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The Effect of Hexyl Side Chains on Molecular Conformations, Crystal Packing, and Charge Transport of Oligothiophenes

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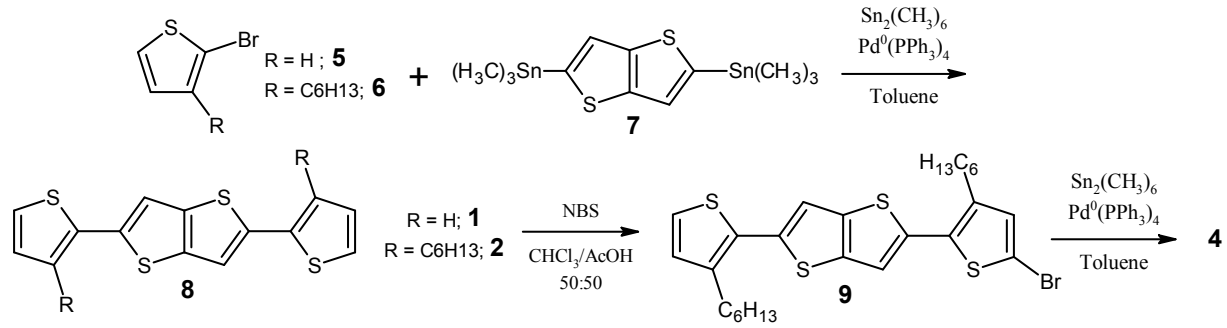
Supporting Information

Contents

Synthesis

Comments:

3-bromothiophene **5**, 2-hexyl-3-bromothiophene **6**, and 2,5-di(trimethyltin)-thieno[3,2-b]thiophene **7** are commercially available. 2,5-Bis-(thiophen-2-yl)thieno[3,2-b]thiophene (**1**) 5-(triisopropylthiophe-2-yl) thieno[3,2-b]thiophene **10** was synthesized according to literature procedure.[1,2] THF was dried over sodium and distilled. Suitable crystals for SCXRD were obtained though slow evaporation from Hexanes.



Scheme S1. Synthesis of **1-H** (**1**), **1-C$_6$** (**2**) and **2-C$_6$** (**4**).

2,5-Bis-(thiophen-2-yl)thieno[3,2-b]thiophene (**1**)[1]

2-bromothiophene (**5**) (0.772 g, 4.74 mmol), 2,5-bis-(trimethyltin)thieno[3,2-b]thiophenes (**7**) (1.03 g, 2.22 mmol), and Tetrakis(triphenylphosphine)palladium(0) (0.124 g, 0.107 mmol) were combined with toluene (100 mL) under N_2. The reaction was stirred and refluxed 15 hrs. After cooling to room temperature, methanol 50 mL was added and the product (**1**) was collected by gravity filtration and recrystallized twice with acetone to yield **1** (0.283 g, 42%) as a yellow-brown powder. Crystals suitable for X-ray analysis were grown in physical vapor transport. ^{1}H NMR shifts available in literature.[1]

2,5-Bis-(3-hexylthiophen-2-yl)thieno[3,2-b]thiophene (**2**)

Follows similar procedure to literature.[1,3,4] 2-bromo-3-hexylthiophene (0.58 g, 2.35 mmol), 2,5-bis-(trimethyltin)thieno[3,2-b]thiophene (0.5 g, 1.07 mmol), and Tetrakis(triphenylphosphine)palladium(0) (0.062 g, 0.0536 mmol) were combined with toluene (100 mL) under N_2. The reaction was stirred and refluxed 15 hrs. Toluene was removed under reduce pressure and hexanes was added. After gravity filtration, the mother liquor was collected and the compound (**2**, yellow solid) was purified by column chromatography on silica gel (hexanes). This yielded **2** (0.26 g, 52%) ^{1}H NMR (500 MHz, $CDCL_3$, δ) 7.26 (s, 2H), 7.24 (d, 2H), 6.99 (d, 2H), 2.83 (t, 4H), 1.71 (m, 4H), 1.42-1.28 (m, 12H), 0.92 (t, 6H)

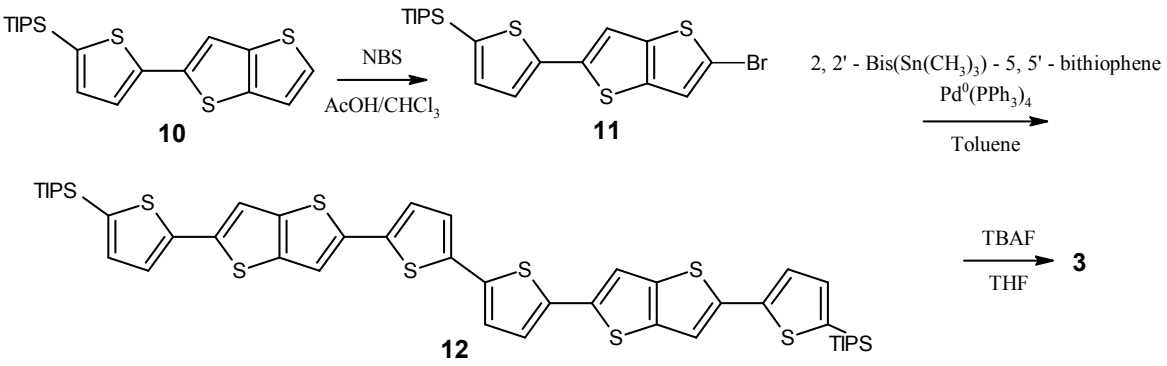
2-(3-hexyl-5-bromothiophen-2-yl)-5-(3-hexylthiophen-2-yl)-thieno[3,2-b]thiophene (**9**)

2 (0.85 g, 1.80 mmol) was added to a stirring mixture of glacial acetic acid and chloroform (100 ml, 50:50. N-bromo-succinimide (0.33 g, 1.85 mmol) was added after **1** completely dissolved. The reaction was left in the absence of light at room temperature under N_2 to react for 15 hrs. To the reaction 100 ml of water was added and the product was extracted with hexanes. The organic layer was reduced under vacuum and the product was purified by column chromatography (hexanes). Since the material elutes close to the di-brominated product and unreacted product, purification was challenging. This yielded **9**

(0.50g, 50%). ^{1}H NMR (500 MHz, $CDCL_3$, δ) 7.23 (s, 1H), 7.22 (d, 1H), 7.19 (s, 1H), 6.98 (d, 1H), 6.93 (s, 1H), 2.80 (t, 2H), 2.74 (t, 2H), 1.63 (m, 4H), 1.42-1.28 (m, 12H), 0.92 (t, 6H)

2,5-Bis-(3-hexylthiophen-2-yl)thieno[3,2-b]thiophene dimer (**4**)

9 (0.50 g, 0.91 mmol), hexamethylditin (0.139 g, 0.425 mmol), and Tetrakis(triphenylphosphine) palladium(0) (0.05 g, 0.0432 mmol) were combined with toluene (100 mL) under N_2. The reaction was stirred and refluxed 15 hrs. Toluene was removed under vacuum and hot hexanes was added. The compound (**4**, orange powder, red crystal) was purified by column chromatography on silica gel (hexanes). This yielded **4** (0.196 g, 45%). ^{1}H NMR (500 MHz, $CDCL_3$, δ) 7.27 (s, 4H), 7.25 (d, 2H), 7.06 (s, 2H), 7.00 (d, 2H), 2.84 (m, 8H), 1.71 (m, 8H), 1.42-1.28 (m, 24H), 0.92 (t, 12H)



Scheme S2. Synthesis of **2-H** (**3**)

2-(5-triisopropylsilyl-thiophen-2-yl)-thieno[3,2-b]thiophene (**10**)

Synthesis of this compound is reported in literature.[2]

2-Bromo-5-(5-triisopropylsilyl-thiophen-2-yl)-thieno[3,2-b]thiophene (**11**)

10 (.20 g, 0.53 mmol) and N-bromo-succinimide (0.096 g, 0.53 mmol) was added to a stirring mixture of glacial acetic acid and chloroform (100 ml, 50:50 by vol). The reaction was left in the absence of light at room temperature under N_2 to react for 15 hrs. To the reaction 100 ml of water was added and the product was extracted with hexanes. The organic layer was reduced under vacuum and the product was purified by column chromatography (hexanes). This yielded **11** (0.2, 81%). ^{1}H NMR (400 MHz, $CDCL_3$, δ) 7.33 (d, 1H), 7.32 (s, 1H), 7.30 (s, 1H), 7.22 (d, 1H), 1.34 (m, 3H), 1.13 (d, 27H)

2,5-bis-(5-triisopropylsilyl-thiophen-2-yl)-thieno[3,2-b]thiophene Dimer (**12**)

11 (.20 g, 0.44 mmol) and 5,5'-bis-(trimethylstanyl)-2,2'-bithiophene and Tetrakis(triphenylphosphine) palladium(0) (0.01 g, 0.008 mmol) were combined with toluene (80 mL) under N_2. The reaction was stirred and refluxed 15 hrs. Product was recovered by precipitation into methanol followed by vacuum filtration. Recrystalized 2x from Toluene gave a red powder. This yielded **12** (0.15 g, 38%). Lack of solubility prevented NMR analysis. Confirmation of product by MALDI-ToF shows the correct 917.8 m/z (expected m/z 919.6).

