Supporting Information

Porous High Valence Metal-Organic Framework Featuring Open Coordination Sites for Effective Water Adsorption

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Table S1 Crystal data and structure refinement details for **HV-MOF-1**.

Compound	**HV-MOF-1**
Formula	$C_{21}H_{23}ErN_4O_{11}$
Formula weight	674.69
Crystal system	Triclinic
Space group	*P*-1
a/ Å	9.862(2)
b/ Å	11.693(2)
c/ Å	13.404(3)
α/°	66.91(3)
β/°	86.98(3)
γ/°	76.69(3)
T/K	293 (2)
μ (mm^{-1})	0.095
Cryst dimensions	0.21×0.10×0.10
No. of reflns collected	5055
No. of unique reflns	3747
No. of params	320
Goodness-of-fit on F^2	0.969
R_1, wR_2 ($I>2\sigma(I)$)	0.0624, 0.1334
R_1, wR_2 (all data)	0.0953, 0.1467
CCDC No	1864545

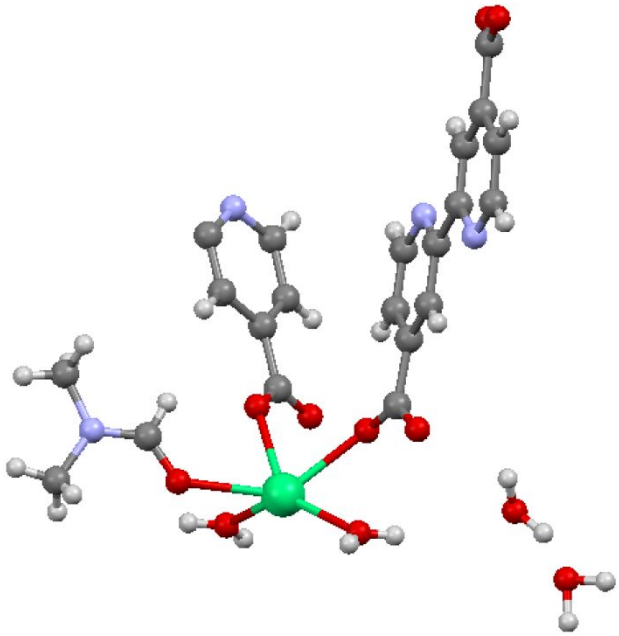

Figure S1. The asymmetric unit of **HV-MOF-1**.

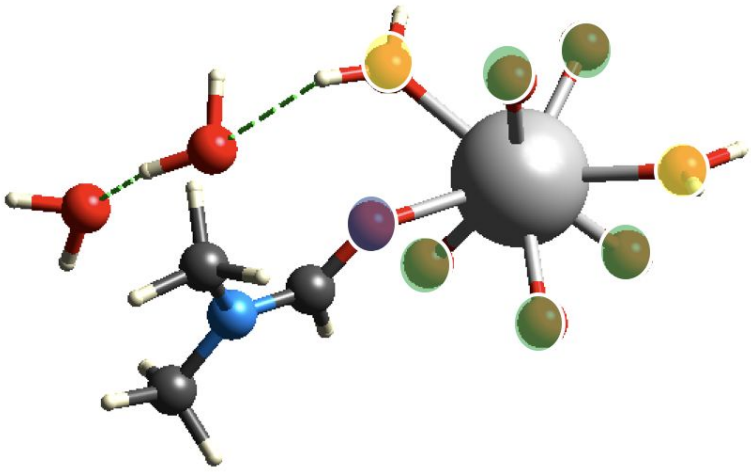

Figure S2. The stretch direction of the two lattice H_2O (in yellow shadow), DMF (in blue shadow) and dcbp molecules (in green shadow) around the Er^{3+} anions.

