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A series of metal-organic frameworks containing diverse secondary building units derived from a flexible triazine-based tetracarboxylic ligand

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Table S1 Selected bond lengths(Å) and bond angles(°) for complex **1-5**

		1	
Zn(1)-O(5)	2.003(2)	O(7)-Zn(1)-O(9)	104.43(9)
Zn(1)-O(3)^{a}	2.007(2)	O(7)-Zn(1)-O(5)	107.75(9)
Zn(1)-O(9)	2.029(2)	O(7)-Zn(1)-O(3)^{a}	143.64(9)
Zn(1)-O(4)^{a}	2.354(2)	O(7)-Zn(1)-O(4)^{a}	92.48(8)
Zn(1)-O(7)	1.956(2)	O(9)-Zn(1)-O(4)^{a}	93.05(8)
Zn(2)-O(1)^{c}	2.099(2)	O(1)^{c}-Zn(2)-O(2)^{c}	59.19(9)
Zn(2)-O(2)^{c}	2.294(3)	O(6)-Zn(2)-O(10)	103.49(9)
Zn(2)-O(6)	1.988(2)	O(6)-Zn(2)-O(8)^{b}	119.70(9)
Zn(2)-O(8)^{b}	2.013(2)	O(6)-Zn(2)-O(1)^{c}	108.44(9)
Zn(2)-O(10)	2.027(2)	O(6)-Zn(2)-O(2)^{c}	98.82(9)
O(3)^{a}-Zn(1)-O(4)^{a}	59.79(8)	O(8)^{b}-Zn(2)-O(1)^{c}	90.10(9)
O(3)^{a}-Zn(1)-O(9)	100.38(9)	O(8)^{b}-Zn(2)-O(10)	98.91(9)
O(5)-Zn(1)-O(4)^{a}	158.24(8)	O(8)^{b}-Zn(2)-O(2)^{c}	137.54(9)
O(5)-Zn(1)-O(9)	89.63(9)	O(10)-Zn(2)-O(2)^{c}	87.84(9)
O(5)-Zn(1)-O(3)^{a}	98.48(9)	O(10)-Zn(2)-O(1)^{c}	136.63(10)
		2	
Zn(1)-O(3)^{a}	2.068(4)	O(3)^{b}-Zn(1)-O(9)	90.69(18)
Zn(1)-O(3)^{b}	2.068(4)	O(3)^{a}-Zn(1)-O(9)	89.31(18)
Zn(1)-O(9)^{c}	2.093(5)	O(3)^{b}-Zn(1)-O(9)^{c}	89.31(18)
Zn(1)-O(9)	2.093(5)	O(3)^{b} -Zn(1)-O(8)	88.4(2)
Zn(1)-O(8)^{c}	2.121(5)	O(8)-Zn(1)-O(8)^{c}	180.0(3)
Zn(1)-O(8)	2.121(5)	O(9)-Zn(1)-O(8)^{c}	96.97(18)
Zn(1)-Zn(2)^{d}	3.3909(6)	O(9)^{c}-Zn(1)-O(8)	96.97(18)
Zn(1)-Zn(3)	2.9764(11)	O(9)^{c}-Zn(1)-O(9)	180.0
Zn(2)^{d}- Zn(3)	3.4252(8)	O(9)-Zn(1)-O(8)	83.03(18)
Zn(2)-O(1)^{a}	1.974(6)	O(9)^{c}-Zn(1)-O(8)^{c}	83.03(18)
Zn(2)-O(2)^{a}	2.488(8)	O(9)^{d}-Zn(2)-O(1)^{a}	122.5(2)
Zn(2)-O(6)	1.990(5)	O(9)^{d}-Zn(2)-O(6)	120.74(19)
Zn(2)-O(7)^{e}	2.029(5)	O(1)^{a}-Zn(2)-O(6)	107.7(2)
Zn(2)-O(9)^{d}	1.958(4)	O(9)^{d}-Zn(2)-O(7)^{e}	105.36(19)
Zn(3)-O(4)^{b}	1.954(5)	O(1)^{a}-Zn(2)-O(7)^{e}	100.1(2)
Zn(3)-O(5)	1.914(5)	O(6)-Zn(2)-O(7)^{e}	93.7(2)
Zn(3)-O(8)	2.131(5)	O(9)^{d}-Zn(2)-O(2)^{a}	90.3(3)
Zn(3)-O(9)	1.994(5)	O(1)^{a}-Zn(2)-O(2)^{a}	57.3(3)
Zn(3)-O(11)	2.039(10)	O(6)-Zn(2)-O(2)^{a}	92.1(3)
O(3)^{a}-Zn(1)-O(8)^{c}	88.4(2)	O(7)^{e}-Zn(2)-O(2)^{a}	157.4(2)
O(3)^{b}-Zn(1)-O(8)^{c}	91.6(2)	O(5)-Zn(3)-O(4)^{b}	120.2(3)
O(3)^{a}-Zn(1)-O(3)^{b}	180.000(1)	O(5)-Zn(3)-O(9)	119.5(2)
O(3)^{a}-Zn(1)-O(9)^{c}	90.69(18)	O(4)^{b}-Zn(3)-O(9)	102.6(2)
O(3)^{a}-Zn(1)-O(8)	91.6(2)	O(5)-Zn(3)-O(11)	72.8(6)
O(5)-Zn(3)-O(8)	127.4(2)	O(4)^{b}-Zn(3)-O(11)	165.0(6)