2,5-Bis-(thiophen-2-yl)thieno[3,2-b]thiophene Dimer (**3**)

Deprotection of **12** (.1 g, 0.11 mmol) was perfomed by tetrabutylamoniumfluoride (8 eqv, 1M in THF) in a refluxing THF solution overnight. The product precipitated out of solution and was collected by vacuum filtration and washed with Hot Toluene and Hot THF. This yielded **3** as a red/orange powder (56 mg, 85%).This product was entirely insoluble except in boiling trichlorobenzene. Confirmation of product by MALDI-ToF shows the correct 605.5 m/z (expected m/z 606.9).

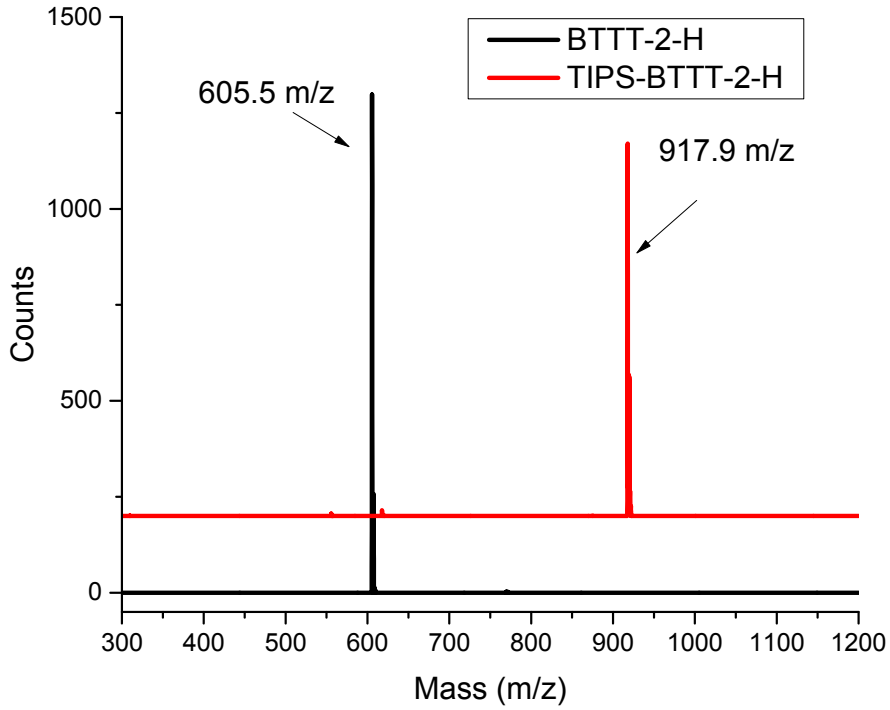


Figure S1 MALDI-ToF of TIPS-BTTT-2-H (**12**) and BTTT-2-H (**3**)

Chemistry References

(1) Zhang, X.; Johnson, J. P.; Kampf, J. W.; Matzger, A. J. Ring fusion effects on the solid-state properties of α-oligothiophenes. *Chem. Mater.* **2006**, *18*, 3470.

(2) Henssler, J. T.; Zhang, X.; Matzger, A. J. Thiophene/Thieno [3, 2-b] thiophene Co-oligomers: Fused-Ring Analogues of Sexithiophene. *J. Org. Chem.* **2009**, *74*, 9112.

(3) Zhang, L.; Colella, N. S.; Liu, F.; Trahan, S.; Baral, J. K.; Winter, H. H.; Mannsfeld, S. C.; Briseno, A. L. Synthesis, electronic structure, molecular packing/morphology evolution, and carrier mobilities of pure oligo-/poly (alkylthiophenes). *J. Am. Chem. Soc.* **2012**, *135*, 844.

(4) Zhang, L.; Liu, F.; Diao, Y.; Marsh, H. S.; Colella, N. S.; Jayaraman, A.; Russell, T. P.; Mannsfeld, S. C.; Briseno, A. L. The good host: formation of discrete one-dimensional fullerene "channels" in well-ordered poly (2, 5-bis (3-alkylthiophen-2-yl) thieno [3, 2-b] thiophene) oligomers. *J. Am. Chem. Soc.* **2014**, *136*, 18120.

Cyclic Voltammetry and UV-Vis

Cyclic voltammograms (CVs) were recorded on a 1000B model electrochemical workstation using glassy carbon discs as the working electrode, Pt wire as the counter electrode, Ag/Ag+ electrode as the reference electrode, and ferrocene/ferrocenium as an internal potential marker. 0.1 M tetrabutylammonium hexafluorophosphate (TBAPF6) dissolved in acenitrile was employed as the supporting electrolyte.

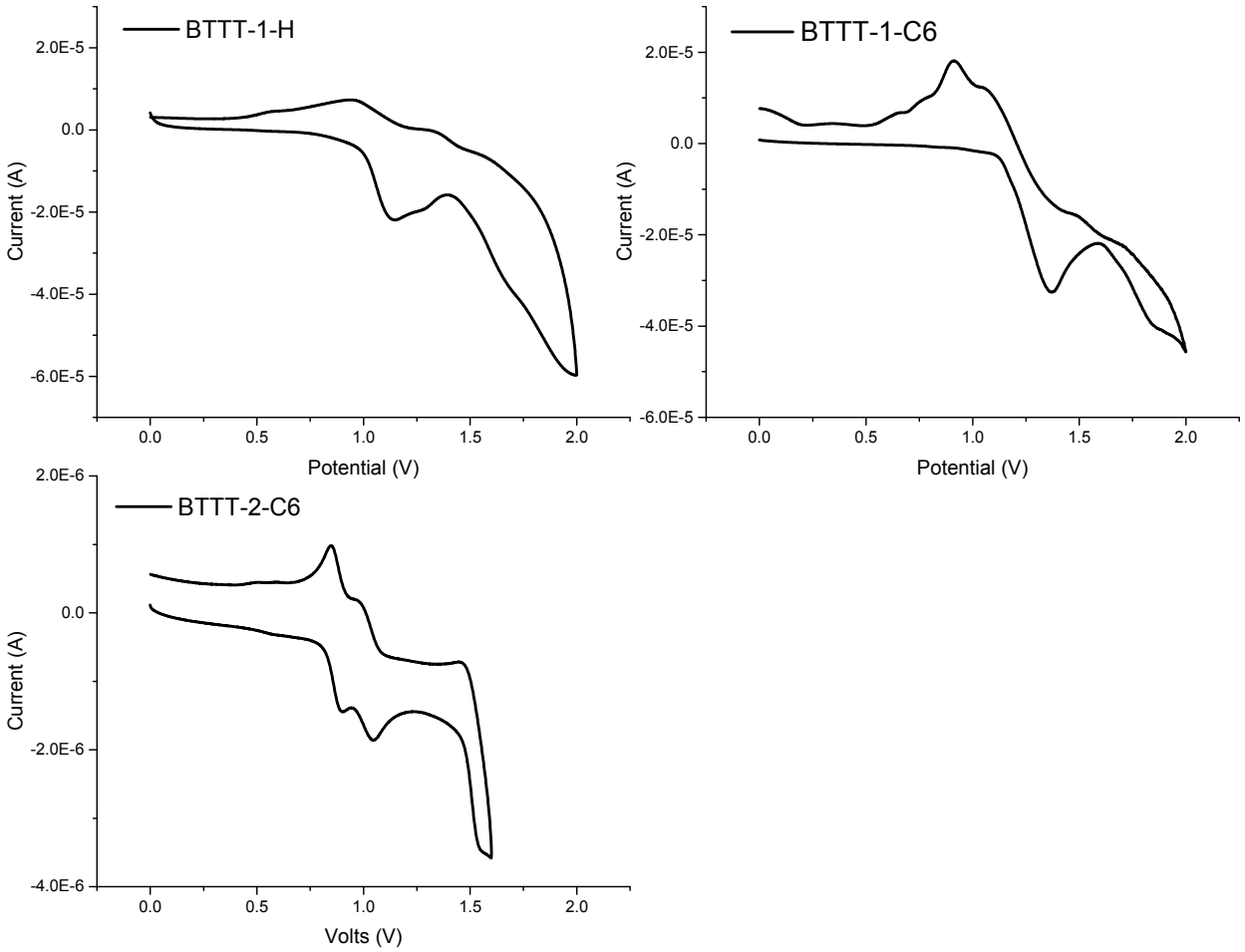


Figure S2. CV of BTTT oligomers in DCM with 0.1M Tetra-n-butylammonium hexafluorophosphate.

