ELECTRONIC SUPPORTING INFORMATION

A conical intersection model to explain aggregation induced emission in diphenyl dibenzofulvene

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Computational Details

The complete active space for DPDBF comprises 26 π orbitals (14 orbitals on the DBF moiety and 12 on the phenyl substituents). At the TD-DFT level (ωB97DX functional,[SI1] see Table SI3) the three lowest lying excited states arise from excitations in the DBF ring. Therefore, the orbitals from the two phenyl substituents can be excluded from the active space. The resulting (14,14) active space (14 electrons in 14 orbitals) was used for the MS-CASPT2 calculations (see Figure SI1). These calculations were carried out sateaverageing over four roots with equal weights in the CASSCF reference calculation, using an IPEA[SI2] parameter of 0.0 and an imaginary level shift[SI3] of 0.1. To reduce the computational effort further, the occupied and virtual orbitals of lowest and highest energy, respectively, were removed from the (14,14) active space for the CASSCF optimizations, leaving an active space of 12 electrons in 12 orbitals. The MS-CASPT2 calculations were carried out with an ANO-S basis set (3s2p1d for carbon and 2s1p for hydrogen), and the CASSCF optimizations with 6-31G*. The optimized structures are displayed in Figure SI2, and the Cartesian coordinates of the structures are given in the final section of this Electronic Supporting Information.

The MS-CASPT2 energies in solution are approximated from the gas phase energies by adding a solvent-induced correction calculated with the CPCM model.[SI4, 5] The correction is equal to the difference between the CASSCF(12,12)/6-31G* energies in the gas phase and calculated with CPCM, following Equation SI1:

$$E^{CPCM}_{MS-CASPT2} = E^{gas}_{MS-CASPT2} + E^{CPCM}_{CASSCF(12,12)} - E^{gas}_{CASSCF(12,12)} \qquad \text{(SI1)}$$

The results for the critical points (gas phase energies and solvent induced corrections) are listed in Table SI1. In all CPCM calculations (except for the vertical absorption, see below) the reaction field is equilibrated with respect to the state-averaged density because otherwise the CASSCF calculations do not converge. For consistency with the MS-CASPT2 calculations, the density is averaged over four states. The relative energies of the structures are obtained with respect to the ground state energy at the ground state minimum, calculated this way. For the vertical absorptions, the CPCM energies at the ground state minimum are recalculated under non-equilibrium conditions, equilibrating the reaction field with respect to the ground state density. For the vertical emission data, the ideal approach would be to recompute the ground-state energy with the reaction field optimized with respect to the emitting state. However, the PCM correction is obtained from the state-averaged calculation since the reaction field is optimized with respect to the average density also here. This approach is accurate enough for our purposes because the solvent induced shifts are small. For instance, the solvent induced shifts for the vertical absorption of S_1 are -0.012 eV (equilibrium conditions) and -0.028 eV (non-equilibrium); the shifts for S_2 are -0.007 eV (equilibrium) and -0.009 eV (non-equilibrium). The difference between the shifts in both regimes is less than 0.02 eV, which is a perfectly acceptable error.

The computed solvent-induced shifts can be compared with the dipole moments of the relevant states. These data (dipole moments along the C_1-C_6 axis) are given for **S_0-Min^{Ac}** in Table SI1. The largest change in the dipole moment with respect to the ground state is found for S_1 and is 0.63 au at the CASSCF level. This corresponds to a moderate charge transfer of approximately 0.2 electrons from the tricyclic unit to the C_1-C_6 bond, assuming that both units are separated by 3 bohr (see the orbitals in Scheme 1). The calculated shift of -0.028 eV (non-equilibrium conditions) is in agreement with this moderate charge transfer character. For comparison, the S_2 excitation induces almost no change in the dipole moment, and the computed shift is smaller (-0.009 eV). Table SI1 also shows that the dipole moments at the MS-CASPT2 level differ only by up to 0.1 au from the CASSCF values, which validates our approach of calculating the solvent-induced shifts at the CASSCF level.

