Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Using diketopyrrolopyrrole to tune doubly excitation and control internal conversion

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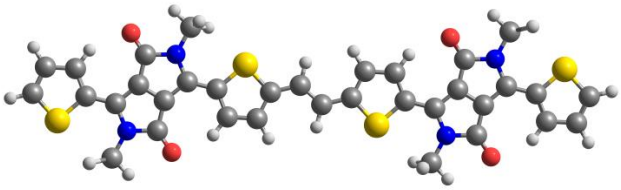
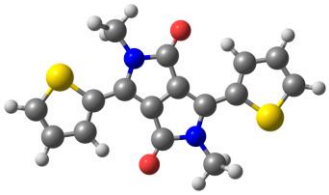
1 DFT and TDDFT calculations

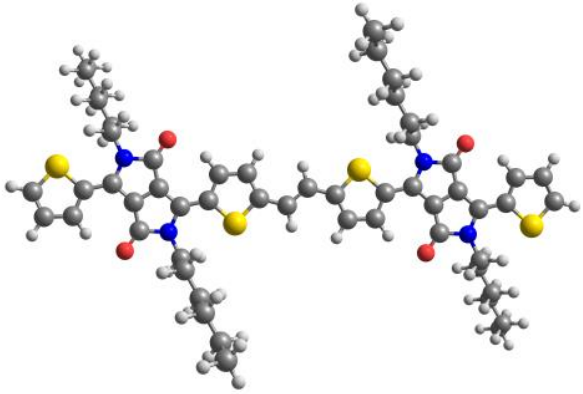
In Figure S1 we show the optimized ground state structures at B3LYP-D3/6-31G(d,p) level for the dimer (T-DPP-T=T-DPP-T) and monomer (T-DPP-T) with the alkyl chains (1b and 1d) and without alkyl chains (1**a** and 1**c**). Vertical excitation and emission energies, oscillator strengths, and the main transitions calculated for these structures are presented in Table S1. For comparison, Table S2 also shows these data calculated at and CAM-B3LYP-D3/6-31G(d,p) level (optimization and excitation energies).



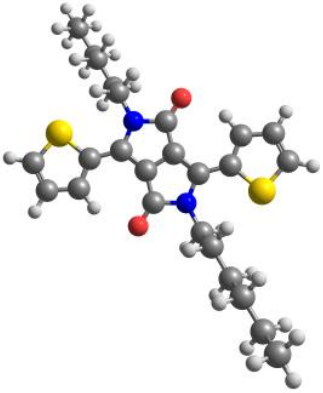
1**a**) R = CH_3



1**c**) R = CH_3



1**b**) R = $(CH_2)_5CH_3$



1**d**) R = $(CH_2)_5CH_3$

*Figure S1. Optimized S_0 minima of dimer (T-DPP-T=T-DPP-T) and monomer (T-DPP-T) with (2**a** and 2**b**) and without alkyl chains (1**a** and 1**b**) at B3LYP-D3/6-31G(d,p) level.*

Table S1. Vertical excitation (S0min) and emission energies (S1 min), in eV, and oscillator strengths for the structures presented in Figure S1 computed at B3LYP-D3/6-31G(d,p) level. Reference values for excited state absorption of monomer and dimer were extracted from Ref. 1.

		T-DPP-T			T-DPP-T=T-DPP-T		
R =		**EE**	***f***	**Transitions**	**EE**	***f***	**Transitions**
CH_3 ($S_{0\ min}$)	S_1	2.41	0.47	H→L (0.71) H ← L (0.13)	1.72	2.10	H→L (0.71) H ← L (-0.11)
	S_2	3.27	0.00	H-1→ L(0.67) H→ L+1 (0.22)	1.91	0.00	H-1 → L (0.60) H → L+1 (-0.35)
CH_3 ($S_{1\ min}$)	S_1	2.18	0.49	H→L (0.71) H ← L (-0.15)	1.56	2.28	H→L (0.72) H ← L (-0.14)
	S_2	3.17	0.00	H→L+1 (0.60) H-1 → L(0.28)	1.72	0.00	H-1 → L (-0.60) H → L+1 (-0.34)
$(CH_2)_5CH_3$ ($S_{0\ min}$)	S_1	2.39 2.2 [a]	0.49	H→L (0.71) H ← L (-0.13)	1.70 1.75[a]	2.09	H→L (0.71) H ← L (-0.13)
	S_2	3.20	0.00	H-1→ L(0.68) H → L+1 0.16)	1.90	0.00	H-1→ L(0.61) H → L+1 (-0.34)
$(CH_2)_5CH_3$ ($S_{1\ min}$)	S_1	2.16	0.50	H→L (0.71) H ← L (-0.15)	1.53	2.28	H→L (0.72) H ← L (-0.14)
	S_2	3.14	0.00	H→L+1 (0.56) H-1 → L(0.34)	1.71	0.00	H-1 → L (-0.62) H → L+1 (-0.34)

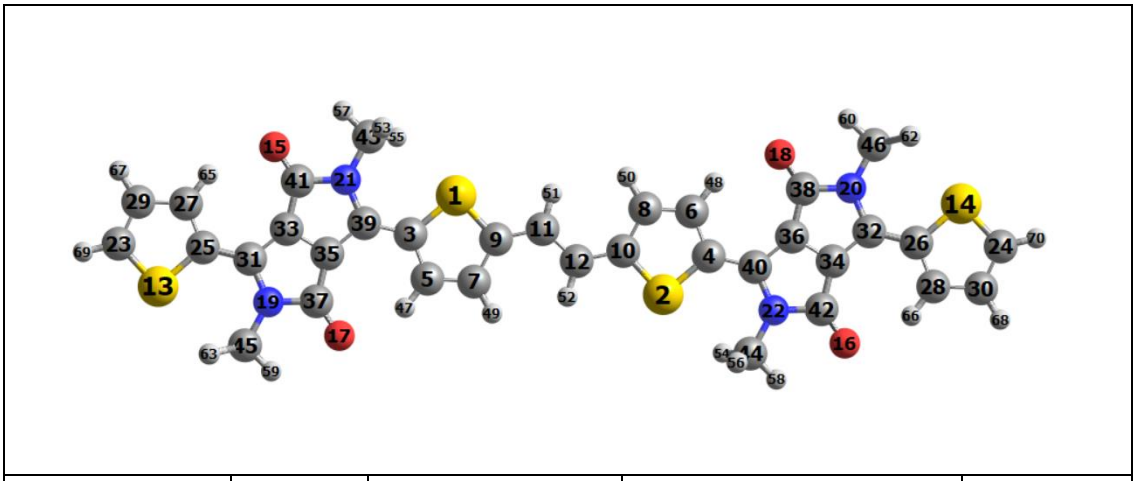
*Adiabatic energies for the bright state (S1) are the following: for the monomer: 2.29 and 2.27 eV for R= **CH_3** *and* ***R*=$(CH_2)_5CH_3$** and for the dimer: 1.63 and 1.61 eV for R= **CH_3** *and* ***R*=$(CH_2)_5CH_3$**. [a] Ref. 1.

Table S2. Excitation energies (in eV) and oscillator strengths for the structures presented in Figure S1 computed at CAM-B3LYP-D3/6-31G(d,p) level. Reference values for excited state absorption of monomer and dimer were extracted from Ref. [1].

		T-DPP-T			T-DPP-T=T-DPP-T		
R =		**EE**	***f***	**Transitions**	**EE**	***f***	**Transitions**
CH_3 ($S_{0\ min}$)	S_1	2.72	0.53	H→L (0.71)	2.27	2.24	H→L (0.64)
	S_2	3.68	0.00	H-1→ L (0.67)	2.66	0.00	H-1 → L (0.53)
CH_3 ($S_{1\ min}$)	S_1	2.38	0.54	H→L (0.71)	1.89	2.45	H→L (0.66)
	S_2	3.69	0.00	H→L (0.68)	2.45	0.00	H-1 → L (0.60)
$(CH_2)_5CH_3$ ($S_{0\ min}$)	S_1	2.72 2.2[a]	0.55	H→L (0.71)	2.26	2.24 1.75[a]	H→L (0.64)
	S_2	3.63	0.00	H-1→ L (0.69)	2.65	0.00	H-1 → L (0.53)
$(CH_2)_5CH_3$ ($S_{1\ min}$)	S_1	2.36	0.56	H→L (0.71)	1.87	2.25	H→L (0.67)
	S_2	3.64	0.00	H-1→ L (0.68)	2.43	0.00	H-1 → L (0.60)

*Adiabatic energies for the bright state (S1) are the following: for the monomer: 2.54 and 2.52 eV for R= **CH_3** *and* ***R*=$(CH_2)_5CH_3$** and for the dimer: 2.08 and 2.06 eV for R= **CH_3** and R=**$(CH_2)_5CH_3$**. [a]Ref. 1

Table S3. Bond lengths at ground state minimum at B3LYP-D3/6-31G(d,p) geometry. Due to C_{2h} symmetry, structural parameters are equivalent in both sides of the molecule.



d (A)	T=T	DPP-T=T-DPP	T-DPP-T=T-DPP-T	T-DPP-T
C11-C12	1.354	1.360	1.361	-
C10-C8	1.382	1.391	1.392	1.371
C6-C4	1.371	1.395	1.397	1.388
C40-C36	-	1.395	1.398	1.394
C34-C32	-	1.369	1.396	1.394
C26-C28	-	-	1.389	1.388
C30-C24	-	-	1.371	1.371
A(3-5-7-9)	113.088	0.000	0.001	-
A(7-9-11-12)	-177.918	-0.009	-0.019	-
A(11-12-10-8)	1.768	0.007	0.017	-
A(11-12-10-2)	178.171	-179.993	-179.986	-
A(1-9-11-12)	179.989	179.979	179.979	-
A(10-8-6-4)	-0.076	0.000	0.000	0.000
A(9-11-12-10)	179.523	-179.999	-179.999	-
A(40-36-34-32)	-	-179.991	-179.99	179.992
A(34-32-26-28)	-	-	0.01	-0.001
A(26-28-30-24)	-	-	0.00	0.001

Table S4. Excitation energies (eV) and oscillator strengths calculated using different basis sets.

	Transition	B3LYP-D3/6-31G(d,p)		B3LYP-D3/6-311+G(d,p)	
T-DPP-T		**EE**	***f***	**EE**	***f***
S_0 min	$S_0 \rightarrow S_1$	2.41	0.47	2.30	0.66
S_1 min	$S_0 \leftarrow S_1$	2.18	0.49	2.08	0.67
T-DPP-T=T-DPP-T					
S_0 min	$S_0 \rightarrow S_1$	1.72	2.10	1.66	2.35
S_1 min	$S_0 \leftarrow S_1$	1.56	2.28	1.50	2.54

Table S5. Excitation energies (eV) and oscillator strengths computed in vacuum and using implicit PCM/ethanol.

