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

Shinae Kim, Justin Conrad, Garrett Tow, Edward Maginn, Mark S. Gordon

In this study, hydrogen bonding and chemical interactions of ethylammonium nitrate (EAN) complex are investigated in theoretical perspective. EAN is a nitrate salts, which are widely utilized in energetics, are the suitable candidate as a noble propellant using the concept of deep eutectic solvents. Additional hydrogen bond donor(1-amino1,2,3-triazole) was added to EAN to investigate the changes in hydrogen bonding and energetics in the mixture using quantum mechanical methods.

The interaction energies between the ion pair and the hydrogen donor, as well as the long-range and short-range interactions were calculated 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 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 present in EAN-(1-AT) systems.