

Supplementary Information for

Synthesis and Helical Supramolecular Organization of Discotic Liquid Crystalline Dibenzo[*hi, st*]ovalene

Qiang Chen,^{#a} Wojciech Zajaczkowski,^{#a} Johannes Seibel,^{#b} Steven De Feyter,^b
Wojciech Pisula,^{*ac} Klaus Müllen,^{*ad} and Akimitsu Narita^{*ae}

^aMax Planck Institute for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany

^bKU Leuven, Department of Chemistry, Division of Molecular Imaging and Photonics,
Celestijnenlaan 200F, 3001 Leuven, Belgium

^cLodz University of Technology, Department of Molecular Physics, Faculty of
Chemistry, Zeromskiego 116, 90-924, Lodz, Poland

^dInstitute of Physical Chemistry, Johannes Gutenberg-University, Duesbergweg 10-14,
55128, Mainz, Germany

^eOrganic and Carbon Nanomaterials Unit, Okinawa Institute of Science and
Technology Graduate University, Okinawa 904-0495, Japan

Correspondence and requests for materials should be addressed to K. Müllen (email: muellen@mpip-mainz.mpg.de) or to A. Narita (email: narita@mpip-mainz.mpg.de)

Table of Content

| | |
|--|----|
| Supplementary Figures and Tables | S3 |
| Additional STM Images | S4 |
| NMR and Mass Spectra..... | S6 |

Supplementary Figures and Tables

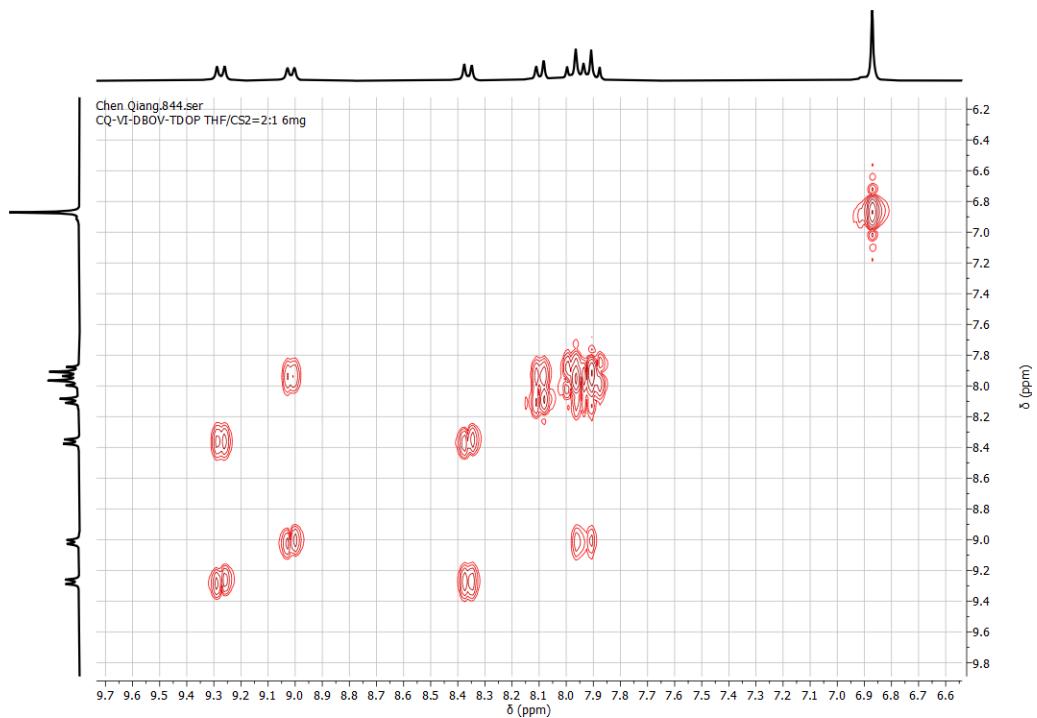


Figure S1. ^1H , ^1H -COSY spectra of DBOV-TDOP in $[\text{D}_8]\text{THF:CS}_2 = 2:1$ (300 MHz, 298K).