O(4)[b]-Zn(3)-O(8)	94.4(2)	O(9)-Zn(3)-O(11)	74.3(6)
O(9)-Zn(3)-O(8)	85.16(18)	O(11)-Zn(3)-O(8)	70.9(6)
		3	
Zn(1)-O(1)[a]	1.9145(19)	O(1)[a]-Zn(1)-O(11)	103.34(9)
Zn(1)-O(8)	1.9585(19)	O(8)-Zn(1)-O(11)	98.13(8)
Zn(1)-O(5)	1.974(2)	O(5)-Zn(1)-O(11)	101.30(9)
Zn(1)-O(11)	1.995(2)	O(4)[b]-Zn(2)-O(3)[c]	147.40(9)
Zn(2)-O(4)[b]	1.960(2)	O(4)[b]-Zn(2)-O(12)	99.50(10)
Zn(2)-O(3)[c]	1.977(2)	O(3)[c]-Zn(2)-O(12)	95.47(10)
Zn(2)-O(12)	2.065(3)	O(4)[b]-Zn(2)-O(6)	115.52(9)
Zn(2)-O(6)	2.064(2)	O(3)[c]-Zn(2)-O(6)	91.87(9)
Zn(2)-O(13)	2.433(2)	O(12)-Zn(2)-O(6)	94.24(9)
O(1)[a]-Zn(1)-O(8)	123.69(9)	O(4)[b]-Zn(2)-O(13)	80.88(7)
O(1)[a]-Zn(1)-O(5)	120.43(9)	O(3)[c]-Zn(2)-O(13)	82.61(7)
O(8)-Zn(1)-O(5)	104.94(9)	O(12)-Zn(2)-O(13)	176.66(8)
		O(6)-Zn(2)-O(13)	88.56(8)
		4	
Cd(1)-O(16)[a]	2.237(3)	O(16)[a]-Cd(1)-O(14)[a]	119.75(12)
Cd(1)-O(26)	2.267(4)	O(26)-Cd(1)-O(14)[a]	86.78(15)
Cd(1)-O(14)[a]	2.287(3)	O(14)[a]-Cd(1)-O(28)	83.68(12)
Cd(1)-O(28)	2.292(3)	O(26)-Cd(1)-O(28)	90.53(16)
Cd(1)-O(27)	2.296(4)	O(16)[a]-Cd(1)-O(28)	156.36(13)
Cd(1)-O(5)	2.365(3)	O(16)[a]-Cd(1)-O(27)	86.19(13)
Cd(2)-O(6)	2.231(3)	O(28)-Cd(1)-O(27)	99.09(14)
Cd(2)-O(1)	2.275(3)	O(16)[a]-Cd(1)-O(5)	75.85(12)
Cd(2)-O(15)[a]	2.278(4)	O(14)[a]-Cd(1)-O(27)	86.92(14)
Cd(2)-O(13)[b]	2.297(3)	O(16)[a]-Cd(1)-O(26)	87.93(15)
Cd(2)-O(2)	2.464(4)	O(26)-Cd(1)-O(5)	98.41(15)
Cd(2)-O(16)[a]	2.611(4)	O(26)-Cd(1)-O(27)	167.84(16)
Cd(2)-O(14)[b]	2.6839(4)	O(4)-Cd(3)-O(10)[c]	88.03(12)
Cd(3)-O(4)	2.213(3)	O(4)-Cd(3)-O(11)[d]	104.72(14)
Cd(3)-O(7)	2.306(3)	O(10)[c]-Cd(3)-O(11)[d]	118.44(12)
Cd(3)-O(8)	2.405(3)	O(4)-Cd(3)-O(7)	106.95(13)
Cd(3)-O(10)[c]	2.245(3)	O(10)[c]-Cd(3)-O(7)	107.67(13)
Cd(3)-O(11)[d]	2.275(3)	O(11)[d]-Cd(3)-O(7)	124.00(13)
Cd(3)-O(12)[d]	2.596(3)	O(4)-Cd(3)-O(8)	161.72(13)
Cd(4)-O(3)	2.347(3)	O(10)[c]-Cd(3)-O(8)	92.58(12)
Cd(4)-O(9)[d]	2.267(3)	O(11)[d]-Cd(3)-O(8)	91.04(13)
Cd(4)-O(12)[d]	2.243(3)	O(7)-Cd(3)-O(8)	55.55(12)
Cd(4)-O(23)	2.254(4)	O(4)-Cd(3)-O(12)[d]	91.34(11)
Cd(4)-O(24)	2.284(4)	O(10)[c]-Cd(3)-O(12)[d]	170.84(11)
Cd(4)-O(25)	2.280(3)	O(11)[b]-Cd(3)-O(12)[d]	52.98(11)
O(14)[a]-Cd(1)-O(5)	163.91(12)	O(7)-Cd(3)-O(12)[d]	81.25(12)
O(28)-Cd(1)-O(5)	81.06(12)	O(8)-Cd(3)-O(12)[d]	90.89(12)

