Supplementary Material (ESI) for CrystEngComm

A series of coordination polymers based on 5,5'-(ethane-1,2-diyl)-bis(oxy)diisophthalic acid and structurally related N-donor ligands: syntheses, structures and properties

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Table S1. Selected bond distances (Å) and angles (°) for **1**.

Ni(1)-O(4)#1	1.9665(18)	Ni(1)-O(1)	2.0057(19)
Ni(1)-O(10)#2	2.0790(17)	Ni(1)-O(8)#3	2.1086(19)
Ni(1)-O(7)#3	2.1136(19)	Ni(1)-O(9)#2	2.2079(19)
Ni(2)-O(3)#1	1.9983(18)	Ni(2)-O(2)	2.0448(18)
Ni(2)-O(3W)	2.053(2)	Ni(2)-O(1W)	2.0653(18)
Ni(2)-O(2W)	2.073(2)	Ni(2)-O(10)#2	2.1079(18)
O(4)#1-Ni(1)-O(1)	96.69(9)	O(4)#1-Ni(1)-O(10)#2	101.87(8)
O(1)-Ni(1)-O(10)#2	100.18(7)	O(4)#1-Ni(1)-O(8)#3	154.02(8)
O(1)-Ni(1)-O(8)#3	92.96(9)	O(10)#2-Ni(1)-O(8)#3	100.06(7)
O(4)#1-Ni(1)-O(7)#3	93.09(7)	O(1)-Ni(1)-O(7)#3	97.66(8)
O(10)#2-Ni(1)-O(7)#3	155.11(8)	O(8)#3-Ni(1)-O(7)#3	61.66(7)
O(4)#1-Ni(1)-O(9)#2	92.51(9)	O(1)-Ni(1)-O(9)#2	160.40(7)
O(10)#2-Ni(1)-O(9)#2	60.87(7)	O(8)#3-Ni(1)-O(9)#2	86.11(8)
O(7)#3-Ni(1)-O(9)#2	99.09(8)	O(3)#1-Ni(2)-O(2)	96.55(9)
O(3)#1-Ni(2)-O(3W)	89.44(9)	O(2)-Ni(2)-O(3W)	173.93(8)
O(3)#1-Ni(2)-O(1W)	172.83(8)	O(2)-Ni(2)-O(1W)	86.35(8)
O(3W)-Ni(2)-O(1W)	87.58(9)	O(3)#1-Ni(2)-O(2W)	82.53(8)
O(2)-Ni(2)-O(2W)	90.21(9)	O(3W)-Ni(2)-O(2W)	89.64(10)
O(1W)-Ni(2)-O(2W)	90.93(8)	O(3)#1-Ni(2)-O(10)#2	96.89(7)
O(2)-Ni(2)-O(10)#2	87.20(8)	O(3W)-Ni(2)-O(10)#2	93.03(9)
O(1W)-Ni(2)-O(10)#2	89.78(7)	O(2W)-Ni(2)-O(10)#2	177.26(8)

Symmetry transformations used to generate equivalent atoms:
#1 –x + 1/2, y - 1/2, -z + 3/2; #2 –x + 1/2, y - 1/2, -z + 1/2; #3 x + 1, y, z + 1.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Ni(1)-N(1)	2.0411(18)	Ni(1)-O(1)	2.0441(16)
Ni(1)-N(4)#1	2.061(2)	Ni(1)-O(1W)	2.1504(17)
Ni(1)-O(10)#2	2.1686(18)	Ni(1)-O(9)#2	2.1821(17)
Ni(2)-N(5)	2.018(2)	Ni(2)-N(8)#3	2.024(2)
Ni(2)-O(8)	2.0533(16)	Ni(2)-O(3)	2.0832(16)
Ni(2)-O(4)	2.1839(16)	Ni(2)-O(7)	2.2701(15)
N(1)-Ni(1)-O(1)	98.22(7)	N(1)-Ni(1)-N(4)#1	96.23(8)
O(1)-Ni(1)-N(4)#1	88.67(7)	N(1)-Ni(1)-O(1W)	89.38(7)
O(1)-Ni(1)-O(1W)	88.41(7)	N(4)#1-Ni(1)-O(1W)	174.00(7)
N(1)-Ni(1)-O(10)#2	97.63(7)	O(1)-Ni(1)-O(10)#2	164.06(6)
N(4)#1-Ni(1)-O(10)#2	91.26(8)	O(1W)-Ni(1)-O(10)#2	90.10(7)
N(1)-Ni(1)-O(9)#2	156.22(7)	O(1)-Ni(1)-O(9)#2	103.55(6)
N(4)#1-Ni(1)-O(9)#2	93.76(8)	O(1W)-Ni(1)-O(9)#2	81.83(7)
O(10)#2-Ni(1)-O(9)#2	60.55(6)	N(5)-Ni(2)-N(8)#3	96.16(8)
N(5)-Ni(2)-O(8)	103.27(7)	N(8)#3-Ni(2)-O(8)	93.28(8)
N(5)-Ni(2)-O(3)	94.18(8)	N(8)#3-Ni(2)-O(3)	95.97(8)
O(8)-Ni(2)-O(3)	159.24(7)	N(5)-Ni(2)-O(4)	155.47(8)
N(8)#3-Ni(2)-O(4)	91.67(7)	O(8)-Ni(2)-O(4)	99.42(6)
O(3)-Ni(2)-O(4)	61.82(7)	N(5)-Ni(2)-O(7)	89.21(7)
N(8)#3-Ni(2)-O(7)	154.09(8)	O(8)-Ni(2)-O(7)	60.85(6)
O(3)-Ni(2)-O(7)	108.94(7)	O(4)-Ni(2)-O(7)	93.83(6)

