

Supplemental Information

Synthesis and Physical Properties of Brominated Hexacene and Hole Transfer Property of Thin-film Transistor

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Physical property at solution state

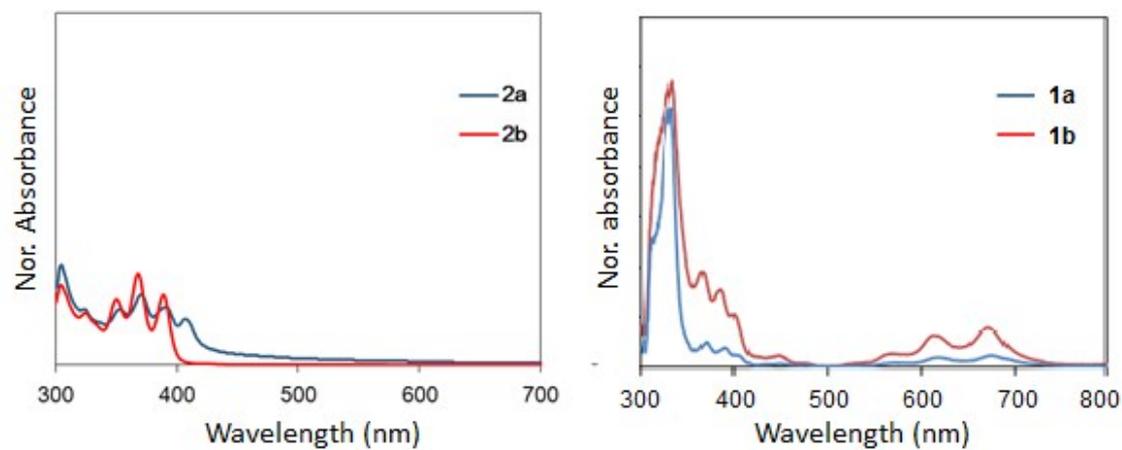


Figure S1. Absorption spectra of (left) **2a** and **2b** in 1,2,4-trichlorobenzene, and (right) after heated at 230 °C for **1a** and **1b**. Note that spectra of **1a** and **1b** should contain some decomposed species such dimerization.

