Br(2)	108.03(7)	C(6F)-N(1F)-Fe(3)	123.2(2)
O(123)-Fe(2)-Br(2)	115.00(6)	C(2F)-N(1F)-Fe(3)	119.4(2)
O(1C)-Fe(2)-Br(2)	106.80(7)		
N(22B)-Fe(2)-Br(2)	97.44(7)		
O(123)-Fe(3)-O(23B)	87.36(9)		

**Table S13.** Selected bond lengths (Å) and bond angles (°) for complex **3**·2Et<sub>2</sub>O

Fe(1)-O(1A)	1.898(5)	Fe(7)-O(2M)	1.933(4)
Fe(1)-O(2B)	1.930(4)	Fe(7)-F(67)	1.969(4)
Fe(1)-F(41)	1.971(4)	Fe(7)-F(78)	1.974(4)
Fe(1)-F(12)	1.977(4)	Fe(7)-N(22L)	2.118(6)
Fe(1)-N(22A)	2.156(5)	Fe(7)-N(1Q)	2.158(6)
Fe(1)-N(1E)	2.165(6)	Fe(8)-O(1M)	1.896(5)
Fe(2)-O(1B)	1.899(5)	Fe(8)-O(2J)	1.922(5)
Fe(2)-O(2C)	1.939(5)	Fe(8)-F(78)	1.967(4)
Fe(2)-F(12)	1.973(4)	Fe(8)-F(85)	1.974(4)
Fe(2)-F(23)	1.981(4)	Fe(8)-N(22M)	2.141(6)
Fe(2)-N(1F)	2.126(4)	Fe(8)-N(1R)	2.174(6)
Fe(2)-N(22B)	2.136(6)	O(1A)-Fe(1)-O(2B)	102.1(2)
Fe(3)-O(1C)	1.909(5)	O(1A)-Fe(1)-F(41)	169.95(19)
Fe(3)-O(2D)	1.937(5)	O(2B)-Fe(1)-F(41)	87.80(18)

Fe(3)-F(23)	1.972(4)	O(1A)-Fe(1)-F(12)	94.52(19)
Fe(3)-F(34)	1.991(4)	O(2B)-Fe(1)-F(12)	87.81(18)
Fe(3)-N(22C)	2.121(6)	F(41)-Fe(1)-F(12)	87.33(17)
Fe(3)-N(1G)	2.150(6)	O(1A)-Fe(1)-N(22A)	86.0(2)
Fe(4)-O(1D)	1.906(5)	O(2B)-Fe(1)-N(22A)	171.3(2)
Fe(4)-O(2A)	1.943(5)	F(41)-Fe(1)-N(22A)	84.13(19)
Fe(4)-F(41)	1.957(4)	F(12)-Fe(1)-N(22A)	88.45(18)
Fe(4)-F(34)	1.969(4)	O(1A)-Fe(1)-N(1E)	89.9(2)
Fe(4)-N(1H)	2.139(6)	O(2B)-Fe(1)-N(1E)	93.3(2)
Fe(4)-N(22D)	2.152(6)	F(41)-Fe(1)-N(1E)	88.0(2)
Fe(5)-O(1J)	1.882(5)	F(12)-Fe(1)-N(1E)	175.1(2)
Fe(5)-O(2K)	1.940(5)	N(22A)-Fe(1)-N(1E)	89.8(2)
Fe(5)-F(85)	1.986(4)	O(1B)-Fe(2)-O(2C)	101.7(2)
Fe(5)-F(56)	1.992(4)	O(1B)-Fe(2)-F(12)	168.74(19)
Fe(5)-N(22J)	2.124(6)	O(2C)-Fe(2)-F(12)	89.50(18)
Fe(5)-N(1N)	2.157(6)	O(1B)-Fe(2)-F(23)	90.7(2)
Fe(6)-O(1K)	1.898(5)	O(2C)-Fe(2)-F(23)	87.81(18)
Fe(6)-F(56)	1.950(4)	F(12)-Fe(2)-F(23)	91.05(17)
Fe(6)-O(2L)	1.956(5)	O(1B)-Fe(2)-N(1F)	89.4(2)
Fe(6)-F(67)	1.995(4)	O(2C)-Fe(2)-N(1F)	98.7(2)
Fe(6)-N(22K)	2.138(6)	F(12)-Fe(2)-N(1F)	87.57(19)
Fe(6)-N(1P)	2.149(6)	F(23)-Fe(2)-N(1F)	173.35(19)
Fe(7)-O(1L)	1.919(5)	O(1B)-Fe(2)-N(22B)	85.8(2)
O(2C)-Fe(2)-N(22B)	171.1(2)	C(1A)-O(1A)-Fe(1)	131.5(5)
F(12)-Fe(2)-N(22B)	83.14(19)	O(1J)-Fe(5)-O(2K)	100.8(2)
F(23)-Fe(2)-N(22B)	87.28(19)	O(1J)-Fe(5)-F(85)	169.92(19)
N(1F)-Fe(2)-N(22B)	86.1(2)	O(2K)-Fe(5)-F(85)	89.24(18)
O(1C)-Fe(3)-O(2D)	98.9(2)	O(1J)-Fe(5)-F(56)	93.7(2)
O(1C)-Fe(3)-F(23)	167.1(2)	O(2K)-Fe(5)-F(56)	87.27(19)
O(2D)-Fe(3)-F(23)	93.56(18)	F(85)-Fe(5)-F(56)	87.85(16)
O(1C)-Fe(3)-F(34)	94.6(2)	O(1J)-Fe(5)-N(22J)	85.8(2)
O(2D)-Fe(3)-F(34)	85.28(19)	O(2K)-Fe(5)-N(22J)	172.9(2)
F(23)-Fe(3)-F(34)	89.56(17)	F(85)-Fe(5)-N(22J)	84.2(2)
O(1C)-Fe(3)-N(22C)	85.4(2)	F(56)-Fe(5)-N(22J)	89.78(19)
O(2D)-Fe(3)-N(22C)	169.9(2)	O(1J)-Fe(5)-N(1N)	90.5(2)
F(23)-Fe(3)-N(22C)	82.75(19)	O(2K)-Fe(5)-N(1N)	96.0(2)
F(34)-Fe(3)-N(22C)	85.32(19)	F(85)-Fe(5)-N(1N)	87.3(2)
O(1C)-Fe(3)-N(1G)	87.6(2)	F(56)-Fe(5)-N(1N)	174.1(2)