Table S1. Opto-electronic data

Material	λ_{max} Soln[a] [nm]	λ_{max} Film[b] [nm]	OG[c] [eV]	IP[d] [eV]	EA[e] [eV]	HOMO[f] [eV]	LUMO[f] [eV]
1-H	373	331	3.0	-5.4	-2.6	-5.10	-2.07
2-H	450	382	2.4	N/A	N/A	-4.90	-2.10
1-C_6	350	343	3.0	-5.4	-2.4	-5.16	-1.35
2-C_6	421	432	2.5	-5.2	-2.6	-5.02	-1.80

[a] Absorptions were measured from thin films on glass. [b] Absorptions measured from methylene chloride solution. [c] Determined from onset of absorption in the solution UV-Vis. [d] Determined by cyclic voltammetry (CV) in chloroform. [e] Estimated from the sum of OG and IP. [f] Computed using B97d/def2-QZVP//B97d/def2-TZV

Crystal data and Structure Refinement of **1-H, 1-C_6, 2-C_6**

Table S2. Crystal data and structure refinement for k13159. **1-C6**

Identification code	k13159
Empirical formula	C26 H32 S4
Formula weight	472.75
Temperature	90(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/n
Unit cell dimensions	a = 11.7048(2) A alpha = 90 deg. b = 7.8063(2) A beta = 98.5108(8) deg. c = 13.3837(3) A gamma = 90 deg.
Volume	1209.42(5) A^3
Z, Calculated density	2, 1.298 Mg/m^3
Absorption coefficient	0.405 mm^-1
F(000)	504
Crystal size	0.320 x 0.200 x 0.070 mm
Theta range for data collection	2.159 to 27.513 deg.
Limiting indices	-15<=h<=15, -10<=k<=10, -17<=l<=17
Reflections collected / unique	21245 / 2769 [R(int) = 0.0420]
Completeness to theta = 25.242	100.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2769 / 36 / 147
Goodness-of-fit on F^2	1.105
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.1042
R indices (all data)	R1 = 0.0544, wR2 = 0.1120
Extinction coefficient	n/a
Largest diff. peak and hole	0.498 and -0.412 e.A^-3

Table S3. Crystal data and structure refinement for x14067. **2-C6**

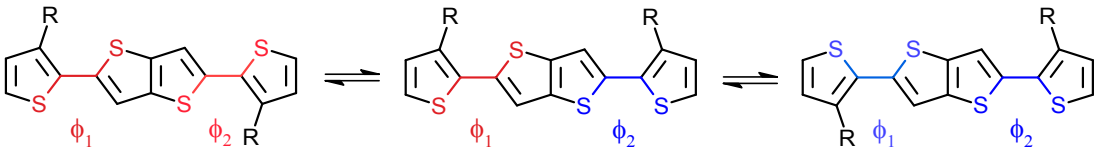
Identification code	x14067
Empirical formula	C52 H62 S8
Formula weight	943.49
Temperature	90(2) K
Wavelength	1.54178 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 5.2285(3) A alpha = 110.465(4) deg. b = 21.9986(15) A beta = 94.335(4) deg. c = 22.2284(14) A gamma = 93.072(4) deg.
Volume	2379.7(3) A^3
Z, Calculated density	2, 1.317 Mg/m^3
Absorption coefficient	3.738 mm^-1
F(000)	1004
Crystal size	0.130 x 0.060 x 0.030 mm
Theta range for data collection	2.132 to 67.477 deg.
Limiting indices	-6<=h<=2, -26<=k<=26, -26<=l<=26
Reflections collected / unique	32315 / 8154 [R(int) = 0.0540]
Completeness to theta = 67.477	95.0 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8154 / 299 / 627
Goodness-of-fit on F^2	1.072
Final R indices [I>2sigma(I)]	R1 = 0.0925, wR2 = 0.2147
R indices (all data)	R1 = 0.1183, wR2 = 0.2340
Extinction coefficient	n/a
Largest diff. peak and hole	0.712 and -0.536 e.A^-3

Table S4. Crystal data and structure refinement for x14080. **1-H**

Identification code	x14080
Empirical formula	C14 H8 S4
Formula weight	304.44
Temperature	90(2) K
Wavelength	1.54178 A
Crystal system, space group	Triclinic, P-1
Unit cell dimensions	a = 5.7171(3) A alpha = 87.647(5) deg. b = 8.6010(6) A beta = 77.952(4) deg. c = 13.2287(8) A gamma = 82.023(4) deg.
Volume	629.96(7) A^3
Z, Calculated density	2, 1.605 Mg/m^3
Absorption coefficient	6.713 mm^-1
F(000)	312
Crystal size	0.270 x 0.130 x 0.002 mm
Theta range for data collection	3.416 to 68.275 deg.
Limiting indices	-6<=h<=2, -10<=k<=10, -15<=l<=15
Reflections collected / unique	7897 / 2255 [R(int) = 0.0479]
Completeness to theta = 67.679	98.1 %
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2255 / 470 / 203
Goodness-of-fit on F^2	1.160
Final R indices [I>2sigma(I)]	R1 = 0.0475, wR2 = 0.1381
R indices (all data)	R1 = 0.0549, wR2 = 0.1441
Extinction coefficient	n/a
Largest diff. peak and hole	0.372 and -0.298 e.A^-3

Computational Chemistry

Table S5. The computed relative free energies, SCCS dihedral angles (ϕ_1 and ϕ_2) of 1-H, 1-Me, and 1-Et.



	anti-anti		*anti-syn*		*syn-syn*	
1-R	*ΔG_{rel} (kcal·mol⁻¹)*	*SCCS (ϕ_1, ϕ_2)*	*ΔG_{rel} (kcal·mol⁻¹)*	*SCCS (ϕ_1, ϕ_2)*	*ΔG_{rel} (kcal·mol⁻¹)*	*SCCS (ϕ_1, ϕ_2)*
1-H	*0.0*	*168, 168*	*0.8*	*173, 32*	*1.5*	*33, 33*
1-Me	*0.8*	*149, 149*	*0.3*	*145, 38*	*0.0*	*38, 38*
1-Et	*1.0*	*139, 139*	*0.5*	*139, 40*	*0.0*	*39, 39*

Computed using B97d/def2-QZVP//B97d/def2-TZV.

The optical band gap was determined by using the absorption edge from the solution spectra. Cyclic voltammetry was performed in dichloromethane with 0.1 M $TBAPF_6$ as the electrolyte and a scan rate of 100 mV/s to determine the ionization potentials (IP) of the oligomers. SI2 shows a summary of the electrochemically determined IP from the onset of oxidation as compared to ferrocene. The electron affinity (EA) was calculated by the sum of the IP and the optical gap (OG).

Table S6. B3LYP/6-311G(d,p) optimized Cartesian coordinates

1-H

C	3.75500	0.18400	0.00600
C	4.56100	1.27700	0.22700
C	5.95000	0.98100	0.16000
C	6.20000	-0.33400	-0.10900
S	4.73400	-1.23600	-0.30700
C	2.30900	0.10700	0.00100
C	1.50700	-0.98000	0.26200
S	1.35400	1.54700	-0.38800
C	0.13100	-0.66200	0.16400
C	-0.13100	0.66200	-0.16400
C	-1.50700	0.98000	-0.26200
C	-2.30900	-0.10700	-0.00100
S	-1.35400	-1.54700	0.38800
C	-3.75500	-0.18400	-0.00600
C	-4.56100	-1.27700	-0.22700
S	-4.73400	1.23600	0.30700
C	-5.95000	-0.98100	-0.16000
C	-6.20000	0.33400	0.10900
H	4.16700	2.25800	0.45700
H	6.73000	1.71400	0.31700
H	7.15200	-0.83200	-0.20600
H	1.90100	-1.94900	0.53700
H	-1.90100	1.94900	-0.53700
H	-4.16700	-2.25800	-0.45700
H	-6.73000	-1.71400	-0.31700
H	-7.15200	0.83200	0.20600

1-H (cation)

C	3.71200	0.18000	0.04700
C	4.53500	1.30800	0.07700
C	5.90200	1.00000	0.08800
C	6.13800	-0.35900	0.06700
S	4.69200	-1.28300	0.03400
C	2.29600	0.12700	0.03000
C	1.48200	-1.01900	-0.00000
S	1.34000	1.62100	0.04400
C	0.13500	-0.69700	-0.01100
C	-0.13500	0.69700	0.01100
C	-1.48200	1.01900	0.00000
C	-2.29600	-0.12700	-0.03000
S	-1.34000	-1.62100	-0.04400
C	-3.71200	-0.18000	-0.04700
C	-4.53500	-1.30800	-0.07700
S	-4.69200	1.28300	-0.03400
C	-5.90200	-1.00000	-0.08800
C	-6.13800	0.35900	-0.06700
H	4.15000	2.31900	0.09000
H	6.69200	1.73700	0.11000
H	7.09200	-0.86600	0.06900
H	1.88100	-2.02300	-0.01300
H	-1.88100	2.02300	0.01300
H	-4.15000	-2.31900	-0.09000
H	-6.69200	-1.73700	-0.11000
H	-7.09200	0.86600	-0.06900

