

Supporting Information

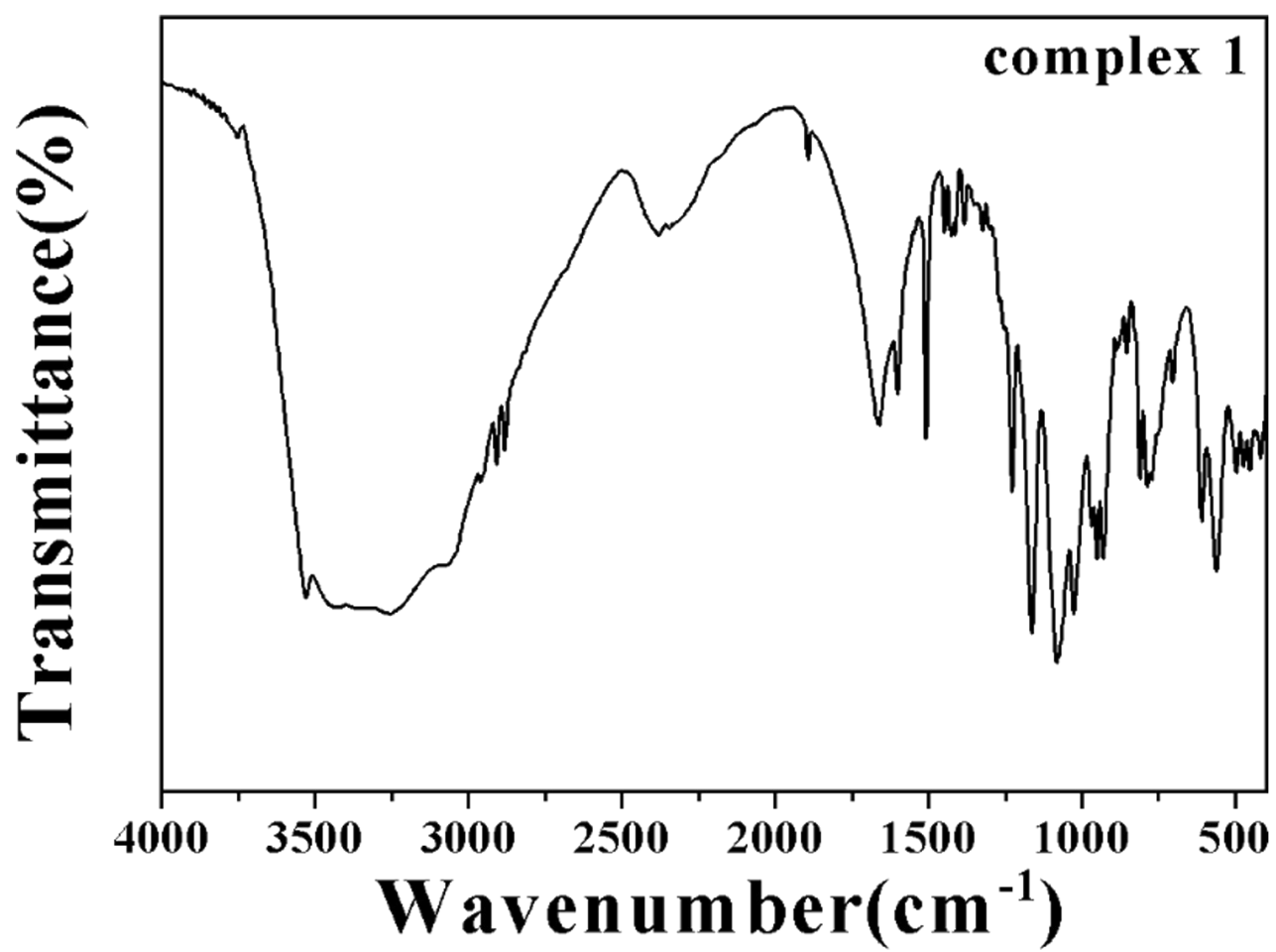
Synthesis, crystal structures, and Magnetic Properties of