

Supporting Materials

Auxiliary ligand-controlled photochromism and decolourization of two bipyridinium-based metal-organic hybrid materials with various water clusters

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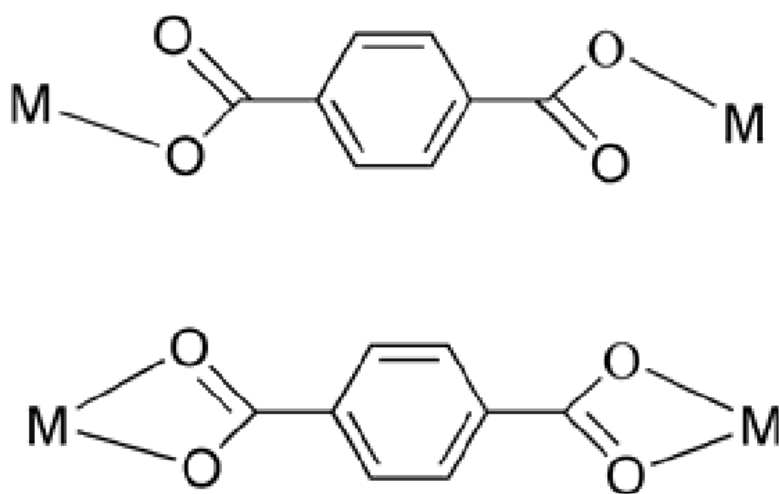


Fig. S1 The coordination modes of the p-BDC ligands in compound **1**.

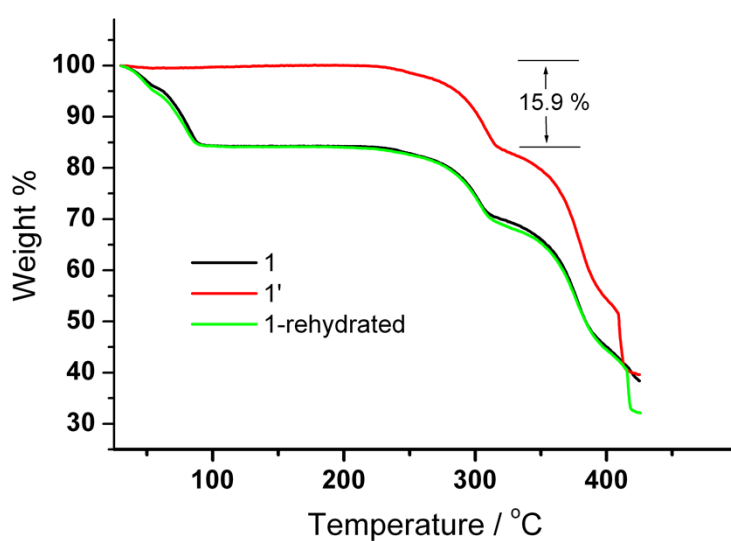


Fig. S2 The TGA curves of **1** (black line), dehydrated sample **1'** (red line) and the sample exposed to humid air for 48 hours (green line).

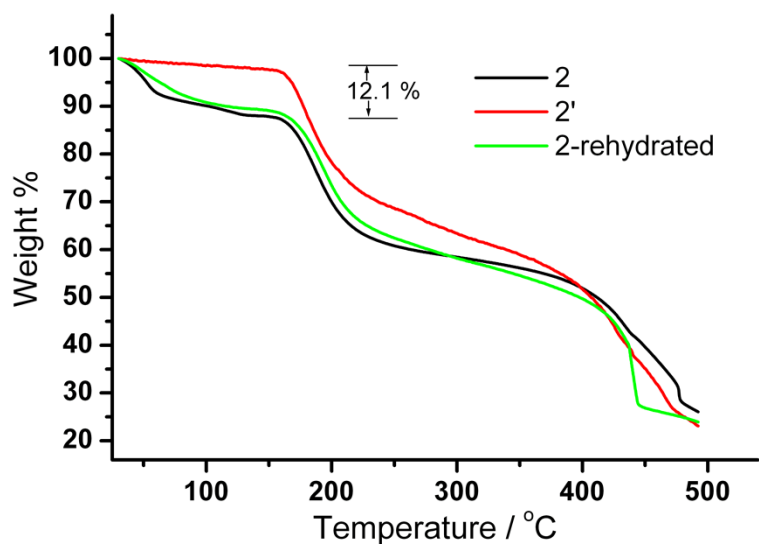


Fig. S3 The TGA curves of **2** (black line), dehydrated sample **2'** (red line) and the sample exposed to humid air for 120 hours (green line).