1-C_6

S	-2.48600	4.16200	-0.67300
S	-0.10600	1.99700	0.57800
C	-0.49500	-0.40100	-0.29900
C	-1.74100	0.25300	-0.47400
H	-2.61800	-0.19300	-0.92200
C	-1.70600	1.56000	-0.05300
C	-2.78000	2.54100	-0.06000
C	-4.08700	2.40200	0.36500
C	-4.83700	3.60700	0.19000
H	-5.87800	3.70100	0.47500
C	-4.11700	4.63200	-0.34400
H	-4.44100	5.63800	-0.56300
C	-4.67900	1.16000	0.97900
H	-5.25200	1.44900	1.86900
H	-3.87600	0.50400	1.32600
C	-5.60700	0.37500	0.03100
H	-6.41500	1.03200	-0.31200
H	-5.05000	0.09200	-0.86900
C	-6.20500	-0.87700	0.68200
H	-6.75900	-0.58600	1.58400
H	-5.39300	-1.53100	1.02300
C	-7.13300	-1.66700	-0.24900
H	-6.58000	-1.95400	-1.15300

H	-7.94800	-1.01500	-0.58700
C	-7.72700	-2.92300	0.39800
H	-6.91100	-3.57400	0.73600
H	-8.28100	-2.63700	1.30000
C	-8.64900	-3.70700	-0.54000
H	-9.49400	-3.09400	-0.86700
H	-9.05400	-4.59700	-0.05100
H	-8.11400	-4.03600	-1.43700
S	2.48200	-4.17500	0.58300
S	0.11300	-1.99900	-0.63400
C	0.50100	0.39900	0.24500
C	1.74700	-0.25600	0.42000
H	2.62300	0.19100	0.87000
C	1.71200	-1.56300	-0.00200
C	2.78600	-2.54300	0.00400
C	4.09900	-2.39900	-0.39900
C	4.84500	-3.60800	-0.23600
H	5.88900	-3.69800	-0.50800
C	4.11600	-4.64200	0.26900
H	4.43600	-5.65200	0.47300
C	4.70400	-1.14600	-0.97900
H	5.29800	-1.42000	-1.85900
H	3.90800	-0.48600	-1.33400
C	5.60800	-0.37700	0.00400
H	6.41200	-1.03700	0.35000
H	5.03000	-0.11600	0.89900
C	6.21300	0.89200	-0.60700
H	6.78800	0.62300	-1.50200
H	5.40400	1.54800	-0.95200
C	7.11500	1.66600	0.36100
H	6.54200	1.92900	1.25900
H	7.92800	1.01200	0.70200
C	7.71400	2.94000	-0.24500
H	6.90200	3.59300	-0.58600
H	8.29000	2.67800	-1.14100
C	8.61100	3.70900	0.73000
H	9.45300	3.09400	1.06200
H	9.02200	4.61100	0.26900
H	8.05500	4.01500	1.62100

1-C_6-cation

S	2.40400	4.18600	0.58800
S	-0.00900	2.07600	-0.33100
C	0.54700	-0.43200	0.13100
C	1.77800	0.20500	0.20200
H	2.71400	-0.27700	0.43800
C	1.66600	1.59100	0.00300
C	2.70900	2.56100	-0.02600
C	4.05100	2.41000	-0.41400
C	4.77700	3.61000	-0.23300
H	5.82100	3.71700	-0.49700
C	4.03500	4.63600	0.29700
H	4.36500	5.63400	0.54300

C	4.67400	1.17700	-1.00800
H	5.29100	1.48400	-1.85900
H	3.90400	0.51800	-1.41400
C	5.56400	0.40000	-0.01200
H	6.35300	1.06400	0.35800
H	4.97600	0.11900	0.87000
C	6.19400	-0.85000	-0.63600
H	6.77800	-0.55800	-1.51700
H	5.40000	-1.51300	-1.00600
C	7.09200	-1.62500	0.33500
H	6.51000	-1.91000	1.22100
H	7.89000	-0.96500	0.69600
C	7.71700	-2.88100	-0.28300
H	6.91900	-3.54100	-0.64500
H	8.30000	-2.59600	-1.16700
C	8.61200	-3.64900	0.69300
H	9.44100	-3.02700	1.04400
H	9.04100	-4.53700	0.22300
H	8.05000	-3.97800	1.57300
S	-2.40400	-4.18600	-0.58800
S	0.00900	-2.07600	0.33100
C	-0.54700	0.43200	-0.13100
C	-1.77800	-0.20500	-0.20200
H	-2.71400	0.27700	-0.43800
C	-1.66600	-1.59100	-0.00300
C	-2.70900	-2.56100	0.02600
C	-4.05100	-2.41000	0.41400
C	-4.77700	-3.61000	0.23300
H	-5.82100	-3.71700	0.49700
C	-4.03500	-4.63600	-0.29700
H	-4.36500	-5.63400	-0.54300
C	-4.67400	-1.17700	1.00800
H	-5.29100	-1.48400	1.85900
H	-3.90400	-0.51800	1.41400
C	-5.56400	-0.40000	0.01200
H	-6.35300	-1.06400	-0.35800
H	-4.97600	-0.11900	-0.87000
C	-6.19400	0.85000	0.63600
H	-6.77800	0.55800	1.51700
H	-5.40000	1.51300	1.00600
C	-7.09200	1.62500	-0.33500
H	-6.51000	1.91000	-1.22100
H	-7.89000	0.96500	-0.69600
C	-7.71700	2.88100	0.28300
H	-6.91900	3.54100	0.64500
H	-8.30000	2.59600	1.16700
C	-8.61200	3.64900	-0.69300
H	-9.44100	3.02700	-1.04400
H	-9.04100	4.53700	-0.22300
H	-8.05000	3.97800	-1.57300

2-C_6

S	11.73500	0.55300	1.76300
C	13.19400	-0.10100	1.10900

H	14.13300	0.07400	1.61000
C	12.95600	-0.79600	-0.03600
H	13.73700	-1.28100	-0.60900
C	11.58200	-0.82400	-0.43000
C	10.77000	-0.13100	0.45500
C	9.34100	0.12800	0.46800
S	8.23700	-0.51700	-0.76600
C	8.65100	0.88200	1.39600
H	9.13100	1.37100	2.23200
C	7.26400	0.93800	1.13100
C	6.86700	0.23900	-0.00100
C	5.48400	0.32700	-0.29100
H	4.99600	-0.12900	-1.14100
C	4.80700	1.09900	0.62600
S	5.89700	1.70700	1.88800
C	3.37500	1.34600	0.68400
C	2.66100	2.51100	0.89300
C	1.25600	2.28900	0.86500
H	0.53700	3.08500	1.02100
C	0.87700	0.98700	0.63500
S	2.29400	-0.02200	0.45400
C	-0.45500	0.43100	0.54900
C	-0.84600	-0.88700	0.58400
H	-0.13900	-1.70000	0.70200
C	-2.25000	-1.10000	0.49300
C	-2.94900	0.08700	0.38600
S	-1.85600	1.46200	0.36700
C	-4.37700	0.34900	0.29600
S	-5.39200	-0.48200	-0.89800
C	-5.09900	1.28200	1.00500
H	-4.65900	1.88900	1.78400
C	-6.45900	1.31700	0.61500
C	-6.79400	0.42100	-0.39000
C	-8.16100	0.42800	-0.75800
H	-8.57600	-0.19700	-1.53000
C	-8.89800	1.34000	-0.02800
S	-7.86500	2.20100	1.13700
C	11.15500	-1.57900	-1.66500
H	11.98200	-1.54800	-2.38300
H	10.31700	-1.08100	-2.15900
C	10.79300	-3.05300	-1.39100
H	9.97000	-3.09600	-0.67000
H	11.64700	-3.54400	-0.90900
C	10.40800	-3.82000	-2.66000
H	9.55000	-3.32700	-3.13500
H	11.23100	-3.76200	-3.38300
C	10.06600	-5.29200	-2.40100
H	9.23800	-5.35000	-1.68300
H	10.92100	-5.78300	-1.91800
C	9.69000	-6.06800	-3.66800
H	8.83500	-5.57800	-4.15100
H	10.51800	-6.00900	-4.38600
C	9.35100	-7.53700	-3.40100
H	10.19800	-8.06200	-2.94900

