Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1996, 35(8), 2292-2300, DOI:10.1021/ic9508334

Table S1. Analytical Data for compounds 2-6

compd	Calcd(%)				Found (%)			
	C	H	N	Fe	C	H	N	Fe
$[FeZnL(\mu\text{-}OAc)(OAc)(H_2L)](ClO_4).H_2O$ (2)	42.82	5.61	7.14	7.12	42.92	5.72	6.98	7.02
$[FeNiL(\mu\text{-}OAc)(OAc)(H_2O)](ClO_4).2H_2O$ (3)	42.21	5.78	7.03	7.02	42.42	5.64	7.13	7.15
$[FeCoL(\mu\text{-}OAc)(OAc)(H_2O)](ClO_4).2H_2O$ (4)	42.20	5.78	7.03	7.01	41.93	5.70	7.13	7.13
$[FeMnL(\mu\text{-}OAc)(OAc)(H_2O)](ClO_4).2H_2O$ (5)	42.41	5.81	7.07	7.05	42.15	5.85	6.96	6.98
$[\{FeCoL(\mu\text{-}OAc)(OAc)\}_2(\mu\text{-}O)](ClO_4)_2.3H_2O$ (6)	43.23	5.53	7.20	7.18	42.97	5.48	7.13	7.27

Table S2. Anisotropic displacement parameters [$Å^2$ x 10^3] for 6.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Co(1)	56(1)	38(1)	41(1)	2(1)	-1(1)	-8(1)
Fe(1)	44(1)	34(1)	37(1)	-2(1)	3(1)	-3(1)
O(1)	48(3)	43(3)	32(3)	0(2)	-5(2)	-2(2)
O(2)	56(3)	33(2)	37(3)	-3(2)	-1(2)	-5(2)
O(3)	41(3)	45(3)	49(3)	0(3)	-8(2)	-3(3)
O(4)	45(3)	63(4)	51(3)	2(3)	3(3)	-5(3)
O(5)	56(5)	37(4)	42(4)	0	0	0(4)
O(6)	62(4)	44(3)	51(3)	-1(3)	-15(3)	7(3)
O(7)	145(8)	97(6)	76(5)	36(4)	-3(5)	28(5)
N(1)	53(4)	46(4)	48(4)	-2(3)	7(3)	4(3)
N(2)	89(6)	61(4)	43(4)	-4(4)	14(4)	-26(4)
N(3)	70(5)	58(5)	47(4)	8(3)	9(4)	-15(4)
N(4)	97(6)	43(4)	56(5)	5(4)	-10(4)	-17(4)
C(1)	54(5)	55(5)	44(5)	-11(4)	-6(4)	-15(5)
C(2)	47(6)	131(10)	89(8)	25(7)	-7(6)	0(6)
C(3)	36(4)	57(5)	61(5)	0(4)	-5(4)	0(4)
C(4)	53(5)	41(4)	54(5)	-10(4)	-10(4)	5(4)
C(5)	53(5)	54(5)	62(6)	-9(4)	-22(5)	4(4)
C(6)	71(7)	66(6)	59(6)	-15(5)	-14(5)	14(5)
C(7)	83(7)	63(6)	39(5)	-9(4)	0(5)	13(5)
C(8)	64(6)	41(4)	43(4)	-5(4)	3(4)	-5(4)
C(9)	75(6)	55(5)	42(5)	-3(4)	14(5)	-7(5)
C(10)	53(5)	33(3)	41(4)	4(4)	-6(4)	2(4)
C(11)	114(9)	126(10)	51(6)	-12(6)	-35(6)	6(8)
C(12)	82(7)	63(6)	39(5)	-3(4)	-2(5)	2(5)
C(13)	42(5)	54(5)	46(5)	-4(4)	3(4)	12(4)
C(14)	78(6)	57(6)	38(5)	-12(4)	-18(5)	14(5)
C(15)	65(6)	54(6)	77(7)	-26(5)	-20(5)	10(5)
C(16)	64(6)	48(5)	73(6)	-7(5)	-4(5)	-2(5)
C(17)	72(6)	39(4)	48(5)	-5(4)	-3(4)	-3(4)
C(18)	99(8)	31(4)	69(6)	2(4)	-6(6)	-11(5)
C(19)	53(5)	41(4)	48(5)	-10(4)	-5(4)	-4(4)
C(20)	114(9)	72(7)	88(8)	-22(6)	-34(7)	-7(6)
C(21)	61(7)	177(13)	60(6)	-20(8)	14(5)	-15(8)
C(22)	86(10)	279(21)	84(10)	-17(12)	21(8)	-22(12)
C(23)	68(8)	177(14)	121(10)	-92(10)	45(7)	-19(8)
C(24)	80(7)	105(9)	52(6)	-3(5)	20(5)	-38(6)
C(25)	136(11)	99(9)	76(8)	11(6)	30(7)	-67(8)
C(26)	104(9)	68(6)	81(7)	-8(6)	15(6)	-49(6)
C(27)	98(9)	55(6)	60(6)	-2(5)	-17(6)	13(6)
C(28)	101(10)	115(10)	102(9)	0(8)	-54(8)	36(8)
Cl(1)	104(3)	179(4)	96(3)	-67(3)	-7(2)	12(3)
O(111)	260(29)	223(26)	63(12)	14(14)	-16(15)	-40(23)
O(112)	204(23)	68(13)	201(23)	-33(13)	-23(18)	-11(13)
O(12)	119(10)	283(17)	208(14)	-14(12)	-16(9)	39(10)
O(14)	181(10)	137(8)	97(6)	-18(6)	-24(6)	-38(7)