O(2D)-Fe(3)-N(1G)	90.5(2)	N(22J)-Fe(5)-N(1N)	86.4(2)
F(23)-Fe(3)-N(1G)	89.1(2)	O(1K)-Fe(6)-F(56)	167.9(2)
F(34)-Fe(3)-N(1G)	175.5(2)	O(1K)-Fe(6)-O(2L)	98.8(2)
N(22C)-Fe(3)-N(1G)	98.7(2)	F(56)-Fe(6)-O(2L)	93.20(19)
O(1D)-Fe(4)-O(2A)	101.9(2)	O(1K)-Fe(6)-F(67)	93.56(19)
O(1D)-Fe(4)-F(41)	90.57(19)	F(56)-Fe(6)-F(67)	88.97(16)
O(2A)-Fe(4)-F(41)	88.28(18)	O(2L)-Fe(6)-F(67)	85.25(18)
O(1D)-Fe(4)-F(34)	166.9(2)	O(1K)-Fe(6)-N(22K)	84.6(2)
O(2A)-Fe(4)-F(34)	91.21(19)	F(56)-Fe(6)-N(22K)	83.6(2)
F(41)-Fe(4)-F(34)	90.11(17)	O(2L)-Fe(6)-N(22K)	173.3(2)
O(1D)-Fe(4)-N(1H)	91.1(2)	F(67)-Fe(6)-N(22K)	88.81(19)
O(2A)-Fe(4)-N(1H)	90.7(2)	O(1K)-Fe(6)-N(1P)	91.2(2)
F(41)-Fe(4)-N(1H)	178.2(2)	F(56)-Fe(6)-N(1P)	87.4(2)
F(34)-Fe(4)-N(1H)	88.5(2)	O(2L)-Fe(6)-N(1P)	89.3(2)
O(1D)-Fe(4)-N(22D)	84.8(2)	F(67)-Fe(6)-N(1P)	173.3(2)
O(2A)-Fe(4)-N(22D)	173.2(2)	N(22K)-Fe(6)-N(1P)	96.4(2)
F(41)-Fe(4)-N(22D)	90.40(19)	O(1L)-Fe(7)-O(2M)	102.52(19)
F(34)-Fe(4)-N(22D)	82.1(2)	O(1L)-Fe(7)-F(67)	167.03(18)
N(1H)-Fe(4)-N(22D)	90.4(2)	O(2M)-Fe(7)-F(67)	90.45(17)
Fe(2)-F(12)-Fe(1)	122.15(18)	O(1L)-Fe(7)-F(78)	90.96(19)
Fe(3)-F(23)-Fe(2)	122.26(19)	O(2M)-Fe(7)-F(78)	86.96(18)
Fe(4)-F(34)-Fe(3)	123.0(2)	F(67)-Fe(7)-F(78)	89.87(17)
Fe(4)-F(41)-Fe(1)	122.36(19)	O(1L)-Fe(7)-N(22L)	84.1(2)
O(2M)-Fe(7)-N(22L)	172.5(2)	O(2J)-Fe(8)-N(22M)	172.9(2)
F(67)-Fe(7)-N(22L)	83.01(19)	F(78)-Fe(8)-N(22M)	83.06(19)
F(78)-Fe(7)-N(22L)	89.4(2)	F(85)-Fe(8)-N(22M)	87.42(18)
O(1L)-Fe(7)-N(1Q)	89.7(2)	O(1M)-Fe(8)-N(1R)	91.3(2)
O(2M)-Fe(7)-N(1Q)	90.5(2)	O(2J)-Fe(8)-N(1R)	90.3(2)
F(67)-Fe(7)-N(1Q)	90.0(2)	F(78)-Fe(8)-N(1R)	87.18(19)
F(78)-Fe(7)-N(1Q)	177.5(2)	F(85)-Fe(8)-N(1R)	175.01(19)
N(22L)-Fe(7)-N(1Q)	93.1(2)	N(22M)-Fe(8)-N(1R)	94.2(2)
O(1M)-Fe(8)-O(2J)	100.5(2)	Fe(6)-F(56)-Fe(5)	123.57(19)
O(1M)-Fe(8)-F(78)	167.6(2)	Fe(7)-F(67)-Fe(6)	122.61(19)
O(2J)-Fe(8)-F(78)	91.77(18)	Fe(8)-F(78)-Fe(7)	123.7(2)
O(1M)-Fe(8)-F(85)	93.53(18)	Fe(8)-F(85)-Fe(5)	121.61(19)
O(2J)-Fe(8)-F(85)	87.60(18)	C(1J)-O(1J)-Fe(5)	130.9(5)
F(78)-Fe(8)-F(85)	88.36(16)		
O(1M)-Fe(8)-N(22M)	84.8(2)		

**Table SI4.** Selected bond lengths (Å) and bond angles (°) for complex **4**.

Fe(1)-O(42)#1	2.116(4)	Fe(2)-O(30)	2.027(4)
Fe(1)-O(32)#1	1.958(4)	Fe(2)-O(45)	1.922(4)
Fe(1)-O(4)	1.867(4)	Fe(2)-N(53)	2.099(5)
Fe(1)-O(12)	2.042(4)	Fe(3)-O(4)	1.942(4)
Fe(1)-O(21)	2.062(4)	Fe(3)-O(31)	2.069(4)
Fe(1)-O(42)	2.062(4)	Fe(3)-O(32)	2.005(4)
Fe(2)-O(4)	1.901(4)	Fe(3)-O(33)	2.008(4)
Fe(2)-O(13)	2.073(4)	Fe(3)-N(41)	2.102(5)
Fe(2)-O(22)	2.037(4)	Fe(3)-O(54)	1.960(4)
O(42)#1-Fe(1)-O(32)#1	85.81(15)	O(4)-Fe(2)-O(13)	92.04(15)
O(42)#1-Fe(1)-O(4)	91.61(15)	O(4)-Fe(2)-O(22)	94.16(16)
O(32)#1-Fe(1)-O(4)	173.51(16)	O(13)-Fe(2)-O(22)	88.12(17)
O(42)#1-Fe(1)-O(12)	172.31(15)	O(4)-Fe(2)-O(30)	90.44(16)
O(32)#1-Fe(1)-O(12)	86.82(16)	O(13)-Fe(2)-O(30)	174.90(17)
O(4)-Fe(1)-O(12)	95.50(16)	O(22)-Fe(2)-O(30)	87.26(17)
O(42)#1-Fe(1)-O(21)	88.69(15)	O(4)-Fe(2)-O(45)	168.91(17)
O(32)#1-Fe(1)-O(21)	89.62(16)	O(13)-Fe(2)-O(45)	86.23(16)
O(4)-Fe(1)-O(21)	96.28(16)	O(22)-Fe(2)-O(45)	96.73(16)
O(42)#1-Fe(1)-O(42)	82.32(16)	O(30)-Fe(2)-O(45)	92.18(16)
O(32)#1-Fe(1)-O(42)	84.12(15)	O(4)-Fe(2)-N(53)	85.52(17)
O(4)-Fe(1)-O(42)	89.64(16)	O(13)-Fe(2)-N(53)	90.30(18)
O(12)-Fe(1)-O(21)	93.44(16)	O(22)-Fe(2)-N(53)	178.37(18)
O(12)-Fe(1)-O(42)	94.77(15)	O(30)-Fe(2)-N(53)	94.34(19)
O(21)-Fe(1)-O(42)	169.38(15)	O(45)-Fe(2)-N(53)	83.54(17)
O(4)-Fe(2)-O(13)	92.04(15)	O(4)-Fe(3)-O(31)	91.72(16)
O(4)-Fe(2)-O(22)	94.16(16)	O(4)-Fe(3)-O(32)	96.55(16)
O(13)-Fe(2)-O(22)	88.12(17)	O(31)-Fe(3)-O(32)	81.77(16)
O(4)-Fe(2)-O(30)	90.44(16)	O(4)-Fe(3)-O(33)	161.79(16)
O(13)-Fe(2)-O(30)	174.90(17)	O(31)-Fe(3)-O(33)	105.51(17)
O(22)-Fe(2)-O(30)	87.26(17)	O(32)-Fe(3)-O(33)	91.81(16)

