Electronic Supplementary Material (ESI) for Nanoscale.

The Crucial Role of a Spacer Material on the Efficiency of Charge Transfer Processes in Organic Donor-Acceptor Junction Solar Cells

Supplementary Information

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Computational details

The two types of trimer structures are shown in Figure 1a (standard trimer) and Figure 1b,c (extended trimer). All structures were optimized as isolated complexes using DFT together with the Perdew–Burke–Ernzerhof (PBE)[1] functional, the SV(P)[2] basis, and the Multipole-Accelerated Resolution of the Identity for the Coulomb energy (MARI-J).[3] Empirical dispersion corrections were added by means of the D3[4] approach. Excited states were calculated using the long-range separated density functional, CAM-B3LYP, and two basis sets, 6-31G[5] and 6-31G*[6, 7]. D3 dispersion corrections were used for the CAM-B3LYP TD-DFT calculations as well.

Full geometry optimizations of the standard and extended trimer structures would lead to distorted geometries which do not resemble the intended structural arrangements of a donor-spacer-C_{60} interface since geometrical restrictions of the surrounding environment are missing. To achieve the desired model arrangement, geometry optimization was performed in steps and by freezing a few selected atoms (see Figure 1) to restrict the structural manifold. For the standard trimer, the C_{60} and T3 monomers were combined and optimized freezing selected atoms. To this C_{60}-T3 structure, P3HT was added as shown in Figure 1a. The whole complex (C_{60}-T3-P3HT) was then optimized. The frozen atoms were located at the end of the chains and at the opposite side of C_{60}, respectively, so that the subunits had sufficient flexibility to come in contact allowing the intersystem distances to be optimized. For the extended trimer, an analogous restricted geometry optimization technique was used as shown in Figure 2b, c.

Since the main objective of this investigation was to determine the relative stability of the CT states with excitations from the π-conjugated polymers to the C_{60}s and the local excitations in the polymers, excitations within the fullerenes were suppressed in most of the calculations by freezing in the TD-DFT calculations the occupied orbitals located on the C_{60} units. Otherwise, about a dozen of local excitations per C_{60} unit would have impeded the already expensive calculations and would not have allowed the focus on the actual states of interest. In practice, all the core orbitals along with twenty percent of the highest occupied orbitals, which were localized at the C_{60} and $(C_{60})_3$ units, were kept frozen. Comparison between full and frozen orbital calculations have been performed as well, showing good agreement in energetic ordering of the remaining states in the two calculations.

Solvent effects were taken into account using the conductor-like polarizable continuum model (C-PCM)[8]. Environmental effects on the electronically excited states were investigated on

the basis of the linear response (LR)[9, 10] and state-specific (SS)[11] approaches. In the LR approach, Hartree and exchange-correlation (XC) potentials are linearly expanded with respect to the variation of the time-dependent density of the ground state. In the SS method, the solvation field adapts to changes in the solute wave function for electronic excitations where the energy correction from fast electronic relaxation of the solvent is state-dependent. SS is considered more accurate for describing the excited electronic states[12-14] with charge distributions significantly different from the ground state such as with polar solvents or CT states in the solute. The SS method is computationally significantly more demanding though and requires that each state be calculated independently. As such, only five states were calculated using the CAM-B3LYP/6-31G* method for the extended trimer which contained, however, representatives of the most important excitation types. For the extended trimer using the CAM-B3LYP/6-31G method, twenty states were calculated, and for the standard trimer using both basis sets, ten states were considered. Dichloromethane (dielectric constant, ε=8.93, refractive index, n=1.42) was chosen to act as a modestly polar environment.

Table S1: Excitation energies Ω of the isolated standard C60-T3-P3HT system using the CAM-B3LYP/6-31G approach

Exc.	Ω(eV)	f	CT	Direction of CT	Location of exciton
S_1	2.69	2.08	0.00		P3HT
S_2	2.83	0.00	0.97	P3HT→C_{60}	
S_3	2.84	0.00	1.00	P3HT→C_{60}	
S_4	2.85	0.00	0.99	P3HT→C_{60}	
S_5	2.87	0.00	0.99	T3→C_{60}	
S_6	2.87	0.00	0.99	T3→C_{60}	
S_7	2.93	0.00	0.99	T3→C_{60}	
S_8	3.41	1.18	0.01		T3
S_9	3.47	0.10	0.00		P3HT
S_{10}	3.63	0.00	0.97	P3HT→C_{60}	
S_{11}	3.63	0.00	1.00	P3HT→C_{60}	
S_{12}	3.65	0.00	0.99	P3HT→C_{60}	
S_{13}	3.92	0.02	0.00		P3HT
S_{14}	3.92	0.02	0.94	T3→C_{60}	
S_{15}	3.93	0.01	0.94	T3→C_{60}	
S_{16}	4.10	0.00	0.98	P3HT→C_{60}	
S_{17}	4.11	0.00	0.98	P3HT→C_{60}	
S_{18}	4.12	0.00	0.99	P3HT→C_{60}	
S_{19}	4.14	0.02	0.95	T3→C_{60}	
S_{20}	4.16	0.00	0.99	T3→C_{60}	

