Supporting Information

New Hybrid Organic-Zincophosphate Frameworks: Single-Crystal-to-Single-Crystal Structural Transformation and Remarkable Thermal and Chemical Stabilities

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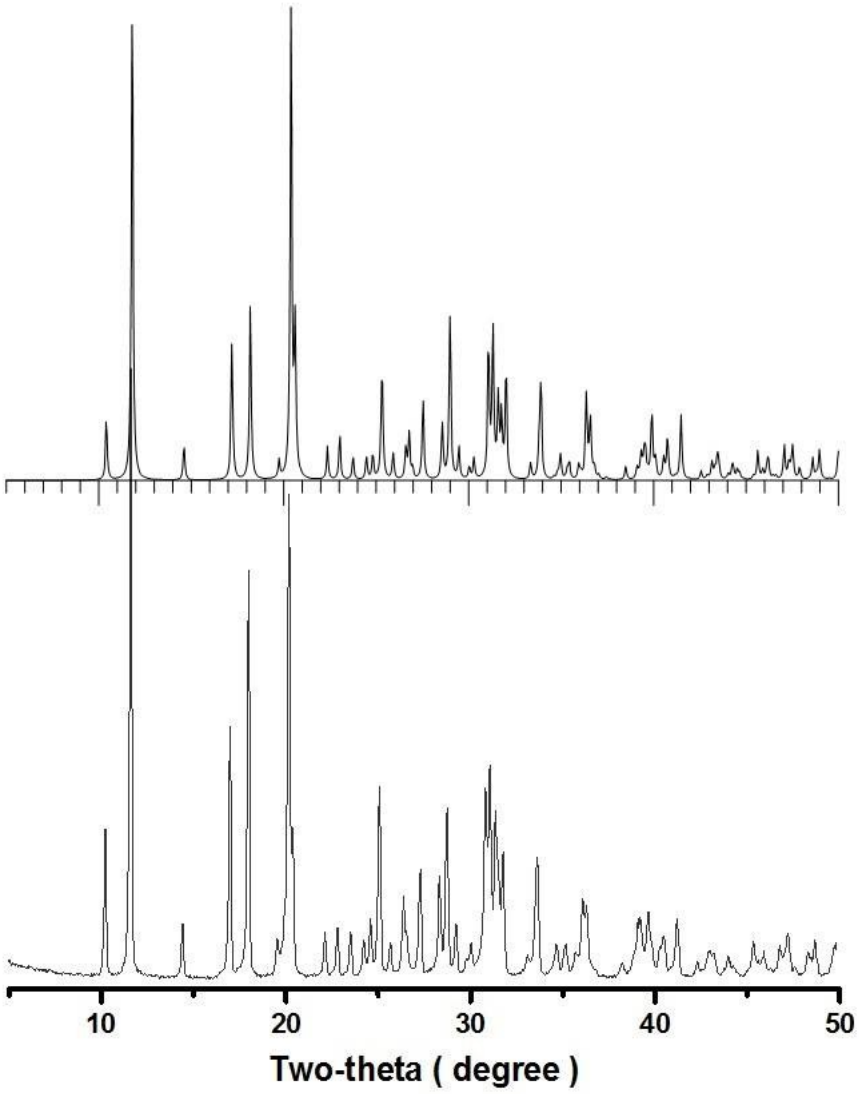

Fig. S1 X-ray powder pattern of $Zn_{1.5}(H_2O)(C_2H_5N_5)(PO_4)$ (bottom). Simulated powder pattern from the atomic coordinates derived by single-crystal X-ray diffraction (top).