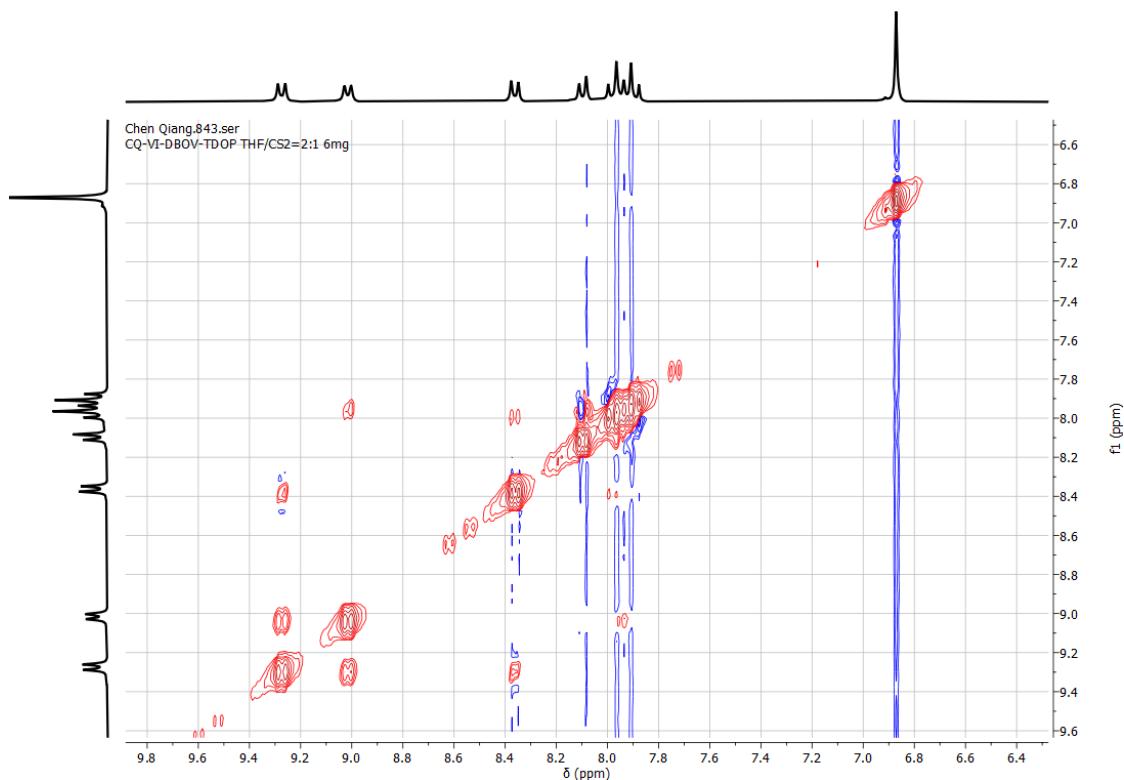


Figure S2. ^1H , ^1H -NOESY spectrum of DBOV-TDOP in $[\text{D}_8]\text{THF:CS}_2 = 2:1$ (300 MHz, 298K).

