Dielectric and thermal characterization of S-ibuprofen

A. C. Rodrigues[a], M. T. Viciosa[b], N. T. Correia[a,c]

[a]*Requimte/CQFB, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Campus de Caparica, 2829-516 Caparica, Portugal*

[b]*CQFM – Centro de Química-Física Molecular and IN – Institute of Nanoscience and Nanotechnology, Instituto Superior Técnico, Universidade Técnica de Lisboa, Avenida Rovisco Pais, 1049-001 Lisboa*

[c]*UMET, UMR 8207, Université Lille1, UFR de Physique, Bât. P5, Cité scientifique, 59655 Villeneuve d'Ascq Cedex, France*

andreia.rodrigues@dq.fct.unl.pt

Ibuprofen is a non-steroidal worldwide used pharmaceutical compound which belongs to the category of 2-arylpropanoic acid, showing analgesic, antipyretic and anti-inflammatory properties. Commonly, it is commercially available as a racemic crystalline compound of S-(+)-ibuprofen and R-(-)-ibuprofen. The S-(+) conformation corresponding to the pharmacological active form is the aim of the present work based on Differential Scanning Calorimetry and Dielectric Relaxation Spectroscopy complementary measurements; the latter technique was used in order to study the molecular mobility (10^{-1} Hz to 10^{6} Hz) in the glassy and in the supercooled liquid state; results will be compared with those previously published for the racemic compound [1]. After melting the crystalline starting material (T_m = 52 ºC), a cooling rate of 10 ºC.min^{-1} from 80 ºC down to -130 ºC was enough to avoid crystallization: no exothermic peaks were observed in the thermogram and a clear heat capacity jump, signature of the glass transformation was detected. On the subsequent heating scan at 10 ºC.min^{-1}, the onset glass transition temperature was determined at T_g = -46 ºC; on further heating (at the same heating rate) S-ibuprofen persists in the supercooled state. Lower cooling rates were also tested (≥2 ºC.min^{-1}) with no observation of melt-crystallization. Similarly to the racemic compound (T_m = 74ºC; T_g = -47 ºC), S-ibuprofen can be classified as a very good glass-former. Also, concerning the molecular mobility, both in the glassy and in the metastable supercooled liquid state, S-(+)-ibuprofen doesn't show significant differences when compared with the racemic compound. Ongoing studies are being focused on the hypothesis of cold-crystallization occurring under specific conditions, which in the case of racemic ibuprofen leads to the formation of a metastable polymorphic variety.

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References

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