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, $[Ag_2(2\text{-ntz})_2]_n$(**1**) and $[Ag_2(BTOF)]_n$(**2**) have been prepared under hydrothermal conditions. Single-crystal X-ray analysis reveals that the Ag^+centersin both Ag(Ⅰ)-MOFs are three-coordinated. Compound **1** features a 3D framework (ρ_1=2.805 g·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 (ρ_2=3.101 g·cm^{-3}) formed by $BTOF^{2-}$ ligands linking metal ions with aquinquedentatechelating-bridging coordinationmode. TG-DSC curves demonstrate that both compounds **1** and **2** keep stable until 240 ℃, 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 formationare 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 velocityand detonationpressureof 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(H_2BTOF)

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