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Electronic Spectra of Some Molecules with Five Membered Rings

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ABSTRACT

RINDO/s -Method has been used to account for the electronic spectra of molecules with five membered rings like Cyclopentadiene(C2H5), Imidazole(C3H4N2) and Furfural (C5H4O2). Bonding and chemical efficiency of these compounds where measured at NTP laboratory conditions for manufacturing of various targeted drugs and polymers. Actually, polyatomic molecules containing a specific functional group produce electronic absorption spectra which show some interesting similarities. Extensive investigations have been carried out on molecules containing some groups like carbonyl group and azole group and the similarities found have been attributed to the effects of functional groups. As expected, Imidazole and Furfural should have loan pair of electrons on Nitrogen atom and consequently their spectra should show the presence of an σ -> π^* transition as a lowest energy transition. This result is in line with our predicted spectra of these molecules. These compounds have importance in organic chemistry. The study of these properties requires a correct understanding of the physical, chemical and other allied problems, their causes and solutions. So, any contribution of investigations on this line will be of considerable importance.

Keywords: Cyclopentadiene (C2H5), Imidazole (C3H4N2), Furfural (C5H4O2), RINDO/s method

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