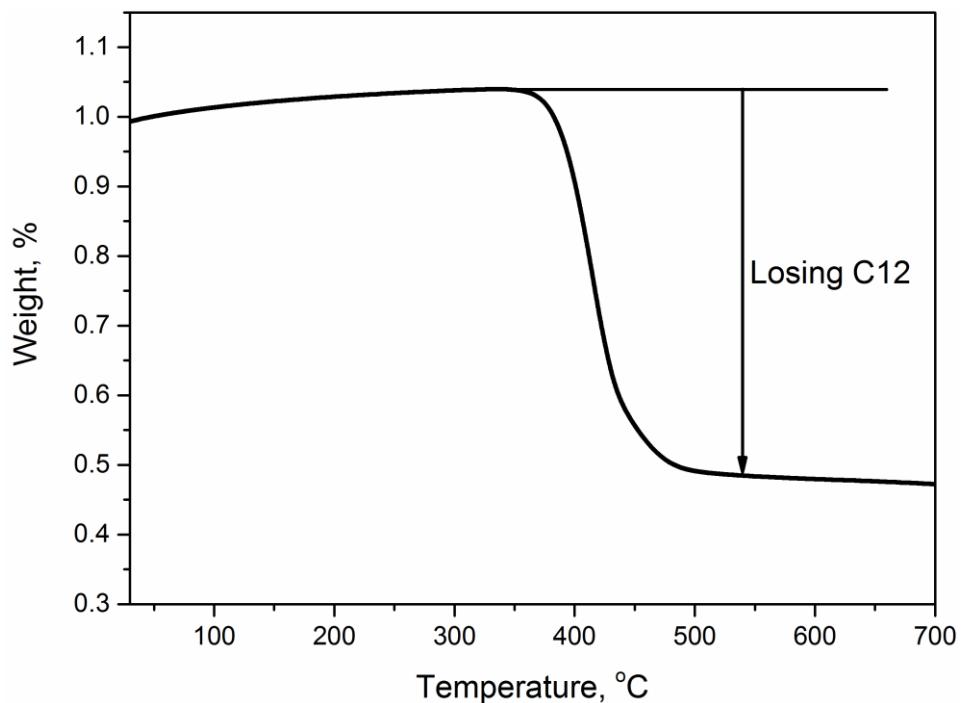


Figure S3. Thermogravimetric analysis (TGA) spectrum of **DBOV-TDOP**.

Additional STM Images

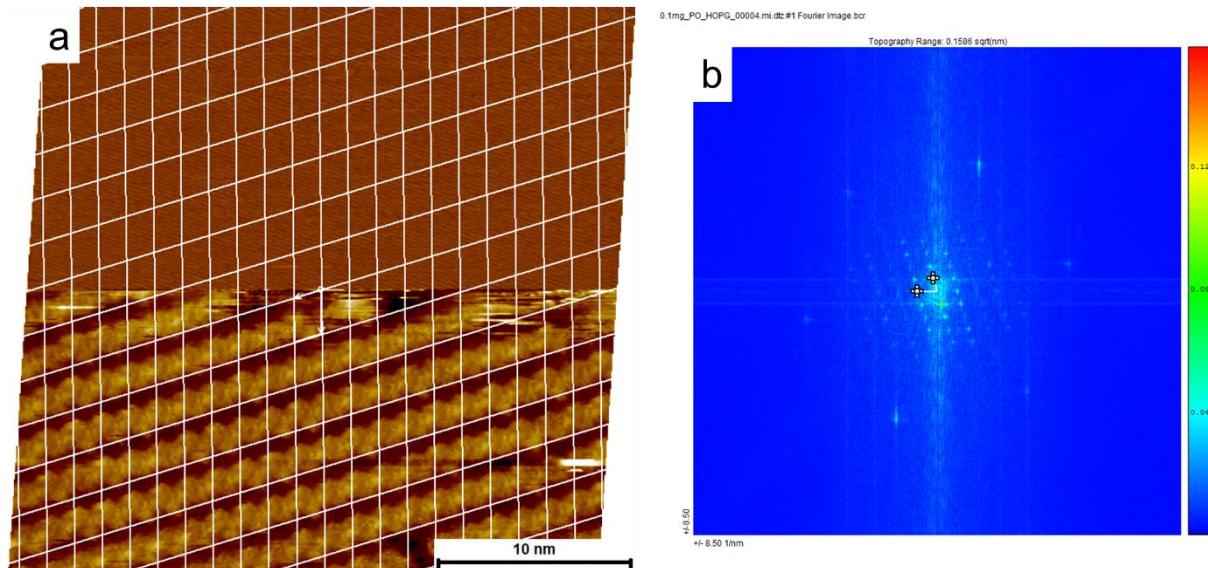


Figure S4. Example for the drift correction and unit cell determination. In the top half of a the HOPG surface lattice is imaged ($V_{\text{bias}} = -0.001$ V, $I_{\text{set}} = 1.0$ nA) and in the bottom part the molecular layer ($V_{\text{bias}} = -1.1$ V, $I_{\text{set}} = 70$ pA). The HOPG is used to correct for drift and the Fast-Fourier Transform (b) to determine the unit cell in the corrected image.

