Supplementary Material (ESI) for CrystEngComm

A series of Cu(II) and Cd(II) coordination polymers constructed by 3,5-dinitrosalicylic acid and flexible bis(triazole) ligands containing different spacers

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

Cu(1)-O(1)	1.9493(18)	Cu(1)-O(23)	1.893(2)
Cu(1)-O(24)	1.9091(19)	Cu(1)-N(1)	1.947(3)
Cu(2)-O(2)	1.928(2)	Cu(2)-O(3)	1.9416(17)
Cu(2)-O(8)	1.9936(17)	Cu(2)-N(6)#1	1.989(3)
Cu(3)-O(9)	1.911(2)	Cu(3)-O(10)	1.9041(18)
Cu(3)-O(15)	1.9674(17)	Cu(3)-N(7)	1.966(2)
Cu(4)-O(16)	1.930(2)	Cu(4)-O(17)	1.9227(18)
Cu(4)-O(22)	2.0188(18)	Cu(4)-O(1W)	2.261(2)
Cu(4)-N(12)#2	1.983(3)		
O(23)-Cu(1)-O(24)	92.32(9)	O(23)-Cu(1)-N(1)	173.85(11)
O(24)-Cu(1)-N(1)	90.75(10)	O(23)-Cu(1)-O(1)	87.26(8)
O(24)-Cu(1)-O(1)	175.15(10)	N(1)-Cu(1)-O(1)	90.13(10)
O(2)-Cu(2)-O(3)	90.88(8)	O(2)-Cu(2)-N(6)#1	166.22(10)
O(3)-Cu(2)-N(6)#1	88.79(9)	O(2)-Cu(2)-O(8)	87.66(8)
O(3)-Cu(2)-O(8)	178.35(9)	N(6)#1-Cu(2)-O(8)	92.44(9)
O(10)-Cu(3)-O(9)	91.83(8)	O(10)-Cu(3)-N(7)	89.19(9)
O(9)-Cu(3)-N(7)	177.53(10)	O(10)-Cu(3)-O(15)	179.26(10)
O(9)-Cu(3)-O(15)	87.62(8)	N(7)-Cu(3)-O(15)	91.37(9)
O(17)-Cu(4)-O(16)	90.92(8)	O(17)-Cu(4)-N(12)#2	87.23(9)
O(16)-Cu(4)-N(12)#2	168.55(10)	O(17)-Cu(4)-O(22)	174.19(10)
O(16)-Cu(4)-O(22)	88.83(8)	N(12)#2-Cu(4)-O(22)	91.87(9)
O(17)-Cu(4)-O(1W)	97.24(10)	O(16)-Cu(4)-O(1W)	93.40(10)
N(12)#2-Cu(4)-O(1W)	98.04(11)	O(22)-Cu(4)-O(1W)	88.57(9)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$ -x, -y+1, -z+1; $^{\#2}$ -x, -y+2, -z+2.

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

Cu(1)-O(23)	1.884(3)	Cu(1)-O(24)	1.906(3)
Cu(1)-N(1)	1.955(3)	Cu(1)-O(1)	1.960(3)
Cu(2)-O(3)	1.910(3)	Cu(2)-O(2)	1.916(3)
Cu(2)-N(7)	1.966(4)	Cu(2)-O(8)	1.974(3)
Cu(3)-O(9)	1.890(3)	Cu(3)-O(10)	1.904(3)
Cu(3)-N(6)#1	1.942(4)	Cu(3)-O(15)	1.972(3)
Cu(4)-O(16)	1.916(3)	Cu(4)-O(17)	1.941(3)
Cu(4)-O(22)	1.974(2)	Cu(4)-N(12)#2	1.973(4)
Cu(4)-O(1W)	2.311(3)		
O(23)-Cu(1)-O(24)	92.69(12)	O(23)-Cu(1)-N(1)	176.50(14)
O(24)-Cu(1)-N(1)	89.18(13)	O(23)-Cu(1)-O(1)	83.84(12)
O(24)-Cu(1)-O(1)	176.51(12)	N(1)-Cu(1)-O(1)	94.30(13)
O(3)-Cu(2)-O(2)	91.04(12)	O(3)-Cu(2)-N(7)	85.92(13)

O(2)-Cu(2)-N(7)	170.66(13)	O(3)-Cu(2)-O(8)	176.29(14)
O(2)-Cu(2)-O(8)	86.63(12)	N(7)-Cu(2)-O(8)	96.82(13)
O(9)-Cu(3)-O(10)	92.98(12)	O(9)-Cu(3)-N(6)#1	175.01(18)
O(10)-Cu(3)-N(6)#1	88.97(15)	O(9)-Cu(3)-O(15)	86.12(13)
O(10)-Cu(3)-O(15)	178.76(14)	N(6)#1-Cu(3)-O(15)	91.99(16)
O(16)-Cu(4)-O(17)	90.87(12)	O(16)-Cu(4)-O(22)	88.28(12)
O(17)-Cu(4)-O(22)	174.75(13)	O(16)-Cu(4)-N(12)#2	164.45(14)
O(17)-Cu(4)-N(12)#2	87.95(14)	N(12)#2-Cu(4)-O(22)	94.24(14)
O(16)-Cu(4)-O(1W)	96.75(13)	O(17)-Cu(4)-O(1W)	92.21(12)
O(22)-Cu(4)-O(1W)	82.75(11)	N(12)#2-Cu(4)-O(1W)	98.79(15)

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

Table S3a. Selected bond distances (Å) and angles (°) for **3**.

Cu(1)-O(2)	1.8940(17)	Cu(1)-O(3)	1.9134(18)
Cu(1)-N(1)	1.969(2)	Cu(1)-O(8)	2.0274(18)
Cu(2)-O(9)	1.9125(19)	Cu(2)-O(10)	1.941(2)
Cu(2)-N(4)	1.972(2)	Cu(2)-O(1)#1	2.0101(18)
Cu(2)-O(1W)	2.297(2)		
O(2)-Cu(1)-O(3)	91.89(8)	O(2)-Cu(1)-N(1)	177.24(9)
O(3)-Cu(1)-N(1)	89.28(9)	O(2)-Cu(1)-O(8)	85.26(7)
O(3)-Cu(1)-O(8)	176.88(8)	N(1)-Cu(1)-O(8)	93.51(8)
O(9)-Cu(2)-O(10)	90.24(8)	O(9)-Cu(2)-N(4)	164.95(9)
O(10)-Cu(2)-N(4)	88.69(9)	O(9)-Cu(2)-O(1)#1	87.06(8)
O(10)-Cu(2)-O(1)#1	176.75(9)	N(4)-Cu(2)-O(1)#1	94.39(9)
O(9)-Cu(2)-O(1W)	96.49(10)	O(10)-Cu(2)-O(1W)	95.37(9)
N(4)-Cu(2)-O(1W)	98.56(10)	O(1)#1-Cu(2)-O(1W)	83.15(8)

Symmetry transformations used to generate equivalent atoms: [#1] x, -y+1/2, -z+1/2.