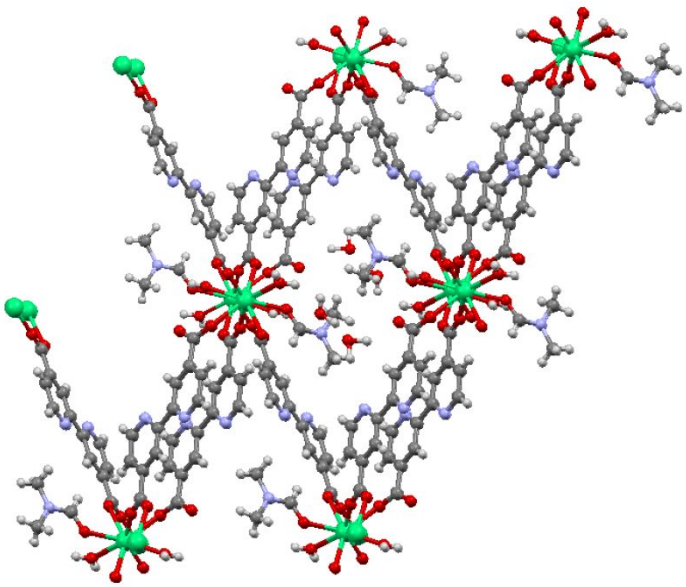

Figure S3. Illustration of the stretch direction for all of the solvent molecules both coordinated and un-coordinated around the diamond-like pores.

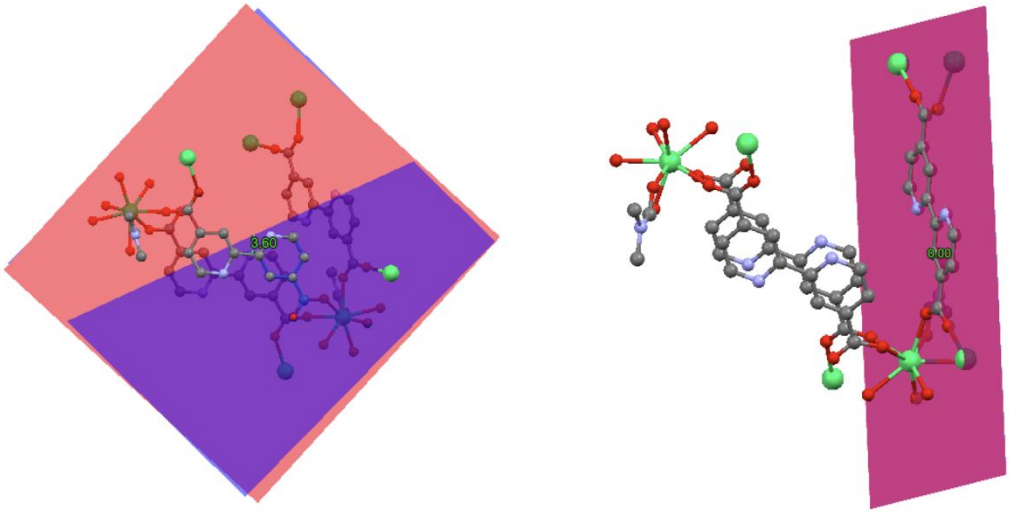

Figure S4. The co-planar of pyridine rings for three-dentate (left) and four-dentate motif (right), with dihedral angle of 3.6º and 0º, respectively.

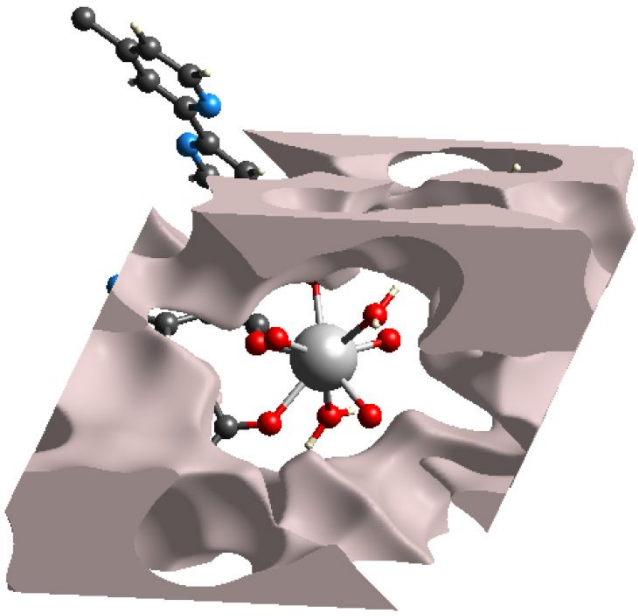

Figure S5. Crystal voids calculations of **HV-MOF-1**.

