Supporting Information

Five discrete and polymeric complexes formed from cobalt(II), 4,4′-bipyridine and 2-sulfoterephthalate: synthetic, crystallographic and magnetic studies

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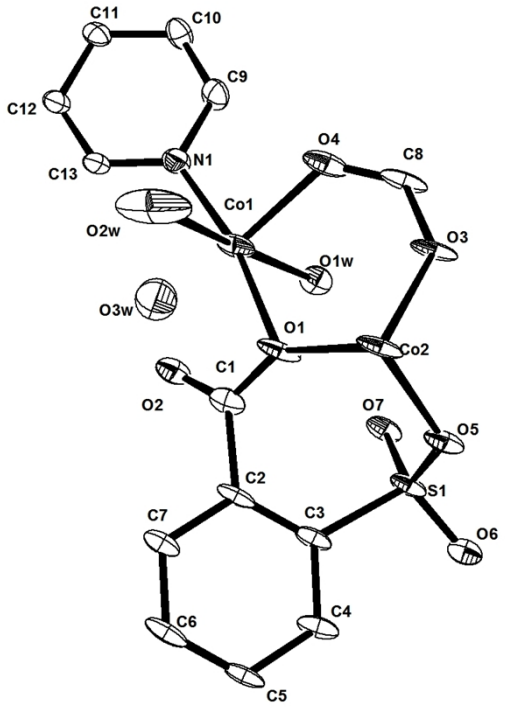


Figure S1. Ortep view (20% ellipsoid probability) of the asymmetric unit of compound **1**. Hydrogen atoms have been omitted for clarity.

Table S1. H-bonding in $\{[Co_3(2\text{-stp})_2(bipy)(H_2O)_4]\cdot 2H_2O\}_n$

Intramonomeric H-bonding	
D-H···A (Å)	**D-H···A (°)**
O1W···O7 2.767(9)	O1W-H2W···O7 171.9(9)
O2W···O3W 2.953(9) O2W'···O3W 2.438(9)	-
O6···O3W 2.953(2)	-

Intermonomeric H-bonding	
D-H···A (Å)	**D-H···A (°)**
O1W···O6[a] 2.742(9)	-
O2W···O2W[b] 2.801(9)	-
O3W···O3W[c] 3.167(9)	-

[a] -x+1/2,+y+1/2,-z+1/2;[b] -x, -y, -z; [c] -x,+y,-z-1/2

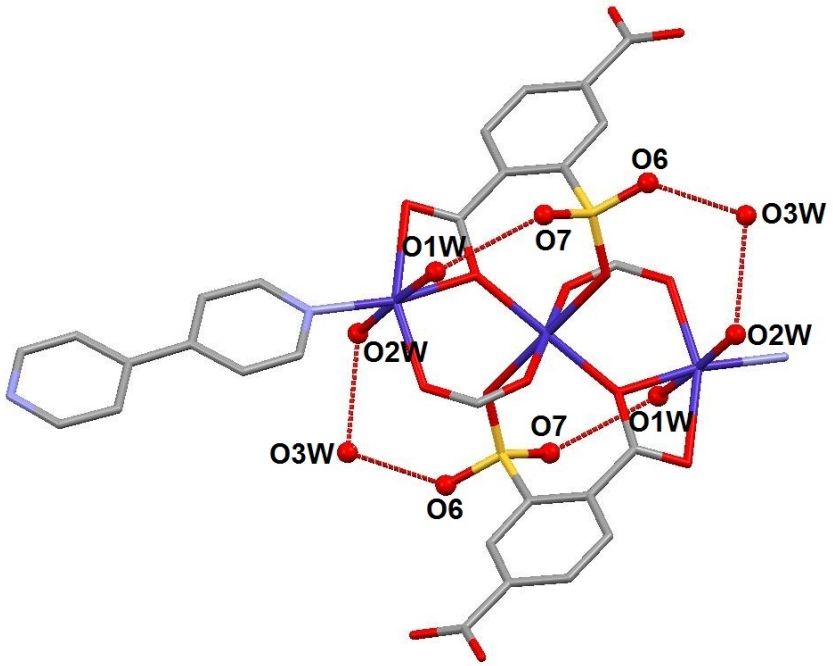


Figure S2. Intra-monomeric H-bonds (as red lines) in **$[Co_3(2\text{-stp})_2(bipy)(H_2O)_4]\cdot 2H_2O$**. The atoms belonging to adjacent monomers necessary to complete the coordination environment around the metal centers have been also included. Hydrogen atoms have been omitted for clarity.