Table S2: Excitation energies Ω of the isolated standard C60-T3-P3HT system using the CAM-B3LYP/6-31G* approach

Exc.	Ω (eV)	f	CT	Direction of CT	Location of exciton
S_1	2.62	2.04	0.00		P3HT
S_2	2.91	0.00	0.97	P3HT→C_{60}	
S_3	2.91	0.00	1.00	P3HT→C_{60}	
S_4	2.92	0.00	0.99	P3HT→C_{60}	
S_5	2.93	0.00	0.99	T3→C_{60}	
S_6	2.94	0.00	0.99	T3→C_{60}	
S_7	2.99	0.00	0.99	T3→C_{60}	
S_8	3.33	1.16	0.01		T3
S_9	3.39	0.10	0.00		P3HT
S_{10}	3.70	0.00	0.97	P3HT→C_{60}	
S_{11}	3.70	0.00	1.00	P3HT→C_{60}	
S_{12}	3.71	0.00	0.99	P3HT→C_{60}	
S_{13}	3.87	0.02	0.00		P3HT
S_{14}	3.99	0.02	0.94	T3→C_{60}	
S_{15}	3.99	0.03	0.94	T3→C_{60}	
S_{16}	4.20	0.03	0.95	T3→C_{60}	
S_{17}	4.23	0.00	0.98	P3HT→C_{60}	
S_{18}	4.24	0.00	0.98	P3HT→C_{60}	
S_{19}	4.25	0.00	0.99	P3HT→C_{60}	
S_{20}	4.27	0.00	0.99	T3→C_{60}	

Table S3: Lowest excitation energies Ω of the isolated components P3HT, T3 and C60 using the CAM-B3LYP/6-31G* approach.

Exc.	Ω (eV)	f
	P3HT	
S_1	2.62	2.10
S_2	3.39	0.00
S_3	3.87	0.02
S_4	4.06	0.14
S_5	4.49	0.01
S_6	4.63	0.00
S_7	4.84	0.04
S_8	4.86	0.00
S_9	4.89	0.00
S_{10}	4.93	0.01
	T3	
S_1	3.30	1.09
S_2	4.54	0.00
S_3	4.91	0.00
S_4	5.07	0.00
S_5	5.13	0.00
S_6	5.15	0.01
S_7	5.24	0.01
S_8	5.30	0.06
S_9	5.41	0.00
S_{10}	5.43	0.02
	C60	
S_1	2.47	0.00
S_2	2.47	0.00
S_3	2.47	0.00
S_4	2.53	0.00
S_5	2.53	0.00
S_6	2.53	0.00
S_7	2.56	0.00
S_8	2.56	0.00
S_9	2.56	0.00
S_{10}	2.57	0.00

Table S4: Excitation energies Ω of the standard C60-T3-P3HT system the using the CAM-B3LYP/6-31G* approach in the LR environment

Exc.	Ω (eV)	f	CT	Direction of CT	Location of exciton
S_1	2.53	2.22	0.00		P3HT
S_2	3.12	0.00	0.97	P3HT→C_{60}	
S_3	3.12	0.00	1.00	P3HT→C_{60}	
S_4	3.13	0.00	0.99	P3HT→C_{60}	
S_5	3.22	0.60	0.57	T3→C_{60}	
S_6	3.23	0.14	0.90	T3→C_{60}	
S_7	3.24	0.48	0.56	T3→C_{60}	
S_8	3.27	0.10	0.00		P3HT
S_9	3.29	0.02	0.99	T3→C_{60}	
S_{10}	3.87	0.01	0.00		P3HT
S_{11}	3.91	0.00	0.97	P3HT→C_{60}	
S_{12}	3.91	0.00	1.00	P3HT→C_{60}	
S_{13}	3.92	0.00	0.99	P3HT→C_{60}	
S_{14}	3.98	0.19	0.00		P3HT
S_{15}	4.28	0.01	0.85	T3→C_{60}	
S_{16}	4.29	0.13	0.86	T3→C_{60}	
S_{17}	4.37	0.00	1.00	P3HT→T3	
S_{18}	4.45	0.00	0.97	P3HT→C_{60}	
S_{19}	4.45	0.00	0.99	P3HT→C_{60}	
S_{20}	4.46	0.00	0.99	P3HT→C_{60}	

