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Influence of the number of halogen substituents and their type on the electrostatic potential of TNB molecules

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It is known that positive potentials above the central regions of molecular surfaces are indicators of the sensitivity towards detonation of molecules.[1] The higher the value is, the more sensitive the molecule is considered to be. The presence of halogens in the molecule significantly affects the charge distribution, and thus the sensitivity. However, the exact influence depends on the type of halogen due to their different strength of electron-withdrawing effect.[2]

In this work, electrostatic potential maps were calculated for the optimized geometries of 1-halo-2,4,6-trinitrobenzene, 1,3-dihalo-2,4,6-trinitrobenzene and 1,3,5-trihalo-2,4,6 -trinitrobenzene. The geometry optimizations were obtained using the PBEPBE/6-311G** level of theory in the Gaussian program. Calculations were made with and without the inclusion of GD3BJ dispersion. The wfn files used in the WFA-SAS program to obtain electrostatic potential maps for the mentioned molecules were obtained using the same combination of method and basis set.

The results showed that within groups of molecules containing the same number of halogen substituents, the value of the positive potential above the central region of the molecule is the highest in cases where the substituent is fluorine. There is a decrease in value as the substituents change in the direction from fluorine to iodine, with the largest decrease being recorded in the case of 1,3,5-trihalo-2,4,6-trinitrobenzene. The obtained results are in accordance with the strength of electron-withdrawing effect of the halogen elements. There is also a noticeable trend of the increase in positive electrostatic potential values with the increase in the number of halogen substituents (with the exception of the sequence in which chlorine is the substituent).

References

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