DFT results

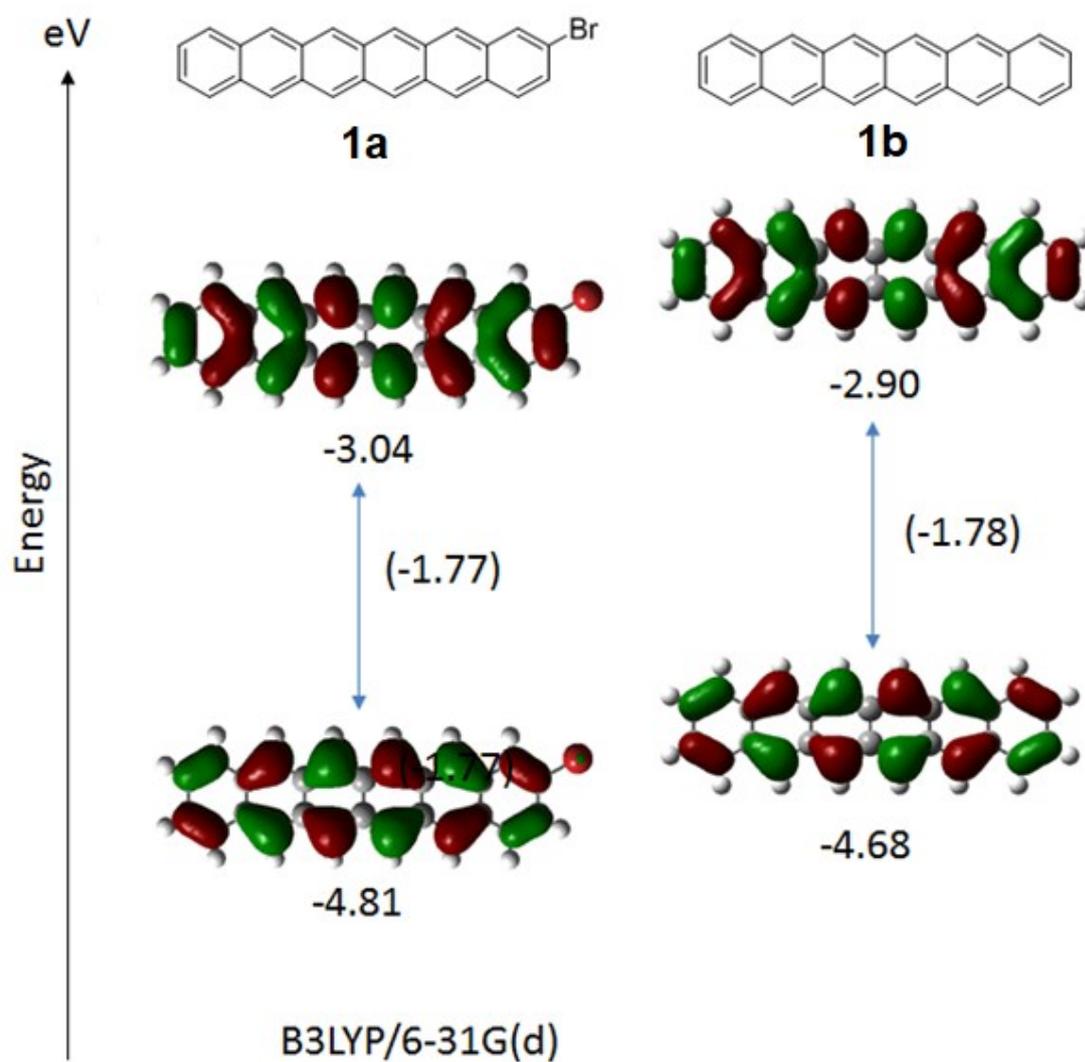


Figure S2. Energy diagram of **1a** and **1b**. The energy was estimated by B3LYP/6-31G(g) level.

Physical property at film state

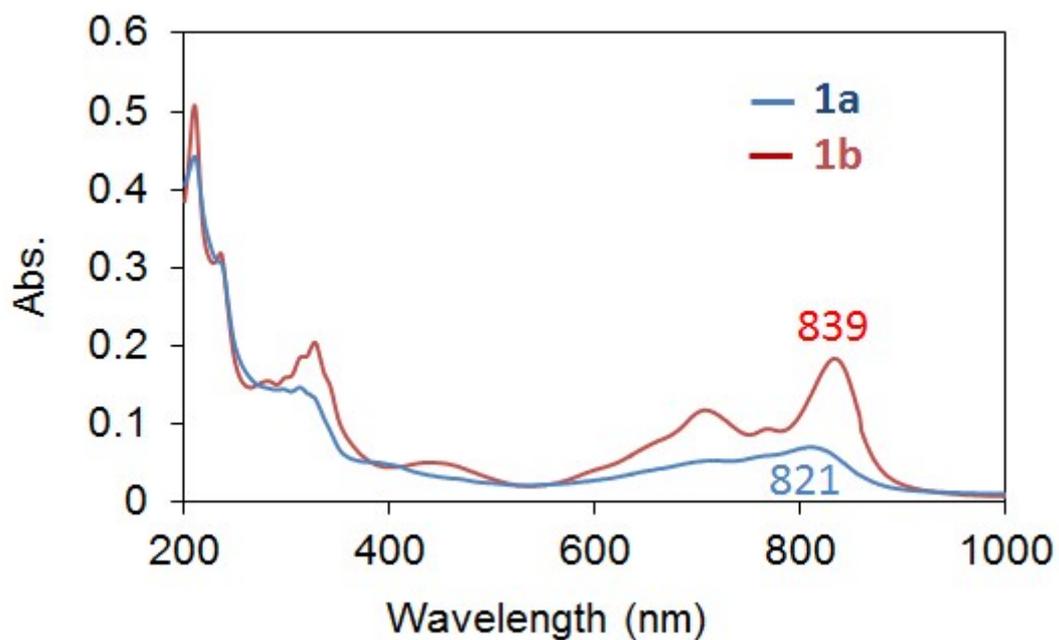


Figure S3. Absorption spectra of vacuum deposited film **1a** and **1b** on quartz plate.