seven transition metal phosphonates

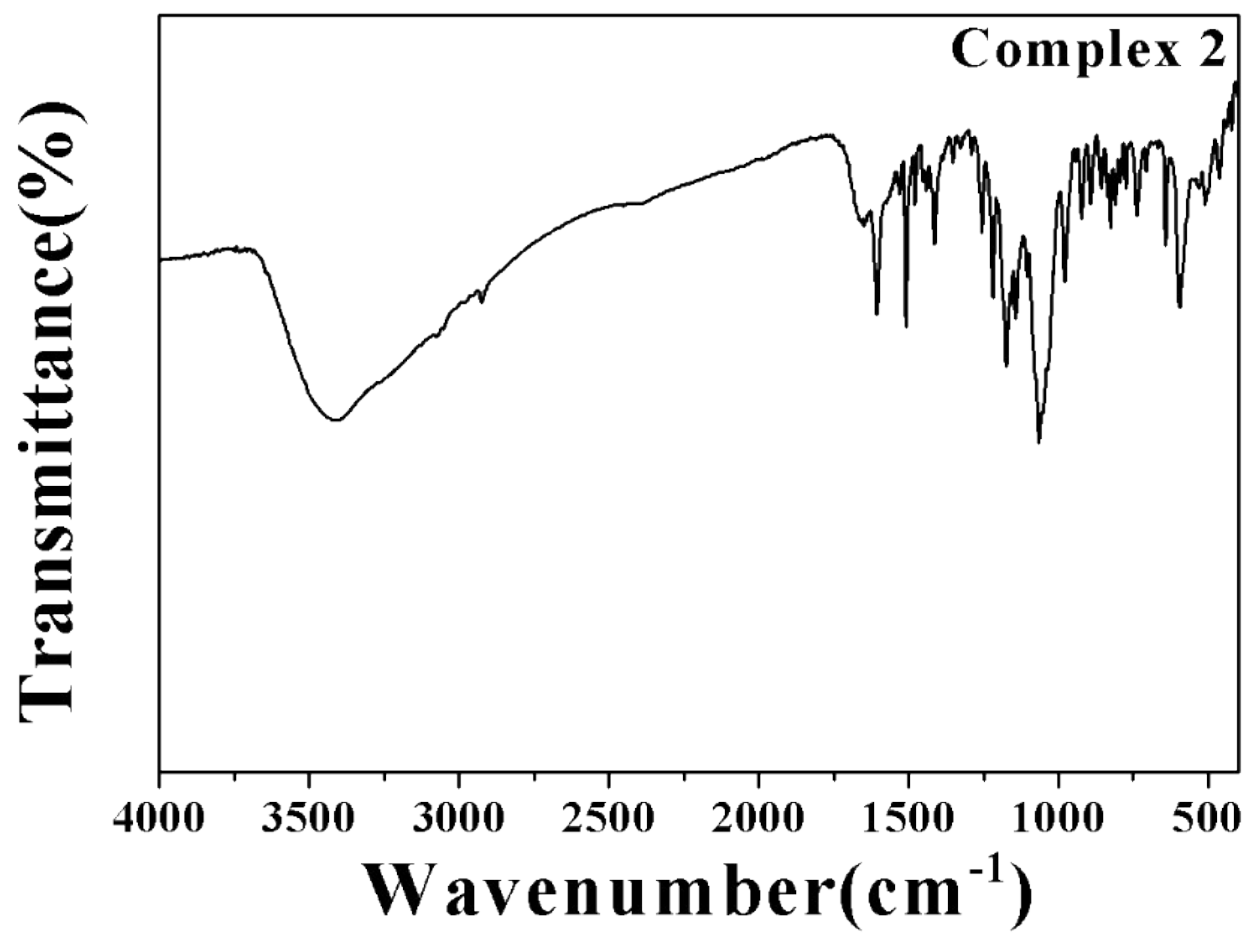
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