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Spectroscopic studies and Hartree-Fock ab initio calculations of a substituted amide of pyrazine-2-carboxylic acid - $C_{16}H_{18}ClN_3O$

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Abstract: A substituted amide of pyrazine-2-carboxylic acid was prepared and the IR spectrum was recorded and analysed. The compound prepared was identified by NMR and mass spectra. The vibrational frequencies of the title compound were computed using the Hartree-Fock level of theory using the 6-31G* basis set and compared with the experimental data. The red shift of the NH stretching frequency indicates weakening of the NH bond. The splitting of the NH stretching bond is due to Davidov coupling between neighbouring units. The first hyperpolarizability, infrared intensities, and Raman activities are reported. Methyl substitution affects all the carbon-nitrogen and carbon-carbon bond lengths of the pyrazine ring of the title compound in comparison with the corresponding bonds of pyrazine. An increase in conjugation enhances the infrared intensity of the carbonyl stretching vibration.

Key Words: Amides of pyrazine carboxylic acid; IR; Hartree-Fock ab initio calculations, hyperpolaziability.

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