X-shaped bolapolyphiles combining benzothiadiazole with fluorinated aromatics for organic semiconductors

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Liquid crystal molecules gained a lot of attention for semiconductors due to their special properties such as self-organization and high charge carrier mobility. Especially molecules with benzothiadiazole (BT) have shown its high potential characteristics as an excellent acceptor [1] and fluorination of aromatic groups lead to lower HOMO-LUMO gaps [2]. Furthermore, liquid crystals forming nano-segregated columnar phases such as X-shaped molecules [3] can form well-ordered donor-acceptor system due to its driving forces from amphiphilicity, which is critical for semiconductor applications [4].

Herein we designed and synthesized new X-shaped molecules based on BT unit. These compounds were characterized by differential scanning calorimetry, polarizing microscopy and X-ray diffraction. Depending on the chain length and temperature, different phases were observed. Compounds with short branched chains show a hexagonal columnar phase (Col_{hex}/*p6mm)* with triangular honeycomb structure. The shortest derivative with linear chains exhibits a rectangular columnar phase (Col_{rec}/*c2mm*) and on increasing the chain length and volume by using branched chains, square columnar phases (Col_{squ}/*p4mm*) replace Col_{hex}/*p6mm*. Due to the importance of aromatic fluorination and BT unit in lowering HOMO-LUMO gap values, UV-vis and fluorescence spectra were conducted for a selected sample. The result was compared to parent compounds without fluorinated aromatics and BT unit. The result shows that both, fluorination of aromatic groups and BT units, have the effect of lowering the HOMO-LUMO gap.

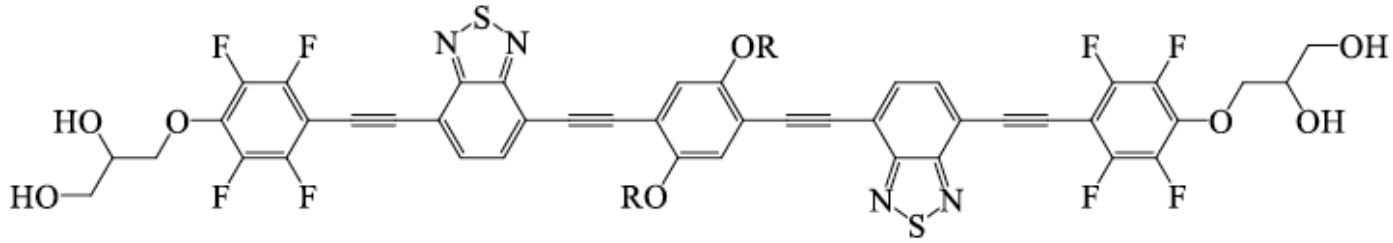

Figure 1. Molecular structure of the reported X-shaped molecules with BT and fluorinated aromatic units (R = linear or branched alkyl chains)

Reference

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