Dottorato di Ricerca in Fisica dell'Università degli Studi di Messina
5 Maggio 2011, ore 15.00, Aula E. Majorana, Dip.to di Fisica,
V.le F. Stagno d'Alcontres 31, S. Agata, Messina

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Seminar title:
Vibrational dynamics and chiral recognition in Ibuprofen/β-cyclodextrins inclusion complexes: FTIR-ATR and numerical simulation results

Abstract

Cyclodextrins are supramolecular host systems able to encapsulate molecules in their hydrophobic cavity via noncovalent interactions. Their chiral recognition properties, not fully characterized yet, are of great relevance in pharmaceutical industry.

Here, we studied how the vibrational properties are affected by the chiral recognition process, upon selection of the non-steroidal anti-inflammatory drug Ibuprofen (IBP) in its chiral (R)- and (S)-, and racemic (R, S)- forms, as model guest, and native and modified β-cyclodextrins (β-CDs) as model host. The changes induced, as a consequence of complexation, on the vibrational spectrum of IBP, have been studied, in solid phase, by attenuated total reflection Fourier transform infrared FTIR-ATR. The recorded spectra have been compared with the wavenumbers and IR intensities as obtained by simulation for the free and complexed guest molecule. By the temperature-dependent analysis of the vibrational spectra in the C=O stretching region, the complexation mechanism has been discussed. It turned out to be enthalpy-driven, with enantiomers of IBP giving rise to more stable inclusion complexes with respect to the racemate. This combined experimental-numerical approach gave crucial information on the expected different "host-guest" interactions that drive the chiral recognition process, helpful to put into evidence differences in the conformational properties of the complexes, that are retained a prerequisite for chiral recognition.