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Vibrational spectral investigation on xanthine and its derivatives—theophylline, caffeine and theobromine

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Abstract

A normal coordinate analysis has been carried out on four compounds having a similar ring structure with different side chain substitutions, which are xanthine, caffeine, theophylline, and theobromine. Xanthine is chemically known as 2,6-dihydroxy purine. Caffeine, theophylline and theobromine are methylated xanthines. Considering the methyl groups as point mass, the number of normal modes of vibrations can be distributed as $\Gamma_{\text{vib}} = 27\,\text{A}' + 12\,\text{A}''$ based on C_s point group symmetry associated with the structures. In the present work 15 A′ and 12 A″ normal modes are considered. A new set of orthonormal symmetry co-ordinates have been constructed. Wilson's *F–G* matrix method has been adopted for the normal coordinate analysis. A satisfactory vibrational band assignment has been made by employing the FTIR and FT Raman spectra of the compounds. The potential energy distribution is calculated with the arrived values of the force constants and hence the agreement of the frequency assignment has been checked.

Keywords: Vibrational spectra; Normal coordinate analysis; FTIR spectra; FT Raman spectra; Xanthine; Caffeine; Theophylline; Theobromine

1. Introduction

Xanthine derivatives are the naturally occurring drugs which find use as central nervous system stimulants. Xanthine is chemically represented as 2,6-dihydroxy purine. Caffeine, theophylline and theobromine are methyl derivatives of xanthine. Chemically caffeine is 1,3,7-trimethyl xanthine; theophylline 1,3-dimethyl xanthine and theobromine 3,7-dimethyl xanthine. Theophylline, caffeine and theobromine have different biochemical effects and are present in different ratios in the different plant sources. They are easily oxidised to uric acid and methyl uric acids. Caffeine occurs naturally in coffee, tea, cola nuts, mate and guarana; theophylline is found in tea whereas theobromine is present in cocoa bean, cola nuts and tea.

Spectroscopic investigations on pharmaceutical samples are of importance in the present. Vibrational spectral studies of pyrimidine and its substituents are extensively studied by many scientists [1,2]. The five membered heterocyclic compounds such as imidazoles are studied by Sathyanarayana et al. [3]. Spectroscopic investigations on samples of pharmaceutical importance have been carried out by many workers [4,5]. Among the biomolecules, N-heterocyclic compounds are of considerable importance as they are of considerable pharmaceutical importance. The vibrational spectral analysis of caffeine and theophylline have been reported already [1]. However, the normal coordinate analysis and the potential energy distribution (PED) associated with each vibrational mode of xanthine and its derivatives have not been carried out fully. An attempt has been made in this work to study four derivatives of purine viz. xanthine, caffeine, theophylline and theobromine.

In the present work, the vibrational spectral analysis have been carried out on four compounds viz., xanthine and its derivatives. Using a normal coordinate analysis, the potential energy constants have been evaluated on the basis of general

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valence force field, applying Wilson's *F–G* matrix method [6].

2. Experimental

Xanthine and its derivatives caffeine, theophylline and theobromine are white crystalline solids. The samples of high grade purity had been obtained from Hi-media chemicals, Mumbai, India and used as such. The FTIR spectra of the compounds have been recorded using Bruker IFS 66 V spectrophotometer over the region 4000–400 cm^{-1}. The FT Raman spectra are recorded using Bruker FRA 106 FT Raman spectrophotometer in the region 3500–50 cm^{-1}. The FTIR and FT Raman spectra of the compounds xanthine, caffeine, theophylline and theobromine are presented in Figs. 1–4, respectively.

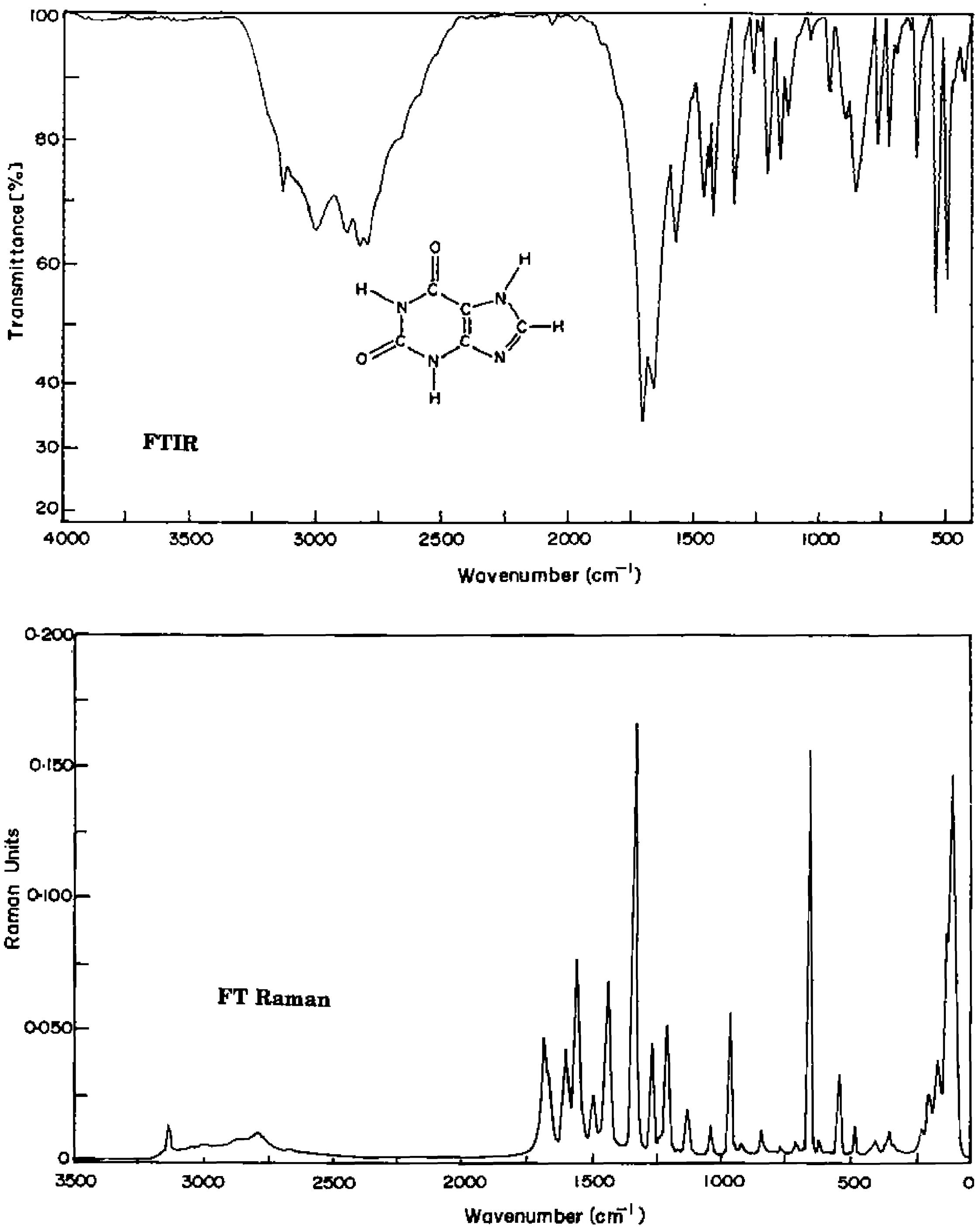

Fig. 1. Vibrational spectra of xanthine.