Supplementary material

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Copper(II) and cobalt(II) complexes based on bis-benzimidazolyl ligand with 1,2-bis(2'-ethoxy)phenyl linker: synthesis, crystal structure and conformations

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1. CCDC for complexes 1-7.

CCDC 941767-941773 for **1-7** contain the supplementary crystallographic data. These data can be obtained free of charge via http//www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge, CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk. Supplementary data and Figures associated with this article can be found, in the online version.

2. The plots of $\chi_m T$ vs T for complexes 1-7.

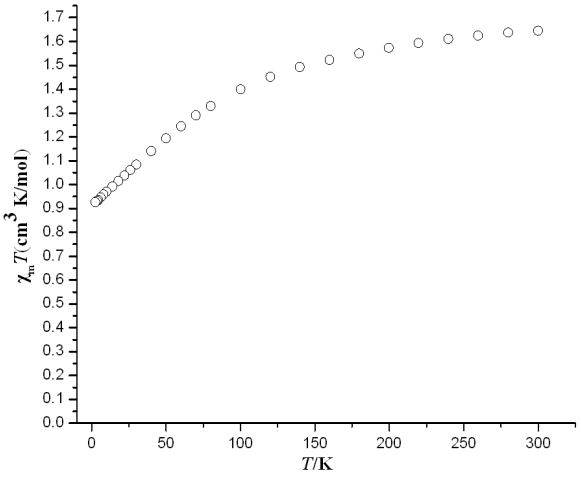

Fig. S1 The plot of $\chi_m T$ versus T for **1**

