

Ligand-induced isomerization, from 3D to 2D→3D POMOFs constructed by Keggin type of silicotungstate anions, Cu(I) and 1,n-di(4H-1,2,4-triazol-4-yl)benzene (n = 3, 4) ligands

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Table S1. Selected bonds lengths (Å) and angles (°) for complexes **1** and **2**.

Bonds (Å)	1	Bonds (Å)	2
O7—Cu1	2.66 (2)	Cu1—N19	1.947(1)
Cu1—N11	1.95 (2)	Cu1—N7	1.984(1)
Cu1—N3 ⁱ	1.97 (2)	Cu1—N1	2.111(2)
Cu1—N2	2.00 (2)	Cu1—O29	2.569(1)
Cu2—N5	2.003 (2)	Cu2—N20	1.868 (2)
Cu2—N6 ⁱⁱ	2.021 (2)	Cu2—N13	1.951 (2)
Cu2—N9 ⁱⁱⁱ	2.071 (2)	Cu2—N2	1.999 (1)
Cu2—N8	2.105 (2)	Cu3—N16 ^v	1.917 (1)
		Cu3—N4	1.934 (1)
		Cu3—N10 ^{iv}	2.112 (2)
		Cu4—N17 ⁱⁱ	1.914 (2)
		Cu4—N22 ⁱ	1.945 (2)
		Cu4—N11 ⁱⁱⁱ	2.013 (1)
		Cu4—O22	2.455 (1)
Bond angles (°)	1	Bond angles (°)	2
N11—Cu1—N3 ⁱ	128.0 (9)	N19—Cu1—N7	141.0 (6)
N11—Cu1—N2	111.9 (8)	N19—Cu1—N1	113.0 (5)
N3 ⁱ —Cu1—N2	119.3 (9)	N7—Cu1—N1	104.2 (6)
N5—Cu2—N6 ⁱⁱ	115.9 (7)	N20—Cu2—N13	136.8 (6)
N5—Cu2—N9 ⁱⁱⁱ	108.2 (7)	N20—Cu2—N2	113.9 (6)
N6 ⁱⁱ —Cu2—N9 ⁱⁱⁱ	118.2 (7)	N13—Cu2—N2	109.2 (6)
N5—Cu2—N8	113.0 (7)	N16 ^v —Cu3—N4	142.0 (6)
N6 ⁱⁱ —Cu2—N8	104.9 (7)	N16 ^v —Cu3—N10 ^{iv}	112.2 (6)
N9 ⁱⁱⁱ —Cu2—N8	94.6 (7)	N4—Cu3—N10 ^{iv}	105.7 (6)
N11—Cu1—N3 ⁱ	128.0 (9)	N17 ⁱⁱ —Cu4—N22 ⁱ	134.4 (6)
		N17 ⁱⁱ —Cu4—N11 ⁱⁱⁱ	113.5 (6)
		N22 ⁱ —Cu4—N11 ⁱⁱⁱ	111.9 (6)

Symmetry code:

1, (i) 1.75-y, -0.25+x, 0.75-z; (ii) 0.25+y, 1.25-x, 0.25+z; (iii) 1.25-y, -0.25+x, -0.25+z; (iv) 2-x, 1-y, 1-z.

2, (i) 2-x, -y, 1-z; (ii) 2-x, -y, -z; (iii) 1-x, 1-y, 1-z; (iv) x, y, -1+z; (v) -1-x, 1+y, z.