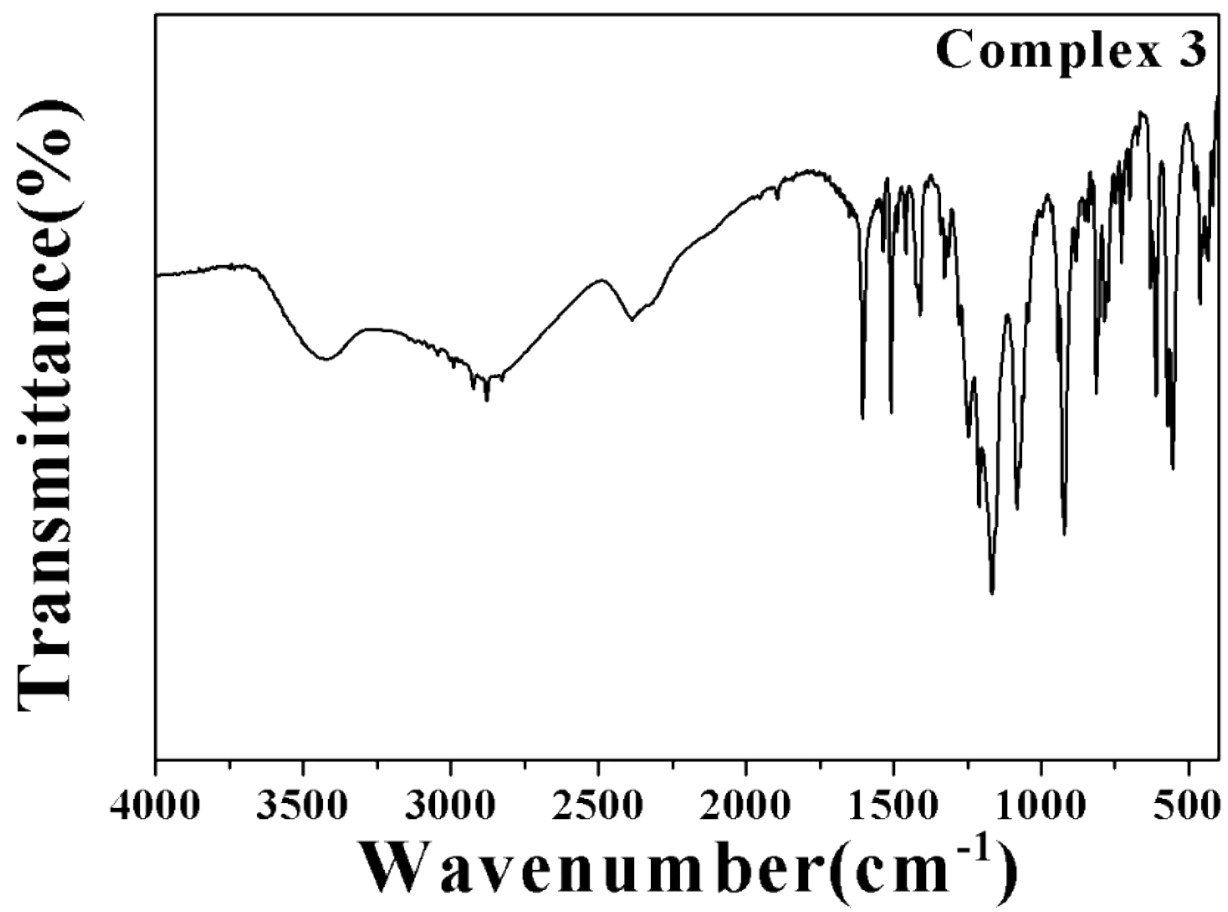
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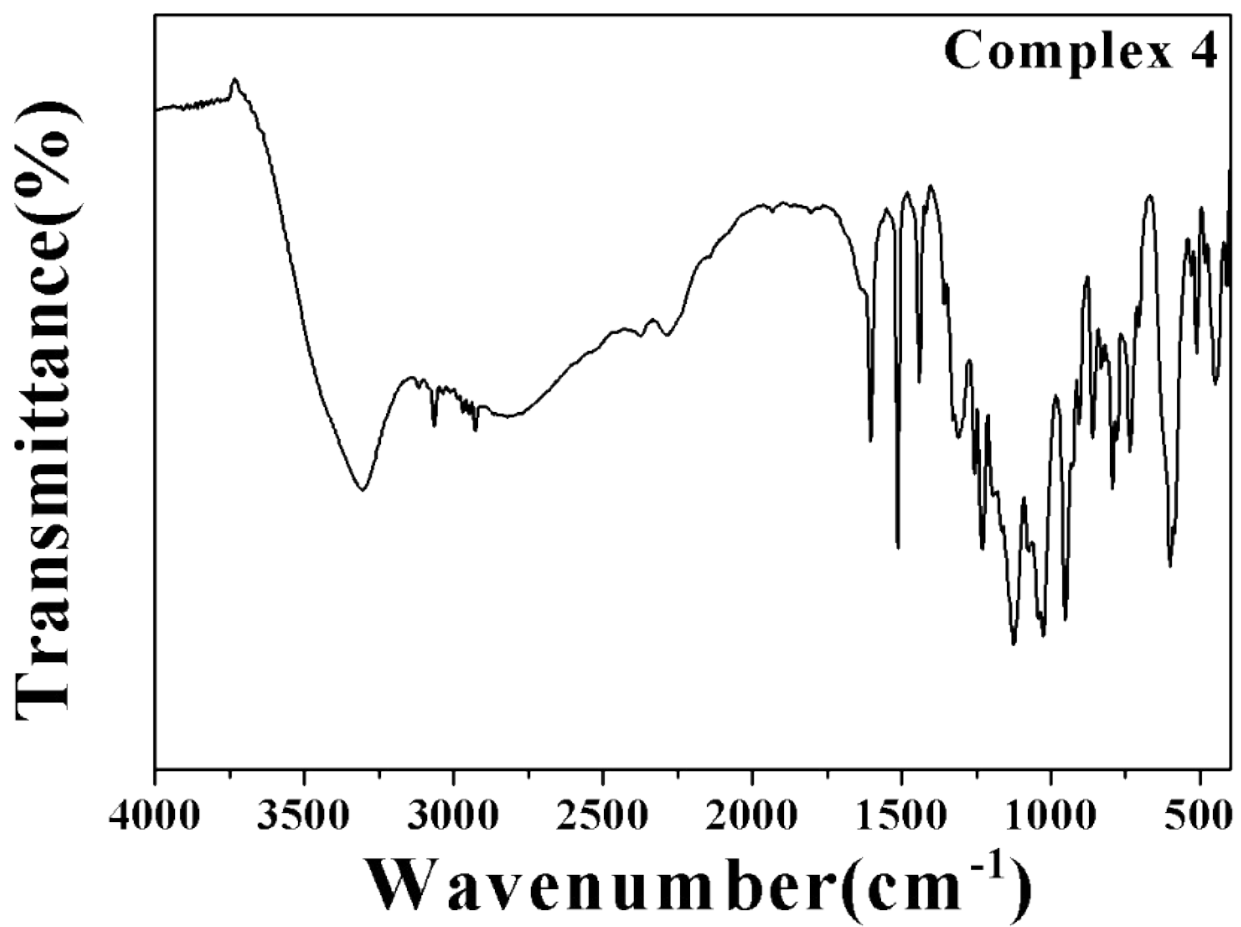