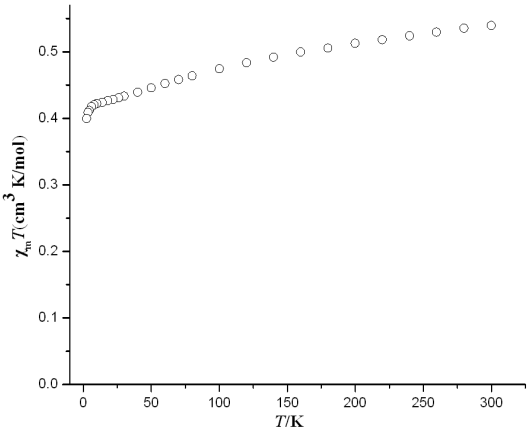

Fig. S2 The plot of $\chi_m T$ versus T for **2**

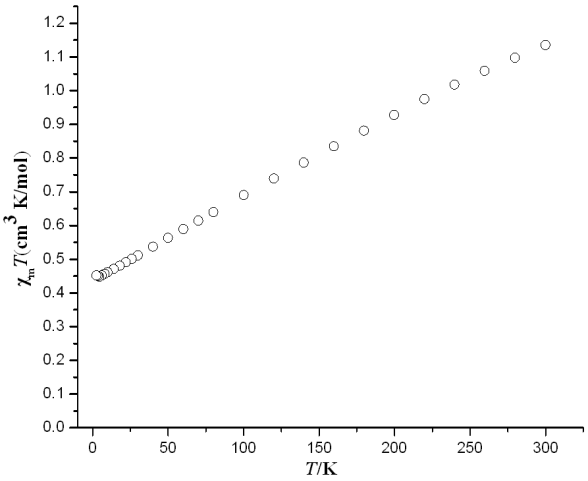

Fig. S3 The plot of $\chi_m T$ versus T for **3**

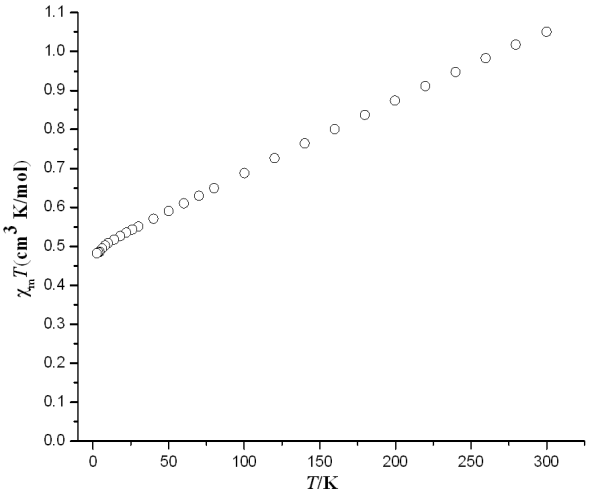

Fig. S4 The plot of $\chi_m T$ versus T for **4**

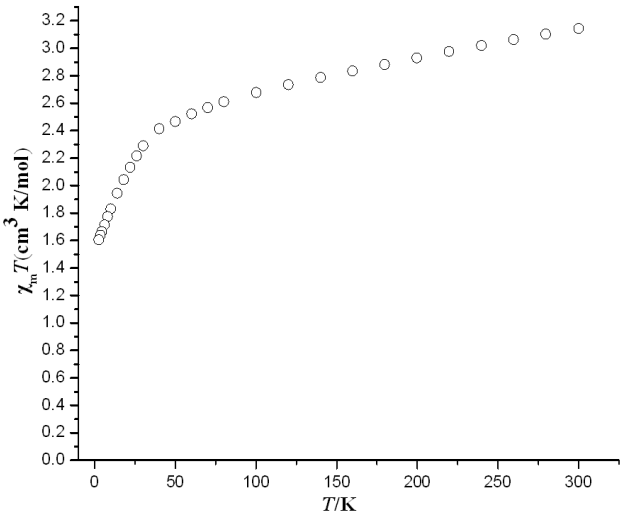

Fig. S5 The plot of $\chi_m T$ versus T for **5**

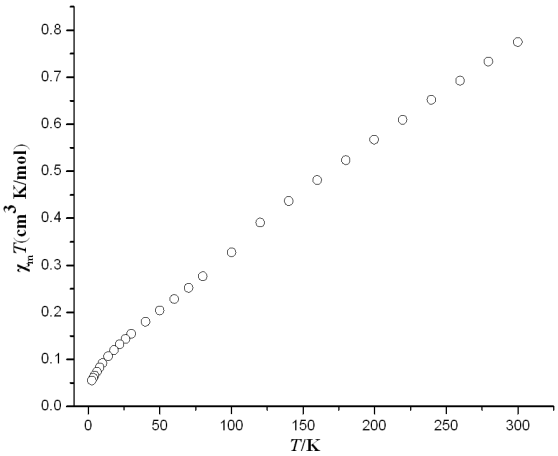

Fig. S6 The plot of $\chi_m T$ versus T for **6**

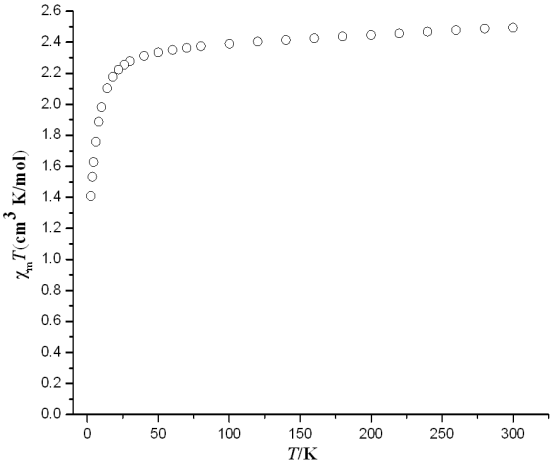

Fig. S7 The plot of $\chi_m T$ versus T for **7**

3. The simulated and the experimental PXRD patterns for complexes 1-7.

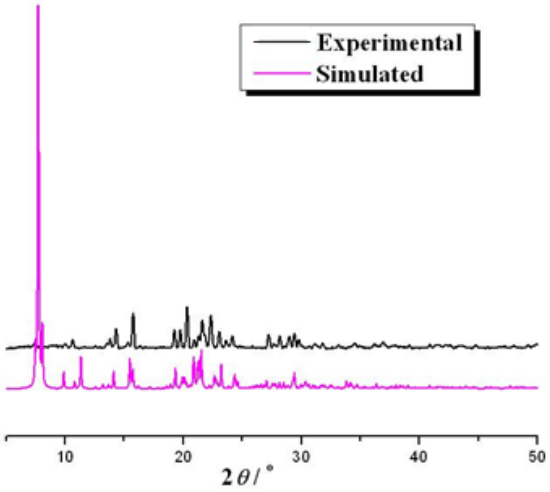

Fig. S8 The simulated (purple) and the experimental (black) PXRD patterns of **1**.

