VIRTUAL

ISXB4

4TH INTERNATIONAL SYMPOSIUM ON HALOGEN BONDING

2 – 5 November 2020
Virtual event
Hosted by Stellenbosch University,
South Africa

2020

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Programme & Abstract Book

2 - 5 November 2020

Presented as a Virtual Event from Stellenbosch, South Africa

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Quantum Chemical Study of Influence of Halogen Bonds on the Sensitivity of Organic Explosives

A. B. Đunović[1], D. Ž. Veljković[1]
[1] *University of Belgrade – Faculty of Chemistry, Belgrade, Serbia*

E-mail: aleksandra.djunovic@gmail.com

Predicting the properties of new energetic materials using computer simulations is the ultimate goal of many theoretical studies. [1] One of the most important tools for revealing the sensitivity of the energetic molecules is Molecular Electrostatic Potential (MEP). It is known that molecules of classical C,H,N,O-explosives have strongly positive electrostatic potential above the central areas of the molecular surfaces. [2] Values of electrostatic potentials on the surface of energetic molecules could be adjusted by introducing electron-donating groups in the molecules but also by non-covalent bonding. [2] While it is known that hydrogen bonds do affect the electrostatic potential and sensitivity of the energetic molecules, [3] influence of halogen bonds in halogen-containing energetic molecules is yet to be revealed.
In this work, Cambridge Structural Database (CSD) was searched for the crystal structures of halogen-containing molecules of explosives. Halogen bonding patterns were analyzed in extracted crystal structures. Based on the analysis of crystal structures, model systems for quantum chemical calculations were made. Quantum chemical calculations were used to calculate electrostatic potential maps of selected molecules and to examine the influence of halogen bonding on the electrostatic potential in the central areas of the studied energetic molecules. Results of this study could be of great importance for the development of the new rules for the design of halogen-containing energetic materials with improved sensitivity toward detonation.

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