Supporting Information

The impact of molecular stacking interactions on the electronic structure and charge transport properties in distyrylbenzene-(DSB) based D-A complexes: a theoretical study

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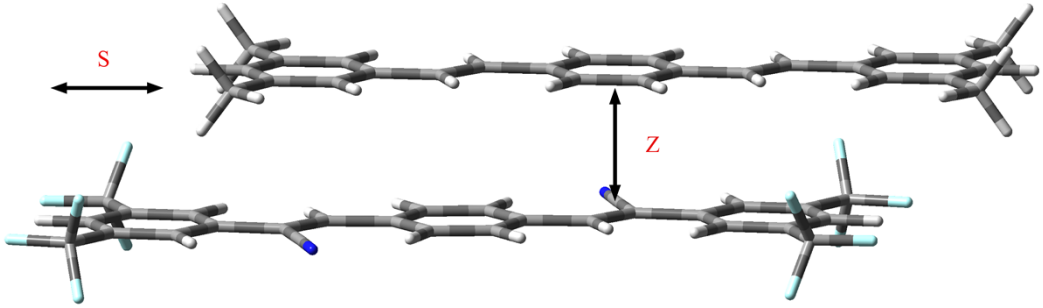


Fig. S1 Schematic diagram of the displacement patterns in cofacial D-A pair.

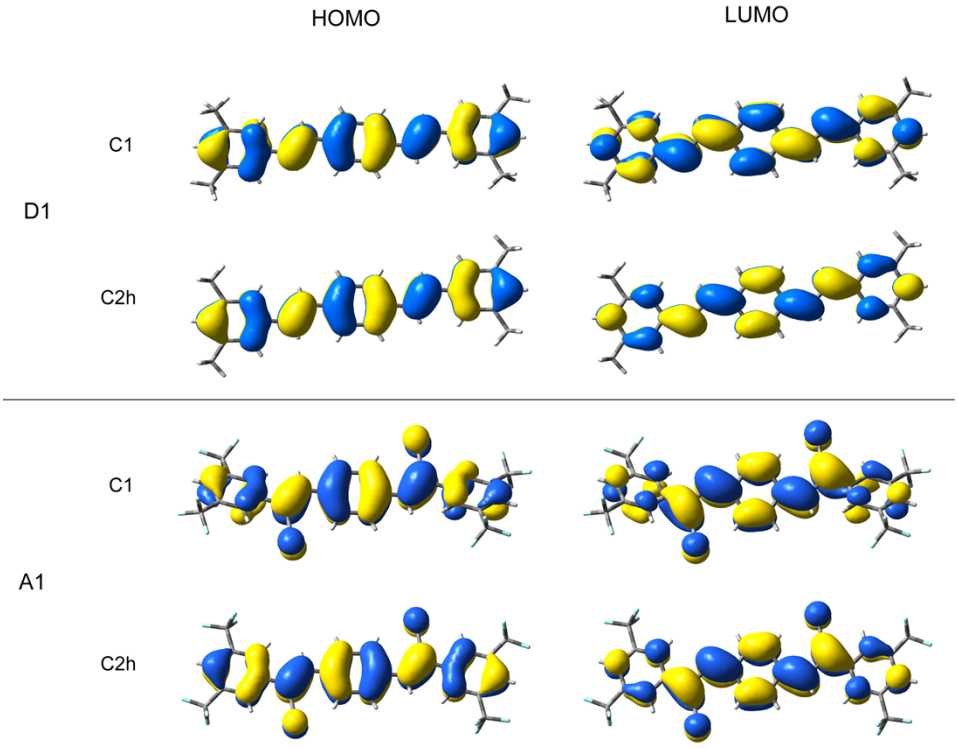


Fig. S2 HOMOs and LUMOs of D1 and A1 with the C_1 symmetrical structure (ground state) and C_{2h} symmetrical structure.

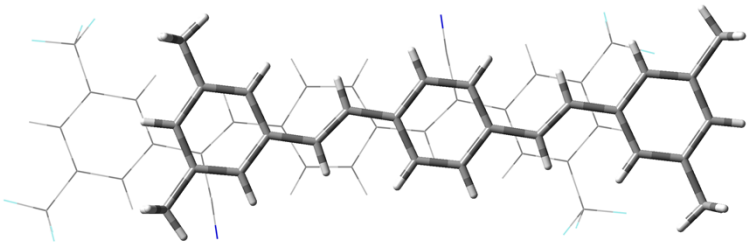


Fig. S3 Molecular packing crystal structure of top view for D-A complexes in experiment.