O(4)-Fe(2)-O(45)	168.91(17)	O(4)-Fe(3)-N(41)	84.51(16)
O(13)-Fe(2)-O(45)	86.23(16)	O(31)-Fe(3)-N(41)	162.28(17)
O(22)-Fe(2)-O(45)	96.73(16)	O(32)-Fe(3)-N(41)	81.47(16)
O(30)-Fe(2)-O(45)	92.18(16)	O(33)-Fe(3)-N(41)	80.76(17)
O(4)-Fe(2)-N(53)	85.52(17)	O(4)-Fe(3)-O(54)	90.72(16)
O(13)-Fe(2)-N(53)	90.30(18)	O(31)-Fe(3)-O(54)	94.75(17)
O(22)-Fe(2)-N(53)	178.37(18)	O(32)-Fe(3)-O(54)	172.01(17)
O(30)-Fe(2)-N(53)	94.34(19)	O(33)-Fe(3)-O(54)	82.16(17)
O(45)-Fe(2)-N(53)	83.54(17)	N(41)-Fe(3)-O(54)	102.59(17)
O(4)-Fe(3)-O(31)	91.72(16)	O(4)-Fe(1)-O(12)	95.50(16)
O(4)-Fe(3)-O(32)	96.55(16)	O(42)#1-Fe(1)-O(21)	88.69(15)
O(31)-Fe(3)-O(32)	81.77(16)	O(32)#1-Fe(1)-O(21)	89.62(16)
O(4)-Fe(3)-O(33)	161.79(16)	O(4)-Fe(1)-O(21)	96.28(16)
O(31)-Fe(3)-O(33)	105.51(17)	O(42)#1-Fe(1)-O(42)	82.32(16)
O(32)-Fe(3)-O(33)	91.81(16)	O(32)#1-Fe(1)-O(42)	84.12(15)
O(4)-Fe(3)-N(41)	84.51(16)	O(4)-Fe(1)-O(42)	89.64(16)
O(31)-Fe(3)-N(41)	162.28(17)	O(12)-Fe(1)-O(21)	93.44(16)
O(32)-Fe(3)-N(41)	81.47(16)	O(12)-Fe(1)-O(42)	94.77(15)
O(33)-Fe(3)-N(41)	80.76(17)	O(21)-Fe(1)-O(42)	169.38(15)
O(4)-Fe(3)-O(54)	90.72(16)	O(4)-Fe(2)-O(13)	92.04(15)
O(31)-Fe(3)-O(54)	94.75(17)	O(4)-Fe(2)-O(22)	94.16(16)
O(32)-Fe(3)-O(54)	172.01(17)	O(13)-Fe(2)-O(22)	88.12(17)
O(33)-Fe(3)-O(54)	82.16(17)	O(4)-Fe(2)-O(30)	90.44(16)
N(41)-Fe(3)-O(54)	102.59(17)	O(13)-Fe(2)-O(30)	174.90(17)
Fe(3)-O(4)-Fe(2)	115.53(18)	O(22)-Fe(2)-O(30)	87.26(17)
Fe(3)-O(4)-Fe(1)	121.11(19)	O(4)-Fe(2)-O(45)	168.91(17)
Fe(2)-O(4)-Fe(1)	121.3(2)	O(13)-Fe(2)-O(45)	86.23(16)
O(42)#1-Fe(1)-O(32)#1	85.81(15)	O(22)-Fe(2)-O(45)	96.73(16)
O(4)-Fe(3)-O(54)	90.72(16)	O(30)-Fe(2)-O(45)	92.18(16)
O(31)-Fe(3)-O(54)	94.75(17)	O(4)-Fe(2)-N(53)	85.52(17)
O(32)-Fe(3)-O(54)	172.01(17)	O(13)-Fe(2)-N(53)	90.30(18)
O(33)-Fe(3)-O(54)	82.16(17)	O(22)-Fe(2)-N(53)	178.37(18)
N(41)-Fe(3)-O(54)	102.59(17)	O(30)-Fe(2)-N(53)	94.34(19)
Fe(3)-O(4)-Fe(2)	115.53(18)	O(45)-Fe(2)-N(53)	83.54(17)
Fe(3)-O(4)-Fe(1)	121.11(19)	Fe(1)-Fe(3)-O(4)	28.81(11)



Fe(2)-O(4)-Fe(1)	121.3(2)	Fe(1)-Fe(3)-O(31)	110.90(12)
O(42)#1-Fe(1)-O(32)#1	85.81(15)	O(4)-Fe(3)-O(31)	91.72(16)
O(4)-Fe(3)-O(54)	90.72(16)	Fe(1)-Fe(3)-O(32)	78.55(11)
O(31)-Fe(3)-O(54)	94.75(17)	O(4)-Fe(3)-O(32)	96.55(16)
O(32)-Fe(3)-O(54)	172.01(17)	O(31)-Fe(3)-O(32)	81.77(16)
O(33)-Fe(3)-O(54)	82.16(17)	Fe(1)-Fe(3)-O(33)	140.32(12)
N(41)-Fe(3)-O(54)	102.59(17)	O(4)-Fe(3)-O(33)	161.79(16)
Fe(3)-O(4)-Fe(2)	115.53(18)	O(31)-Fe(3)-O(33)	105.51(17)
Fe(3)-O(4)-Fe(1)	121.11(19)	O(32)-Fe(3)-O(33)	91.81(16)
Fe(2)-O(4)-Fe(1)	121.3(2)	Fe(1)-Fe(3)-N(41)	59.86(12)
O(42)#1-Fe(1)-O(4)	91.61(15)	O(4)-Fe(3)-N(41)	84.51(16)
O(32)#1-Fe(1)-O(4)	173.51(16)	O(31)-Fe(3)-N(41)	162.28(17)
O(42)#1-Fe(1)-O(12)	172.31(15)	O(32)-Fe(3)-N(41)	81.47(16)
O(32)#1-Fe(1)-O(12)	86.82(16)	O(33)-Fe(3)-N(41)	80.76(17)
O(4)-Fe(1)-O(12)	95.50(16)	Fe(1)-Fe(3)-O(54)	109.44(13)
O(42)#1-Fe(1)-O(21)	88.69(15)	O(4)-Fe(3)-O(54)	90.72(16)
O(32)#1-Fe(1)-O(21)	89.62(16)	O(31)-Fe(3)-O(54)	94.75(17)
O(4)-Fe(1)-O(21)	96.28(16)	O(32)-Fe(3)-O(54)	172.01(17)
O(42)#1-Fe(1)-O(42)	82.32(16)	O(33)-Fe(3)-O(54)	82.16(17)
O(32)#1-Fe(1)-O(42)	84.12(15)	N(41)-Fe(3)-O(54)	102.59(17)
O(4)-Fe(1)-O(42)	89.64(16)	Fe(3)-O(4)-Fe(2)	115.53(18)
O(12)-Fe(1)-O(21)	93.44(16)	Fe(3)-O(4)-Fe(1)	121.11(19)
O(12)-Fe(1)-O(42)	94.77(15)	Fe(2)-O(4)-Fe(1)	121.3(2)
O(21)-Fe(1)-O(42)	169.38(15)		