Table S3b. Hydrogen bonds for **3** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1A)···N(2)#4	0.839(18)	2.24(2)	3.034(3)	157(4)
O(1W)-H(1B)···O(7)#5	0.831(18)	2.43(2)	3.214(3)	157(4)

Symmetry transformations used to generate equivalent atoms: [#4] -x, -y+1, -z; [#5] -x+1/2, y+1/2, -z+1/2.

Table S4a. Selected bond distances (Å) and angles (°) for **4**.

Cu(1)-O(2)	1.922(2)	Cu(1)-O(3)	1.9443(18)
Cu(1)-N(1)	1.983(3)	Cu(1)-O(8)#1	2.0006(18)
Cu(1)-O(1W)	2.307(2)	Cu(2)-O(9)	1.888(2)
Cu(2)-O(10)	1.9031(18)	Cu(2)-N(6)#2	1.945(2)

Cu(2)-O(1)	1.9954(17)		
O(2)-Cu(1)-O(3)	89.52(8)	O(2)-Cu(1)-N(1)	157.55(9)
O(3)-Cu(1)-N(1)	86.76(9)	O(2)-Cu(1)-O(8)#1	88.13(8)
O(3)-Cu(1)-O(8)#1	171.54(9)	N(1)-Cu(1)-O(8)#1	98.44(9)
O(2)-Cu(1)-O(1W)	102.67(9)	O(3)-Cu(1)-O(1W)	91.20(9)
N(1)-Cu(1)-O(1W)	99.53(10)	O(8)#1-Cu(1)-O(1W)	81.39(8)
O(9)-Cu(2)-O(10)	92.32(8)	O(9)-Cu(2)-N(6)#2	176.03(9)
O(10)-Cu(2)-N(6)#2	90.99(9)	O(9)-Cu(2)-O(1)	84.46(8)
O(10)-Cu(2)-O(1)	176.72(8)	N(6)#2-Cu(2)-O(1)	92.24(9)

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

Table S4b. Hydrogen bonds for **4** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1B)···O(4)#2	0.840(17)	2.19(2)	2.991(3)	160(3)
O(1W)-H(1A)···O(13)#3	0.834(17)	2.33(3)	2.993(3)	137(3)

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

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

Cu(1)-O(2)	1.899(4)	Cu(1)-O(3)	1.901(4)
Cu(1)-O(8)	1.913(4)	Cu(1)-N(1)	1.978(4)
Cu(2)-O(8)	1.912(4)	Cu(2)-O(10)	1.912(4)
Cu(2)-N(2)	1.988(5)	Cu(2)-O(1W)	2.358(4)
Cu(2)-O(11)	1.920(4)	Cu(3)-N(6)#1	1.977(4)
Cu(3)-O(9)	1.983(3)	Cu(3)-O(2W)	2.292(8)
O(2)-Cu(1)-O(3)	93.50(17)	O(2)-Cu(1)-O(8)	92.73(16)
O(3)-Cu(1)-O(8)	173.46(16)	O(2)-Cu(1)-N(1)	178.86(16)
O(3)-Cu(1)-N(1)	86.34(18)	O(8)-Cu(1)-N(1)	87.39(17)
O(8)-Cu(2)-O(10)	93.86(16)	O(8)-Cu(2)-O(11)	171.34(16)
O(10)-Cu(2)-O(11)	92.44(17)	O(8)-Cu(2)-N(2)	87.03(17)
O(10)-Cu(2)-N(2)	173.52(16)	O(11)-Cu(2)-N(2)	86.05(18)
O(8)-Cu(2)-O(1W)	91.68(15)	O(10)-Cu(2)-O(1W)	94.35(15)
O(11)-Cu(2)-O(1W)	93.75(16)	N(2)-Cu(2)-O(1W)	92.03(16)
N(6)#1-Cu(3)-N(6)#2	162.7(3)	N(6)#2-Cu(3)-O(9)	89.05(17)
N(6)#2-Cu(3)-O(9)#3	92.07(17)	O(9)#3-Cu(3)-O(9)	172.6(2)
N(6)#1-Cu(3)-O(2W)	98.64(15)	O(9)-Cu(3)-O(2W)	86.28(12)

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

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

Cu(1)-O(3)	1.962(5)	Cu(1)-O(2)	1.991(5)
Cu(1)-O(1)#1	1.994(6)	Cu(1)-N(4)	2.023(5)
Cu(1)-N(1)	2.209(6)		
O(3)-Cu(1)-O(2)	90.22(19)	O(3)-Cu(1)-O(1)#1	175.6(2)
O(2)-Cu(1)-O(1)#1	87.4(2)	O(3)-Cu(1)-N(4)	89.7(2)
O(2)-Cu(1)-N(4)	163.3(2)	O(1)#1-Cu(1)-N(4)	91.6(2)
O(3)-Cu(1)-N(1)	94.2(2)	O(2)-Cu(1)-N(1)	96.3(2)
O(1)#1-Cu(1)-N(1)	89.7(2)	N(4)-Cu(1)-N(1)	100.4(2)

Symmetry transformations used to generate equivalent atoms: [#1] x-1/4, -y+3/4, -z+3/4.

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

Cu(1)-O(3)	1.905(3)	Cu(1)-O(2)	1.909(3)
Cu(1)-N(1)	1.947(3)	Cu(1)-O(1)#1	1.992(3)
O(3)-Cu(1)-O(2)	90.84(11)	O(3)-Cu(1)-N(1)	89.29(13)
O(2)-Cu(1)-N(1)	178.50(13)	O(3)-Cu(1)-O(1)#1	176.92(12)
O(2)-Cu(1)-O(1)#1	86.22(11)	N(1)-Cu(1)-O(1)#1	93.67(13)

Symmetry transformations used to generate equivalent atoms: [#1] -x+3/4, y+1/4, -z+3/4.

