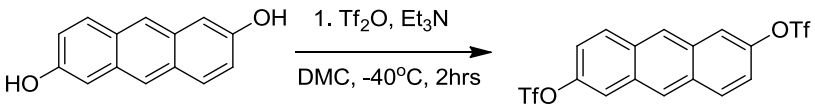
Supporting Information

Oligofuran-Containing Molecules for Organic Electronics

Ori Gidron,[a] Afshin Dadvand,[b] Emily Wei-Hsin Sun,[b] Insik Chung,[b] Linda J. W. Shimon,[c] Michael Bendikov,[a,] and Dmitrii F. Perepichka,[b,]**

[a] Department of Organic Chemistry and [c] Department of Chemical Research Support, Weizmann Institute of Science, Rehovot 76100, Israel and [b] Department of Chemistry and Centre for Self-Assembled Chemical Structures (CSACS), McGill University, Montreal, Canada.

Synthetic Procedure



2,6-bis(trifluoromethanesulfonyloxy)anthracene (**3**) The synthetic procedure is similar to that previously reported.[1] To 50 mL two neck round bottom flask fitted with magnetic bar, thermometer and nitrogen inlet was added 2,6-dihydroxyanthracene (0.13 g, 0.62 mmol), dry dichloromethane (10 mL) and triethylamine (0.59 g, 5.86 mmol). After cooling down to –40°C (acetonitrile/dry ice), triflic anhydride (0.44 g, 1.56 mmol) was slowly added dropwise via syringe. The reaction mixture was stirred for 2 hours at –40°C and the cooling bath was removed to allow warming up to room temperature. Dichloromethane (20 mL) was added and the resulted solution was washed with water (50 mL). The organic layer was separated, dried over $MgSO_4$ and the evaporated under reduced pressure to afford brownish solid. The crude product was purified by column chromatography (silica, hexane/EtOAc) to afford white solid (0.29 g, 85 %). Spectroscopic data are in good agreement with literature data. (Mery,S.; Haristoy, D.; Nicoud, J.-F.; Guillon, D.; Monobeb, H.; Shimizub, Y. *J. Mater. Chem.* **2003**, 13, 1622–1630).

X-ray structural analysis of DHS-2F (CCDC reference number 905238). Compound **DHS-2F** was crystallized from hexane to give yellow needles. Crystal data: $C_{36}H_{42}O_2$, 0.24 × 0.02 × 0.02 mm^3, triclinic, *P1*, a = 5.4160(4)Å, b =

16.0287(12) Å, c = 18.6890(18) Å, α = 155.342(2)° β = 91.826(4)° γ = 94.608(3)° from 9796 reflections, T = 100(2) K, V = 1457.6(2) $Å^3$, Z = 2, Fw = 506.70, Dc = 1.154 $Mg.m^{-3}$, μ = 0.069 mm^{-1}. *Data collection and processing:* Bruker KappaAPEXII diffractometer, MoKα (λ = 0.71073 Å), graphite monochromator, MiraCol optics, $-6 \leq h \leq 6$, $-19 \leq k \leq 19$, $-22 \leq l \leq 22$, 2θmax = 52.22°, frame scan width = 0.5°, scan speed 1.0° per 240 s, typical peak mosaicity 0.6°, 22005 reflections collected, 9796 independent reflections (R-int = 0.035). The data were processed with Bruker Apex2. *Solution and refinement:* Structure solved with Bruker Shelxs. Full matrix least-squares refinement based on F^2 SHELXL-97, 689 parameters with 3 restraints gave final R_1 = 0.0442 (based on F^2) for data with $I > 2\sigma(I)$ and R_1 = 0.0726 on 9796 reflections, goodness-of-fit on F^2 = 1.005, largest electron density peak = 0.181e/$Å^3$ and hole -0.211 e/$Å^3$.

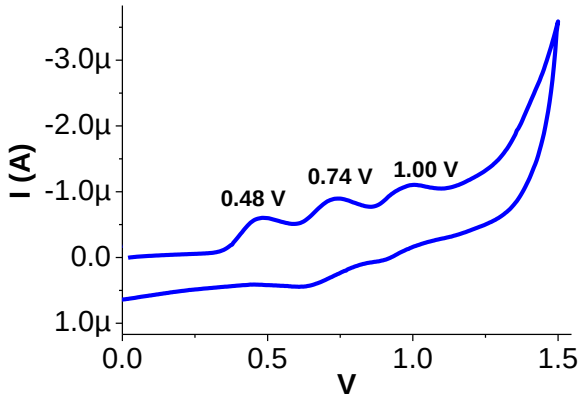


Figure S1. Cyclic voltammogram of **DH2F-Ant** *vs.* SCE in dichloroethane with 0.1M $Bu_4N^+BF_4$, measured at scan rates of 50 mV s^{-1}.

