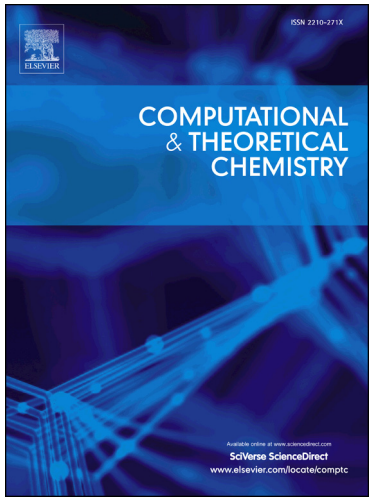

Quantum-Chemical Design of Tetrazolo[1,5-*b*][1,2,4,5]tetrazine Based Nitrogen-rich Energetic Materials

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Quantum-Chemical Design of Tetrazolo[1,5-*b*][1,2,4,5]tetrazine Based Nitrogen-rich Energetic Materials

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Abstract

The molecular structures of azole substituted tetrazolo[1,5-*b*][1,2,4,5]tetrazine (AsTT) derivatives were designed and fully optimized at the B3PW91/6-31G(d,p) level of theory. Isodesmic reaction was constructed to predict gas phase heat of formation (HOF) and heat of sublimation derived from Politzer approach was used to calculate HOF at condensed phase. The presence of nitrogen-rich AsTT backbone is found promising in increasing the HOF values. Politzer approach also extended to predict the densities of these derivatives from the calculated surface electrostatic properties. Kamlet-Jacobs equations were used to calculate detonation performances based on predicted solid phase heats of formation, densities and gaseous detonation products. The charge distribution on molecular surface and free space per molecule in the unit cell were used to analyze the sensitivity. The explosive power and power index were calculated to assess the potential of designed compounds. According to our calculations, the designed AsTT derivatives possess interesting explosive properties and could be the potential addition in high energy materials (HEMs).

Keywords: Tetrazole; Density functional theory; Heat of formation; Power index; Detonation properties.