Table S3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 6.

	x	y	z	U(eq)
H(1)	6151(4)	1423(2)	1000(2)	80
H(2)	5267(4)	1969(3)	-146(2)	80
H(3)	4180(4)	930(3)	2189(2)	80
H(4)	4290(5)	247(2)	1616(2)	80
H(2A)	2108(5)	1483(4)	901(4)	133
H(2B)	2340(5)	1640(4)	394(4)	133
H(2C)	2297(5)	2033(4)	793(4)	133
H(3A)	6216(4)	2404(3)	1200(3)	62
H(3B)	6847(4)	2035(3)	1356(3)	62
H(5)	6794(5)	2133(3)	2159(3)	68
H(7)	4936(6)	1839(3)	2900(3)	74
H(9A)	3763(5)	1630(3)	2516(3)	69
H(9B)	3662(5)	1852(3)	2014(3)	69
H(11A)	6892(7)	2162(5)	2979(3)	145
H(11B)	6377(7)	1768(5)	3222(3)	145
H(11C)	6145(7)	2323(5)	3236(3)	145
H(12A)	4580(5)	1460(3)	-569(3)	74
H(12B)	4051(5)	1691(3)	-188(3)	74
H(14)	3904(5)	759(3)	-696(3)	69
H(16)	3682(5)	-290(3)	251(3)	74
H(18A)	4257(6)	-230(3)	977(3)	79
H(18B)	4952(6)	129(3)	989(3)	79
H(20A)	3210(7)	-454(4)	-511(4)	137
H(20B)	3691(7)	-201(4)	-903(4)	137
H(20C)	2889(7)	8(4)	-770(4)	137
H(21A)	6568(6)	2172(5)	433(4)	119
H(21B)	7135(6)	1791(5)	642(4)	119
H(22A)	6910(7)	1275(7)	153(5)	180
H(22B)	6773(7)	1749(7)	-137(5)	180
H(23A)	5747(6)	1051(5)	117(5)	147
H(23B)	5904(6)	1270(5)	-378(5)	147
H(24A)	2769(6)	1131(4)	1852(3)	95
H(24B)	2933(6)	989(4)	2372(3)	95
H(25A)	3330(7)	206(4)	2142(4)	125
H(25B)	2495(7)	299(4)	1975(4)	125
H(26A)	3151(6)	-76(4)	1381(3)	101
H(26B)	2943(6)	458(4)	1219(3)	101
H(28A)	6655(7)	757(4)	1715(4)	159
H(28B)	6535(7)	286(4)	2020(4)	159
H(28C)	6581(7)	802(4)	2259(4)	159

Table S4. Bond lengths [A] and angles [°] for 6.

