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Oral -Confinement effects in the molecular dynamics of ibuprofen studied by DRS

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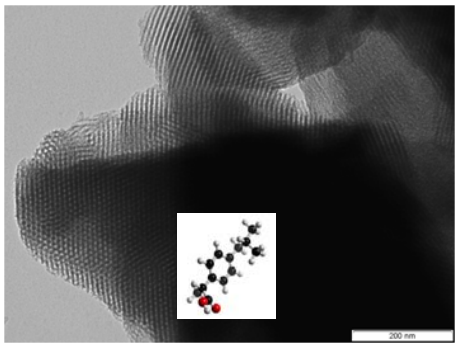
In this work, dielectric relaxation spectroscopy was applied to study the molecular mobility of racemic Ibuprofen confined to MCM-41 molecular sieves (100% Si chemical composition) with a hexagonal structure of cylindrical pores of 3.6 nm diameter.



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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