Theoretical Study of Deep Eutectic Propellant (DeEP):
Hydrogen Bonding Analysis of Ethylammonium Nitrate (EAN) based system

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In this study, hydrogen bonding and chemical interactions of ethylammonium nitrate (EAN) and 1-Amino-1,2,3-triazole (1-AT) complex are investigated in theoretical perspective. EAN-(1-AT) complex is a suitable candidate as a deep eutectic propellant. The 1-AT molecules were added to EAN in order to investigate the changes in hydrogen bonding and interaction energies of the eutectic mixture.

The interaction energies (including long-range and short-range interactions) between the ion pair as well as the interaction energies between ions and 1-AT were computed using the Effective Fragment Potential (EFP) method. The Resolution-of-Identity (RI) applied second order Møller-Plesset Perturbation Theory (RI-MP2), and coupled cluster theory (RI-CCSD(T)) were also used to calculate total interaction energies as a benchmark for the EFP results.

The total EFP interaction energy is in a good agreement with the RI- MP2 and RI-CCSD(T) results. Oriented Quasi-atomic orbitals (QUAO) and kinetic bond order (KBO) analysis elucidated that there are network of hydrogen bonding in EAN-(1-AT) systems. The hydrogen bonding network in EAN-(1-AT) system is constructed with N-H and O-H interactions.

All the calculations in this study are done using General Atomic and Molecular Electronic Structure Software (GAMESS) package.

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