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

Cu(1)-O(2)	1.9107(19)	Cu(1)-O(3)	1.9292(19)
Cu(1)-N(6)#1	1.995(2)	Cu(1)-N(1)	2.008(2)
Cu(1)-O(1)#2	2.300(2)		
O(2)-Cu(1)-O(3)	91.66(8)	O(2)-Cu(1)-N(6)#1	161.48(10)
O(3)-Cu(1)-N(6)#1	86.17(9)	O(2)-Cu(1)-N(1)	89.36(9)
O(3)-Cu(1)-N(1)	177.45(9)	N(6)#1-Cu(1)-N(1)	92.11(10)
O(2)-Cu(1)-O(1)#2	99.75(8)	O(3)-Cu(1)-O(1)#2	91.80(8)
N(6)#1-Cu(1)-O(1)#2	98.71(8)	N(1)-Cu(1)-O(1)#2	90.33(9)

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

Table S9a. Selected bond distances (Å) and angles (°) for **9**.

Cd(1)-O(1)#1	2.2669(14)	Cd(1)-N(1)	2.2828(16)
Cd(1)-O(2)	2.2922(13)	Cd(1)-O(1W)	2.2967(16)
Cd(1)-O(3)	2.3032(14)	Cd(1)-O(2)#2	2.3581(14)
O(1)#1-Cd(1)-N(1)	83.69(6)	O(1)#1-Cd(1)-O(2)	92.39(5)
N(1)-Cd(1)-O(2)	169.87(6)	O(1)#1-Cd(1)-O(1W)	101.43(6)
N(1)-Cd(1)-O(1W)	88.67(6)	O(2)-Cd(1)-O(1W)	101.28(5)
O(1)#1-Cd(1)-O(3)	167.57(5)	N(1)-Cd(1)-O(3)	108.41(6)
O(2)-Cd(1)-O(3)	75.20(5)	O(1W)-Cd(1)-O(3)	82.09(6)

O(1)#1-Cd(1)-O(2)#2	96.63(5)	N(1)-Cd(1)-O(2)#2	92.11(6)
O(2)-Cd(1)-O(2)#2	79.03(5)	O(1W)-Cd(1)-O(2)#2	161.90(5)
O(3)-Cd(1)-O(2)#2	80.50(5)		

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

Table S9b. Hydrogen bonds for **9** (Å and °).

D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O(1W)-H(1B)···O(3)#4	0.833(16)	1.869(17)	2.690(2)	168(3)
O(1W)-H(1A)···O(4)#5	0.846(16)	2.223(17)	3.044(2)	164(2)

Symmetry transformations used to generate equivalent atoms: #4 x+1, y, z; #5 -x, -y+1, -z+1.

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

Cd(1)-O(2)	2.2580(18)	Cd(1)-O(3)#1	2.2787(19)
Cd(1)-N(1)	2.295(3)	Cd(1)-N(6)#2	2.305(3)
Cd(1)-O(2)#1	2.330(2)	Cd(1)-N(7)	2.331(3)
O(2)-Cd(1)-O(3)#1	150.65(8)	O(2)-Cd(1)-N(1)	121.68(9)
O(3)#1-Cd(1)-N(1)	87.58(9)	O(2)-Cd(1)-N(6)#2	94.71(9)
O(3)#1-Cd(1)-N(6)#2	88.10(9)	N(1)-Cd(1)-N(6)#2	88.01(11)
O(2)-Cd(1)-O(2)#1	75.20(7)	O(3)#1-Cd(1)-O(2)#1	75.53(7)
N(1)-Cd(1)-O(2)#1	163.11(8)	N(6)#2-Cd(1)-O(2)#1	91.20(10)
O(2)-Cd(1)-N(7)	91.34(9)	O(3)#1-Cd(1)-N(7)	87.63(9)
N(1)-Cd(1)-N(7)	87.09(11)	N(6)#2-Cd(1)-N(7)	173.62(10)
O(2)#1-Cd(1)-N(7)	92.31(9)		

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

Table S11. Selected bond distances (Å) and angles (°) for **11**.

Cd(1)-O(3)	2.252(6)	Cd(1)-N(6)#1	2.255(9)
Cd(1)-O(3)#1	2.264(6)	Cd(1)-O(4)	2.269(6)
Cd(1)-N(1)	2.296(10)		
O(3)-Cd(1)-N(6)#1	158.3(3)	O(3)-Cd(1)-O(3)#1	97.5(3)
N(6)#1-Cd(1)-O(3)#1	91.3(3)	N(6)#1-Cd(1)-O(4)	86.6(3)
O(3)-Cd(1)-O(4)	76.7(2)	O(3)#1-Cd(1)-O(4)	153.4(2)
O(3)-Cd(1)-N(1)	95.2(3)	N(6)#1-Cd(1)-N(1)	97.3(3)
O(3)#1-Cd(1)-N(1)	120.5(3)	O(4)-Cd(1)-N(1)	86.1(3)