O(27)-Cd(1)-O(5)	90.47(14)	O(12)^{d}-Cd(4)-O(23)	90.23(15)
O(6)-Cd(2)-O(1)	111.52(15)	O(12)^{d}-Cd(4)-O(9)^{d}	118.03(12)
O(6)-Cd(2)-O(15)^{a}	99.22(16)	O(23)-Cd(4)-O(9)^{d}	83.91(16)
O(1)-Cd(2)-O(15)^{a}	123.49(13)	O(12)^{d}-Cd(4)-O(25)	159.23(12)
O(6)-Cd(2)-O(13)^{b}	89.88(13)	O(23)-Cd(4)-O(25)	90.12(16)
O(1)-Cd(2)-O(13)^{b}	100.43(12)	O(9)^{d}-Cd(4)-O(25)	82.64(12)
O(15)^{a}-Cd(2)-O(13)^{b}	126.61(12)	O(12)^{d}-Cd(4)-O(24)	83.83(13)
O(6)-Cd(2)-O(2)	165.55(15)	O(23)-Cd(4)-O(24)	165.98(17)
O(1)-Cd(2)-O(2)	55.08(12)	O(9)^{d}-Cd(4)-O(24)	87.68(14)
O(15)^{a}-Cd(2)-O(2)	93.60(13)	O(25)-Cd(4)-O(24)	99.93(14)
O(13)^{b}-Cd(2)-O(2)	87.78(12)	O(12)^{d}-Cd(4)-O(3)	79.32(11)
O(6)-Cd(2)-O(16)^{a}	85.20(12)	O(23)-Cd(4)-O(3)	105.92(16)
O(1)-Cd(2)-O(16)^{a}	83.27(12)	O(9)^{d}-Cd(4)-O(3)	160.54(12)
O(15)^{a}-Cd(2)-O(16)^{a}	52.60(11)	O(25)-Cd(4)-O(3)	80.63(12)
O(13)^{b}-Cd(2)-O(16)^{a}	174.69(11)	O(24)-Cd(4)-O(3)	85.49(13)
O(2)-Cd(2)-O(16)^{a}	97.48(12)		
		5	
Cd(1)-O(1)^{a}	2.312(4)	Cd(4)-O(19)	2.440(6)
Cd(1)-O(10)^{b}	2.334(5)	O(1)^{a}-Cd(1)-O(9)^{b}	142.78(16)
Cd(1)-O(7)	2.332(4)	O(10)^{b}-Cd(1)-O(7)	87.9(2)
Cd(1)-O(9)^{b}	2.341(5)	O(10)^{b}-Cd(1)-O(9)^{b}	55.53(18)
Cd(1)-O(8)^{c}	2.397(4)	O(7)-Cd(1)-O(9)^{b}	94.66(17)
Cd(1)-O(5)	2.448(4)	O(1)^{a}-Cd(1)-O(8)^{c}	81.34(14)
Cd(1)-O(2)^{a}	2.570(4)	O(7)-Cd(1)-O(8)^{c}	160.51(14)
Cd(2)-O(8)^{c}	2.217(4)	O(1)^{a}-Cd(1)-O(5)	87.97(13)
Cd(2)-O(16)^{d}	2.257(4)	O(10)^{b}-Cd(1)-O(5)	80.43(17)
Cd(2)-O(17)	2.263(5)	O(9)^{b}-Cd(1)-O(8)^{c}	84.47(16)
Cd(2)-O(4)^{e}	2.299(5)	O(10)^{b}-Cd(1)-O(8)^{c}	107.3(2)
Cd(2)-O(18)	2.358(5)	O(1)^{a}-Cd(1)-O(7)	87.88(15)
Cd(2)-O(5)	2.398(4)	O(1)^{a}-Cd(1)-O(10)^{b}	161.55(17)
Cd(3)-O(6)	2.259(4)	O(9)^{b}-Cd(1)-O(5)	118.26(16)
Cd(3)-O(3)^{e}	2.264(5)	O(8)^{c}-Cd(1)-O(5)	68.59(13)
Cd(3)-O(14)	2.331(4)	O(1)^{a}-Cd(1)-O(2)^{a}	53.09(13)
Cd(3)-O(13)	2.489(5)	O(10)^{b}-Cd(1)-O(2)^{a}	141.59(17)
Cd(3)-O(15)^{e}	2.368(4)	O(7)-Cd(1)-O(2)^{a}	73.51(14)
Cd(3)-O(16)^{e}	2.413(4)	O(9)^{b}-Cd(1)-O(2)^{a}	92.09(16)
Cd(3)-O(20)	2.314(7)	O(8)^{c}-Cd(1)-O(2)^{a}	87.05(14)
Cd(4)-O(6)	2.509(4)	O(5)-Cd(1)-O(2)^{a}	137.42(13)
Cd(4)-O(11)^{f}	2.332(7)	O(7)-Cd(1)-O(5)	127.49(13)
Cd(4)-O(12)^{f}	2.304(7)	O(8)^{c}-Cd(2)-O(18)	88.45(17)
Cd(4)-O(13)^{g}	2.561(4)	O(17)-Cd(2)-O(4)^{e}	83.92(18)
Cd(4)-O(14)	2.311(4)	O(16)^{d}-Cd(2)-O(4)^{e}	94.04(17)
Cd(4)-O(15)	2.318(4)	O(8)^{c}-Cd(2)-O(16)^{d}	100.91(16)
O(4)^{e}-Cd(2)-O(5)	85.00(15)	O(6)-Cd(3)-O(13)	134.47(14)

