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Posters

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The poster sessions will take place in the ILL/ESRF library on

- Wednesday March 3 from **13h00** to **14h00** and from **17h20** to **19h30**
- Thursday March 4 from **13h00** to **13h50**
- Friday March 5 from **13h20** to **15h20**

N. CORREIA

1) Confining effects in the molecular dynamics of ibuprofen investigated by dielectric relaxation spectroscopy

2) Cellulose Acetate membranes characterized by Dielectric Relaxation Spectroscopy

CONFINING EFFECTS IN THE MOLECULAR DYNAMICS OF IBUPROFEN INVESTIGATED BY DIELECTRIC RELAXATION SPECTROSCOPY

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Among the pharmaceutical compounds, those that are glass formers can play a crucial role concerning the therapeutic activity. In fact, a growing interest is devoted to the development of amorphous solid pharmaceuticals since the amorphous form of a drug often shows an improved solubility, accelerated dissolution and bioavailability promoting therapeutic activity when compared to the ordered crystalline material. However, the amorphous solid state is out of equilibrium, and therefore unstable. Thus confinement in nanoporous host systems emerged recently as a strategy to overcome this problem and as a way to increase the lifetime of amorphous drugs for real-life applications. For instance, in ibuprofen, it was observed that when encapsulated in MCM-41 molecular sieves, it does not crystallize, being at room temperature in the supercooled liquid state as confirmed by NMR and X-ray diffraction.

In this work, dielectric relaxation spectroscopy was applied to study the molecular mobility of Ibuprofen confined to MCM-41 molecular sieves (100% Si chemical composition) with a hexagonal structure of cylindrical pores of 3.6 nm diameter. A complex relaxation map including two secondary relaxations in the glassy state, γ and β, a main α process associated with the dynamic glass transition of the bulk-like molecules and a *surface* process is given for the first time. The β-relaxation speeds up, and its activation energy is lower than for the bulk, being also identified as the genuine Johari-Goldstein process. The temperature dependence of the relaxation time of the α process does not obey a VFTH law, oppositely to the bulk. Instead an apparent Arrhenius behavior is found, and thus an acceleration of the molecular dynamics of the bulk-like molecules is observed, which is interpreted as a confinement effect. Moreover, it is concluded that the molecular dynamics is determined by a counterbalance of the confinement and an adsorption effect. The latter is observed by the *surface* process which has an essentially lower molecular dynamics than the one found for the bulk relaxation processes. The temperature dependence of the *surface* process relaxation times follows a VFTH-equation, being attributed to the glass transition of the Ibuprofen molecules linked via weak hydrogen bonding to the inner pore surface.

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