

Preparation, Detonation and Safety Performance of the Solvent-Free Energetic Ag(I)-MOFs

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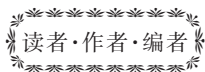
Abstract: Based on energetic ligands 3,5-dinitro-1-*H*-1,2,4-triazole and 3,4-bis(1-*H*-5-tetrazolyl)furoxan, two solvent-free energetic Ag(I)-MOFs, [Ag₂(2-ntz)₂]_n(**1**) and [Ag₂(BTOF)]_n(**2**) have been prepared under hydrothermal conditions. Single-crystal X-ray analysis reveals that the Ag⁺ centers in both Ag(I)-MOFs are three-coordinated. Compound **1** features a 3D framework ($\rho_1=2.805\text{ g}\cdot\text{cm}^{-3}$) constructed by 2-ntz⁻ ligands bridging metal ions with a μ_3 -1,2,4 mode. Compound **2** presents a 2D folded layer structure ($\rho_2=3.101\text{ g}\cdot\text{cm}^{-3}$) formed by BTOF²⁻ ligands linking metal ions with aquinquentatechelating-bridging coordination mode. TG-DSC curves demonstrate that both compounds **1** and **2** keep stable until 240 °C, exhibiting high thermal stability. The heats of combustion of **1** and **2** are determined by oxygen-bomb calorimeter, and the corresponding standard molar enthalpies of formation are determined to be (1375.74±1.27) kJ·mol⁻¹ and (1647.42±1.46) kJ·mol⁻¹, respectively. The detonation and safety performance analyses show that the heat of detonation, detonation velocity and detonation pressure of compounds **1** and **2** are, respectively calculated as 5.55 kJ·g⁻¹ and 3.78 kJ·g⁻¹, 8.97 km·s⁻¹ and 7.69 km·s⁻¹, as well as 44.87 GPa and 34.37 GPa. Both compounds **1** and **2** are insensitive to impact and friction, and are good high energy yet low sensitivity materials.

Key words: energetic metal-organic frameworks (E-MOFs); 3,5-dinitro-1-*H*-1,2,4-triazole; 3,4-bis(1-*H*-5-tetrazolyl)furoxan (H₂BTOF)

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含能材料的损伤特征与点火过程有密切的联系,炸药、推进剂的内部损伤及其对力学特性、安全特性和点火行为的影响规律受到了含能材料学界的高度重视,为推动这一重要研究方向的学术交流,本刊特设立“损伤与点火”专栏。专栏主要征集炸药、推进剂等含能材料的损伤观测与多尺度表征技术、含损伤的本构方程、准静态与动态损伤演化规律、损伤与破坏的宏(细)观模式、损伤对起爆、爆炸、爆轰成长以及非冲击起爆行为的影响等方向的原创性研究论文。来稿请注明“损伤与点火”专栏。

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