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

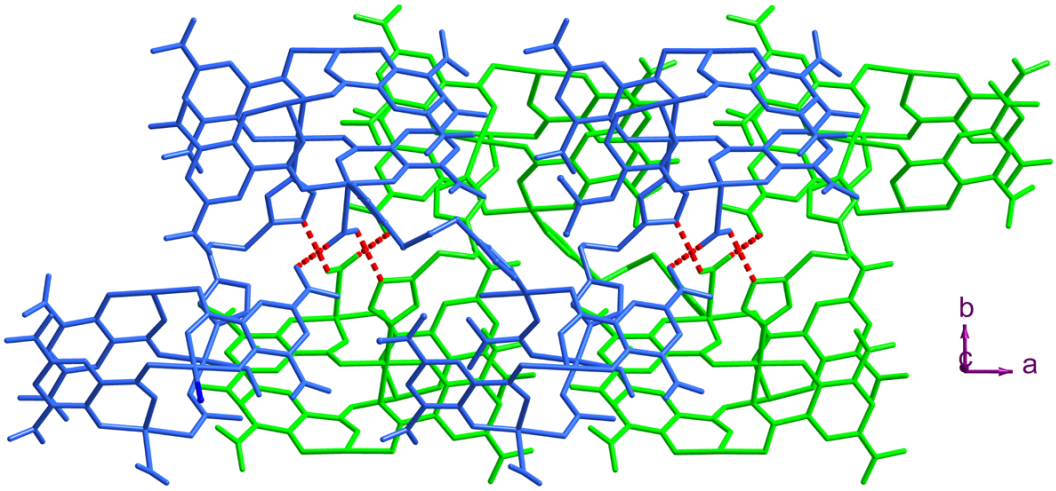
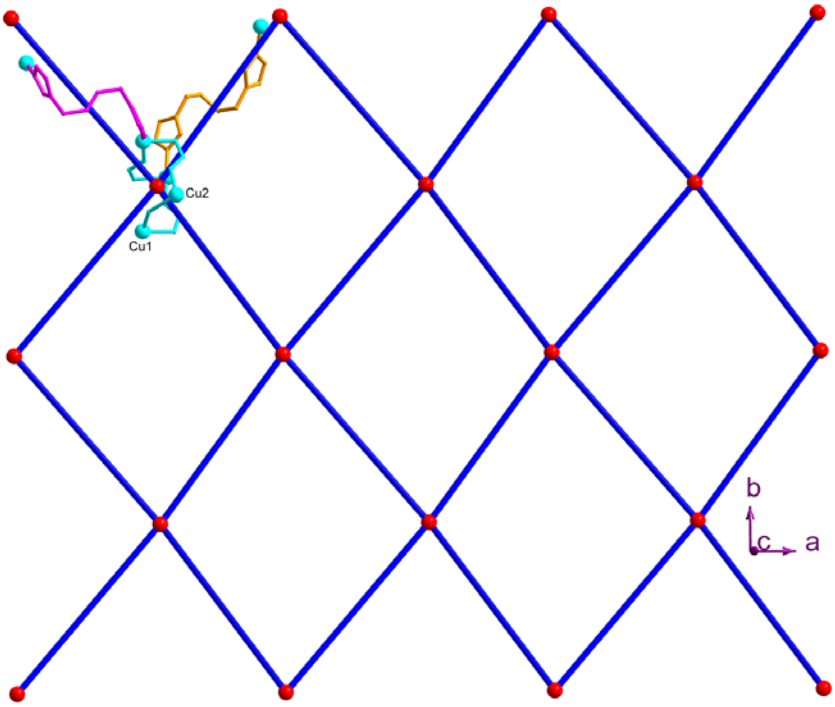
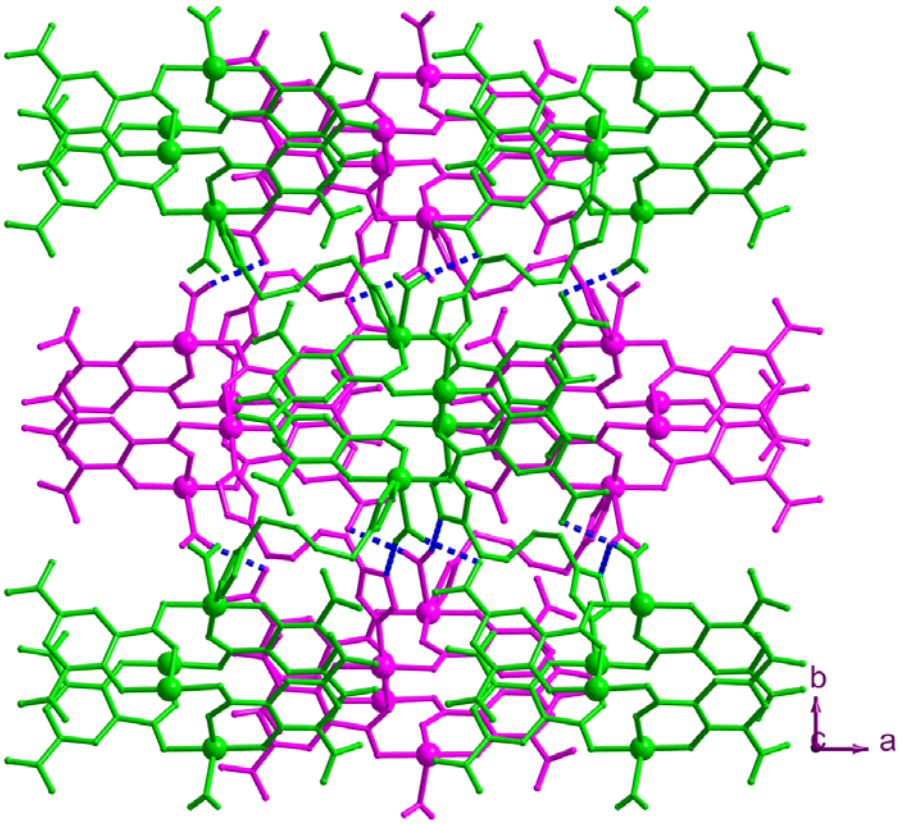


Fig. S1 The 3D supramolecular architecture constructed by hydrogen-bonding interactions in **2**.



(a)



(b)

Fig. S2. (a) View of the 4^4 network of **3**. (b) The 3D supramolecular architecture of **3** constructed by hydrogen-bonding interactions.