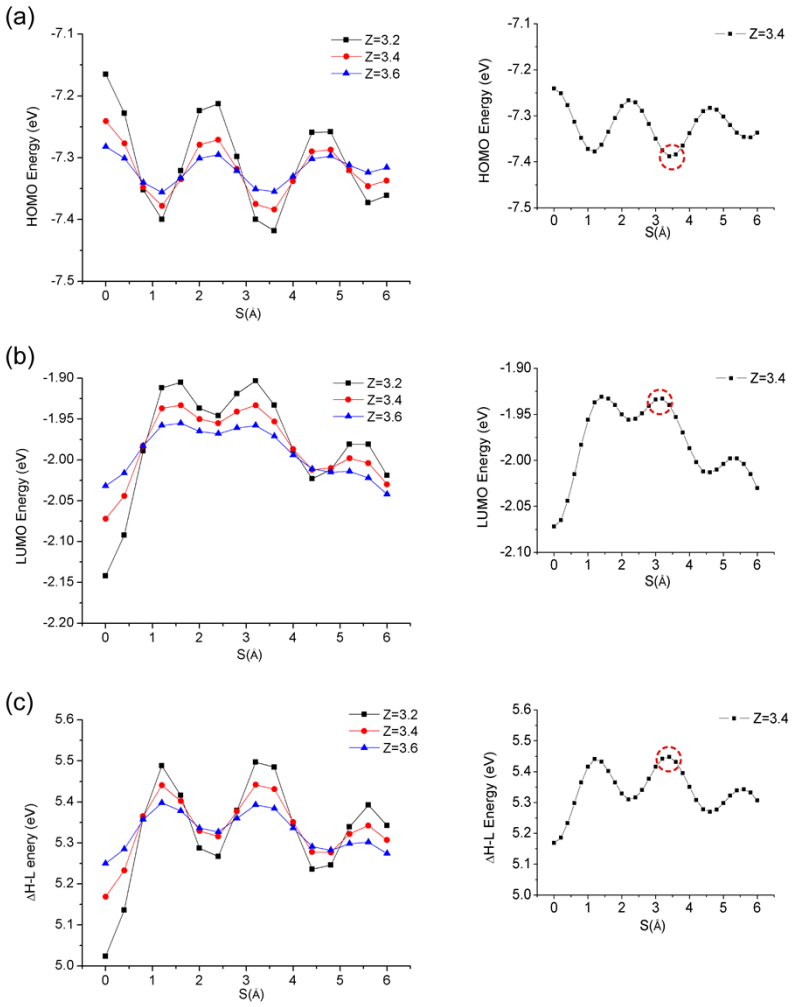


Fig. S4 Evolution of the HOMO (a), LUMO (b) and HOMO-LUMO gap energy (c) for D1-A1 pair as a function of the horizontal displacement S for the fixed vertical separation Z of 3.2 Å, 3.4 Å and 3.6 Å.