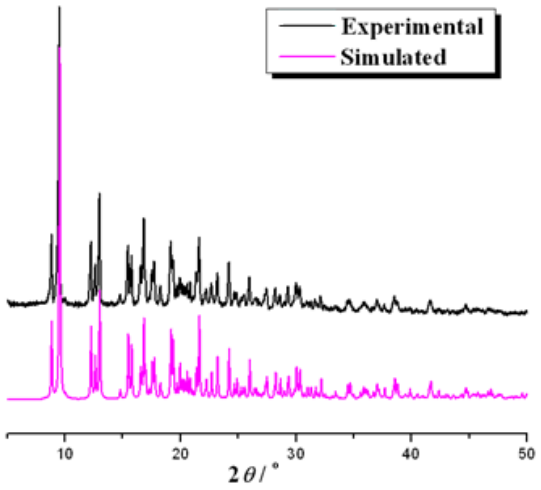

Fig. S9 The simulated (purple) and the experimental (black) PXRD patterns of **2**.

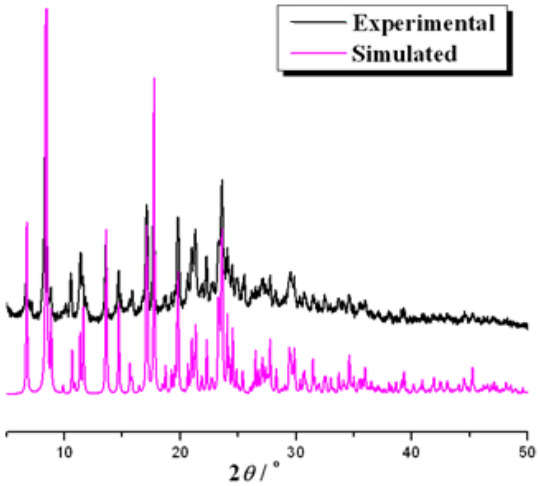

Fig. S10 The simulated (purple) and the experimental (black) PXRD patterns of **3**.

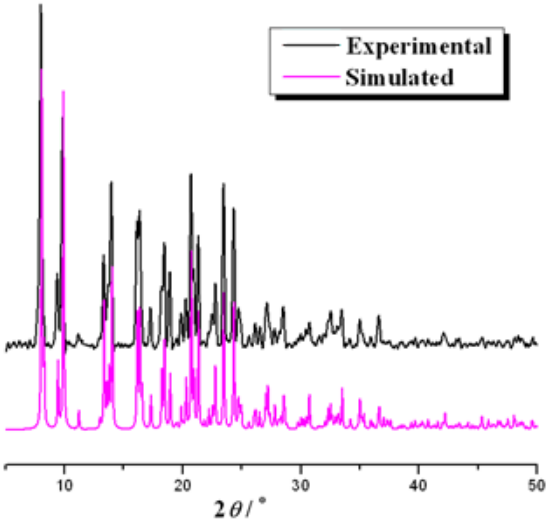

Fig. S11 The simulated (purple) and the experimental (black) PXRD patterns of **4**.

