Supplementary Materials

Synthesis, Structural Features, and Catalytic Activity of a New Iron(II) 3D Metal-Organic Framework Driven by an Ether-Bridged Pyridine-Dicarboxylate

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Supplementary materials contain:

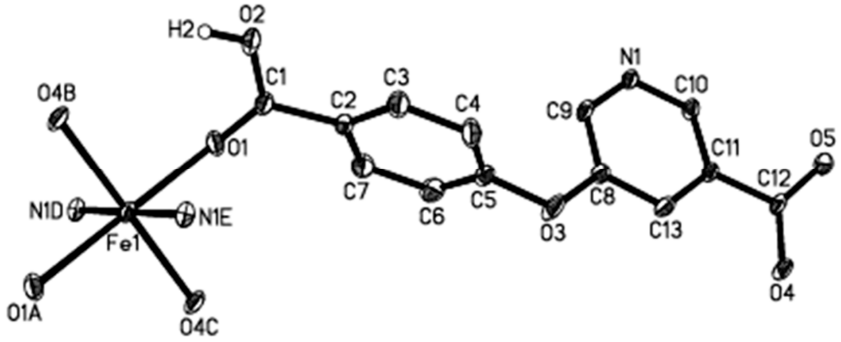

Figure S1 Drawing of the asymmetric unit of compound **1** with 30% probability thermal ellipsoids; H atoms are omitted for clarity except the H of the COOH group. Symmetry code: A = $-x + 1, -y + 1, -z$; B = $x, y, z - 1$; C = $-x + 1, -y + 1, -z + 1$; D = $-x + 1/2, y + 1/2, -z + 1/2$; E = $x + 1/2, -y + 1/2, z - 1/2$.

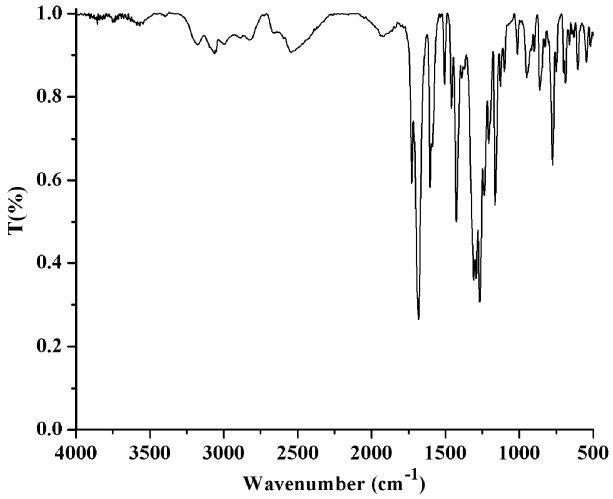

Figure S2 FT-IR spectrum for H_2cpna.

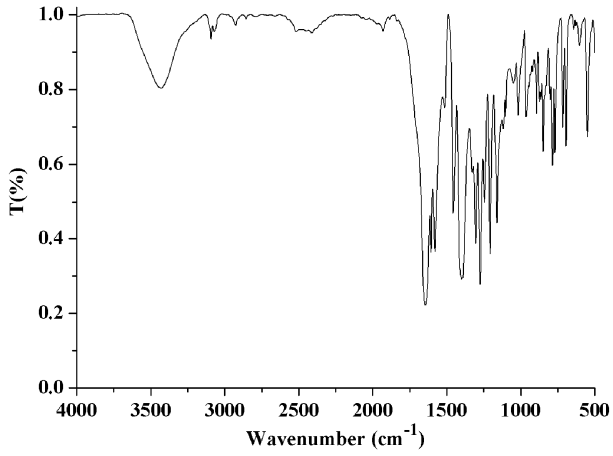

Figure S3 FT-IR spectrum for compound **1**.

Stability study of the compound 1 in CH_3CN-H_2O: the compound **1** (taking 30 mg) was dispersed in 100 mL CH_3CN-H_2O (v:v=2:1) under stirring for 6 h at 60 °C, and then the obtained solid was collected by filtration. It was dried and used to run PXRD. The filtrate was analyzed by UV-vis spectrophotometry. The PXRD patterns of the samples after immersing in CH_3CN-H_2O match well with the plots simulated from the single-crystal X-ray data (Figure S4), thus confirming that the compound is stable in CH_3CN-H_2O. No changes were found in the solid-state UV-vis spectra of compound **1** (Figure S6). However, in the presence of oxidant (H_2O_2 or $K_2S_2O_8$) the CP **1** starts to dissolve. Some peaks in the UV-vis spectrum of the CH_3CN/H_2O solution (filtrate) obtained after dissolving **1** can be attributed to soluble Fe-cpna species derived from **1**.

