ELECTRONIC SUPPORTING INFORMATION

Unravelling the mechanism of water sensing by the Mg^{2+} dihydroxy-terephthalate MOF (AEMOF-1′)

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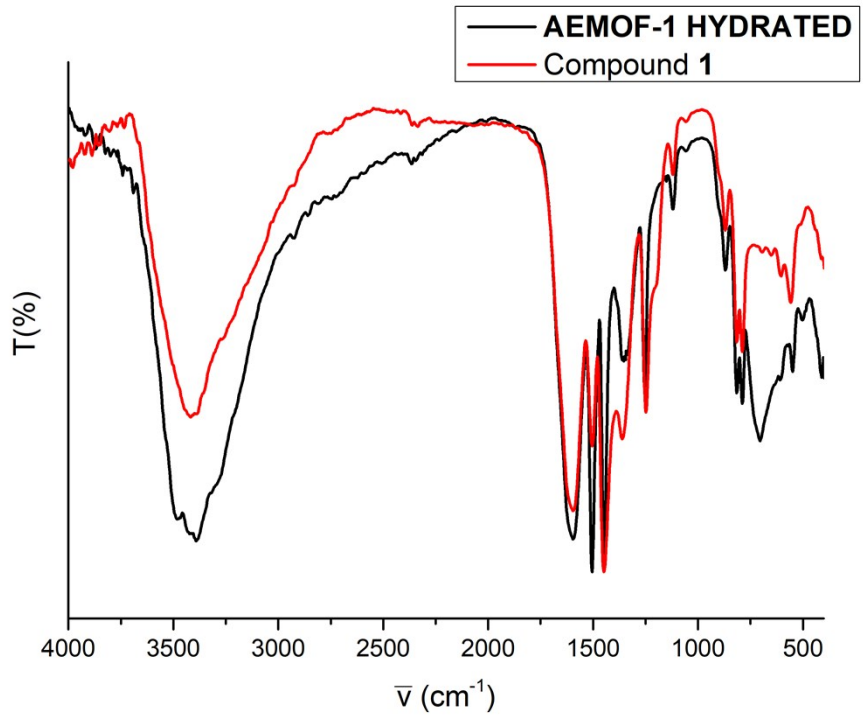


Fig. S1. IR spectra of **AEMOF-1 hydrated** and compound **1**.

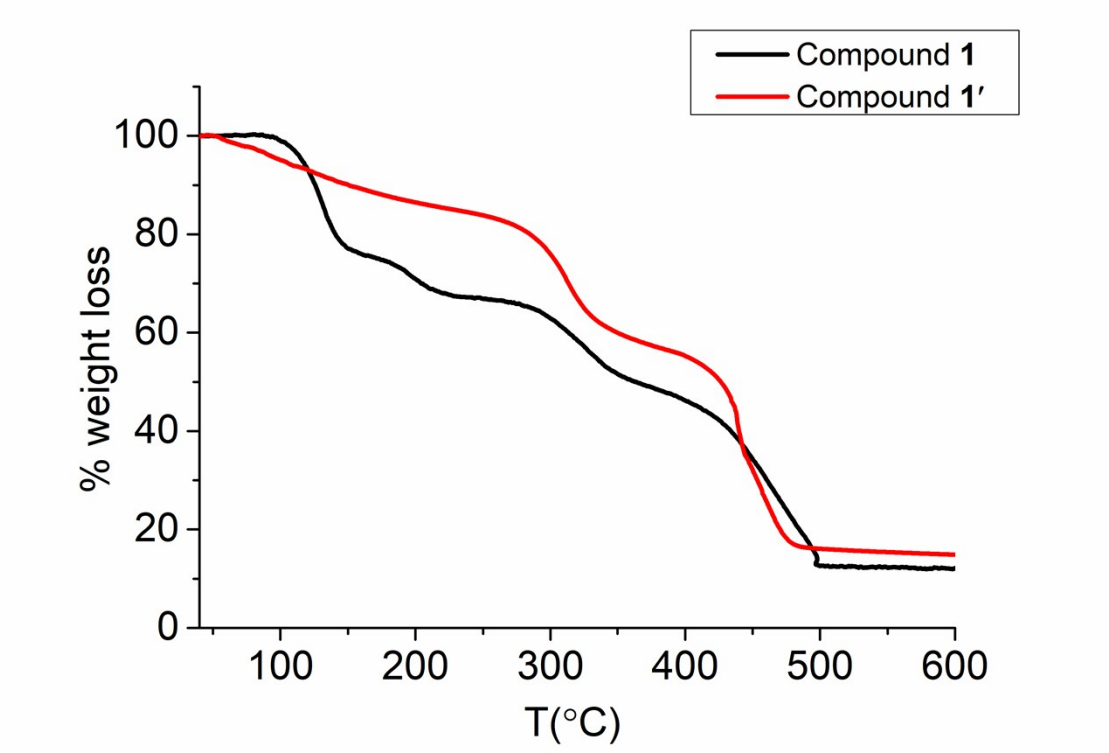


Fig. S2. TGA data for compounds **1** and **1′**.