In our discussion, we compare the experimental absorption and emission maxima with the computed vertical excitations at the ground and excited state minima, respectively, although these quantities do not correspond exactly to each other. Thus, the absorption maximum may be red shifted by 0.1 – 0.3 eV with respect to the vertical absorption because of the different force constants for the two states (including Duschinsky rotations), whereas the emission maximum may be blue shifted with respect to the vertical emission value for the same reason.[SI6] These differences have not been considered here because the expected shifts are small, and the calculation of the force constants for our systems is very expensive. We also note that asymmetries in the spectral line shape may also contribute to the shifts. In addition, for emission spectra the maxima in the wave length and frequency domains may differ by additional small amounts.

For the solid, we employed a cell model containing 24 DPDBF units. The starting structure is taken from the x-ray crystal structure.[SI7] The calculations were carried out at the ONIOM(CAS(12,12,nr=2)/6-31G*:UFF) level, where UFF stands for the Universal Force Field.[SI8] The QM part is composed by the central DPDBF unit (see Figure 4), mechanically embedded in the rigid MM part. The conical intersection optimization in the solid is carried out using the procedure described in Ref. SI8.[SI9] The final energies are obtained using the ONIOM extrapolation formula (Equation SI2): [SI10]

$$E_{MS-CASPT2}^{ONIOM} = E_{MS-CASPT2}^{model} + E_{UFF}^{real} - E_{UFF}^{model} \tag{SI2}$$

In Equation SI2, the model and real superscripts refer to the QM system and the whole crystal cell, respectively. The results are given in Table SI2.

To validate our approach, where a single DPDBF molecule is treated quantum mechanically, we have estimated the intermolecular exciton couplings with TD-DFT calculations on the DPDBF monomer and a hexamer (see Table SI3). We have used the ωB97XD functional, which contains the long range correction necessary to avoid spurious charge transfer excitations. The ω parameter was set to 0.1. This value gives the best compromise between obtaining accurate vertical excitations for the monomer, which requires small ω values, and avoiding spurious charge transfer states for the hexamer. For the monomer, the calculated vertical excitations are 3.70 eV and 4.23 eV for S_1 and S_2, respectively. These values show a significant deviation from the MS-CASPT2 data, but here we center on the coupling values, which can be estimated from the TD-DFT results for the hexamer. In this case we obtain two groups of six excitations each: the first group ranges from 3.68 eV to 3.78 eV, and the second one appears between 4.05 eV to 4.20 eV. According to a natural transition orbital analysis,[SI11] the first group of excitations corresponds to S_1-type excitations localized by more than 99 % on a single DPDBF unit. For the second group, the excitations are linear combinations of monomer S_2 excitations (see Figure SI3 for a representative example). However the small energy range of 0.15 eV covered by the six S_2-like states indicates that the couplings between the monomers are of the order of less than 0.1 eV. This lies well below the relaxation energy of S_2 in the monomer, which is approximately 0.5 eV (see Table 1). Thus, the S_2-like excitations will localize upon relaxation on a single DPDBF unit, and exciton formation can be excluded. Therefore, the relaxation can be well described with the hybrid QM:MM approach used here.

To characterize the seam (Figure 3), conical intersections on the seam were optimized freezing the dihedral angle φ to values between 0° and 90° in intervals of 10°. At these structures, the C_1-C_6 bond is substantially stretched, and the optimizations are carried out with a (12,12) active space that includes 10 π orbitals on the DBF fragment and the σ and σ^* orbitals of the C_1-C_6 bond. The MS-CASPT2 energies (see Table SI4) are calculated in the gas phase with a (16,14) active space that includes twelve π orbitals and the σ/σ^* orbital pair. Because of the different active space used for these calculations compared to the other critical points (Table SI2), the energies of the seam structures are given relative to the MS-CASPT2/CASSCF(16,14) energy of the seam minimum (φ=90°).