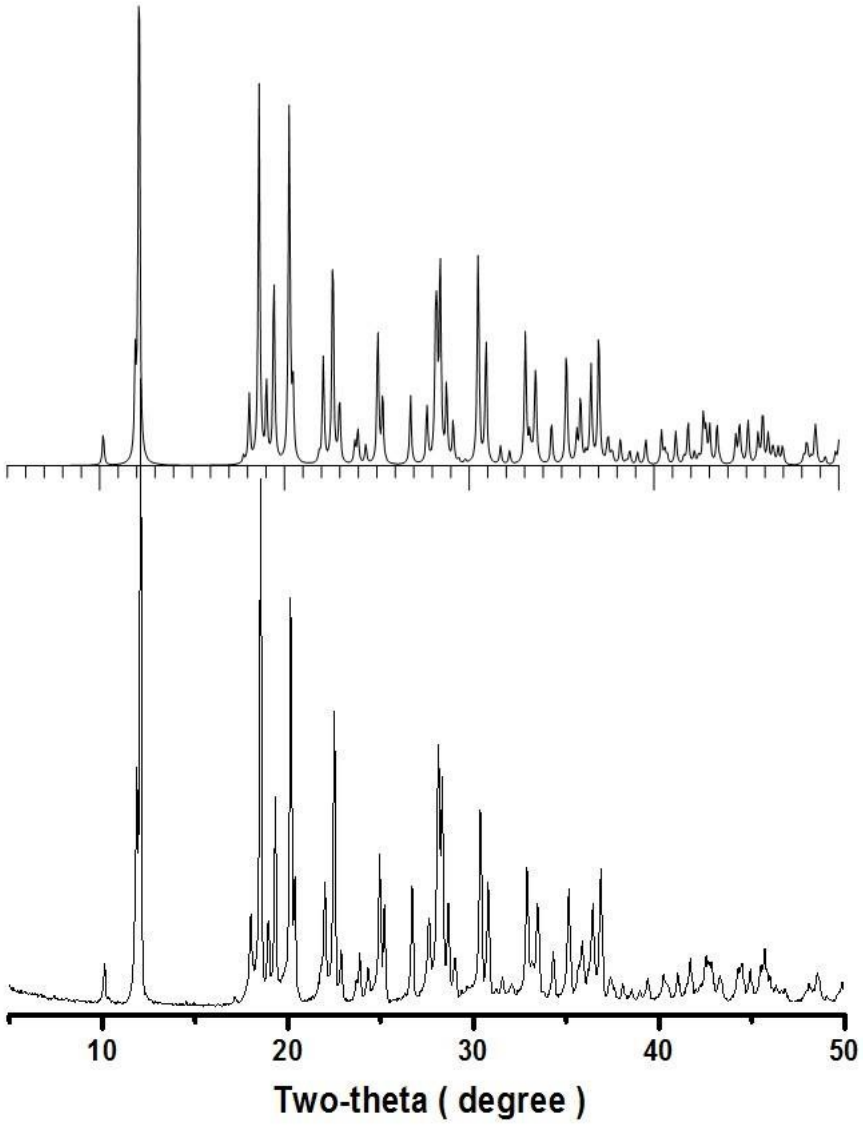

Fig. S2 X-ray powder pattern of $Zn_{1.5}(C_2H_5N_5)(PO_4)$ (bottom). Simulated powder pattern from the atomic coordinates derived by single-crystal X-ray diffraction (top).