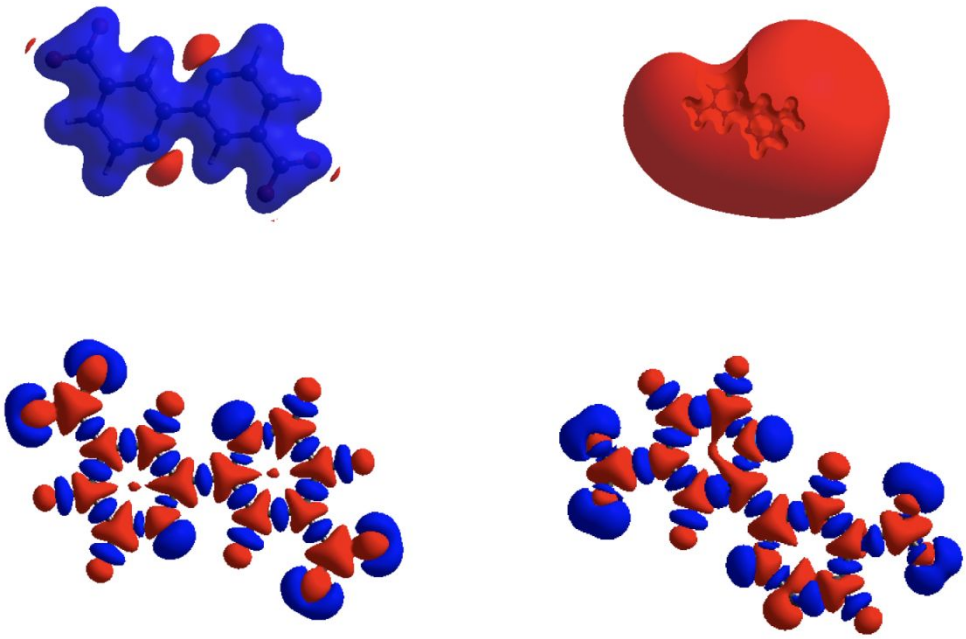

Figure S6. Comparison between the Electrostatic potentials (upper) and Promolecule density of dcbp molecules in different bridging motifs.