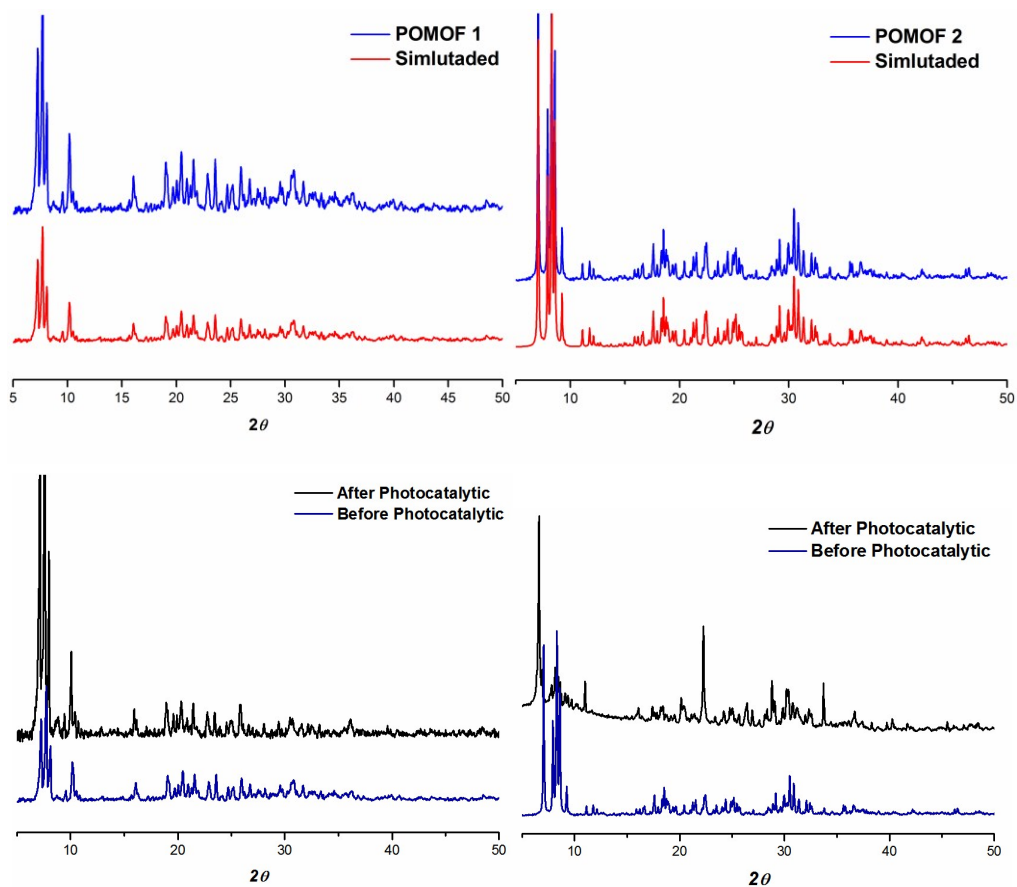


Fig. S1 The simulative and experimental XRPD patterns of POMOF **1** and **2** (upside). The XRPD patterns of POMOF **1** and **2** before and after photocatalytic (underside).

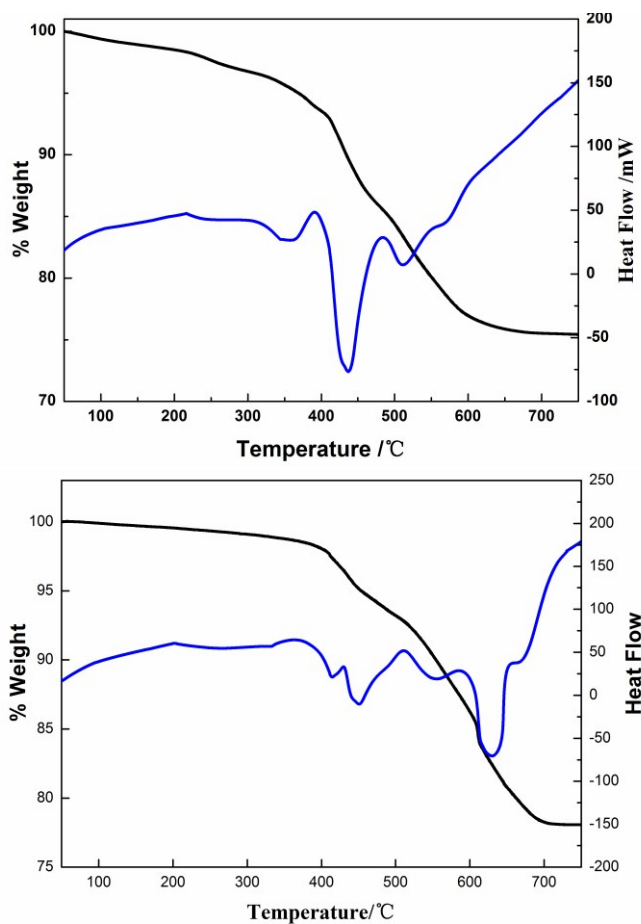


Fig. S2 Thermogravimetric analyses (TGA) of POMOFs 1 and 2.

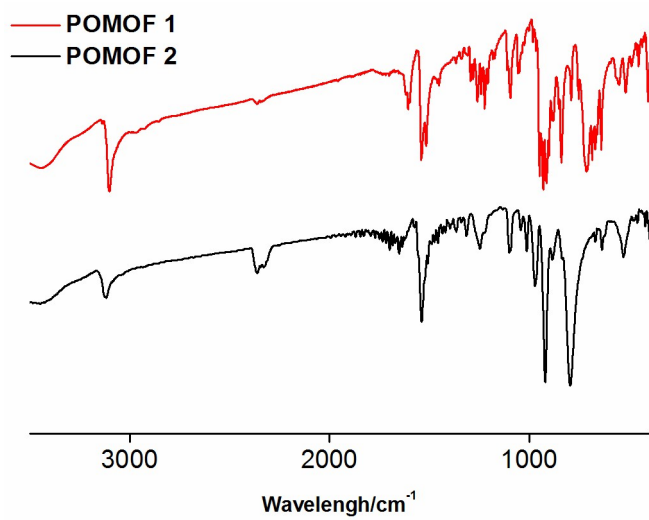


Fig. S3 IR spectra of POMOFs 1 and 2.