The TGA data for compound **1** reveal weight losses starting from ~ 100^{0}C and ending at ~ 600 ^{0}C. These weight losses are attributed to the removal of water molecules and the decomposition of the H_2dhtp^{2-} ligands. The calculated and found total weight loss for **1**, considering the removal of six water molecules and one H_2dhtp^{2-} ligand (with the TGA residue being MgO), are 87.7 and 87.9 % respectively.

The TGA data for compound **1′** indicate continuous weight losses starting from ~ 40 ^{0}C and ending at ~ 600 ^{0}C. The calculated and found total weight loss for **1′**, considering the removal of two coordinating water molecules and one H_2dhtp^{2-} ligand (with the TGA residue being MgO), are 84.3 and 85.1 % respectively.

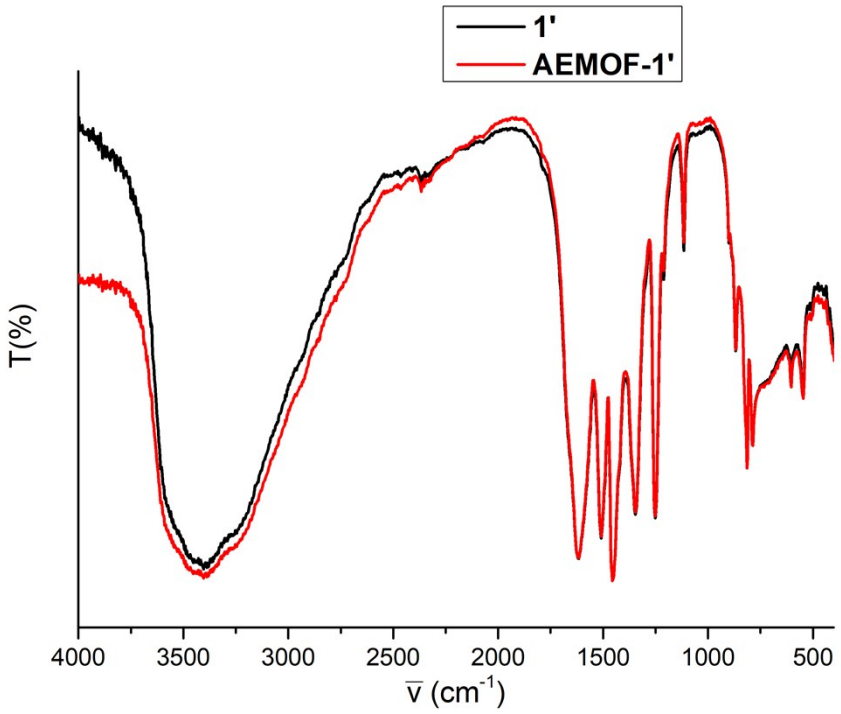


Fig. S3. IR spectra of **AEMOF-1´** and **1´**.