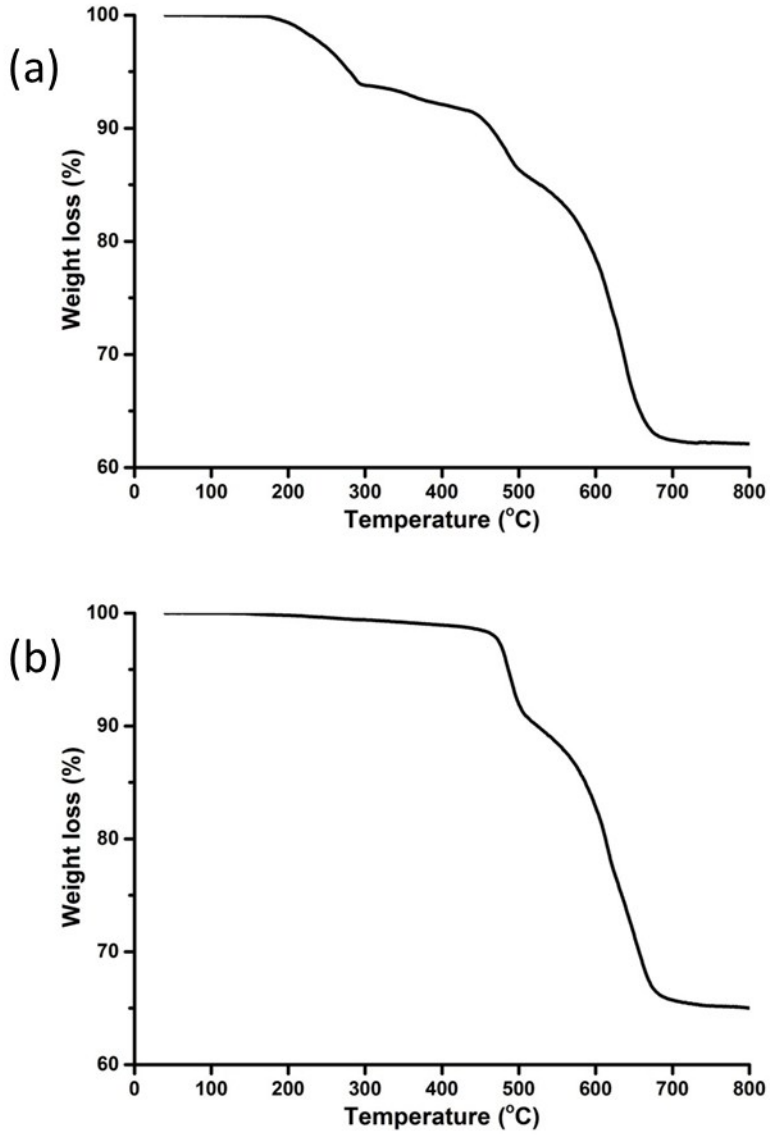

Fig. S3 TGA curve for $Zn_{1.5}(H_2O)(C_2H_5N_5)(PO_4)$ (1) and $Zn_{1.5}(C_2H_5N_5)(PO_4)$ (2) measured in O_2 at 5 °C/min.