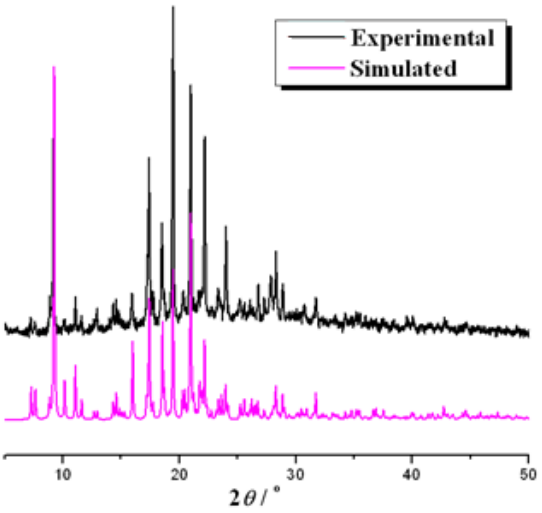

Fig. S12 The simulated (purple) and the experimental (black) PXRD patterns of **5**.

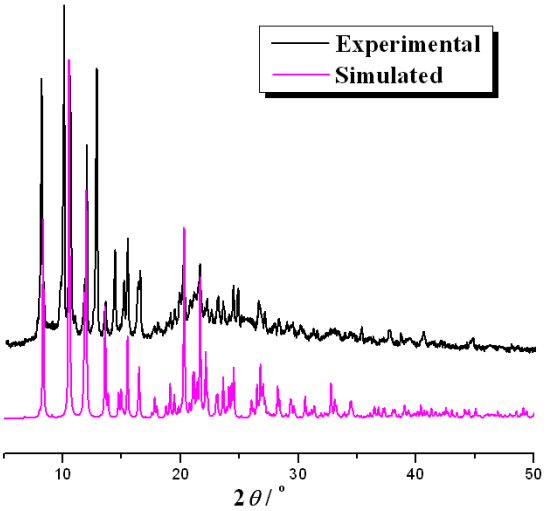

Fig. S13 The simulated (purple) and the experimental (black) PXRD patterns of **6**.

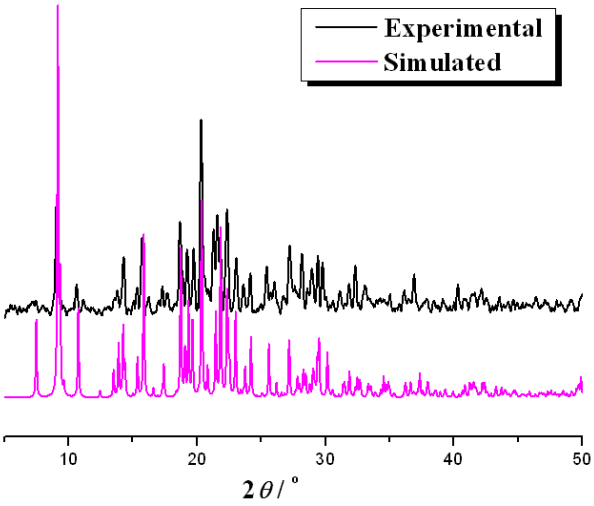

Fig. S14 The simulated (purple) and the experimental (black) PXRD patterns of **7**.

4. The curves of thermogravimetric analysis for complexes 1-7

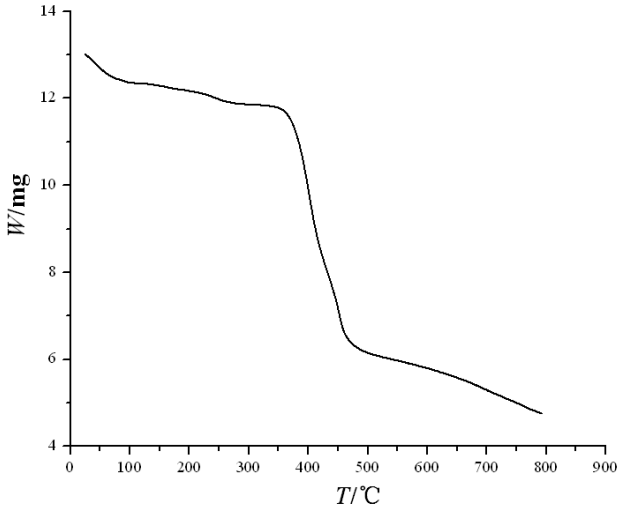

Fig. S15 TG curve from room temperature to 800 ˚C for **1**.

