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The chelate complexes as an improved high-energy compounds

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Recent studies in high-energy material design revealed that coordination compounds show excellent detonation performances. Earlier experimental studies found that the nitro-acetylacetonato aluminum (III) complex easily combusts in the air when heated.[1] These findings indicate that the nitro-acetylacetonato metal derivatives may act as potential energetic compounds. The intensive theoretical studies of classical explosives formerly revealed that the impact sensitivity of high-energy molecules could be predicted by analysis of molecular electrostatic potential over the C–NO_2 bonds.[2] This concept is applied here.

In order to investigate their energetic properties, we calculated the molecular electrostatic potential and bond dissociation energies for the weakest C-NO_2 bonds for several nitro-tris(acetylacetonato) complexes. The results show good agreement between bond dissociation energies calculated for the weakest C-NO_2 bonds and a slightly positive electrostatic potential above the observed C-NO_2 bonds. The bond dissociation energies for studied complexes are close to the BDE value calculated for the 1,3,5-triamino-2,4,6-trinitrobenzene classified as a significant low-sensitive explosive. We also noticed that the metal ion replacement may be used for fine-tuning of the electrostatic potential above the middle regions of the nitro-chelate rings. However, the presented results show that these compounds have moderate sensitivity, and that the positive electrostatic potential above the central area of the nitro-chelate rings could be used for the assessment of detonation properties of chelate energetic molecules.

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