Title:	Vibrational spectroscopic and density functional theory studies of chloranil-imidazole interaction
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Abstract:	The present work reports vibrational spectra and density functional theory calculations for chloranil, imidazole and their complexes. Th experimentally observed infrared and Raman bands have been assigned with the help of calculated vibrational frequencies and poten energy distribution analysis. Some bands of chloranil and imidazole have been found to shift on the complex formation due to partial electronic charge transfer from imidazole to chloranil. The charge transfer between these molecules is also corroborated by the electr absorption spectroscopy and calculations. The theoretical values of the interaction energy of various possible chloranil-imidazole interactions suggest that the two molecules interact preferably via N and H atoms of imidazole and CO group of chloranil with their molecular planes almost perpendicular to each other.
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