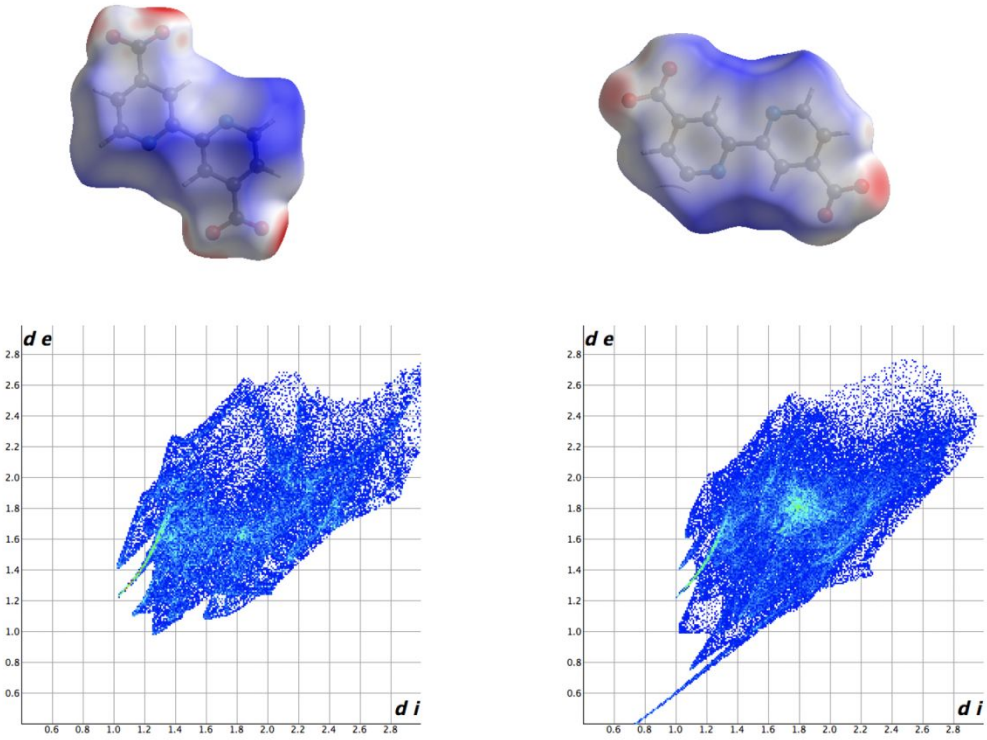

Figure S7. Comparison between the 3-D d_{norm} Hirshfeld surfaces and 2-D fingerprint plots for dcbp molecules in different bridging motifs.

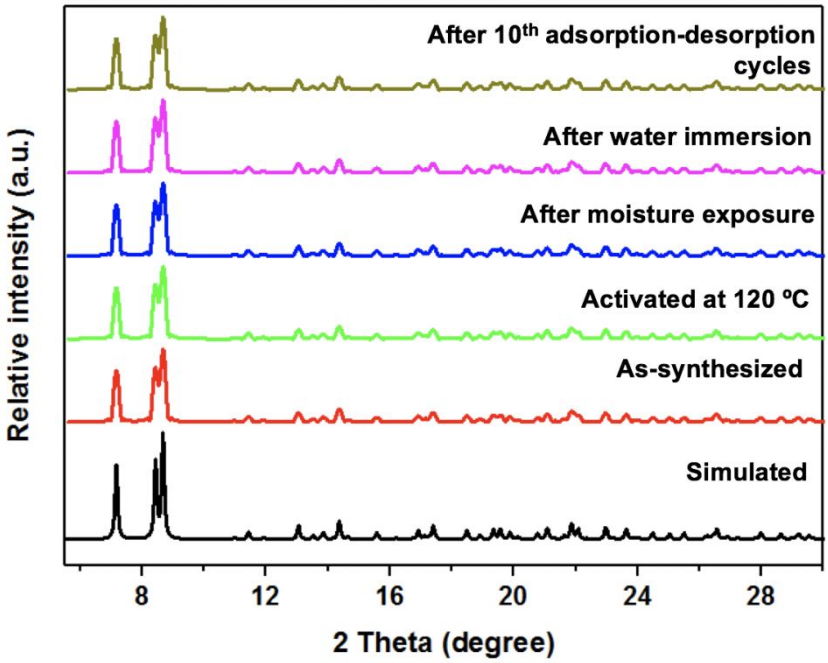

Figure S8. PXRD patterns of **HV-MOF-1** in different adsorption-desorption states.

