Powder X-ray Diffraction Study of Dimeric Discotic Liquid Crystals

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Discotic liquid crystal usually self-assemble into columnar structure, which possess one dimensional charge mobility and can be good candidate for the optical device, such as light emitting diodes, field effect transistors and solar cells. Nevertheless, the long-range ordered superstructure often exists only in mesophase. Behind the mesophase, the stacking gradually becomes disorder unless forms the glassyl material, which the whole structure including flexible side chain was frozen into qusi-solid during supercooling process. Moreover, low molar mass glassyl molecule are well-known for more clear optical property and eaiser prosess in application.

$$C_6H_{13}O$$
 OC_6H_{13} OC_6H_{13}

HDBP(6,12,6): $R_1 = C_6 H_{13}$, $R_2 = C_{12} H_{24}$

Scheme 1: The synthesis of hexaalkoxydibenzo[a,c]phenazines **HDBP(6,12,6)**

X-ray diffraction

X-ray diffraction studies of **HDBP(6,12,6)**, confirmed their columnar hexagonal mesophase assignment made by POM. The lattice constant, discdisc intramolecular distant and alkyl halo from the XRD provided further informations on the packing of the discogens within the mesophase (Table 1). The synthesized discogens showed a disc-discintramolecular distant of around 3.50 Å. Further, **HDBP**(6,12,6) have a calculated lattice constants of 21.99Å at colh. Thus, the rectangular lattice parameter could be also calculated to a = 34.44 Å and b = 23.06Å. Unfortunately, the other high order reflections do not appear so that it is difficult to assign the 2D rectangular symmetry. Moreover, The transformation between the hexagonal structure and the rectangular structure was depicted in the Fig. 1.

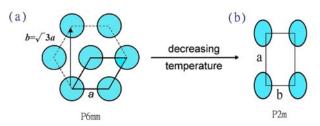


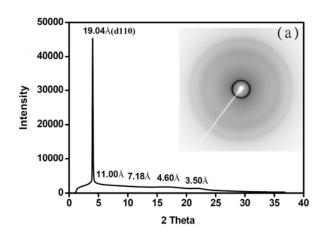
Fig. 1: Figure shows the relation between pesudohexagonal (a) and rectangular structure (b) with decreasing temperature.

In summary, a series of novel dimmers based on dibenzo[a,c]phenazine discogen have successfully been synthesized. **HDBP**(6,12,6) possessed glassy state while

Table 1:
Variable-Temperature
XRD
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compd.	temp.(⁰ C)	d-spacing(A)	Miller indices(hkl)	lattice constants(A)
HDBP(6,12,6)	120	19.04	(100)	a=21.99
		11.00	(110)	
		7.18	(210)	
		4.60	alkyl halo	
		3.50	core-core	
	30	19.16	(110)	a=34.44
		17.22	(200)	b=23.06
		4.50	alkyl halo	
		3.53	core-core	



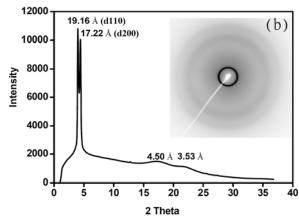


Fig. 2: Powder X-ray diffractogram of **HDBP**(6,12,6) at (a) Colho phase at 120 °C (b) Colro phase at room temperature, (c) after four months, it still remains liquid crystalline. supercooling process, which would be good candidates for optical device. These thermal properties of new dimmers with dipolar moment in centre core also can provide the scientist more insight into dimmeric liquid crystal system.