Table S5: Excitation energies Ω of the standard C60-T3-P3HT system the using the CAM-B3LYP/6-31G approach in the LR environment

Exc.	Ω (eV)	f	CT	Direction of CT	Location of exciton
S_1	2.60	2.26	0.0		P3HT
S_2	3.08	0.00	0.97	P3HT→C_{60}	
S_3	3.08	0.00	1.00	P3HT→C_{60}	
S_4	3.09	0.00	0.98	P3HT→C_{60}	
S_5	3.20	0.01	0.99	T3→C_{60}	
S_6	3.21	0.01	0.99	T3→C_{60}	
S_7	3.27	0.02	0.99	T3→C_{60}	
S_8	3.32	1.21	0.01		T3
S_9	3.35	0.09	0.00		P3HT
S_{10}	3.87	0.00	0.97	P3HT→C_{60}	
S_{11}	3.88	0.00	1.00	P3HT→C_{60}	
S_{12}	3.89	0.00	0.98	P3HT→C_{60}	
S_{13}	3.92	0.01	0.00		P3HT
S_{14}	4.08	0.20	0.00		P3HT
S_{15}	4.28	0.05	0.91	T3→C_{60}	
S_{16}	4.28	0.04	0.91	T3→C_{60}	
S_{17}	4.35	0.00	1.00	P3HT→C_{60}	
S_{18}	4.35	0.00	0.98	P3HT→C_{60}	
S_{19}	4.36	0.00	0.99	P3HT→C_{60}	
S_{20}	4.40	0.00	1.00	P3HT→T3	

Table S6: Excitation energies Ω of the standard C60-T3-P3HT system using the CAM-B3LYP/6-31G* approach in the SS environment

Exc.	Ω (eV)	f	Direction of CT	Location of Exciton
S_1	1.29	0.00	P3HT→C_{60}	
S_2	1.29	0.00	P3HT→C_{60}	
S_3	1.29	0.00	P3HT→C_{60}	
S_4	1.29	0.00	P3HT→C_{60}	
S_5	1.88	0.00	T3→C_{60}	
S_6	1.88	0.00	T3→C_{60}	
S_7	1.88	0.00	T3→C_{60}	
S_8	1.88	0.00	T3→C_{60}	
S_9	1.90	0.00	T3→C_{60}	
S_{10}	2.63	2.04		P3HT

Table S7: Excitation energies Ω of the standard C60-T3-P3HT system using the CAM-B3LYP/6-31G approach in the SS environment

Exc.	Ω (eV)	f	CT	Direction of CT	Location of Exciton
S_1	1.23	0.00	1.00	P3HT→C_{60}	
S_2	1.23	0.00	1.00	P3HT→C_{60}	
S_3	1.24	0.00	1.00	P3HT→C_{60}	
S_4	1.84	0.00	1.00	T3→C_{60}	
S_5	1.84	0.00	1.00	T3→C_{60}	
S_6	1.86	0.00	1.00	T3→C_{60}	
S_7	2.06	0.00	1.00	P3HT→C_{60}	
S_8	2.06	0.00	1.00	P3HT→C_{60}	
S_9	2.07	0.00	1.00	P3HT→C_{60}	
S_{10}	2.70	2.07	0.00		P3HT

Table S8: Excitation energies Ω of the isolated standard C60-T3-P3HT system using the CAM-B3LYP/6-31G* approach (only core orbitals were frozen)

Exc.	Ω (eV)	f	CT	Direction of CT	Location of exciton
S_1	2.47	0.00	0.01		C60
S_2	2.47	0.00	0.00		C60
S_3	2.48	0.00	0.01		C60
S_4	2.52	0.00	0.01		C60
S_5	2.53	0.00	0.00		C60
S_6	2.53	0.00	0.01		C60
S_7	2.56	0.00	0.01		C60
S_8	2.56	0.00	0.01		C60
S_9	2.57	0.00	0.00		C60
S_{10}	2.57	0.00	0.00		C60
S_{11}	2.62	2.03	0.00		P3HT
S_{12}	2.84	0.00	0.01		C60
S_{13}	2.85	0.00	0.01		C60
S_{14}	2.85	0.00	0.01		C60
S_{15}	2.86	0.00	0.01		C60
S_{16}	2.86	0.00	0.01		C60
S_{17}	2.91	0.00	1.00	P3HT$\rightarrow$$C_{60}$	
S_{18}	2.91	0.00	1.00	P3HT$\rightarrow$$C_{60}$	
S_{19}	2.92	0.00	1.00	P3HT$\rightarrow$$C_{60}$	
S_{20}	2.93	0.00	1.00	T3$\rightarrow$$C_{60}$	

