Ab initio Crystal Structure and Charge Density Distribution of a Highly Energetic 2,4-dinitrobenzoic Acid Molecule

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Abstract: The energetic parameters, such as density, bond strength, and sensitivity of explosives/propellants decide their detonation power and safety. Experimentally, optimization of these parameters is found to be a difficult task; therefore, prior to synthesis, it makes sense to estimate these parameters by computational techniques, ab initio crystal structure prediction, and quantum chemical calculation coupled with the AIM analysis. Here, we predict the density of an energetic 2,4-dinitrobenzoic acid (DNBA) molecule from different ab initio crystal structure models and validate the results through comparisons with experimental data. The bond topological characterization reveals that the C—NO_2 bonds are the weakest bonds and are identified as sensitive bonds in the molecule. The bond sensitivity is estimated from Murray's method. The impact sensitivity of this molecule is also calculated. Large negative electrostatic potential regions are found near the NO_2 and carboxylic groups, which are the reactive sites of the molecule.

Keywords: energetic material, crystal structure prediction, electron density, Laplacian of electron density, electrostatic potential, impact sensitivity.

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