Symmetry transformations used to generate equivalent atoms:

#1 x, -y + 1/2, z - 1/2; #2 -x, y + 1/2, -z + 1/2; #3 –x + 1,y - 1/2,-z + 1/2.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Co(1)-O(8)#4	1.989(3)	Co(1)-O(1)	2.010(2)

Co(1)-N(1)	2.020(4)	Co(1)-N(4)#5	2.036(4)
Co(2)-N(5)	2.016(4)	Co(2)-O(4)#1	2.032(3)
Co(2)-O(10)#2	2.064(4)	Co(2)-O(3)	2.067(3)
Co(2)-O(9)#3	2.187(4)	Co(2)-O(9)#2	2.393(4)
O(8)#4-Co(1)-O(1)	99.98(13)	O(8)#4-Co(1)-N(1)	115.64(16)
O(1)-Co(1)-N(1)	111.64(14)	O(8)#4-Co(1)-N(4)#5	97.71(15)
O(1)-Co(1)-N(4)#5	115.88(15)	N(1)-Co(1)-N(4)#5	114.46(17)
N(5)-Co(2)-O(4)#1	94.53(14)	N(5)-Co(2)-O(10)#2	110.39(15)
O(4)#1-Co(2)-O(10)#2	98.87(14)	N(5)-Co(2)-O(3)	97.99(15)
O(4)#1-Co(2)-O(3)	161.39(12)	O(10)#2-Co(2)-O(3)	89.63(13)
N(5)-Co(2)-O(9)#3	89.37(15)	O(4)#1-Co(2)-O(9)#3	83.06(13)
O(10)#2-Co(2)-O(9)#3	159.82(12)	O(3)-Co(2)-O(9)#3	83.37(12)
N(5)-Co(2)-O(9)#2	169.05(15)	O(4)#1-Co(2)-O(9)#2	86.40(12)
O(10)#2-Co(2)-O(9)#2	58.75(12)	O(3)-Co(2)-O(9)#2	83.92(12)
O(9)#3-Co(2)-O(9)#2	101.57(12)		

Symmetry transformations used to generate equivalent atoms:

#1 –x + 3, -y, -z +3; #2 x - 1, y, z; #3 –x + 4, -y, -z + 3; #4 x - 1, y, z - 1; #5 –x + 4, -y + 2, -z + 2.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Co(1)-O(1)	2.007(4)	Co(1)-O(9)#1	2.088(4)
Co(1)-O(2W)	2.107(4)	Co(1)-N(1)	2.126(4)
Co(1)-O(3)#2	2.155(4)	Co(1)-O(1W)	2.171(3)
Co(2)-O(10)#1	2.031(3)	Co(2)-O(8)#3	2.058(3)
Co (2)-O(2)	2.091(3)	Co(2)-N(7)	2.132(4)
Co(2)-N(6)#4	2.145(4)	Co(2)-O(1W)	2.229(3)
O(1)-Co(1)-O(9)#1	100.42(16)	O(1)-Co(1)-O(2W)	174.32(16)
O(9)#1-Co(1)-O(2W)	85.22(16)	O(1)-Co(1)-N(1)	89.99(17)
O(9)#1-Co(1)-N(1)	88.43(16)	O(2W)-Co(1)-N(1)	89.51(17)