Table S9: Excitation energies Ω of the isolated extended $(C60)_3$-$(T3)_3$-P3HT system using the CAM-B3LYP/6-31G* approach

Exc.	Ω (eV)	f	CT	Direction of CT	Location of exciton
1 ^{1}A	2.33	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
2 ^{1}A	2.37	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
3 ^{1}A	2.38	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
4 ^{1}A	2.56	0.01	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
5 ^{1}A	2.59	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
6 ^{1}A	2.62	0.00	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
7 ^{1}A	2.67	1.92	0.00		P3HT
8 ^{1}A	2.74	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
9 ^{1}A	2.75	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
10 ^{1}A	2.76	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
11 ^{1}A	2.78	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
12 ^{1}A	2.79	0.00	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
13 ^{1}A	2.80	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
14 ^{1}A	2.81	0.00	0.98	$(T3)_3 \rightarrow (C_{60})_3$	
15 ^{1}A	2.82	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
16 ^{1}A	2.82	0.00	1.00	$P3HT \rightarrow (C_{60})_3$	
17 ^{1}A	2.83	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
18 ^{1}A	2.85	0.00	1.00	$P3HT \rightarrow (C_{60})_3$	
19 ^{1}A	2.89	0.00	1.00	$P3HT \rightarrow (C_{60})_3$	
20 ^{1}A	2.96	0.00	0.97	$(T3)_3 \rightarrow (C_{60})_3$	
21 ^{1}A	2.96	0.00	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
22 ^{1}A	2.97	0.00	0.98	$(T3)_3 \rightarrow (C_{60})_3$	
23 ^{1}A	3.02	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
24 ^{1}A	3.04	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
25 ^{1}A	3.05	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
26 ^{1}A	3.06	0.00	1.00	$P3HT \rightarrow (C_{60})_3$	
27 ^{1}A	3.07	0.00	1.00	$P3HT \rightarrow (C_{60})_3$	
28 ^{1}A	3.08	0.00	1.00	$P3HT \rightarrow (C_{60})_3$	
29 ^{1}A	3.10	0.00	0.10		$(T3)_3$
30 ^{1}A	3.14	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
31 ^{1}A	3.15	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
32 ^{1}A	3.15	0.00	1.00	$P3HT \rightarrow (C_{60})_3$	
33 ^{1}A	3.16	0.00	1.00	$P3HT \rightarrow (C_{60})_3$	

34 ^{1}A	3.16	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
35 ^{1}A	3.17	0.00	1.00	P3HT$\rightarrow(C_{60})_3$	
36 ^{1}A	3.26	0.07	0.03		$(T3)_3$
37 ^{1}A	3.28	0.00	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
38 ^{1}A	3.29	0.00	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
39 ^{1}A	3.29	0.00	0.97	$(T3)_3 \rightarrow (C_{60})_3$	
40 ^{1}A	3.43	1.38	0.03		P3HT/$(T3)_3$

Table S10: Excitation energies Ω of the isolated extended $(C60)_3$-$(T3)_3$-P3HT system using the CAM-B3LYP/6-31G approach

Exc.	Ω (eV)	f	CT	Direction of CT	Location of exciton
S_1	2.24	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_2	2.28	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_3	2.30	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_4	2.47	0.01	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
S_5	2.51	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_6	2.54	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_7	2.68	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_8	2.69	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_9	2.70	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{10}	2.71	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{11}	2.72	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{12}	2.73	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{13}	2.73	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	
S_{14}	2.74	1.96	0.00		P3HT
S_{15}	2.75	0.00	0.98	$(T3)_3 \rightarrow (C_{60})_3$	
S_{16}	2.75	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{17}	2.76	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	
S_{18}	2.77	0.00	0.97	$(T3)_3 \rightarrow (C_{60})_3$	
S_{19}	2.79	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	
S_{20}	2.92	0.00	0.98	$(T3)_3 \rightarrow (C_{60})_3$	
S_{21}	2.92	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{22}	2.93	0.00	0.97	$(T3)_3 \rightarrow (C_{60})_3$	
S_{23}	2.96	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{24}	2.97	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{25}	2.99	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{26}	3.00	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	
S_{27}	3.01	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	
S_{28}	3.02	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	
S_{29}	3.07	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{30}	3.08	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{31}	3.09	0.00	1.00	$(T3)_3 \rightarrow (C_{60})_3$	
S_{32}	3.10	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	
S_{33}	3.11	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	
S_{34}	3.11	0.00	1.00	P3HT$\rightarrow (C_{60})_3$	

S_{35}	3.15	0.00	0.11		$(T3)_3$
S_{36}	3.23	0.00	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
S_{37}	3.23	0.00	0.99	$(T3)_3 \rightarrow (C_{60})_3$	
S_{38}	3.24	0.00	0.97	$(T3)_3 \rightarrow (C_{60})_3$	
S_{39}	3.32	0.10	0.03		$(T3)_3$
S_{40}	3.49	1.97	0.08		$(T3)_3$