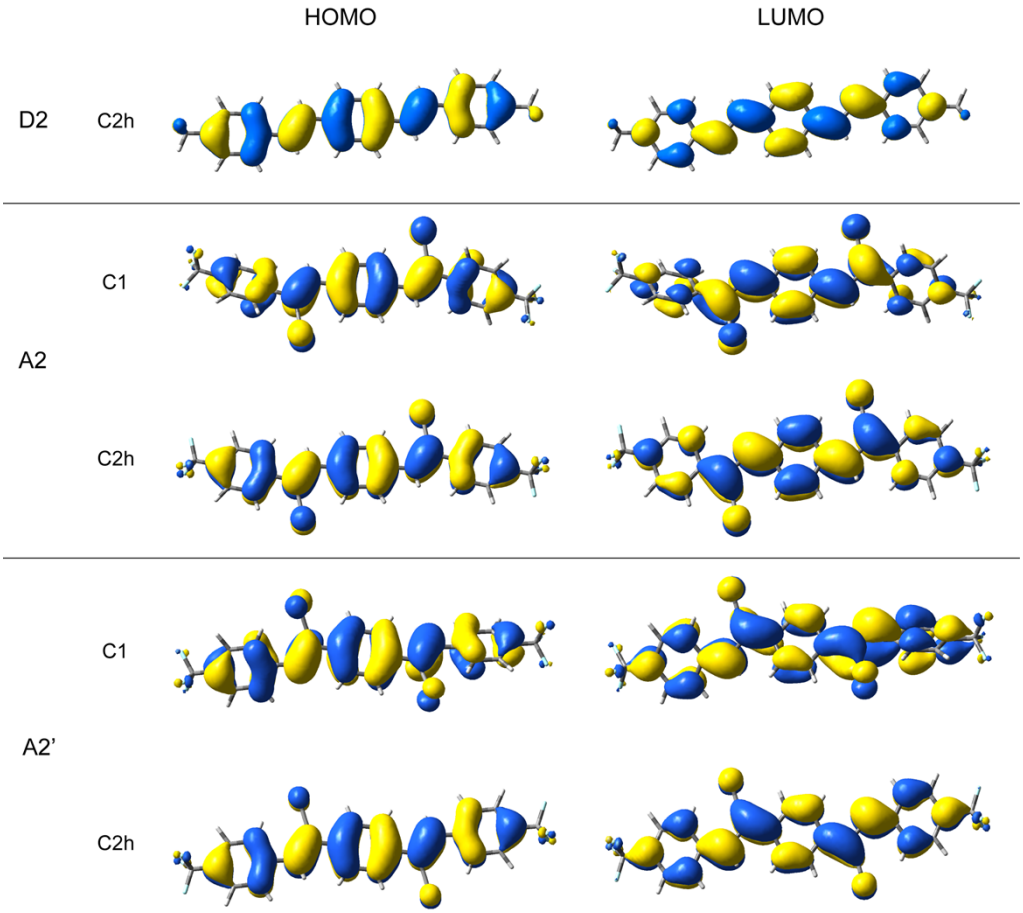


Fig. S5 HOMOs and LUMOs of D2 and A2 with the C1 symmetrical structure (in ground state) and C2h symmetrical structure.