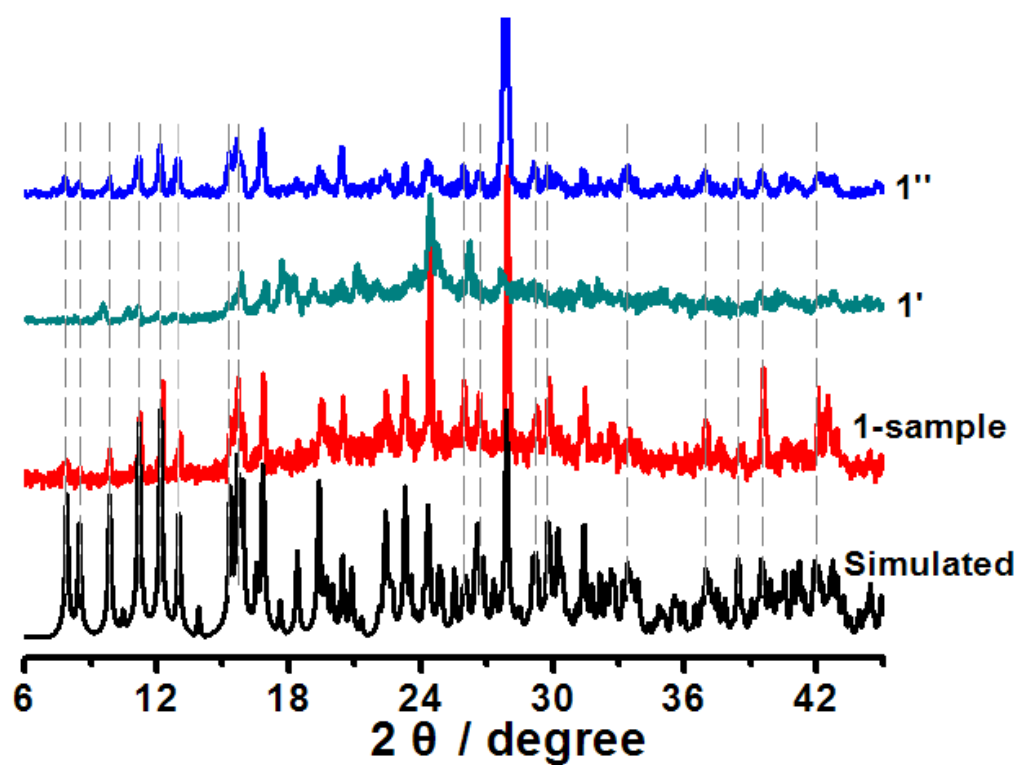


Fig. S4 The PXRD patterns of **1**. Black: simulated one; red: as-synthesized sample **1**; green: dehydrated sample **1'**; blue: the sample exposed to humid air for 48 hours.

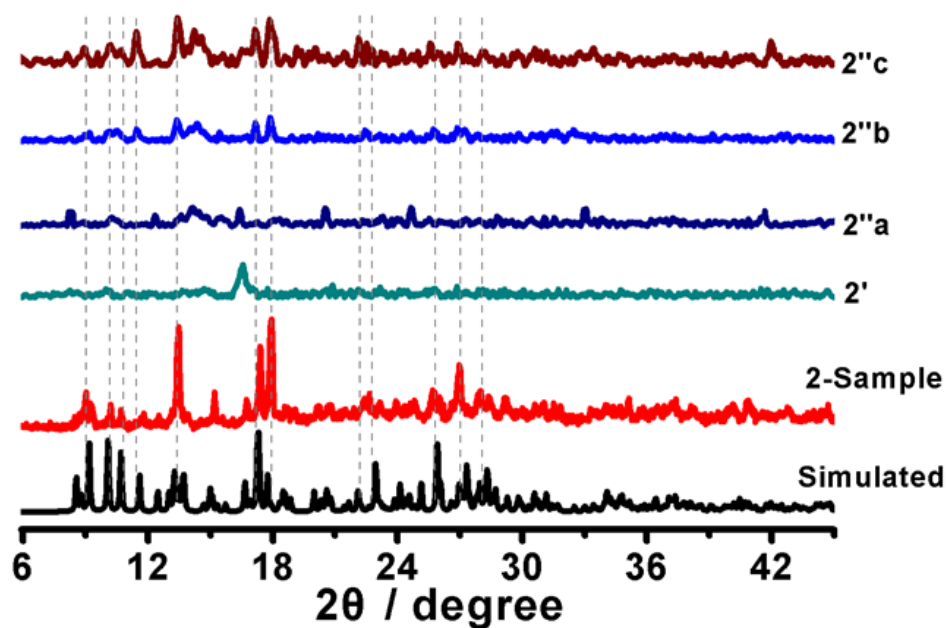


Fig. S5 The PXRD patterns of **2**. Black: simulated one; red: as-synthesized sample **2**; green: dehydrated sample **2'**; dark blue: the sample exposed to humid air for 48 hours; blue: the sample exposed to humid air for 72 hours; brown: the sample exposed to humid air for 120 hours.