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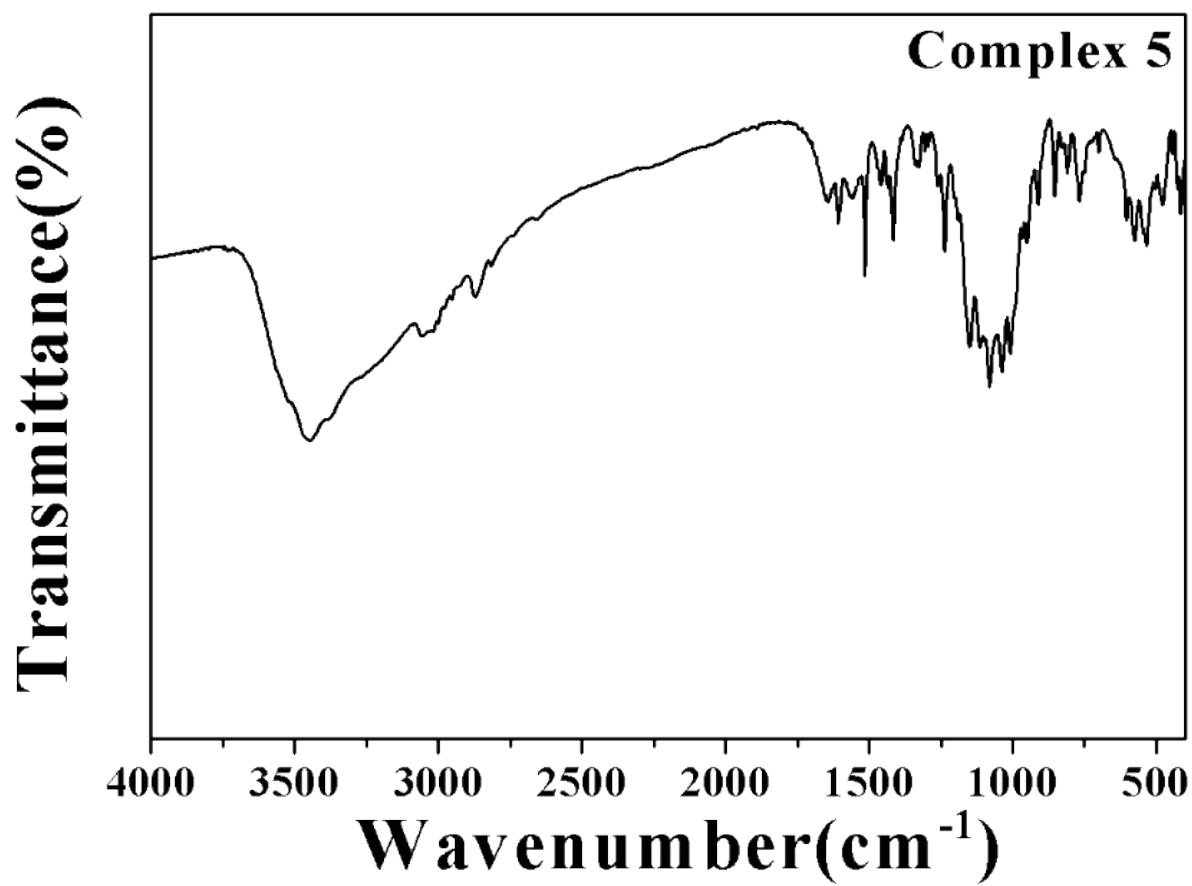