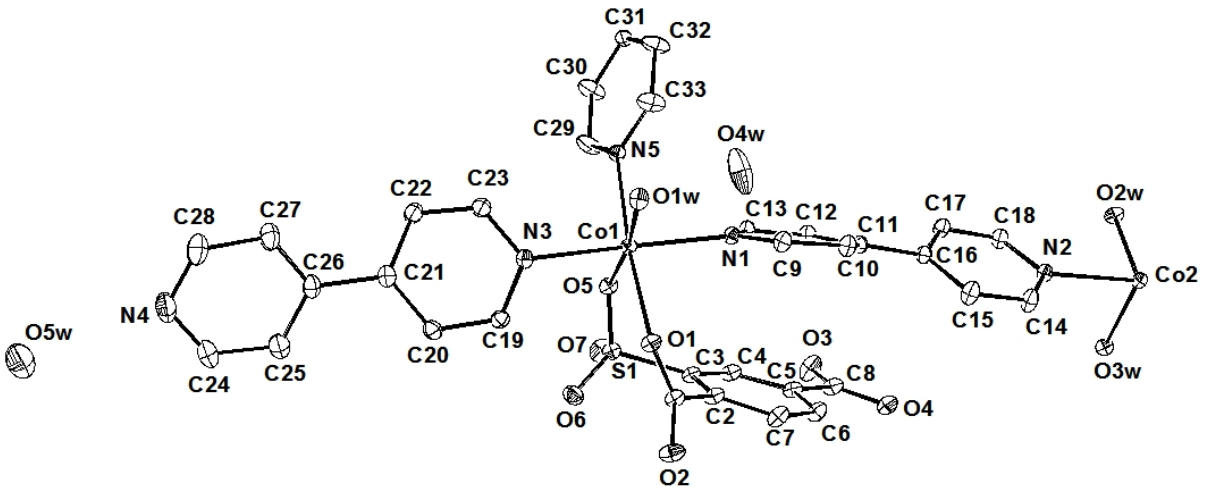


Figure S3. Ortep view (20% ellipsoid probability) of the asymmetric unit of compound **2**. Hydrogen atoms have been omitted for clarity.

Table S2. H-bonding in **{[Co_3(2-stp)$_2$(bipy)$_5$(H_2O)$_6$]·4H_2O}$_n$**.

Intra-monomeric H-bonding	
D-H···A (Å)	**D-H···A (°)**
O1W···O4W 2.674(3)	O1W-H1W···O4W 135.22(9)
O5W···N4 2.947(5)	O5W-H9W···N4 158.83(9)
Inter-monomeric H-bonding	
D-H···A (Å)	**D-H···A (°)**

O5W···O7[a] 2.980(4)	O5W-H10W···O7 142.05(8)
O2W···O1[a] 2.672(2)	O2W-H4W···O1 161.22(9)
O3W···O2[a] 2.621(3)	O3W-H5W···O2 175.35(9)
O4W···O3W[b] 2.850(3)	O4W-H7W···O3W 155.58(9)
O4W···O4[b] 2.764(3)	O4W-H8W···O4 147.59(9)
O1W···O3[b] 2.681(3)	O1W-H2W···O3 147.69(8)
O2W···O4[c] 2.743(3)	O2W-H3W···O4 151.85(9)
O3W···O4[c] 2.688(3)	O3W-H6W···O4 168.57(9)

[a] x+1, y-1, z; [b] x, y-1, z; [c] x-1, y, z;