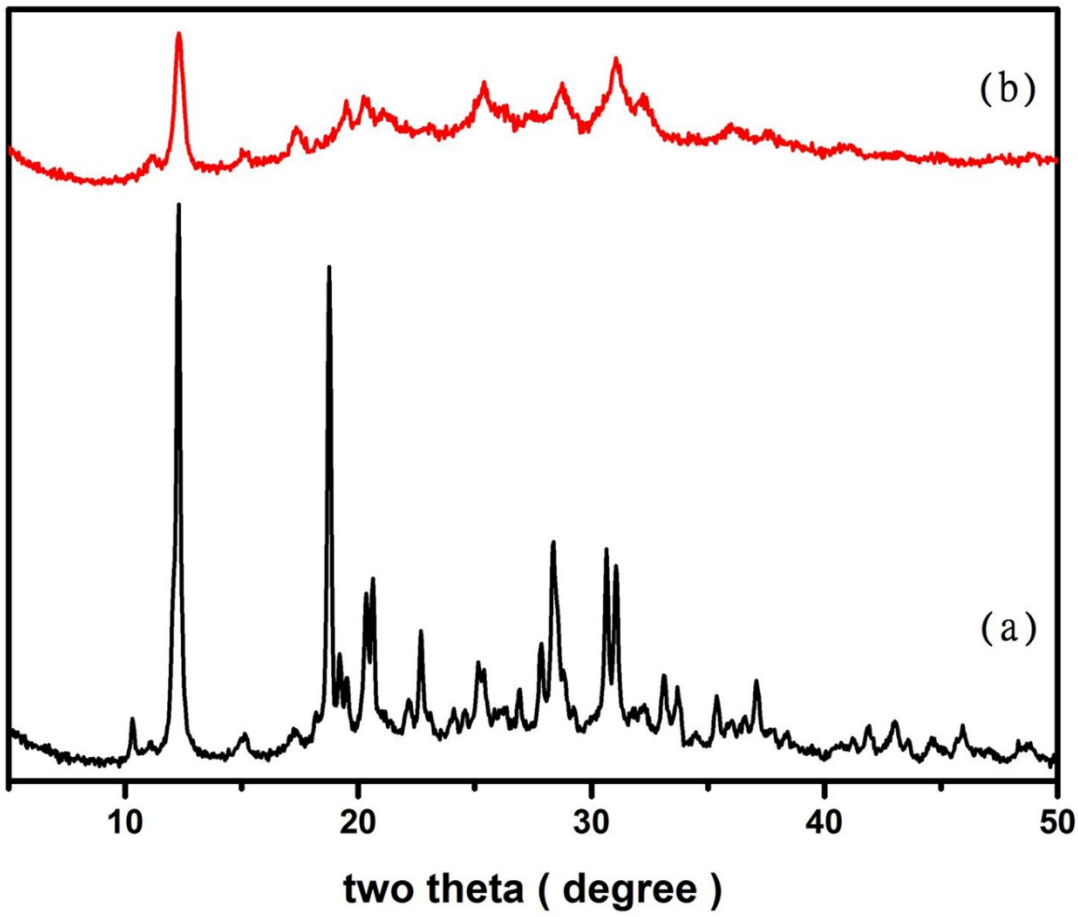

Fig. S4 The X-ray powder patterns for 2 collected during the thermal-stability studies: holding for 20 min at 450℃ (a) and 500℃ (b).

