Energetic Windmill: Computational insight into planar guanidine-based nitroazole-substituted compounds as energetic materials

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Abstract

In this work, we designed a series of energetic materials with a windmill-like structure based on guanidine and nitroazole, and optimized them at the B3LYP/6-311G** level using density functional theory (DFT). According to the optimization results, 6 molecules with planar structures were screened out from 28 molecules and their regularities were summarized. We calculated their geometry, natural bond orbital (NBO) charge, frontier molecular orbital, molecular surface electrostatic potential, and thermochemical parameters. In addition, their properties such as density, enthalpy of formation, detonation velocity, detonation pressure and impact sensitivity are also predicted. The result shows that this series of compounds is a promising new type of energetic material, especially compound 1 has superior detonation velocity and detonation pressure (D=9720m/s, P=41.9GPa).

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