			Transition	T-DPP-T		T-DPP-T=T-DPP-T	
				EE	***f***	**EE**	***f***
B3LYP-D3/ 6-311+G(d,p)	vacuum	**$S_{0\ min}$**	$S_0 \rightarrow S_1$	2.30	0.66	1.66	2.35
	vacuum	**$S_{1\ min}$**	$S_0 \leftarrow S_1$	2.08	0.67	1.50	2.54
	Ethanol	**$S_{0\ min}$**	$S_0 \rightarrow S_1$	2.21	0.80	1.59	2.62
	Ethanol	**$S_{1\ min}$**	$S_0 \leftarrow S_1$	1.97	0.82	1.35	2.90
PBE0-D3/ 6-311+G(d,p)	vacuum	**$S_{0\ min}$**	$S_0 \rightarrow S_1$	2.37	0.68	1.76	2.43
	vacuum	**$S_{1\ min}$**	$S_0 \leftarrow S_1$	2.14	0.69	1.57	2.61
	Ethanol	**$S_{0\ min}$**	$S_0 \rightarrow S_1$	2.28	0.82	1.69	2.68
	Ethanol	**$S_{1\ min}$**	$S_0 \leftarrow S_1$	2.03	0.84	1.41	2.94
ωB97XD/ 6-311+G(d,p)	vacuum	**$S_{0\ min}$**	$S_0 \rightarrow S_1$	2.63	0.69	2.28	2.41
	vacuum	**$S_{1\ min}$**	$S_0 \leftarrow S_1$	2.28	0.71	1.92	2.62
	Ethanol	**$S_{0\ min}$**	$S_0 \rightarrow S_1$	2.53	0.81	2.20	2.59
	Ethanol	**$S_{1\ min}$**	$S_0 \leftarrow S_1$	2.15	0.84	1.74	2.87

2 Spin-flip calculations

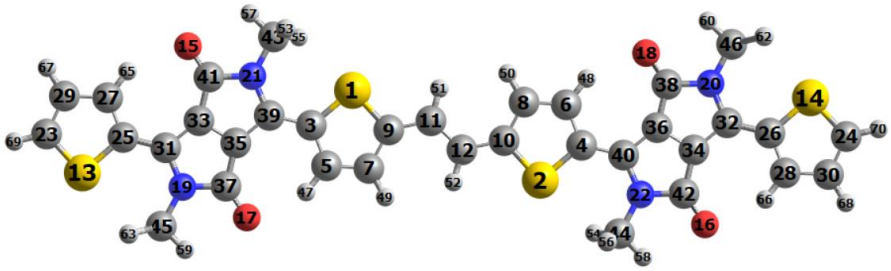
Initial assignment of the spin-flip states was done initially in the ground state geometry. Excitation energies, spin contamination and analysis of the main configurations (coefficients > 0.1) suggest that the states of interest are roots 3 and 4 of all molecules.

Table S6. Excitation energies, $\langle S^2 \rangle$ and configurations in ground state minimum at ROHF-SF-TD-DFT/BHHLYP/6-31G(d,p).

	Symmetry	**Excitation Energy (eV)**	$\langle S^2 \rangle$	CSF Coeff Configs
T-DPP-T=T-DPP-T				
Root 1	1^1A_g	-1.389	0.1235	175 -0.172714 175 -> 176 177 -0.941851 177 -> 176 353 -0.119927 176 -> 177 529 0.114157 175 -> 178 531 0.191440 177 -> 178
Root 3	2^1A_g	0.583	0.8469	175 0.720998 175 -> 176 177 -0.211737 177 -> 176 353 -0.364559 176 -> 177 531 -0.504891 177 -> 178
Root 4	1^1B_u	0.679	0.1710	176 -0.647489 176 -> 176 352 0.309140 175 -> 177 354 0.653843 177 -> 177 530 0.164195 176 -> 178

T-DPP-T				
Root 1	1^1A_g	-1.455058	0.0192	86 -0.982589 86 -> 85 171 -0.150000 85 -> 86
Root 3	2^1A	1.301203	0.0631	85 -0.696529 85 -> 85 172 0.676063 86 -> 86 257 -0.144130 85 -> 87 344 -0.133907 86 -> 88
Root 4	3^1A	1.917730	0.9646	80 0.279278 80 -> 85 84 -0.357509 84 -> 85 169 0.175416 83 -> 86 171 -0.285962 85 -> 86 256 0.111256 84 -> 87 258 0.774350 86 -> 87 341 -0.102813 83 -> 88 343 0.148196 85 -> 88
T=T				
Root 1	1^1A_g	-2.388625	0.0296	51 0.982829 51 -> 50 101 0.114058 50 -> 51
Root 3	1^1B_u	1.475532	0.0533	50 -0.684904 50 -> 50 100 -0.136572 49 -> 51 102 0.692810 51 -> 51
Root 4	2^1A_g	2.046341	0.9126	47 -0.122273 47 -> 50 49 0.678000 49 -> 50 97 -0.129335 46 -> 51 101 0.318032 50 -> 51 153 -0.599532 51 -> 52 305 -0.124283 50 -> 55
DPP-T=T-DPP				
Root 1	1^1A_g	-1.055466	0.1830	133 0.209015 133 -> 134 135 -0.908315 135 -> 134 269 -0.175996 134 -> 135 403 0.159651 133 -> 136 405 -0.240429 135 -> 136
Root 3	2^1A_g	0.657221	0.7874	133 0.721625 133 -> 134 135 0.222709 135 -> 134 267 -0.114929 132 -> 135 269 0.444107 134 -> 135 403 0.136570 133 -> 136 405 -0.414688 135 -> 136
Root 4	1^1B_u	0.933346	0.3368	132 0.161534 132 -> 134 134 -0.586358 134 -> 134 268 -0.491516 133 -> 135 270 0.580754 135 -> 135 404 -0.109425 134 -> 136 540 -0.124333 135 -> 137

Table S7. Bond lengths at ground state minimum with C_{2h} symmetry (at TDDFT/B3LYP-D3 and SF-TDDFT/BHHLYP) and the dark and bright states minima (at SF-TDDFT/BHHLYP level) of T-DPP-T=T-DPP-T. Due to the molecular symmetry, all dihedral angles are 0.000 degrees.



d (A)	GS – DFT	GS-SF	DS	BS
C11-C12	1.361	1.348	1.390	1.377
C10-C8	1.392	1.375	1.414	1.377
C6-C4	1.397	1.377	1.414	1.377
C40-C36	1.398	1.372	1.432	1.406
C34-C32	1.396	1.373	1.409	1.390
C26-C28	1.389	1.373	1.379	1.379
C30-C24	1.371	1.357	1.359	1.359

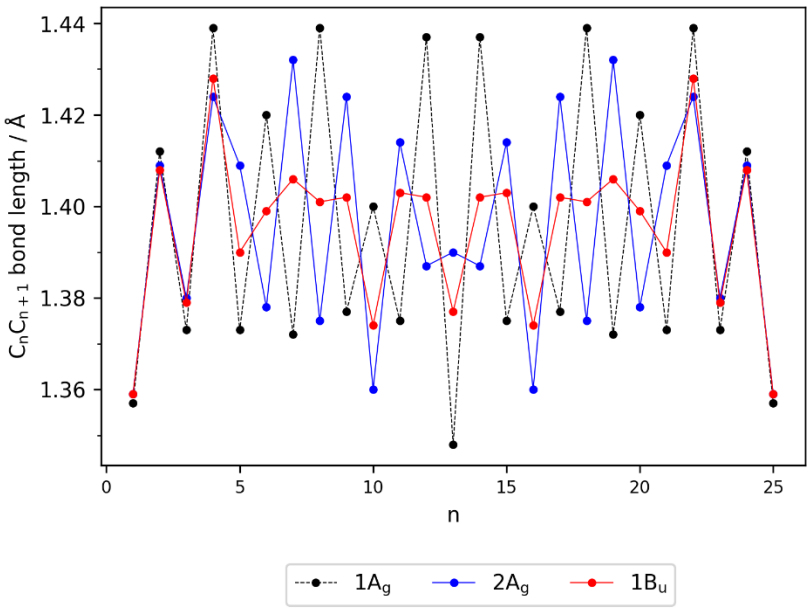


Figure S2. Calculated bond lengths for T-DPP-T=T-DPP-T at the $1A_g$, $2A_g$ and B_u equilibrium geometries at SF-TDDFT/BHHLYP level. Although the bond length alternation is strongly affected method,[2,3] the observed pattern should remain.

3 DFT/MRCI

Table S8. Excitation energies (EE) in eV, symmetry, oscillator strength (f) and main contributions (coefficients^2 > 0.1) at the S_0 geometry with DFT/MRCI level.

		f	Sym	EE	%D	
T-DPP-T	S_1	0.59	2A	2.32	7.4	0.858600 | H→L
	S_2	0.00	3A	3.25	39.4	0.443458 | H→L+1 0.213980 | H^2→L^2
T=T	S_1	1.04	1Bu	3.60	3.9	0.910941 | H→ L
	S_2	0.00	2Ag	4.43	35.9	0.298078 | H-3 → L 0.242948 | H → L+1 0.196941 | H^2 → L^2
DPP-T=T-DPP	S_1	0.00	2Ag	1.85	53.8	0.266024 | H-1 → L 0.194180 | H-1 H → L L+1 0.184540 | H^2 → L^2
	S_2	1.35	1Bu	1.92	16.4	0.688579 | H → L
T-DPP-T=T-DPP-T	S_1	0.00	2Ag	1.57	57.0	0.253327 | H-1 H → L L+1 0.196445 | H-1 → L 0.162040 | H^2 → L^2
	S_2	2.10	1Bu	1.66	10.4	0.723315 | H→ L
ET1	S_1	1.62	1Bu	2.97	5.1	0.875894 | H → L+1
	S_2	0.00	2Ag	3.42	39.9	0.283525 | H → L+2 0.215599 | H-1 → L+1 0.193882 | H^2 → $L+1^2$
ET2	S_1	2.23	1Bu	2.59	6.0	0.838826 | H → L+1
	S_2	0.00	2Ag	2.84	43.8	0.230741 | H → L+2 0.196001 | H^2 → $L+1^2$ 0.191085 | H-1 → L+1 0.103149 | H-1 H → L+1 L+2
ET3	S_1	2.74	1Bu	2.30	7.0	0.796665 | H → L+1
	S_2	0.00	2Ag	2.37	47.3	0.193171 | H → L+2 0.186338 | H^2 → $L+1^2$ 0.148485 | H-1 → L+1 0.124637 | H-1 H → L+1 L+2
ET4	S_1		2Ag	2.00	50.5	0.175091 | H^2 → $L+1^2$ 0.152426 | H → L+2 0.145571 | H-1 H → L+1 L+2 0.108631 | H-1 → L+1
	S_2	3.25229	1Bu	2.07	8.2	0.749399 | H → L+1

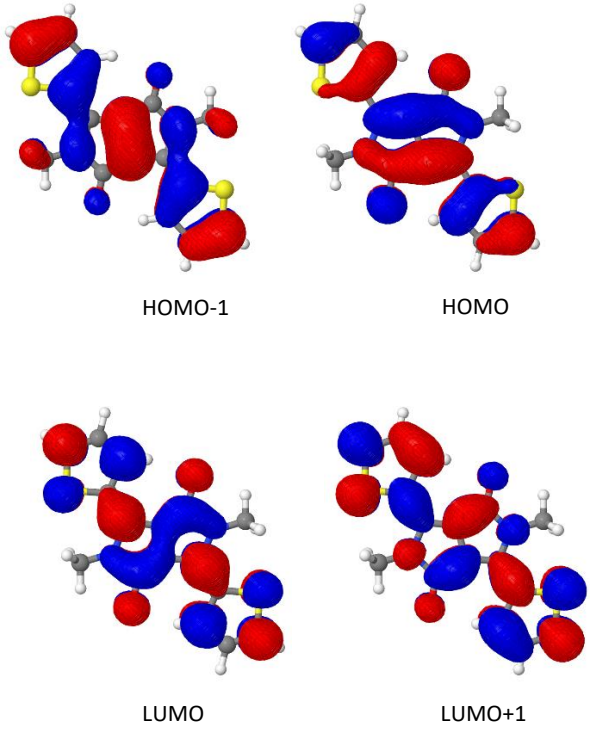


Figure S3. Molecular orbitals of T-DPP-T at the ground state geometry at DFT/MRCI def2-SV(P).