O(1)-Co(1)-O(3)#2	83.71(15)	O(9)#1-Co(1)-O(3)#2	173.85(15)
O(2W)-Co(1)-O(3)#2	90.62(15)	N(1)-Co(1)-O(3)#2	87.01(16)
O(1)-Co(1)-O(1W)	90.53(14)	O(9)#1-Co(1)-O(1W)	93.00(13)
O(2W)-Co(1)-O(1W)	89.82(14)	N(1)-Co(1)-O(1W)	178.36(15)
O(3)#2-Co(1)-O(1W)	91.50(13)	O(10)#1-Co(2)-O(8)#3	173.73(14)
O(10)#1-Co(2)-O(2)	92.38(15)	O(8)#3-Co(2)-O(2)	91.81(15)
O(10)#1-Co(2)-N(7)	86.68(16)	O(8)#3-Co(2)-N(7)	88.92(15)
O(2)-Co(2)-N(7)	86.66(15)	O(10)#1-Co(2)-N(6)#4	88.54(16)
O(8)#3-Co(2)-N(6)#4	87.07(16)	O(2)-Co(2)-N(6)#4	177.43(15)
N(7)-Co(2)-N(6)#4	90.99(17)	O(10)#1-Co(2)-O(1W)	91.47(13)
O(8)#3-Co(2)-O(1W)	92.93(13)	O(2)-Co(2)-O(1W)	93.48(13)
N(7)-Co(2)-O(1W)	178.14(15)	N(6)#4-Co(2)-O(1W)	88.90(14)

Symmetry transformations used to generate equivalent atoms:

#1 -x, -y + 1, -z + 1; #2 –x + 1, -y + 1, -z + 1; #3 x + 1/2, -y + 1/2, -z + 1; #4 x - 1/2, y - 1/2, -z + 1/2.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Ni(1)-O(1)	2.016(3)	Ni(1)-O(1)#1	2.016(3)
Ni(1)-N(1)	2.037(14)	Ni(1)-N(1)#1	2.037(14)
Ni(1)-O(1W)#1	2.125(3)	Ni(1)-O(1W)	2.125(3)
Ni(2)-O(6)	1.989(6)	Ni(2)-O(4)#2	2.002(3)
Ni(2)-O(4)#3	2.002(3)	Ni(2)-O(3)	2.009(3)
Ni(2)-O(3)#4	2.009(3)		
O(1)-Ni(1)-O(1)#1	180.00(7)	O(1)-Ni(1)-N(1)	98.9(3)
O(1)#1-Ni(1)-N(1)	81.1(3)	O(1)-Ni(1)-N(1)#1	81.1(3)
O(1)#1-Ni(1)-N(1)#1	98.9(3)	N(1)-Ni(1)-N(1)#1	180.000(3)
O(1)-Ni(1)-O(1W)#1	88.80(14)	O(1)#1-Ni(1)-O(1W)#1	91.20(14)
N(1)-Ni(1)-O(1W)#1	84.2(3)	N(1)#1-Ni(1)-O(1W)#1	95.8(3)
O(1)-Ni(1)-O(1W)	91.20(14)	O(1)#1-Ni(1)-O(1W)	88.80(14)

N(1)-Ni(1)-O(1W)	95.8(3)	N(1)#1-Ni(1)-O(1W)	84.2(3)
O(1W)#1-Ni(1)-O(1W)	180.0	O(6)-Ni(2)-O(4)#2	95.39(16)
O(6)-Ni(2)-O(4)#3	95.39(16)	O(4)#2-Ni(2)-O(4)#3	89.1(2)
O(6)-Ni(2)-O(3)	98.22(16)	O(4)#2-Ni(2)-O(3)	166.37(15)
O(4)#3-Ni(2)-O(3)	89.15(18)	O(6)-Ni(2)-O(3)#4	98.22(16)
O(4)#2-Ni(2)-O(3)#4	89.15(17)	O(4)#3-Ni(2)-O(3)#4	166.37(15)
O(3)-Ni(2)-O(3)#4	89.4(3)		

Symmetry transformations used to generate equivalent atoms:

#1 –x + 3/2, -y + 3/2, -z + 1; #2 –x + 2, -y + 2, -z + 2; #3 –x + 2, y, -z + 2; #4 x, -y + 2, z.

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Zn(1)-O(1)	1.938(4)	Zn(1)-O(11)	1.950(4)
Zn(1)-N(1)	1.985(5)	Zn(1)-O(4)#5	1.990(4)
Zn(2)-O(12)	1.949(4)	Zn(2)-O(8)	2.001(4)
Zn(2)-N(4)#4	2.004(4)	Zn(2)-O(10)#3	2.061(3)
Zn(2)-O(7)	2.431(4)	Zn(3)-O(11)#1	1.896(4)
Zn(3)-O(12)	1.917(3)	Zn(3)-O(3)#2	1.963(4)
Zn(3)-O(9)#3	1.980(4)		
O(1)-Zn(1)-O(11)	106.00(16)	O(1)-Zn(1)-N(1)	120.80(19)
O(11)-Zn(1)-N(1)	106.41(19)	O(1)-Zn(1)-O(4)#5	114.81(18)
O(11)-Zn(1)-O(4)#5	97.96(15)	N(1)-Zn(1)-O(4)#5	107.99(17)
O(12)-Zn(2)-O(8)	128.01(14)	O(12)-Zn(2)-N(4)#4	109.95(18)
O(8)-Zn(2)-N(4)#4	110.53(17)	O(12)-Zn(2)-O(10)#3	102.78(15)
O(8)-Zn(2)-O(10)#3	102.90(15)	N(4)#4-Zn(2)-O(10)#3	97.42(16)
O(12)-Zn(2)-O(7)	87.52(14)	O(8)-Zn(2)-O(7)	58.27(14)
N(4)#4-Zn(2)-O(7)	94.40(16)	O(10)#3-Zn(2)-O(7)	160.54(15)
O(11)#1-Zn(3)-O(12)	119.01(15)	O(11)#1-Zn(3)-O(3)#2	107.92(17)
O(12)-Zn(3)-O(3)#2	115.72(17)	O(11)#1-Zn(3)-O(9)#3	106.68(17)