O(17)-Cd(2)-O(5)	167.78(15)	O(3)^{e}-Cd(3)-O(13)	78.80(18)
O(16)^{d}-Cd(2)-O(5)	85.97(14)	O(20)-Cd(3)-O(13)	89.5(3)
O(8)^{c}-Cd(2)-O(5)	72.43(13)	O(14)-Cd(3)-O(13)	53.68(15)
O(4)^{e}-Cd(2)-O(18)	75.12(18)	O(15)^{d}-Cd(3)-O(13)	74.30(15)
O(17)-Cd(2)-O(18)	90.6(2)	O(6)-Cd(4)-O(13)^{g}	114.77(16)
O(16)^{d}-Cd(2)-O(18)	169.06(18)	O(12)^{f}-Cd(4)-O(14)	106.1(2)
O(18)-Cd(2)-O(5)	91.54(16)	O(12)^{f}-Cd(4)-O(15)	89.2(3)
O(8)^{c}-Cd(2)-O(4)^{e}	151.75(16)	O(14)-Cd(4)-O(15)	84.29(16)
O(16)^{d}-Cd(2)-O(17)	89.70(19)	O(12)^{f}-Cd(4)-O(11)^{f}	54.7(3)
O(8)^{c}-Cd(2)-O(17)	119.67(16)	O(14)-Cd(4)-O(11)^{f}	122.6(2)
O(16)^{d}-Cd(3)-O(13)	128.00(14)	O(15)-Cd(4)-O(11)^{f}	138.1(2)
O(20)-Cd(3)-O(16)^{d}	83.3(3)	O(12)^{f}-Cd(4)-O(19)	158.4(3)
O(3)^{e}-Cd(3)-O(16)^{d}	105.54(18)	O(14)-Cd(4)-O(19)	90.82(19)
O(15)^{d}-Cd(3)-O(16)^{d}	54.09(14)	O(15)-Cd(4)-O(19)	79.04(18)
O(6)-Cd(3)-O(14)	80.81(15)	O(11)^{f}-Cd(4)-O(19)	126.4(2)
O(6)-Cd(3)-O(16)^{d}	94.89(14)	O(12)^{f}-Cd(4)-O(6)	128.5(2)
O(14)-Cd(3)-O(15)^{d}	126.18(16)	O(14)-Cd(4)-O(6)	76.13(14)
O(20)-Cd(3)-O(15)^{d}	87.9(3)	O(15)-Cd(4)-O(6)	140.89(17)
O(3)^{e}-Cd(3)-O(15)^{d}	90.96(19)	O(11)^{f}-Cd(4)-O(6)	80.25(19)
O(6)-Cd(3)-O(15)^{d}	148.05(14)	O(19)-Cd(4)-O(6)	67.90(16)
O(20)-Cd(3)-O(14)	79.6(3)	O(12)^{f}-Cd(4)-O(13)^{g}	84.6(2)
O(3)^{e}-Cd(3)-O(14)	91.6(2)	O(14)-Cd(4)-O(13)^{g}	155.59(17)
O(14)-Cd(3)-O(16)^{d}	162.84(17)	O(15)-Cd(4)-O(13)^{g}	73.77(16)
O(6)-Cd(3)-O(3)^{e}	106.50(17)	O(11)^{f}-Cd(4)-O(13)^{g}	81.5(2)
O(6)-Cd(3)-O(20)	80.1(3)	O(19)-Cd(4)-O(13)^{g}	74.84(18)
O(3)^{e}-Cd(3)-O(20)	168.1(3)		