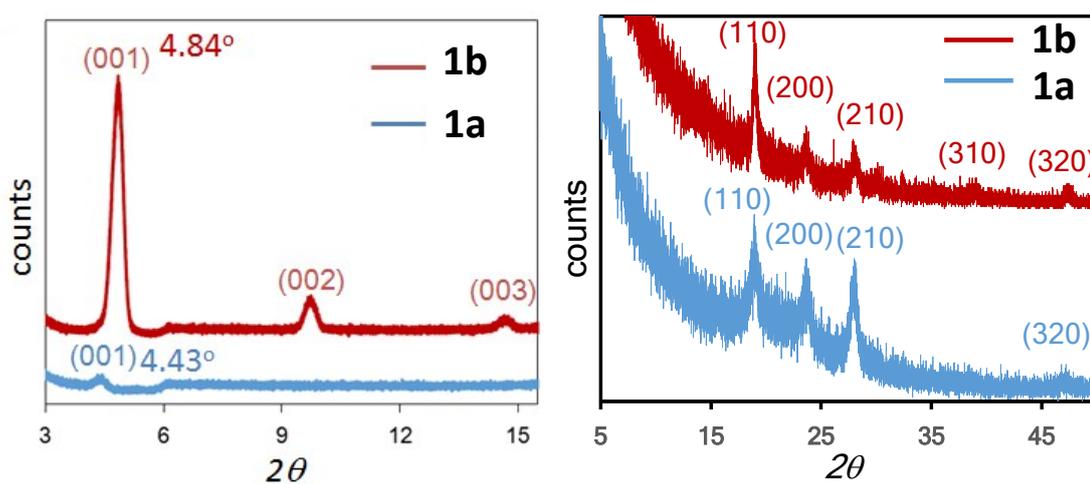


Figure S4. XRD (left: out-of-plane, right: in-plane) results of films **1a** and **1b**.

NMR spectra

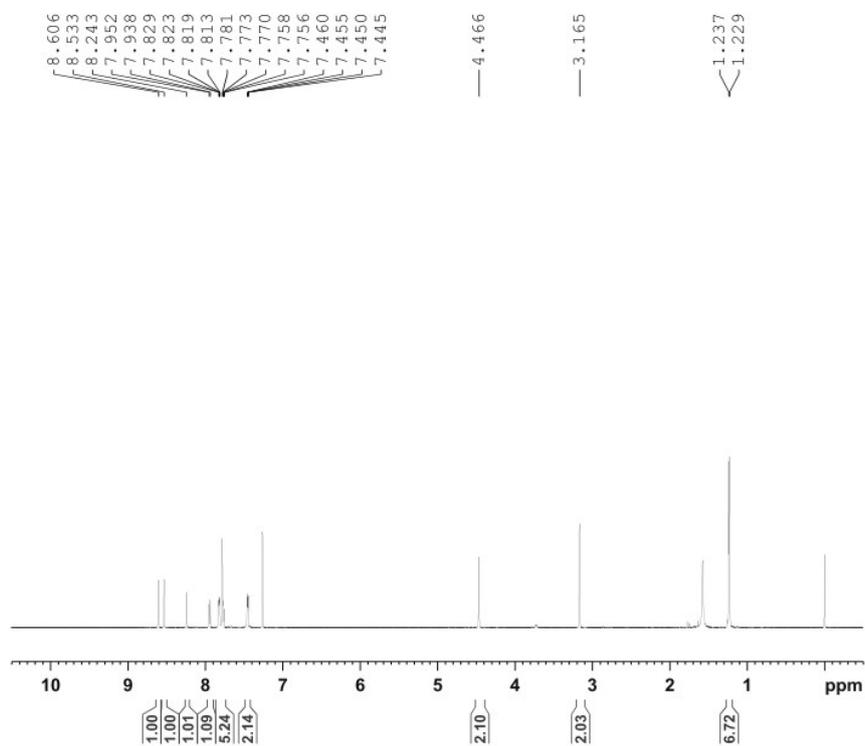


Fig S5. ¹H NMR spectra of **8** (600 MHz).