O(12)-Zn(3)-O(9)#3	105.21(16)	O(3)#2-Zn(3)-O(9)#3	100.15(18)

Symmetry transformations used to generate equivalent atoms:

#1 x - 1, y + 1, z - 1; #2 x, y + 1, z - 1; #3 x, y + 1, z; #4 x, y, z - 1; #5 x + 1, y, z.

Table S7. Selected bond distances (Å) and angles (°) for **7**.

Ni(1)-O(1)	2.059(2)	Ni(1)-N(6)#1	2.071(3)
Ni(1)-O(3)#2	2.080(2)	Ni(1)-N(1)	2.087(3)
Ni(1)-O(2W)	2.106(2)	Ni(1)-O(1W)	2.113(2)
O(1)-Ni(1)-N(6)#1	91.62(10)	O(1)-Ni(1)-O(3)#2	179.80(9)
N(6)#1-Ni(1)-O(3)#2	88.56(10)	O(1)-Ni(1)-N(1)	89.58(10)
N(6)#1-Ni(1)-N(1)	178.42(11)	O(3)#2-Ni(1)-N(1)	90.24(10)
O(1)-Ni(1)-O(2W)	92.19(8)	N(6)#1-Ni(1)-O(2W)	88.66(10)
O(3)#2-Ni(1)-O(2W)	87.74(8)	N(1)-Ni(1)-O(2W)	90.27(10)
O(1)-Ni(1)-O(1W)	86.97(8)	N(6)#1-Ni(1)-O(1W)	89.64(10)
O(3)#2-Ni(1)-O(1W)	93.10(8)	N(1)-Ni(1)-O(1W)	91.45(10)
O(2W)-Ni(1)-O(1W)	178.08(9)		

Symmetry transformations used to generate equivalent atoms:

#1 x + 1, -y + 1/2, z + 1/2; #2 –x + 3, y + 1/2, -z + 5/2.

Table S8. Selected bond distances (Å) and angles (°) for **8**.

Zn(1)-O(6)	1.960(3)	Zn(1)-O(1)	1.962(3)
Zn(1)-N(1)	2.022(4)	Zn(1)-N(6)#1	2.050(4)
Zn(2)-O(3)	1.946(3)	Zn(2)-O(9)#2	1.993(3)
Zn(2)-N(12)#3	1.999(4)	Zn(2)-N(7)	2.011(4)
O(6)-Zn(1)-O(1)	119.24(16)	O(6)-Zn(1)-N(1)	101.41(17)
O(1)-Zn(1)-N(1)	127.94(15)	O(6)-Zn(1)-N(6)#1	96.43(18)
O(1)-Zn(1)-N(6)#1	99.46(16)	N(1)-Zn(1)-N(6)#1	107.21(17)
O(3)-Zn(2)-O(9)#2	108.71(15)	O(3)-Zn(2)-N(12)#3	109.11(17)
O(9)#2-Zn(2)-N(12)#3	116.74(15)	O(3)-Zn(2)-N(7)	100.30(17)

O(9)#2-Zn(2)-N(7)	112.78(17)	N(12)#3-Zn(2)-N(7)	107.89(17)

Symmetry transformations used to generate equivalent atoms:
#1 –x + 3/2, y + 1/2, -z + 1/2; #2 x, y, z - 1; #3 –x + 3/2, y + 1/2, -z - 1/2.

Table S9. Selected bond distances (Å) and angles (°) for **9**.

Co(1)-O(1)	2.061(4)	Co(1)-N(1)	2.066(5)
Co(1)-O(2W)	2.095(4)	Co(1)-O(4)#1	2.160(4)
Co(1)-O(1W)	2.166(4)	Co(1)-O(3)#1	2.216(4)
O(1)-Co(1)-N(1)	108.91(19)	O(1)-Co(1)-O(2W)	93.93(17)
N(1)-Co(1)-O(2W)	93.9(2)	O(1)-Co(1)-O(4)#1	94.12(15)
N(1)-Co(1)-O(4)#1	156.22(18)	O(2W)-Co(1)-O(4)#1	90.32(16)
O(1)-Co(1)-O(1W)	87.59(16)	N(1)-Co(1)-O(1W)	87.9(2)
O(2W)-Co(1)-O(1W)	177.14(15)	O(4)#1-Co(1)-O(1W)	87.15(15)
O(1)-Co(1)-O(3)#1	153.73(15)	N(1)-Co(1)-O(3)#1	96.84(19)
O(2W)-Co(1)-O(3)#1	89.33(16)	O(4)#1-Co(1)-O(3)#1	59.77(14)
O(1W)-Co(1)-O(3)#1	88.25(15)		

Symmetry transformations used to generate equivalent atoms:

#1 x, y - 1, z.