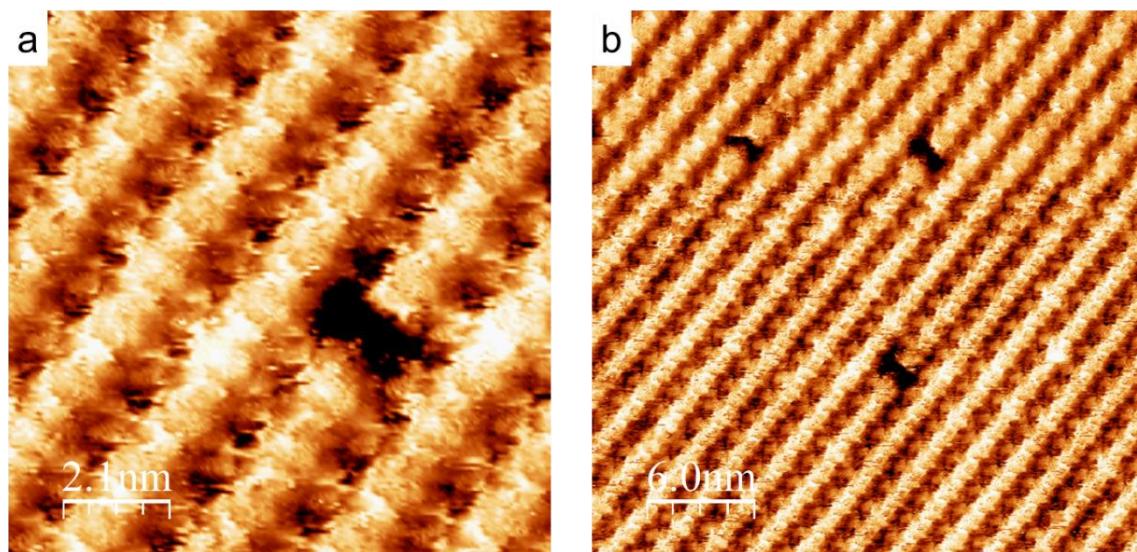


Figure S5. Additional STM images illustrating the molecular assembly in the second layer structure through single-molecules defects. Imaging parameters: a) $V_{\text{bias}} = -1.1$ V, $I_{\text{set}} = 80$ pA, b) $V_{\text{bias}} = -1.1$ V, $I_{\text{set}} = 80$ pA.

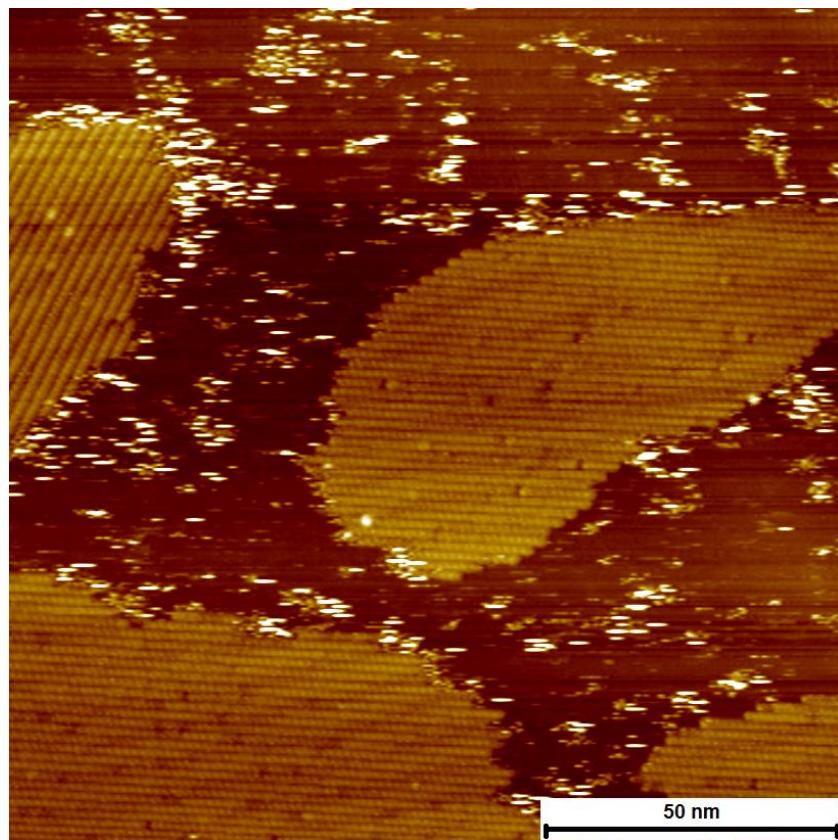


Figure S6. Additional STM image showing the increase in non-covered areas at lower concentrations ($c = 6 \times 10^{-6}$ mol/L). Imaging parameters: $V_{\text{bias}} = -1.1$ V, $I_{\text{set}} = 80$ pA.