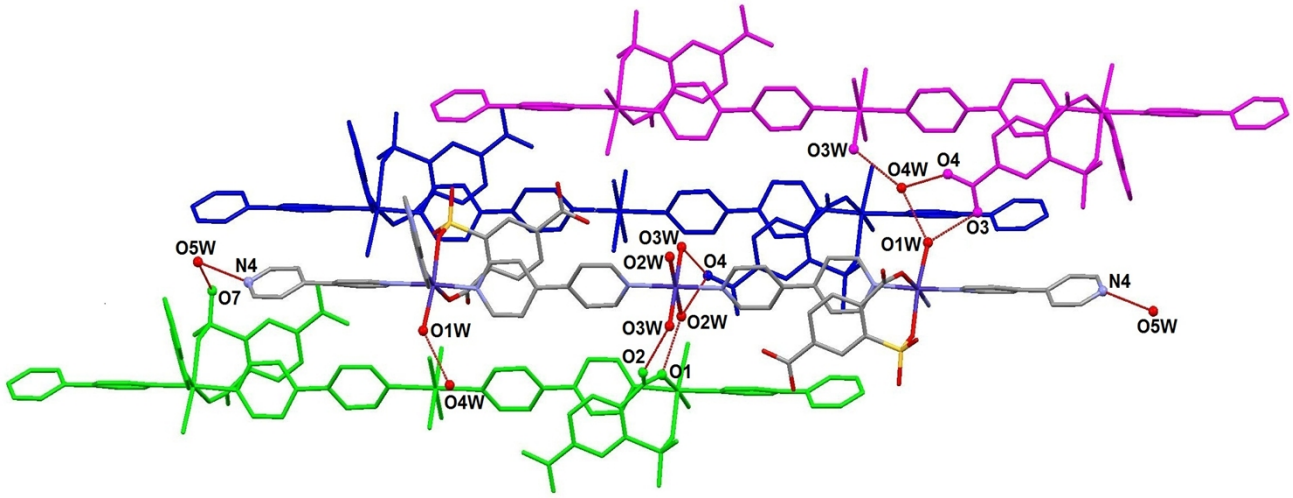


Figure S4. View of the H-bonding network in **2** (H-bonds are shown as red lines). The colored molecules are in the positions obtained applying the operations a (green), b

(magenta) and c (blue) (see Table S2) on the general coordinates. Hydrogen atoms have been omitted for clarity.

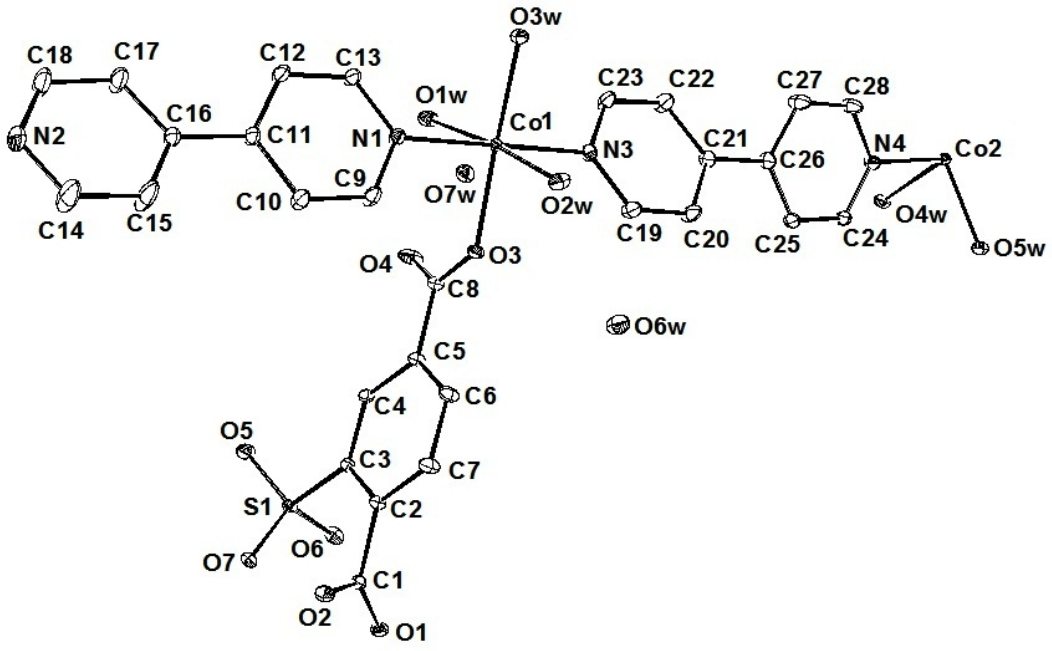


Figure S5. Ortep view (20% ellipsoid probability) of the asymmetric unit of compound **3**. Hydrogen atoms have been omitted for clarity.

