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لتركيب الإلكتروني والطيف لبعض مشتقات ٢ -مركبتوكوانزولين

Document Language	:	Arabic
Abstract	:	The present work presents a detailed and through investigation of the electronic structure and spectra of a series of 2-mercaptoquinazolin-4-one , S-alkyl (aryl) derivatives and N,S-dialkyl (diaryl) derivatives of 2-mercaptoquinazolin-4-one . The ultimate aim , however , is to pinpoint those structural factors that underlie the biological activity of this class of compounds . The ground state geometry of 2-mercaptoquinazolinone was determined using RHF method with 6-311G** basis set. The effect of substituents of different electron-donating (accepting) strengths on the geometry and the electronic structural features of 2-mercaptoquinazolin-4-one was examined . Substituents studied in the present work are methyl , ethyl , allyl , benzyl , dimethylmalonate , acetylacetone and P-methoxyacetophenone . The tautomeric equilibria in 2-mercaptoquinazolin-4-one were explored. All tautomeric forms were considered . The present investigation indicates that 2-mercaptoquinazolin-4-one exists in solution as a statistical mixture of oxo-thiol and oxo-thione forms . In the present work a complete and thorough survey of PA and PDE on each of the possible sites in 2-mercaptoquinazolin-4-one has been performed . 2-Mercptoquinazolin-4-one behave as acids where they possess high tendency to loss proton from SH and N8 atoms . Comparison between the experimentally observed and theoretically computed spectra in addition to a quantitative assignment of all transitions observed , were given using INDO and MINDO/3 methods . The computed state dipole moments are used to indicate the polarity of the excited stats and hence predict thier solvent dependence.
Supervisor	:	أ.د. سعد الله بن قاري عزيز ، أ.د. حسين محمد مصطفى
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