Unique structure of transition metal hydrazine perchlorate primary explosives and the ways to work with them

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Abstract

Two new primary explosives of nickel and cobalt hydrazine perchlorates, were synthesized and characterized by X-ray single crystal diffraction. Elemental analysis and explosives sensitivity tests were conducted. Structures obtained by X-ray diffraction experiment contain ionic polymeric structures uncharacter-istic of currently studied explosives.

DFT calculations on the compounds of interest predict heats of explosion comparable those for known powerful primary explosives.

Relevance

Research in the field of energetic materials is of utmost importance for national security as it allows for better, faster and more accurate response in event of any hostile act as well as helps with its prevention or mitigation of effects.

Understanding the intricacies of the relationship between structural and physical properties and not just macroscopic properties of explosive materials is a matter of importance.

Knowing the exact atomic coordinates of the components of a structure is a starting point, which allows for implementation of state-of-the-art computational techniques for prediction of energy liberated in the process of explosion.

Technical Approach

As a result of the current investigation we report the synthesis, preliminary elemental, structural studies and DFT calculations of two metal based primary explosives, which offer high density, and sensitivity for primary explosives with detonation energies in line with other known powerful secondary explosives.

We succeeded in the preparation and characterization of nickel hydrazine pechlorate (NHP) and its cobalt analog CHP.

In both of the substances metal atoms are connected by a single hydrazine molecule (Figure 1a, b) forming a continuous metal hydrazine polymer. No cross-linking was observed between the threads of the polymetal hydrazinate.

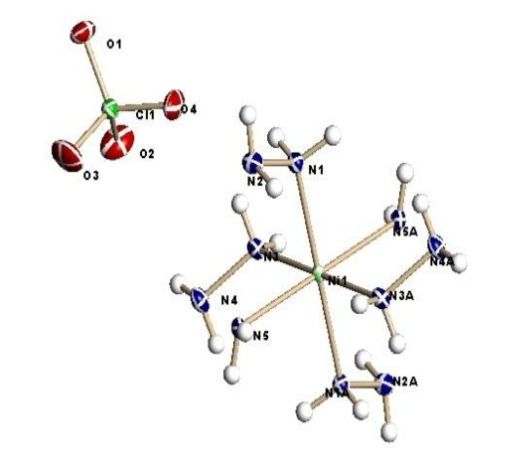

Figure 1.a Monomeric unit of nickel hydrazine perchlorate polymer

Sensitivity studies proved that NHP was not viable for any practical application, however, properties of CHP appear much more promising.

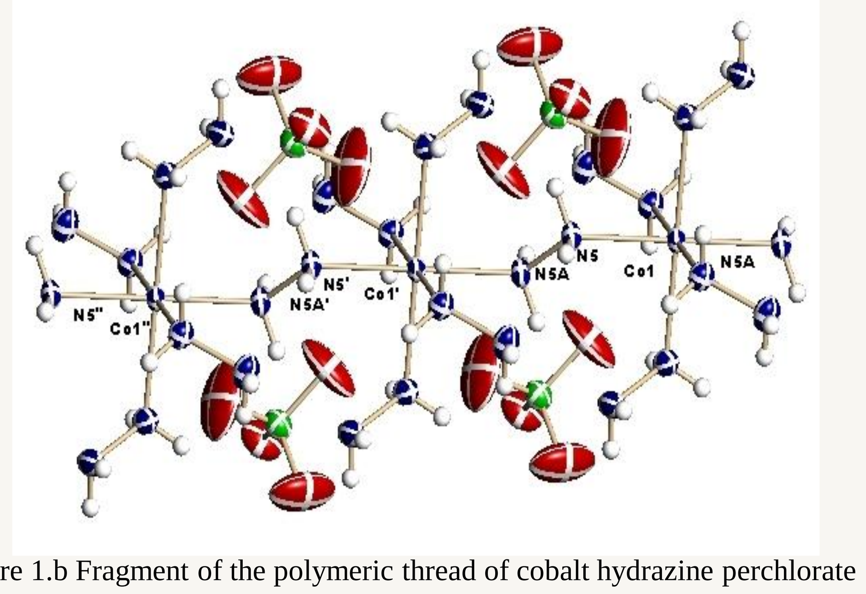

Figure 1.b Fragment of the polymeric thread of cobalt hydrazine perchlorate

Flame, spark and impact sensitivity of CHP is comparable to those of lead or silver azide[1,2], while apparently providing more power.

Observed power and sensitivity of the compounds led to interest in determining the heat of explosion for target molecules.