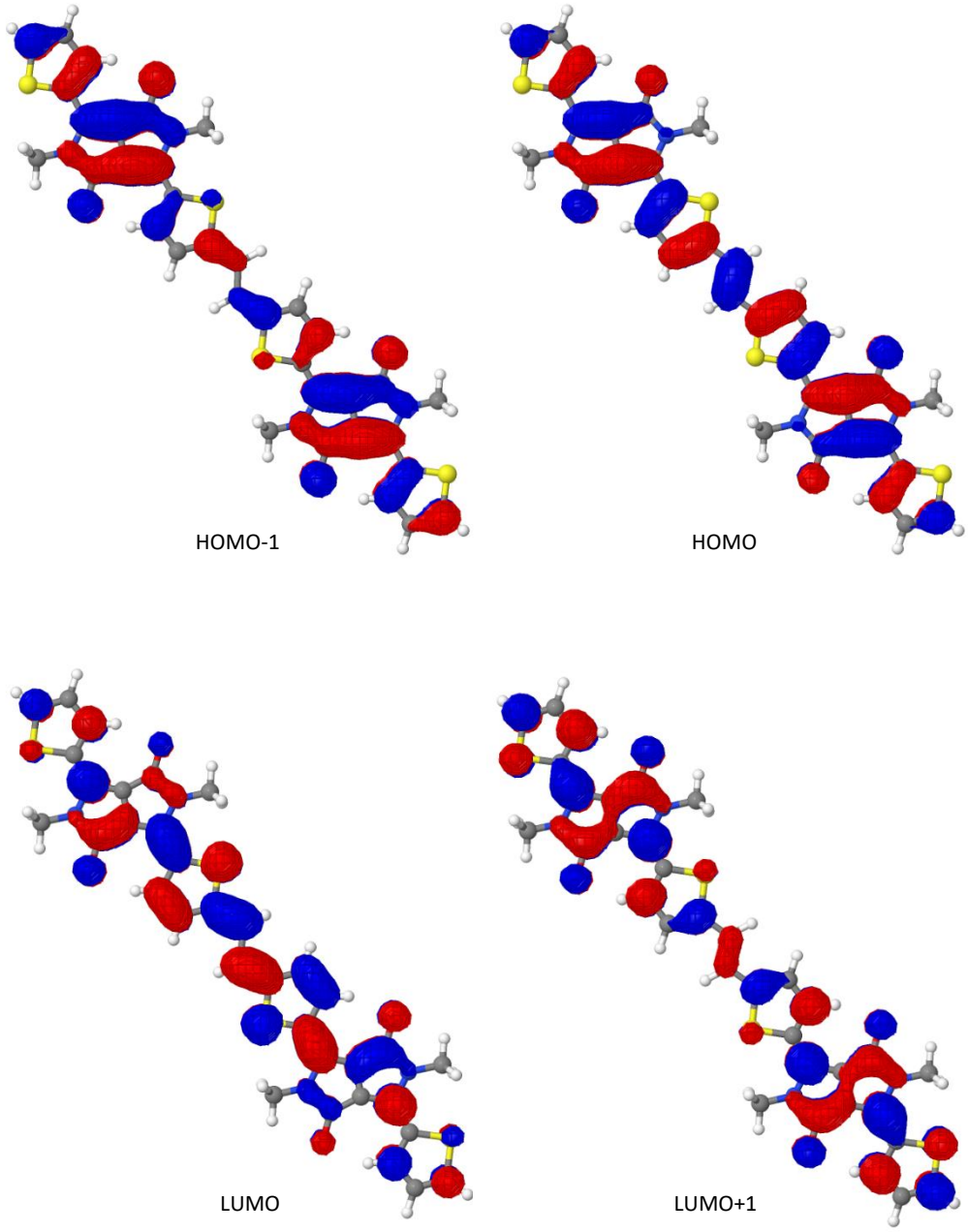


Figure S4. Molecular orbitals of T-DPP-T=T-DPP-T at the ground state geometry at DFT/MRCI def2-SV(P)

4 Wavefunction analysis

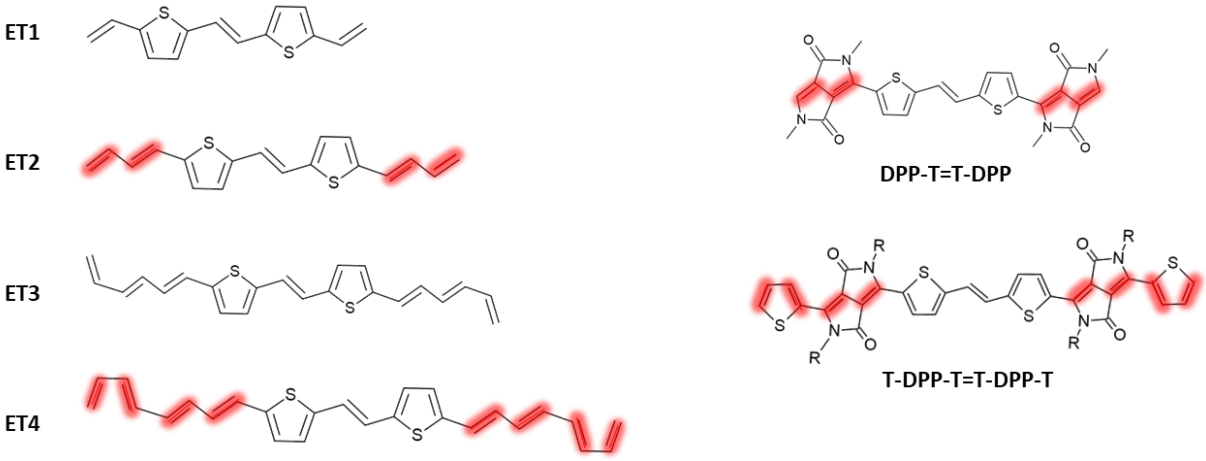


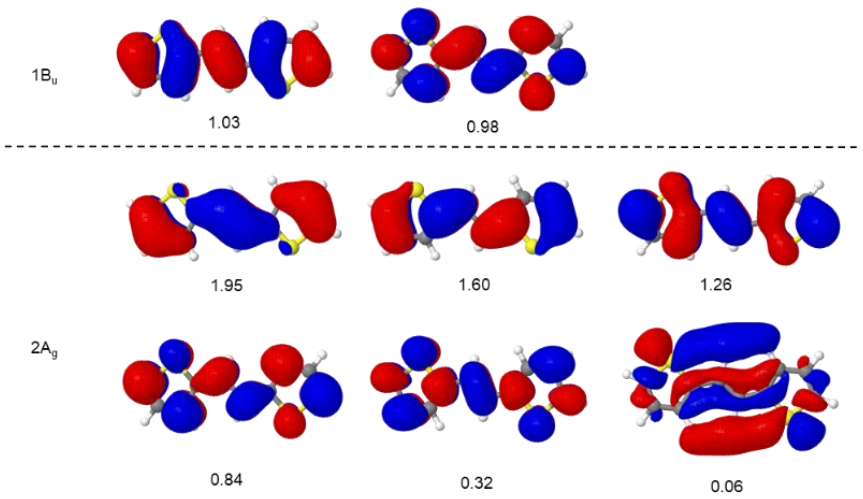
Figure S5. Molecular structures used to investigate the effect of increase the conjugation.

Table S9. Excitation energies (eV), Ω-values, promotion number (p), excitation number (η), number of unpaired electrons ($n_{n,nl}$), LUNO and LUNO+1 occupations (y_0 and y_1, respectively) at DFT/MRCI def2-SV(P) level.

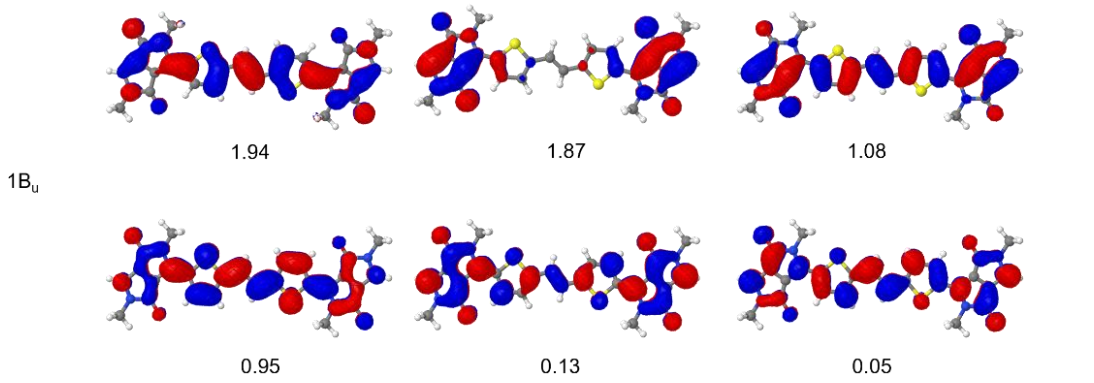
	Sym	**EE**	**Ω**	***p***	***η***	$n_{n,nl}$	y_0	y_1
T=T	$2A_g$	4.428	0.611	1.505	1.235	2.559	0.839	0.321
	$1B_u$	3.600	0.927	1.095	0.917	2.017	0.984	0.040
ET1-T=T-ET1	$2A_g$	3.425	0.56	1.608	1.257	2.558	0.758	0.391
	$1B_u$	2.971	0.904	1.127	0.907	2.037	0.979	0.060
ET1-T=T-ET2	$2A_g$	2.837	0.501	1.728	1.289	2.585	0.786	0.371
	$1B_u$	2.595	0.883	1.160	0.890	2.067	0.973	0.081
ET1-T=T-ET3	$2A_g$	2.371	0.44	1.857	1.320	2.627	0.783	0.378
	$1B_u$	2.297	0.861	1.200	0.871	2.110	0.964	0.104
ET1-T=T-ET4	$2A_g$	2.005	0.376	1.978	1.351	2.716	0.791	0.391
	$1B_u$	2.070	0.835	1.243	0.848	2.166	0.952	0.129
DPP-T=T-DPP	$2A_g$	1.846	0.372	1.930	1.329	2.617	0.956	0.236
	$1B_u$	1.923	0.758	1.410	0.941	2.135	0.946	0.129
T-DPP-T=T-DPP-T	$2A_g$	1.566	0.331	1.966	1.340	2.690	0.864	0.320
	$1B_u$	1.658	0.814	1.251	0.854	2.157	0.938	0.134
T-DPP-T	2A	2.322	0.884	1.128	0.916	2.025	0.991	0.047
	3A	3.248	0.57	1.500	1.227	2.636	0.725	0.574