References

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Table SI1: CASSCF(14,14)/ANO-S, CASPT2, and MS-CASPT2 energies for the critical points in the gas phase and in acetonitrile (see Equation SI1).

Structure	State	CASSCF(14,14)/ ANO-S (gas) Energy [au]	CASPT2/ANO-S (gas) Energy [au]	MS-CASPT2/ANO-S (gas) Energy [au]	CASSCF(12,12)/ 6-31G* (gas) Energy [au]	CASSCF(12,12)/ 6-31G* (CPCM) Energy [au]	CPCM shift[a] Energy [au]	MS-CASPT2/ ANO-S (CPCM)[b] Energy [eV]
S_0-Min^{Ac}	S_0	-995.3804571 (0.22)[c]	-998.5683413	-998.5684222 (0.23)[c]	-995.19858	-995.20761 (-995.20746)[d]	-0.00903 (-0.008882)[e]	0.00
	S_1	-995.2293015 (-0.41)[c]	-998.4464124	-998.4544622 (-0.52)[c]	-995.04259	-995.05059 (-995.05104)[d]	-0.00801 (-0.008452)[e]	3.13
	S_2	-995.2103261 (0.19)[c]	-998.4212522	-998.4211713 (0.17)[c]	-995.01401	-995.02271 (-995.02262)[d]	-0.00870 (-0.008609)[e]	4.02
	S_3	-995.194348 (-0.17)[c]	-998.4199046	-998.4118548 (-0.06)[c]	-995.01154	-995.01962 (-995.01984)[d]	-0.00808 (-0.008296)[e]	4.29
S_1-Min^{Ac}	S_0	-995.3154976	-998.5233689	-998.5265545	-995.12992	-995.13914	-0.00923	1.13
	S_1	-995.2723029	-998.4743006	-998.4744067	-995.09421	-995.10177	-0.00757	2.59
	S_2	-995.2019733	-998.424349	-998.4295424	-995.02094	-995.02877	-0.00784	3.81
	S_3	-995.1948446	-998.432728	-998.4242429	-995.01636	-995.02727	-0.01091	3.87
S_2-Min^{Ac}	S_0	-995.3470513	-998.5501807	-998.5510586	-995.17669	-995.18515	-0.00846	0.48
	S_1	-995.2473167	-998.4619651	-998.4622364	-995.07321	-995.08122	-0.00801	2.91
	S_2	-995.2213073	-998.4400297	-998.4395961	-995.05041	-995.05872	-0.00831	3.52
	S_3	-995.1962634	-998.4250153	-998.4242997	-995.00869	-995.01674	-0.00804	3.94
(S_1/S_0)-CI^{Ac}	S_0	-995.2661922	-998.4574647	-998.4724211	-995.05775	-995.06516	-0.00741	2.65
	S_1	-995.2653351	-998.472309	-998.4574701	-995.0564	-995.06508	-0.00867	3.02
	S_2	-995.1767083	-998.3931433	-998.3931378	-994.98109	-994.99802	-0.01693	4.55
	S_3	-995.1634564	-998.3728088	-998.3726966	-994.96886	-994.97676	-0.00789	5.35

[a] Difference between CPCM and gas phase CASSCF(12,12) energies. [b] Energies for structures other than **S_0-Min^{Ac}** calculated relative to the ground state CPCM energy of **S_0-Min^{Ac}** obtained with the equilibrium approximation; the corresponding CASSCF(12,12)/6-31G*(PCM) energy is -995.2076067 au. [c] In brackets, dipole moment of the states along the C_1-C_6 axis, referred to the center of mass, in au. [d] CPCM energies calculated using the non-equilibrium approximation for the vertical excitations; CPCM energies in the equilibrium regime in brackets (reaction field equilibrated with respect to the averaged density). [e] CPCM shifts in the equilibrated regime in brackets.

Table SI2: CASSCF(14,14)/ANO-S, CASPT2, and MS-CASPT2 energies for the critical points in the crystal (see Equation SI2).