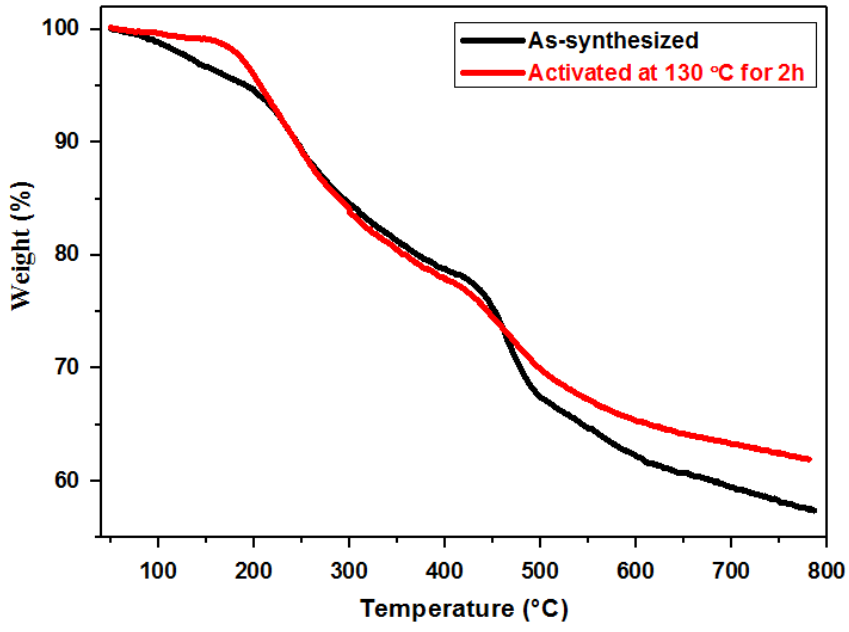

Figure S9. Comparison between the TGA profiles of **HV-MOF-1** in different water adsorption-desorption states

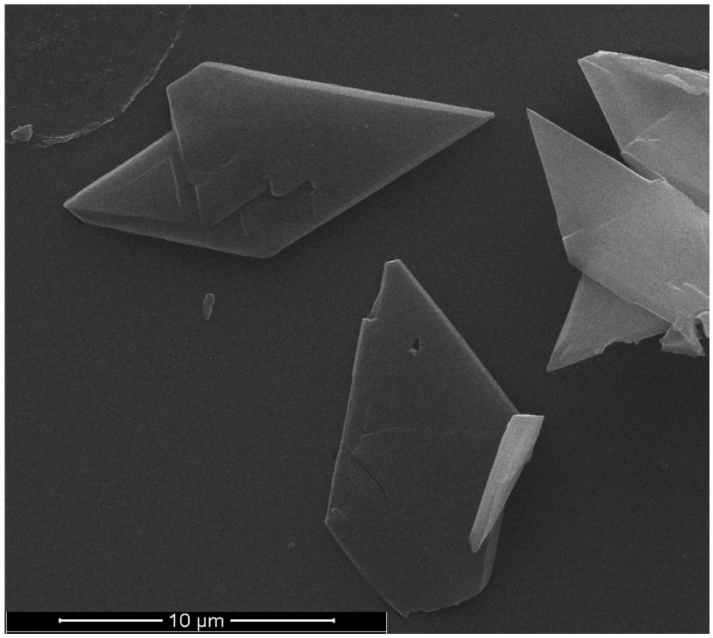

Figure S10. SEM image of the activated **HV-MOF-1** species.

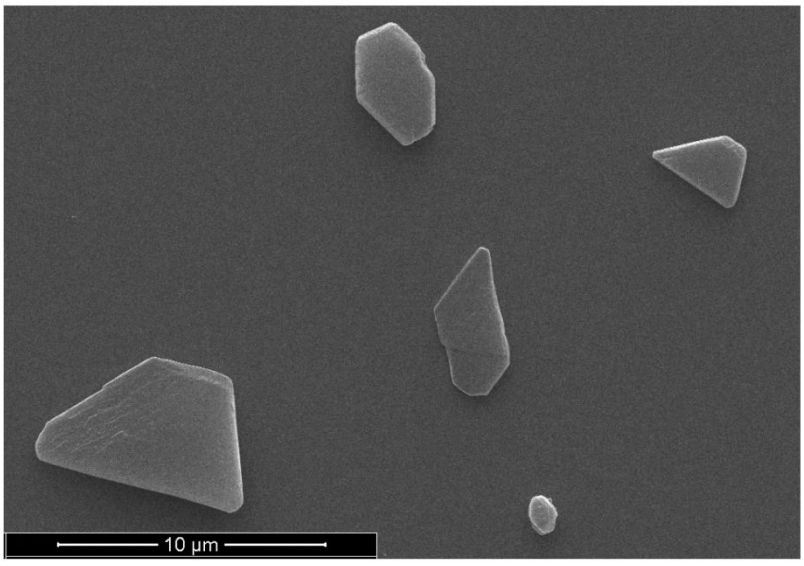

Figure S11. SEM image of the activated **HV-MOF-1** species after immersion in water for more than 24h.