

## CORRELATION BETWEEN MOLECULAR ELETRONIC STRUCTURE, SENSITIVY TO EXPLOSION AND CHEMICAL STABILITY OF ENERGETIC MATERIALS: NITRAMINES

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**Abstract:** Military explosives have extreme mechanical demands hence must withstand impact without initiating their detonation / deflagration. They also must have chemical stability during storage to resist to deterioration resulting from temperature variations and humidity. Among the different types of explosives, nitramines are a promising class of energetic materials for military used due to its great insensitivity and high energy content; e.g., nitroguanidine is a member of the class already in use. In this work, 21 nitramines molecules were investigated. Their geometries were optimized using the DFT/B3LYP//6-311+G(d) method and the Gaussian 09 program. Their molecular electronic densities were decomposed using two different atom-centered partition methods, the distributed multipole analysis (DMA) and the deformed atoms in molecules (DAM). From the partitioned electronic densities, mathematical relations were found between molecular properties and sensitivity to explosion of the nitramines following the approaches developed in our group for nitroaromatics [1,2]. Chemical stability employing this approach was also investigated. The results will be presented at the conference.

Key-words: Nitramines, electronic structure, impact sensitivity, chemical stability.

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## **References:**

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