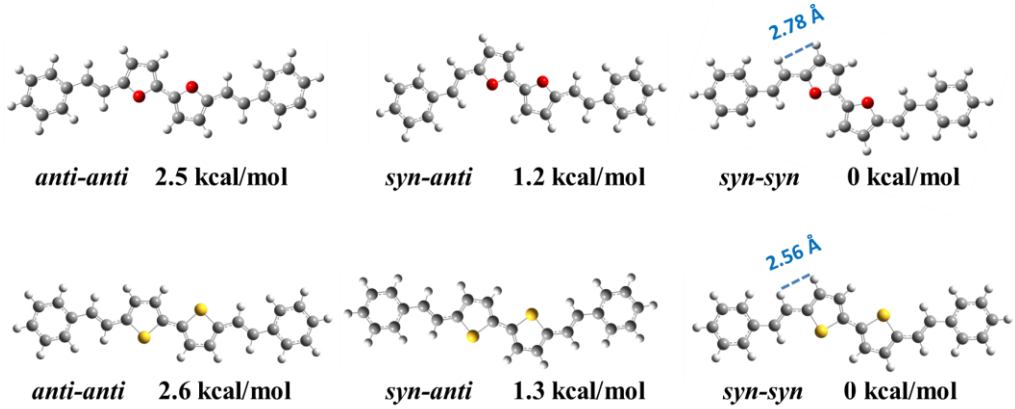


Figure S2. Calculated (B3LY/6-31G(d)) geometries and corresponding energies (in kcal/mol vs. *syn-syn* conformation) of different conformations of **DS-2F** (top) and **DS-2T** (bottom).

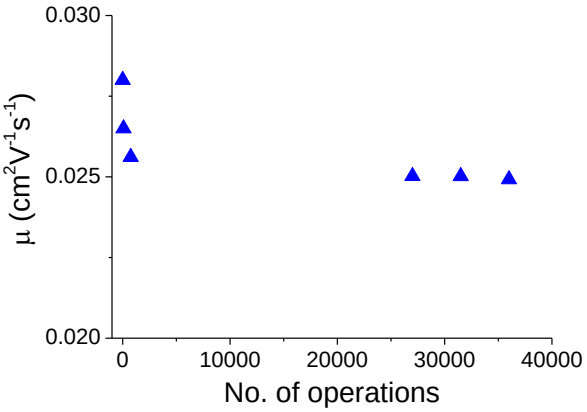


Figure S3. Bias stress measurements of FETs of **DH-7F** on Si/SiO_2/PMMA, (each operation presents a sweep of V_G from 0 to –75 V, keeping V_{DS} = –75 V).

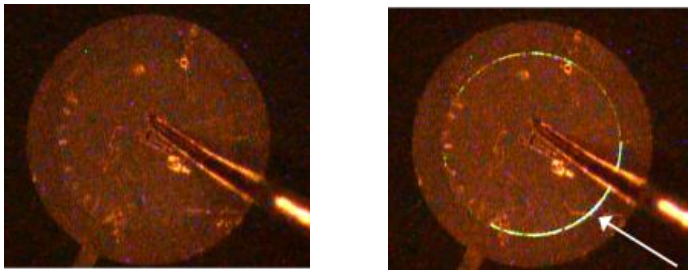


Figure S4. Electroluminescence of a bottom-contact OFET based on **DH-7F** under external illumination. The left image shows the device without applying bias, and the right image shows electroluminescence appearing in the vicinity of the cathode upon biasing of the gated device (indicated by the white arrow).

Table S1. Absolute energies (Hartrees) for calculated structures.

Compound Name	Energy (HF)	Compound Name	Energy (HF)
DS-2F (*syn-syn*)	-1075.80195341	**DS-2T** (*syn-syn*)	-1721.74878460
DS-2F (*syn-anti*)	-1075.79998497	**DS-2T** (*syn-anti*)	-1721.74667006
DS-2F (*anti-anti*)	-1075.79790707	**DS-2T** (*anti-anti*)	-1721.74465133
DS-4F(*anti-anti*)	-1533.47872489	**DS-4T**(*anti-anti*)	-2825.37519366
D2F-Ant	-1454.88441998	**D2T-Ant**	-2746.78687140

1 Y. Goto, K. Nakajima, N. Mizoshita, M. Suda, N. Tanaka, T. Hasegawa, T. Shimada, T. Tani and S. Inagaki, *Microporous Mesoporous Mater.*, 2009, **117**, 535-540.