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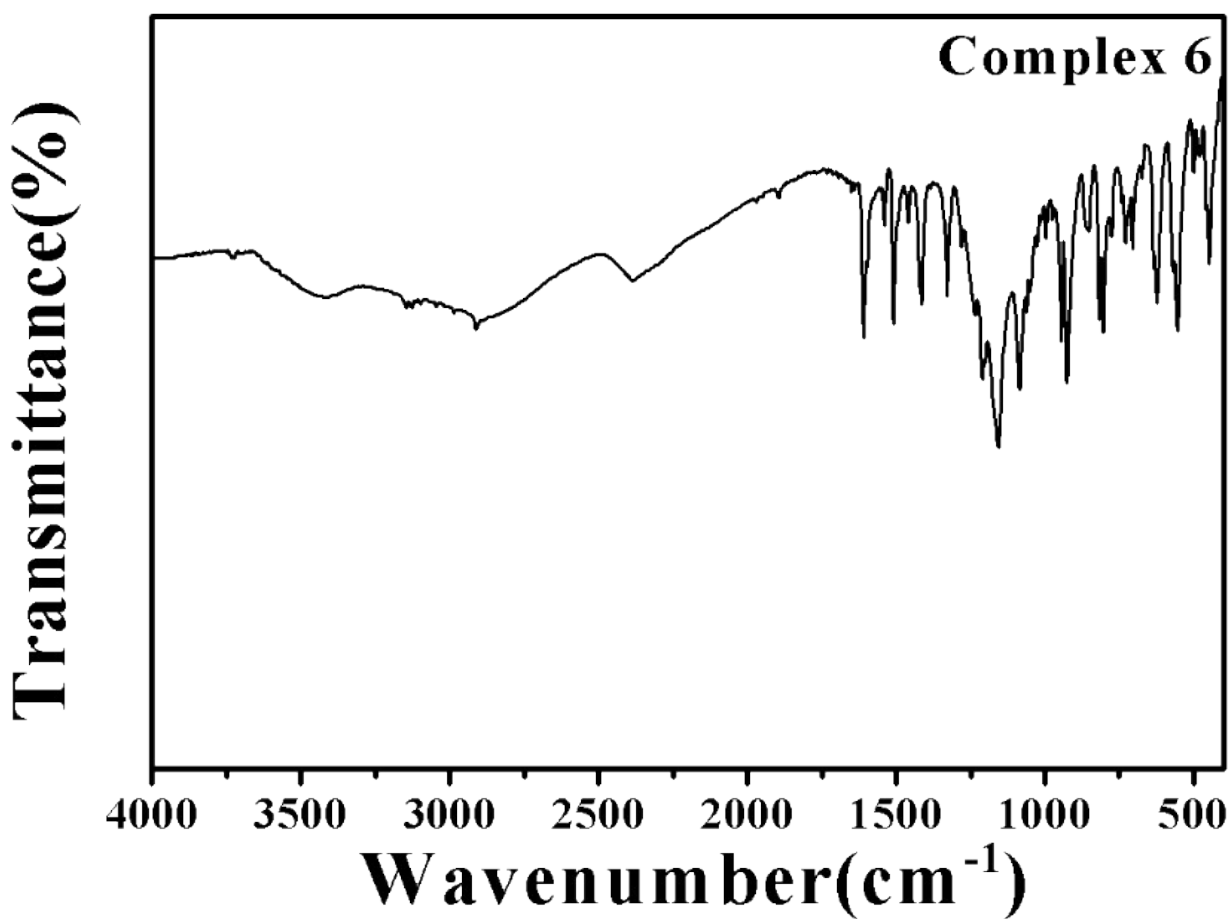


Figure S1. IR spectra of the complexes 1-6.