NMR and Mass Spectra

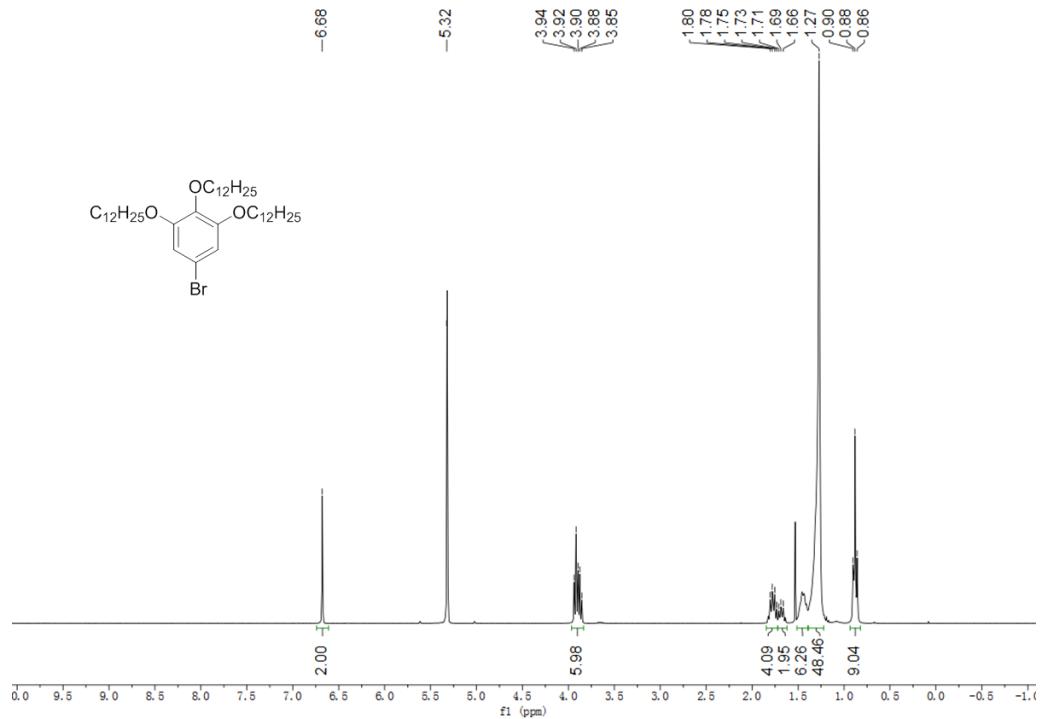


Figure S7. ¹H NMR spectrum of compound S-6 in CD₂Cl₂ (300 MHz, 298 K).