Table S10. Selected bond distances (Å) and angles (°) for **10**.

Zn(1)-O(1)	1.947(5)	Zn(1)-N(1)	2.014(7)
Zn(1)-O(3)#1	2.017(6)	Zn(1)-N(6)#2	2.040(7)
Zn(1)-O(4)#1	2.480(8)		
O(1)-Zn(1)-N(1)	114.0(3)	O(1)-Zn(1)-O(3)#1	102.2(3)
N(1)-Zn(1)-O(3)#1	137.2(3)	O(1)-Zn(1)-N(6)#2	99.0(3)
N(1)-Zn(1)-N(6)#2	96.4(3)	O(3)#1-Zn(1)-N(6)#2	99.8(3)
O(1)-Zn(1)-O(4)#1	138.5(3)	N(1)-Zn(1)-O(4)#1	81.0(3)

O(3)#1-Zn(1)-O(4)#1	56.5(2)	N(6)#2-Zn(1)-O(4)#1	118.4(3)

Symmetry transformations used to generate equivalent atoms:

#1 –x + 3/2, y + 1/2, -z + 3/2; #2 –x + 1, y, -z + 1/2.

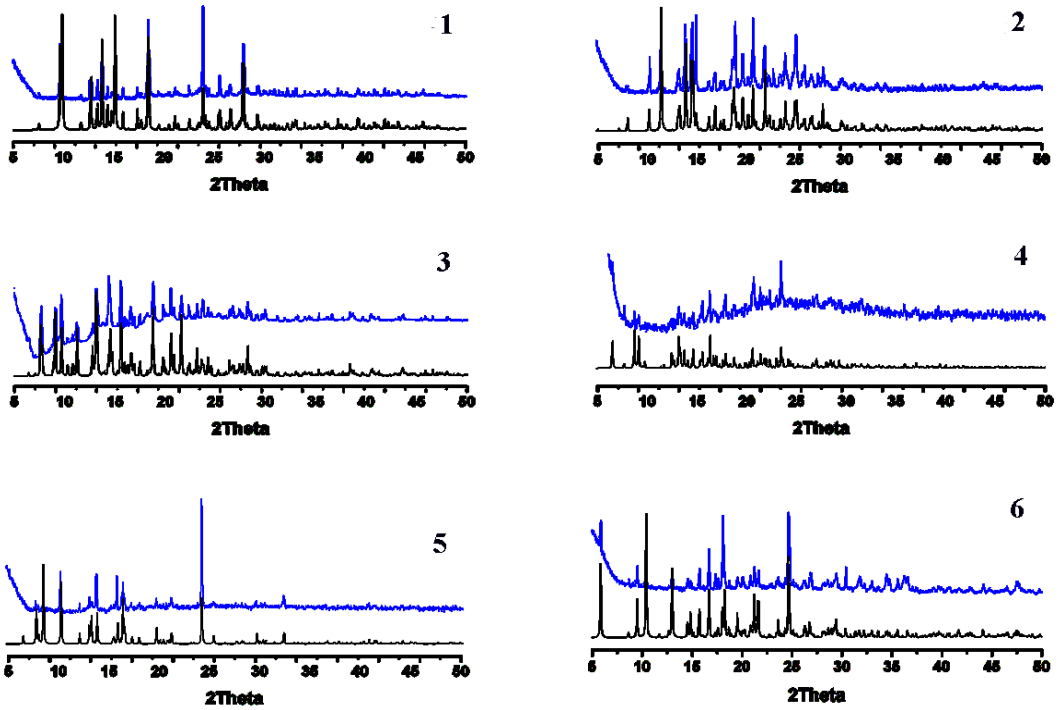

Fig. S1 The simulated (black) and experimental (blue) PXRD patterns for compounds **1**-**6**.