Table S11: Excitation energies Ω of the extended C60-T3-P3HT system using the CAM-B3LYP/6-31G approach in the SS environment

Exc.	Ω (eV)	f	CT	Direction of CT	Location of exciton
S_1	1.59	0.00	1.00	P3HT→$(C_{60})_3$	
S_2	1.59	0.00	1.00	P3HT→$(C_{60})_3$	
S_3	1.60	0.00	1.00	P3HT→$(C_{60})_3$	
S_4	1.61	0.00	1.00	P3HT→$(C_{60})_3$	
S_5	1.77	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_6	1.77[a]	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_7	1.88	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_8	1.91	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_9	1.91	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{10}	1.91	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{11}	1.91	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{12}	2.10	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{13}	2.10	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{14}	2.10	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{15}	2.12	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{16}	2.12	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{17}	2.13	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{18}	2.13	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{19}	2.21[b]	0.00	1.00	$(T3)_3$→$(C_{60})_3$	
S_{20}	2.75	1.92	0.00		P3HT

[a]Excitation energy averaged over two oscillating energies: 1.77 eV and 1.76 eV, [b]Excitation energy averaged over three oscillating energies: 2.12 eV, 2.21 eV, 2.29 eV

Cartesian coordinates of the standard thiophene trimer optimized using the PBE/SV(P) method

C	3.1788433	-3.3404777	8.7294822
C	2.1629913	1.9236048	4.2388618
C	4.1932961	-2.6019358	9.3660229
C	3.1778863	2.6620684	4.8745973
C	0.9111888	0.5207736	9.4177558
C	5.6498111	-2.2595722	5.0899862
C	0.7072100	1.5797260	8.5142357
C	5.4457160	-1.2004282	4.1863733
C	5.2231193	1.7759497	8.8185697
C	6.1760029	1.2165311	7.9477714
C	1.7887723	-2.9153880	8.8404798
C	3.3868397	-3.8532528	7.3812431
C	0.9038546	1.6708448	4.9280168
C	3.8543610	-1.4115747	10.1364448
C	2.5027054	0.7326668	3.4705591
C	5.4522949	-2.3493070	8.6766978
C	2.9698170	3.1748710	6.2229336
C	4.5678397	2.2365672	4.7631986
C	0.4723816	-0.8257546	9.0736018
C	4.6001638	-3.2476720	5.3034574
C	0.0560245	1.3304607	7.2343982
C	2.1723050	0.4125604	10.1403882
C	4.1847892	-1.0928887	3.4645885
C	6.3001643	-2.0096791	6.3699936
C	1.7564833	2.5685534	8.3008657
C	5.8842093	0.1463539	4.5304211
C	0.1827602	-2.2568749	7.0684542
C	2.1226607	-3.3960890	5.2954145
C	-0.1614767	-0.4822977	5.5540328
C	4.5756743	0.9416625	9.8234645
C	1.7802812	-1.6217357	3.7794169
C	6.5163764	-0.1971328	8.0505971
C	4.2335543	2.7169456	8.3085353
C	6.1731903	1.5774043	6.5354837
C	4.8957248	1.0877906	4.0196072
C	1.7544677	2.9302593	6.8884018
C	5.6527671	-2.8441248	7.3752138
C	3.8442756	0.3225384	3.3604780
C	2.5127749	-1.0013486	10.2433980
C	0.7034818	2.1651094	6.2296245
C	4.6023063	-3.6095170	6.7161106
C	1.4615750	-1.7665152	9.5838030
C	6.5119545	0.3871767	5.7658266
C	2.9740209	2.4637688	8.9981774
C	6.7240987	-0.7097519	6.7018760
C	3.1709557	-2.0460747	3.6713027
C	3.1855132	1.3668032	9.9342626
C	-0.3683533	0.0303108	6.9025884
C	3.3826240	-3.1430356	4.6062261
C	-0.1559445	-1.0668030	7.8383930
C	5.2186901	2.4858739	6.0433069
C	4.2315761	3.0660226	6.9455455
C	5.8917711	-1.0023745	9.0206871
C	1.4527560	-0.2566492	3.6857552
C	4.9044900	-0.4228600	9.9228900

