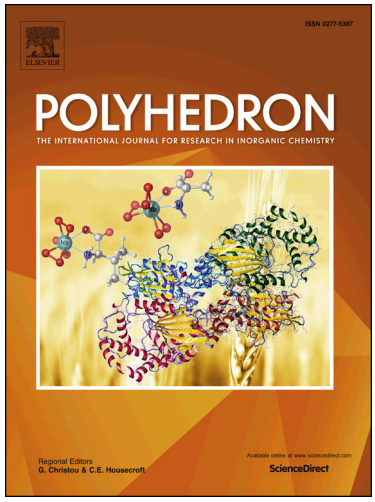

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1D Energetic Metal–organic Frameworks Assembled with Energetic Combination of Furazan and Tetrazole

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Abstract: Two novel 1D Cd(II) energetic MOFs $[Cd(NH_2NH_2)(AFT)_2 \cdot 0.7H_2O]_n$ (**1**) and $[Cd(ODH)_{1.5}(AFT)_2 \cdot 5H_2O]_n$ (**2**), combining the advantages of tetrazole-ring and furazan-ring, were successfully synthesized based on 2D energetic MOF $[Cd(H_2O)_2(AFT)_2]_n$ (**3**, AFT=4-amino-3-(5-tetrazolate)-furazan, ODH=$NH_2NHCOCONHNH_2$= oxalyl-dihydrazide). The crystal structures were determined by single-crystal X-ray diffraction, and fully characterized by elemental analysis and FT-IR spectroscopy. The thermal stability and impact sensitivity were also investigated. For **1**, 1D energetic MOF had an outstanding thermal stability (T_p>300 ^oC) and insensitivity (IS>24.5 J). In addition, the non-isothermal kinetics parameters, critical temperature of thermal explosion, entropy of activation, enthalpy of activation and free energy of activation were discussed in detail. For **2**, it was revealed that the each Cd(II) cation is located in a unique hepta-coordination environment. Noticeably, tetrazole-ring of AFT group presents typical monodentate coordination mode, and ODH molecule presents typical tridentate and tetradentate coordination modes, featuring a one-dimensional chain structure. Therefore, the reasonable assembly strategy plays a decisive role in energetic properties of MOF-based energetic materials.

Keywords: Tetrazole; Furazan; MOF; Crystal structure; Thermal behaviour