VERSITA doi: 10.2478/auoc-2014-0001
Ovidius University Annals of Chemistry Volume 25, Number 1, pp. 5-10, 2014

Investigation of hydrogen bonding between nitrosamine and sulfuric acid using Density Functional Theory

Sadeghali BAVAFA* and Mona MAHBOUBI

University of Applied Science and Technology of Chabahar, Chabahar Free Trad Zone, 9971763444, Iran and International University of Chabahar (IUC), Chabahar, Iran

Abstract DFT calculations were performed to analyze those interactions; B3LYP and B3PW91 methods were applied and the following basis sets were used: 6-311++G(2d, 2p), 6-311++G(3df, 3pd) and aug-cc-pVDZ. The natural bond orbital (NBO) analysis and atom in molecules (AIM) theory were applied to understand the nature of the interactions. The most stable complex NS1 with an eight-membered cyclic structure contains two O–H···O and N–H···O hydrogen bonding interactions. From the values of ρ(r) at O···H critical points, it can be concluded that the H-boding in eight-membered cyclic NS1 is stronger than other. The elongation of the O–H bond length is caused by the electron-density transfer to the O–H antibonding orbital.

Keywords: DFT, H-bonding, AIM, NBO, nitrosamine, sulfuric acid

ISSN-1223-7221