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Sensitivity and Performance of Azole Based Energetic Materials[1]

ZIJUN YU, ELLIOT BERNSTEIN, Colorado State University — Imidazole, pyrazole, 1,2,3-triazole, 1,2,4-triazole, and tetrazole based energetic materials are theoretically investigated by employing density functional theory (DFT). Heats of formation ($\Delta_f H^0$s) for the studied compounds (298 K) in the gas phase are determined at the B3P86/6-311G (d, p) theory level through isodesmic reactions. The bond dissociation energies (BDEs) corresponding to NO_2, NH_2, CH_3, and Cl removal from carbon or nitrogen positions of the azole ring are also calculated at the B3P86/6-311G (d, p) theory level. The substituent effect of electron-withdrawing (NO_2, Cl) and electron-donating (NH_2, CH_3) groups on the $\Delta_f H^0$s and BDEs is discussed. Both electron-withdrawing groups and electron-donating groups (except the CH_3 group) dramatically increase the $\Delta_f H^0$s of these energetic materials when the substituent is at an N position on the azole ring. For substitution at a C atom on the azole ring, electron-withdrawing and electron-donating groups have different effects on the $\Delta_f H^0$s for different azole compounds. A correlation is developed for this series of energetics between impact sensitivity $h_{50\%}$ and the defined sensitivity index (SI): based on this empirical relationship and its extrapolation, the impact sensitivities of compounds for which experiments are not available are provided. The promising energetic compounds in each group, which have potentially good energetic performance and low sensitivity, are 1-amino-2,4,5-trinitroimidazole, 1-amino-3,4,5-trinitropyrazole, 1,4-dinitro-1,2,3-triazole, 1,3-dinitro-1,2,4-triazole, 1-nitrotetrazole.

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