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Abstract	:	The present work presents a detailed and through investigations of the electronic structure and spectra of 1-phenyl-3-trifluoromethyl-4-phenylazo-5-pyrazolone and 1-pheny-3-amino-4-phenylazo-5-pyrazolone derivatives. The ultimate aim however, is to pinpoint those structural factors that underlie the industrial activity of these classes of dyes. The ground state geometry of 3-trifluoromethyl and 3-amino pyrazolone were determined using RHF with 6-31G* and 6-311G** basis sets. The tautomeric equilibria of 3-amino and 3-trifluoromethylpyrazolone were explored. All tautomeric forms were considered. The present investigation indicates that the cyclic hydroazopyrazolone is the most stable tautomer over keto-azo and enol-azo tautomers. The effect of substituents of different electron-donating (accepting) strengths on the geometry and electronic structural features of the studied dyes were examined using AM1-MO method. The results of AM1-MO are interpreted via ionization potential, electron affinity, net charge and dipole moments. The electronic absorption spectra in the UV and visible regions were measured using polar (methanol) and non-polar (dioxane) solvents. Comparison between the experimentally observed and theoretically computed spectra in addition to a quantitative assignment of all transitions observed were given.
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