Symmetry codes:(**1**) a -x,-y,-z; b -x+1,-y,-z+1; c -x+2,-y+1,-z+1;
(**2**) a x-1/2,-y-3/2,z+1/2 ; b -x+3/2,y-1/2,-z-1/2; c -x+1,-y-2,-z; d -x+1,-y-1,-z; e x,y+1,z;
(**3**) a -x+1/2,-y+3/2,-z;b -x+1/2,y+1/2,-z+1/2; c x+1/2,y+1/2,z;
(**4**) a x,-y+5/2,z+1/2; b -x+1,-y+3,-z; c -x+2,-y+2,-z+1; d x,-y+5/2,z-1/2;
(**5**) a -x+2,y-1/2,-z+3/2;b -x+1,-y+1,-z+1;c x,-y+1/2,z+1/2;d x,-y+3/2,z+1/2; e -x+2,y+1/2,-z+3/2;
f -x+1,y-1/2,-z+1/2; g x,-y+3/2,z-1/2

Figure S1 Comparison of experimental and calculated powder X-ray diffraction patterns of complex **1**.

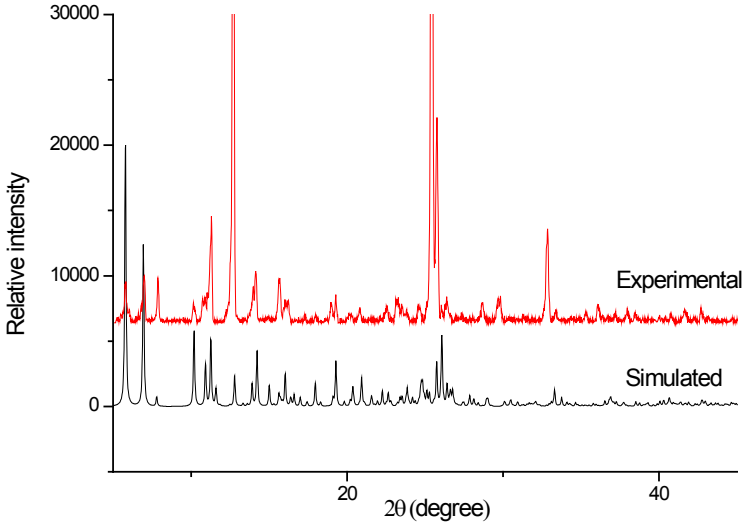

Figure S2 Comparison of experimental and calculated powder X-ray diffraction patterns of complex **2**.

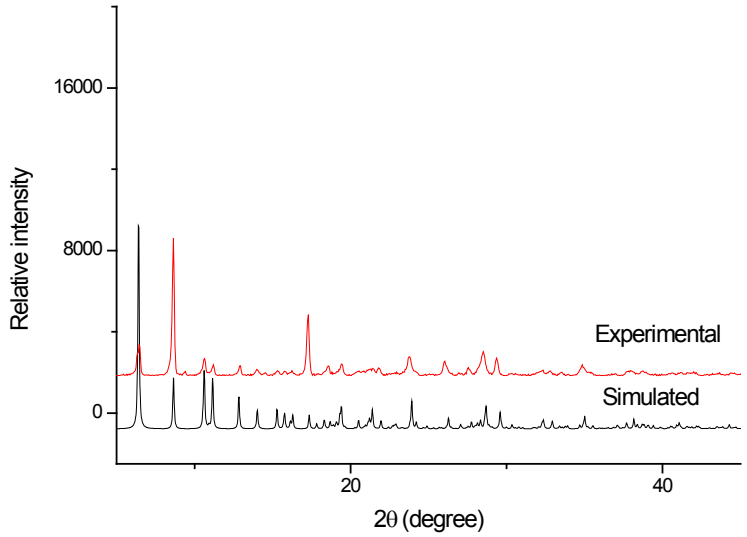

Figure S3 Comparison of experimental and calculated powder X-ray diffraction patterns of complex **3**.

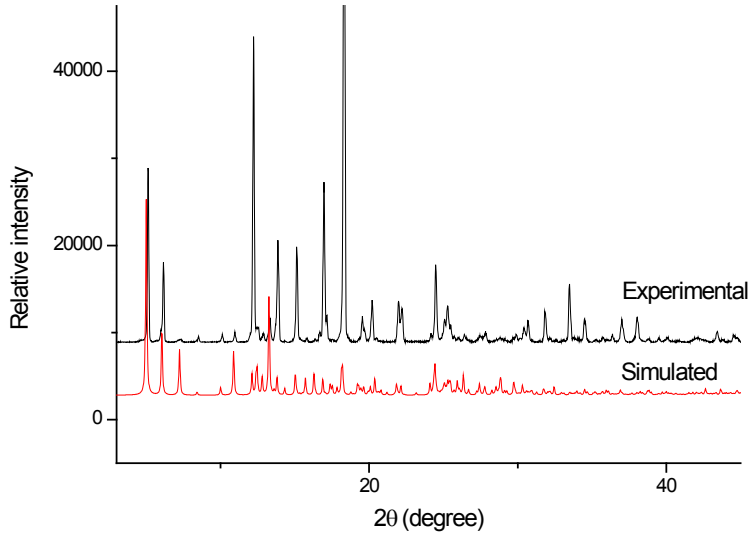

Figure S4 Comparison of experimental and calculated powder X-ray diffraction patterns of complex **4**.

