

## Unsymmetrically substituted perylene bisimides exhibiting liquid crystalline and self-assembly properties

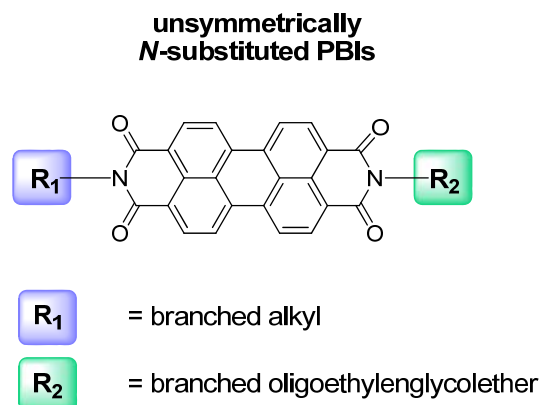
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**Abstract:** Perylene bisimide (“perylene-tetracarboxydiimide”, PBI) derivatives represent an important class of n-type semiconductor materials exhibiting a relatively high electron affinity among large-band-gap materials. They are promising candidates for application in organic electronic devices. The solid-state packing of the perylene bisimide derivatives plays a major role in improving the device performance. For instance an increase in exciton diffusion length and an improvement in charge carrier mobility can be achieved by increased ordering of perylene molecules. Inducing liquid crystallinity is an elegant way of improving organization because it promotes  $\pi$ - $\pi$  stacking, allows for dynamic reorganization, and facilitates the processing of thin films, which is not feasible with organic single crystals or insoluble compounds. We recently synthesized highly soluble, unsymmetrically *N*-substituted perylene bisimide derivatives bearing branched alkyl chains and branched oligoethyleneglycol ethers (Figure 1).

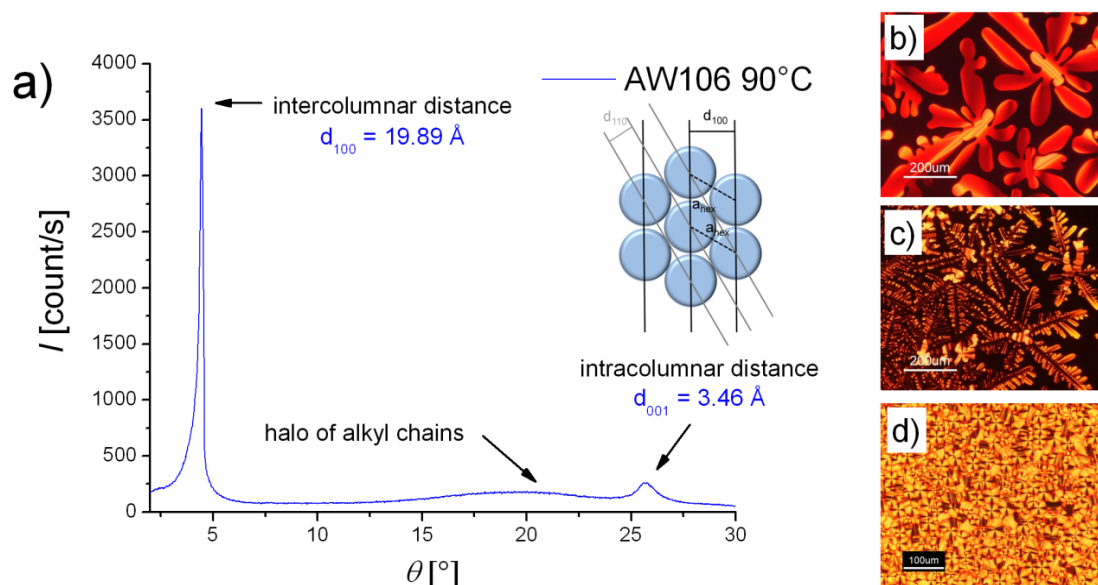


**Figure 1.** Schematic representation of chemical structure of unsymmetrically *N*-substituted perylene bisimides

Thermotropic behavior of PBIs was studied by differential scanning calorimetry. The respective PBIs show hexagonally ordered columnar mesophases (Col<sub>h</sub>) in a wide temperature range, dependent on the size of the *N*-substituents (Table 1). The molecular order within observed columnar hexagonal mesophases was determined by a combination of polarization microscopy and X-ray diffraction experiments (Figure 2). Detailed studies of charge transport and charge transfer in combination with suitable electron donor molecules is currently underway. The synthesis, characterization and liquid crystalline properties will be the content of this presentation.

**Table 1.** Thermal behavior of selected PBIs as investigated by differential scanning calorimetry, phase transition temperatures with corresponding transitions enthalpies of selected PBIs.

PBI	M g mol <sup>-1</sup>	T <sub>dec</sub> °C	T / ΔH °C / kJmol <sup>-1</sup>
1	991.3	323.1	Cr 51.0 (10.7) → LC <sub>1</sub> 63.2 (0.24) → LC <sub>2</sub> 107.7 (3.0) → I I 105.0 (-2.9) → LC <sub>2</sub> 58.7 (-0.23) → LC <sub>1</sub> 23.5 (-7.6) → Cr
2	947.0	323.5	26.6 br (-4.2) → Cr 78.2 (15.8) → LC 145.8 (3.5) I I 141.7 (-3.3) → LC 39.8 (-1.8) → Cr 21.9 (-3.7) → Cr
3	879.1	looki	K 77.6 (16.8) → LC 154.4 (3.6) → I I 146.1 (-3.8) → LC



**Figur**

**e 2.** a) X-ray diffraction of Col<sub>ho</sub> perylene bisimide AW106 in the mesophase (90 °C). The inset shows the columnar hexagonal packing parameters. b-d) Optical microscopic images of the hexagonal columnar mesophase Col<sub>ho</sub> textures (crossed polarizers) of different PBIs showing dendritic growth aggregates and spherulitic-like texture with maltese crosses.

#### References:

1. André Wicklein, Suhrit Ghosh, Michael Sommer, Frank Würthner and Mukundan Thelakkat

Self-Assembly of Semiconductor Organogelator for Nanostructured Organic Bulk Heterojunction

Chem. Mater. 2008 Submitted

2. André Wicklein, and Mukundan Thelakkat

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