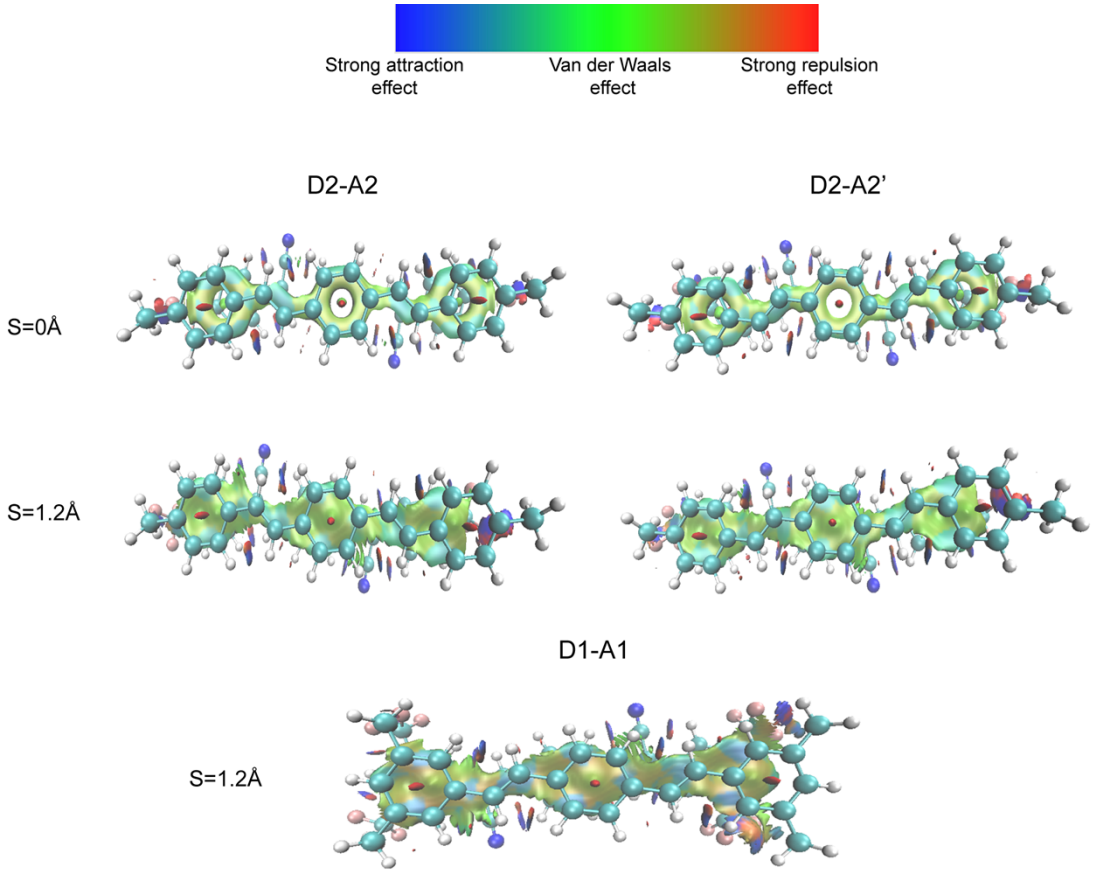


Fig. S6 Visualization of the weak interactions for D2-A2 pair, D2-A2' pair in real space at the configuration of S=0 Å and S=1.2 Å with fixed Z=3.6 Å, and for D1-A1 pair at the configuration of S=1.2 Å, Z= 3.4 Å. The scale runs from -0.01 (min) to 0.01 (max).

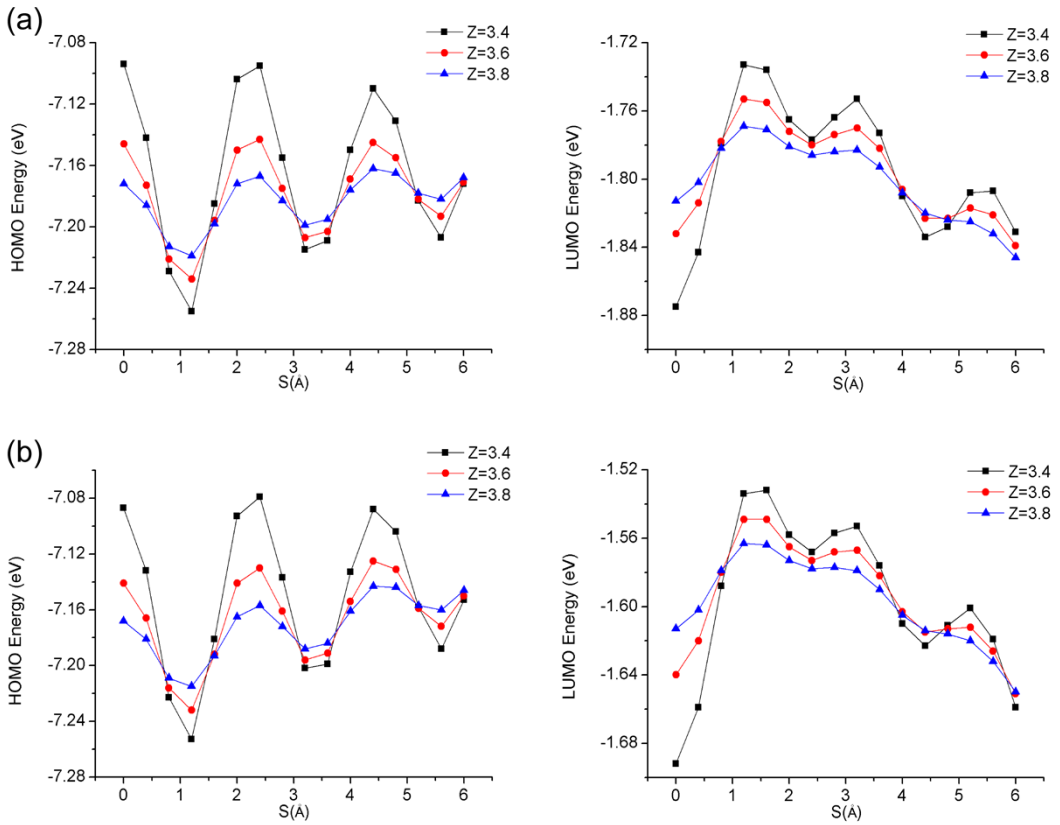


Fig. S7 Evolution of the HOMO energies and LUMO energies for D2-A2 pair (a) and D2-A2' pair (b) as a function of the horizontal displacement S for the fixed vertical separation Z of 3.4 Å, 3.6 Å and 3.8 Å.

