Solvent Effect on the Structures and Magnetic Properties of Two Doubly Interpenetrated Metal-Organic Frameworks

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Supporting Information

Table S1. Selected bond lengths (Å) and angles (º) for **1-H_2O**

Co1—O5	1.995 (9)	Co1—N1	2.120 (8)	Co1—N5B	2.180 (8)
Co1—O7A	2.052 (8)	Co1—O1	2.177 (8)	Co1—O2	2.191 (8)
Co2—O6	1.989 (8)	Co2—N6	2.135 (9)	Co2—O3D	2.176 (9)
Co2—O8A	2.038 (8)	Co2—N10C	2.163 (9)	Co2—O4D	2.244 (9)
O5—Co1—O7A	122.6 (4)	N1—Co1—O1	85.5 (4)	O5—Co1—O2	88.7 (4)
O5—Co1—N1	89.8 (4)	O5—Co1—N5B	95.1 (4)	O7A—Co1—O2	148.5 (4)
O7A—Co1—N1	89.3 (4)	O7A—Co1—N5B	88.3 (4)	N1—Co1—O2	94.5 (4)
O5—Co1—O1	147.0 (4)	N1—Co1—N5B	175.1 (5)	O1—Co1—O2	59.2 (3)
O7A—Co1—O1	90.1 (4)	O1—Co1—N5B	90.3 (4)	N5B—Co1—O2	85.4 (4)
O6—Co2—O8A	123.5 (4)	N6—Co2—N10C	175.9 (4)	O6—Co2—O4D	88.2 (4)
O6—Co2—N6	92.8 (3)	O6—Co2—O3D	146.7 (4)	O8A—Co2—O4D	148.0 (4)
O8A—Co2—N6	87.6 (3)	O8A—Co2—O3D	89.6 (4)	N6—Co2—O4D	86.9 (4)
O6—Co2—N10C	91.3 (4)	N6—Co2—O3D	91.8 (4)	N10C—Co2—O4D	92.5 (4)
O8A—Co2—N10C	90.8 (4)	N10C—Co2—O3D	84.4 (4)	O3D—Co2—O4D	59.1 (3)

Symmetry codes: A: *x*, *y*-1, *z*; B: *x*+1/2, -*y*+3/2, *z*; C: *x*-1/2, -*y*+3/2, *z*; D: *x*, *y*, *z*+1.

Table S2. Selected bond lengths (Å) and angles (º) for **2-MeOH**

Co1—O1	1.989 (3)	Co1—O7B	2.122 (3)	Co1—N5C	2.150 (3)
Co1—O3A	2.033 (3)	Co1—N1	2.126 (3)	Co1—O8B	2.277 (3)
Co2—O5	1.949 (3)	Co2—O2	1.998 (3)	Co2—N10D	2.233 (3)
Co2—O4A	1.964 (3)	Co2—N6	2.184 (3)		
O1—Co1—O3A	117.74 (12)	O7B—Co1—N1	94.29 (13)	O1—Co1—O8B	91.09 (12)
O1—Co1—O7B	149.47 (12)	O1—Co1—N5C	91.23 (13)	O3A—Co1—O8B	151.17 (11)
O3A—Co1—O7B	92.31 (11)	O3A—Co1—N5C	88.01 (12)	O7B—Co1—O8B	59.04 (10)
O1—Co1—N1	90.73 (13)	O7B—Co1—N5C	84.11 (12)	N1—Co1—O8B	88.37 (12)
O3A—Co1—N1	90.92 (12)	N1—Co1—N5C	178.04 (13)	N5C—Co1—O8B	91.78 (12)
O5—Co2—O4A	118.57 (13)	O4A—Co2—N6	91.28 (12)	O4A—Co2—N10D	89.60 (12)
O5—Co2—O2	113.79 (14)	O2—Co2—N6	92.05 (12)	O2—Co2—N10D	85.32 (12)
O4A—Co2—O2	127.51 (12)	O5—Co2—N10D	91.78 (13)	N6—Co2—N10D	177.22 (13)
O5—Co2—N6	90.12 (13)				

Symmetry codes: A: *x*, *y*-1, *z*; B: *x*+1/2, -*y*+3/2, *z*-1/2; C: *x*-1/2, -*y*+3/2, *z*-1/2; D: *x*+1/2, -*y*+3/2, *z*+1/2.