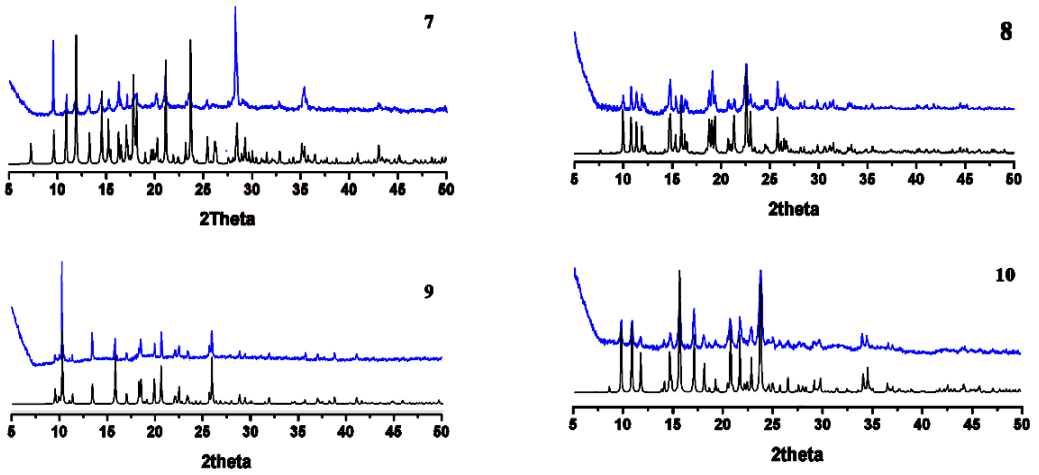

Fig. S2 The simulated (black) and experimental (blue) PXRD patterns for compounds **7**-**10**.

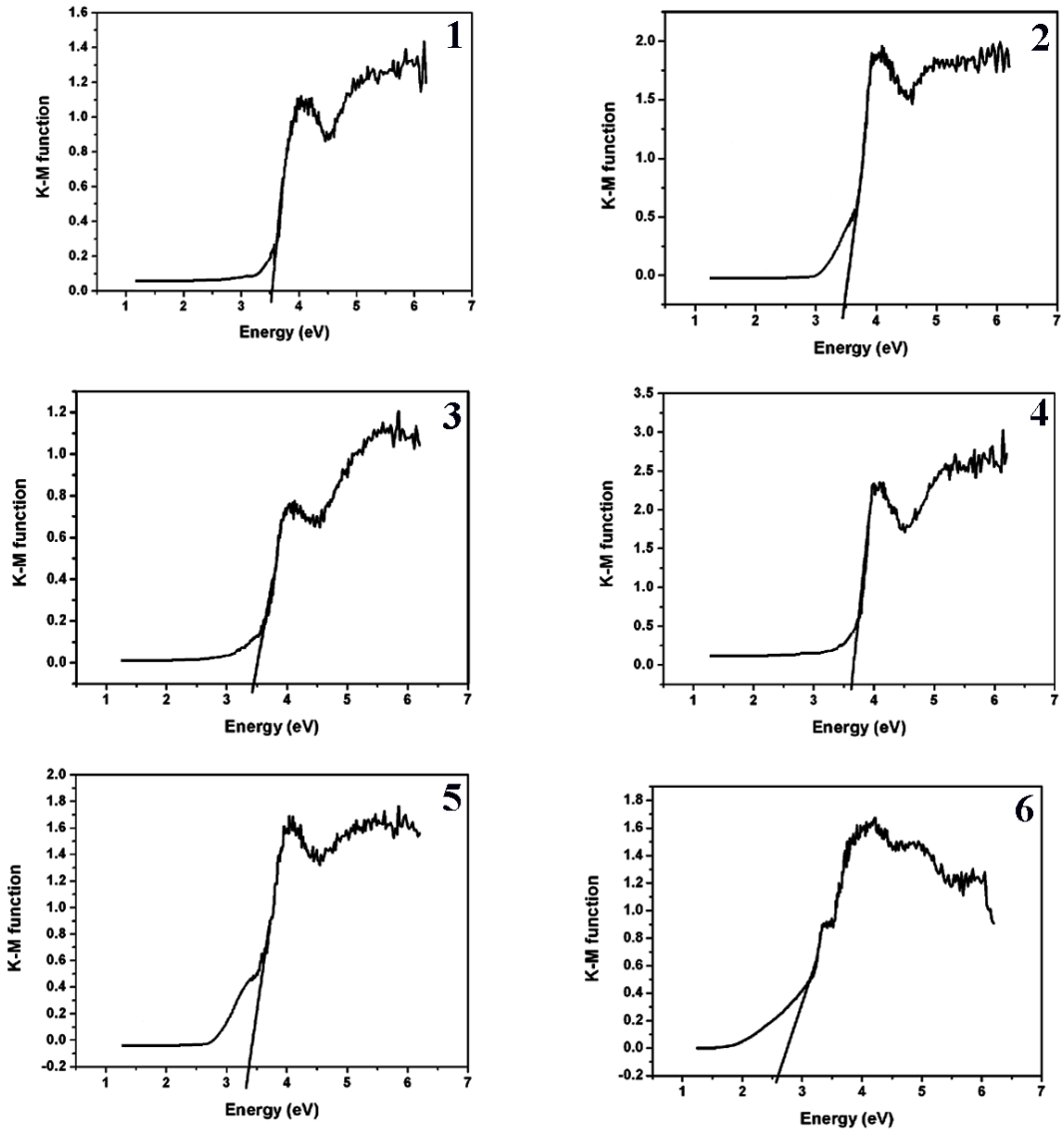

Fig. S3 UV-Vis-NIR diffuse reflectance spectra of K-M functions *vs* energy (eV) of compounds **1**-**6**.