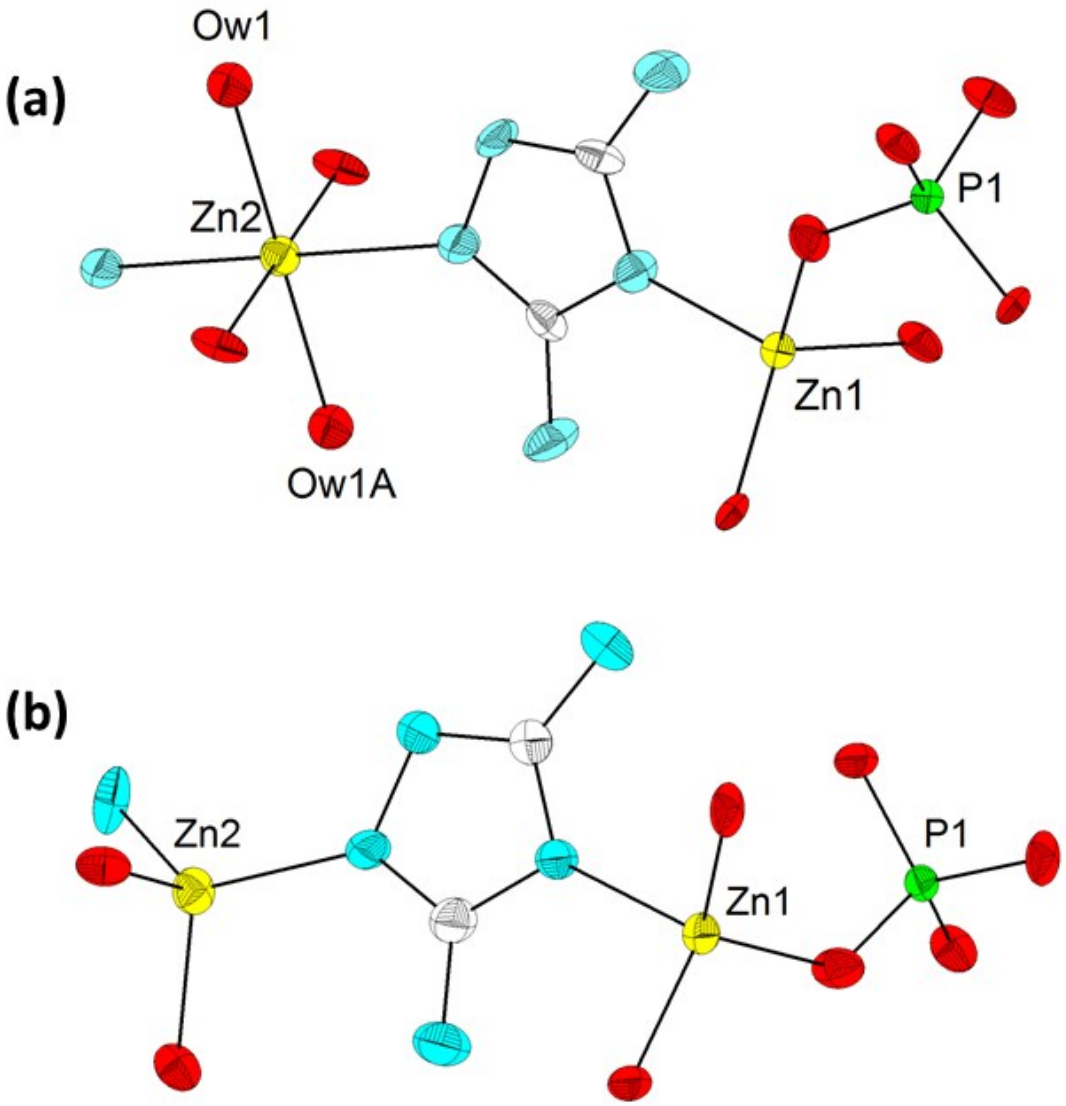

Fig. S5 The ORTEP diagrams for the coordination environments of Zn and P in the structures of **1** and **2**. Yellow ellipsoids, Zn atoms; green ellipsoids, P atoms; red ellipsoids, O atoms and water oxygen atoms; light blue ellipsoids, N atoms; white ellipsoids, C atoms. Thermal ellipsoids are shown at 70% probability.

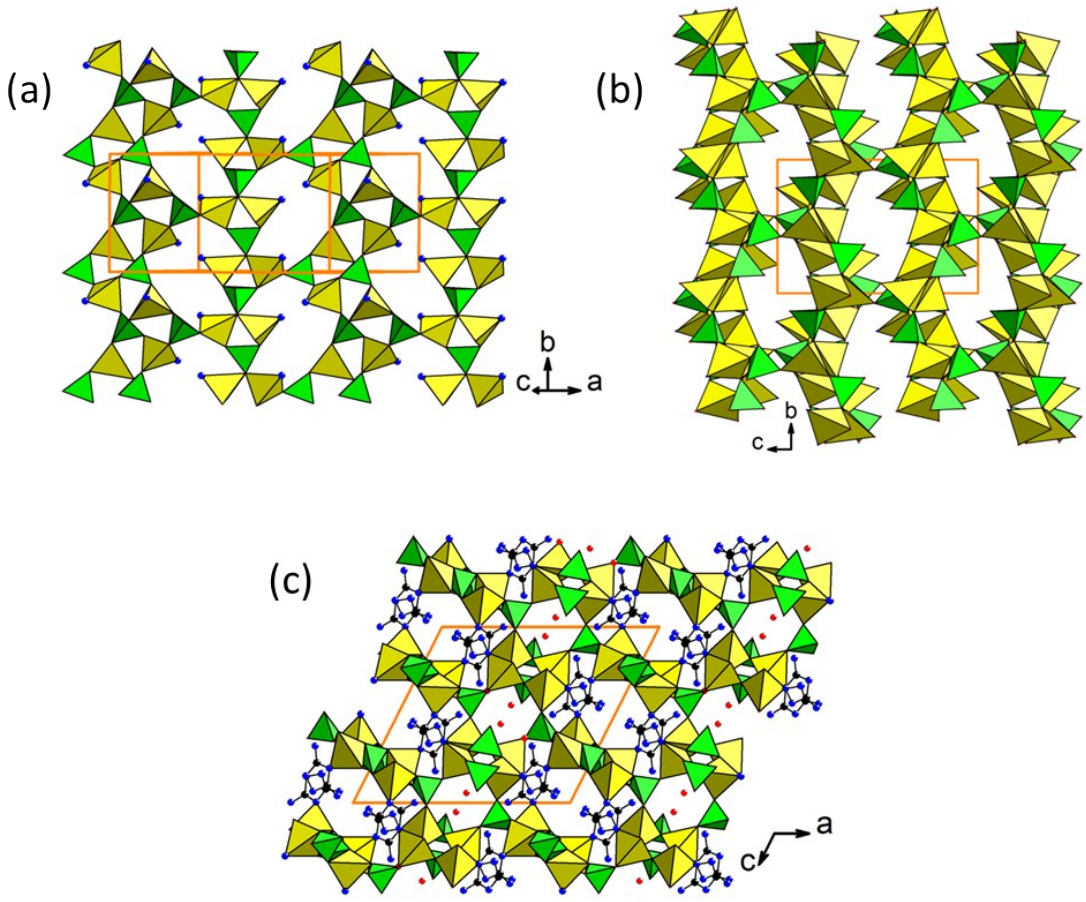

Fig. S6 Perspective view of the structure of $Zn_4(C_2H_5N_5)_2(HPO_4)(PO_4)_2 \cdot H_2O$: (a) The inorganic layer with 3-, 4-, and 10-membered rings. (b) Two zincophosphate sheets linked to each other to form a 3D inorganic framework through the linkage of zinc and phosphate tetrahedra. (c) The 3,5-diamino-1,2,4-triazole ligands in a bidentate fashion coordinate to zinc atoms and extend away from 3D inorganic framework as pendent ligands.