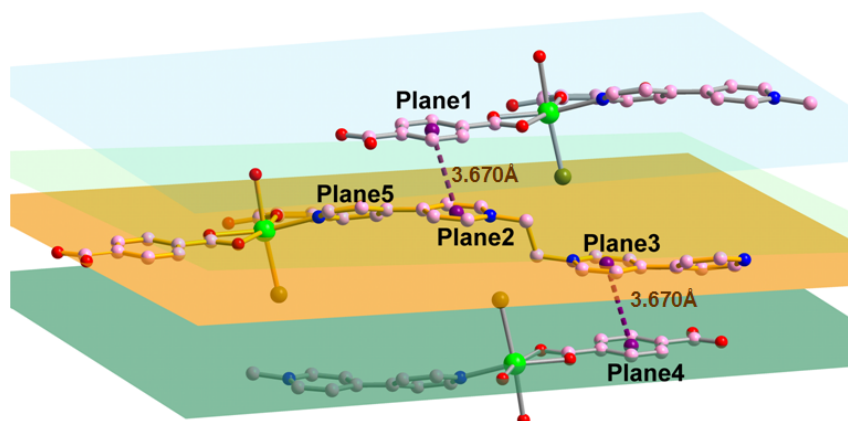


Fig. S6 The orientation of the pyridinium ring and the *p*-BDC²⁻ group in compound **1**.

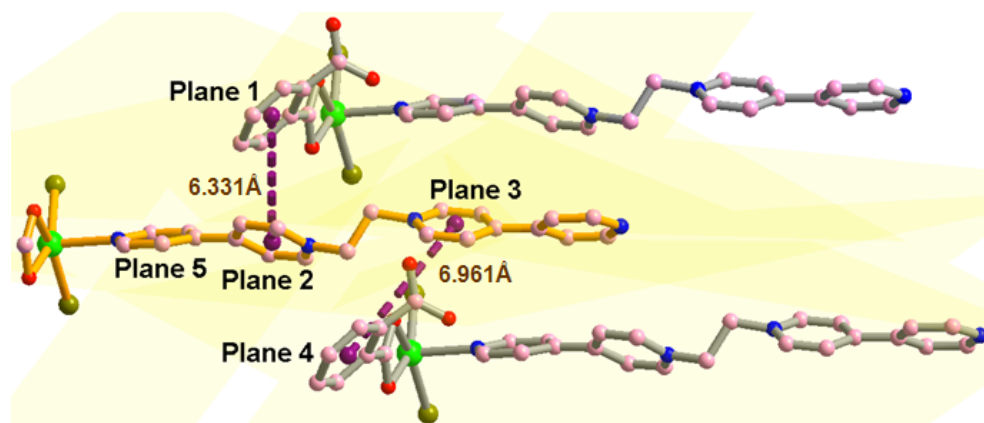


Fig. S7 The orientation of the pyridinium ring and the *p*-BDC²⁻ group in compound **2**.

Table S1 Hydrogen-bond parameters in compound **1**.

D-H...A	d(D-H) (Å)	D(H...A) (Å)	D(D...A) (Å)	∠D-H...A (°)
O1W-H1A...O3W	0.820	2.053	2.873	179.7
O1W-H1B...O2W	0.816	1.926	2.732	169.3
O2W-H2A...O5W	0.819	2.018	2.806	161.5
O5W-H5A...O3W	0.820	2.013	2.818	167.2
O5W-H5B...O6W	0.821	2.200	2.794	129.4
O6W-H6B...O4W	0.820	1.987	2.737	151.8
O6W-H6B...O5W	0.820	2.138	2.956	174.5
O2W-H2B...O2	0.819	2.075	2.892	174.1
O3W-H3A...O1	0.823	2.049	2.856	166.4
O3W-H3B...O4	0.824	1.969	2.773	164.9
O4W-H4A...O3	0.821	1.975	2.767	161.7
O4W-H4B...O1	0.823	2.029	2.776	150.7

Table S2 Hydrogen-bond parameters in compound **2**

D-H...A	d(D-H) (Å)	D(H...A) (Å)	D(D...A) (Å)	∠D-H...A (°)
O1W-H1A...O2W	0.845	2.096	2.790	136.2
O2W-H2B...O8W	0.849	2.022	2.811	154.1
O3W-H3A...O2W	0.850	2.066	2.905	168.9
O3W-H3B...O4W	0.850	2.009	2.845	167.6
O4W-H4A...O6W	0.848	1.974	2.811	168.8
O4W-H4B...O7W	0.852	1.890	2.741	176.0
O5W-H5A...O4W	0.850	1.943	2.778	166.7
O5W-H5B...O1W	0.850	1.974	2.750	151.3
O6W-H6A...O3W	0.843	2.037	2.856	163.7
O6W-H6B...O1W	0.853	1.863	2.691	163.0
O7W-H7A...O6W	0.846	2.000	2.843	174.1
O8W-H8A...O5W	0.851	1.931	2.771	169.3
O1W-H1B...O4	0.835	1.837	2.655	165.9
O2W-H2A...O4	0.854	1.918	2.726	157.4
O7W-H7B...O3	0.864	1.953	2.799	166.2
O8W-H8B...O3	0.855	2.025	2.855	163.7