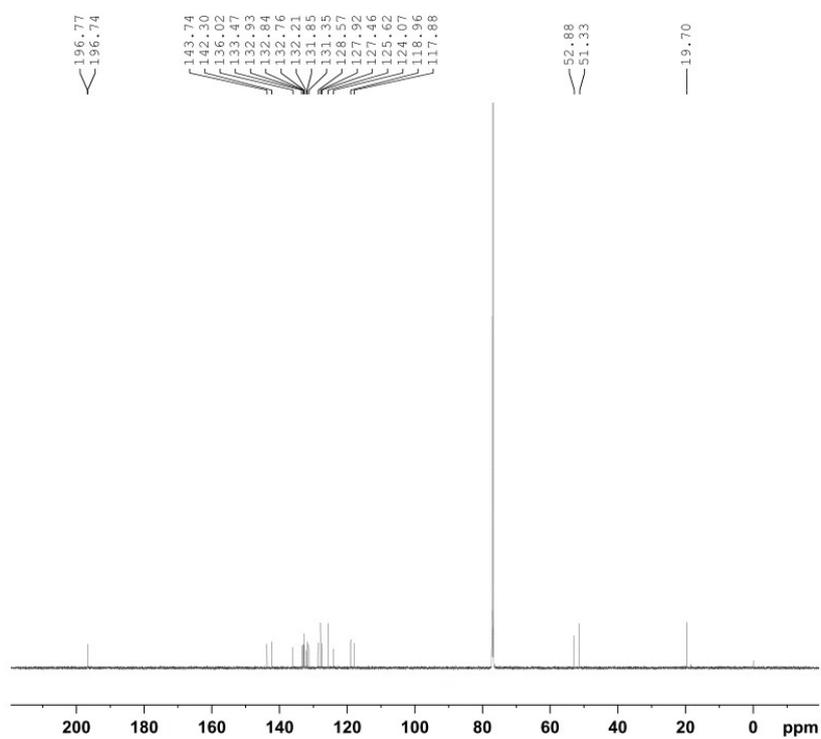


Fig S6. ^{13}C NMR spectra of **8** (125 MHz).

