Theoretical Investigation of Explosive Detection via Halogen Bonding

Arjun Jaini and Carol A. Parish

Department of Chemistry, University of Richmond, VA

There are many kinds of widely available and powerful explosives that are extremely hard to detect due to their low-volatility and non-aromatic structure. A more effective explosive detection method would be extremely valuable in protecting the general public. This project studied the possibility of using halogen bonding as the basis for a molecular recognition device for explosives. A halogen bond is a highly directional non-covalent interaction between a region of positive electrostatic potential on a halogen atom and a Lewis base. The interactions of various halogen systems and explosives, which acted as the Lewis bases, were modeled with density functional theory and a multitude of functionals and basis sets in order to ensure accurate energy calculations. The data collected supports the concept that halogen bonding can be used as the basis for a molecular recognition device for explosives.