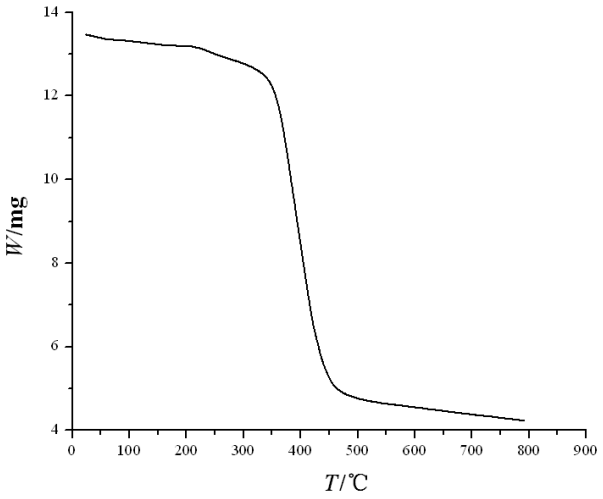

Fig. S16 TG curve from room temperature to 800 ˚C for **2**.

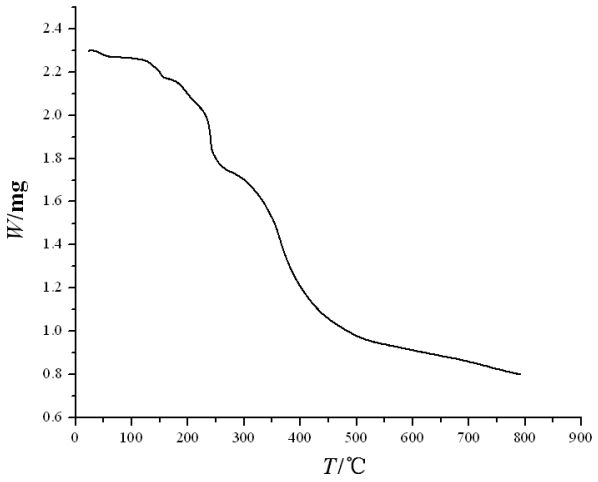

Fig. S17 TG curve from room temperature to 800 ˚C for **3**.

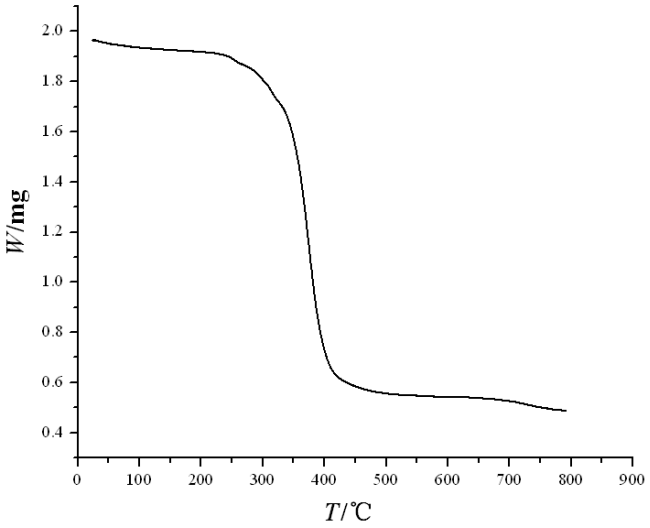

Fig. S18 TG curve from room temperature to 800 ˚C for **4**.

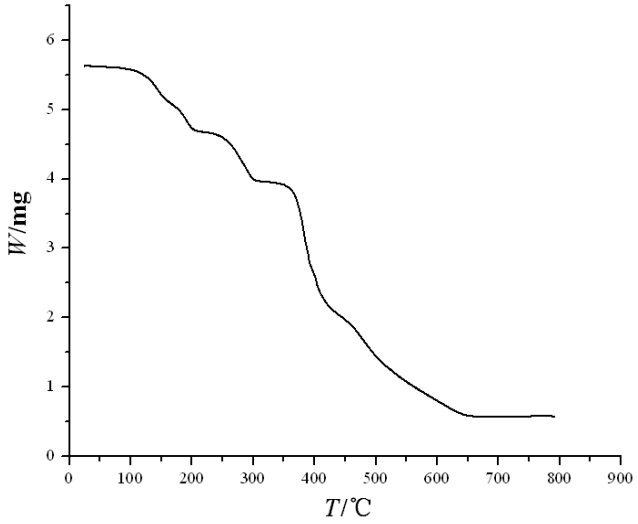

Fig. S19 TG curve from room temperature to 800 ˚C for **5**.

