

Polymorphism on a Liquid Crystal: 4-Cyanophenyl 4-buthylbenzoate (4CBz)

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Liquid crystals are materials that look to be fluid to the naked eye but, under a polarized microscope, a textured, crystalline-like structure appears. Rigid cores and flexible tails within the structure of a molecule are usually prerequisites for this behaviour. On the molecular level, these materials exhibit unique phases, on the cooling sequence: isotropic, nematic, and smectic. Two situations are possible for the last transition: a crystalline phase or an amorphous mesophase, showing molecular motions of a partially disordered material. In some experimental conditions, a direct transition nematic-crystal should be observed.

The compound under study, 4-cyanophenyl 4-buthylbenzoate (4CBz, Fig. 1), was originally produced by Hoffmann-La Roche with the trade name of RO-CM-1500, but nowadays is supplied by Sigma as a crystalline solid with a melting point of 66.6°C, measured by DSC [1, 2].

After the initial melting of the commercial sample, the cooling from the isotropic liquid an isotropic-nematic transition was detected at *ca.* 41°C (without appreciable hysteresis) and, at *ca.* 17°C, a second transition (nematic-crystal) is observed. This new crystal form (kinetically stable during some hours) shows a melting temperature of *ca.* 13°C (53.2°C) lower than the commercial form and a melting enthalpy inferior by a factor of 0.79, being considered as an evidence for a new polymorphic form. Using cooling rates, in the range 5 to 10 K/min, from the isotropic liquid to temperatures below the nematic-crystal transition, new transient polymorphic forms were detected as a function of the heating rate used. The use of a similar thermal protocol, some images of these evolutions were recorded by hot stage microscopy. To the best of our knowledge, the crystal structure of the commercial form is unknown, and was determined in this work, using x-ray crystal diffraction at ambient and low temperature (T= 150K).

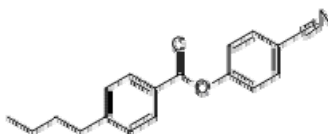


Fig.1. (4-Cyanophenyl) 4-Methylbenzoate (CAS 38690-77-6)

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References

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