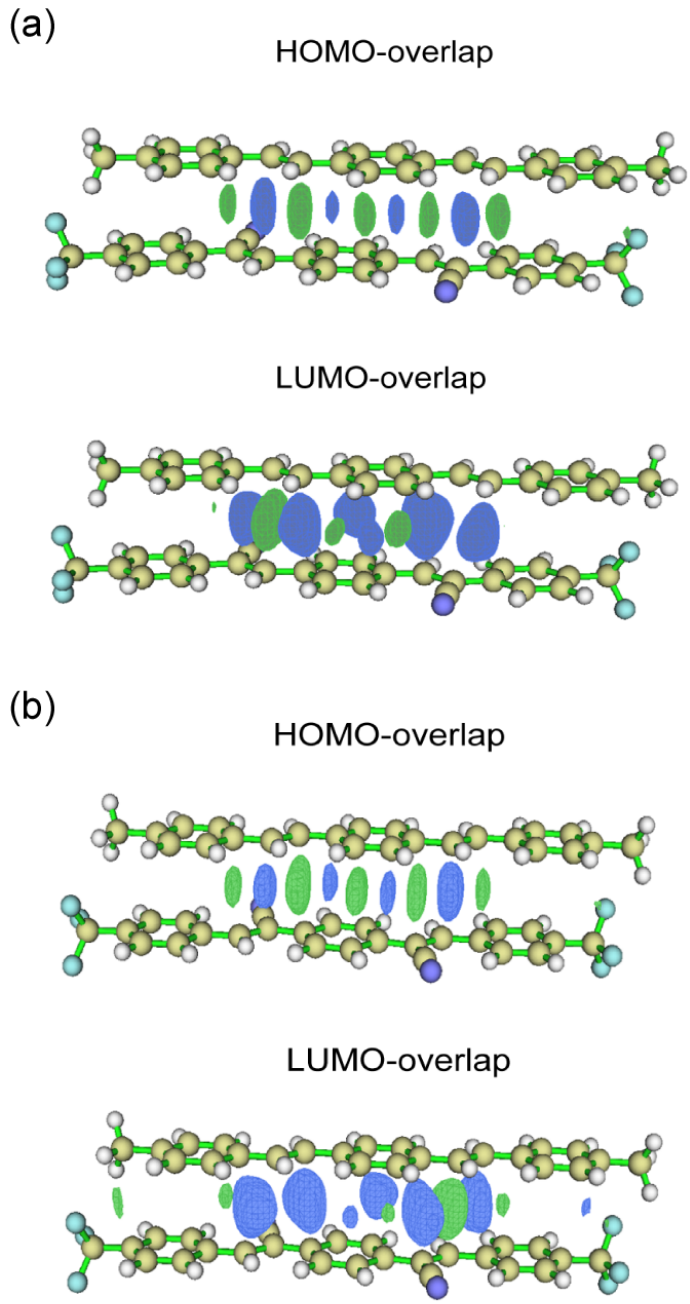


Fig. S8 The visualization of intermolecular orbital (HOMO and LUMO) overlap between (a) D2 and A2 (b) D2 and A2' molecules. Green/Blue isosurface refers to the overlap in the way of same/opposite phase.

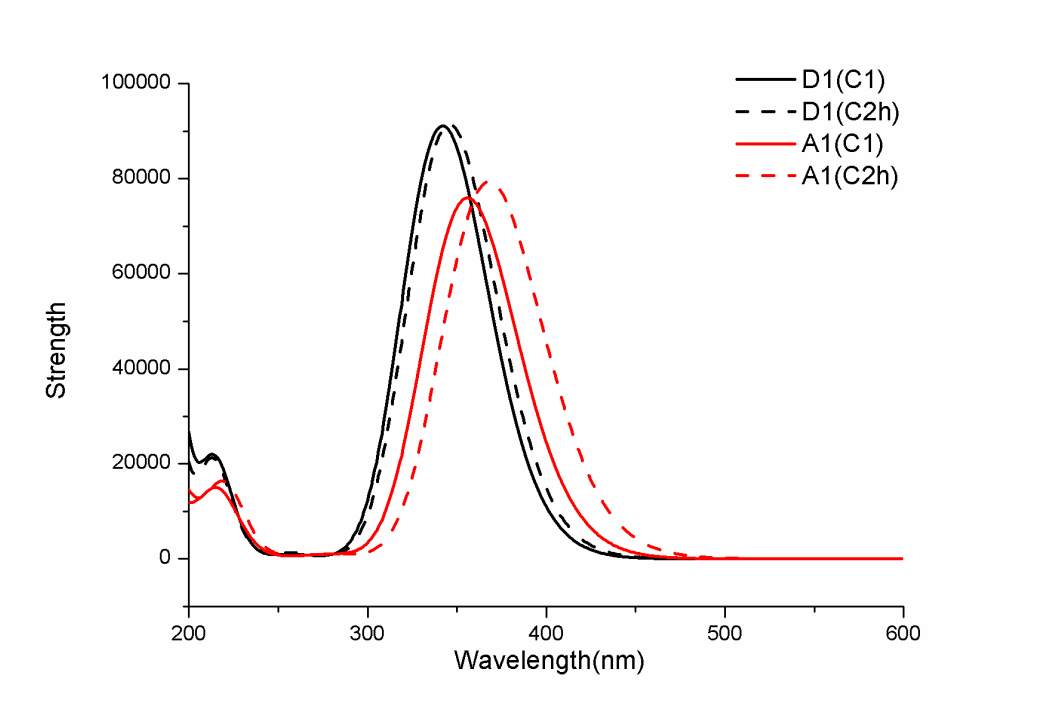
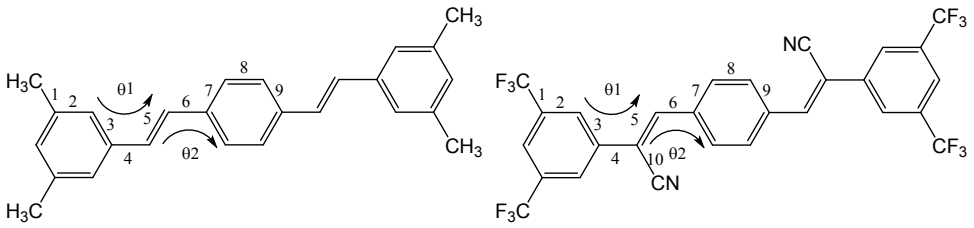