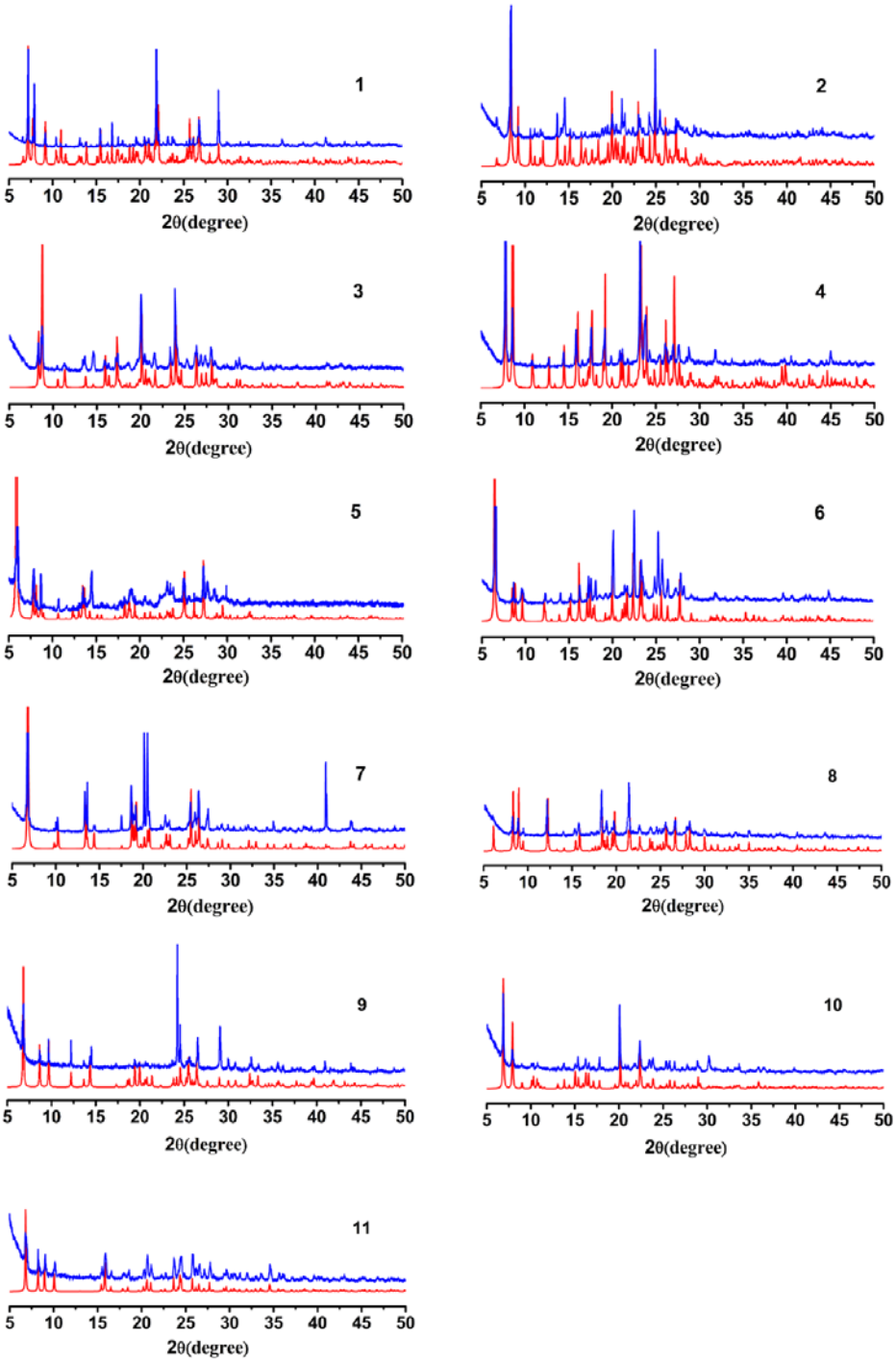
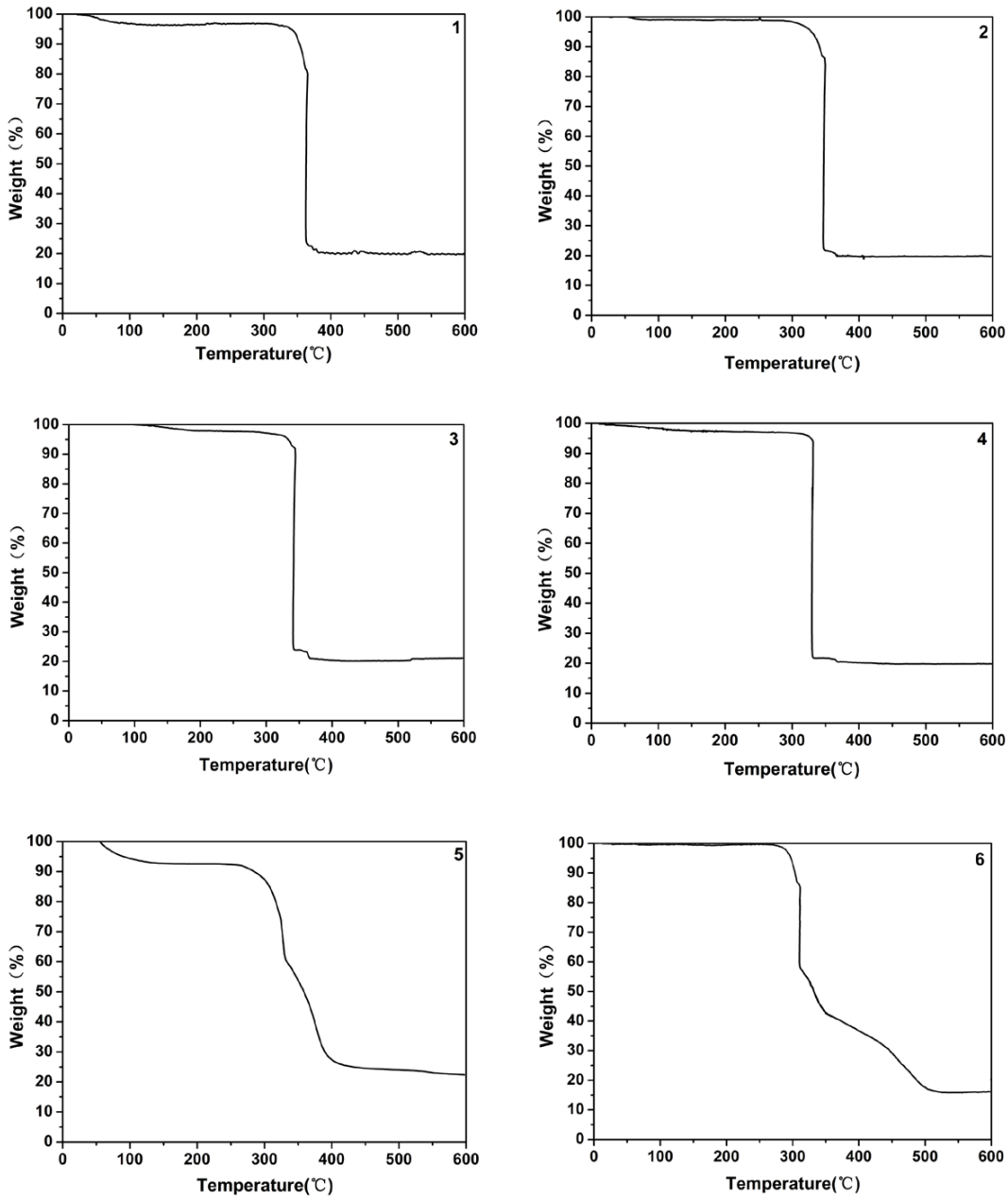