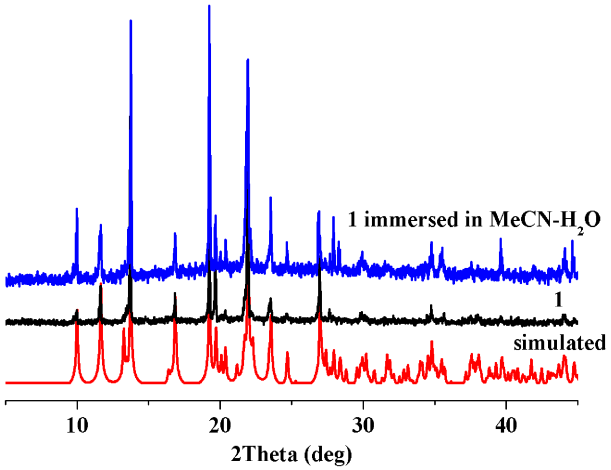

Figure S4 PXRD patterns of **1** at room temperature.

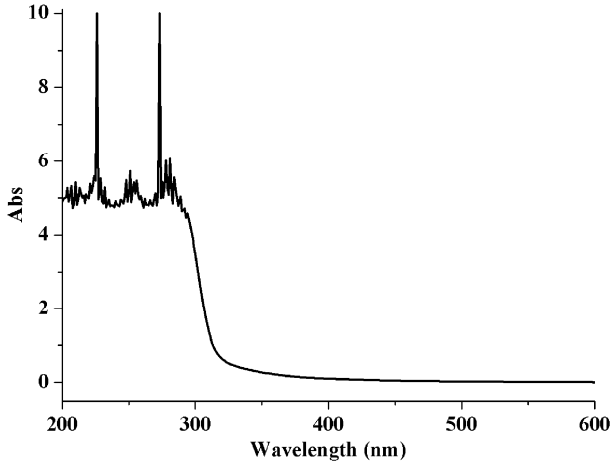

Figure S5 Solution UV-Vis absorption spectrum of the sample obtained upon dissolution of **1** in CH_3CN-H_2O (v:v = 2:1) in the presence of oxidant.

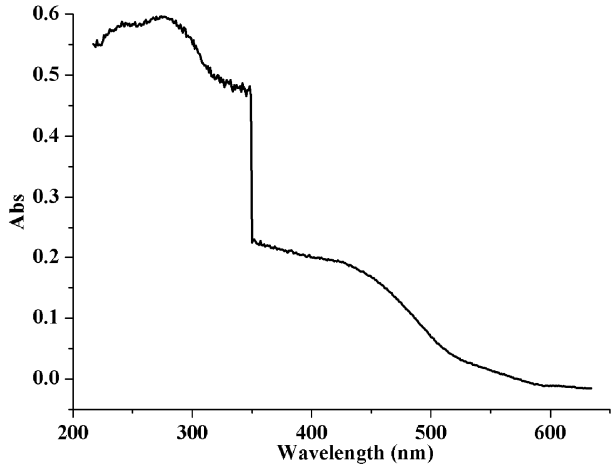

Figure S6 Solid-state UV-Vis absorption spectrum of compound **1**.

Table S1 Selected bond lengths (Å) and bond angles (°) for **1**.

Fe(1)–O(1)	2.183(3)	Fe(1)–O(1)i	2.183(3)	Fe(1)–O(4)ii	2.075(3)
Fe(1)–O(4)iii	2.075(3)	Fe(1)–N(1)iv	2.152(3)	Fe(1)–N(1)v	2.152(3)
O(1)–Fe(1)–O(4)ii	94.32(10)	O(1)–Fe(1)–N(1)iv	86.39(11)	O(1)–Fe(1)–O(4)iii	85.68(10)
O(1)–Fe(1)–N(1)v	93.61(11)	O(4)ii–Fe(1)–N(1)iv	89.63(10)	O(4)ii–Fe(1)–N(1)v	90.37(10)

Symmetry codes: i: $-x + 1, -y + 1, -z$; ii: $x, y, z - 1$; iii: $-x + 1, -y + 1, -z + 1$; iv: $-x+ 1/2, y + 1/2, -z + 1/2$; v: $x + 1/2, -y + 1/2, z - 1/2$.

Table S2 Hydrogen bond parameters in crystal packing [Å, °] of **1**.

Compound	D–H···A	*d*(D–H)	*d*(H···A)	*d*(D···A)	∠DHA	Symmetry code
1	O(2)–H(2)···O(5)	0.82	1.66	2.471	172.0	$x, y, z - 1$

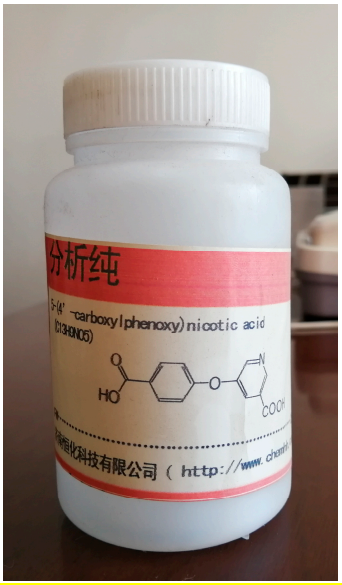

Figure S7. Photograph of the H_2cpna reagent acquired from a commercial supplier (Jinan Henghua Sci. & Tec. Co., Ltd, http://www.chemhh.com, catalogue code: 120511H-1B, purity 98%, CAS: 1777822-70-4).