**Table SI5.** Selected bond lengths (Å) and bond angles (°) for complex **5**·2MeCN.

Fe(1)-O(56)#1	2.103(3)	Fe(3)-O(22)	1.974(4)
Fe(1)-O(42)#1	2.051(3)	Fe(3)-O(31)	2.056(4)
Fe(1)-O(8)#1	2.048(4)	Fe(3)-O(51)	1.947(3)
Fe(1)-Fe(1)#1	3.1352(14)	Fe(3)-N(55)	2.087(4)
Fe(1)-O(4)#1	1.867(3)	O(4)-Fe(5)	1.898(3)
Fe(1)-Fe(5)#1	3.2587(10)	Fe(5)-O(6)	2.043(4)
Fe(1)-O(2)	1.996(3)	Fe(5)-O(17)	1.956(4)
Fe(1)-O(56)	2.096(4)	Fe(5)-N(21)	2.094(4)
O(2)-Fe(3)	2.030(3)	Fe(5)-O(29)	2.045(4)
Fe(3)-O(4)	1.976(3)	Fe(5)-O(40)	2.018(4)
Fe(3)-Fe(5)	3.2648(10)	O(2)-Fe(3)-O(51)	93.30(15)
O(56)#1-Fe(1)-(42)#1	170.73(14)	O(4)-Fe(3)-O(51)	165.04(15)
O(56)#1-Fe(1)-O(8)#1	92.72(14)	O(22)-Fe(3)-O(51)	84.04(15)
O(42)#1-Fe(1)-O(8)#1	95.19(14)	O(31)-Fe(3)-O(51)	103.24(15)
O(56)#1-Fe(1)-Fe(1)#1	41.60(9)	O(2)-Fe(3)-N(55)	80.46(15)
O(42)#1-Fe(1)-Fe(1)#1	129.78(11)	O(4)-Fe(3)-N(55)	84.21(15)
O(56)#1-Fe(1)-O(4)#1	88.40(14)	O(22)-Fe(3)-N(55)	98.58(16)
O(42)#1-Fe(1)-O(4)#1	95.75(14)	O(31)-Fe(3)-N(55)	164.76(16)
O(8)#1-Fe(1)-O(4)#1	94.69(15)	O(51)-Fe(3)-N(55)	83.61(16)
O(56)#1-Fe(1)-O(2)	83.04(13)	Fe(3)-O(4)-Fe(1)#1	122.47(18)
O(42)#1-Fe(1)-O(2)	92.68(14)	Fe(3)-O(4)-Fe(5)	114.83(17)
O(8)#1-Fe(1)-O(2)	86.06(14)	Fe(1)#1-O(4)-Fe(5)	119.87(18)
Fe(1)#1-Fe(1)-O(2)	82.33(10)	O(4)-Fe(5)-O(6)	94.93(15)
O(4)#1-Fe(1)-O(2)	171.43(15)	O(4)-Fe(5)-O(17)	170.47(15)
O(56)#1-Fe(1)-O(56)	83.39(14)	O(6)-Fe(5)-O(17)	88.18(15)
O(42)#1-Fe(1)-O(56)	88.09(14)	O(4)-Fe(5)-N(21)	87.85(15)
O(8)#1-Fe(1)-O(56)	171.10(14)	O(6)-Fe(5)-N(21)	89.40(16)
O(4)#1-Fe(1)-O(56)	93.21(14)	O(17)-Fe(5)-N(21)	83.16(16)
O(2)-Fe(1)-O(56)	85.53(13)	O(4)-Fe(5)-O(29)	90.14(15)

Fe(1)-O(2)-Fe(3)	121.92(17)	O(6)-Fe(5)-O(29)	173.14(15)
Fe(1)-O(2)-H(21)	113.2	O(17)-Fe(5)-O(29)	87.55(15)
Fe(3)-O(2)-H(21)	110.1	O(4)-Fe(5)-O(40)	95.81(15)
O(2)-Fe(3)-O(4)	93.22(14)	O(6)-Fe(5)-O(40)	88.67(15)
O(2)-Fe(3)-O(22)	177.27(15)	O(17)-Fe(5)-O(40)	93.27(15)
O(4)-Fe(3)-O(22)	89.23(15)	N(21)-Fe(5)-O(29)	95.41(16)
O(2)-Fe(3)-O(31)	85.51(15)	N(21)-Fe(5)-O(40)	176.00(16)
O(4)-Fe(3)-O(31)	90.69(15)	O(29)-Fe(5)-O(40)	86.22(15)
O(22)-Fe(3)-O(31)	95.69(16)		