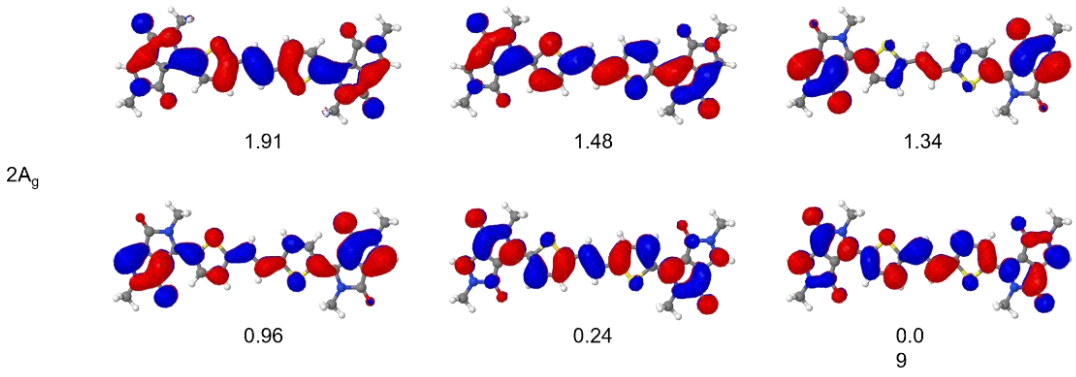
5 Natural orbitals

T=T



DPP-T=T-DPP





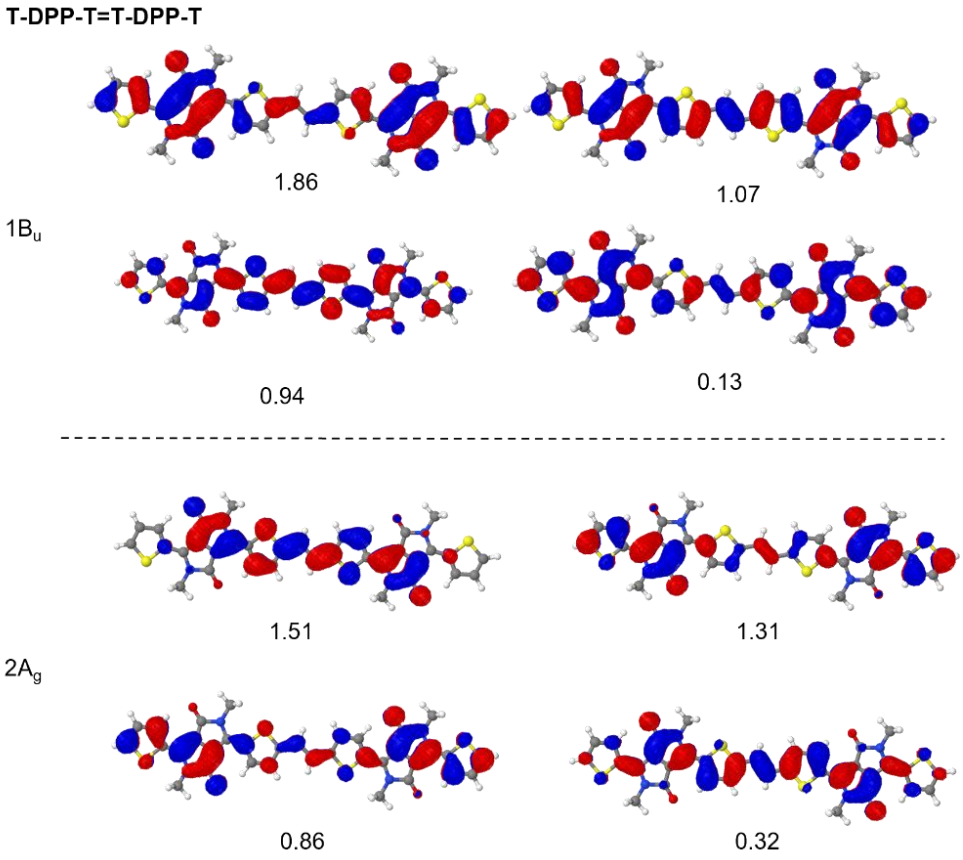


Figure S6. Natural orbitals of T=T, DPP-T=T-DPP and T-DPP-T=T-DPP-T at DFT/MRCI def2SV(P) level.

6 Natural difference orbitals

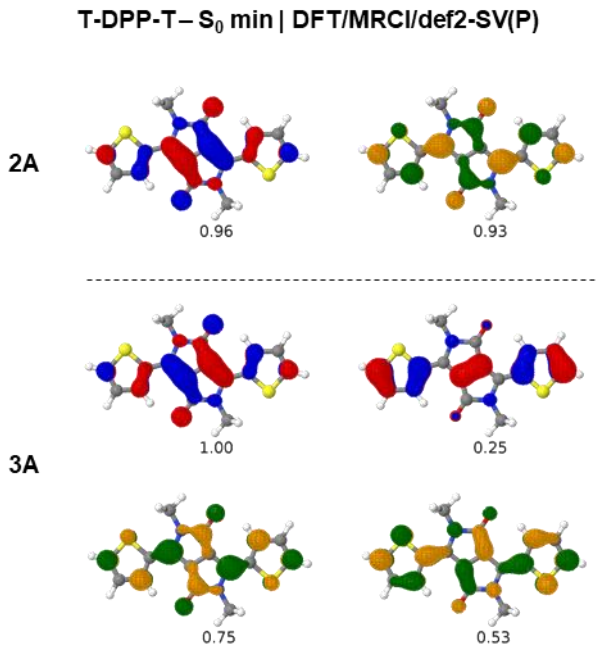


Figure S7. Natural difference orbitals of T-DPP-T at S_0 minimum with DFT/MRCI def2-SV(P) level.

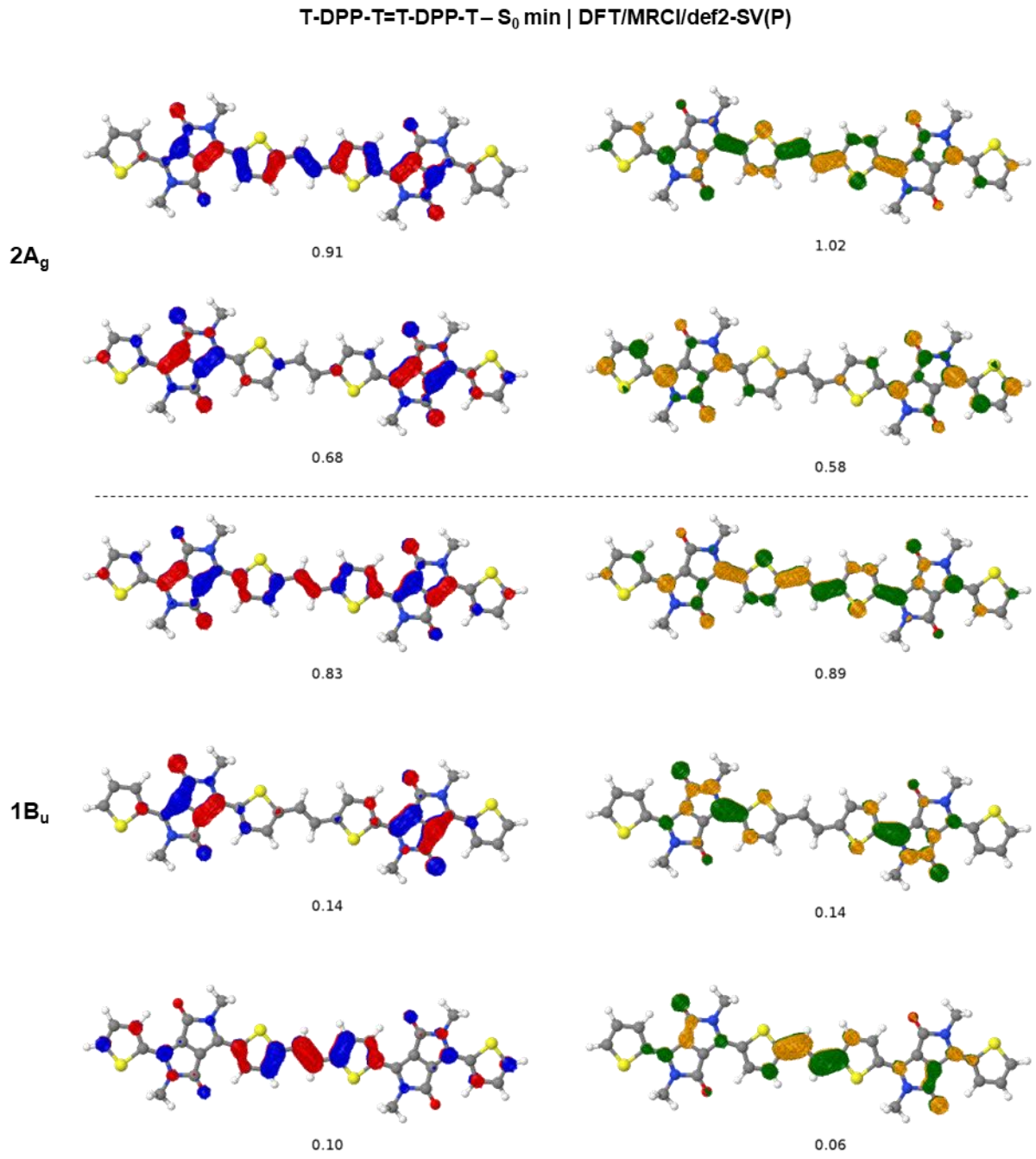


Figure S8. Natural difference orbitals of T-DPP-T=T-DPP-T at S_0 minimum with DFT/MRCI def2-SV(P) level.