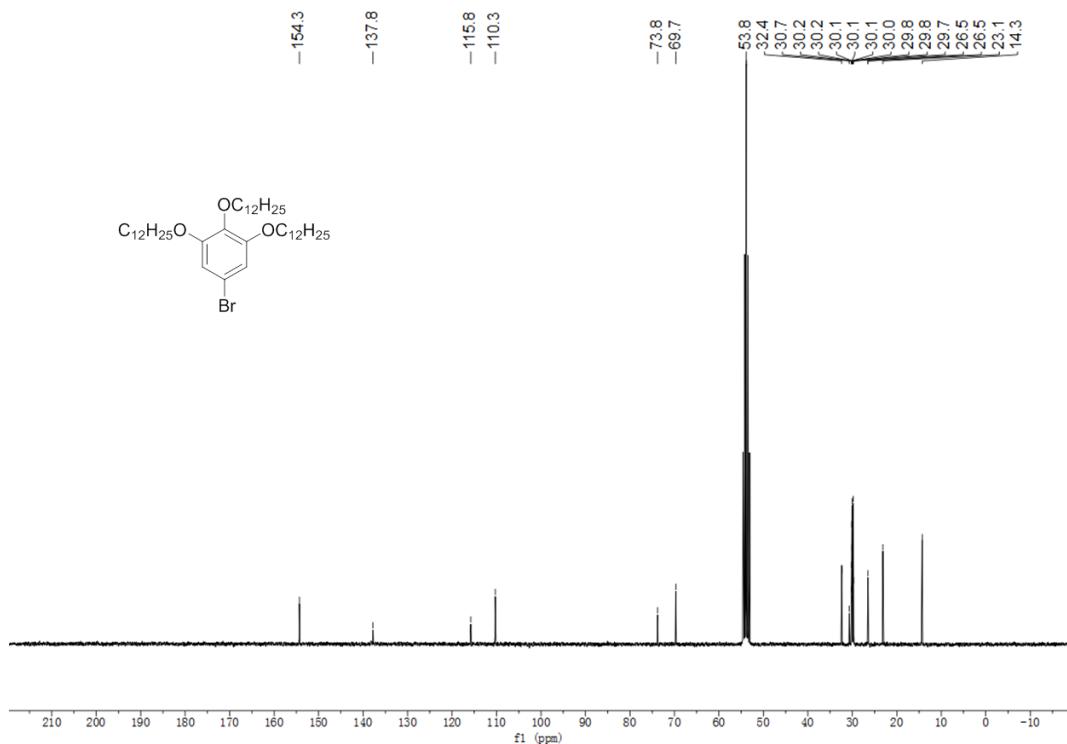


Figure S8. ¹³C NMR spectrum of compound S-6 in CD₂Cl₂ (75 MHz, 298 K).