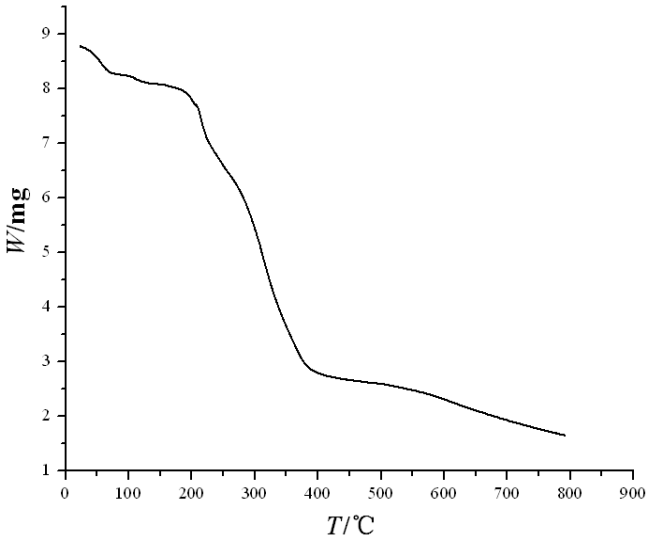

Fig. S20 TG curves from room temperature to 800 ˚C for **6**.

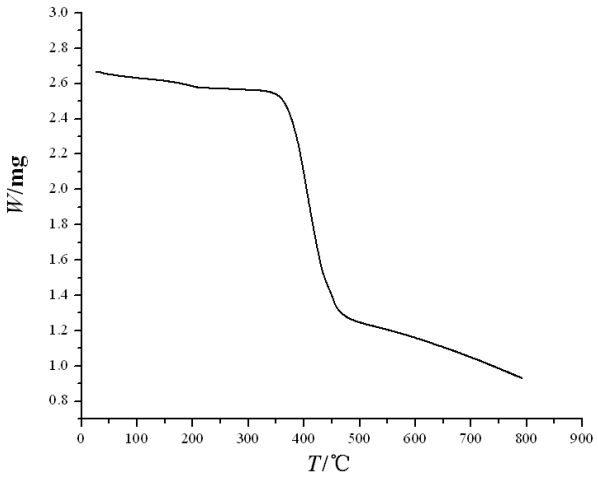

Fig. S21 TG curve from room temperature to 800 ˚C for **7**.

5. Tables of summary of crystallographic data for 1-7

Table S1 Summary of crystallographic data for **1-4**

	1·0.25H_2O	**2**	**3**·DMF	**4**
chemical formula	$C_{24}H_{24}ClCo_{0.5}N_4O_3\cdot0.25H_2O$	$C_{24}H_{22}Cl_2CuN_4O_2$	$C_{24}H_{22}CuN_6O_8$·DMF	$C_{24}H_{22}CuN_4O_6S$
fw	485.89	532.90	659.11	558.06
Cryst syst	Monoclinic	Orthorhombic	Triclinic	Triclinic
space group	*C*2/*c*	P*bca*	*P*$\bar{1}$	*P*$\bar{1}$
a/Å	15.340(1)	18.563(9)	10.323(6)	9.829(4)
b/Å	21.905(1)	12.601(6)	10.989(6)	11.206(5)
c/Å	16.945(1)	19.977(1)	13.345(8)	11.682(5)
α/deg	90	90	79.5(1)	102.8(1)
β/deg	113.4(1)	90	85.1(1)	104.7(1)
γ/deg	90	90	75.5(1)	98.2(1)
V/Å^3	5224.8(6)	4673.1(4)	1440.66(1)	1195.26(9)
Z	8	8	2	2
D_{calcd}, Mg/m^3	1.235	1.515	1.519	1.551
Abs coeff, mm^{-1}	0.484	1.193	0.824	1.050