**Table SI6.** Selected bond lengths (Å) and bond angles (°) for complex **6**·2MeCN.

Fe(1)-O(3)	1.927(5)	Fe(2)#1-O(1)-Fe(2)	105.1(2)
Fe(1)-O(50)	1.948(5)	O(27)-Fe(1)-O(20)	88.6(3)
Fe(1)-O(12)	1.997(7)	O(3)-Fe(1)-N(1)	84.5(2)
Fe(1)-O(27)	2.016(6)	O(50)-Fe(1)-N(1)	84.6(2)
Fe(1)-O(20)	2.048(6)	O(12)-Fe(1)-N(1)	91.2(3)
Fe(1)-N(1)	2.145(7)	O(27)-Fe(1)-N(1)	177.4(2)
Fe(2)-O(50)	1.860(6)	O(20)-Fe(1)-N(1)	89.5(3)
Fe(2)-O(13)	1.979(8)	O(50)-Fe(2)-O(13)	96.8(3)
Fe(2)-O(40)	2.019(7)	O(50)-Fe(2)-O(40)	96.8(3)
Fe(2)-O(33)	2.037(5)	O(13)-Fe(2)-O(40)	164.0(3)
Fe(2)-O(1)#1	2.067(6)	O(50)-Fe(2)-O(33)	95.9(2)
Fe(2)-O(1)	2.073(4)	O(13)-Fe(2)-O(33)	84.5(3)
Fe(3)-O(50)	1.872(5)	O(40)-Fe(2)-O(33)	86.0(3)
Fe(3)-O(34)	2.025(6)	O(50)-Fe(2)-O(1)#1	162.16(19)
Fe(3)-O(19)	2.029(5)	O(13)-Fe(2)-O(1)#1	84.5(3)
Fe(3)-O(26)	2.039(6)	O(40)-Fe(2)-O(1)#1	85.0(3)
Fe(3)-O(41)	2.045(7)	O(33)-Fe(2)-O(1)#1	101.9(2)
Fe(3)-O(60)	2.091(6)	O(50)-Fe(2)-O(1)	87.3(2)
O(1)-Fe(2)#1	2.067(6)	O(13)-Fe(2)-O(1)	94.2(2)
O(3)-Fe(1)-O(50)	169.1(2)	O(40)-Fe(2)-O(1)	94.6(2)
O(3)-Fe(1)-O(12)	88.4(3)	O(33)-Fe(2)-O(1)	176.6(2)
O(50)-Fe(1)-O(12)	91.9(2)	O(1)#1-Fe(2)-O(1)	74.9(2)
O(3)-Fe(1)-O(27)	93.7(2)	O(50)-Fe(3)-O(34)	95.3(2)
O(50)-Fe(1)-O(27)	97.2(2)	O(50)-Fe(3)-O(19)	96.5(2)

O(12)-Fe(1)-O(27)	90.6(3)	O(34)-Fe(3)-O(19)	168.1(2)
O(3)-Fe(1)-O(20)	88.3(2)	O(50)-Fe(3)-O(26)	96.5(3)
O(50)-Fe(1)-O(20)	91.6(2)	O(34)-Fe(3)-O(26)	90.4(3)
O(12)-Fe(1)-O(20)	176.5(2)	O(19)-Fe(3)-O(26)	87.6(2)
O(50)-Fe(3)-O(41)	94.5(3)	Fe(2)-O(50)-Fe(3)	122.0(3)
O(34)-Fe(3)-O(41)	90.8(3)	Fe(2)-O(50)-Fe(1)	117.6(3)
O(19)-Fe(3)-O(41)	89.0(3)	Fe(3)-O(50)-Fe(1)	120.4(3)
O(26)-Fe(3)-O(41)	168.7(3)		
O(50)-Fe(3)-O(60)	178.5(3)		
O(34)-Fe(3)-O(60)	83.8(2)		
O(19)-Fe(3)-O(60)	84.4(2)		
O(26)-Fe(3)-O(60)	84.7(3)		
O(41)-Fe(3)-O(60)	84.3(3)		
N(1)-O(1)-Fe(2)#1	129.6(4)		
N(1)-O(1)-Fe(2)	114.8(4)		

**Table S17.** Selected bond lengths (Å) and bond angles (°) for complex **7·5MeCN**.

Fe(1)-O(11)#1	2.070(4)	O(11)#1-Fe(1)-O(11)	73.64(15)
Fe(1)-Fe(3)	3.2509(11)	Fe(3)-Fe(1)-O(11)	112.04(10)
Fe(1)-O(1)	1.871(4)	O(1)-Fe(1)-O(11)	89.39(15)
Fe(1)-O(11)	2.043(4)	O(11)#1-Fe(1)-O(121)	85.15(16)
Fe(1)-O(121)	2.030(4)	Fe(3)-Fe(1)-O(121)	111.19(11)
Fe(1)-O(151)	2.016(4)	O(1)-Fe(1)-O(121)	94.96(16)
Fe(1)-O(161)	2.058(4)	O(11)-Fe(1)-O(121)	92.72(16)
Fe(2)-Fe(3)	3.3336(11)	O(11)#1-Fe(1)-O(151)	85.18(15)
Fe(2)-O(1)	1.961(4)	Fe(3)-Fe(1)-O(151)	77.26(11)
Fe(2)-O(71)	1.892(4)	O(1)-Fe(1)-O(151)	97.28(16)
Fe(2)-O(122)	2.034(4)	O(11)-Fe(1)-O(151)	94.37(16)
Fe(2)-O(132)	2.013(4)	O(121)-Fe(1)-O(151)	165.91(16)
Fe(2)-O(142)	2.059(4)	O(11)#1-Fe(1)-O(161)	101.64(15)
Fe(2)-N(11)	2.120(5)	Fe(3)-Fe(1)-O(161)	73.43(12)
Fe(3)-O(1)	1.863(4)	O(1)-Fe(1)-O(161)	95.25(16)
Fe(3)-O(17)	2.088(4)	O(11)-Fe(1)-O(161)	174.33(16)
Fe(3)-O(133)	2.032(4)	O(121)-Fe(1)-O(161)	83.65(16)
Fe(3)-O(143)	1.990(4)	O(151)-Fe(1)-O(161)	88.29(17)
Fe(3)-O(153)	2.014(4)	Fe(3)-Fe(2)-O(1)	28.52(11)