H	9.09000	-8.06100	-4.32400
H	8.50200	-7.62900	-2.71600
C	3.24500	3.89300	1.04500
H	4.28500	3.83500	1.37100
H	2.70200	4.42300	1.83600
C	3.17800	4.71900	-0.25500
H	3.72600	4.18700	-1.04000
H	2.13700	4.77900	-0.59600
C	3.74900	6.13100	-0.09200
H	4.78800	6.06200	0.25600
H	3.19800	6.65700	0.69900
C	3.70200	6.96300	-1.37900
H	2.66300	7.03500	-1.72700
H	4.25100	6.43600	-2.17100
C	4.27900	8.37400	-1.21900
H	3.73000	8.90000	-0.42900
H	5.31600	8.30100	-0.87000
C	4.23100	9.19800	-2.50900
H	4.80000	8.71300	-3.30900
H	4.65200	10.19600	-2.36100
H	3.20300	9.32000	-2.86300
C	-2.85900	-2.47400	0.62200
H	-2.28400	-3.17800	0.00900
H	-3.87600	-2.47800	0.22500
C	-2.89200	-2.98000	2.07900
H	-1.87500	-2.97900	2.48800
H	-3.46600	-2.27100	2.68500
C	-3.49800	-4.38200	2.21100
H	-2.92400	-5.08500	1.59200
H	-4.51500	-4.37600	1.80000
C	-3.53700	-4.89400	3.65500
H	-2.51900	-4.90300	4.06400
H	-4.10700	-4.18900	4.27300
C	-4.14900	-6.29300	3.79400
H	-3.58100	-6.99800	3.17500
H	-5.16700	-6.28300	3.38500
C	-4.18500	-6.79700	5.23900
H	-3.17800	-6.84900	5.66500
H	-4.62500	-7.79600	5.30400
H	-4.77700	-6.13100	5.87500
C	-10.31000	1.66600	-0.10500
C	-11.32300	1.08800	-0.86200
C	-12.58700	1.70500	-0.62000
H	-13.50200	1.40100	-1.10900
C	-12.54700	2.71800	0.29200
H	-13.35600	3.33700	0.64600
S	-10.95000	2.96300	0.89300
C	-11.12500	-0.06100	-1.82600
H	-10.41800	0.24600	-2.60800
H	-10.63700	-0.88400	-1.29000
C	-12.39800	-0.58300	-2.50400
H	-13.10300	-0.93600	-1.74400
H	-12.89500	0.24500	-3.02000
C	-12.13900	-1.69400	-3.53500

H	-11.47900	-1.29900	-4.31800
H	-13.08800	-1.92700	-4.03300
C	-11.53600	-3.00200	-2.99600
H	-10.54600	-2.81300	-2.56300
H	-11.36000	-3.67100	-3.84700
C	-12.40500	-3.73500	-1.96600
H	-12.54300	-3.10700	-1.07900
H	-13.40600	-3.89000	-2.38800
C	-11.81600	-5.08300	-1.53900
H	-12.45300	-5.58300	-0.80500
H	-10.82600	-4.95700	-1.08900
H	-11.70500	-5.75500	-2.39600

2-C6 (cation)

S	11.88100	1.12600	1.31400
C	13.33200	0.28500	0.93500
H	14.27500	0.62300	1.34200
C	13.10300	-0.78300	0.11300
H	13.89200	-1.43700	-0.24000
C	11.73800	-0.95900	-0.24500
C	10.92300	0.02100	0.32500
C	9.51000	0.27200	0.22400
S	8.36200	-0.93900	-0.38200
C	8.85400	1.44000	0.60800
H	9.37600	2.30800	0.99000
C	7.47000	1.36200	0.42600
C	7.02300	0.14300	-0.10900
C	5.64500	0.06700	-0.29200
H	5.12900	-0.79400	-0.69800
C	4.98100	1.23800	0.09600
S	6.14300	2.45000	0.69700
C	3.57600	1.45200	0.06700
C	2.80400	2.61300	0.31600
C	1.43400	2.36400	0.21000
H	0.68500	3.13100	0.35900
C	1.08600	1.05200	-0.11500
S	2.53000	0.08000	-0.29800
C	-0.20700	0.50600	-0.29400
C	-0.56200	-0.80100	-0.62200
H	0.17700	-1.57800	-0.78400
C	-1.93500	-1.04500	-0.73300
C	-2.70200	0.11500	-0.48500
S	-1.65000	1.48100	-0.11000
C	-4.10400	0.35700	-0.55200
S	-5.30200	-0.91100	-0.90300
C	-4.74000	1.57100	-0.27300
H	-4.20100	2.46400	0.01800
C	-6.12400	1.49900	-0.41100
C	-6.60700	0.22300	-0.73300
C	-8.00200	0.13800	-0.85100
H	-8.53800	-0.75000	-1.14700
C	-8.62600	1.35400	-0.58400
S	-7.43900	2.62700	-0.23300
C	11.31100	-2.08800	-1.14800

H	12.15300	-2.33800	-1.80000
H	10.50100	-1.76400	-1.81000
C	10.88400	-3.36300	-0.38300
H	10.15100	-3.10500	0.38800
H	11.75600	-3.76700	0.14300
C	10.30000	-4.43700	-1.30900
H	9.46200	-4.00800	-1.87600
H	11.05500	-4.72400	-2.05300
C	9.81800	-5.68700	-0.56400
H	9.06200	-5.39600	0.17800
H	10.65400	-6.12000	-0.00000
C	9.22900	-6.75700	-1.49100
H	8.39300	-6.32400	-2.05600
H	9.98500	-7.04500	-2.23300
C	8.74700	-8.00600	-0.74600
H	9.57200	-8.49100	-0.21400
H	8.31900	-8.73900	-1.43500
H	7.97900	-7.75400	-0.00700
C	3.37800	3.97100	0.64400
H	4.20700	4.18100	-0.04200
H	3.81900	3.93400	1.64900
C	2.38500	5.14200	0.58200
H	1.85000	5.12100	-0.37500
H	1.63300	5.02700	1.37200
C	3.07700	6.50100	0.74600
H	3.89700	6.58200	0.02000
H	3.53900	6.55300	1.74100
C	2.12300	7.68900	0.57000
H	1.37000	7.67000	1.36800
H	1.57400	7.57800	-0.37500
C	2.83200	9.05000	0.58300
H	3.28900	9.20900	1.56800
H	3.65700	9.03400	-0.14000
C	1.89600	10.22000	0.26300
H	1.41900	10.08700	-0.71400
H	2.44000	11.16800	0.24200
H	1.10100	10.30800	1.01200
C	-2.45700	-2.42100	-1.05800
H	-1.68800	-2.94700	-1.63300
H	-3.32800	-2.35500	-1.71600
C	-2.81300	-3.26300	0.18800
H	-1.92800	-3.33900	0.83000
H	-3.57800	-2.74500	0.77600
C	-3.30800	-4.66800	-0.17800
H	-2.51100	-5.20400	-0.71000
H	-4.14700	-4.58600	-0.88100
C	-3.74400	-5.49500	1.03800
H	-2.89900	-5.59400	1.73100
H	-4.52800	-4.95300	1.58400
C	-4.25900	-6.89200	0.66900
H	-3.46600	-7.44200	0.14700
H	-5.08700	-6.79400	-0.04500
C	-4.72600	-7.70300	1.88200
H	-3.91700	-7.82800	2.61000

H	-5.06300	-8.70100	1.58600
H	-5.55900	-7.20800	2.39200
C	-10.01500	1.69800	-0.71000
C	-11.13500	0.86100	-0.73700
C	-12.33900	1.60800	-0.85200
H	-13.32300	1.16000	-0.84700
C	-12.14800	2.95800	-0.95800
H	-12.89700	3.72900	-1.07700
S	-10.48400	3.38200	-0.90100
C	-11.09300	-0.64000	-0.55200
H	-10.68600	-1.10100	-1.46400
H	-10.38100	-0.86900	0.25000
C	-12.44700	-1.30300	-0.25200
H	-12.84900	-0.89800	0.68500
H	-13.15800	-1.04900	-1.04300
C	-12.37600	-2.83300	-0.16400
H	-11.96500	-3.22900	-1.10400
H	-13.40700	-3.20400	-0.12100
C	-11.59900	-3.40500	1.04400
H	-10.80100	-2.71200	1.34400
H	-11.10100	-4.33600	0.75000
C	-12.49400	-3.67900	2.26200
H	-12.94200	-2.73700	2.60300
H	-13.32600	-4.32000	1.94600
C	-11.74900	-4.33800	3.42600
H	-12.42000	-4.53100	4.26900
H	-10.93500	-3.70100	3.79000
H	-11.31200	-5.29500	3.12300

2-H-(*anti-anti*)

S	-11.70400	0.77500	0.52300
C	-13.08300	-0.11400	-0.03400
H	-14.07600	0.22600	0.21900
C	-12.71700	-1.20500	-0.76800
H	-13.42900	-1.89200	-1.20700
C	-11.30900	-1.33100	-0.90800
C	-10.60300	-0.33300	-0.27500
C	-9.17100	-0.13500	-0.20700
S	-8.08400	-1.52600	-0.35500
C	-8.47400	1.03700	-0.02200
H	-8.95800	2.00000	0.07200
C	-7.07500	0.82800	-0.00700
C	-6.68900	-0.49500	-0.18800
C	-5.28900	-0.70000	-0.21200
H	-4.80700	-1.65400	-0.37000
C	-4.59100	0.47500	-0.04000
S	-5.68000	1.85900	0.16400
C	-3.16200	0.67500	-0.00200
C	-2.44200	1.83000	-0.21500
C	-1.04400	1.66200	-0.09400
H	-0.33400	2.46800	-0.21700
C	-0.66300	0.37300	0.21000
S	-2.07700	-0.65700	0.35800