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C     0.4646591    0.3235571    4.5852359
C     2.1248046   -3.7449111    6.6581974
C     1.1378850   -3.1648356    7.5604205
C     1.1328394   -2.4553776    4.7848566
C     0.1801624   -1.8958669    5.6560339
H    -6.0650875    2.7125604  -10.8532304
H    -1.3800760    1.1845181   -7.5117040
H     0.0068568    0.9586814   -5.2741936
H    -5.8144573    2.6281924  -13.3634146
S    -4.0092456    1.5136000   -8.9035757
C    -1.8223752    0.9159620   -6.5402518
C    -1.0787253    0.7892320   -5.3413420
C    -6.1216965    1.5996433  -10.7894357
H    -5.5004859    2.5977017  -15.9054685
H     1.6357431    0.8657088    0.2323183
C    -5.6302500    1.1412700   -9.4453200
S     0.2458709    0.3403016   -2.4062605
C    -3.1838603    0.6499844   -6.3848464
C    -5.8886589    1.5141855  -13.3451263
H    -7.2028625    1.3429161  -10.8576885
C    -1.8513408    0.4225165   -4.2377820
C    -4.2444793    0.6910043   -7.3686391
C    -5.3733720    0.9973138  -11.9954969
C    -1.4438404    0.2113002   -2.8654838
H    -4.2858923    1.2271622  -11.9017870
C    -5.5826059    1.4853137  -15.9067990
H    -6.9755877    1.2807902  -13.4450004
C     0.9716800   -0.0225886    0.3010553
C    -0.1096700    0.0157000   -0.7254500
C    -6.3063718    0.4201528   -8.4722341
S    -3.5325054    0.2434094   -4.7131173
C    -5.5336142    0.1652119   -7.3042301
C    -5.1289946    0.9382520  -14.5462370
H    -4.0388282    1.1442651  -14.4187616
H    -6.6666390    1.2663216  -16.0579095
C    -2.2232074   -0.0904036   -1.7476595
H     0.5082800   -0.0247917    1.3114517
C    -1.4683454   -0.2036647   -0.5484934
H    -5.0890975    1.3692217  -18.0418736
C    -4.7730619    0.9177443  -17.0769111
H    -3.6856092    1.1222917  -16.9498139
H    -7.3464061    0.0841890   -8.6057475
H     3.0804600   -1.0703047    0.8558330
H    -3.3153472   -0.2178138   -1.8011185
H    -5.8994181   -0.4026978   -6.4349046
S     2.0282503   -1.5392970    0.1134278
H    -5.4546791   -0.1137828  -11.9554163
H    -1.9047409   -0.4347481    0.4356666
H    -5.2270602   -0.1741923  -14.5452561
H    -4.8958974   -0.1867399  -17.1560598
H   -11.7860250    5.1898952  -16.0268700
H   -18.5926865    1.6635340  -12.5921539
H    -5.1535970    8.2423002  -19.0021217
H   -19.3799083    1.6577121  -14.1996120
C   -18.9567699    0.9988644  -13.4079196
C   -12.1487150    4.1407320  -16.0485265
H    -6.5915936    7.2386428  -19.3902449
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H	-13.1385820	4.1368388	-16.5597800
C	-5.5341566	7.1999917	-19.0424890
H	-12.3278743	3.8203689	-14.9972206
H	-19.7862224	0.3842989	-12.9992387
H	-5.5510789	6.8059427	-18.0007238
H	-16.4458642	1.7259108	-14.6460102
H	-9.7262165	4.8152660	-17.3856979
H	-3.2062558	7.9096898	-20.5194546
C	-17.8467300	0.1373300	-13.9485700
C	-11.1562079	3.2500067	-16.7459431
C	-16.6527600	0.6486300	-14.5425100
C	-9.9814921	3.7440955	-17.3694868
C	-4.6764948	6.3565353	-19.9470172
C	-3.5340609	6.8629514	-20.6193728
S	-13.8124497	1.4921550	-15.6960936
S	-7.2016281	4.5636349	-18.6710842
S	-0.8410700	7.7106500	-22.0794500
C	-17.8547164	-1.2495278	-13.9473804
C	-11.2811371	1.8537275	-16.8793970
C	-15.7510068	-0.3296243	-14.9697894
C	-4.8992011	4.9960176	-20.2343451
C	-9.1850382	2.7773565	-17.9922541
C	-2.8554013	5.9407419	-21.4201074
C	-12.3169912	0.9482012	-16.4434995
H	-18.6428738	-1.9164591	-13.5708879
C	-14.4428610	-0.1417965	-15.5620853
C	-5.9338277	4.0920759	-19.7938299
C	-7.9606180	2.9785779	-18.7279291
H	1.2050720	7.9204683	-23.4407526
C	0.3988934	7.2220911	-23.1780342
C	-1.6548903	6.1545401	-22.1998726
S	-16.4252100	-1.9255000	-14.6473000
S	-9.9178951	1.1946046	-17.7741163
S	-3.6689682	4.3873948	-21.3324764
C	-12.3409794	-0.4449388	-16.5572180
C	-13.5183167	-1.0721252	-16.0712549
C	-6.1131595	2.7522453	-20.1543382
C	0.2052600	5.9274900	-23.6172200
C	-7.2338535	2.1113250	-19.5663057
C	-0.9629500	5.3021700	-23.0779600
H	-11.5059407	-1.0152687	-16.9940790
H	0.8813968	5.4213832	-24.3235780
H	-5.4337512	2.2332233	-20.8484638
C	-13.7210218	-2.5628201	-16.1071925
C	-1.3680593	3.8926129	-23.4159346
H	-2.4085768	3.8405178	-23.8089542
C	-7.5762894	0.6688544	-19.8207263
H	-14.6475768	-2.8431967	-16.6578357
H	-13.8119471	-2.9941595	-15.0838519
H	-8.6249532	0.5446203	-20.1726956
H	-7.4683698	0.0540386	-18.8979386
H	-1.3258550	3.2228853	-22.5263665
H	-0.6931645	3.4663999	-24.1881172
H	-12.8647905	-3.0623344	-16.6074107
H	-6.9032375	0.2366353	-20.5908281