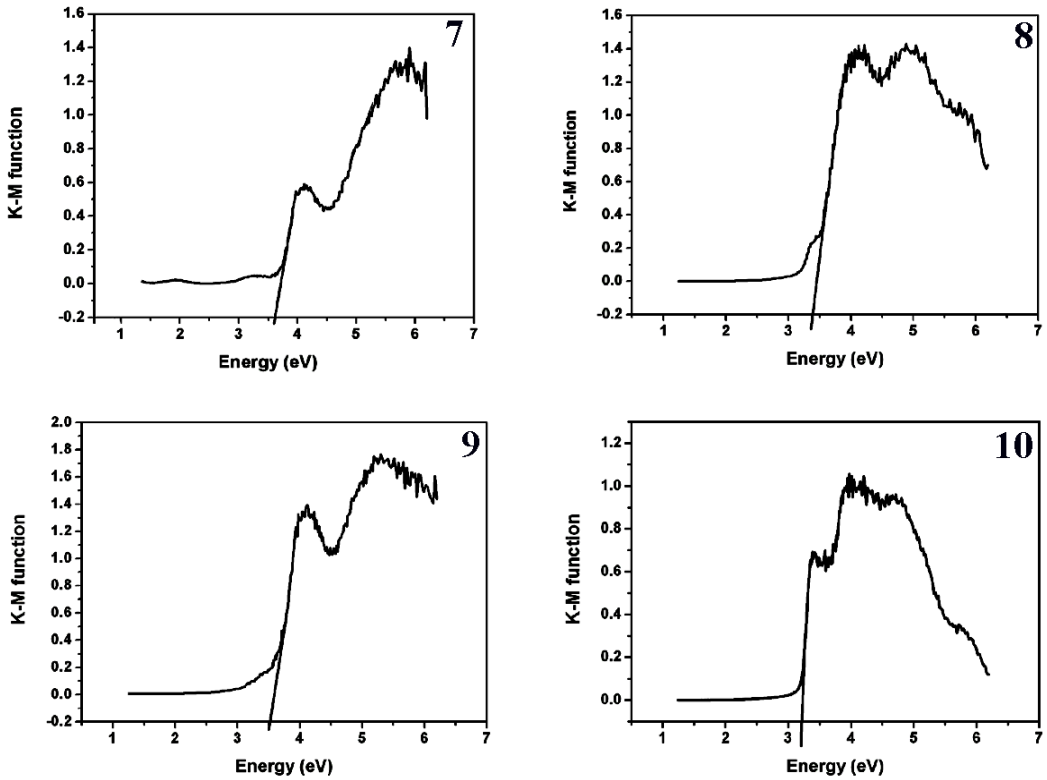

Fig. S4 UV-Vis-NIR diffuse reflectance spectra of K-M functions *vs* energy (eV) of compounds **7**-**10**.