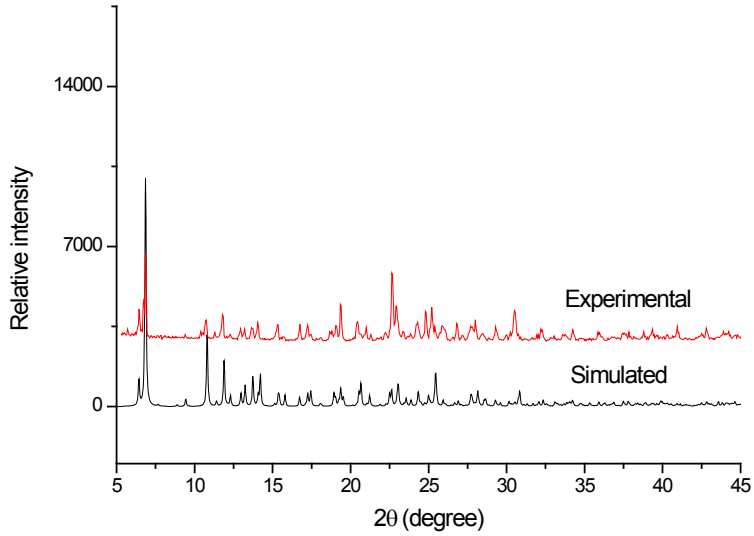

Figure S5 Comparison of experimental and calculated powder X-ray diffraction patterns of complex **5**.