Fe(3)-O(163)	2.026(4)	Fe(3)-Fe(2)-O(71)	152.68(12)
O(11)#1-Fe(1)-Fe(3)	161.81(11)	O(1)-Fe(2)-O(71)	168.05(16)
O(11)#1-Fe(1)-O(1)	163.01(15)	Fe(3)-Fe(2)-O(122)	110.15(11)
Fe(3)-Fe(1)-O(1)	29.41(11)	O(1)-Fe(2)-O(122)	92.65(15)
O(142)-Fe(2)-N(11)	94.35(18)	O(71)-Fe(2)-O(122)	93.94(16)
Fe(1)-Fe(3)-Fe(2)	59.73(2)	Fe(3)-Fe(2)-O(132)	74.22(12)
Fe(1)-Fe(3)-O(1)	29.56(11)	O(1)-Fe(2)-O(132)	94.83(16)
Fe(2)-Fe(3)-O(1)	30.18(11)	O(71)-Fe(2)-O(132)	95.57(17)
Fe(1)-Fe(3)-O(17)	149.48(12)	O(122)-Fe(2)-O(132)	85.97(18)
Fe(2)-Fe(3)-O(17)	150.79(12)	Fe(3)-Fe(2)-O(142)	70.78(11)
O(1)-Fe(3)-O(17)	179.01(16)	O(1)-Fe(2)-O(142)	89.24(16)
Fe(1)-Fe(3)-O(133)	116.52(14)	O(71)-Fe(2)-O(142)	84.56(16)
Fe(2)-Fe(3)-O(133)	73.55(12)	O(122)-Fe(2)-O(142)	177.16(18)
O(1)-Fe(3)-O(133)	95.55(17)	O(132)-Fe(2)-O(142)	91.76(19)
O(17)-Fe(3)-O(133)	85.30(17)	Fe(3)-Fe(2)-N(11)	107.61(12)
Fe(1)-Fe(3)-O(143)	115.24(14)	O(1)-Fe(2)-N(11)	85.02(16)
Fe(2)-Fe(3)-O(143)	76.98(13)	O(71)-Fe(2)-N(11)	85.26(17)
O(1)-Fe(3)-O(143)	96.96(17)	O(122)-Fe(2)-N(11)	87.93(17)
O(17)-Fe(3)-O(143)	83.52(18)	O(132)-Fe(2)-N(11)	173.88(18)
O(133)-Fe(3)-O(143)	90.8(2)	Fe(2)-O(71)-C(71)	132.4(4)
Fe(1)-Fe(3)-O(153)	73.21(12)	Fe(1)-O(121)-C(12)	129.8(4)
Fe(2)-Fe(3)-O(153)	117.83(13)	Fe(2)-O(122)-C(12)	133.5(4)
O(1)-Fe(3)-O(153)	95.73(17)	Fe(2)-O(132)-C(13)	133.1(4)
O(17)-Fe(3)-O(153)	83.40(16)	Fe(3)-O(133)-C(13)	132.9(4)
O(133)-Fe(3)-O(153)	168.47(18)	Fe(2)-O(142)-C(14)	136.1(4)
Fe(1)-Fe(3)-O(163)	76.78(12)	Fe(3)-O(143)-C(14)	130.4(4)
Fe(2)-Fe(3)-O(163)	111.59(13)	Fe(1)-O(151)-C(15)	128.7(4)
O(1)-Fe(3)-O(163)	94.32(17)	Fe(3)-O(153)-C(15)	134.6(4)
O(17)-Fe(3)-O(163)	85.26(17)	Fe(1)-O(161)-C(16)	131.5(4)
O(133)-Fe(3)-O(163)	83.9(2)	Fe(3)-O(163)-C(16)	129.5(4)
O(143)-Fe(3)-O(153)	90.2(2)	Fe(2)-N(11)-O(11)	117.9(3)
O(143)-Fe(3)-O(163)	167.96(19)	Fe(2)-N(11)-C(11)	126.3(4)
O(153)-Fe(3)-O(163)	92.8(2)	Fe(1)-O(11)-N(11)	115.8(3)
Fe(2)-O(1)-Fe(1)	117.67(18)	Fe(3)-O(17)-H(172)	112.1
Fe(2)-O(1)-Fe(3)	121.30(19)	Fe(3)-O(17)-H(171)	114.6
Fe(1)-O(1)-Fe(3)	121.03(19)	H(172)-O(17)-H(171)	119.3
Fe(1)#1-O(11)-Fe(1)	106.36(15)		
Fe(1)#1-O(11)-N(11)	132.6(3)		

**Table S18.** Selected bond lengths (Å) and bond angles (°) for complex **8**·MeOH.

Fe(1)-O(1)#1	1.9800(14)	Na(1)-O(20)#2	2.3192(19)
Fe(1)-N(2)	2.1174(16)	Na(1)-O(4)#3	2.458(3)
Fe(1)-O(2)	2.0194(12)	Na(1)-O(2)	2.451(2)
Fe(1)-O(3)	2.0140(4)	Na(1)-O(4)	2.361(2)
Fe(1)-O(6)	1.9345(14)	Na(1)-O(20)	2.3192(19)
Fe(1)-O(10)	2.0704(12)	O(20)#2-Na(1)-O(20)	111.12(11)
O(1)#1-Fe(1)-N(2)	95.22(6)	O(4)#3-Na(1)-O(20)	121.72(6)
O(1)#1-Fe(1)-O(2)	92.58(6)	O(2)-Na(1)-O(20)	83.50(6)
N(2)-Fe(1)-O(2)	172.01(6)	O(4)-Na(1)-O(20)	97.06(6)
O(1)#1-Fe(1)-O(3)	88.83(6)	Fe(1)-N(2)-C(3)	126.94(14)
N(2)-Fe(1)-O(3)	85.25(6)	Fe(1)-N(2)-O(1)	117.18(11)
O(2)-Fe(1)-O(3)	93.17(7)	C(3)-N(2)-O(1)	115.27(16)
O(1)#1-Fe(1)-O(6)	88.30(6)	N(2)-O(1)-Fe(1)#4	121.93(11)
N(2)-Fe(1)-O(6)	84.94(6)	Na(1)-O(2)-Fe(1)#2	120.54(6)
O(2)-Fe(1)-O(6)	97.07(7)	Na(1)-O(2)-Fe(1)	120.54(6)
O(3)-Fe(1)-O(6)	169.48(7)	Fe(1)#2-O(2)-Fe(1)	101.82(8)
O(1)#1-Fe(1)-O(10)	169.41(6)	Na(1)-O(2)-H(2)	96(3)
N(2)-Fe(1)-O(10)	95.22(6)	Fe(1)#2-O(2)-H(2)	108.3(16)
O(2)-Fe(1)-O(10)	76.94(6)	Fe(1)-O(2)-H(2)	108.3(16)
O(3)-Fe(1)-O(10)	90.26(7)	Fe(1)-O(3)-Fe(1)#4	117.35(3)
O(6)-Fe(1)-O(10)	94.39(7)	Fe(1)-O(3)-Fe(1)#1	117.35(3)
O(20)#2-Na(1)-O(4)#3	121.72(6)	Fe(1)#4-O(3)-Fe(1)#1	117.35(3)
O(20)#2-Na(1)-O(2)	83.50(6)	Na(1)-O(4)-Na(1)#5	140.95(11)
O(4)#3-Na(1)-O(2)	79.95(7)	Na(1)-O(4)-H(4)#2	110(2)
O(20)#2-Na(1)-O(4)	97.06(6)	Na(1)#5-O(4)-H(4)#2	92(2)
O(4)#3-Na(1)-O(4)	99.05(11)		
O(2)-Na(1)-O(4)	179.00(9)		