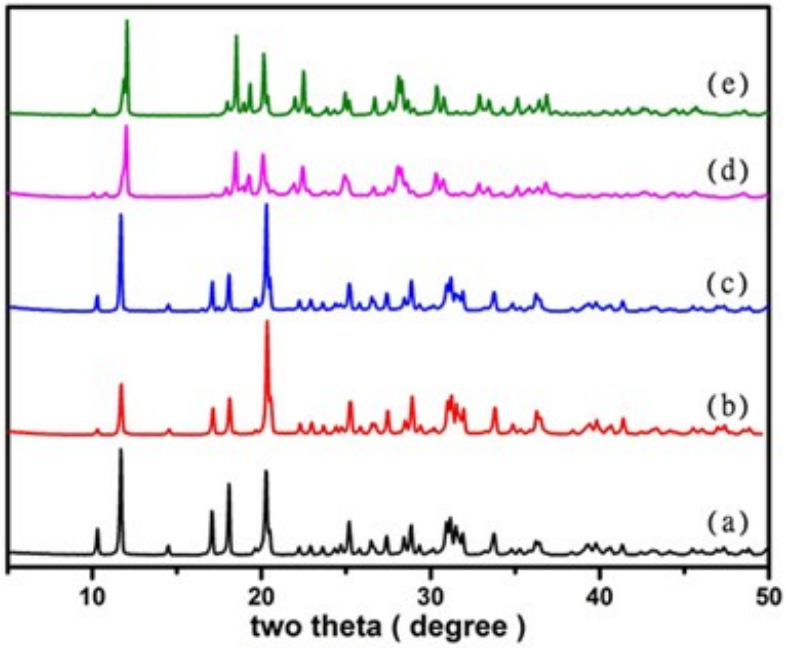

Fig. S7 The X-ray powder patterns of **1** collected during the chemical stability studies: as-synthesized sample of **1** (a); in boiling DMF at 155°C for 1 d (b), 5 d (c), and 7 d (d); and an as-synthesized sample of **2** (e).

