عنوان مقاله:

Computational Analysis on all Di-Fluorobenzenethiol: a DFT-B3LYP Study

محل انتشار:

بیست و یکمین کنفرانس شیمی فیزیک انجمن شیمی ایران (سال: 1397)

تعداد صفحات اصل مقاله: 1

نویسندگان:

Hossein Shirani Il Beigi - *Department of Chemistry, Nazhand Higher Education Institute, Urmia*

Reza Fatollahi Qeshlaq - *Young Researchers and Elite Club, Urmia Branch, Islamic Azad University, Urmia, Iran*

Mahsa Fatollahi Qeshlaq - *University of Tabriz, Tabriz, Iran*

خلاصه مقاله:

Since the discovery of intrinsically conducting polymers, researchers have explored theirunusual electronic properties for a wide range of applications. Due to the presence of aconjugated π-electron backbone, these polymers exhibit electronic properties such as lowionization potential, and high electron affinities. These unique properties make these materialssuitable for applications as organic light emitting diodes, sensors, supercapacitors, organic solarcells and electrochromic displays [1]. The objective of the present research is to study theelectrical and structural properties of all di-fluorobenzenethiol. All of the possible of difluorobenzenethiolstudied in this work are presented in Fig. 1. ( ) The B3LYP method with 6-311+G* basis set calculations by Gaussian 09 have beencarried out successfully to study the structural and the energetical properties of all difluorobenzenethioland electronic, Gibbs and zero-Point energy, HLG, dipole moment and alsoIR and NMR spectra have been calculated. The vibrational analysis showed that all structurescorrespond to local minima in potential energy surface. The electrochemical stability of 3,5-difluorobenzenethiol is greater than other compounds and also the zero-point energy for thismolecule is greater than .other molecules

کلمات کلیدی:

B3LYP, Electrochemical stability