Cartesian coordinates of the extended thiophene trimer optimized using the PBE/SV(P) method

C	-11.1836400	-1.8013000	0.8684000
C	-10.6280537	-0.9349744	-0.0601851
C	-9.2104831	-0.8741190	-0.0092520
C	-8.6575407	-1.6954616	0.9697816
S	-9.9306216	-2.5398714	1.8364912
C	-4.7434830	-1.8515110	1.3130245
C	-5.2863454	-2.6852699	2.2943348
C	-6.7015258	-2.7179561	2.2846980
C	-7.2691183	-1.9095701	1.2957100
S	-6.0186260	-1.0985222	0.3772771
C	-12.6333596	-2.0909184	1.1389842
C	-13.1900418	-1.3834968	2.3926525
C	-14.7155996	-1.4668327	2.5311569
C	-15.2635755	-0.5392801	3.6233554
C	-16.7941829	-0.4963806	3.7222655
C	-17.2952849	0.4899346	4.7814011
C	-0.8433000	-1.4757200	0.9899200
C	-1.4250306	-0.7765564	-0.0564032
C	-2.8417784	-0.8332735	-0.0558998
C	-3.3628855	-1.5750822	1.0026232
S	-2.0662728	-2.1969362	2.0107940
C	0.6108229	-1.6244486	1.2776245
S	1.0615344	-0.8329834	2.8986998
C	-11.5693900	2.3395800	1.5824900
C	-11.0067493	1.7552171	2.7077908
C	-9.5886583	1.6543270	2.6574829
C	-9.0390962	2.1688125	1.4856090
S	-10.3163842	2.7831442	0.4447472
C	-5.1162140	2.2670912	1.0711936
C	-5.6836447	2.5164018	-0.1800481
C	-7.1010226	2.5051149	-0.1713551
C	-7.6506252	2.2510946	1.0874077
S	-6.3737759	2.0459603	2.2731853
C	-13.0274416	2.5248277	1.2602135
C	-13.5281891	1.6145858	0.1164277
C	-15.0543059	1.4717974	0.0347400
C	-15.4954247	0.3941661	-0.9677659
C	-16.9754994	-0.0033645	-0.8797526
C	-17.3287767	-1.1769048	-1.7985268
C	-1.1970700	2.2836200	1.4645700
C	-1.7247741	1.5914280	2.5450929
C	-3.1449950	1.5281360	2.5391377
C	-3.7209193	2.1674215	1.4420365
S	-2.4759110	2.8703974	0.4228568
C	0.2404968	2.5462605	1.1495144
S	0.6056704	2.1445536	-0.6269353
H	-11.2348222	-0.3615929	-0.7757143
H	-8.5965520	-0.2506818	-0.6757671
H	-4.6623365	-3.2628642	2.9935631
H	-7.3077674	-3.3183997	2.9801406
H	-12.8075971	-3.1895281	1.2185077
H	-13.2130485	-1.7531682	0.2497874