7 Mulliken population analysis

First, we partitioned the molecules into different fragments and computed the sum of the contributions of the atoms of fragment I to the attachment ($p_A(A)$), represented as σ_A^I, and to the detachment ($p_D(A)$), represented as σ_D^I. Then, the charge-transfer (δ) character was given by the difference of the absolute value of the collective attachment and detachment densities of that fragment, i.e., $|\sigma_A^I| - |\sigma_A^{II}|$, as shown in Equation 2. When no electron is lost upon photoexcitation, $|\sigma^{AT}| - |\sigma^{DET}|$ should be equivalent for fragments I and II in a two-fragment analysis. δ near zero indicates that no charge-transfer character, while values near 1 would indicate that approximately one electron was transferred.

$$\sigma_I^A = \sum_{A \in I} p_A(A), \sigma_I^D = \sum_{A \in I} p_D(A) \quad (1)$$

$$\delta = |\sigma_A^I| - |\sigma_D^I| \quad (2)$$

This analysis based on the Mulliken population of the attachment and detachment densities is unusual to evaluate charge transfer quantitatively. Therefore, we also performed a similar analysis for 4-(dimethylamino)benzonitrile (DMABN) (Table S8 and S9), which is a well-known example of a charge-transfer character in the excited state.[4–6] Using this approach, the predicted charge-transfer index δ for DMABN is 0.863, nicely agreeing with the charge-transfer index obtained from the one-particle transition density matrix analysis (0.759). Therefore, using the Mulliken population analysis of the detachment and attachment densities seems to be a valid alternative to evaluate the charge-transfer character.

We considered three different fragmentations schemes whenever was possible, as shown in Figure S11. The other two are radial fragmentations: one called "radial_minimal," considering the ethylenic double bond as one fragment and the remaining parts as another fragment; and the other one called "radial_extended", which considers the double bond and the core thiophenes as one fragment and the remaining DPP and thiophene units as another one. δ, σ^A and σ^D are reported in ESI Tables S7 and S8. The “left-right” fragmentation is zero by symmetry reasons, as it should be.

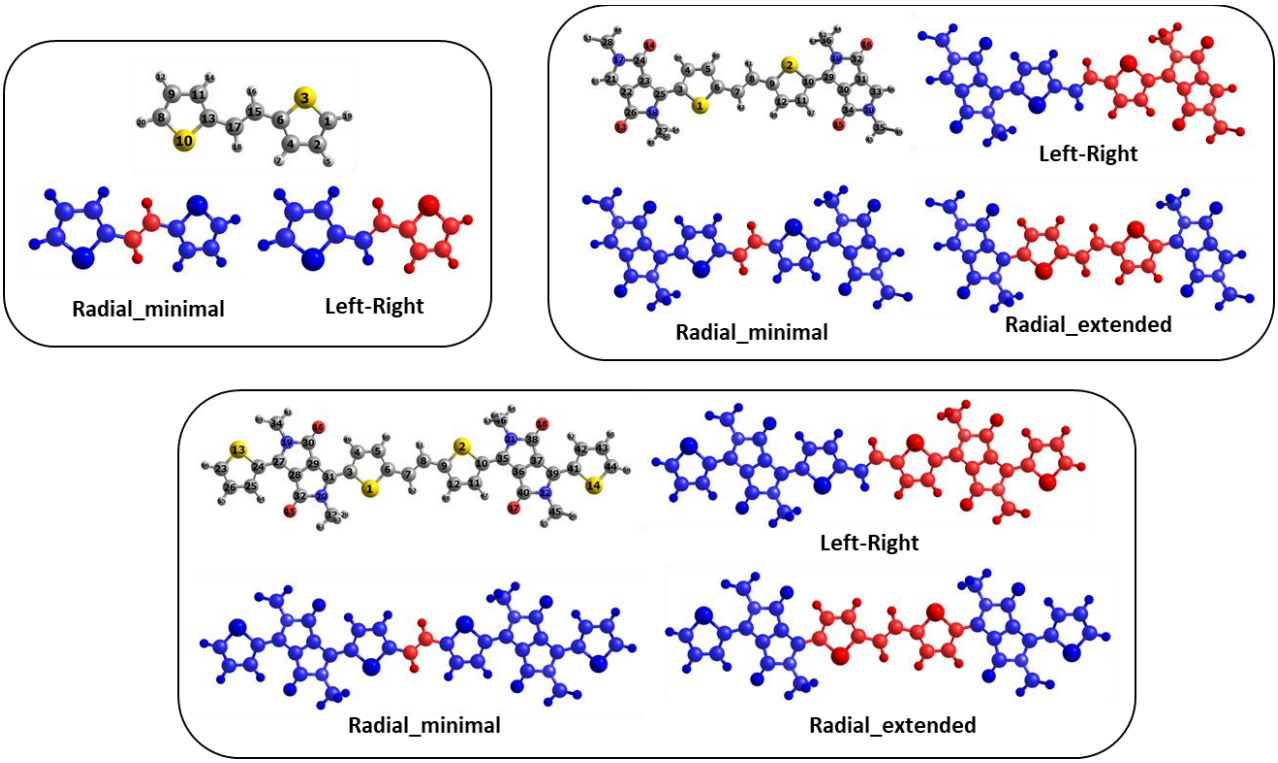


Figure S9. Proposed fragmentations for the Mulliken population analysis.

Table S10. Mulliken population analysis over the detachment (D) and attachment (A) densities[7] within three fragmentations: left-right, radial_minimal and radial_extended (Figure S11). Ground state geometries optimized at B3LYP-D3/6-31G(d,p) and electronic structure calculation at DFT/MRCI def2-SV(P).

		Left-Right		**Radial_minimal**		**Radial_extended**	
		A	**D**	**A**	**D**	**A**	**D**
T=T							
$2A_g$	Frag 1	-0.75260	0.75257	-0.35968	0.33426	-	-
	Frag 2	-0.75260	0.75257	-1.14552	1.17088	-	-
$1B_u$	Frag 1	-0.54753	0.54753	-0.29148	0.25542	-	-
	Frag 2	-0.54753	0.54753	-0.80358	0.83964	-	-
DPP-T=T-DPP							
$2A_g$	Frag 1	-0.96516	0.96515	-0.2083	0.17652	-0.87446	0.79272
	Frag 2	-0.96516	0.96515	-1.7221	1.75378	-1.05586	1.13758
$1B_u$	Frag 1	-0.70510	0.70510	-0.1495	0.11536	-0.63284	0.57190
	Frag 2	-0.70510	0.70510	-1.2607	1.29484	-0.77736	0.83830
T-DPP-T=T-DPP-T							
$2A_g$	Frag 1	-0.9828	0.98274	-0.17006	0.14584	-0.73518	0.68732
	Frag 2	-0.9828	0.98274	-1.79546	1.81964	-1.23034	1.27816
$1B_u$	Frag 1	-0.6254	0.62535	-0.11870	0.09236	-0.49736	0.46078
	Frag 2	-0.6254	0.62535	-1.13202	1.15834	-0.75336	0.78992

DMABN							
2A	Frag 1	1.028	-0.165				
	Frag 2	0.354	-1.217				
3A	Frag 1	0.030	-0.036				
	Frag 2	1.046	-1.040				

Table S11. δ_{AD} for symmetric "left-right", "radial_minimal" and "radial_extended" fragmentations as depicted in Figure S11. Ground state geometries optimized at B3LYP-D3/6-31G(d,p) and electronic structure calculation at DFT/MRCI def2-SV(P).

		Left-Right	**Radial_minimal**	**Radial_extended**
T=T				
$2A_g$	Frag 1	0.00003	0.02542	
	Frag 2	0.00003	-0.02536	
$1B_u$	Frag 1	0.00000	0.03606	
	Frag 2	0.00000	-0.03606	
DPP-T=T-DPP				
$2A_g$	Frag 1	0.00001	0.03174	0.08174
	Frag 2	0.00001	-0.03172	-0.08172
$1B_u$	Frag 1	0.00000	0.03410	0.06094
	Frag 2	0.00000	-0.03410	-0.06094
T-DPP-T=T-DPP-T				
$2A_g$	Frag 1	0.00002	0.02422	0.04786
	Frag 2	0.00002	-0.02418	-0.04782
$1B_u$	Frag 1	0.00001	0.02634	0.03658
$2A_g$	Frag 1	0.00001	-0.02632	-0.03656
DMABN				
2A	Frag 1	0.86300		
	Frag 2	-0.86300		
3A	Frag 1	-0.00600		
	Frag 2	0.00600		

8 Cartesian coordinates

T-DPP-T=T-DPP-T | B3LYP-D3/6-31G(d,p) C_1 – Ground State

70
symmetry c1

S	-3.091460000	-1.445690000	0.571030000
S	3.085790000	1.393610000	0.560230000
C	-4.435220000	-0.308730000	0.572570000
C	-3.945900000	0.999380000	0.571140000
C	-2.547770000	1.079850000	0.568940000
C	-1.907960000	-0.155870000	0.568590000
C	-0.508930000	-0.481260000	0.566590000
C	0.503250000	0.429170000	0.564870000
C	1.902290000	0.103780000	0.562850000
C	4.429550000	0.256640000	0.558750000
C	3.940220000	-1.051470000	0.560240000
C	2.542100000	-1.131930000	0.562520000
S	-11.943040000	1.162900000	0.580700000
S	11.937330000	-1.215050000	0.544300000
O	-8.471040000	-2.947940000	0.580330000
O	-6.561110000	2.661030000	0.573120000
O	6.555410000	-2.713130000	0.556460000
O	8.465380000	2.895830000	0.550500000
N	-8.673100000	1.653590000	0.576670000
N	-6.358910000	-1.943330000	0.576540000
N	6.353250000	1.891230000	0.554700000
N	8.667410000	-1.705700000	0.551950000
C	-13.100660000	-0.119290000	0.583340000
C	-10.599830000	0.017530000	0.580470000
C	-11.087830000	-1.282930000	0.582390000
C	-12.501360000	-1.352880000	0.584000000
C	-9.203240000	0.365780000	0.578490000
C	-8.119910000	-0.514870000	0.577910000
C	-6.909770000	0.227470000	0.575680000
C	-7.237600000	1.634330000	0.574830000
C	-5.825550000	-0.654610000	0.574830000
C	-7.792970000	-1.922820000	0.578530000
C	-5.658210000	-3.214640000	0.576830000
C	-9.374080000	2.924860000	0.576680000
C	5.819880000	0.602520000	0.556270000
C	6.904090000	-0.279570000	0.554800000
C	8.114230000	0.462760000	0.552240000
C	7.787310000	1.870710000	0.552130000
C	9.197550000	-0.417900000	0.550450000
C	7.231900000	-1.686430000	0.554710000

C	10.594150000	-0.069660000	0.547530000
C	11.082170000	1.230790000	0.546610000
C	12.495700000	1.300720000	0.543400000
C	13.094980000	0.067120000	0.541840000
C	9.368380000	-2.976970000	0.551440000
C	5.652560000	3.162550000	0.555480000
H	4.605380000	-1.908740000	0.559610000
H	2.004730000	-2.072570000	0.563970000
H	-4.611060000	1.856650000	0.571680000
H	-2.010390000	2.020480000	0.567610000
H	0.252770000	1.487430000	0.564960000
H	-0.258450000	-1.539520000	0.566440000
H	5.030570000	3.277150000	-0.337070000
H	6.421590000	3.936380000	0.553990000
H	8.599710000	-3.751070000	0.553820000
H	9.991270000	-3.090100000	1.443460000
H	10.421460000	2.091260000	0.548170000
H	13.050130000	2.231580000	0.542280000
H	14.151190000	-0.165630000	0.539410000
H	-9.995910000	3.038260000	-0.316060000
H	-8.605410000	3.698950000	0.575390000
H	-6.427220000	-3.988470000	0.578880000
H	-5.036280000	-3.328480000	1.469510000
H	-10.427100000	-2.143390000	0.582520000
H	-13.055780000	-2.283750000	0.585600000
H	-14.156880000	0.113440000	0.584240000
H	9.987230000	-3.091670000	-0.343190000
H	5.033520000	3.277650000	1.450020000
H	-9.993990000	3.039270000	1.470600000
H	-5.039100000	-3.330470000	-0.317570000

