Studies of Self-Assembled Supra-Structures of H-Bonded Superdiscs and Macrocyclic Liquid Crystals by X-ray Diffraction

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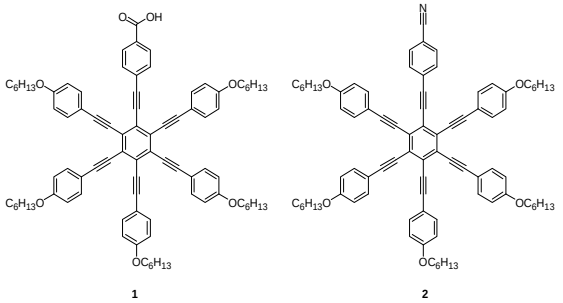
Covalent interactions have been conventionally ulitized for constructing molecules with desired functionalities, for example, materials for information display. On the contrary, specific intermolecular interactions, such as hydrogen bondings, have been overlooked as a power tool for assembling architechtures that can not be easily achieved by the conventional covalent approaches. Recently, demands of anisotropic properties of bulk materials have urged the development of constructing molecular skeletons by specific interactions. Hydrogen bonding has been the most studied interaction among various specific interactions since it is well studied among them. In order to utilize this powerful tool to accomplish infinite two- or three-dimensional networks, we have aimed on self-assembled organizations based on disc-like molecules. The infinite structures are to be realized from simple systems like hydrogen bonded hetero-dimers. Accordingly, we have prepared disc-like hydrogen donors and disc-like hydrogen acceptors. Their optical and mesogenic properties have been investigated. Moreover, these two have been subjected to hydrogen bonding studies. Herein, the mesogenic as well as preliminary powder X-ray diffraction studies of a disc-like hydrogen donor, compound **1**, and a disc-like hydrogen acceptor,



Scheme 1. Sturctures of the discotic molecules **1** and compound **2**, are reported (Scheme 1).

The mesogenic properties of compounds **1** and **2** were studied using differential scanning calorimetry (DSC) and polarized optical microscopy (POM). studies of the two single components and the complex. As shown in Fig. 3, the signals corresponding to the aromatic region of compound **1** have shifted to the downfiled region after complexation.

In order to detail the structural information of the hydrogen bonded complex, powder X-ray diffractions (XRD) were performed. At this stage, only the XRD of compound **1** was investigated. Both the columnar and nematic phases were explored by XRD. As showin Fig. 1, two sharp signals in the small angle region and two broad halos in the wide angle regime were observed for the columnar mesophase of **1**. The two small angle signals are indexed to the 200 and 110 reflections of a rectangular columnar arrangement. The calculated d-spacings are 22.3 and 21.7 Å respectively. The two halos in the wide angle region correspond to 4.8 and 3.6 Å. The halo at 4.8 Å originates from the molten side cahins and the halo at 3.6 Å is attributed to the intracolumnar distance. At higher temperature, one broad signal in the small angle region and a halo in the wide angle part were observed as shown in Fig. 2. The calculated d-spacing of the small angle peak is of 23.8 Å which approximates the core dimension. The halo at 4.6 Å is typical for chain correlation. The diffractogram resembles that of the typical discotic nematic phase. Based on the POM and XRD results, a discotic nematic phase is assigned.

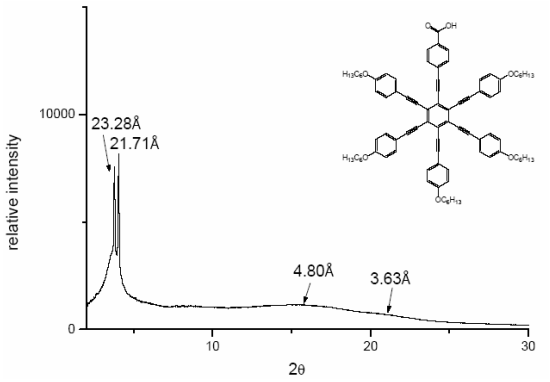


Figure 1. XRD pattern for compound **1** in the columnar mesophase temperature range.

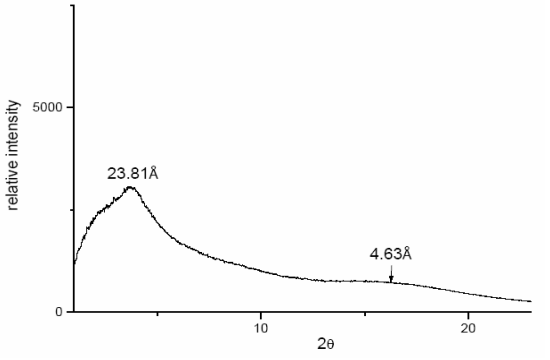


Figure 2. XRD pattern for compound **1** in the nematic mesophase temperature range.

In future, XRD studies of the complex as well as other hydrogen bonded systems currently developed in our laboratory are to be investigated to probe the possible long range ordering of these systems.