**Table S19.** Selected bond lengths (Å) and bond angles (°) for complex **9**.

O(1)-Fe(1)	1.907(8)	O(67)-Fe(3)	2.075(7)
O(1)-Na(1)	2.746(9)	O(67)-Fe(4)	2.073(7)
N(9)-Fe(1)	2.108(9)	O(69)-Fe(2)	1.999(7)
O(10)-Fe(3)	1.964(7)	O(69)-Fe(5)	2.008(7)
O(11)-Fe(1)	1.973(8)	O(70)-Fe(1)	2.048(7)
N(12)-Fe(2)	2.146(9)	O(70)-Fe(2)	2.055(7)
O(20)-Fe(2)	1.916(8)	O(70)-Fe(3)	2.079(7)
O(21)-Fe(2)	1.964(7)	O(71)-Fe(1)	1.984(7)
N(22)-Fe(3)	2.124(8)	O(71)-Fe(6)	1.992(7)
O(30)-Fe(3)	1.913(7)	O(71)-Na(1)	2.341(8)
O(31)-Fe(4)	1.946(7)	O(72)-Fe(4)	1.967(7)
O(31)-Na(2)	2.376(8)	O(72)-Fe(5)	1.977(7)
N(39)-Fe(4)	2.093(8)	O(72)-Fe(6)	1.954(6)
O(40)-Fe(5)	2.001(7)	O(73)-Fe(3)	2.005(7)
O(41)-Fe(4)	2.022(7)	O(73)-Fe(4)	2.036(7)
N(42)-Fe(6)	2.115(8)	O(73)-Na(2)	2.352(8)
O(50)-Fe(6)	1.952(7)	O(74)-Na(2)	2.249(10)
O(50)-Na(1)	2.502(9)	O(76)-Na(2)#1	2.378(9)
O(51)-Fe(5)	1.941(7)	O(76)-Na(2)	2.339(9)
N(59)-Fe(5)	2.120(9)	O(78)-Na(1)	2.302(10)
O(60)-Fe(6)	1.977(7)	O(80)-Na(1)	2.359(10)
O(61)-Fe(2)	2.060(7)	Fe(1)-Na(1)	3.417(5)
O(61)-Fe(5)	2.106(7)	Fe(4)-Fe(6)	3.380(2)
O(63)-Na(1)	2.495(11)	Fe(4)-Na(2)	3.235(5)
O(65)-Fe(1)	2.081(7)	Fe(5)-Fe(6)	3.378(2)
O(65)-Fe(6)	2.095(7)	Fe(6)-Na(1)	3.335(5)
C(2)-O(1)-Fe(1)	132.0(7)	O(69)-Fe(2)-O(21)	96.1(3)
C(2)-O(1)-Na(1)	135.2(7)	N(12)-Fe(2)-O(20)	86.5(3)
Fe(1)-O(1)-Na(1)	92.7(3)	O(61)-Fe(2)-O(20)	94.7(3)
C(8)-N(9)-Fe(1)	124.3(7)	O(70)-Fe(2)-O(20)	171.4(3)
O(10)-N(9)-Fe(1)	120.7(6)	O(69)-Fe(2)-O(20)	97.3(3)
N(9)-O(10)-Fe(3)	121.9(6)	O(21)-Fe(2)-O(20)	90.1(3)
N(12)-O(11)-Fe(1)	123.5(6)	N(22)-Fe(3)-O(70)	85.2(3)

O(11)-N(12)-Fe(2)	118.8(6)	N(22)-Fe(3)-O(67)	88.9(3)
C(13)-N(12)-Fe(2)	124.7(8)	O(70)-Fe(3)-O(67)	87.1(3)
C(19)-O(20)-Fe(2)	129.8(7)	N(22)-Fe(3)-O(73)	165.7(3)
N(22)-O(21)-Fe(2)	123.0(6)	O(70)-Fe(3)-O(73)	89.5(3)
O(21)-N(22)-Fe(3)	120.4(6)	O(67)-Fe(3)-O(73)	77.5(3)
C(23)-N(22)-Fe(3)	123.2(7)	N(22)-Fe(3)-O(10)	93.8(3)
C(29)-O(30)-Fe(3)	133.1(7)	O(70)-Fe(3)-O(10)	86.3(3)
C(32)-O(31)-Fe(4)	131.7(7)	O(67)-Fe(3)-O(10)	172.7(3)
C(32)-O(31)-Na(2)	129.2(7)	O(73)-Fe(3)-O(10)	99.2(3)
Fe(4)-O(31)-Na(2)	96.4(3)	N(22)-Fe(3)-O(30)	88.3(3)
C(38)-N(39)-Fe(4)	126.1(8)	O(70)-Fe(3)-O(30)	173.0(3)
O(40)-N(39)-Fe(4)	117.6(6)	O(67)-Fe(3)-O(30)	95.3(3)
N(39)-O(40)-Fe(5)	120.4(5)	O(73)-Fe(3)-O(30)	97.4(3)
N(42)-O(41)-Fe(4)	120.5(5)	O(10)-Fe(3)-O(30)	91.5(3)
O(41)-N(42)-Fe(6)	117.6(6)	N(39)-Fe(4)-O(67)	90.1(3)
C(43)-N(42)-Fe(6)	126.2(8)	N(39)-Fe(4)-O(73)	166.8(3)
C(49)-O(50)-Fe(6)	130.7(7)	O(67)-Fe(4)-O(73)	76.9(3)
C(49)-O(50)-Na(1)	132.2(7)	N(39)-Fe(4)-O(41)	98.3(3)
Fe(6)-O(50)-Na(1)	96.2(3)	O(67)-Fe(4)-O(41)	171.6(3)
C(52)-O(51)-Fe(5)	132.3(7)	O(73)-Fe(4)-O(41)	94.7(3)
C(58)-N(59)-Fe(5)	126.3(8)	N(39)-Fe(4)-O(72)	87.7(3)
O(60)-N(59)-Fe(5)	120.1(6)	O(67)-Fe(4)-O(72)	92.7(3)
N(59)-O(60)-Fe(6)	119.0(5)	O(73)-Fe(4)-O(72)	94.9(3)
C(62)-O(61)-Fe(2)	123.6(7)	O(41)-Fe(4)-O(72)	88.0(3)
C(62)-O(61)-Fe(5)	124.1(7)	N(39)-Fe(4)-O(31)	87.3(3)
Fe(2)-O(61)-Fe(5)	98.4(3)	O(67)-Fe(4)-O(31)	95.0(3)
C(64)-O(63)-Na(1)	133.6(10)	O(73)-Fe(4)-O(31)	91.7(3)
Na(1)-O(63)-H(631)	100.5	O(41)-Fe(4)-O(31)	85.1(3)
C(66)-O(65)-Fe(1)	122.3(6)	O(72)-Fe(4)-O(31)	170.8(3)
C(66)-O(65)-Fe(6)	122.7(6)	N(59)-Fe(5)-O(61)	87.6(3)
Fe(1)-O(65)-Fe(6)	97.6(3)	N(59)-Fe(5)-O(69)	163.4(3)
C(68)-O(67)-Fe(3)	122.4(6)	O(61)-Fe(5)-O(69)	75.7(3)
C(68)-O(67)-Fe(4)	122.3(7)	N(59)-Fe(5)-O(40)	102.5(3)
Fe(3)-O(67)-Fe(4)	98.7(3)	O(61)-Fe(5)-O(40)	169.8(3)
Fe(2)-O(69)-Fe(5)	103.8(3)	O(69)-Fe(5)-O(40)	94.1(3)



