SUPPLEMENTARY MATERIAL

OPTOELECTRONIC PROPERTIES OF TRIPHENYLAMINE BASED DYES FOR SOLAR CELL APPLICATIONS. A DFT STUDY

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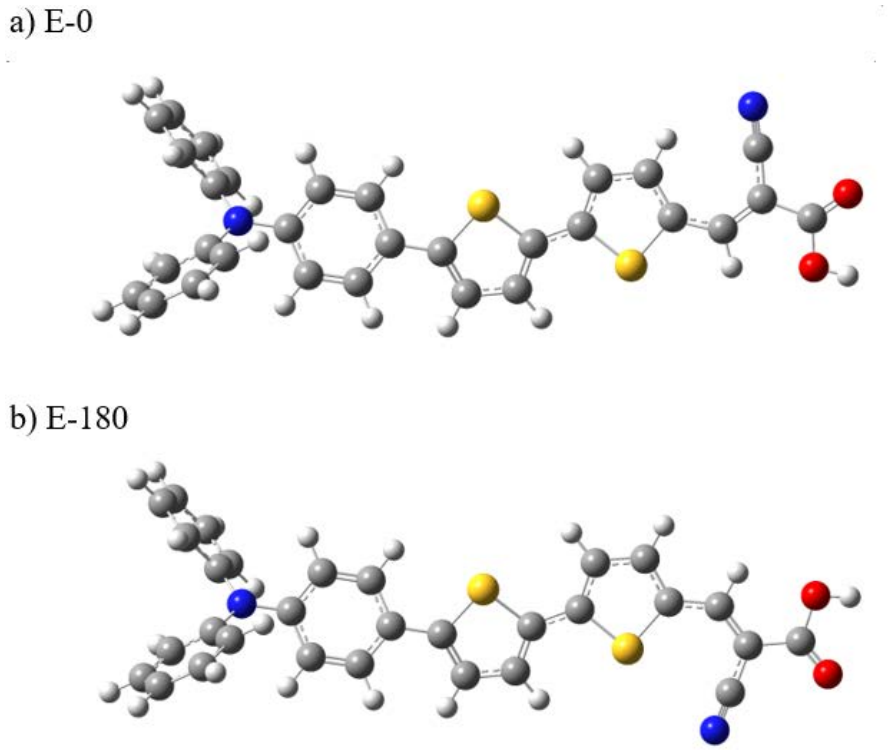

***Figure 1S**. Stable conformers a) E-0 and b) E-180 of D1, where the numbers represent the dihedral angle values.*

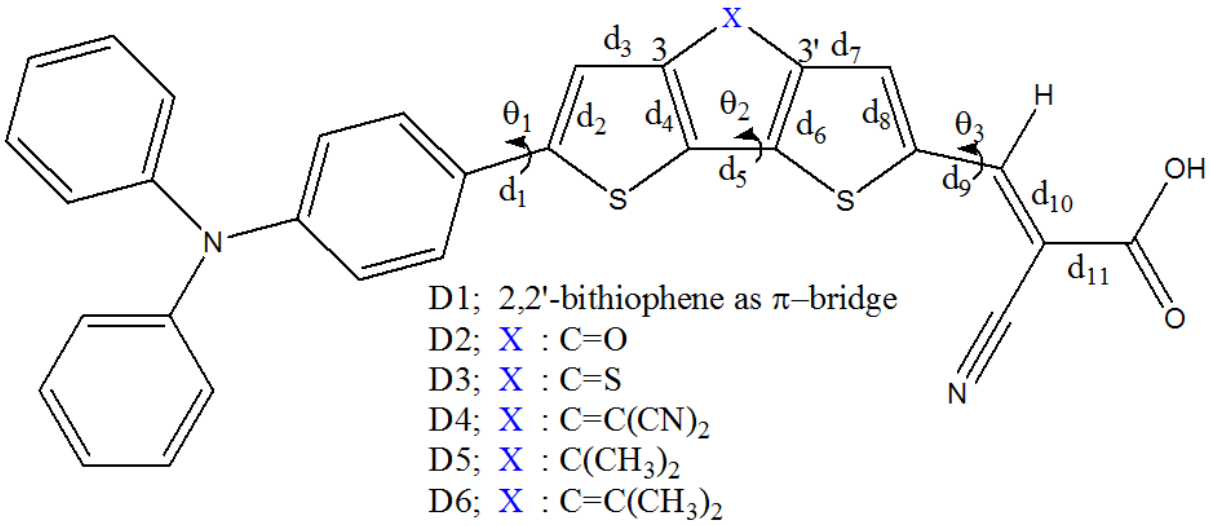

***Figure 2S**. The selected bond lengths participate in intramolecular charge transfer from TPA to the terminal acceptor cyanoacrylic acid and dihedral angles between rings.*

Table 1S: Optimized selected conjugated bond lengths (Å) and dihedral angles (°) of studied dyes, in neutral and doped (p,n) states calculated at the CPCM-B3LYP/6-311G(d,p) level of theory.

