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Influence of the presence of halogen substituents on high-energy properties of nitroaromatic molecules

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Sensitivity towards detonation of high energetic materials (HEMs) and the positive potential in the central regions of their molecular surfaces are directly related. The presence of halogen atoms in HEMs creates the possibility for halogen bonding which can be used for modifying of electrostatic potential values [1]. Also, it has been noticed that the substitution of hydrogen atoms by halogen atoms in molecules like nitromethane leads to a decrease of bond dissociation energy values (BDE) for the C–N bond [2].

In this paper, the geometries and potentials in the central regions of molecular surfaces of 1,4-dihalo-5,8-dinitronaphthalene and 2,3-dihalo-5,8-dinitronaphthalene were analyzed. Optimal geometries and maps of electrostatic potential (MEP) were calculated using PBEPBE/6-311G** level of theory. The WFA-SAS program was used to obtain MEP for the mentioned molecules. Bond dissociation energies for optimized geometries were calculated using SAPT program.

Results showed that the potentials above the central regions of molecular sufaces in the 2,3-dihalo-5,8-dinitronaphthalene molecules are higher than in the case of 1,4-dihalo-5,8-dinitronaphthalene analogues. The most significant difference was detected in the case of molecules with chlorine as a substituent (up to 3 kcal/mol). However, the dissociation energies of C–N bonds are higher for all 2,3-substituted dinitronaphthalenes compared to 1,4-substituted analogues. There is a decrease in BDE values in both cases, but it is more significant for the 1,4-substituted dinitronaphthalenes, where the BDE value for 1,4-difluoro-5,8-dinitronaphthalene is more than 7 kcal/mol higher compared to the BDE for iodine analogue.

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