Fe(1)-O(70)-Fe(2)	117.2(3)	N(59)-Fe(5)-O(72)	85.6(3)
Fe(1)-O(70)-Fe(3)	116.9(3)	O(61)-Fe(5)-O(72)	90.8(3)
Fe(2)-O(70)-Fe(3)	116.8(3)	O(69)-Fe(5)-O(72)	95.4(3)
Fe(1)-O(71)-Fe(6)	104.4(3)	O(40)-Fe(5)-O(72)	89.1(3)
Fe(1)-O(71)-Na(1)	104.1(3)	N(59)-Fe(5)-O(51)	87.4(3)
Fe(6)-O(71)-Na(1)	100.3(3)	O(61)-Fe(5)-O(51)	94.6(3)
Fe(1)-O(71)-H(711)	113.2	O(69)-Fe(5)-O(51)	92.9(3)
Fe(6)-O(71)-H(711)	107.9	O(40)-Fe(5)-O(51)	86.8(3)
Na(1)-O(71)-H(711)	124.6	O(72)-Fe(5)-O(51)	171.0(3)
Fe(4)-O(72)-Fe(5)	117.5(3)	N(42)-Fe(6)-O(65)	90.1(3)
Fe(4)-O(72)-Fe(6)	119.0(3)	N(42)-Fe(6)-O(71)	166.4(3)
Fe(5)-O(72)-Fe(6)	118.4(3)	O(65)-Fe(6)-O(71)	76.4(3)
Fe(3)-O(73)-Fe(4)	102.4(3)	N(42)-Fe(6)-O(60)	100.6(3)
Fe(3)-O(73)-Na(2)	122.4(3)	O(65)-Fe(6)-O(60)	169.3(3)
Fe(4)-O(73)-Na(2)	94.7(3)	O(71)-Fe(6)-O(60)	92.9(3)
Fe(3)-O(73)-H(731)	114.8	N(42)-Fe(6)-O(72)	86.6(3)
Fe(4)-O(73)-H(731)	113.4	O(65)-Fe(6)-O(72)	90.8(3)
Na(2)-O(73)-H(731)	107.3	O(71)-Fe(6)-O(72)	95.1(3)
C(75)-O(74)-Na(2)	142.0(9)	O(60)-Fe(6)-O(72)	90.6(3)
Na(2)-O(74)-H(741)	88.5	N(42)-Fe(6)-O(50)	86.7(3)
Na(2)#1-O(76)-C(77)	128.2(7)	O(65)-Fe(6)-O(50)	91.5(3)
Na(2)#1-O(76)-Na(2)	92.0(3)	O(71)-Fe(6)-O(50)	91.9(3)
C(77)-O(76)-Na(2)	115.6(7)	O(60)-Fe(6)-O(50)	88.4(3)
C(79)-O(78)-Na(1)	120.2(7)	O(72)-Fe(6)-O(50)	173.0(3)
Na(1)-O(78)-H(781)	123.5	O(78)-Na(1)-O(71)	153.6(4)
C(81)-O(80)-Na(1)	107.8(9)	O(78)-Na(1)-O(80)	92.2(4)
Na(1)-O(80)-H(801)	109.1	O(71)-Na(1)-O(80)	105.2(3)
N(9)-Fe(1)-O(65)	91.1(3)	O(78)-Na(1)-O(63)	117.6(4)
N(9)-Fe(1)-O(70)	84.8(3)	O(71)-Na(1)-O(63)	80.9(3)
O(65)-Fe(1)-O(70)	87.6(3)	O(80)-Na(1)-O(63)	95.1(4)
N(9)-Fe(1)-O(71)	167.5(3)	O(78)-Na(1)-O(50)	94.0(3)
O(65)-Fe(1)-O(71)	76.8(3)	O(71)-Na(1)-O(50)	71.6(3)
O(70)-Fe(1)-O(71)	91.1(3)	O(80)-Na(1)-O(50)	170.5(4)
N(9)-Fe(1)-O(11)	95.6(4)	O(63)-Na(1)-O(50)	75.7(3)
O(65)-Fe(1)-O(11)	171.8(3)	O(78)-Na(1)-Fe(6)	126.2(3)

O(70)-Fe(1)-O(11)	88.3(3)	O(71)-Na(1)-Fe(6)	35.98(18)
O(71)-Fe(1)-O(11)	96.1(3)	O(80)-Na(1)-Fe(6)	140.6(3)
N(9)-Fe(1)-O(1)	89.1(3)	O(63)-Na(1)-Fe(6)	75.8(2)
O(65)-Fe(1)-O(1)	92.8(3)	O(50)-Na(1)-Fe(6)	35.57(18)
O(70)-Fe(1)-O(1)	173.9(3)	O(78)-Na(1)-O(1)	94.6(3)
O(71)-Fe(1)-O(1)	94.9(3)	O(71)-Na(1)-O(1)	68.1(3)
O(11)-Fe(1)-O(1)	91.9(3)	O(80)-Na(1)-O(1)	84.8(4)
N(9)-Fe(1)-Na(1)	139.9(2)	O(63)-Na(1)-O(1)	147.7(3)
O(65)-Fe(1)-Na(1)	78.6(2)	O(50)-Na(1)-O(1)	101.8(3)
O(70)-Fe(1)-Na(1)	132.5(2)	O(78)-Na(1)-Fe(1)	125.1(3)
O(71)-Fe(1)-Na(1)	41.6(2)	Fe(6)-Na(1)-O(1)	83.86(19)
O(11)-Fe(1)-Na(1)	98.9(3)	O(76)-Na(2)-O(73)	90.5(3)
O(1)-Fe(1)-Na(1)	53.4(2)	O(76)-Na(2)-O(74)	101.5(4)
N(12)-Fe(2)-O(61)	91.3(3)	O(73)-Na(2)-O(74)	107.3(4)
N(12)-Fe(2)-O(70)	85.3(3)	O(76)-Na(2)-O(31)	162.6(3)
O(61)-Fe(2)-O(70)	87.9(3)	O(73)-Na(2)-O(31)	74.4(3)
N(12)-Fe(2)-O(69)	167.9(3)	O(74)-Na(2)-O(31)	91.5(4)
O(61)-Fe(2)-O(69)	77.0(3)	O(76)-Na(2)-O(76)#1	88.0(3)
O(70)-Fe(2)-O(69)	91.3(3)	O(73)-Na(2)-O(76)#1	95.1(3)
N(12)-Fe(2)-O(21)	95.3(3)	O(74)-Na(2)-O(76)#1	155.4(4)
O(61)-Fe(2)-O(21)	172.0(3)	O(31)-Na(2)-O(76)#1	84.8(3)
O(70)-Fe(2)-O(21)	88.2(3)		