Table S3. Relevant H-bonding in **$[Co_3(2\text{-stp})_2(bipy)_4(H_2O)_{10}]\cdot 8H_2O$**.

D-H···A (Å)	D-H···A (°)
O2W···O6W 2.753(2)	O2W-H4W···O6W 170(2)
O3W···O7W[a] 2.719(2)	O3W-H5W···O7W 160(2)
O2W···O4[a] 2.808(2)	O2W-H3W···O4 172(3)
O6W···O6[a] 2.808(2)	O6W-H12W···O6 172(3)
O3W···O2[b] 2.736(2)	O3W-H6W···O2 173(2)

O1W···O7[b] 2.740(2)	O1W-H2W···O7 172(3)
O7W···O5[b] 2.819(2)	O7W-H13W···O5 166(3)
O4W···O1[c] 2.731(2)	O4W-H8W···O1 176(3)
O5W···O7[c] 2.692(2)	O5W-H9W···O7 172(4)
O4W···O2[d] 2.835(2)	O4W-H7W···O2 156(3)
O5W···O2[e] 2.721(2)	O5W-H10W···O2 164(3)

[a] x-1,+y,+z; [b] x-1/2,-y+1/2,+z-1/2; [c] -x+2,-y+1,-z; [d] x,+y,+z-1; [e] -x+1,-y+1,-z.

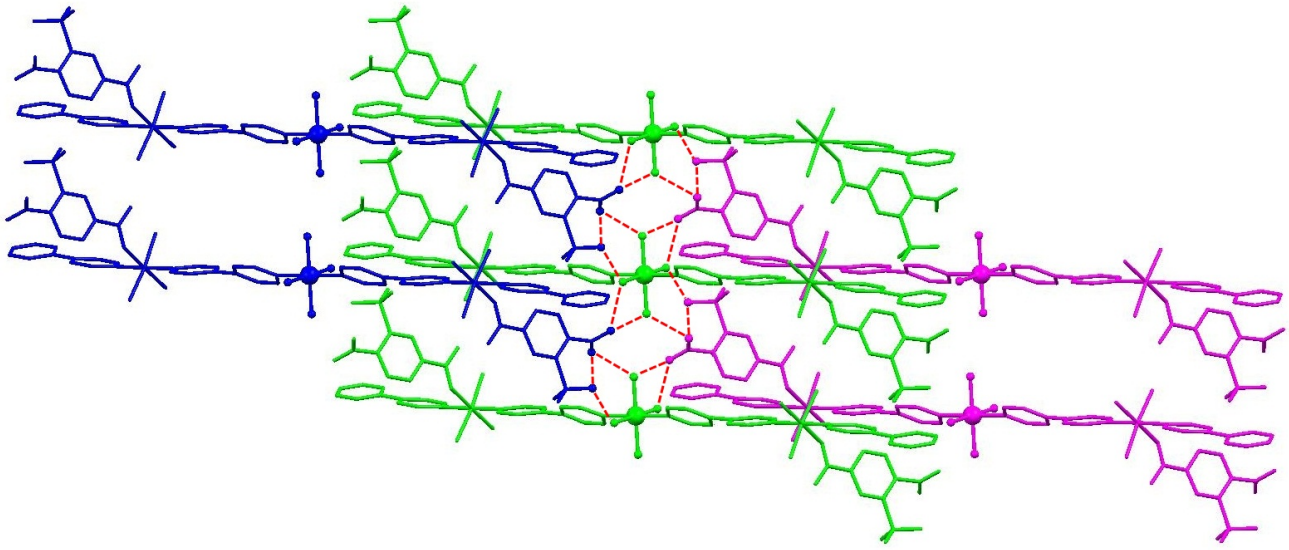
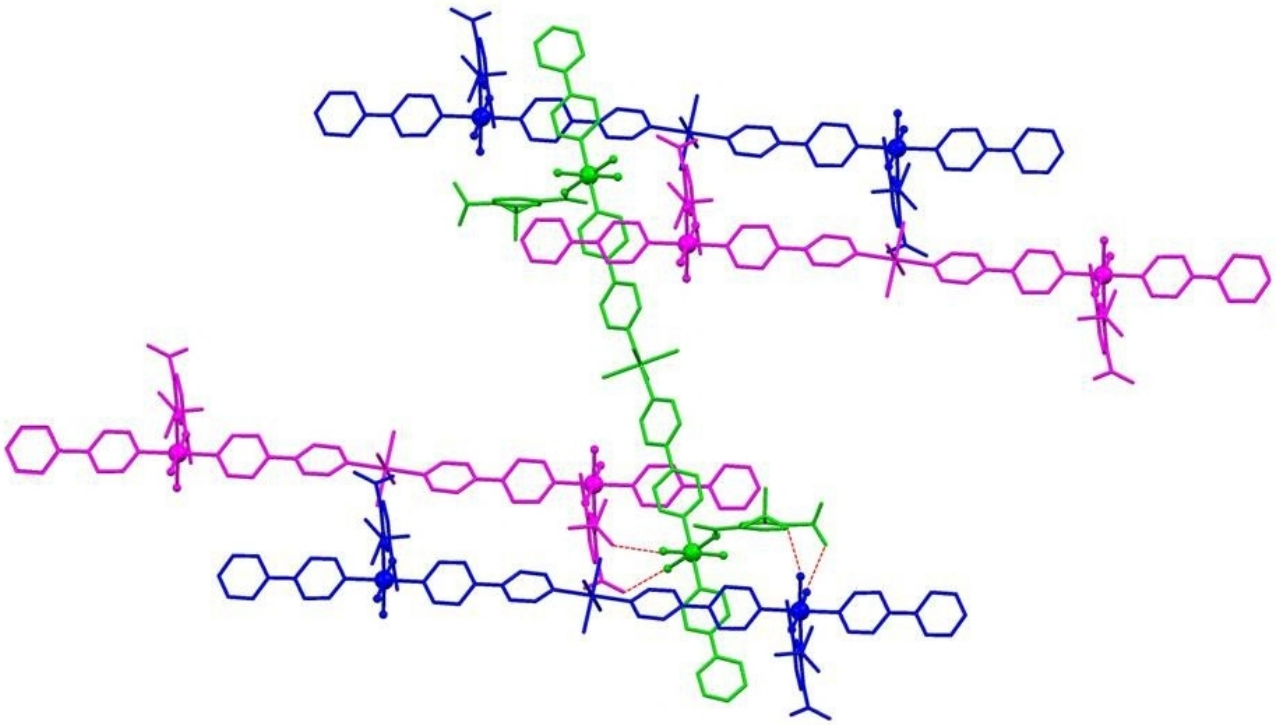