F(000)	2024	2184	682	574
Cryst size, mm	0.22 × 0.20 × 0.18	0.22 × 0.21 × 0.20	0.24 × 0.20 × 0.19	0.22 × 0.18 × 0.17
θ_{min}, θ_{max}, deg	2.61, 25.01	2.04 , 25.01	1.55, 25.01	1.86, 25.00
T /K	296(2)	296(2)	296(2)	296(2)
no. of data collected	12834	21911	7385	6047
no. of unique data	4532	4115	5046	4167
no. of refined params	308	305	399	313
goodness-of-fit on F^2 [a]	1.013	1.049	1.053	1.018
Final *R* indices[b] [$I > 2\sigma(I)$]				
*R*1	0.0630	0.0337	0.0285	0.0789
*wR*2	0.2143	0.0828	0.0759	0.2051
R indices (all data)				
*R*1	0.0766	0.0440	0.0321	0.0846
*wR*2	0.2283	0.0897	0.0781	0.2110

[a] Goof = $[\Sigma\omega(F_o^2 - F_c^2)^2/(n-p)]^{1/2}$, where *n* is the number of reflection and *p* is the number of parameters refined. [b] R1 = $\Sigma(||F_o| - |F_c||)/\Sigma|F_o|$; wR2 = $1/[\sigma^2(F_o^2) + (0.0691P) + 1.4100P]$ where $P = (F_o^2 + 2F_c^2)/3$.

Table S2 Summary of crystallographic data for **5**-**7**

	5·2DMF	**6**·CH_3OH·1.75H_2O	**7**
chemical formula	$C_{32}H_{26}CoN_4O_6$ ·2DMF	$C_{28}H_{27}CuN_4O_6$ ·CH_3OH·1.75H_2O	$C_{24}H_{22}Cl_2CoN_4O_2$
fw	767.69	642.65	528.29
Cryst syst	Monoclinic	Monoclinic	Triclinic

space group	$P2_1/n$	$C2/c$	$P\bar{1}$
a/Å	12.794(5)	21.696(1)	9.706(5)
b/Å	16.935(7)	16.665(1)	10.761(5)
c/Å	18.010(8)	17.179(1)	13.131(6)
α/deg	90	90	112.4(1)
β/deg	104.7(1)	102.0(2)	96.6(1)
γ/deg	90	90	103.7(1)
V/Å^3	3774.1(3)	6075.8(9)	1198.16(1)
Z	4	8	2
D_{calcd}, Mg/m^3	1.351	1.405	1.464
Abs coeff, mm^{-1}	0.514	0.777	0.968
F(000)	1604	2684	542
Cryst size, mm	0.19 × 0.15 × 0.14	0.25 × 0.23 × 0.20	0.25 × 0.16 × 0.15
θ_{min}, θ_{max}, deg	1.76, 25.01	1.55, 25.01	2.11, 25.01
T /K	296(2)	296(2)	296(2)
no. of data collected	19055	14826	6157
no. of unique data	6654	5324	4206
no. of refined params	482	396	298
goodness-of-fit on F^2 [a]	1.045	1.025	1.047
Final R indices[b] [$I > 2\sigma(I)$]			
$R1$	0.0452	0.0610	0.0283
$wR2$	0.1273	0.1554	0.0725
R indices (all data)			
$R1$	0.0612	0.1087	0.0320
$wR2$	0.1409	0.1853	0.0748

[a] Goof = $[\Sigma\omega(F_o^2 - F_c^2)^2/(n-p)]^{1/2}$, where n is the number of reflection and p is the number of parameters refined. [b] R1 = $\Sigma(||F_o| - |F_c||)/\Sigma|F_o|$; wR2 = $1/[\sigma^2(F_o^2)$ +

$(0.0691P) + 1.4100P]$ where $P = (F_o^2 + 2F_c^2)/3$.