Thermospectroscopic studies in the stretching region of betaxolol and betaxolol hydrochloride

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The infrared spectra recorded at different temperatures give valuable informations on the structure of solid organic crystals in particular, regarding hydrogen bonding network. In fact, while the external applied temperature is an excelent tool to point out the hydrogen bond feature, infrared spectroscopy is privileged technique to characterize this type of bonds. For these reasons thermospectrophotometry is among the methods commonly used in solid state research.

In the present paper FTIR spectra of betaxolol and betaxolol hydrochloride at diferent temperatures from -170 ºC to melting point are presented. For the latter compound, spectra for heating and cooling runs are given. The spectra for the compounds dissolved in CCl_4 at 25 ºC are also presented.

The stretching vibration spectra were resolved into Lorentzian curves by peak fitting and the characteristic parameters for the bands assigned to bonds involving the NH and OH groups are determined. Phase transitions were detected for the systems under consideration from the variation of the band parameters with the temperature.

The spectral data obtained allow to point out some important structural features. Four hydrogen bond systems are present in betaxolol in solid state at temperature below 55 ºC. For temperature above this limit a more stable form defined by three hydrogen bonds is dominant. Fusion is almost a silent transformation on the spectroscopic view point.

In betaxolol hydrochloride four hydrogen bonds were found at wavenumbers near the values observed for betaxolol. As temperature increases a change in the parameter patterns occurs between 55 and 65 ºC giving rise to a thermally stable crystalline form. Betaxolol fusion of the salt is not detected by infrared spectroscopy.

For betaxolol hydrochloride infrared spectra were taken on the cooling of the melt down to -170 ºC and re-heating the solid again to the liquid state. The structure modifications occuring during the thermal cycle are reported by the variation of the maximum wavenumber, width at half-height and the intensity of the individual bands.

The thermal behavior of the betaxolol hydrochloride is interpreted on the grounds structure determined by X-ray.