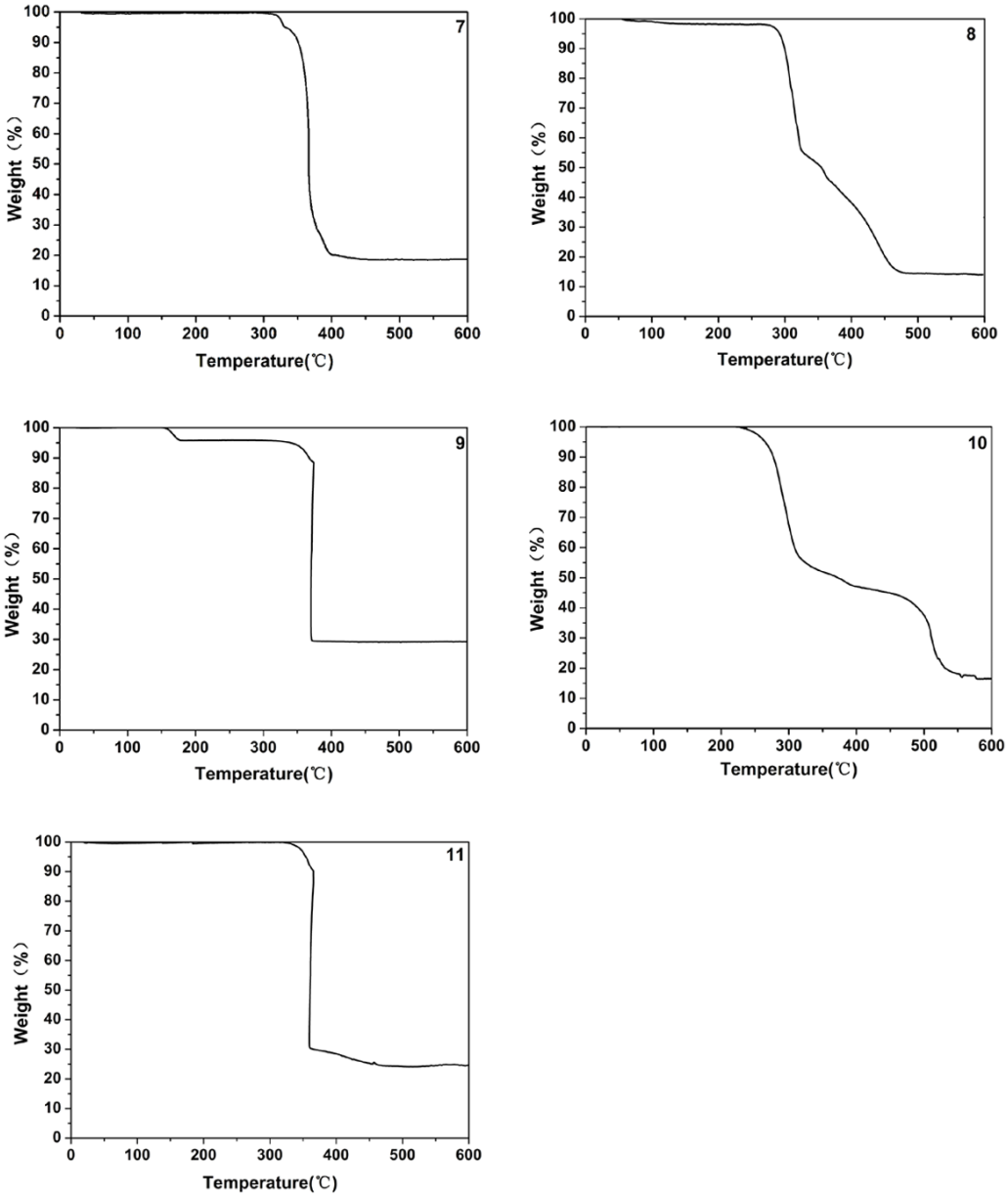


