Theoretical Studies on the Salts Formed by Triazoles with Nitrate and Dinitramide

*Xueli Zhang Xuedong Gong

Department of Chemistry, Nanjing University of Science and Technology, Nanjing 210094 (P.R. China)

*Corresponding author:532191322@qq.com

Bases 1,2,4-trizole (A) and 1,2,3-trizole (B) and acids HNO_3 (I) and $HN(NO_2)_2$ (II) react to produce energetic salts. In this study, the reactions of these bases and acids were studied at the B97d/aug-cc-pvdz level. All reactions were exothermic and spontaneous. For the reactions of the same acid, the $\Delta_r G_m$ is more negative, the produced salt has higher decomposition temperature. The quantum theory of atoms in molecules (QTAIM) was used to study the intramolecular hydrogen bond interactions. The order of contributions to the total hydrogen bond energies ($E_{H,tots}$) is: NO_3^- > $N(NO_2)_2^-$ and 1,2,3-trizolium > 1,2,4-trizolium. The lattice energy (H_L), the energy gap between frontier orbits (E_g), and the second-order perturbation energy (E_2) were also calculated for better understanding the intramolecular interactions between the cations and anions. These results show that A series salts have stronger intramolecular interactions than B series. HNO_3 is more helpful for forming stronger interactions than $HN(NO_2)_2$.

Keywords: Energetic salts, Hydrogen bond, Intramolecular interaction, DFT