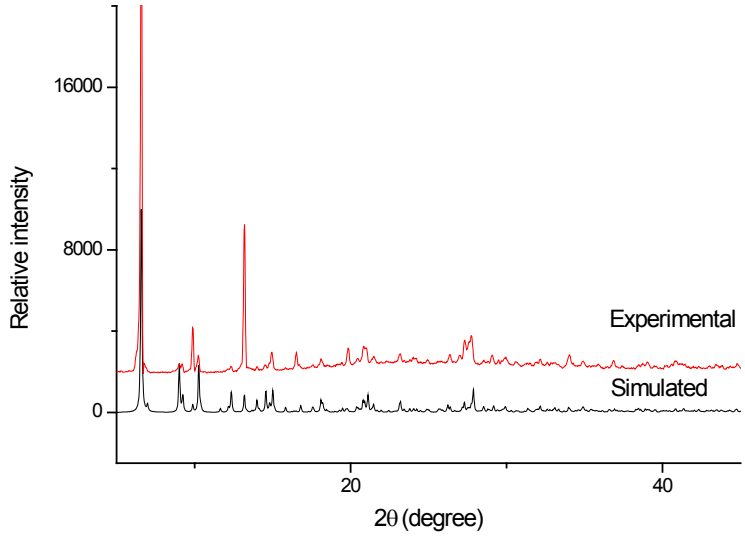

Figure S6 MS spectra of H4CCTA

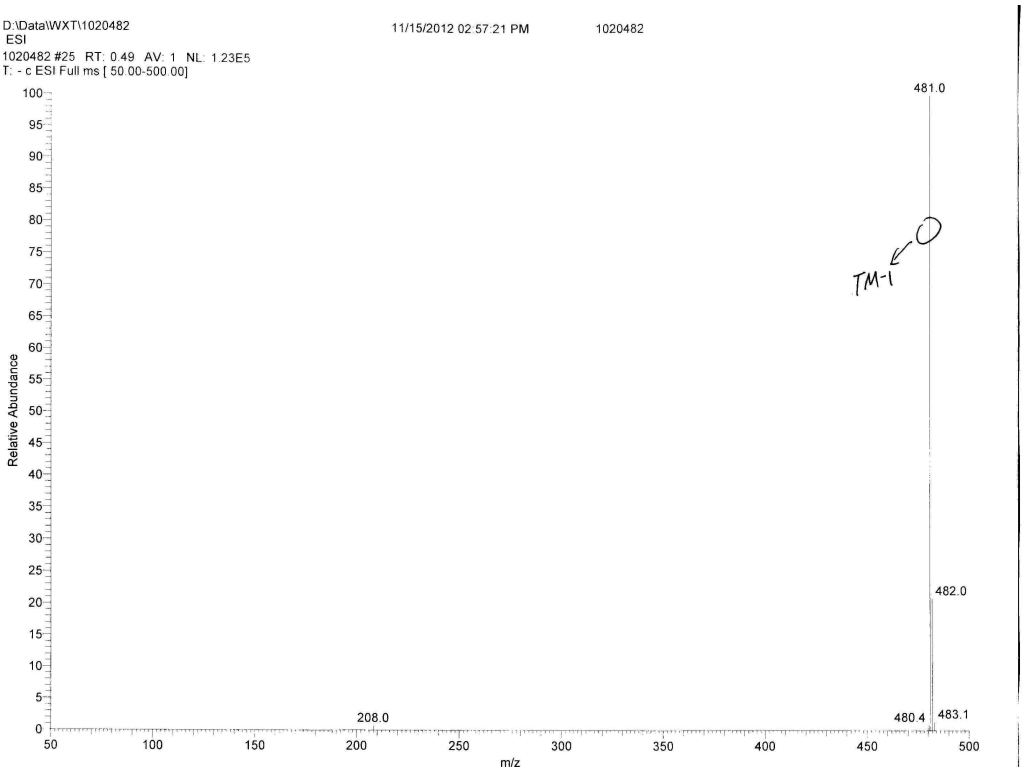

