Electronic Supplementary information

Table S1. Hydrogen bond interactions for compounds **1-6**.

D-H···A	D-H (Å)	H···A (Å)	D···A (Å)	D-H···A (º)
[$CoL_2(H_2O_2)$].MeOH (1)				
O(7)-H(7A)···O(6)#1	0.92(2)	1.89(2)	2.803(7)	171(6)
O(7)-H(7B)···O(3)#2	0.93(2)	1.81(3)	2.683(7)	156(6)
O(8)-H(8A)···O(1S)	0.92(2)	1.77(3)	2.663(10)	165(7)
O(8)-H(8B)···O(2)#3	0.91(2)	1.84(3)	2.707(7)	159(7)
O(1S)-H(1S)···O(6)#1	0.97(2)	1.78(5)	2.730(9)	164(16)
C(6)-H(6)···O(8)#4	0.93	2.57	3.459(9)	160
C(5)-H(5)···O(5)#4	0.93	2.65	3.497(8)	151
C(8)-H(8)···O(1S)#5	0.93	2.59	3.360(11)	141
C(13)-H(13)···O(3)#6	0.93	2.45	3.364(8)	168
C(1S)-H(1S1)···O(1)#7	0.96	2.60	3.430(16)	145
[$CoL_2(H_2O)(MeOH]$ (2)				
O(7)-H(7A)···O(6)#1	0.88(4)	1.84(4)	2.714(4)	177(4)
O(8)-H(8A)···O(3)#2	0.79(5)	1.92(6)	2.709(5)	171(6)
O(8)-H(8B)···O(6)#3	0.88(5)	1.97(5)	2.834(5)	165(5)
C(13)-H(13)···O(5)#3	0.93	2.41	3.333(5)	172
C(5)-H(5)···O(3)#4	0.93	2.64	3.527(6)	159
[CuL_2(N-MeIm)$_2$] (3)				
C(7)-H(7)…O(3)#2	0.93	2.40	3.329(6)	175
C(13)-H(13)···O(3)#3	0.93	2.52	3.165(5)	126
C(14)-H(14a)···O(2)#4	0.96	2.60	3.444(6)	147
[CoL_2(bipy)] (4)				
C(12)-H(12)···O(2)#2	0.93	2.46	3.219(15)	139
C(7)-H(7)···O(3)#3	0.93	2.59	3.503(10)	166
C(14)-H(14)···O(1)#4	0.93	2.60	3.333(11)	136
[ZnL_2(bipy)] (5)				
C(12)-H(12)···O(2)#2	0.93	2.44	3.215(8)	141
C(7)-H(7)···O(3)#3	0.93	2.60	3.506(6)	166
C(14)-H(14)···O(1)#4	0.93	2.57	3.300(6)	135
[CdL_2(bipy)] (6)				
C(13)-H(13)···O(2)#2	0.93	2.41	3.326(3)	167
C(7)-H(7)···O(2)#3	0.93	2.58	3.499(3)	168
C(14)-H(14)···O(3)#4	0.93	2.43	3.344(3)	167

Symmetry transformations:

(**1**) #1 -x+2, -y, -z+1; #2 y+1, -x+0.5 ,-z+1.5; #3 -x+1.5, -y+0.5 ,z; #4: y+0.5, -x+1, z+0.5; #5: -y+1.5, x-1, -z+1.5; #6: -y+1, x-0.5, z-0.5; #7: y+1, -x+1.5, -z+1.5. (**2**) #1: -x+1, -y+1, -z; #2: x, y+1, z; #3: -x+2, -y+1, -z; #4: -x+2, -y-1, -z+1. (**3**) #2: x, y-1, z; #3: -x+2, -y+1, -z+2; #4: x+1, y-1, z. (**4**) #2: x, y, z+1; #3: x, y+0.5, z+0.5; #4: x, y-0.5, z+0.5. (**5**) #2: x, y, z+1; #3: x, y-0.5, z+0.5; #4: x, y+0.5, z+0.5. (**6**) #2: x+0.5, y+0.5, -z+1.5; #3: x+1, y, z; #4: x+0.5, -y, z+0.5.

Table S2. O···C=O interactions for compounds **1** and **2**.