C	0.66300	-0.16300	0.40100
C	1.04800	-1.33500	1.01400
H	0.34100	-2.02000	1.46400
C	2.44700	-1.53400	1.04100
C	3.16400	-0.51700	0.44800
S	2.07300	0.70000	-0.19100
C	4.59300	-0.37400	0.31000
S	5.63500	-1.80500	0.40200
C	5.32400	0.77500	0.09800
H	4.87400	1.75500	0.03100
C	6.71200	0.51400	0.01700
C	7.05700	-0.82300	0.17300
C	8.44900	-1.07800	0.13100
H	8.90400	-2.05000	0.26400
C	9.17900	0.07100	-0.06600
S	8.13500	1.49400	-0.21500
C	10.61500	0.22100	-0.16600
C	11.39000	1.32400	0.11100
C	12.77900	1.10800	-0.09600
H	13.53800	1.85900	0.08100
C	13.06200	-0.15600	-0.52800
H	14.02300	-0.59100	-0.75400
S	11.62400	-1.10500	-0.71200
H	10.97500	2.25300	0.47900
H	2.92000	-2.38400	1.51400
H	-2.90900	2.77300	-0.46600
H	-10.82900	-2.11500	-1.47800

2-H-(anti-anti)

S	-11.65000	1.08500	-0.01000
C	-13.03500	0.05700	-0.00300
H	-14.02100	0.49500	-0.00600
C	-12.69500	-1.27000	0.00700
H	-13.42300	-2.07000	0.01300
C	-11.29700	-1.47400	0.01000
C	-10.56800	-0.29800	0.00100
C	-9.14300	-0.13000	0.00100
S	-8.08400	-1.55100	-0.00400
C	-8.42100	1.05600	0.00400
H	-8.88800	2.03100	0.00700
C	-7.03900	0.82900	0.00300
C	-6.67300	-0.52800	-0.00100
C	-5.29700	-0.75400	-0.00100
H	-4.83100	-1.73000	-0.00400
C	-4.56700	0.43700	0.00200
S	-5.63700	1.85600	0.00500
C	-3.15900	0.60000	0.00200
C	-2.42600	1.79300	0.00600
C	-1.05000	1.60800	0.00500
H	-0.34000	2.42500	0.00800
C	-0.65500	0.26600	0.00100
S	-2.07100	-0.77800	-0.00200
C	0.65500	-0.26600	-0.00100
C	1.05000	-1.60800	-0.00500

H	0.34000	-2.42500	-0.00800
C	2.42600	-1.79300	-0.00600
C	3.15900	-0.60000	-0.00200
S	2.07100	0.77800	0.00200
C	4.56700	-0.43700	-0.00200
S	5.63700	-1.85600	-0.00500
C	5.29700	0.75400	0.00100
H	4.83100	1.73000	0.00200
C	6.67300	0.52800	0.00000
C	7.03900	-0.82900	-0.00300
C	8.42100	-1.05600	-0.00400
H	8.88800	-2.03100	-0.00700
C	9.14300	0.13000	-0.00100
S	8.08400	1.55100	0.00300
C	10.56800	0.29800	-0.00200
C	11.29700	1.47400	-0.01500
C	12.69500	1.27000	-0.01200
H	13.42300	2.06900	-0.02100
C	13.03500	-0.05700	0.00400
H	14.02100	-0.49500	0.01000
S	11.65000	-1.08500	0.01600
H	10.83800	2.45400	-0.02800
H	2.89700	-2.76700	-0.01000
H	-2.89700	2.76700	0.00900
H	-10.83800	-2.45400	0.01800

Table S7. Snapshots of MD from different crystallographic directions.

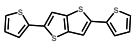
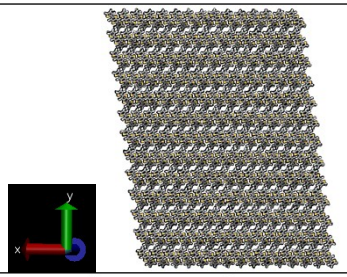
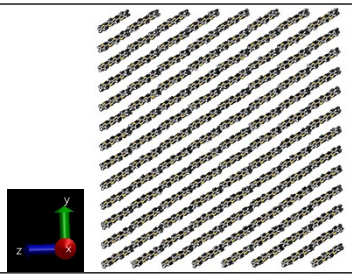
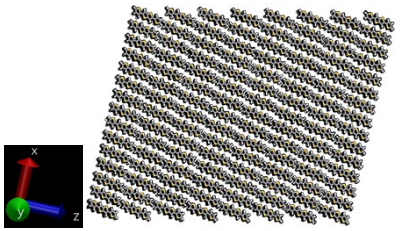
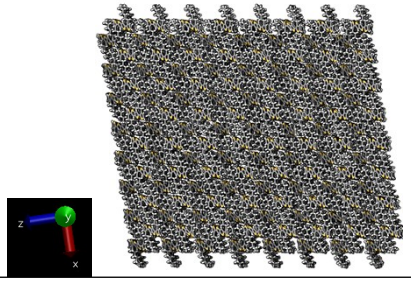
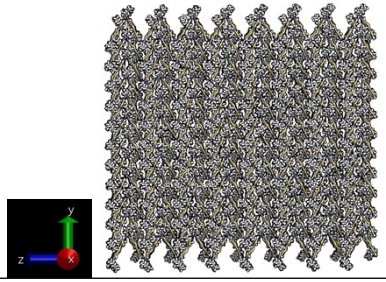
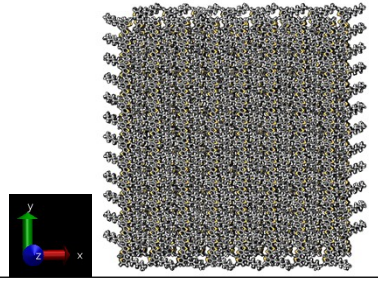
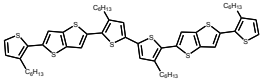
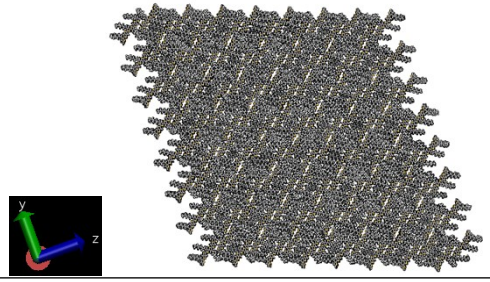
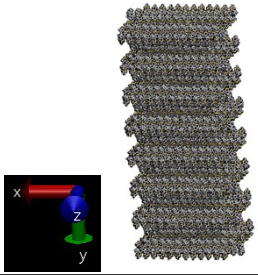
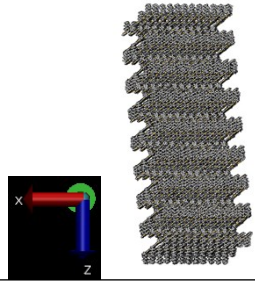
1-H				
1-C6				
2-C6				

Figure S2. Site-energy difference distributions.