Table S1 Crystallographic data for complexes 1 - 6.

	1	2	3	4	5	6
CCDC	1835239	1812308	1812312	1812305	1812303	1812304
No.						
Empirical	C ₁₈ H ₃₄ N ₂ O ₁₈	C ₉ H ₁₄ NO ₇ P ₂ F	C ₁₈ H ₃₁ N ₂ O ₁₈	C ₂₄ H ₃₂ N ₄ O ₁	C ₁₄ H ₁₆ N ₂ O ₆	C ₁₄ H ₁₆ N ₂ O ₆
formula	P ₄ F ₂ Co ₃	Cu	P ₄ F ₂ Fe ₃	₁ P ₂ FCu ₂	P ₂ FCo	P ₂ FNi
Formula	905.14	392.70	892.88	760.58	448.16	447.92
weigh						
T/K	173	173	173	173	173	173
Crystal	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	monoclinic

system						
Space	P 21/c	P 21/c	I 2/a	P 21/c	P -1	C 2/m
group						
a/Å	12.752(1)	14.537(1)	10.5218(7)	5.9865(4)	8.3161(9)	13.195(1)
b/Å	12.516(1)	10.4704(8)	9.8194(6)	23.413(1)	8.5014(7)	9.851(1)
c/Å	9.514(1)	9.1811(7)	28.815(2)	21.723(1)	13.377(1)	13.688(2)
α°	90	90	90	90	95.080(3)	90
β°	92.796(4)	99.314(3)	91.524(3)	91.934(3)	105.064(4)	112.336(4)
γ°	90	90	90	90	107.257(3)	90
V/Å ³	1516.7(3)	1379.05(19)	2976.1(3)	3043.0(3)	857.96(14)	1645.6(3)
Z	2	4	4	4	2	4
D _{calc} /g	1.982	1.891	1.993	1.660	1.735	1.808
cm ⁻³						
μ /mm ⁻¹	1.929	1.859	1.756	1.573	1.232	1.421
F(000)	918.0	796.0	1812.0	1556.0	456.0	916.0
h, k, l	15, 15, 11	17, 12, 10	12, 11, 34	7, 27, 25	9, 10, 15	15, 11, 16
max						
S	1.015	1.060	1.036	1.049	1.067	1.032
R ₁ , wR ₂	0.0497,	0.0377,	0.0486,	0.0634,	0.0395,	0.0454,
[I > 2 σ (I)]	0.0869	0.0794	0.0979	0.1278	0.0670	0.0886

Table S2. Selected bond lengths (Å) and bond angles (°) for complex 1 - 6.