DPP-T=T-DPP | B3LYP-D3/6-31G(d,p) C_1 – Ground State

56
symmetry c1

S	-3.064050000	-1.435340000	0.570680000
S	3.113080000	1.397130000	0.559850000
C	-4.405580000	-0.297920000	0.572120000
C	-3.917880000	1.009580000	0.570650000
C	-2.518850000	1.089760000	0.568480000
C	-1.881600000	-0.146610000	0.568200000
C	-0.481160000	-0.473750000	0.566270000
C	0.530190000	0.435550000	0.564390000
C	1.930630000	0.108400000	0.562430000
C	4.454610000	0.259710000	0.558410000
C	3.966910000	-1.047790000	0.559910000
C	2.567880000	-1.127970000	0.562140000

O	-8.459980000	-2.917000000	0.580070000
O	-6.528270000	2.696480000	0.572850000
O	6.577320000	-2.734690000	0.556410000
O	8.509000000	2.878810000	0.550050000
N	-8.635780000	1.671120000	0.576630000
N	-6.332900000	-1.928720000	0.576140000
N	6.381930000	1.890510000	0.554340000
N	8.684810000	-1.709320000	0.551980000
C	-9.138990000	0.389940000	0.578410000
C	-8.090920000	-0.491360000	0.577690000
C	-6.871530000	0.253180000	0.575350000
C	-7.199270000	1.665040000	0.574680000
C	-5.799650000	-0.639670000	0.574410000
C	-7.775230000	-1.908080000	0.578310000
C	-5.635870000	-3.201380000	0.576200000
C	-9.407220000	2.899000000	0.576640000
C	5.848680000	0.601460000	0.555950000
C	6.920560000	-0.291380000	0.554620000
C	8.139950000	0.453160000	0.552030000
C	7.824260000	1.869880000	0.551830000
C	9.188020000	-0.428130000	0.550450000
C	7.248310000	-1.703240000	0.554710000
C	9.456260000	-2.937190000	0.551110000
C	5.684890000	3.163170000	0.554950000
H	4.631990000	-1.905790000	0.559320000
H	2.029790000	-2.068110000	0.563540000
H	-4.582960000	1.867580000	0.571170000
H	-1.980760000	2.029900000	0.567130000
H	0.281020000	1.494070000	0.564300000
H	-0.231990000	-1.532280000	0.566350000
H	5.063760000	3.282080000	-0.337830000
H	6.458080000	3.933390000	0.553360000
H	8.743510000	-3.763190000	0.553240000
H	10.088590000	-3.005470000	1.442160000
H	-10.038610000	2.967270000	-0.315070000
H	-8.694460000	3.724990000	0.575230000
H	-6.409070000	-3.971590000	0.578100000
H	-5.014810000	-3.319840000	1.469090000
H	10.084650000	-3.006710000	-0.342620000
H	5.066690000	3.282820000	1.449660000
H	-10.036550000	2.968530000	1.469710000
H	-5.017610000	-3.321480000	-0.318410000
H	-10.205970000	0.212160000	0.580030000
H	10.254990000	-0.250350000	0.548330000

T=T | B3LYP-D3/6-31G(d,p) C_1 – Ground State

20
symmetry c1

C	-4.371690000	-0.613990000	-0.258210000
C	-4.006350000	0.104170000	0.850530000
S	-2.996720000	-1.017640000	-1.231140000
C	-2.607190000	0.337970000	0.926710000
H	-4.716530000	0.457110000	1.589500000
C	-1.897310000	-0.204750000	-0.127590000
H	-2.136940000	0.891860000	1.730670000
C	4.369840000	0.754860000	0.232360000
C	3.994210000	0.123790000	-0.924880000
S	3.001420000	1.101680000	1.235980000
C	2.592190000	-0.086870000	-1.014690000
H	4.698620000	-0.179840000	-1.690800000
C	1.890850000	0.383430000	0.079370000
H	2.113090000	-0.567100000	-1.859750000
C	-0.478630000	-0.191350000	-0.415970000
H	-0.174580000	-0.669970000	-1.344380000
C	0.473170000	0.361190000	0.372020000
H	0.170120000	0.830070000	1.305710000
H	-5.362190000	-0.926340000	-0.558150000
H	5.364200000	1.034670000	0.550900000

T-DPP-T | B3LYP-D3/6-31G(d,p) C_1 – Ground State

34
symmetry c1

S	3.197861000	1.372216000	0.560516000
C	2.043684000	0.086699000	0.563012000
C	4.544121000	0.230903000	0.558653000
C	4.060183000	-1.070523000	0.560042000
C	2.646590000	-1.144891000	0.562517000
S	12.061802000	-1.212843000	0.544736000
O	6.684379000	-2.728094000	0.556224000
O	8.575221000	2.888051000	0.550290000
N	6.466632000	1.873201000	0.554518000
N	8.793095000	-1.713418000	0.551796000
C	5.940764000	0.583205000	0.556058000
C	7.024913000	-0.293669000	0.554549000
C	8.234923000	0.453521000	0.551999000
C	7.902937000	1.858983000	0.551934000
C	9.319048000	-0.423433000	0.550301000
C	7.356800000	-1.699119000	0.554501000
C	10.715769000	-0.071279000	0.547509000
C	11.199905000	1.230068000	0.546468000
C	12.613575000	1.304102000	0.543532000
C	13.216213000	0.072365000	0.542306000

C	9.498174000	-2.982215000	0.551233000
C	5.761449000	3.141937000	0.555253000
H	4.723362000	-1.929094000	0.559231000
H	2.095109000	-2.077514000	0.563855000
H	5.138559000	3.253791000	-0.336993000
H	6.527782000	3.918408000	0.553599000
H	8.731788000	-3.758636000	0.553351000
H	10.121324000	-3.093837000	1.443322000
H	10.536884000	2.088744000	0.547770000
H	13.165287000	2.236591000	0.542369000
H	14.273038000	-0.157571000	0.540123000
H	10.117631000	-3.095130000	-0.343266000
H	5.141700000	3.254498000	1.449594000
H	0.986829000	0.316430000	0.564720000

T-DPP-T=T-DPP-T | B3LYP-D3/6-31G(d,p) C_{2h} – Ground State

70

S	-0.97476	3.25640	0.00000
S	0.97476	-3.25640	0.00000
C	-2.71596	3.51400	0.00000
C	-3.37470	2.28243	0.00000
C	-2.51139	1.17967	0.00000
C	-1.16110	1.51589	0.00000
C	0.00744	0.68064	0.00000
C	-0.00744	-0.68064	0.00000
C	1.16110	-1.51589	0.00000
C	2.71596	-3.51400	0.00000
C	3.37470	-2.28243	0.00000
C	2.51139	-1.17967	0.00000
S	-8.78021	8.17856	0.00000
S	8.78021	-8.17856	0.00000
O	-3.40053	8.28730	0.00000
O	-6.34984	3.14829	0.00000
O	6.34984	-3.14829	0.00000
O	3.40053	-8.28730	0.00000
N	-6.98870	5.39935	0.00000
N	-2.75953	6.03804	0.00000
N	2.75953	-6.03804	0.00000
N	6.98870	-5.39935	0.00000
C	-8.58224	9.89465	0.00000
C	-7.03310	7.92664	0.00000
C	-6.37906	9.15205	0.00000
C	-7.26022	10.25955	0.00000
C	-6.37208	6.64804	0.00000
C	-4.99526	6.41648	0.00000

C	-4.75316	5.01759	0.00000
C	-6.02588	4.33438	0.00000
C	-3.37470	4.78630	0.00000
C	-3.72230	7.10108	0.00000
C	-1.34224	6.35207	0.00000
C	-8.40616	5.08565	0.00000
C	3.37470	-4.78630	0.00000
C	4.75316	-5.01759	0.00000
C	4.99526	-6.41648	0.00000
C	3.72230	-7.10108	0.00000
C	6.37208	-6.64804	0.00000
C	6.02588	-4.33438	0.00000
C	7.03310	-7.92664	0.00000
C	6.37906	-9.15205	0.00000
C	7.26022	-10.25955	0.00000
C	8.58224	-9.89465	0.00000
C	8.40616	-5.08565	0.00000
C	1.34224	-6.35207	0.00000
H	4.45768	-2.21549	0.00000
H	2.86232	-0.15470	0.00000
H	-4.45768	2.21549	0.00000
H	-2.86232	0.15470	0.00000
H	-0.96740	-1.19159	0.00000
H	0.96740	1.19159	0.00000
H	0.84602	-5.96220	0.89355
H	1.26945	-7.44061	0.00000
H	8.47944	-3.99721	0.00000
H	8.90189	-5.47645	-0.89333
H	5.29660	-9.22427	0.00000
H	6.92752	-11.29066	0.00000
H	9.45464	-10.53391	0.00000
H	-8.90189	5.47645	0.89333
H	-8.47944	3.99721	0.00000
H	-1.26945	7.44061	0.00000
H	-0.84602	5.96220	-0.89355
H	-5.29660	9.22427	0.00000
H	-6.92752	11.29066	0.00000
H	-9.45464	10.53391	0.00000
H	8.90189	-5.47645	0.89333
H	0.84602	-5.96220	-0.89355
H	-8.90189	5.47645	-0.89333
H	-0.84602	5.96220	0.89355

DPP-T=T-DPP | B3LYP-D3/6-31G(d,p) C_{2h} – Ground State

S	-0.983600000	3.252310000	0.000000000
S	0.983600000	-3.252310000	0.000000000
C	-2.724230000	3.504580000	0.000000000
C	-3.381180000	2.273390000	0.000000000
C	-2.514970000	1.171850000	0.000000000
C	-1.166490000	1.512890000	0.000000000
C	0.005910000	0.679980000	0.000000000
C	-0.005910000	-0.679980000	0.000000000
C	1.166490000	-1.512890000	0.000000000
C	2.724230000	-3.504580000	0.000000000
C	3.381180000	-2.273390000	0.000000000
C	2.514970000	-1.171850000	0.000000000
O	-3.445880000	8.277110000	0.000000000
O	-6.373720000	3.112760000	0.000000000
O	6.373720000	-3.112760000	0.000000000
O	3.445880000	-8.277110000	0.000000000
N	-7.000680000	5.371050000	0.000000000
N	-2.778170000	6.028700000	0.000000000
N	2.778170000	-6.028700000	0.000000000
N	7.000680000	-5.371050000	0.000000000
C	-6.373720000	6.596440000	0.000000000
C	-5.019330000	6.394510000	0.000000000
C	-4.769940000	4.987720000	0.000000000
C	-6.045010000	4.298540000	0.000000000
C	-3.391140000	4.775590000	0.000000000
C	-3.748610000	7.095940000	0.000000000
C	-1.362920000	6.348960000	0.000000000
C	-8.431640000	5.136200000	0.000000000
C	3.391140000	-4.775590000	0.000000000
C	4.769940000	-4.987720000	0.000000000
C	5.019330000	-6.394510000	0.000000000
C	3.748610000	-7.095940000	0.000000000
C	6.373720000	-6.596440000	0.000000000
C	6.045010000	-4.298540000	0.000000000
C	8.431640000	-5.136200000	0.000000000
C	1.362920000	-6.348960000	0.000000000
H	4.464530000	-2.203730000	0.000000000
H	2.863250000	-0.146130000	0.000000000
H	-4.464530000	2.203730000	0.000000000
H	-2.863250000	0.146130000	0.000000000
H	-0.964160000	-1.194110000	0.000000000
H	0.964160000	1.194110000	0.000000000
H	0.863250000	-5.963560000	0.893750000
H	1.297640000	-7.438370000	0.000000000
H	8.578730000	-4.055160000	0.000000000
H	8.900640000	-5.562990000	-0.892390000