X=O···C=O	**O···C (Å)**	**XOC (º)**
[$CoL_2(H_2O)_2$].MeOH (1)		
C(4)=O(3)···[C(11)=O(4)]#8	3.047(8)	92.8(4)
[$CoL_2(H_2O)$(MeOH] (2)		
C(14)=O(6)···[C(11)=O(4)]#5	3.184(5)	92.1(3)

Symmetry transformations: (**1**) #8: -y+0.5, x-1, -z+1.5. (**2**) #5: -x+1, -y+1, -z.

Table S3. π-π Interactions for compounds **1-6.**[a]

π-π	**Cg-Cg[a](Å)**	**alpha[b]**	**beta[c]**	**gamma[d]**	**Cg(I)_J[e]**	**Cg(J)_I[f]**
[$CoL_2(H_2O)_2$].MeOH (1)						
π[C5-C10]···π[C5-C10]#9	3.711	5.09	26.17	26.17	3.331	3.331
π[C5-C10]···π[C15-C20]#10	3.638	6.78	15.22	20.52	3.408	3.511
π[C15-C20]···π[C15-C20]#11	3.746	1.59	22.84	22.84	3.452	3.452
[$CoL_2(H_2O)$(MeOH] (2)						
π[C5-C10] ···π[C1-C4,C9,C10]#7	3.688	0.68	19.63	19.78	3.470	3.473
π[C5-C10]···π[C5-C10]#7	3.865	0.00	26.03	26.03	3.473	3.473
π[C5-C10]···π[C5-C10]#8	4.114	0.00	32.43	32.43	3.472	3.472
π[C15-C20]···π[C15-C20]#9	3.664	0.00	21.95	21.95	3.399	3.399
π[C11-C14,C19,C20]···π[C11-C14,C19,C20]#10	3.506	0.00	18.50	18.50	3.325	3.325
[CuL_2(N-MeIm)$_2$] (3)						
π[C5-C10]···π[C5-C10]#5	3.805	0.00	22.39	22.39	3.518	3.518
π[imidazol]···π[imidazol]#6	3.755	0.00	19.75	19.75	3.534	3.534
[CoL_2(bipy)] (4)						
π[C5-C10]···π[C5-C10]#5	4.288	21.18	27.69	36.16	3.463	3.798
π[C5-C10]···π[C1-C4, C9,C10]#5	4.048	23.18	22.53	1.60	4.046	3.739
[ZnL_2(bipy)] (5)						
π[C5-C10]···π[C5-C10]#5	4.274	20.35	27.74	36.22	3.467	3.804
π[C5-C10]···π[C1-C4, C9,C10]#5	4.023	21.48	20.81	1.65	4.021	3.760
[CdL_2(bipy)] (6)						
π[C1-C4,C9,C10]···π[C1-C4,C9,C10]#5	3.754	0.03	15.52	15.52	3.617	3.617
π[C1-C4,C9,C10]···π[C5-C10]#5	3.873	2.17	22.72	21.17	3.612	3.572

[a] Centroid-Centroid distance. [b] Dihedral angle between the ring planes. [c] Angle between the centroid vector Cg(I)…Cg(J) and the normal to the plane I. [d] Angle between the centroid vector Cg(I)…Cg(J) and the normal to the plane J. [e] Perpendicular distance of Cg(I) on ring plane J. [f] Perpendicular distance of Cg(J) on ring plane I.

Symmetry transformations:

(**1**) #9: -x+1.5, -y+0.5, z; #10: -y+0.5, x-1, -z+1.5; #11: -x+1.5, -y-0.5, z. (**2**) #7: -x+2, -y, -z+1; #8: -x+1, -y, -z+1; #9: -x+1, -y+2, -z; #10: -x+1, -y+3, -z. (**3**) #5: -x+2, -y, -z+2; #6: -x+3, -y+1, -z+1. (**4**) #5: -x+0.5, y, z+0.5. (**5**) #5: -x+0.5, y, z+0.5. (**6**) #5: -x+1, -y, -z+1; #6: x, -y-0.5, -z+1.

Table S4. C-H···π interactions for compound **3.**[a]

C-H···π	**H···Cg (Å)**	**C···Cg (Å)**	**C-H-Cg (º)**	**D_{min} (Å)**
[CuL_2(N-MeIm)$_2$] (3)				
C(6)-H(6)···π[imidazol]#5	2.95	3.818	156	3.032, C13

[a] Cg: centroid; D_{min}: minimum C(H)-C(ring) distance.
Symmetry transformations: (**3**) #5: -x+2, -y, -z+2.