Abstract

Aminoethanol, a molecule with both amino and hydroxyl group on vicinal carbon atoms, has been studied in the literature. Due to the presence of the amino and hydroxyl groups, it has been an interesting molecule to study for the hydrogen bonding point of view as an interplay of inter and intramolecular hydrogen bonding can be observed in aminoethanol, an aspect that has not been well addressed in the previous work. The intermolecular hydrogen bonding of the aminoethanol - water system is also interesting to study as there are several isomers of this system.

Matrix Isolation infrared spectroscopy has been used to study the conformations of the aminoethanol in argon and nitrogen matrices. Lowest energy conformation has been observed in both the matrices. The conformations of aminoethanol have been studied computationally using different levels of theories, AIM and NBO analysis.

The aminoethanol water complexes have also been studied computationally, and the optimized structures for the water complexes corresponding to the lowest energy structure are presented. The orbital interaction analysis has also been performed to understand the role of orbital interactions in the structure of the complexes.