

INFRARED SPECTROSCOPY IN THE STUDY OF TERFENADINE PHASE TRANSITIONS

J. Canotilho², M. Ermelinda Eusébio¹, Felisbela S. Costa², A. T. de Sousa², J. Simões Redinha¹ and M. Luísa P. Leitão¹

¹*Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade de Coimbra, 3004-535 Coimbra, Portugal*

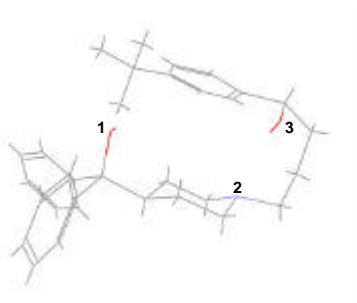
²*Faculdade de Farmácia, Universidade de Coimbra, 3000-295 Coimbra, Portugal*

Phase transitions are important doors to understand the structure of substances in different states of matter. Several techniques can be used for this purpose each of them pointing out specific aspects of the problem.

Infrared spectroscopy is one of the most important methods for the knowledge of structures in particular when hydrogen bonds are present. Indeed the establishment of a hydrogen bond, HB, is followed by modification of the spectral pattern of the groups involved relatively to those found where these bonds are not present. In the stretching vibration region a shift of the maxima towards lower frequencies of the absorption bands due to the groups involved in HB and an increase of the band width and the intensity are observed.

The aim of the present work is the study of the structural forms of terfenadine by using the stretching vibration absorption modes.

Besides a large non-polar part, the terfenadine molecule has two hydroxyl groups (1;3) and one nitrogen atom (2) which can participate in *intra*- and *intermolecular* hydrogen bonds. Another type of hydrogen bond can further result from the interaction of the hydroxyl with phenyl groups.



1-(4-tert-butylphenyl)-4-[4'-(diphenyl-hydroxymethyl)-1'-piperidyl] butan-1-ol

The terfenadine specimens under study were obtained from crystallization in solution in several solvents and in different experimental conditions giving rise to crystalline, amorphous and solvate states.

Infrared spectra of these solids and of those formed by phase transition upon heating were recorded. Glasses obtained from the melt on cooling were also studied by this spectroscopic technique.

The stretching region exhibits broad and complex OH absorption bands which were decomposed into three to five Hertzian shape bands by a curve fitting procedure. Peak maximum shift, peak half-width, and peak area were determined at different temperatures for each component. A discussion on the structure of the phases and the changes of state for terfenadine is undertaken based on OH stretching vibration modes.