Table S3. Crystal data and structure refinement for **1-H_2O** and **2-MeOH**

Complex	**1-H_2O**	**2-MeOH**
Empirical formula	$C_{40}H_{28}Co_2N_{10}O_{10}$	$C_{41}H_{32}Co_2N_{10}O_{10}$
Formula weight	926.58	942.63
Crystal system	orthorhombic	Monoclinic
Space group	*Pna*2_1	*P*2_1/*n*
a (Å)	29.144(6)	17.497(4)
b (Å)	10.411(2)	10.171(2)
c (Å)	14.792(3)	23.344(5)
β (°)		90.54(3)
Volume (Å^3)	4488.2(16)	4154.2(14)
Z	4	4
D_{calc} (g/cm^3)	1.371	1.507
θ range for data collection	1.5 to 25.00	1.5 to 25.25
Reflections collected	20019	23652
Independent reflections	7052 (Rint =0.141)	7490 (Rint =0.053)
Data/restraints/ parameters	7052/290/569	7490/20/568
Goodness of fit (GOF)	1.007	1.022
Final *R* indices[$I > 2\sigma(I)$]	0.1057	0.0587
R indices (all data)	0.2230	0.1199
Largest diff. peak and hole (e/Å^3)	0.464/-0.469	0.621/-0.342

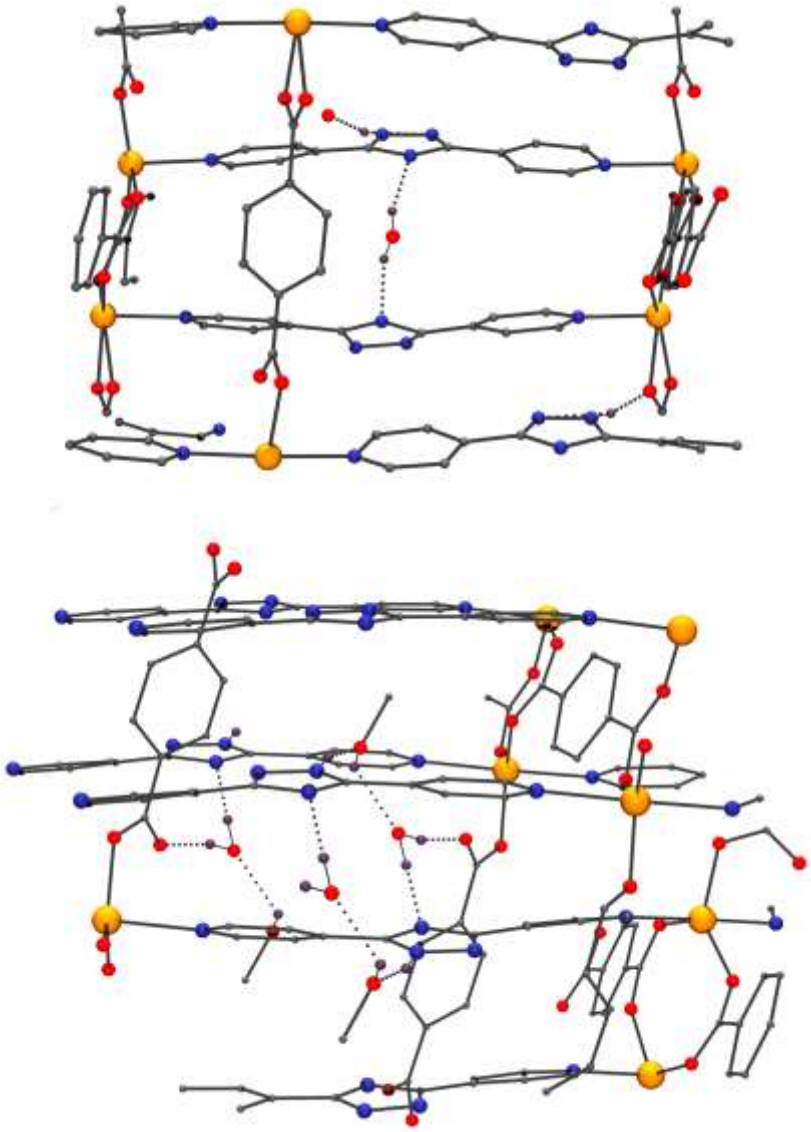

Fig. S1. H-bonds promoted by the solvent molecules in **1-H_2O** (top) and **2-MeOH** (bottom). In **1-H_2O** the water molecules interact by means of two H-bonds with the triazole rings whereas in **2-MeOH** interact with one triazole ring and the non-coordinated O-atom of the carboxylato function. Linkage with the second triazole ring is mediated by the H-bonds established by the water-methanol and methanol-triazole bonds. The triazole rings are pillared in **1-H_2O** whereas they are deplaced in **2-MeOH**.

