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Original Article

Theoretical study on the electronic spectra in cyclic 1,2-diketones

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Abstract

The structural and electronic properties of some α-diketones have been investigated theoretically by performing both Hartree–Fock and density functional theory calculations at HF/6-31G(d,p) and B3LYP/6-31G(d,p) levels of theory.

The electronic spectra were calculated by ZINDO and TD methods at each level of theory. The wavelength of the $n \rightarrow \pi^*$ electronic transitions was correlated with the torsion angle between the two carbonyl groups in these compounds. The study revealed that the $n \rightarrow \pi^*$ electronic transitions in the studied compounds are functions of the torsion angles between the two carbonyl groups within the linkage CO–CO.

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Keywords

Cyclic 1,2-diketones; $n \rightarrow \pi^*$ Electronic spectra; CO–CO torsion angle

1. Introduction