

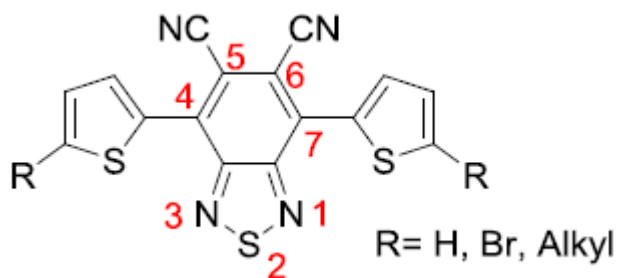
Liquid Crystals of Hexasubstituted Benzenes bearing ultra strong dipole moments

T. Nevolianis^{1*}, J. Wudarczyk², K. Müllen², G. Papamokos¹, G. Floudas¹

¹Department of Physics, University of Ioannina, P.O. Box 1186, 45110, Ioannina, Greece

²Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Hexasubstituted benzenes bearing dipole moments exceeding 10 debye have been recently reported in the literature via functionalization of diaminophthalonitrile to its brominated and tetracyanated derivatives.[1] By their transformation into dithienyl derivatives (4,7-di(thiophen-2-yl)benzo[c]-[1,2,5]thiadiazole-5,6-dicarbonitrile – Figure 1) the cyano groups further increase the electron-withdrawing ability of the acceptor. In this work we study three rod-like liquid crystals (Fig. 1, R=C₆H₁₃, C₁₆H₃₃ and R=C₆H₁₃ with hydrogens at positions 5 and 6 instead of the CN) bearing strong dipole moments perpendicularly to the molecular axes. We investigated them by means of X-ray diffraction (XRD) and Polarizing Optical Microscopy (POM) to determine the unit cell structure and liquid crystalline textures respectively. Differential Scanning Calorimetry (DSC) and Dielectric Spectroscopy (DS) were employed to identify phase transitions from the heat of fusion and temperature dependence of the dielectric permittivity, respectively. For the monomers carrying either CN groups or hydrogens at positions 5 and 6 and for R=H, C₆H₁₃, C₁₆H₃₃, the energetics and their dipole moments, total molecular polarizabilities (α), and first order hyperpolarizabilities (β) are reported via state of the art DFT calculations. Such molecules may lead to enhanced charge separation efficiency by decreasing the exciton binding energy and thus become potentially applicable to organic photovoltaics. [2]



[1] J. Wudarczyk, G. Papamokos, V. Margaritis, D. Schollmeyer, F. Hinkel, M. Baumgarten, G. Floudas and K. Müllen *Ang. Chem. Int. Ed.* **2016**, 55, 3220-3223.

[2] N. Camaioni, R. Po, *J. Phys. Chem. Lett.* **2013**, 11, 1821-1828.