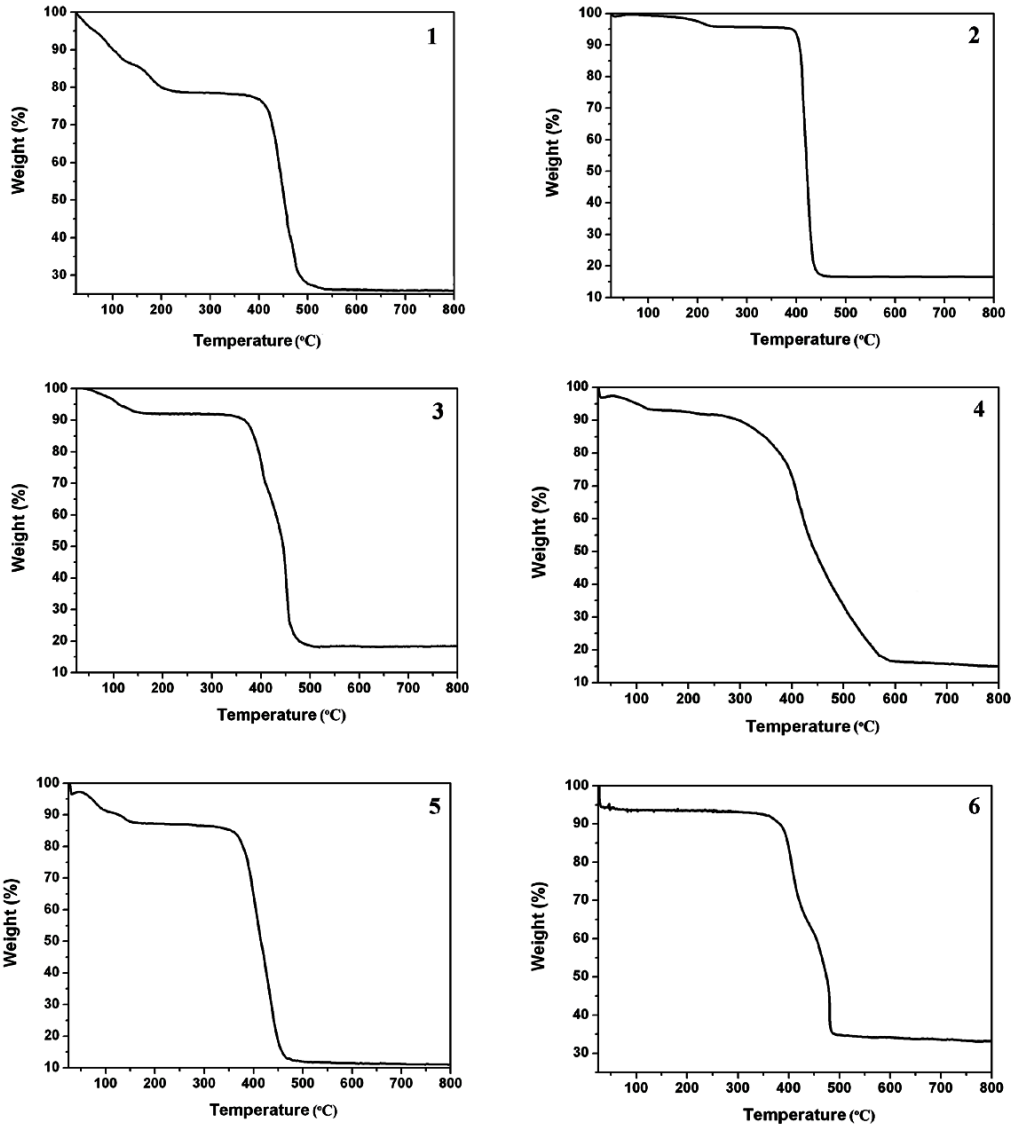

Fig. S5 The TGA curves of compounds **1**-**6**.

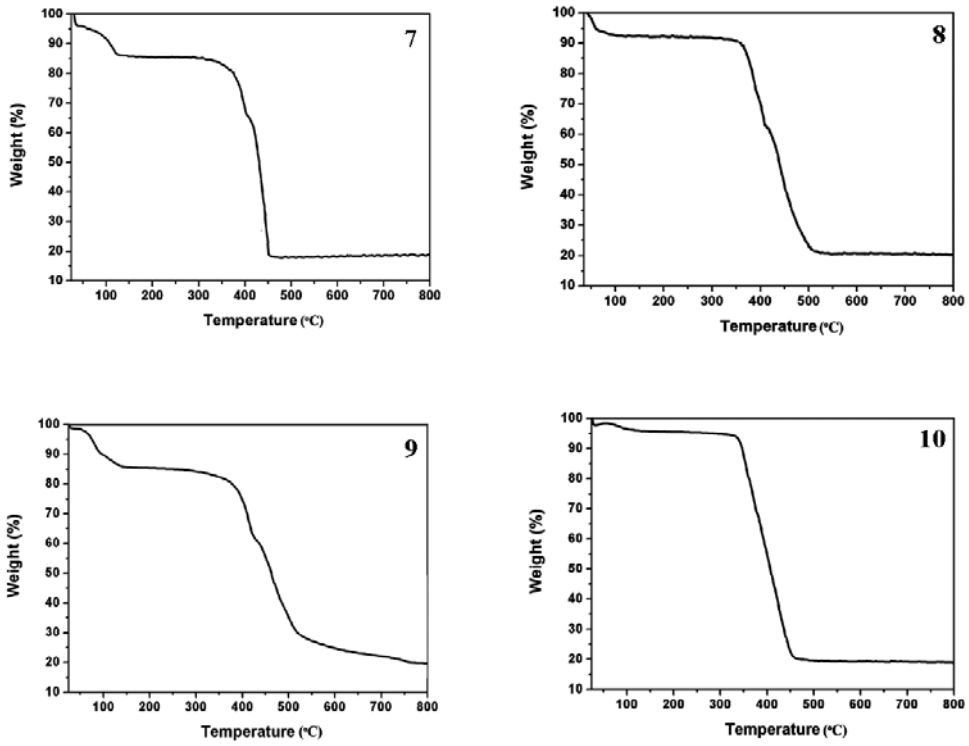

Fig. S6 The TGA curves of compounds **7**-**10**.