Figure S6. Hydrogen bonds formed by the water molecules surrounding Co2 (represented as red dotted lines) highlighted for one group of metal centers.



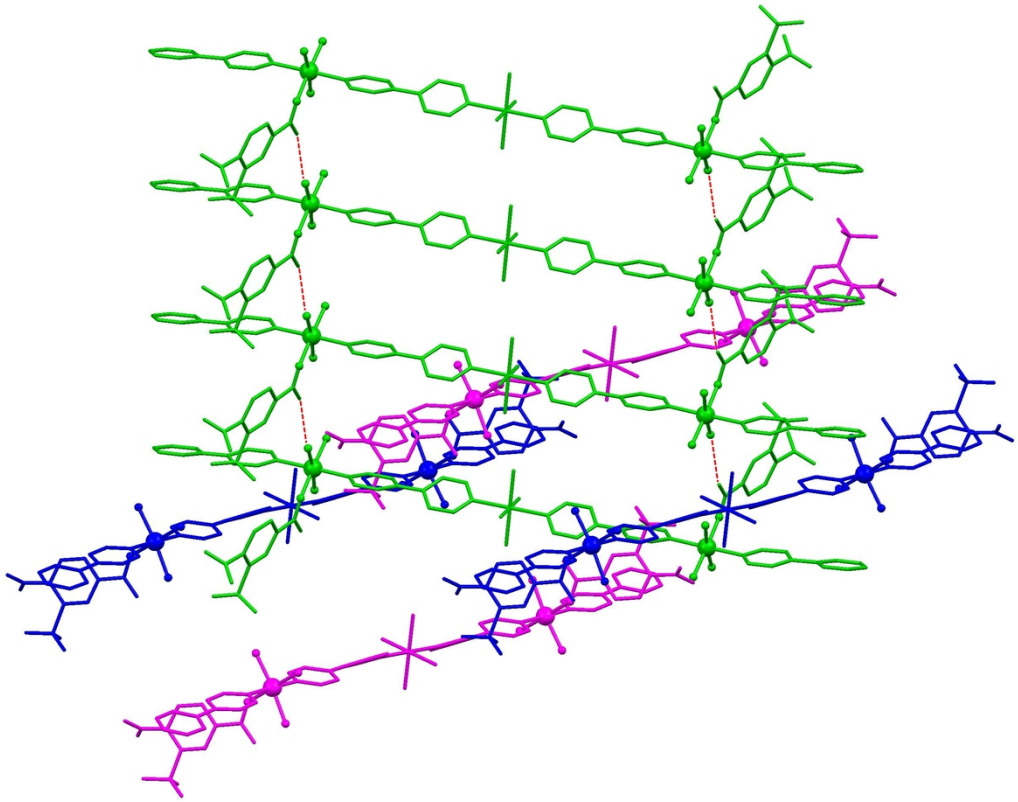


Figure S7. Two perspective views of the hydrogen bonds formed by the water molecules surrounding Co1 (represented as red dotted lines) highlighted for one group of metal centers.

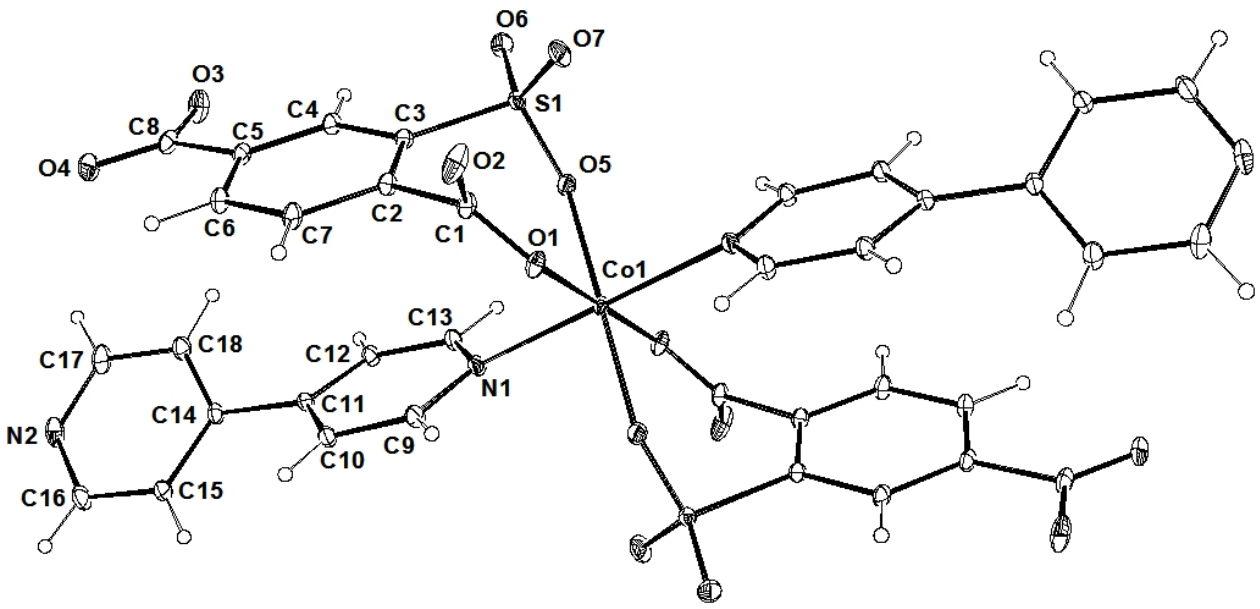


Figure S8. Ortep view (20% ellipsoid probability) of the symmetry-generated complex **4** **[Co(2-stpH$_2$)$_2$(bipy)$_2$]**. The carboxylic hydrogen atoms which could not be located in the difference Fourier map are not shown.