Powder X-ray Diffraction Studies of Self-Assembled Supra-Structures of H-Bonded Superdiscs and Helical Discotic Liquid-Crystalline Hexabenzocoronenes

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Large polycyclic aromatic hydrocarbons have been the focus of considerable research interests during the past several years. Recently, scientists have taken the family of substituted hexa-*peri*-hexabenzocoronenes (HBCs) seriously which have been studied intensively by Müllen and his co-workers. As we can known, HBCs are particularly promising for not only their large aromatic cores permit one of the highest values for the intrinsic charge carrier mobility.

Herein, we will detail the first study of the self-assembly and electronic properties of a new type of hexabenzocoronene whose aromatic core is distorted away from planarity by steric congestion in its proximal carbon atoms. These compounds will exhibit helical molecular structures (Figure 1). The helical configuration should lead to complementary intermolecular stacking. Powder X-ray diffraction these compounds will provide information about the detailed molecular packing patterns. Furthermore, X-ray diffractions will also disclose the inter- and intra-columnar structures. The resulting closer molecular packing will provide higher charge carrier mobilities. Moreover, These HBC's derivatives should pack into chiral columns.

The mesogenic properties of compounds **1** was studied using differential scanning calorimetry (DSC) and polarized optical microscopy (POM). In the lower temperature regime, a columnar liquid crystalline phase was temporarily assigned based on its fan-shaped texture. (Fig. 1) . In order to detail the structural information of the hexabenzocoronenes, powder X-ray diffractions (XRD) were performed. At this stage, the XRD of compound **1** was investigated. The columnar phase was explored by XRD. As showin Fig 2, one 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 small angle signal is indexed to the 200 reflection of a rectangular columnar arrangement. The calculated d-spacing is 23.8 Å respectively. The two halos in the wide angle region correspond to 4.8 and 3.6 Å. 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.

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.

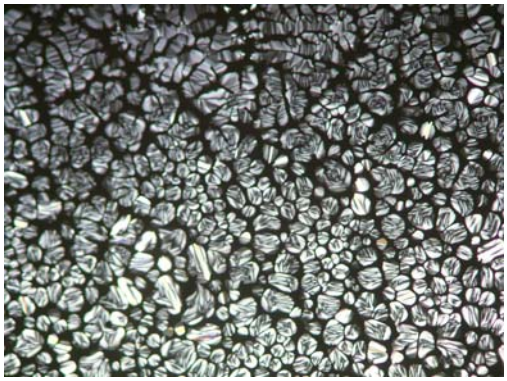

Figure 1. Optical texture of compound **1** in the columnar mesophase temperature range.

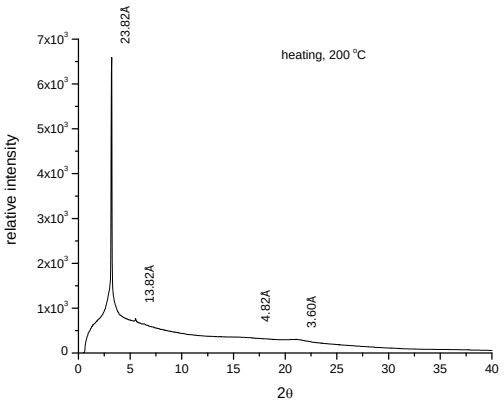

Figure 2. XRD pattern for compound **1** in its liquid crystalline temperature range.