Dyes	d_1	d_2	d_3	d_4	d_5	d_6	d_7	d_8	d_9	d_{10}	d_{11}	θ_1	θ_2	θ_3
D1	1.461	1.379	1.410	1.380	1.439	1.389	1.399	1.390	1.422	1.368	1.481	25.7	169.2	179.4
$D1^+$	1.431	1.401	1.389	1.399	1.425	1.395	1.394	1.395	1.431	1.362	1.494	5.7	179.3	180.0
$D1^-$	1.444	1.389	1.398	1.399	1.410	1.406	1.381	1.415	1.392	1.406	1.450	4.4	179.7	180.0
Δ^+	0.030	-0.022	0.021	-0.019	0.014	-0.006	0.005	-0.005	-0.009	0.006	-0.013	20.0	10.1	0.6
Δ^-	0.017	-0.010	0.012	-0.019	0.029	-0.017	0.018	-0.025	0.030	-0.038	0.031	21.3	10.5	0.5
D2	1.458	1.385	1.405	1.386	1.446	1.395	1.392	1.398	1.420	1.368	1.481	25.0	0.0	179.9
$D2^+$	1.430	1.406	1.384	1.403	1.431	1.402	1.390	1.400	1.429	1.362	1.495	5.0	0.0	180.0
$D2^-$	1.449	1.386	1.399	1.419	1.402	1.430	1.374	1.416	1.392	1.397	1.456	9.2	0.0	179.9
Δ^+	0.028	-0.021	0.021	-0.017	0.015	-0.007	0.002	-0.002	-0.009	0.006	-0.014	20.0	0.0	0.1
Δ^-	0.009	-0.001	0.006	-0.033	0.044	-0.035	0.018	-0.018	0.028	-0.029	0.025	15.8	0.0	0.0
D3	1.458	1.383	1.407	1.392	1.441	1.402	1.394	1.396	1.42	1.368	1.481	25.1	0.0	180.0
$D3^+$	1.430	1.404	1.386	1.410	1.425	1.409	1.393	1.398	1.429	1.362	1.495	3.9	0.0	179.9
$D3^-$	1.456	1.378	1.411	1.425	1.398	1.435	1.383	1.408	1.398	1.389	1.461	17.5	0.0	179.9
Δ^+	0.028	-0.021	0.021	-0.018	0.016	-0.007	0.001	-0.002	-0.009	0.006	-0.014	21.2	0.0	0.0
Δ^-	0.002	0.005	-0.004	-0.033	0.043	-0.033	0.011	-0.012	0.022	-0.021	0.020	7.6	0.0	0.1
D4	1.457	1.384	1.411	1.394	1.436	1.404	1.400	1.395	1.422	1.367	1.482	24.4	0.0	180.0
$D4^+$	1.432	1.402	1.392	1.411	1.423	1.409	1.398	1.397	1.430	1.362	1.495	4.2	0.0	180.0

$D4^-$	1.457	1.377	1.416	1.424	1.398	1.434	1.389	1.405	1.401	1.386	1.464	17.0	0.0	179.9
Δ^+	0.025	-0.018	0.019	-0.017	0.013	-0.005	0.002	-0.002	-0.008	0.005	-0.013	20.2	0.0	0.0
Δ^-	0.000	0.007	-0.005	-0.030	0.038	-0.030	0.011	-0.010	0.021	-0.019	0.018	7.4	0.0	0.0
D5	1.460	1.385	1.408	1.386	1.431	1.396	1.392	1.401	1.417	1.371	1.478	25.9	0.0	179.9
$D5^+$	1.428	1.408	1.385	1.408	1.413	1.405	1.390	1.403	1.427	1.364	1.494	3.7	0.0	179.9
$D5^-$	1.439	1.401	1.391	1.405	1.406	1.412	1.377	1.425	1.389	1.408	1.448	4.8	0.0	179.8
Δ^+	0.032	-0.023	0.023	-0.022	0.018	-0.009	0.002	-0.002	-0.010	0.007	-0.016	22.2	0.0	0.0
Δ^-	0.021	-0.016	0.017	-0.019	0.025	-0.016	0.015	-0.024	0.028	-0.037	0.030	21.1	0.0	0.1
D6	1.460	1.382	1.417	1.397	1.423	1.407	1.399	1.399	1.417	1.371	1.478	27.3	0.0	179.9
$D6^+$	1.429	1.406	1.393	1.422	1.403	1.417	1.397	1.400	1.427	1.364	1.493	4.7	0.0	179.8
$D6^-$	1.442	1.394	1.401	1.422	1.395	1.429	1.382	1.421	1.390	1.404	1.451	8.3	0.0	179.9
Δ^+	0.031	-0.024	0.024	-0.025	0.020	-0.011	0.002	-0.002	-0.011	0.007	-0.016	22.6	0.0	0.1
Δ^-	0.018	-0.012	0.015	-0.025	0.028	-0.022	0.017	-0.022	0.027	-0.033	0.027	19.0	0.0	0.0

$\Delta^+ = d - d^+$ (bond lengths) $\theta - \theta^+$ (dihedral angles)

$\Delta^- = d - d^-$ (bond lengths) $\theta - \theta^-$ (dihedral angles)

Table 2S: Maximum absorption wavelengths (λ_{max}/ nm), oscillator strengths (ƒ) and major contributions to the absorption band, of the studied dyes obtained at the CPCM-TD-CAM-B3LYP/6-311(d,p) level of theory.

Dyes	λ_{max} /nm	ƒ	Major contributions to the absorption band
D1	430.2	1.569	HOMO-1→LUMO (32%), HOMO→LUMO (60%)
D2	528.5	0.578	HOMO-1→LUMO (35%), HOMO→LUMO (53%)
D3	411.1	0.525	HOMO-1→LUMO (34%), HOMO→LUMO (36%), HOMO→LUMO+1(10%)
D4	407.9	0.340	HOMO-1→LUMO (40%), HOMO→LUMO (38%)
D5	453.7	1.662	HOMO-1→LUMO (24%), HOMO→LUMO (70%)
D6	468.1	1.407	HOMO-1→LUMO (24%), HOMO→LUMO (69%)