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A NOVEL COORDINATED ENERGETIC COMPOUND LEADING A PROMISING CONCEPT OF PROPELLANT FORMULA DESIGNING

Abstract

Both combustion catalysis and composition formula of solid propellant were always related to mercury- or lead-based compounds, which has caused serious environment damages. But now, a batch of non-lead energetic materials are regarded as promising candidates for traditional ones. Imidazole (IMI), a pentacyclic heterocycle containing two nitrogen atoms and three carbon atoms, were chosen as precursors. Crystalline complex [Mn(IMI)6](NO3)2(compound 1) were synthesized by specific steps. The optimized structure was characterized to be associated with a true local energy minimum on the potential energy surface without any imaginary frequency component. The X-ray single crystal diffraction illustrate that the title complex belongs to the rhombohedral system, space group R-3. In compound 1, every Mn2+ ion was hexa-coordinated with six IMI groups, which is presented as the lowest steric hindrance status. The DSC result shows only one exothermal decomposition with peak temperature at 267.2 C. Non–isothermal kinetic and thermodynamic parameters were obtained via Kissinger's method as well as Ozawa's method. The critical temperature of thermal explosion, S, H, and G were calculated as 209.1 C, -69.52 J•K-1•mol-1, 114.89kJ•mol-1, 129.23kJ•mol-1, respectively. Additionally, the sensitivities towards impact, friction and static electricity were measured to be obtuse via relevant standard. The combustion catalysis of solid propellant, in previous engineering applications, were inert catalyst in a sense. However, introducing of heterocyclic coordination complex to propellant has changed the contradictory situation. Experimental results indicated that nitrogen-rich heterocyclics could make a great contribution to improving molecule's heat of formation and thermal stability. Mn2+, a metal element with high catalytic activity, were innovatively coordinated with heterocyclic, which can effectively adjust the combustion performance of propellants by improving oxidation reaction rate. Propellant combustion are catalyzed by [Mn(IMI)6](NO3)2, meanwhile [Mn(IMI)6](NO3)2 will decompose due to the heat of combustion itself. Actually, many researchers had proved that the reaction activity of metal cations from coordinated compounds obviously exceeded ones from normal compounds. That's the exact reason why [Mn(IMI)6](NO3)2 is a promising component of composite solid propellant. In considerate of such excellent properties, not limited to [Mn(IMI)6](NO3)2, many other heterocycle coordinated complex, owning similar performances in structure, could be pulled into solid propellant formula research.