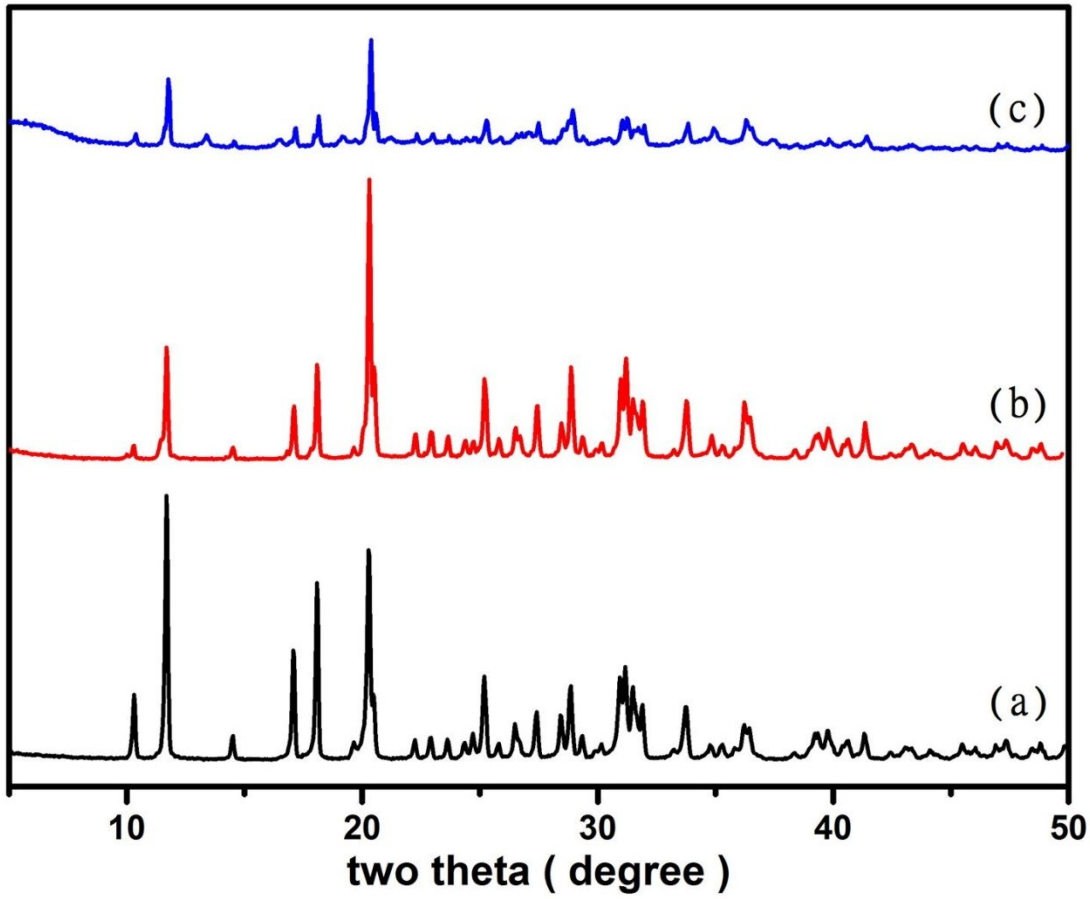

Fig. S8 The X-ray powder patterns of 1 for the chemical stability studies: as-synthesized sample of 1 (a), in aqueous sodium hydroxide at 100℃ for 1 d (b), 5 d (c).