Co(1)-O(6)	1.914(5)	Co(1)-O(4)	1.914(6)
Co(1)-N(4)	1.946(7)	Co(1)-O(1)	1.947(5)
Co(1)-O(2)	1.955(5)	Co(1)-N(3)	1.971(7)
Fe(1)-O(5)	1.7895(12)	Fe(1)-O(1)	1.990(5)
Fe(1)-O(3)	2.084(5)	Fe(1)-N(2)	2.135(7)
Fe(1)-O(2)	2.140(5)	Fe(1)-N(1)	2.163(6)
O(1)-C(10)	1.363(8)	O(2)-C(19)	1.381(8)
O(3)-C(1)	1.258(9)	O(4)-C(1)	1.268(9)
O(5)-Fe(1)#1	1.7897(12)	O(6)-C(27)	1.283(11)
O(7)-C(27)	1.229(12)	N(1)-C(21)	1.468(11)
N(1)-C(3)	1.495(10)	N(2)-C(12)	1.476(11)
N(2)-C(23)	1.527(14)	N(3)-C(9)	1.490(10)
N(3)-C(24)	1.491(11)	N(4)-C(26)	1.471(12)
N(4)-C(18)	1.482(11)	C(1)-C(2)	1.492(12)
C(3)-C(4)	1.503(11)	C(4)-C(10)	1.389(11)
C(4)-C(5)	1.403(10)	C(5)-C(6)	1.387(12)
C(6)-C(7)	1.375(12)	C(6)-C(11)	1.509(12)
C(7)-C(8)	1.385(11)	C(8)-C(10)	1.397(10)
C(8)-C(9)	1.502(11)	C(12)-C(13)	1.515(11)
C(13)-C(14)	1.393(10)	C(13)-C(19)	1.402(10)
C(14)-C(15)	1.370(12)	C(15)-C(16)	1.395(12)
C(15)-C(20)	1.525(11)	C(16)-C(17)	1.374(11)
C(17)-C(19)	1.398(10)	C(17)-C(18)	1.486(11)
C(21)-C(22)	1.40(2)	C(22)-C(23)	1.46(2)
C(24)-C(25)	1.535(14)	C(25)-C(26)	1.500(13)
C(27)-C(28)	1.503(14)	Cl(1)-O(131)	1.30(2)
Cl(1)-O(12)	1.310(12)	Cl(1)-O(14)	1.354(9)
Cl(1)-O(132)	1.41(2)	Cl(1)-O(112)	1.61(2)
Cl(1)-O(111)	1.66(2)	O(111)-O(132)	1.67(3)
O(112)-O(131)	1.58(3)	O(131)-O(132)	0.88(3)
WA2-WA3#2	1.10(3)	WA3-WA2#2	1.10(3)

O(6)-Co(1)-O(4)	174.6(2)	O(6)-Co(1)-N(4)	88.0(3)
O(4)-Co(1)-N(4)	94.0(3)	O(6)-Co(1)-O(1)	87.3(2)
O(4)-Co(1)-O(1)	90.6(2)	N(4)-Co(1)-O(1)	175.3(3)
O(6)-Co(1)-O(2)	86.1(2)	O(4)-Co(1)-O(2)	88.8(2)
N(4)-Co(1)-O(2)	95.0(3)	O(1)-Co(1)-O(2)	83.8(2)
O(6)-Co(1)-N(3)	97.8(3)	O(4)-Co(1)-N(3)	87.2(3)
N(4)-Co(1)-N(3)	89.5(3)	O(1)-Co(1)-N(3)	92.0(2)
O(2)-Co(1)-N(3)	174.1(3)	O(5)-Fe(1)-O(1)	104.7(2)
O(5)-Fe(1)-O(3)	93.3(2)	O(1)-Fe(1)-O(3)	85.6(2)
O(5)-Fe(1)-N(2)	95.9(3)	O(1)-Fe(1)-N(2)	159.3(2)
O(3)-Fe(1)-N(2)	95.1(3)	O(5)-Fe(1)-O(2)	174.5(2)
O(1)-Fe(1)-O(2)	78.2(2)	O(3)-Fe(1)-O(2)	82.2(2)
N(2)-Fe(1)-O(2)	81.4(2)	O(5)-Fe(1)-N(1)	95.0(2)
O(1)-Fe(1)-N(1)	85.1(2)	O(3)-Fe(1)-N(1)	168.9(2)
N(2)-Fe(1)-N(1)	91.5(3)	O(2)-Fe(1)-N(1)	89.9(2)
C(10)-O(1)-Co(1)	114.0(4)	C(10)-O(1)-Fe(1)	130.0(4)
Co(1)-O(1)-Fe(1)	100.6(2)	C(19)-O(2)-Co(1)	120.4(4)
C(19)-O(2)-Fe(1)	126.4(4)	Co(1)-O(2)-Fe(1)	95.3(2)
C(1)-O(3)-Fe(1)	129.0(5)	C(1)-O(4)-Co(1)	128.2(5)
Fe(1)-O(5)-Fe(1)#1	169.5(4)	C(27)-O(6)-Co(1)	128.8(7)
C(21)-N(1)-C(3)	107.2(7)	C(21)-N(1)-Fe(1)	113.1(6)
C(3)-N(1)-Fe(1)	110.1(5)	C(12)-N(2)-C(23)	111.4(7)
C(12)-N(2)-Fe(1)	111.2(5)	C(23)-N(2)-Fe(1)	111.8(7)
C(9)-N(3)-C(24)	110.3(7)	C(9)-N(3)-Co(1)	112.9(5)
C(24)-N(3)-Co(1)	115.4(5)	C(26)-N(4)-C(18)	114.4(7)
C(26)-N(4)-Co(1)	115.5(6)	C(18)-N(4)-Co(1)	112.1(5)
O(3)-C(1)-O(4)	125.3(8)	O(3)-C(1)-C(2)	118.3(8)