Figure S7 ^{1}H NMR of H4CCTA

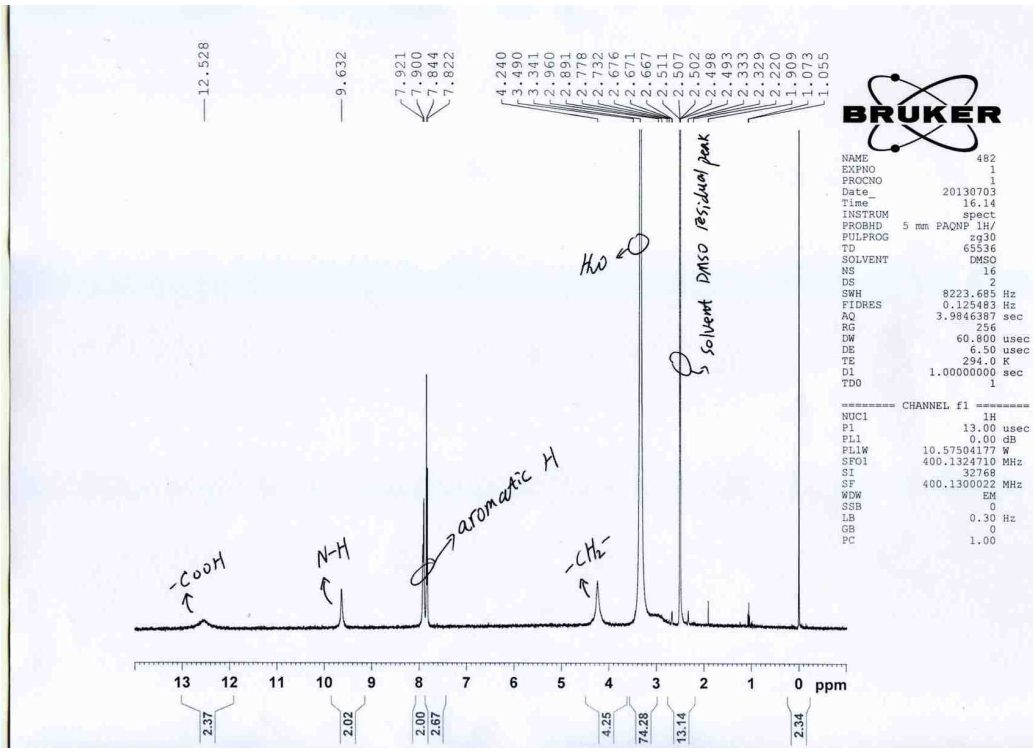

Figure S8 TG curves for complexes 1-5