

29/05/2015

New Procedure to Obtain Liquid Crystals



Currently, liquid crystals are of considerable interest due mainly to their applications in electronics and optics (TV, mobile phones or table screen). These materials are formed by sets of molecules that are organised in different ways depending on their composition. This study shows how the inclusion in these molecules of a group called polar atoms can affect the way they interact with each other and thus their organisation and behaviour as liquid crystals.

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Liquid crystals are an intermediate state of matter, situated between a solid (ordered internal structure) and a liquid (disordered internal structure). Consequently, liquid crystals combine some solid state properties such as molecular order, with other liquid ones, such as fluidity. In this state of matter, called mesophase, molecules may be arranged in layers or stacked in columns, generating diverse types of mesophases.

We can distinguish two ways of producing a mesophase (or liquid crystals): by the action of temperature, to obtain thermotropic liquid crystals; or by the action of temperature and also the presence of a solvent, to obtain lyotropic liquid crystals. The thermotropic liquid crystals are the most common industrially applied because of their properties, and therefore those studied in our research group.

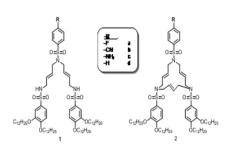


Figure 1. Open precursors 1 and macrocycles 2.

We have studied the preparation liquid characterisation of crystals whose structures are shown in Figure 1. Four of them have open structures, 1, and four others closed, cycles 2. All these structures have a common part; two hexagonal rings of six members (aromatic rings) containing two chains of 12 carbon atoms. The other aromatic ring contains polar groups (-F, -CN, -NH2) which were introduced in order to promote interactions between molecules (intermolecular interactions). The same molecules were also prepared with a hydrogen atom as a model to compare

properties.

mesophase.

All molecules prepared present thermotropic liquid crystal behaviour; that is, the molecules organise themselves when heated. These materials were studied using laboratory techniques such as Polarized Optical Microscopy (POM, Figure 2), Differential Scanning Calorimetry (DSC) and X-Ray Diffraction (XRD).

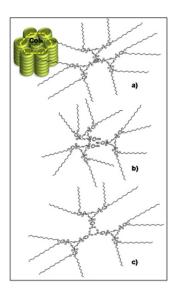
From our results we can draw the following conclusions:

a) Polar groups play an important role in the organisation of the molecules when they are heated. These molecules organise themselves into types of discs, which then stack themselves forming columns. In turn, these columns are arranged among them forming hexagons (Figure 3). This type of organisation is what is known as hexagonal columnar Figure 2. Optical micrograph of compound 1d



showing a Colhmesophase, at 38°C, on cooling cycle.

- b) Each disc forming columns comprises three identical molecules interacting with each other through the polar groups introduced into said molecules, orienting them toward the centre of the disc. The long chains are oriented towards the outside of the disc, and can interact with other chains of the upper and lower discs.
 - c) The stability of these columnar mesophases was much higher than that observed for the corresponding compounds devoid of polar groups.
 - d) The presence of chains of 12 carbon atoms coating the outside part of columns was also an important parameter, not only for the presence of a high number of intermolecular interactions, but also because they are fluid and disordered in the liquid crystals state, allowing the highly dynamic nature of columnar phases. The variation of the molecular



architecture allowed control of thermotropic properties and the design of discotic mesophases (a type of mesophase in which molecules are arranged following a disk shape), appearing at different temperature ranges. Up to a limit, a greater number of intermolecular interactions produce a clear increase in the temperature range in which the molecules present liquid crystal behaviour.

Figure 3. Three examples of the proposed models for the hexagonal columnar mesophases where the difference lies in the intermolecular interactions; a) π - π stacking; b)dipole-dipole; and c) hydrogen-bonding interactions.

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References

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