bond		bond angles (°)			
lengths (Å)					
Complex 1					
Co1-O2	2.0816(3)	O6 ⁱ -Co1-O6 ⁱⁱ	180.000	O4 ⁱⁱ -Co2-O5 ^{iv}	85.36(1)
Co1-O8	2.1516(4)	O6 ⁱ -Co1-O2	90.60(1)	O4 ⁱⁱ -Co2-O7	86.69(1)
Co1-O6	2.0591(3)	O6 ⁱ -Co1-O2	89.40(1)	O5 ^{iv} -Co2-O7	167.47(1)

Co2-O3	2.2080(4)	O6 ⁱ -Co1-O2 ⁱⁱⁱ	89.40(1)	O4 ⁱⁱ -Co2-O3 ^{iv}	174.18(1)
Co2-O4	2.0360(3)	O6 ⁱⁱ -Co1-O2 ⁱⁱⁱ	90.60(1)	O5 ^{iv} -Co2-O3 ^{iv}	95.91(1)
Co2-O5	2.0825(3)	O2-Co1-O2 ⁱⁱⁱ	180.000	O7-Co2-O3 ^{iv}	92.97(1)
Co2-O7	2.0901(4)	O6 ⁱ -Co1-O8 ⁱⁱⁱ	92.07(1)	O4 ⁱⁱ -Co2-O3	97.97(1)
Co2-N1	2.2772(4)	O6 ⁱⁱ -Co1-O8 ⁱⁱⁱ	87.93(1)	O5 ^{iv} -Co2-O3	96.88(1)
		O2-Co1-O8 ⁱⁱⁱ	86.01(1)	O7-Co2-O3	93.79(1)
		O2 ⁱⁱⁱ -Co1-O8 ⁱⁱⁱ	93.99(1)	O3 ^{iv} -Co2-O3	76.25(1)
		O6 ⁱ -Co1-O8	87.93(1)	O4 ⁱⁱ -Co2-N1 ^{iv}	100.42(1)
		O6 ⁱⁱ -Co1-O8	92.07(1)	O5 ^{iv} -Co2-N1 ^{iv}	80.75(1)
		O2-Co1-O8	93.99(1)	O7-Co2-N1 ^{iv}	91.21(1)
		O2 ⁱⁱⁱ -Co1-O8	86.01(1)	O3 ^{iv} -Co2-N1 ^{iv}	85.40(1)
		O8 ⁱⁱⁱ -Co1-O8	180.000	O3-Co2-N1 ^{iv}	161.20(1)
		O2-Ni1-O7	88.28(15)		
Complex 2					
Cu1-O1	1.930(3)	O1-Cu1-O5	174.32(11)	O4 ⁱ -Cu1-N1	173.18(11)
Cu1-O5	1.941(3)	O1-Cu1-O4 ⁱ	94.14(11)	O1-Cu1-O6 ⁱⁱ	85.55(9)
Cu1-O4 ⁱ	1.960(3)	O5-Cu1-O4 ⁱ	90.79(11)	O5-Cu1-O6 ⁱⁱ	97.89(9)
Cu1-O1	2.060(3)	O1-Cu1-N1	88.31(11)	O4 ⁱ -Cu1-O6 ⁱⁱ	82.54(9)
Cu1-O6 ⁱⁱ	2.423(2)	O5-Cu1-N1	87.11(11)	N1-Cu1-O6 ⁱⁱ	91.31(10)
Complex 3					
Fe1-O8	1.976(2)	O8-Fe1-O2	89.53(12)	O9-Fe1-O6 ⁱⁱ	90.97(13)
Fe1-O2	2.041(3)	O8-Fe1-O4 ⁱ	91.58(12)	O6-Fe1-O6 ⁱⁱ	80.27(13)
Fe1-O4 ⁱ	2.059(3)	O2-Fe1-O4 ⁱ	177.73(14)	O1 ⁱ -Fe2-O1	142.1(2)
Fe1-O9	2.071(4)	O8-Fe1-O9	93.17(13)	O1 ⁱ -Fe2-O7	108.96(10)
Fe1-O6	2.110(3)	O2-Fe1-O9	91.72(13)	O1-Fe2-O7	108.96(10)
Fe1-O6 ⁱⁱ	2.131(3)	O4 ⁱ -Fe1-O9	90.20(13)	O1 ⁱ -Fe2-O3 ⁱⁱⁱ	93.39(13)
Fe2-O1 ⁱ	2.013(3)	O8-Fe1-O6	95.59(12)	O1-Fe2-O3 ⁱⁱⁱ	87.30(13)
Fe2-O1	2.013(3)	O2-Fe1-O6	90.02(13)	O7-Fe2-O3 ⁱⁱⁱ	88.94(9)

Fe2-O7	2.039(5)	O4 ⁱ -Fe1-O6	87.90(13)	O1 ⁱ -Fe2-O3 ^{iv}	87.30(13)
