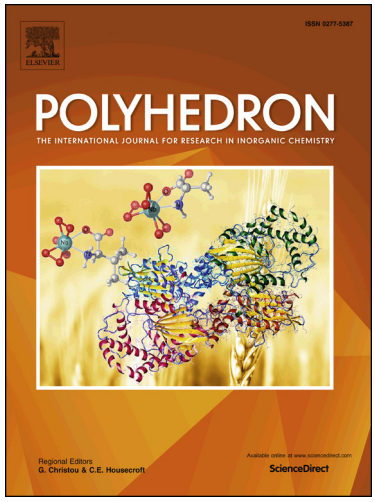

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Building Polynitrogen Clusters with Metal-Metal Multiple Bonds

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Abstract: Metal-metal multiple bonds based polynitrogen complex clusters may become a class of high-energy, insensitive and green primary explosives. Five complexes containing chromium (Cr≡Cr), molybdenum (Mo≡Mo), tungsten (W≡W), technetium (Tc≡Tc) and rhenium (Re≡Re) metal multiple bonds with pentazole ligands were theoretically built. The metal-metal multiple bonds, metal-pentazole coordination bonds, molecular static and dynamic polarizability were investigated with density functional theory M06-L/LanL2DZ, The Wiberg bond order sequence of metal-metal is Mo–Mo > Cr–Cr > W–W > Re–Re > Tc–Tc Bidentate coordination bonds were formed between each metal-metal edge and two pentazole ligands, which strengthen the coordination bonds, and Wiberg bond order sequence of metal-pentazole is Re–N > W–N > Tc–N > Mo–N > Cr–N. The gaseous and solid phase formation enthalpies, enthalpies of sublimation and theoretical density of five complexes were predicted. As candidates for primary explosives, their detonation heats were calculated and the descending order is $Re_4(N_5)_8$ > $W_4(N_5)_8$ > $Tc_4(N_5)_8$ > $Mo_4(N_5)_8$ > $Cr_4(N_5)_8$. M_4N_{40} clusters may be a class of promising green primary explosives.

Keywords: metal-metal multiple bonds; bidentate complex; primary explosives; detonation heat; dynamic polarizability

Introduction

The search for high-energy, insensitive and green primary explosives is always ongoing. The conventional primary explosives usually contain toxic elements such as lead, mercury, and perchlorate, which are harmful to biosome and ecological environment. In this work we designed five high-energy compounds which contain only two elements in one compound, single metallic element and nitrogen. The decomposed products are nitrogen and a pure metal, with little damage to environment, these compounds are green energetic materials.