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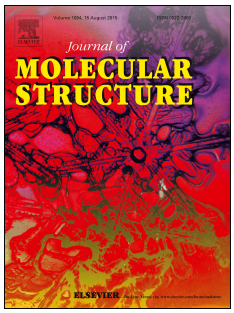

Synthesis and spectral investigations of pyridinium picrate

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Synthesis and Spectral investigations of Pyridinium picrate

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ABSTRACT
This article describes the vibrational spectra of a crystalline compound called "Pyridinium Picrate. The vibrational spectra measurements were recorded as a function of temperature by both FT-IR and Raman spectroscopy. The presence of various functional groups and modes of their vibrations were assigned and followed evolutions. The stability of the crystalline compound arising from has been analyzed using DSC analysis. This crystal composed of two symmetry groups C_{2v} and P_{-1} respectively named phase I and II, this transition was followed by a function of temperature and XRD, is agreement with crystal structure data. In the present investigation, IR and Raman spectroscopy were employed for the identification of the transitions phase of this dimorphic. Essentially studied by Raman low frequency, the shift, disappearance and appearance of the peaks are used for the determination of the phase transition by the characteristic bands NO_2, C–H deformation and C–O stretching, these results reveal a reversibility of this structural transition, depending on the operating conditions.
Keywords: Pyridinium Picrate, phase transition, FT-Raman, FT-IR, XRD, DSC.

1. INTRODUCTION

Many active ingredients have several polymorphic forms, with one of them only being the desired form to be formulated in the drug. It is thus imperative to control within the mixture which form is present. Being non-invasive, and very chemically selective to discriminate polymorphs, Raman spectroscopy is well adapted to determine within tablets or capsules which form(s) are included. The structural phase transitions alter the crystal's vibrational behavior, so that: Raman spectra show changes across those transitions; Raman spectroscopy provides a convenient proxy for structural phase changes. Doubling of features, frequency shifts, line width changes, are the typical signatures of structural transitions (Soft modes signal softening of restoring forces typical of many structural transitions. The pyridinium Picrate properties has allowed to intervene in various fields such as biology, optics, catalysis and as purification in the pharmaceutical industry, hence the importance of knowing the polymorphic behavior of the active substance to optimize operation and storage conditions so that only the desired shape will be present in these processes, or the importance of the thermal stability of this dimorphic compound (two phase).

The work presented in this article is an contribution to the study of phenomena related to dimorphic of an organic salt called [$(C_6H_2N_3O_7)^-.(C_5H_6N)^+$] " Picrate Pyridine ", by comparing the behavior of its two forms, respectively named phase I and II, to provide additional structural and spectral data with previous results of other authors, by monitoring the behavior and activity of any group spectroscopy essential to the understanding of its mechanism of structural changes to tackle the question of reversibility in this transition. To do this, a particular technique was preferred; Raman spectroscopy has the ability to provide guests with information on the molecule structure, its binding mode and the presence or absence of an interaction, which makes particularly interesting target for certain influenced by phase transition phenomena particular groupings. To complete the data structural studies of this dimorphic, because of our knowledge, the vibration spectra of crystals PicPy has never been a comprehensive spectral study. The unusual work is essentially based on the diffraction XRD, on which, we refer in this study.

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