H	-8.900640000	5.562990000	0.892390000
H	-8.578730000	4.055160000	0.000000000
H	-1.297640000	7.438370000	0.000000000
H	-0.863250000	5.963560000	-0.893750000
H	8.900640000	-5.562990000	0.892390000
H	0.863250000	-5.963560000	-0.893750000
H	-8.900640000	5.562990000	-0.892390000
H	-0.863250000	5.963560000	0.893750000
H	-6.946940000	7.513760000	0.000000000
H	6.946940000	-7.513760000	0.000000000

T=T | B3LYP-D3/6-31G(d,p) C_{2h} – Ground State

20

C	-0.01755	4.43069	0.00000
C	-1.27849	3.89326	0.00000
S	1.19646	3.19516	0.00000
C	-1.27849	2.47268	0.00000
H	-2.18010	4.49505	0.00000
C	-0.01181	1.91969	0.00000
H	-2.18255	1.87511	0.00000
C	0.01755	-4.43069	0.00000
C	1.27849	-3.89326	0.00000
S	-1.19646	-3.19516	0.00000
C	1.27849	-2.47268	0.00000
H	2.18010	-4.49505	0.00000
C	0.01181	-1.91969	0.00000
H	2.18255	-1.87511	0.00000
C	0.41348	0.53576	0.00000
H	1.48799	0.36586	0.00000
C	-0.41348	-0.53576	0.00000
H	-1.48799	-0.36586	0.00000
H	0.26649	5.47371	0.00000
H	-0.26649	-5.47371	0.00000

ET1 | SF-TDDFT BHLYP collinear /6-31G(d,p) C_{2h} - Ground State

28

S	0.972570000	3.267690000	0.000000000
S	-0.972570000	-3.267690000	0.000000000
C	2.704530000	6.033260000	0.000000000
C	-2.704530000	-6.033260000	0.000000000
C	3.321720000	4.841940000	0.000000000
C	-3.321720000	-4.841940000	0.000000000
C	-0.005800000	0.678410000	0.000000000
C	0.005800000	-0.678410000	0.000000000

C	1.165720000	1.520340000	0.000000000
C	2.510690000	1.191480000	0.000000000
C	3.365350000	2.315800000	0.000000000
C	2.704530000	3.530360000	0.000000000
C	-1.165720000	-1.520340000	0.000000000
C	-2.510690000	-1.191480000	0.000000000
C	-3.365350000	-2.315800000	0.000000000
C	-2.704530000	-3.530360000	0.000000000
H	3.272110000	6.956990000	0.000000000
H	1.621900000	6.125630000	0.000000000
H	4.410780000	4.812830000	0.000000000
H	-3.272110000	-6.956990000	0.000000000
H	-1.621900000	-6.125630000	0.000000000
H	-4.410780000	-4.812830000	0.000000000
H	-0.964780000	1.191850000	0.000000000
H	0.964780000	-1.191850000	0.000000000
H	2.867830000	0.168440000	0.000000000
H	4.448090000	2.250410000	0.000000000
H	-2.867830000	-0.168440000	0.000000000
H	-4.448090000	-2.250410000	0.000000000

ET2 | SF-TDDFT BHLYP collinear /6-31G(d,p) C_{2h} - Ground State

36

S	-1.146200000	3.211110000	0.000000000
S	1.146200000	-3.211110000	0.000000000
C	-4.812710000	4.970660000	0.000000000
C	4.812710000	-4.970660000	0.000000000
C	-3.484770000	4.700430000	0.000000000
C	3.484770000	-4.700430000	0.000000000
C	-0.028190000	0.678620000	0.000000000
C	0.028190000	-0.678620000	0.000000000
C	-1.238260000	1.460280000	0.000000000
C	-2.568710000	1.062530000	0.000000000
C	-3.484770000	2.131740000	0.000000000
C	-2.889770000	3.385200000	0.000000000
C	1.238260000	-1.460280000	0.000000000
C	2.568710000	-1.062530000	0.000000000
C	3.484770000	-2.131740000	0.000000000
C	2.889770000	-3.385200000	0.000000000
C	-5.355450000	6.311490000	0.000000000
H	-5.531170000	4.152110000	0.000000000
H	-2.793950000	5.542650000	0.000000000
C	5.355450000	-6.311490000	0.000000000
H	5.531170000	-4.152110000	0.000000000

H	2.793950000	-5.542650000	0.000000000
H	0.904340000	1.238640000	0.000000000
H	-0.904340000	-1.238640000	0.000000000
H	-2.869560000	0.021370000	0.000000000
H	-4.559870000	1.995120000	0.000000000
H	2.869560000	-0.021370000	0.000000000
H	4.559870000	-1.995120000	0.000000000
C	-6.668000000	6.600310000	0.000000000
C	6.668000000	-6.600310000	0.000000000
H	-4.632260000	7.127330000	0.000000000
H	-7.421320000	5.816670000	0.000000000
H	-7.026370000	7.624060000	0.000000000
H	4.632260000	-7.127330000	0.000000000
H	7.421320000	-5.816670000	0.000000000
H	7.026370000	-7.624060000	0.000000000

ET3 | SF-TDDFT BHLYP collinear /6-31G(d,p) C_{2h} - Ground State

44

S	1.130830000	3.216970000	0.000000000
S	-1.130830000	-3.216970000	0.000000000
C	4.795820000	4.986310000	0.000000000
C	-4.795820000	-4.986310000	0.000000000
C	3.463520000	4.712430000	0.000000000
C	-3.463520000	-4.712430000	0.000000000
C	0.024990000	0.679320000	0.000000000
C	-0.024990000	-0.679320000	0.000000000
C	1.229990000	1.466230000	0.000000000
C	2.563340000	1.074090000	0.000000000
C	3.474510000	2.145480000	0.000000000
C	2.874670000	3.398910000	0.000000000
C	-1.229990000	-1.466230000	0.000000000
C	-2.563340000	-1.074090000	0.000000000
C	-3.474510000	-2.145480000	0.000000000
C	-2.874670000	-3.398910000	0.000000000
C	5.335050000	6.316140000	0.000000000
H	5.511730000	4.165400000	0.000000000
H	2.772000000	5.553830000	0.000000000
C	-5.335050000	-6.316140000	0.000000000
H	-5.511730000	-4.165400000	0.000000000
H	-2.772000000	-5.553830000	0.000000000
H	-0.910470000	1.234400000	0.000000000
H	0.910470000	-1.234400000	0.000000000
H	2.868080000	0.034070000	0.000000000
H	4.550050000	2.012780000	0.000000000
H	-2.868080000	-0.034070000	0.000000000

H	-4.550050000	-2.012780000	0.000000000
C	6.663390000	6.595770000	0.000000000
C	-6.663390000	-6.595770000	0.000000000
H	4.614870000	7.133950000	0.000000000
H	7.354050000	5.753190000	0.000000000
C	7.281060000	7.916240000	0.000000000
H	-4.614870000	-7.133950000	0.000000000
C	-7.281060000	-7.916240000	0.000000000
C	6.663390000	9.110170000	0.000000000
H	-7.354050000	-5.753190000	0.000000000
C	-6.663390000	-9.110170000	0.000000000
H	-8.370200000	-7.911730000	0.000000000
H	-5.581590000	-9.208680000	0.000000000
H	-7.232200000	-10.033810000	0.000000000
H	8.370200000	7.911730000	0.000000000
H	5.581590000	9.208680000	0.000000000
H	7.232200000	10.033810000	0.000000000

ET4 | SF-TDDFT BHLYP collinear /6-31G(d,p) C_{2h} - Ground State

44

S	1.130830000	3.216970000	0.000000000
S	-1.130830000	-3.216970000	0.000000000
C	4.795820000	4.986310000	0.000000000
C	-4.795820000	-4.986310000	0.000000000
C	3.463520000	4.712430000	0.000000000
C	-3.463520000	-4.712430000	0.000000000
C	0.024990000	0.679320000	0.000000000
C	-0.024990000	-0.679320000	0.000000000
C	1.229990000	1.466230000	0.000000000
C	2.563340000	1.074090000	0.000000000
C	3.474510000	2.145480000	0.000000000
C	2.874670000	3.398910000	0.000000000
C	-1.229990000	-1.466230000	0.000000000
C	-2.563340000	-1.074090000	0.000000000
C	-3.474510000	-2.145480000	0.000000000
C	-2.874670000	-3.398910000	0.000000000
C	5.335050000	6.316140000	0.000000000
H	5.511730000	4.165400000	0.000000000
H	2.772000000	5.553830000	0.000000000
C	-5.335050000	-6.316140000	0.000000000
H	-5.511730000	-4.165400000	0.000000000
H	-2.772000000	-5.553830000	0.000000000
H	-0.910470000	1.234400000	0.000000000
H	0.910470000	-1.234400000	0.000000000
H	2.868080000	0.034070000	0.000000000
H	4.550050000	2.012780000	0.000000000

H	-2.868080000	-0.034070000	0.000000000
H	-4.550050000	-2.012780000	0.000000000
C	6.663390000	6.595770000	0.000000000
C	-6.663390000	-6.595770000	0.000000000
H	4.614870000	7.133950000	0.000000000
H	7.354050000	5.753190000	0.000000000
C	7.281060000	7.916240000	0.000000000
H	-4.614870000	-7.133950000	0.000000000
C	-7.281060000	-7.916240000	0.000000000
C	6.663390000	9.110170000	0.000000000
H	-7.354050000	-5.753190000	0.000000000
C	-6.663390000	-9.110170000	0.000000000
H	-8.370200000	-7.911730000	0.000000000
H	-5.581590000	-9.208680000	0.000000000
H	-7.232200000	-10.033810000	0.000000000
H	8.370200000	7.911730000	0.000000000
H	5.581590000	9.208680000	0.000000000
H	7.232200000	10.033810000	0.000000000