Fig. S3. Simulated (red) and experimental (blue) PXRD patterns of **1**–**11**.

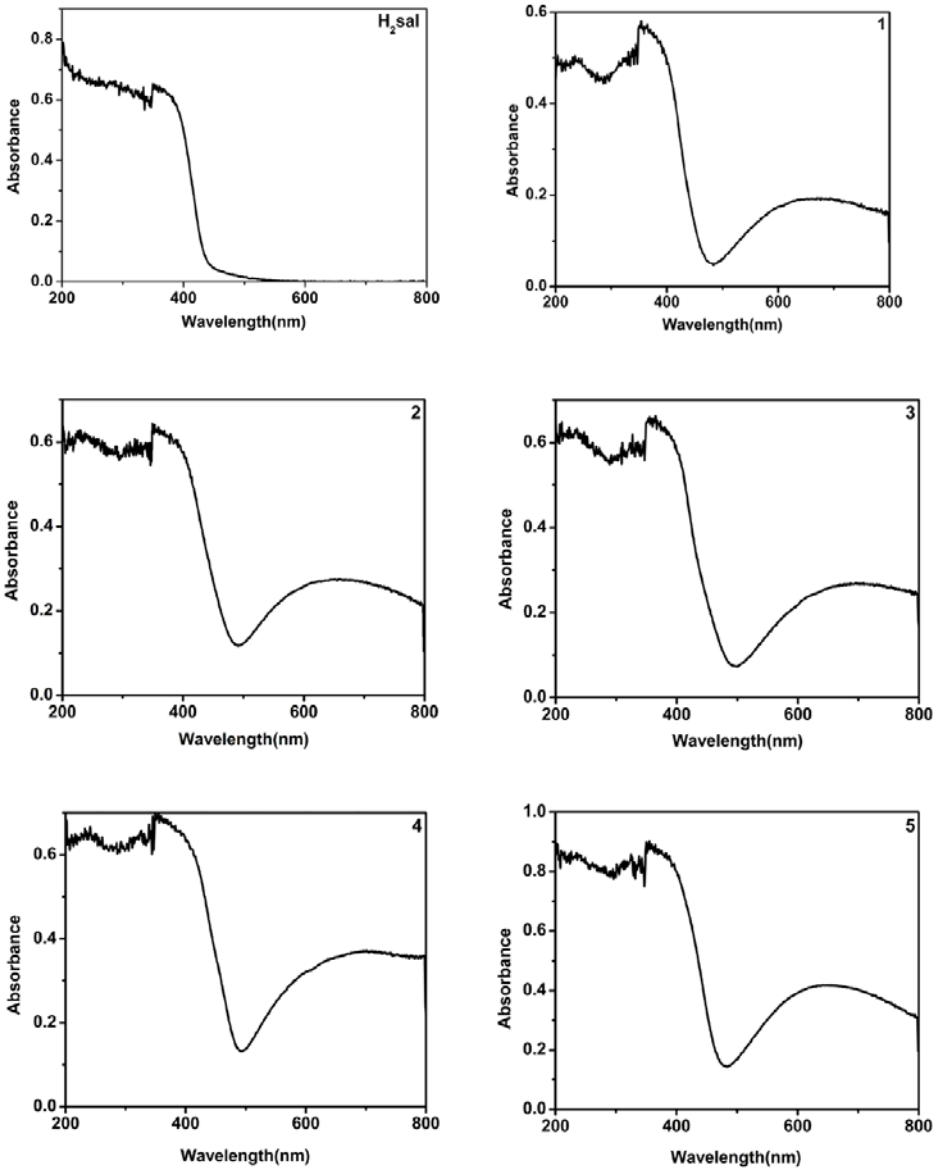


(a)

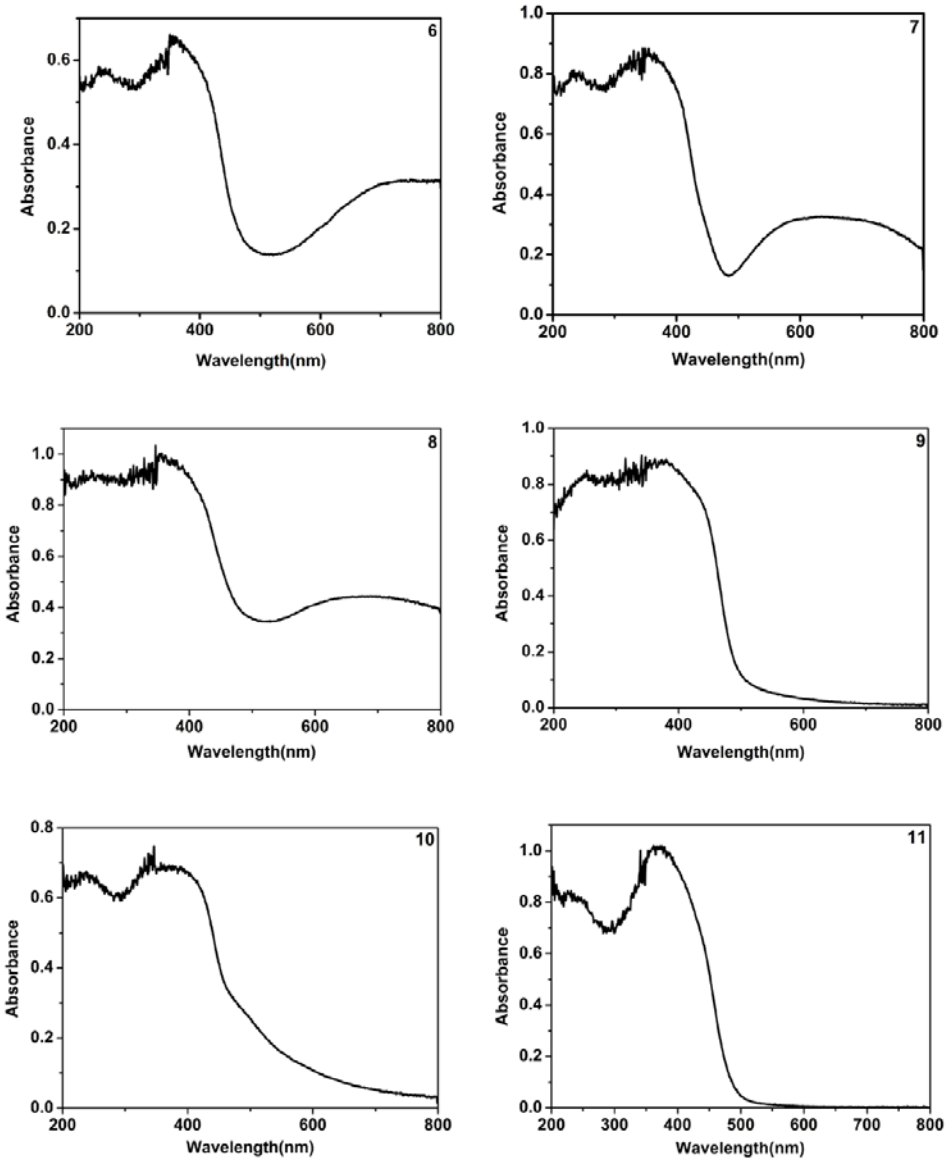


(b)

Fig. S4 TGA curves of compounds (a) **1**–**6** and (b) **7**–**11**.