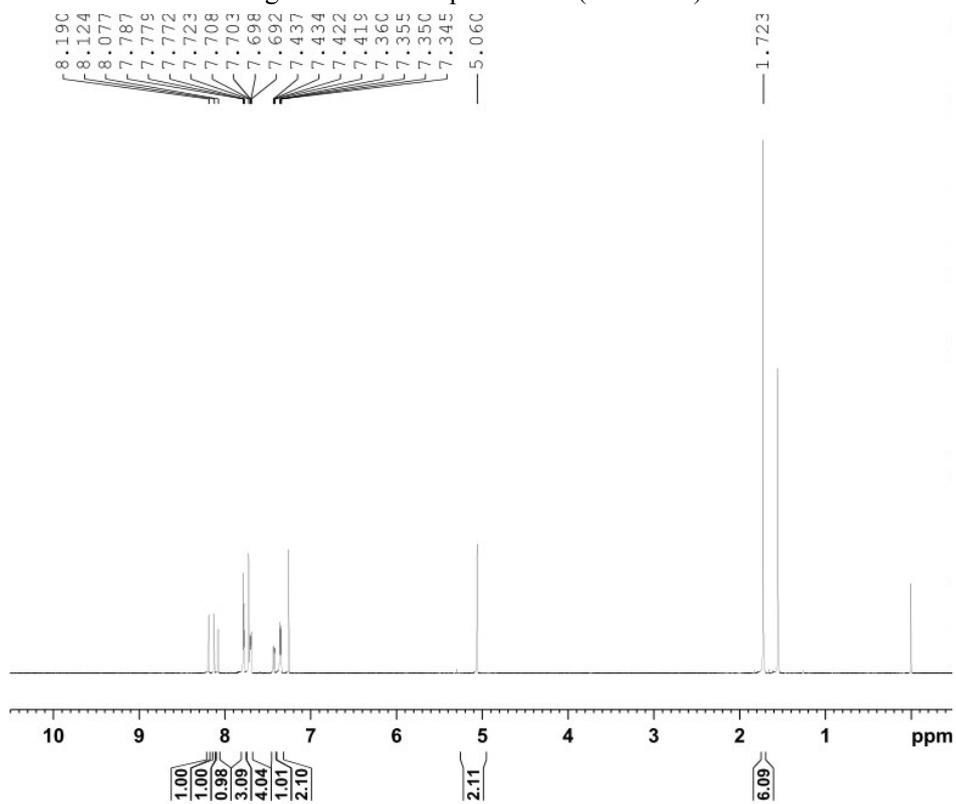


Fig S7. ^{13}C NMR spectra of **9** (600 MHz).

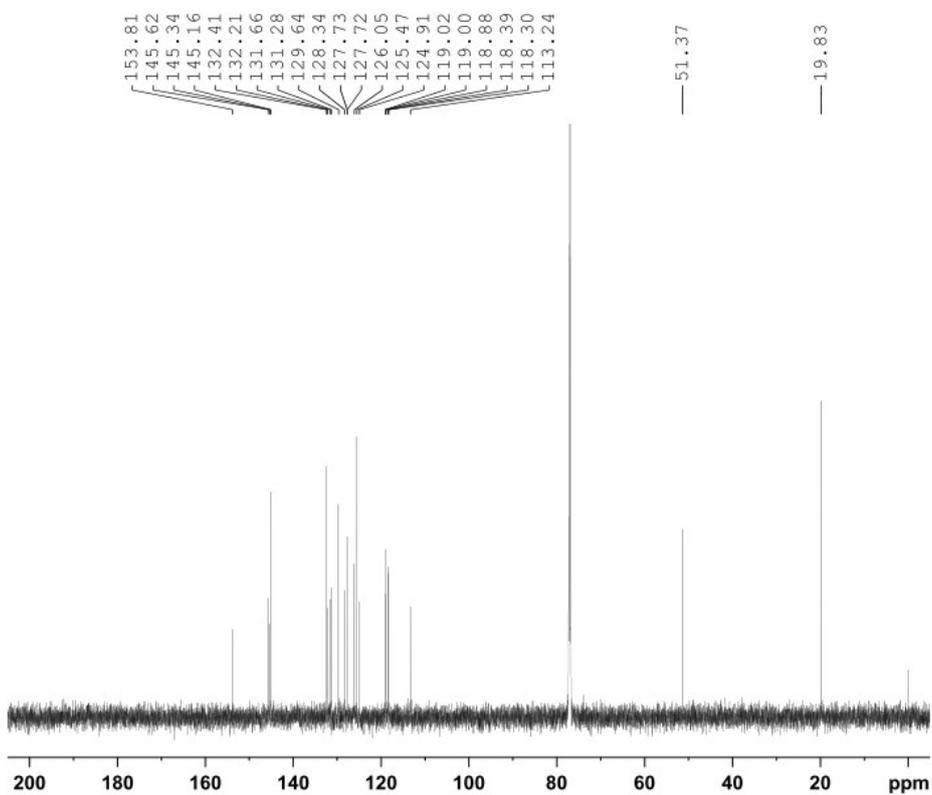


Fig S8. ^{13}C NMR spectra of **9** (125 MHz).