T-DPP-T=T-DPP-T | SF-TDDFT BHLYP collinear /6-31G(d,p) C_{2h} - $2A_g$

70

S	-3.181045000	1.169512000	0.000000000
S	3.181045000	-1.169512000	0.000000000
C	-4.408392000	-0.091907000	0.000000000
C	4.408392000	0.091907000	0.000000000
C	-3.767839000	-1.363531000	0.000000000
C	3.767839000	1.363531000	0.000000000
C	-2.408647000	-1.305111000	0.000000000
C	2.408647000	1.305111000	0.000000000
C	-1.873239000	0.003519000	0.000000000
C	1.873239000	-0.003519000	0.000000000
C	-0.551579000	0.422682000	0.000000000
C	0.551579000	-0.422682000	0.000000000
S	-11.642774000	-2.394075000	0.000000000
S	11.642774000	2.394075000	0.000000000
O	-8.650676000	2.030453000	0.000000000
O	8.650676000	-2.030453000	0.000000000
O	-6.186717000	-3.286992000	0.000000000
O	6.186717000	3.286992000	0.000000000
N	-8.366319000	-2.523232000	0.000000000
N	8.366319000	2.523232000	0.000000000
N	-6.469095000	1.298736000	0.000000000
N	6.469095000	-1.298736000	0.000000000
C	-12.923746000	-1.255509000	0.000000000

C	12.923746000	1.255509000	0.000000000
C	-10.441888000	-1.122431000	0.000000000
C	10.441888000	1.122431000	0.000000000
C	-11.063009000	0.109557000	0.000000000
C	11.063009000	-0.109557000	0.000000000
C	-12.469099000	0.024664000	0.000000000
C	12.469099000	-0.024664000	0.000000000
C	-9.031480000	-1.318961000	0.000000000
C	9.031480000	1.318961000	0.000000000
C	-8.029940000	-0.328195000	0.000000000
C	8.029940000	0.328195000	0.000000000
C	-6.785377000	-0.920583000	0.000000000
C	6.785377000	0.920583000	0.000000000
C	-6.967019000	-2.352271000	0.000000000
C	6.967019000	2.352271000	0.000000000
C	-5.771198000	0.090236000	0.000000000
C	5.771198000	-0.090236000	0.000000000
C	-7.851195000	1.117664000	0.000000000
C	7.851195000	-1.117664000	0.000000000
C	-5.918908000	2.633689000	0.000000000
C	5.918908000	-2.633689000	0.000000000
C	-8.921337000	-3.856610000	0.000000000
C	8.921337000	3.856610000	0.000000000
H	-4.340329000	-2.275167000	0.000000000
H	4.340329000	2.275167000	0.000000000
H	-1.784732000	-2.180729000	0.000000000
H	1.784732000	2.180729000	0.000000000
H	-0.375192000	1.486786000	0.000000000
H	0.375192000	-1.486786000	0.000000000
H	-5.317910000	2.811864000	0.885803000
H	5.317910000	-2.811864000	-0.885803000
H	-5.317910000	2.811864000	-0.885803000
H	5.317910000	-2.811864000	0.885803000
H	-6.759288000	3.314773000	0.000000000
H	6.759288000	-3.314773000	0.000000000
H	-8.081280000	-4.538012000	0.000000000
H	8.081280000	4.538012000	0.000000000
H	-9.522454000	-4.032888000	-0.886046000
H	9.522454000	4.032888000	0.886046000
H	-9.522454000	-4.032888000	0.886046000
H	9.522454000	4.032888000	-0.886046000
H	-10.506319000	1.030878000	0.000000000
H	10.506319000	-1.030878000	0.000000000
H	-13.116653000	0.883153000	0.000000000
H	13.116653000	-0.883153000	0.000000000
H	-13.940964000	-1.597701000	0.000000000

H	13.940964000	1.597701000	0.000000000

T-DPP-T=T-DPP-T | SF-TDDFT BHLYP collinear /6-31G(d,p) C_{2h} - $1B_u$

70

S	-2.974974000	-1.599699000	0.000000000
S	2.974974000	1.599699000	0.000000000
C	-4.366768000	-0.533974000	0.000000000
C	4.366768000	0.533974000	0.000000000
C	-3.934703000	0.800028000	0.000000000
C	3.934703000	-0.800028000	0.000000000
C	-2.568492000	0.949896000	0.000000000
C	2.568492000	-0.949896000	0.000000000
C	-1.861922000	-0.261861000	0.000000000
C	1.861922000	0.261861000	0.000000000
C	-0.479079000	-0.494439000	0.000000000
C	0.479079000	0.494439000	0.000000000
S	-11.864175000	0.646326000	0.000000000
S	11.864175000	-0.646326000	0.000000000
O	-8.243425000	-3.285792000	0.000000000
O	8.243425000	3.285792000	0.000000000
O	-6.602306000	2.346190000	0.000000000
O	6.602306000	-2.346190000	0.000000000
N	-8.643903000	1.260699000	0.000000000
N	8.643903000	-1.260699000	0.000000000
N	-6.200449000	-2.216772000	0.000000000
N	6.200449000	2.216772000	0.000000000
C	-12.965601000	-0.665162000	0.000000000
C	12.965601000	0.665162000	0.000000000
C	-10.491572000	-0.435717000	0.000000000
C	10.491572000	0.435717000	0.000000000
C	-10.926148000	-1.744498000	0.000000000
C	10.926148000	1.744498000	0.000000000
C	-12.328950000	-1.866198000	0.000000000
C	12.328950000	1.866198000	0.000000000
C	-9.121273000	-0.035406000	0.000000000
C	9.121273000	0.035406000	0.000000000
C	-8.002511000	-0.860692000	0.000000000
C	8.002511000	0.860692000	0.000000000
C	-6.841560000	-0.080231000	0.000000000
C	6.841560000	0.080231000	0.000000000
C	-7.229332000	1.302529000	0.000000000
C	7.229332000	-1.302529000	0.000000000
C	-5.713794000	-0.919697000	0.000000000
C	5.713794000	0.919697000	0.000000000
C	-7.609992000	-2.252868000	0.000000000

C	7.609992000	2.252868000	0.000000000
C	-5.452791000	-3.452000000	0.000000000
C	5.452791000	3.452000000	0.000000000
C	-9.390745000	2.495946000	0.000000000
C	9.390745000	-2.495946000	0.000000000
H	-4.637743000	1.616587000	0.000000000
H	4.637743000	-1.616587000	0.000000000
H	-2.081054000	1.907593000	0.000000000
H	2.081054000	-1.907593000	0.000000000
H	-0.156125000	-1.523258000	0.000000000
H	0.156125000	1.523258000	0.000000000
H	-4.833092000	-3.539911000	-0.886448000
H	4.833092000	3.539911000	0.886448000
H	-4.833092000	-3.539911000	0.886448000
H	4.833092000	3.539911000	-0.886448000
H	-6.182858000	-4.250484000	0.000000000
H	6.182858000	4.250484000	0.000000000
H	-8.657983000	3.292059000	0.000000000
H	8.657983000	-3.292059000	0.000000000
H	-10.010475000	2.585164000	0.886439000
H	10.010475000	-2.585164000	-0.886439000
H	-10.010475000	2.585164000	-0.886439000
H	10.010475000	-2.585164000	0.886439000
H	-10.241274000	-2.574602000	0.000000000
H	10.241274000	2.574602000	0.000000000
H	-12.844224000	-2.810007000	0.000000000
H	12.844224000	2.810007000	0.000000000
H	-14.021776000	-0.474534000	0.000000000
H	14.021776000	0.474534000	0.000000000

T-DPP-T | SF-TDDFT BHLYP collinear /6-31G(d,p) C_{2h} - S_1

34

S	3.212250000	1.379170000	0.554590000
C	2.076240000	0.092660000	0.560430000
C	4.565020000	0.253090000	0.560540000
C	4.080940000	-1.056620000	0.562400000
C	2.684780000	-1.130910000	0.562560000
S	12.048150000	-1.219780000	0.543280000
O	6.717590000	-2.703460000	0.556950000
O	8.542670000	2.864460000	0.547520000
N	6.461250000	1.862670000	0.557990000
N	8.799090000	-1.701550000	0.554770000
C	5.921340000	0.600340000	0.553580000
C	7.041880000	-0.287290000	0.548520000

C	8.217810000	0.446610000	0.551340000
C	7.877790000	1.844680000	0.550920000
C	9.337770000	-0.440670000	0.552880000
C	7.381580000	-1.686340000	0.554220000
C	10.694960000	-0.094230000	0.548330000
C	11.178820000	1.216130000	0.547220000
C	12.575210000	1.290100000	0.543410000
C	13.183640000	0.067150000	0.540000000
C	9.492360000	-2.967870000	0.552610000
C	5.764530000	3.126460000	0.558670000
H	4.739630000	-1.907820000	0.558880000
H	2.138280000	-2.056830000	0.565360000
H	5.149890000	3.234320000	-0.326900000
H	6.526610000	3.896910000	0.551160000
H	8.733560000	-3.737050000	0.552120000
H	10.112170000	-3.074780000	1.435350000
H	10.520250000	2.066890000	0.545840000
H	13.121030000	2.216400000	0.544400000
H	14.233410000	-0.149280000	0.540430000
H	10.112310000	-3.073870000	-0.334980000
H	5.147410000	3.233200000	1.444840000
H	1.027060000	0.309530000	0.566370000

T-DPP-T | SF-TDDFT BHLYP collinear /6-31G(d,p) C_{2h} - S_2

34

S	3.211610000	1.392990000	0.562240000
C	2.086590000	0.083760000	0.561760000
C	4.577620000	0.267780000	0.560730000
C	4.090070000	-1.065650000	0.559900000
C	2.707920000	-1.144040000	0.560460000
S	12.048160000	-1.233280000	0.544540000
O	6.706770000	-2.701410000	0.549930000
O	8.552290000	2.860540000	0.551260000
N	6.467780000	1.881670000	0.553410000
N	8.793470000	-1.721490000	0.567310000
C	5.916480000	0.611240000	0.560240000
C	7.046810000	-0.285810000	0.548710000
C	8.212740000	0.445800000	0.543210000
C	7.876200000	1.852860000	0.550760000
C	9.343150000	-0.451160000	0.552430000
C	7.384380000	-1.693440000	0.556670000
C	10.682030000	-0.108910000	0.542430000
C	11.169550000	1.225460000	0.537140000
C	12.552000000	1.303390000	0.540710000
C	13.173350000	0.075580000	0.538440000

C	9.485440000	-2.988070000	0.559420000
C	5.773140000	3.146870000	0.559250000
H	4.756520000	-1.909970000	0.558500000
H	2.164770000	-2.072350000	0.565830000
H	5.160870000	3.262310000	-0.331140000
H	6.537070000	3.914680000	0.557740000
H	8.723450000	-3.754900000	0.545110000
H	10.107590000	-3.103680000	1.439810000
H	10.503410000	2.069370000	0.552560000
H	13.095320000	2.231860000	0.546510000
H	14.226440000	-0.129070000	0.540070000
H	10.096020000	-3.099230000	-0.332710000
H	5.154910000	3.260130000	1.440360000
H	1.033330000	0.288640000	0.562040000

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