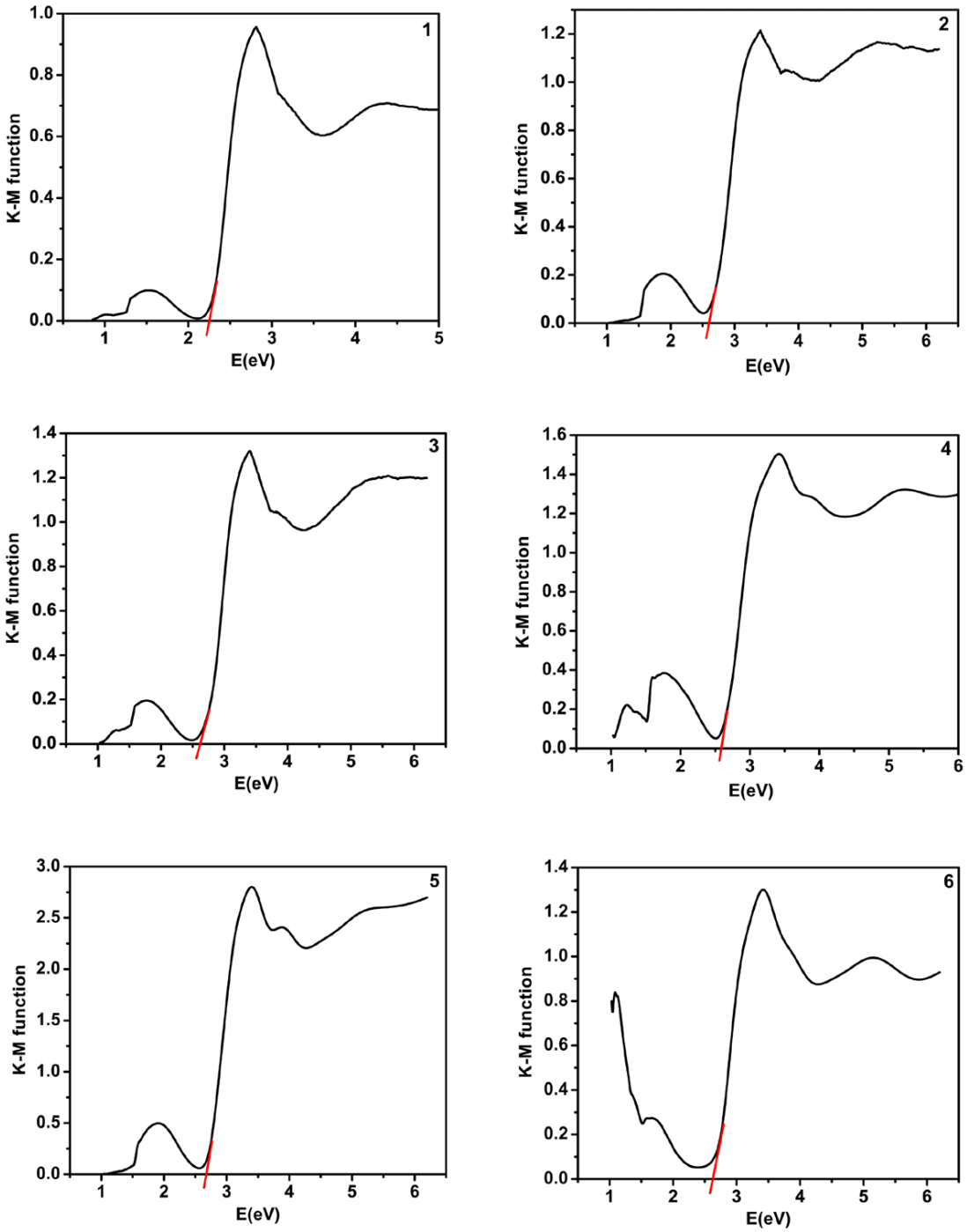


(a)

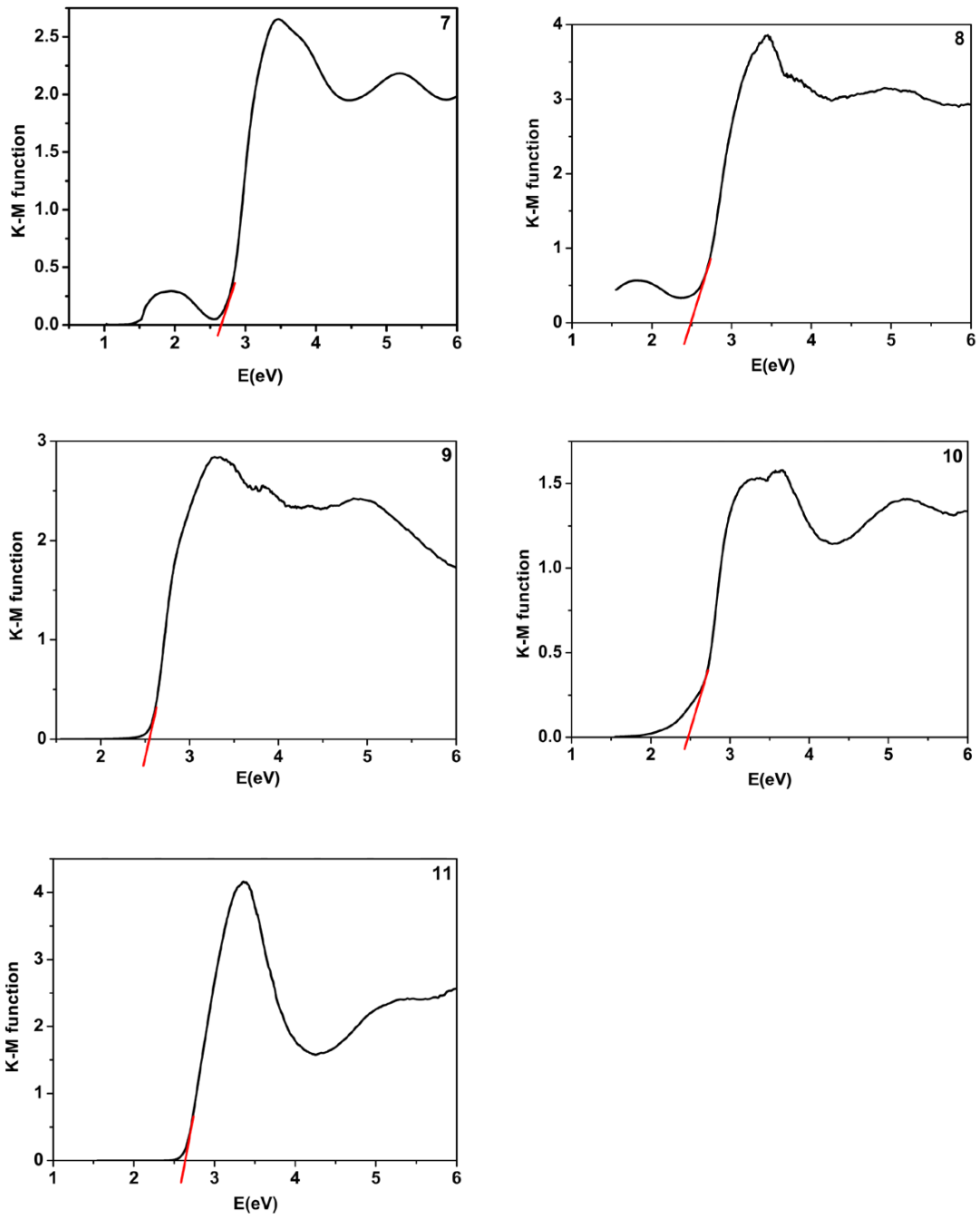


(b)

Fig. S5 UV-vis spectrum of (a) H_2sal and compounds **1**–**5** (b) **6**–**11** in the solid state at room temperature.



(a)



(b)

Fig. S6 Diffuse reflectance UV-vis-NIR spectra of K-M functions *vs* energy (eV) of compounds (a) **1**–**6** and (b) **7**–**11**.