Poster Presentation

MS035.P19

Theoretical investigations on structure and properties of metal substituted pentazole

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Potential high-energy density materials (HEDMs) and new crystalline compounds are great interest of researchers, because they can undergo exothermic reaction (N2) and replacing some C–H units in a molecular or ionic framework by nitrogens. It increases the compound's heat of formation and also its density, because a nitrogen atom has a greater mass but smaller volume than a C–H unit. The alkali metal (M=Li, Na, and K) substituted derivatives of pentazole (N5) and pentazolate anion were studied using density functional theory. The substituted metals improve energy barrier for decomposition of the N5 ring of PhN5 by 19.3-65.0 kJ/mol. M-3 has the ionic N-M bond, which is not found for M-1 and M-2. M-1 and M-2 have similar electrostatic potentials and dispersion interactions between metal and N5 ring. Theoretical study would be using structural predictions, NMR technique, MS spectra, bond length, bond order, density, free energy and molecular structure. The present investigation focuses on nitrogen-rich compounds mainly synthesis of substituted pentazoles, and high-energy density materials are slightly more stable but conversely, more difficult to make. It has applications in explosives, propellants and will be very useful in defence science. Therefore, the design and synthesis of new nitrogen-rich compounds, the alkali metal (M=Li, Na, and K) substituted compounds and HEDMs with high performance properties has been one of the most challenging tasks in this field.

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Keywords: PhN5, Heat of formation, spectroscopy