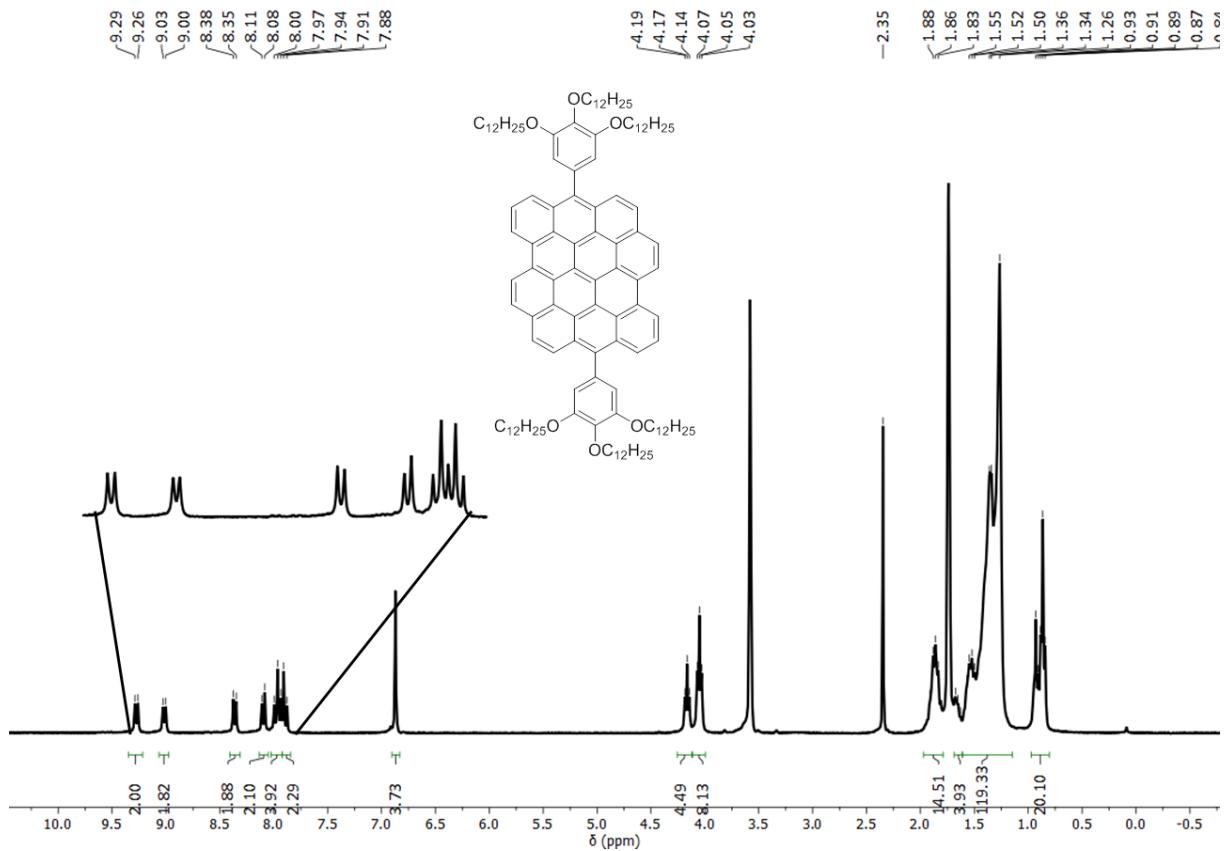


Figure S9. ^1H NMR spectrum of compound **DBOV-TDOP** in $\text{THF}-d_8:\text{CS}_2 = 1:1$ (300 MHz, 298 K).

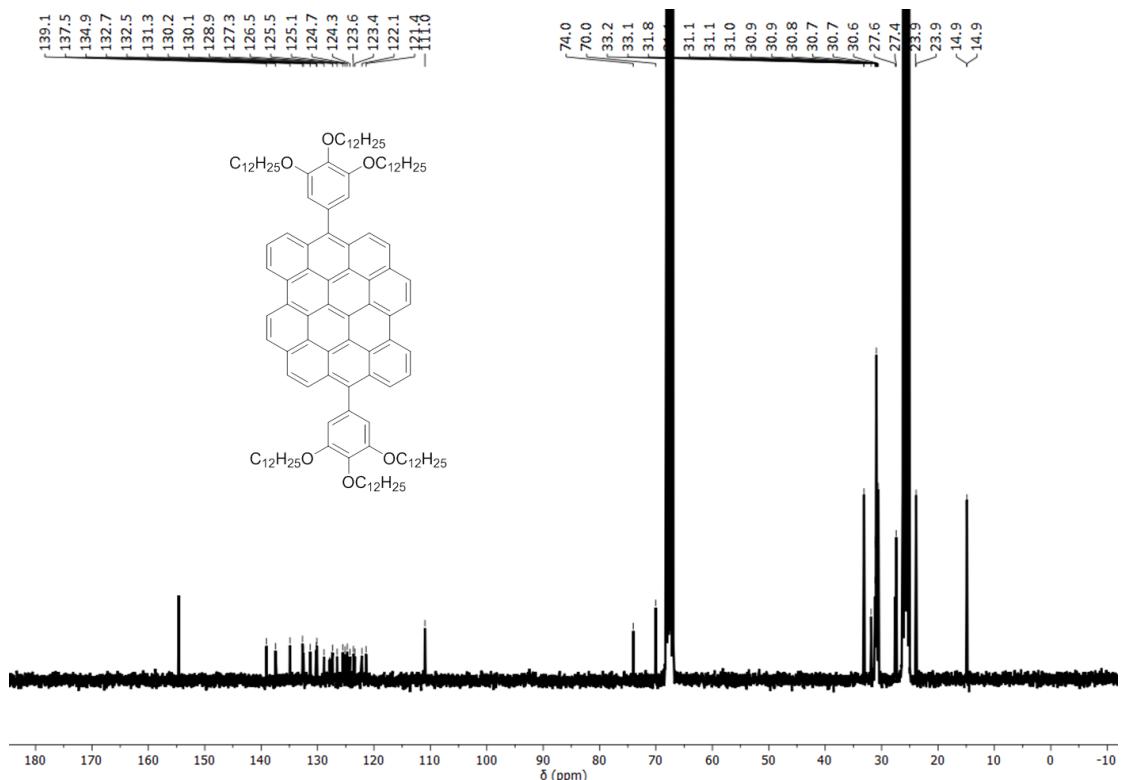


Figure S10. ^{13}C NMR spectrum of compound **DBOV-TDOP** in $\text{THF}-d_8:\text{CS}_2 = 1:1$ (75 MHz, 298 K).