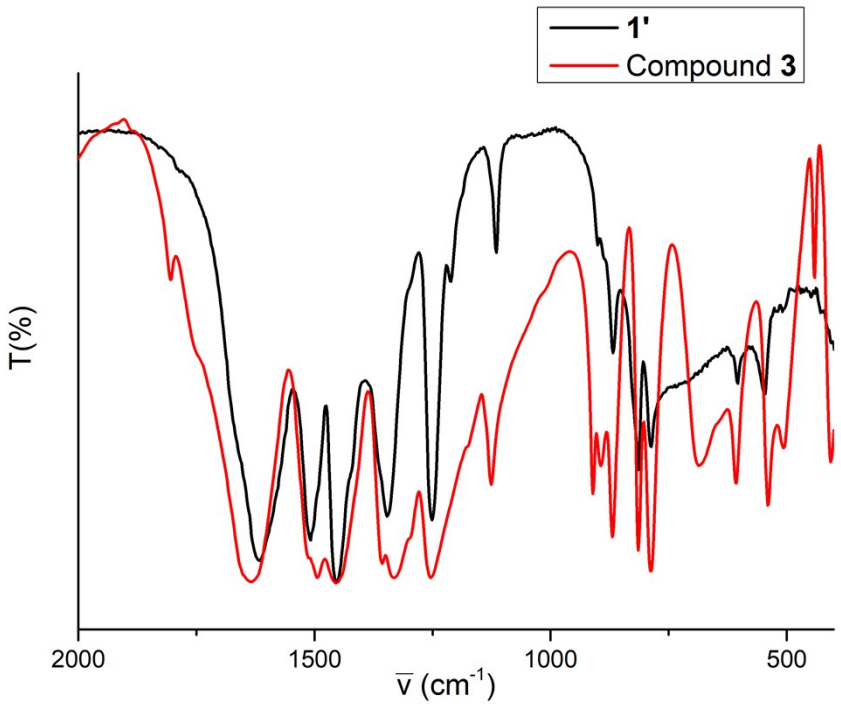
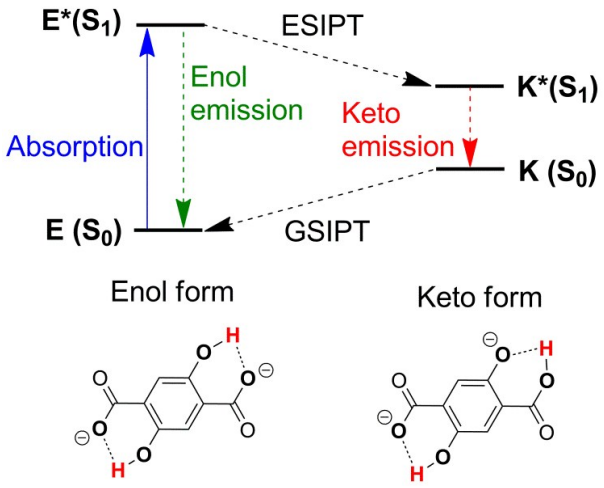


Fig. S4. IR spectra of **1´** and **3**.



Scheme S1. The four level ESIPT photo-cycle involved in the photophysics of AEMOFs. GSIPT stands for ground state intramolecular proton transfer.

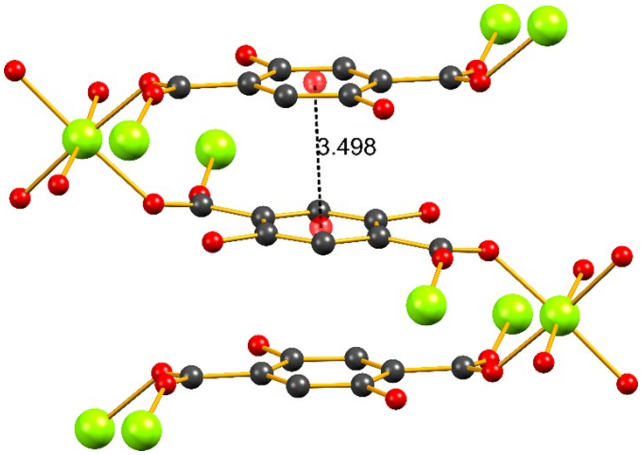


Fig. S5. Representation of the strong π-π interactions in compound **3**.

Table S1. Dimensions of the unique hydrogen bonds (distances in Å and angles in °) for **1**.

D^a – H⋯A^b	D^a ⋯A^b	H⋯A^b	< D^a H A^b
O2T–H1T⋯O3#1	2.609	1.77	170
O2T–H2T⋯O2#2	2.854	2.05	157
O3T'–H3T'⋯O6#3	3.018	2.18	175
O1T–H1T1⋯O4#1	2.704	1.87	179
O1T–H1T2⋯O5#4	2.737	1.91	176
O3T'–H4T'⋯O1W#3	2.787	2.07	164
O1W–H1W⋯O3#5	2.732	1.89	179
O1W–H2W⋯O3T'#6	3.101	2.32	154
O5–H1O5⋯O2	2.528	1.73	152
O6–H1O6⋯O4	2.491	1.74	146

Symmetry transformations used to generate equivalent atoms:
(1) –1+x, y, –1+z; (2) –x, –0.5+y, –z; (3) 1–x, –0.5+y, –z; (4) x, y, –1+z; (5) 1–x, 0.5+y, 1–z; (6) x, 0.5–y, z

[a]D= donor atom

[b]A= acceptor atom