

Structural Analysis of Thermotropic Liquid Crystals using Pair-Angle Distribution Functions

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Thermotropic liquid crystals are a group of pure molecules that experience liquid crystal phases at specific temperatures without the aid of a solvent. Liquid crystals are important due to their properties likened to both solid and liquid phases, such as electrochemically behaving as a solid but flowing like a liquid. These properties are utilised through applications in digital screens in the form of LCDs and biological and chemical sensors [1]. To form the liquid crystals, these macromolecules are inherently disordered, meaning typical crystallographic techniques can be difficult. Hence we are looking to Fluctuation X-ray Scattering (FXS) [2], and a novel analysis technique for it called Pair-Angle Distribution Function (PADF) method [3, 4]. The PADF maps the three- and four-body correlations for atomic distribution and specialises in disordered-ordered systems, where there is typically some nanostructure, such as proteins [5] and liquid crystals.

To investigate the liquid crystal systems, we have taken a collection of calamitic samples, namely n-CB family (n=4-12 sans 10), cholesteryl pelargonate, 4-Isothiocyanatophenyl-4-pentylbicyclo[2.2.2]octane-1-carboxylate (IPOC), 2',3,4-Trifluoro-4"-propyl-1,1':4',1"-terphenyl (TriFPP), and 2',3,4,5-Tetrafluoro-4"-propyl-1,1':4',1"-terphenyl (TetraFPP). We have first investigated their thermal phase behaviour through cross-polarised optical microscopy (CPOM) and differential scanning calorimetry (DSC) experiments over a range of 20-100°C. The calamitic samples were shown to form a combination of nematic, smectic and chiral nematic mesophases, but many samples displayed hysteresis, making the temperatures at which those mesophases were displayed inconsistent with the literature.

For these liquid crystal systems, the structure is important for all applications. While the ordering of liquid crystal phases is generally understood, local molecular coordination is difficult to characterise experimentally because of the liquid-like disorder at short-length scales. As such, we have conducted powder X-ray diffraction experiments to determine the structure of the crystalline state, which thermally leads into the liquid crystal state, to gain insights into this structure. This research will be furthered through molecular dynamics simulations [6] and FXS/PADF, providing novel insights into these materials in the crystalline phase, liquid crystalline phases, and the transitions between them.

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