O(4)-C(1)-C(2)	116.4(8)	N(1)-C(3)-C(4)	115.3(6)
C(10)-C(4)-C(5)	118.0(8)	C(10)-C(4)-C(3)	123.4(7)
C(5)-C(4)-C(3)	118.6(7)	C(6)-C(5)-C(4)	122.9(8)
C(7)-C(6)-C(5)	117.7(8)	C(7)-C(6)-C(11)	120.7(9)
C(5)-C(6)-C(11)	121.5(9)	C(6)-C(7)-C(8)	121.2(8)
C(7)-C(8)-C(10)	120.7(8)	C(7)-C(8)-C(9)	123.0(8)
C(10)-C(8)-C(9)	116.3(7)	N(3)-C(9)-C(8)	111.1(7)
O(1)-C(10)-C(4)	123.6(7)	O(1)-C(10)-C(8)	116.8(7)
C(4)-C(10)-C(8)	119.5(7)	N(2)-C(12)-C(13)	113.6(7)
C(14)-C(13)-C(19)	118.2(7)	C(14)-C(13)-C(12)	116.6(7)
C(19)-C(13)-C(12)	125.2(7)	C(15)-C(14)-C(13)	123.8(8)
C(14)-C(15)-C(16)	116.3(8)	C(14)-C(15)-C(20)	122.2(9)
C(16)-C(15)-C(20)	121.5(9)	C(17)-C(16)-C(15)	122.6(9)
C(16)-C(17)-C(19)	119.8(8)	C(16)-C(17)-C(18)	121.4(7)
C(19)-C(17)-C(18)	118.4(7)	N(4)-C(18)-C(17)	113.3(7)
O(2)-C(19)-C(17)	118.2(7)	O(2)-C(19)-C(13)	122.5(7)
C(17)-C(19)-C(13)	119.2(7)	C(22)-C(21)-N(1)	119.0(11)
C(21)-C(22)-C(23)	122.3(11)	C(22)-C(23)-N(2)	116.4(11)
N(3)-C(24)-C(25)	112.7(9)	C(26)-C(25)-C(24)	114.7(8)
N(4)-C(26)-C(25)	110.3(9)	O(7)-C(27)-O(6)	124.1(10)
O(7)-C(27)-C(28)	120.8(10)	O(6)-C(27)-C(28)	115.0(10)
O(131)-Cl(1)-O(12)	117.7(13)	O(131)-Cl(1)-O(14)	127.8(12)
O(12)-Cl(1)-O(14)	113.2(8)	O(131)-Cl(1)-O(132)	37.6(12)
O(12)-Cl(1)-O(132)	132.1(11)	O(14)-Cl(1)-O(132)	108.6(11)
O(131)-Cl(1)-O(112)	64.6(13)	O(12)-Cl(1)-O(112)	92.8(11)
O(14)-Cl(1)-O(112)	103.2(9)	O(132)-Cl(1)-O(112)	99.7(13)
O(131)-Cl(1)-O(111)	93(2)	O(12)-Cl(1)-O(111)	82.2(12)
O(14)-Cl(1)-O(111)	104.1(10)	O(132)-Cl(1)-O(111)	65.6(12)
O(112)-Cl(1)-O(111)	152.0(11)	Cl(1)-O(111)-O(132)	50.2(11)
O(131)-O(112)-Cl(1)	47.9(11)	O(132)-O(131)-Cl(1)	78(3)
O(132)-O(131)-O(112)	139(3)	Cl(1)-O(131)-O(112)	67.5(14)
O(131)-O(132)-Cl(1)	64(2)	O(131)-O(132)-O(111)	112(3)
Cl(1)-O(132)-O(111)	64.2(12)		

Symmetry transformations used to generate equivalent atoms:

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