Theoretical calculations made at Lawrence Livermore National Laboratory suggest heat of detonation values comparable to CL-20[2] for DFT optimized structures exceeding those for experimentally obtained X-ray crystal structures (Figure 2).

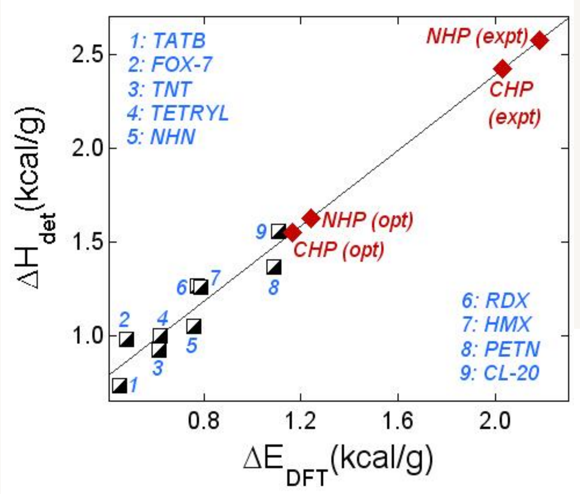

Figure 2.Plot of "T = 0 Energy of detonation" (ΔE_{DFT}) vs the heat of detonation (ΔH_{det})

The difference in heat of detonation of NHP and CHP compared to those of commonly used explosives (Table 1) is notable.

Name of explosive	ΔH_{det}, kcal/g
Nickel hydrazine perchlorate, NHP	1.61-2.55
Cobalt hydrazine perchlorate, CHP	1.55-2.40
Nickel hydrazine nitrate, NHN	1.11
Pentaerythritol tetranitrate, PETN	1.37
Lead azide, LA	0.39
2,4,6-Trinitrotuluene, TNT	0.93
Cyclotrimethylene trinitramine, RDX	1.27
Hexanitrohexaazaisowurtzinta ne, CL-20	1.56

Table 1. Heats of detonation for NHP and CHP in comparison with commonly used primary and secondary explosives.

In the search for reducing the sensitivity of NHP and CHP, substitution of hydrazine with other more stable high-nitrogen-containing ligands at several of the positions was attempted.

We were able to obtain mixed complex of cobalt hydrazine hydrazinecarboxylate perchlorate CHHP (Figure 3).

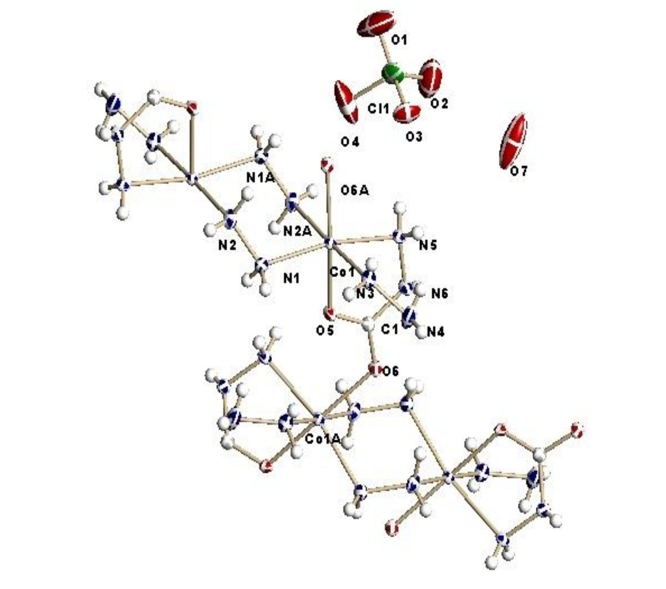

Figure 3. Connectivity of cobalt hydrazine hydrazinecarboxylato perchlorate derived from X-ray experiment.

Evaluation tests conducted with CHHP indicate lower impact sensitivity and temperature of detonation compared to that of CHP.

Accomplishments Through Current Year

Crystal structures and the theoretical computation of heat of detonation for NHP and NHP were determined for the first time.

Future Work

Future work will be focused on studying and broadening the scope of high nitrogen-containing ligands which can be applied to obtain less sensitive explosive complexes or compositions.

Opportunities for Transition to Customer

The described properties should trigger interest in further testing and thorough evaluation of transition metal hydrazine perchlorate primary explosives as well as less sensitive hydrazinecarboxylate per-chlorate compounds.

Applications may be found both in military and civilian use.

Publications Acknowledging DHS Support

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Other References

2. Agrawal, J. P. *High Energy Materials*; Wiley-VCH: Weinheim, 2010.

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