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Tris-(nitroacetylacetonato) complexes as new high-energy materials

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Recent advances in high-energy materials studies have shown that coordination compounds are promising energetic compounds with satisfactory detonation properties and moderate sensitivity. Earlier experimental studies found that the nitro-acetylacetonato aluminum (III) complex easily ignites in the air when heated. Theoretical calculations performed on nitroaromatic explosives revealed that molecular electrostatic potential over the C-NO_2 bonds is a good tool for determining the impact sensitivity of these molecules. Herein, we calculated the molecular electrostatic potential and bond dissociation energies for several nitro-tris(acetylacetonato) complexes. A rough estimation of the electrostatic potential predicts slightly positive electrostatic potentials above the C-NO_2 bonds. These results show that the metal ion replacement may induce the fine adjustment of electrostatic potential above the C-NO_2 bonds in the nitro-chelate complexes. The reported results agree with the calculated bond dissociation energies. These values indicate that introducing the transition metals in the nitro-chelate complexes may increase their sensitivity. However, we also synthesized and characterized the nitro-tris(acetylacetonato) cobalt(III) complex. The UV/VIS and FTIR tests confirmed that the synthesized complex was $Co(acac\text{-}NO_2)_3$. The obtained results agree with the experimental results that Collman et al. reported. The open flame test showed that this complex easily combusts when exposed to the open flame.

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