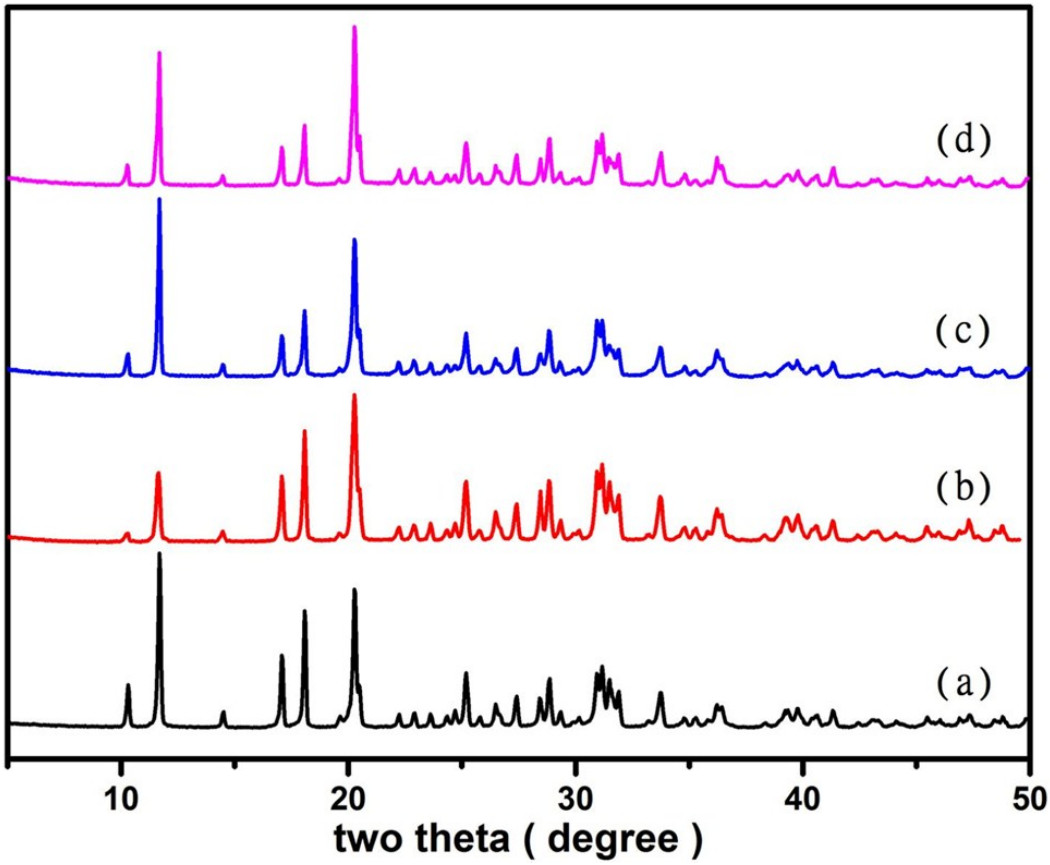

Fig. S9 The X-ray powder patterns of 1 for the chemical stability studies: as-synthesized sample of 1 (a), in boiling methanol at 66℃ for 1 d (b), 5 d (c), 7 d (d).

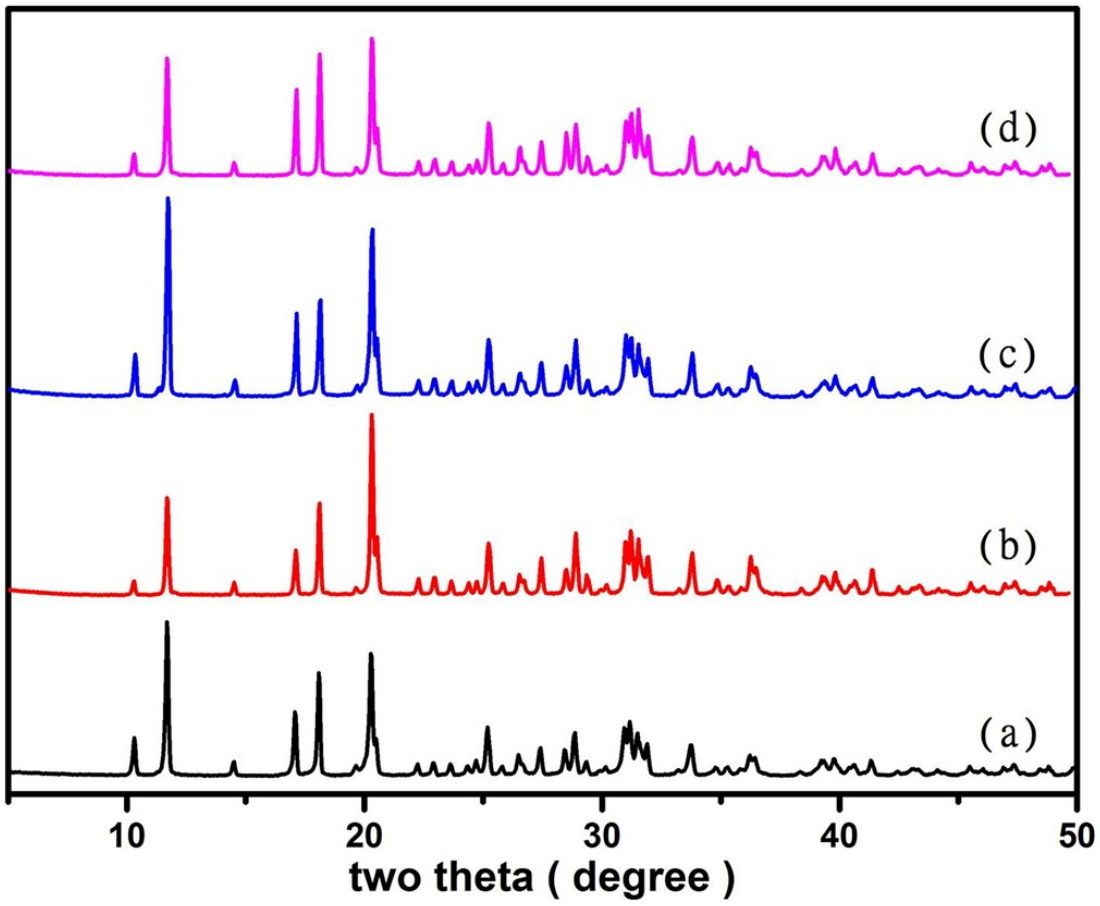

Fig. S10 The X-ray powder patterns of 1 for the chemical stability studies: as-synthesized sample of 1 (a), in boiling pyridine at 116℃ for 1 d (b), 5 d (c), 7 d (d).