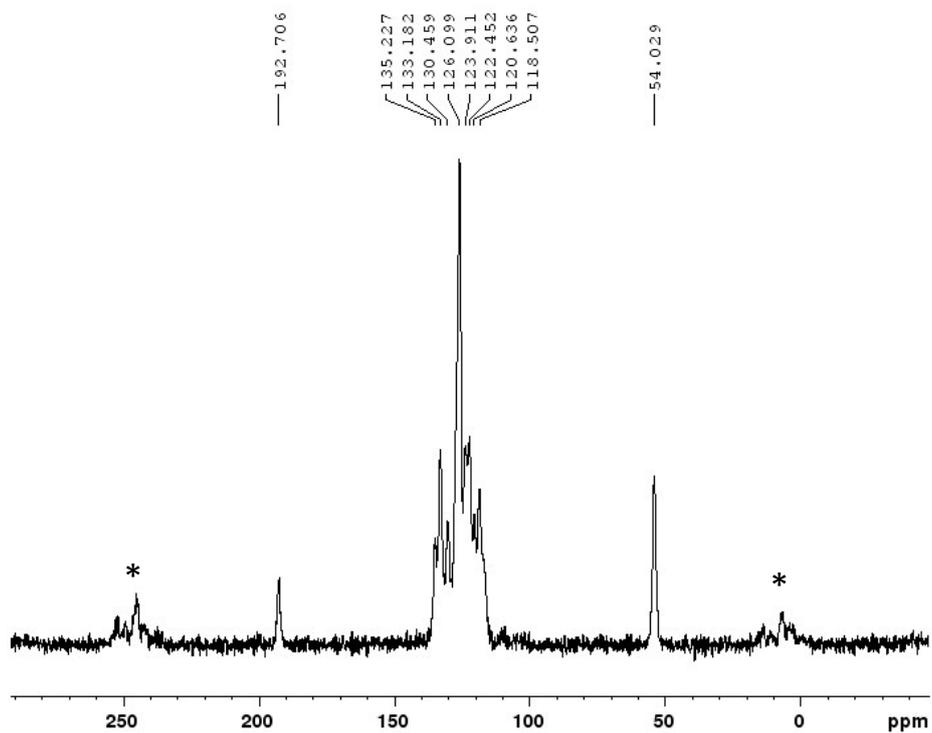


Fig S9. ^{13}C CP/MS NMR spectra of **2a** (100 MHz)

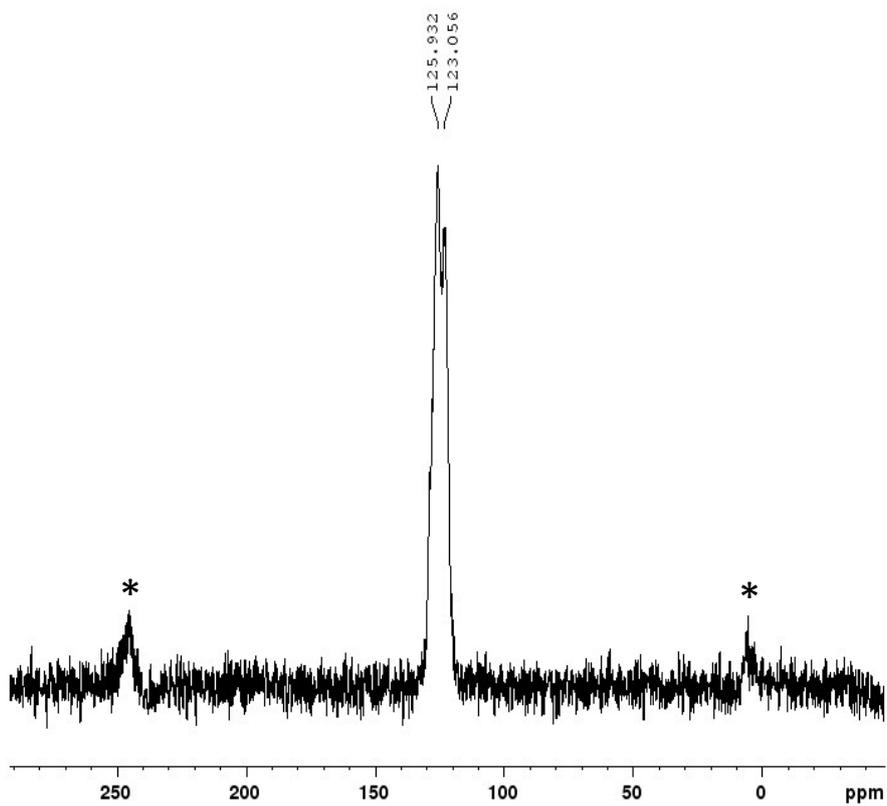


Fig S10. ^{13}C CP/MS NMR spectra of **1a** (100 MHz)