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Document Title : *ELECTRONIC STRUCTURE AND SPECTRA OF SOME THIADIAZOLE DERIVATIVES*

التركيب لإلكتروني و ا لطيف لبعض مشتقات ا لثياديازول

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Abstract : The present work presents a detailed and thorough investigation of the electronic structure and spectra of 1,3,4-thiadiazole derivatives. The ultimate aim, however, is to pinpoint those structural factors that underlie the biological activity of these class of compounds. The ground state geometry of 1,3,4-thiadiazole was determined. AM1-MO method was used since it takes very good account for the directional character of bonding and describes a polar bond much more accurately than do any other semi-empirical methods. The effect of substituents of different electron-donating (accepting) strengths on the geometry and the electronic structural features of 1,3,4-thiadiazole was examined. Substituents studied in the present work are all in the para-position of iminophenyl moiety, namely, Br, CH3 and OCH3 groups. The results of MO-calculations are interpreted via total energy, electronic energy, core-core repulsion energy, ionization potential, electron affinity, dipole moments, heat of formation, net charges and charge density maps of HOMO and LUMO. The electronic absorption spectra in the UV region were measured using polar (methanol) and non-polar (cyclohexane) solvents. Comparison between the experimentally observed and theoretically computed spectra (INDO/S) in addition to a quantitative assignment of all transitions observed, were given. The computed state dipole moment is used to indicate the polarity of the excited state and hence predicts its solvent dependence.

Supervisor : أ. د. حسين محمد أحمد مصطفى ، د. محمد قاضي

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