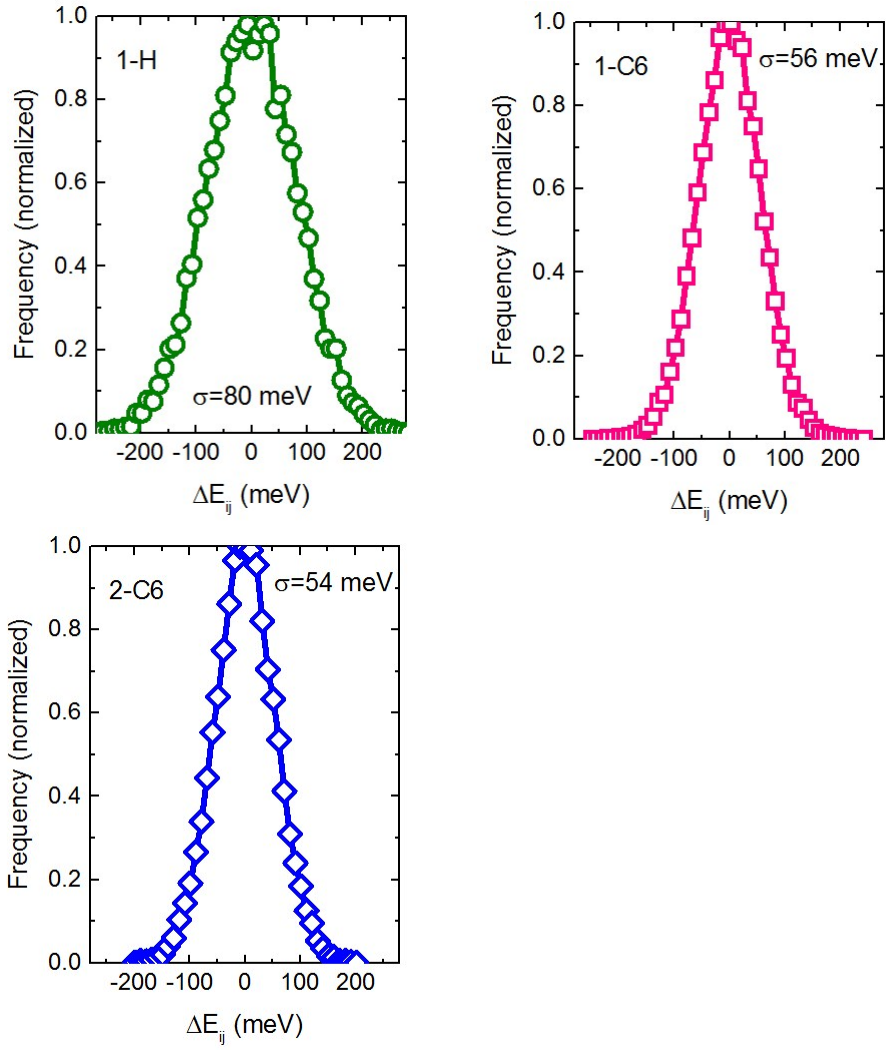
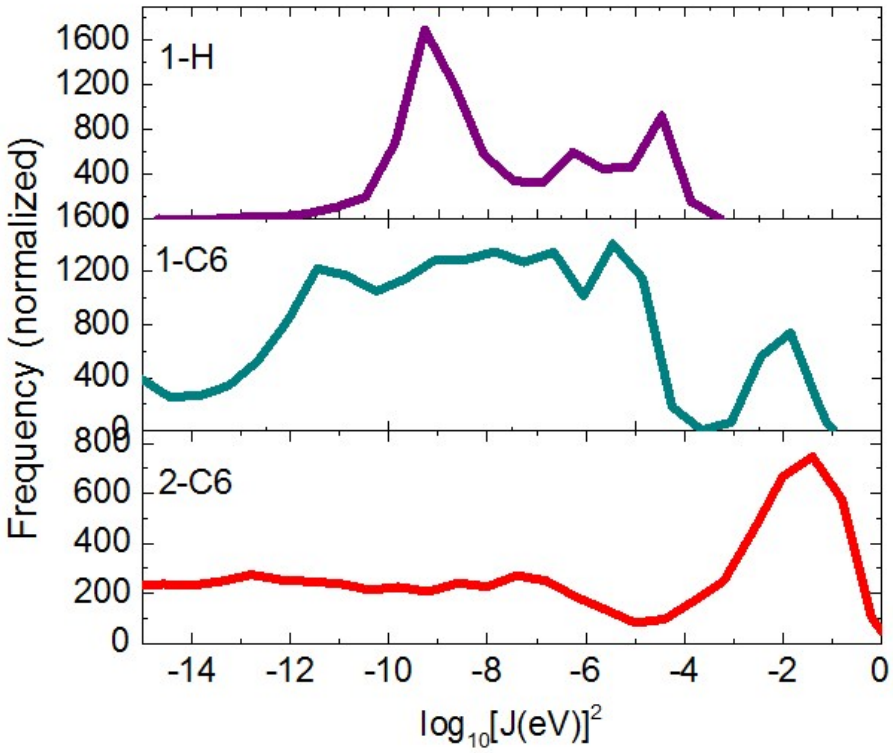


Figure S3. Electronic-coupling, J, distributions.



Details of the kinetic Monte Carlo (kMC) Simulations:

Transfer Rates

We employ the charge-transport simulations procedure implemented in **VOTCA** package developed by Andrienko and co-workers.[1,2] On the basis of the assumption that charges are localized on a single molecule and charge-transfer reactions take place *via* an intersite hopping mechanism, the charge-hopping rate is evaluated by the nonadiabatic, high-temperature limit of the Marcus rate[3,4]

$$k_{ij} = \frac{J_{ij}^2}{\hbar}\sqrt{\frac{\pi}{\lambda k_b T}} exp\left[-\frac{\left(\Delta E_{ij} - \lambda_e\right)^2}{4\lambda k_b T}\right]$$

where T is the temperature, J_{ij} is the transfer integral between the initial and final states. λ_e is the electron-transfer reorganization energy and $\Delta E_{ij} = \varepsilon_i - \varepsilon_j$ is called the site-energy difference of the

transfer reaction. ε_i is the energy difference of the entire system when molecule *i* is charged or neutral. Thus, for reactions involving identical molecules, $\Delta E_{ij}=0$.

Reorganization Energy:

The reorganization energy λ is calculated from adiabatic potential energy surfaces of neutral and cationic states of compounds, using the following expression:

$$\lambda = \left(E^{n}_{q_c} - E^{n}_{q_n}\right) + \left(E^{c}_{q_n} - E^{c}_{q_c}\right)$$

where $E^{n}_{q_n}$ ($E^{c}_{q_n}$) is the energy of the neutral *n* (charged *c*) state of the molecule in its optimized *neutral* geometry and $E^{n}_{q_c}$ ($E^{c}_{q_c}$) is the energy of the neutral *n* (charged *c*) state of the molecule in its optimized *charged* geometry. We used in Gaussian09,[5] to calculate λ for an isolated molecule. We employ the B3LYP hybrid density functional with the 6- 31G(d) basis set.

Site-energies:

A charge-transfer reaction from molecule *i* and *j* is driven by site-energy. Here, we calculate site-energies of the electron transfer from polarizable force-fields with the help of *ab initio* methods. Site-energies include contributions from electrostatic Coulombic interactions (with polarization effects) between atoms and the contributions from the external electric field. Thus, site energy difference is defined as follows:

$$\Delta E_{ij} = \Delta E_{elec.} + \Delta E_{ext.}$$

External electric field contributions are calculated using the expression $\Delta E_{ext.} = q\vec{F}.\vec{d}_{ij}$. Here $\vec{F}$ is the field-vector and $\vec{d}_{ij}$ is the position-vector between molecules *i* and *j*. Polarized Coulombic contributions to site energies are calculated self-consistently using Thole Model.[2,6–7] Partial charges of neutral and charged states are generated via Merz−Singh− Kollman scheme using HF/6-31G(d) method based on B3LYP/6-31G(d,p) optimized geometries, as implemented in Gaussian09.[5] Isotropic atomic polarizabilities of the neutral and charged states are reparameterized for each species as to reproduce the molecular polarizabilities obtained from B3LYP/ 6-31G(d,p) method.[5]

Electronic Coupling

A pair of molecules of whose centroid distance is below 0.8*nm* is determined as neighboring molecular pair. The electronic coupling, J, between these molecular pairs are calculated by the ZINDO method.[2,8]

Energetic disorder

Energetic disorder σ is calculated by fitting the histogram of ΔE_{ij} site-energy differences to a Gaussian-distribution function

$$f(\varepsilon,\sigma) = \frac{1}{2\pi} exp[-\frac{\varepsilon^2}{2\sigma^2}]$$

kMC simulations and electron-mobility

Charge dynamics is simulated using the kinetic Monte Carlo (kMC) technique using the VOTCA package. In this stochastic procedure, a charge-carrier is initially chosen randomly within the system with periodic-boundaries and propagated by hopping between sites, where hopping probabilities (thus the hopping times) are defined by the Marcus rate. The simulations are performed until the results are converged. Charge-carrier mobility is calculated by

$$\mu_e = \frac{v}{|F|},$$

where v is the charge-carrier velocity and F is applied electric field. The reported mobilities are the averages over 10-100 stochastic realizations.

Table S9. Nuclear coordinates for 1-H, 1-Me, 1-Et, in the syn-syn (SS), syn-anti (AS), and anti-anti (AA).

1-Et-AA

C	-3.75800	0.42700	-0.10700
C	-4.77200	-0.24300	0.57900
C	-6.06900	0.28200	0.26900
C	-6.04800	1.33000	-0.62600
S	-4.43000	1.69300	-1.13800
C	-2.31500	0.24400	-0.07600
C	-1.34200	1.23800	-0.09400
S	-1.58200	-1.38000	-0.11800
C	-0.02800	0.70200	-0.13300
C	0.02800	-0.70200	-0.13300
C	1.34200	-1.23800	-0.09400
C	2.31500	-0.24400	-0.07700
S	1.58200	1.38000	-0.11800
C	3.75800	-0.42700	-0.10700
C	4.77200	0.24300	0.57900
S	4.43000	-1.69300	-1.13800
C	6.06900	-0.28200	0.26900
C	6.04800	-1.33000	-0.62600

C	-4.57500	-1.38000	1.55600
C	-4.87700	-2.76200	0.93000
C	4.57500	1.38000	1.55600
C	4.87700	2.76200	0.93000
H	-6.98500	-0.10100	0.71800
H	-6.88600	1.90800	-1.00800
H	-1.59200	2.29700	-0.06300
H	1.59200	-2.29700	-0.06400
H	6.98500	0.10100	0.71800
H	6.88600	-1.90800	-1.00800
H	-3.54700	-1.36600	1.94600
H	-5.24800	-1.22200	2.41500
H	-4.74600	-3.56200	1.67500
H	-5.91100	-2.80100	0.55500
H	-4.20300	-2.96300	0.08400
H	3.54700	1.36600	1.94600
H	5.24800	1.22200	2.41500
H	4.20400	2.96300	0.08400
H	4.74700	3.56200	1.67500
H	5.91100	2.80100	0.55500