Fe2-O3 ⁱⁱⁱ	2.140(3)	O9-Fe1-O6	171.08(13)	O1-Fe2-O3 ^{iv}	93.39(13)
Fe2-O3 ^{iv}	2.140(3)	O8-Fe1-O6 ⁱⁱ	175.86(13)	O7-Fe2-O3 ^{iv}	88.94(13)
		O2-Fe1-O6 ⁱⁱ	90.47(12)	O3 ⁱⁱⁱ -Fe2-O3 ^{iv}	177.89(18)
		O4 ⁱ -Fe1-O6 ⁱⁱ	90.47(12)	O3 ⁱⁱⁱ -Fe2-O3 ^{iv}	177.89(18)
Complex 4					
Cu1-O4	1.941(4)	O4-Cu1-O2	166.85(18)	O6 ⁱⁱ -Cu2-O1	174.69(17)
Cu1-O2	1.946(4)	O4-Cu1-N2	93.41(19)	O6 ⁱⁱ -Cu2-N3 ⁱⁱⁱ	89.32(17)
Cu1-N2	2.006(5)	O2-Cu1-N2	90.78(18)	O1-Cu2-N3 ⁱⁱⁱ	88.59(17)
Cu1-N1	2.050(5)	O4-Cu1-N1	87.35(18)	O6 ⁱⁱ -Cu2-N4	90.57(18)
Cu1-O8	2.266(4)	O2-Cu1-N1	87.41(17)	O1-Cu2-N4	90.14(17)
Cu2-O6 ⁱⁱ	1.940(4)	N2-Cu1-N1	174.9(1)	N3 ⁱⁱⁱ -Cu2-N4	164.6(2)
Cu2-O1	1.953(4)	O4-Cu1-O8	96.46(17)	O6 ⁱⁱ -Cu2-O7	92.92(16)
Cu2-N3 ⁱⁱⁱ	2.028(4)	O2-Cu1-O8	95.73(17)	O1-Cu2-O7	92.21(16)
Cu2-N4	2.039(5)	N2-Cu1-O8	93.40(19)	N3 ⁱⁱⁱ -Cu2-O7	98.38(18)
Cu2-O7	2.168(4)	N1-Cu1-O8	91.52(18)	N4-Cu2-O7	97.01(19)
Cu2 ⁱⁱⁱ -N3	2.028(4)				
Complex 5					
Co1-O2 ⁱⁱ	2.028(2)	O2 ⁱⁱ -Co1-O6 ⁱⁱⁱ	92.54(9)	O6 ⁱⁱⁱ -Co1-N2	85.85(10)
Co1-O6 ⁱⁱⁱ	2.075(2)	O2 ⁱⁱ -Co1-O4	176.41(10)	O4-Co1-N2	92.49(9)
Co1-O4	2.091(2)	O6 ⁱⁱⁱ -Co1-O4	90.93(8)	O1-Co1-N2	92.27(10)
Co1-O1	2.116(2)	O2 ⁱⁱ -Co1-O1	88.36(9)	O2 ⁱⁱ -Co1-N1	98.21(8)
Co1-N2	2.148(2)	O6 ⁱⁱⁱ -Co1-O1	176.80(8)	O6 ⁱⁱⁱ -Co1-N1	91.84(9)
Co1-N1	2.276(2)	O4-Co1-O1	88.23(9)	O4-Co1-N1	82.59(8)
		O2 ⁱⁱ -Co1-N2	86.84(9)	O1-Co1-N1	84.99(9)
				N2-Co1-N1	174.54(9)
Complex 6					
Ni1-N1	2.213(4)	O3 ⁱⁱⁱ -Ni1-O3 ^{iv}	89.55(16)	N2-Ni1-O1	92.00(12)

Ni1-N2	2.095(5)	O3 ⁱⁱⁱ -Ni1-N2	87.59(12)	O1 ⁱ -Ni1-O1	84.35(16)
Ni1-O3 ⁱⁱⁱ	2.040(3)	O3 ^{iv} -Ni1-N2	87.59(12)	O3 ⁱⁱⁱ -Ni1-N1	93.33(11)
Ni1-O3 ^{iv}	2.040(3)	O3 ⁱⁱⁱ -Ni1-O1 ⁱ	177.35(11)	O3 ^{iv} -Ni1-N1	93.33(11)
Ni1-O1 ⁱ	2.098(3)	O3 ^{iv} -Ni1-O1 ⁱ	93.05(11)	N2-Ni1-N1	178.71(18)
Ni1-O1	2.098(3)	N2-Ni1-O1 ⁱ	92.00(12)	O1 ⁱ -Ni1-N1	87.05(11)
		O3 ⁱⁱⁱ -Ni1-O1	93.05(11)	O1-Ni1-N1	87.04(11)
		O3 ^{iv} -Ni1-O1	177.35(11)		