Fig. S9 Computed UV-vis absorption spectra of D1 and A1 monomers with C1 and C2h geometry, respectively.

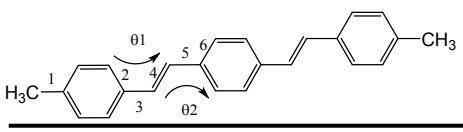
Table S1 Bond lengths (Å), torsion angles (°), the highest occupied molecular orbital (HOMO) energies (eV), the lowest unoccupied molecular orbital (LUMO) energies (eV) and potential difference (ΔE, kcal/mol) in different optimized geometry of **D1** and **A1** and the experimental values.

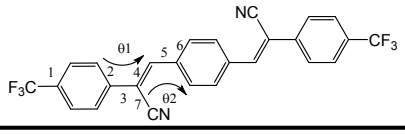


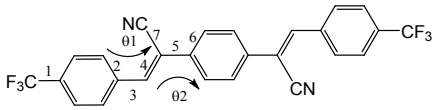
	D1			A1		
	C_1(Ground state)	C_{2h}	Exp	C_1(Ground state)	C_{2h}	Exp
1	1.510	1.510	1.508	1.507	1.508	1.496
2	1.389	1.391	1.387	1.393	1.389	1.379
3	1.408	1.406	1.403	1.399	1.403	1.399
4	1.464	1.464	1.461	1.488	1.489	1.473
5	1.347	1.347	1.331	1.360	1.361	1.349
6	1.461	1.461	1.461	1.456	1.456	1.448
7	1.408	1.408	1.396	1.411	1.412	1.400
8	1.385	1.384	1.381	1.383	1.382	1.371
9	1.406	1.406	1.398	1.409	1.409	1.405
10				1.429	1.430	1.444

θ1	-7.5	0.0	0.6	-31.1	0.0	1.7
θ2	-7.4	0.0	-1.3	-5.6	0.0	-4.7
HOMO	-5.303	-5.278		-6.908	-6.858	
LUMO	-1.921	-1.946		-3.621	-3.697	
ΔE	0.10			84.37		

Table S2 Bond lengths (Å) , torsion angles (°), the highest occupied molecular orbital (HOMO) energies (eV), the lowest unoccupied molecular orbital (LUMO) energies (eV) and potential difference (ΔE, kcal/mol) in different optimized geometry of D2, A2 and A2'.







	D2	A2		A2'	
	C_{2h}(Ground state)	C_1(Ground state)	C_{2h}	C_1(Ground state)	C_{2h}
1	1.508	1.504	1.504	1.505	1.505
2	1.408	1.404	1.406	1.409	1.411
3	1.463	1.487	1.488	1.460	1.460
4	1.347	1.360	1.361	1.359	1.360
5	1.461	1.456	1.456	1.485	1.486
6	1.408	1.411	1.410	1.403	1.406
7		1.429	1.431	1.431	1.432
θ1	0.0	30.7	0.0	-8.5	0.0
θ2	0.0	6.2	0.0	-29.5	0.0
HOMO	-5.271	-6.631	-6.568	-6.629	-6.518
LUMO	-1.942	-3.390	-3.469	-3.076	-3.281
ΔE		1.27		1.13	