1-Et-AS

C	3.76100	-0.39000	-0.09200
C	4.72200	0.39000	0.55100
C	6.05600	-0.01000	0.21100
C	6.11400	-1.07200	-0.66500
S	4.52600	-1.60400	-1.12100
C	2.30800	-0.35100	-0.02100
C	1.43900	-1.43700	0.00300
S	1.41600	1.19100	-0.06100
C	0.07700	-1.03500	0.00200
C	-0.11800	0.35600	-0.01600
C	-1.47800	0.76100	0.04700
C	-2.34500	-0.32500	0.09200
S	-1.45700	-1.87100	0.06100
C	-3.79700	-0.29400	0.11800
C	-4.65100	0.58400	-0.55200
S	-4.71900	-1.45000	1.08300
C	-6.03000	0.31000	-0.27600
C	-6.22600	-0.75600	0.57400
C	4.44100	1.52200	1.51400
C	4.56500	2.91300	0.84800
C	-4.21000	1.69500	-1.47500
C	-4.24500	3.08500	-0.79500
H	6.94100	0.47000	0.62700
H	6.99300	-1.57200	-1.06200
H	1.79400	-2.46500	0.04100
H	-1.82700	1.78900	0.08800
H	-6.84700	0.88100	-0.71600
H	-7.16500	-1.17600	0.92600

H	3.43800	1.40700	1.94800
H	5.16200	1.45900	2.34600
H	4.37500	3.71200	1.58100
H	5.57300	3.05600	0.43000
H	3.84100	3.01800	0.02600
H	-3.19500	1.48700	-1.84300
H	-4.87800	1.71300	-2.35200
H	-3.59000	3.10900	0.08900
H	-3.91700	3.86900	-1.49400
H	-5.26400	3.32500	-0.45600

1-Et-SS

C	3.76300	0.34800	-0.11100
C	4.69300	-0.45800	0.54900
C	6.04000	-0.03400	0.31000
C	6.13900	1.07300	-0.50300
S	4.57600	1.62400	-1.02200
C	2.31600	0.22700	-0.11700
C	1.56400	-0.94300	-0.11200
S	1.27100	1.67200	-0.08500
C	0.16800	-0.68200	-0.08300
C	-0.16800	0.68200	-0.08400
C	-1.56400	0.94300	-0.11200
C	-2.31600	-0.22700	-0.11700
S	-1.27100	-1.67200	-0.08400
C	-3.76300	-0.34800	-0.11100
C	-4.69300	0.45800	0.54900
S	-4.57600	-1.62400	-1.02200
C	-6.04000	0.03400	0.31000
C	-6.13900	-1.07300	-0.50300
C	4.35500	-1.64200	1.42500
C	4.53900	-2.99400	0.69500
C	-4.35500	1.64200	1.42500
C	-4.53900	2.99400	0.69500
H	6.90400	-0.53200	0.74900
H	7.03500	1.59900	-0.82300
H	2.01800	-1.92900	-0.16100
H	-2.01800	1.92900	-0.16100
H	-6.90400	0.53200	0.74900
H	-7.03500	-1.59900	-0.82300
H	5.01000	-1.62600	2.31100
H	3.31900	-1.55200	1.78500
H	4.28300	-3.83400	1.36000
H	3.90200	-3.05100	-0.20000
H	5.58200	-3.11800	0.36500
H	-5.01000	1.62600	2.31100
H	-3.31900	1.55200	1.78500
H	-5.58200	3.11700	0.36500
H	-4.28300	3.83400	1.36000
H	-3.90200	3.05100	-0.20000

1-H-SS

C	3.76600	-0.22700	-0.08900
C	4.51300	-1.27400	-0.62000
C	5.91900	-1.11600	-0.44100
C	6.24900	0.05400	0.21400
S	4.83300	0.96800	0.64400
C	2.32000	-0.10900	-0.07300
C	1.41000	-1.16100	-0.07700
S	1.50200	1.47000	-0.10200
C	0.06800	-0.70000	-0.10800
C	-0.06800	0.70000	-0.10800
C	-1.41000	1.16100	-0.07700
C	-2.32000	0.10900	-0.07300
S	-1.50200	-1.47000	-0.10200
C	-3.76600	0.22700	-0.08900
C	-4.51300	1.27400	-0.62000
S	-4.83300	-0.96800	0.64400
C	-5.91900	1.11600	-0.44200
C	-6.24900	-0.05400	0.21400
H	4.05100	-2.10800	-1.14600
H	6.66200	-1.82700	-0.79900
H	7.23500	0.43500	0.46500
H	1.72000	-2.20200	-0.03100
H	-1.72000	2.20200	-0.03100
H	-4.05100	2.10700	-1.14600
H	-6.66200	1.82700	-0.80000
H	-7.23500	-0.43500	0.46500

1-H-AS

C	-3.77900	0.13400	0.02500
C	-4.65400	1.21100	0.12900
C	-6.02900	0.83400	0.09800
C	-6.20800	-0.52900	-0.02700
S	-4.68800	-1.36900	-0.12700
C	-2.33000	0.13500	0.02500
C	-1.46400	-0.93400	0.23800
S	-1.44200	1.64800	-0.27900
C	-0.10300	-0.53700	0.16900
C	0.09300	0.83000	-0.09300
C	1.45300	1.22400	-0.17500
C	2.31700	0.15400	0.04000
S	1.43000	-1.35700	0.34900
C	3.76700	0.21300	0.05800
C	4.55500	1.31300	0.38300
S	4.78700	-1.14900	-0.40100
C	5.95400	1.06300	0.26700
C	6.23700	-0.22700	-0.13600

H	-4.30800	2.23700	0.24500
H	-6.85400	1.53900	0.17500
H	-7.13800	-1.08900	-0.06800
H	-1.81200	-1.94200	0.45400
H	1.80900	2.22400	-0.40900
H	4.12500	2.25300	0.72400
H	6.72400	1.80000	0.48900
H	7.20800	-0.69100	-0.28700

1-H-AA

C	3.76900	0.16900	0.04000
C	4.58900	1.28000	0.21800
C	5.98100	0.97000	0.18600
C	6.22800	-0.37300	-0.01300
S	4.75200	-1.27800	-0.18300
C	2.32200	0.10100	0.02000
C	1.50600	-1.01700	0.17500
S	1.36500	1.58100	-0.23100
C	0.12900	-0.68300	0.10300
C	-0.12900	0.68300	-0.10200
C	-1.50600	1.01700	-0.17500
C	-2.32200	-0.10100	-0.02000
S	-1.36500	-1.58100	0.23200
C	-3.76900	-0.16900	-0.04000
C	-4.58900	-1.28000	-0.21800
S	-4.75200	1.27800	0.18300
C	-5.98100	-0.97000	-0.18600
C	-6.22800	0.37300	0.01300
H	4.19300	2.28000	0.38700
H	6.77100	1.70900	0.31600
H	7.18500	-0.88400	-0.07100
H	1.90100	-2.01500	0.35300
H	-1.90100	2.01500	-0.35300
H	-4.19200	-2.28000	-0.38700
H	-6.77100	-1.70900	-0.31600
H	-7.18500	0.88400	0.07100

SCF energy: -2130.635872 hartree
zero-point correction: +0.169659 hartree
enthalpy correction: +0.186466 hartree
free energy correction: +0.123565 hartree
quasiharmonic free energy correction: +0.127612 hartree

Et-syn-syn

C	3.76300	0.34800	-0.11100
C	4.69300	-0.45800	0.54900
C	6.04000	-0.03400	0.31000
C	6.13900	1.07300	-0.50300

S	4.57600	1.62400	-1.02200
C	2.31600	0.22700	-0.11700
C	1.56400	-0.94300	-0.11200
S	1.27100	1.67200	-0.08500
C	0.16800	-0.68200	-0.08300
C	-0.16800	0.68200	-0.08400
C	-1.56400	0.94300	-0.11200
C	-2.31600	-0.22700	-0.11700
S	-1.27100	-1.67200	-0.08400
C	-3.76300	-0.34800	-0.11100
C	-4.69300	0.45800	0.54900
S	-4.57600	-1.62400	-1.02200
C	-6.04000	0.03400	0.31000
C	-6.13900	-1.07300	-0.50300
C	4.35500	-1.64200	1.42500
C	4.53900	-2.99400	0.69500
C	-4.35500	1.64200	1.42500
C	-4.53900	2.99400	0.69500
H	6.90400	-0.53200	0.74900
H	7.03500	1.59900	-0.82300
H	2.01800	-1.92900	-0.16100
H	-2.01800	1.92900	-0.16100
H	-6.90400	0.53200	0.74900
H	-7.03500	-1.59900	-0.82300
H	5.01000	-1.62600	2.31100
H	3.31900	-1.55200	1.78500
H	4.28300	-3.83400	1.36000
H	3.90200	-3.05100	-0.20000
H	5.58200	-3.11800	0.36500
H	-5.01000	1.62600	2.31100
H	-3.31900	1.55200	1.78500
H	-5.58200	3.11700	0.36500
H	-4.28300	3.83400	1.36000
H	-3.90200	3.05100	-0.20000

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