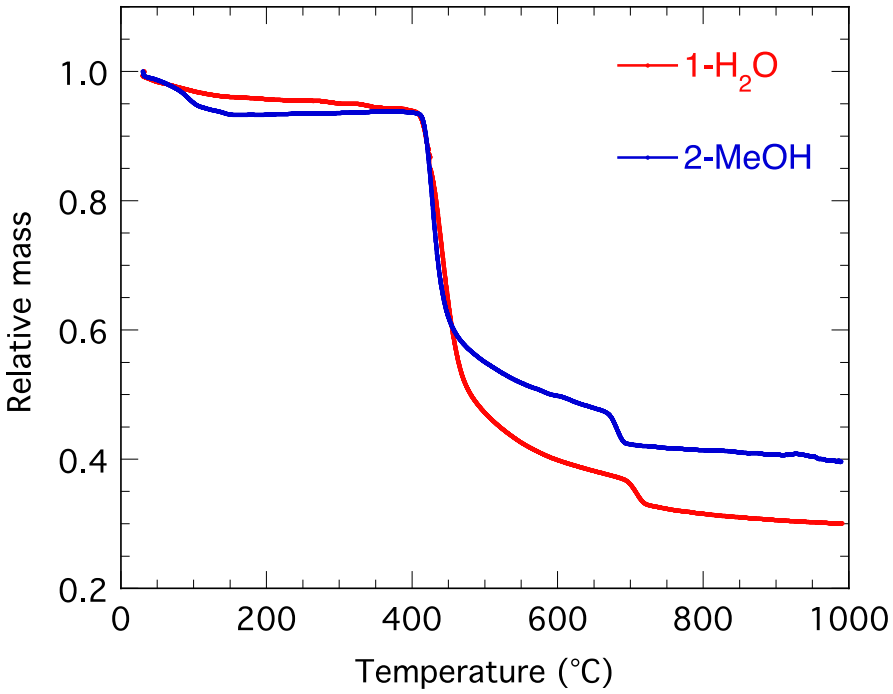

Fig. S2. TGA of **1-H_2O** (red) and **2-MeOH** (blue).

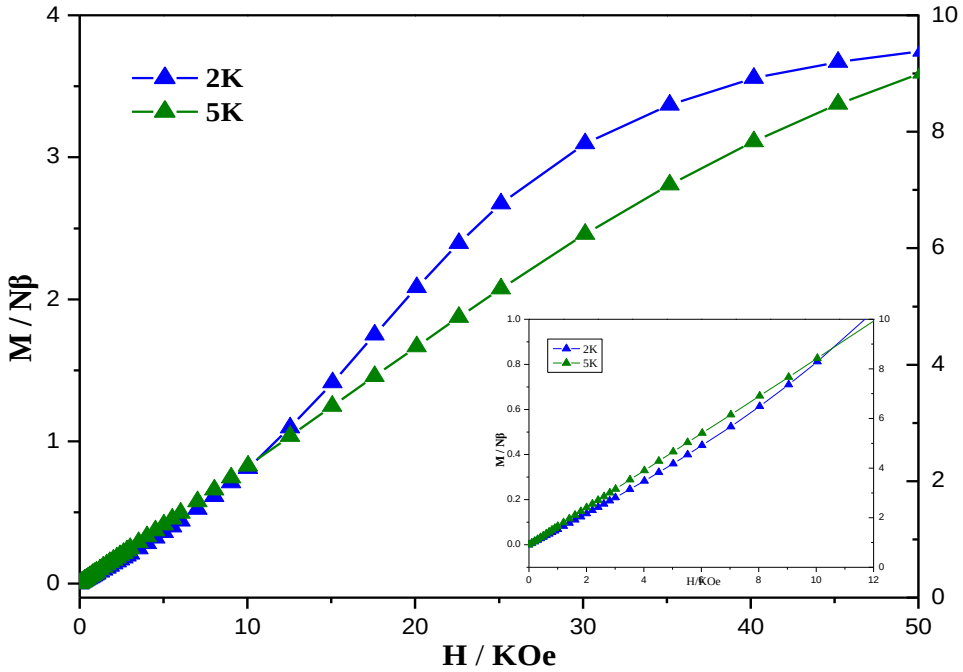

Fig. S3. *M* vs *H* plot for **1-H_2O**. The inset is the blowup of the curves for **1-H_2O** in the lower field region.