

EuroSciCon Conference on

Chemistry 2018

February 19-20, 2018 Paris, France

Ayesha Ashraf, J Org Inorg Chem 2018, Volume: 4 DOI: 10.21767/2472-1123-C1-002

DENSITY FUNCTIONAL THEORY STUDY OF INTERACTION OF SOME HALOGEN ACIDS WITH POLYANILINE EMERALDINE SALT GAS SENSOR

Ayesha Ashraf

University of the Punjab, Lahore, Pakistan

ased on density functional theory (DFT) calculations, the ability of a B conducting polymer; polyaniline emeraldine salt (PAn-ES) as the sensor for HCl and HBr gas molecules have been investigated. The polymer structures are modelled theoretically through oligomer approach. The selectivity and sensitivity of PAn-ES (with 2-8 even number of oligomers) among two of the halogen acids are simulated at UB3LYP/6-31G (d) level. Various features like the energy of interaction, natural bond orbital and Mulliken charge analyses are also in line with the analysis from optimized geometric parameters to calculate the detecting ability of PAn-ES towards halogen acids in terms of charge transfer. Interaction energies between donor and acceptor molecules are calculated and corrected for basis set superposition error (BSSE). Comparatively larger forces of attraction among sensor and analyte were observed in nPAn ES-HBr complex as compared to nPAn ES-HCI. To find out the differences in IP, EA, charge separations between donors and acceptors and electron distribution in the acceptor units, spectral properties were analyzed. It is observed that electronic properties of nPAn ES are sensitive to the interaction of nPAn ES with HBr and HCl by calculating the energy gaps between HOMO and LUMO. The theoretical approach helps to conclude that polyaniline conducting polymers shows more selectivity towards HBr as compared to that for HCl and this outcome agrees with reported results based on experimental observations.

Biography

Ayesha Ashraf has completed her M.Phil from Institute of Chemistry, Pakistan and PhD Studies from University of the Punjab, Pakistan. She has been received 3rd position in M.phil 2011-2013 Fall, Institute of Chemistry, University of the Punjab, Lahore, Pakistan. And DPCC Research scholarship awarded for 201. She has recently published 01 paper in reputed journals in short time.

ayesha.analyst@gmail.com