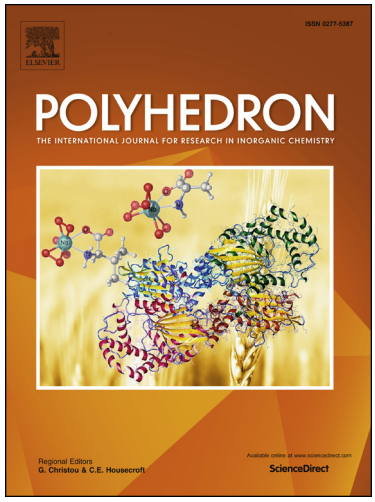

Four new energetic complexes constructed from nickel(II) and 2-(dinitromethylene)-1,3-diazacyclopentane: synthesis, characterization and thermal properties

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Four new energetic complexes constructed from nickel(II) and 2-(dinitromethylene)-1,3-diazacyclopentane: synthesis, characterization and thermal properties

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Abstract

Four new energetic nickel complexes of DNDZ [DNDZ=2-(dinitromethylene)-1,3-diazacyclopentane], $Ni(NH_3)_2(DNDZ)_2$ (**1**), $Ni(CH_3NH_2)_2(DNDZ)_2$ (**2**), $Ni(C_2H_5NH_2)_2(DNDZ)_2$ (**3**) and $Ni(C_3H_7NH_2)_2(DNDZ)_2$ (**4**), have been first synthesized and characterized. The crystal structures studies of **1** and **2** show that the central nickel(II) ion is six-coordinated by two O atoms and two N atoms from two $DNDZ^-$ anions and two N atoms from ammonias (methylamines) to form a distorted octahedral structure. Thermal decomposition processes of the four complexes were studied. The kinetic parameters of the exothermic decomposition process, specific heat capacities and adiabatic times-to-explosion for the four complexes were analyzed. All calculation and research results indicate that these complexes present relatively low thermal stability and easily decompose. Sensitivity tests reveal that the complexes are less sensitive to mechanical stimuli.

Keywords: 2-(Dinitromethylene)-1,3-diazacyclopentane (DNDZ); Nickel complex; Crystal structure; Thermal behavior; Adiabatic time-to-explosion

1. Introduction

The studies of energetic materials have a long history, which can date back to Liebig's and Gay-Lussac's early investigations in the 1820s [1]. With the development energetic compounds, today's researchers mainly devote to designing new energetic compounds with high energy and low sensitivity to enhance detonation and safety properties. Based on the background, many insensitive energetic compounds, like 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), 3-nitro-1,2,4-triazol-5-one(NTO) and *N*-guanylurea dinitramide (GUDN), have been widely investigated and reported [2]. 1,1-Diamino-2,2-dinitroethylene (FOX-7), as a novel high-energy material with high thermal stability and low sensitivity, has been continually studied since first synthesis in 1998 [3]. Molecular structure shows that FOX-7 is a typical "push-pull" nitro-enamine containing a highly polarized carbon-carbon double bond with positive and negative charges being stabilized by amino group and nitro group respectively, and has manifold tautomers and resonances [4]. FOX-7 presents high reactivity to form many new energetic derivatives [5].

2-(Dinitromethylene)-1,3-diazacyclopentane (DNDZ), as a bis nucleophilic substitution derivative of FOX-7, can be prepared by the reaction of FOX-7 and ethanediamine in *N*-methyl pyrrolidone (NMP) at 110°C for 8 h. DNDZ also belongs to "push-pull" nitro-enamine compounds, and has the same characteristics with FOX-7. After

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