H	-12.8835261	-0.3159107	2.3444880
H	-12.6960593	-1.7972721	3.3020750
H	-15.0278434	-2.5186815	2.7330066
H	-15.1861986	-1.1932131	1.5575580
H	-14.8894149	0.4964866	3.4327562
H	-14.8365576	-0.8344004	4.6115817
H	-17.1799526	-1.5199515	3.9431468
H	-17.2219346	-0.2221820	2.7281407
H	-16.9597887	1.5269682	4.5532705
H	-16.9077486	0.2289807	5.7925385
H	-18.4048337	0.5076350	4.8360449
H	-0.8278033	-0.2411477	-0.8078000
H	-3.4781843	-0.3545432	-0.8146993
H	0.9181012	-2.6919377	1.3288492
H	1.1833124	-1.1322343	0.4631718
H	2.3231702	-1.3641601	2.9709948
H	-11.6152876	1.3989729	3.5529410
H	-8.9743664	1.1947647	3.4466354
H	-5.0745240	2.6698329	-1.0838720
H	-7.7227585	2.6599296	-1.0665334
H	-13.2533321	3.5904496	1.0222821
H	-13.5962054	2.2875332	2.1879853
H	-13.0881289	0.6061446	0.2695638
H	-13.1202391	1.9760032	-0.8559272
H	-15.5255077	2.4503045	-0.2201416
H	-15.4410156	1.2011841	1.0457199
H	-14.8810155	-0.5235468	-0.7979803
H	-15.2543385	0.7215724	-2.0069703
H	-17.6205548	0.8759729	-1.1164413
H	-17.2179887	-0.2765079	0.1749699
H	-16.6890450	-2.0613339	-1.5774127
H	-17.1699212	-0.9220263	-2.8709326
H	-18.3855339	-1.4981473	-1.6773895
H	-1.0909096	1.1177517	3.3089480
H	-3.7402415	0.9820032	3.2863997
H	0.5051792	3.6156979	1.3047646
H	0.8721973	1.9162720	1.8129597
H	1.7842739	2.8388198	-0.6955249
S	2.1008674	-3.7497279	-3.7551390
C	1.4641516	-3.1744107	-2.1094144
C	0.0103000	-3.4659800	-1.9524600
C	-0.6028088	-4.2642077	-0.9970881
S	-1.1854151	-2.7247679	-2.9922592
C	-2.0211552	-4.2561401	-1.0732055
C	-2.5139856	-3.4533116	-2.1021040
C	-3.8861906	-3.1641477	-2.4515816
C	-4.3939970	-2.1785958	-3.3012866
S	-5.2022998	-4.0839479	-1.7413648
C	-5.8086170	-2.1565534	-3.3640183
C	-6.4200915	-3.1242832	-2.5626608
C	-7.8255655	-3.3711248	-2.3329328
C	-8.4291664	-4.2193183	-1.4041708
S	-9.0616166	-2.5156309	-3.2426437
C	-9.8483047	-4.1676285	-1.4271811
C	-10.3602900	-3.2789400	-2.3618400
C	-11.7993185	-2.9221539	-2.6168493
C	-12.6445741	-4.0008189	-3.3247475

C	-14.1367337	-3.6386259	-3.3478335
C	-15.0226921	-4.6603378	-4.0725433
C	-16.5202272	-4.3214167	-4.0396368
C	-17.3908640	-5.3165706	-4.8126488
H	-10.4905758	-4.7422903	-0.7427097
H	-7.8474717	-4.8320984	-0.6984946
H	-3.7446003	-1.4762789	-3.8465629
H	-6.3845989	-1.4344855	-3.9626161
H	-11.8589453	-1.9716630	-3.1933065
H	-12.2671983	-2.7053949	-1.6293431
H	-12.5047996	-4.9755993	-2.8026241
H	-12.2658173	-4.1502685	-4.3620074
H	-14.2677845	-2.6357375	-3.8214326
H	-14.4966509	-3.5189170	-2.2970629
H	-14.8654863	-5.6708330	-3.6238819
H	-14.6884496	-4.7477492	-5.1341144
H	-16.6724985	-3.2943647	-4.4486819
H	-16.8659579	-4.2719137	-2.9802438
H	-17.2939776	-6.3470454	-4.4015212
H	-17.1003427	-5.3606210	-5.8872386
H	-18.4666505	-5.0424950	-4.7658156
H	-0.0318175	-4.8253548	-0.2410971
H	-2.6783559	-4.7937069	-0.3733188
H	1.6697488	-2.0826467	-2.0307753
H	2.0232962	-3.6842812	-1.2956407
H	3.3095577	-3.1127590	-3.6560118
C	9.1574028	-8.4794361	-7.1400158
C	10.3317258	-1.7052475	0.1228037
C	8.8055288	-7.9830529	-5.8711388
C	9.5562353	5.4688672	10.0264681
C	10.0373595	-1.4970543	1.4830597
C	9.6468234	4.3986799	9.1180708
C	10.2095159	6.7367649	9.7267548
C	8.2049047	-9.2794774	-7.8997885
C	9.5199693	-2.6223437	-0.6670594
C	10.3932982	4.5582969	7.8763776
C	7.4879902	-8.2690757	-5.3166526
C	8.9188834	-2.1986983	2.1016001
C	10.9301566	6.8909313	8.5280402
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