Crystal structure determination and molecular mobility study in the glass phase of a cholesteric liquid crystal: cholesteryl hydrogen phthalate (CHP)

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The designation of liquid crystal refers to substances that, in condensed phase, display forms of molecular organization sharing characteristics common to the crystalline and the liquid states. This intermediate state, called mesophase, often has the appearance of a translucent liquid, which distinguishes it from "normal" (isotropic) liquids, optically characterized by their transparency. The liquid crystalline mesophases combine characteristics typical of macroscopic crystal phase such as optical, electrical and magnetic anisotropy, with mechanical characteristics of liquids (fluidity).
The compound under study, cholesteryl hydrogen phthalate (CHP, Fig. 1) is sold in the crystalline form. To the best of our knowledge, the crystal structure was not available in the literature and was determined in this work using x-ray crystal diffraction at ambient and low temperature.

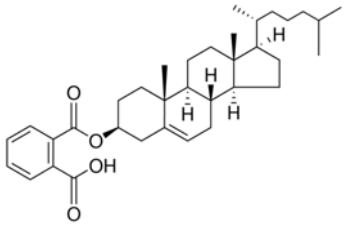

Fig. 1. Cholesteryl Hydrogen Phthalate (CAS 6732-01-0)

The commercial crystalline phase of CHP melts at 168.2ºC (ΔH_{melt} = 60.5 J/g) and displays thermotropic liquid crystalline behavior. Cooling from the isotropic liquid induces an isotropic-cholesteric phase transition at ca. 85ºC and a glass transition is detected at 35ºC (at 10 K/min), avoiding crystallization of the compound [1]. This glass transition is specific of a partially disordered material and differ from the canonical glass transition. The vitreous phase was stable if maintained at temperatures below 65°C, so the study of the molecular mobility in the amorphous solid state seems possible. In contrast, cold crystallization happens if the temperature of the sample reaches 80ºC. On the other hand, there is evidence of polymorphism in this substance; however, this aspect has not yet been studied in depth.
Several images will be presented that have been captured by optical microscopy and illustrate some aspects the thermal behavior observed by DSC.

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[1] G. P. Johari, J. W. Goodby, G. E. Johnson, *Nature* 297 (1982) 315-317.