Investigations on paracetamol by spectral analysis and ultrasonics & microwave measurements

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The pharmaceutical compound, paracetamol can possess two possible structures with, C_{2v} and C_s symmetries, assuming $NHCOCH_3$ as a point mass. The 33 normal modes of vibration under C_{2v} symmetry may be distributed as vib = $12A_1 + 3A_2 + 7B_1 + 11B_2$, while under C_s symmetry as vib = $23A' + 10A''$. All modes of vibration under C_s symmetry are active in both IR and Raman, while A_2 species of C_{2v} is IR inactive. But all other species of C_{2v} are IR and Raman active.

A systematic set of symmetry coordinates for both the symmetries has been constructed and a normal coordinate analysis has been carried out by F-G matrix method and using Wilson's approximation[1]. The potential energy distribution for various normal modes of vibration are calculated for both the symmetries and compared.

Spectroscopic pure samples of paracetamol were obtained from a leading pharmaceutical laboratory, Chennai, India. The FTIR spectrum was recorded in the region 4000-400 cm^{-1}. FT Raman spectrum was recorded over the range of 4000-10 cm^{-1} on Bruker 66v IFS spectrophotometer at RSIC, IIT, Chennai, India. The UV Visible spectra was recorded using UV visible 160A spectrometer.

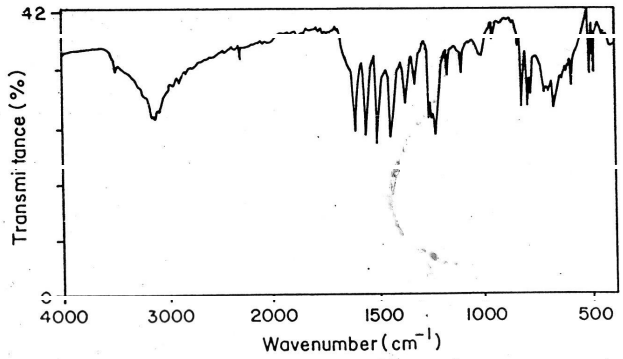

Fig 1. FTIR spectrum of paracetamol

Further, the suitability of the drug for administration was studied by exposing it to various conditions by UV spectral investigations. The samples of the drug were exposed to sunlight, IR radiation, kept at ice point, at room temperature.

The paracetamol compound was taken in liquid state and ultrasonic parameters were measured by using ultrasonic interferometer at 1, 2, 3, 5 and 7 MHz at various temperatures. Microwave measurements were also carried out and the results were briefly discussed. Dielectric behaviour of the compound at various temperature conditions was studied by Roberts and Von Hippel Method[2].

References

1 Wilson E B (Jr), Decius D C & Cross P C, "*Molecular Vibrations*", (McGraw Hill, New York).
2 S. Roberts & A Von Hippel, *J Appl Physics*, 7 (1956) 17.

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