Structure	State	CASSCF(14,14)/ ANO-S Energy [au]	CASPT2/ANO-S Energy [au]	MS-CASPT2/ANO-S Energy [au]	UFF (real) Energy [au]	UFF (model) Energy [au]	MS-CASPT2/ANO-S (ONIOM) Energy [eV]
S_0-Min^{cry}	S_0	-995.3789042	-998.5653131	-998.5653894	4.6855747	0.1717148	0.00
	S_1	-995.2253037	-998.4404335	-998.4489568			3.17
	S_2	-995.2075475	-998.4167387	-998.4166165			4.05
	S_3	-995.1882587	-998.4149882	-998.4065107			4.32
S_1-Min^{cry}	S_0	-995.3355412	-998.5324452	-998.532549	4.7373478	0.2227496	0.91
	S_1	-995.249942	-998.4518771	-998.4519585			3.11
	S_2	-995.1976345	-998.4120511	-998.4119743			4.19
	S_3	-995.1881363	-998.4049787	-998.4048703			4.39
S_2-Min^{cry}	S_0	-995.3627118	-998.5565597	-998.5566094	4.7034132	0.1893640	0.24
	S_1	-995.2379984	-998.4527115	-998.45512			3.01
	S_2	-995.2137185	-998.4282778	-998.4264643			3.79
	S_3	-995.20193	-998.4185933	-998.4179487			4.02
(S_1/S_0)-CI^{cry}	S_0	-995.1890801	-998.3822433	-998.402287	4.7470784	0.2297039	4.53
	S_1	-995.1883768	-998.3927253	-998.373999			5.30
	S_2	-995.0970059	-998.3088331	-998.308801			7.08
	S_3	-995.0870343	-998.2938734	-998.292588			7.52

Table SI3. Time-dependent ωB97DX/6-31G* (ω=0.1) excitation energies of the DPDBF monomer and a hexamer.

	State	Energy [eV]
Monomer	S_0	0.00
	S_1	3.70
	S_2	4.23
	S_3	4.54
Hexamer	S_0	0.00
	S_1	3.68
	S_2	3.72
	S_3	3.73
	S_4	3.76
	S_5	3.77
	S_6	3.78
	S_7	4.05
	S_8	4.11
	S_9	4.16
	S_{10}	4.17
	S_{11}	4.19
	S_{12}	4.20

Table SI4. CASSCF(16,14)/ANO-S, CASPT2, and MS-CASPT2 energies for the optimized points on the S_1/S_0 seam, at different frozen values of φ.

φ [°]	State	CASSCF(14,14)/ ANO-S Energy [au]	CASPT2/ANO-S Energy [au]	MS-CASPT2/ANO-S Energy [au]	MS-CASPT2/ANO-S Energy [eV][a]
90	S_0	-995.2293496	-998.4735650	-998.4735650	0.00
	S_1	-995.2277007	-998.4600379	-998.4600379	
80	S_0	-995.2274165	-998.4702581	-998.4702581	0.09
	S_1	-995.2257155	-998.4569700	-998.4569700	
70	S_0	-995.2206312	-998.4627147	-998.4627147	0.28
	S_1	-995.2191370	-998.4502984	-998.4502984	
60	S_0	-995.2109516	-998.4523572	-998.4523572	0.55
	S_1	-995.2095571	-998.4407521	-998.4407521	
50	S_0	-995.1998140	-998.4406708	-998.4406708	0.86
	S_1	-995.1984428	-998.4296617	-998.4296617	
40	S_0	-995.1885316	-998.4287814	-998.4287814	1.18
	S_1	-995.1871875	-998.4181041	-998.4181041	
30	S_0	-995.1771523	-998.4166968	-998.4166968	1.51
	S_1	-995.1757985	-998.4059987	-998.4059987	
20	S_0	-995.1670162	-998.4049202	-998.4049202	1.84
	S_1	-995.1655874	-998.3937252	-998.3937252	
10	S_0	-995.1586805	-998.3946606	-998.3946606	2.12
	S_1	-995.1571684	-998.3828269	-998.3828269	
0	S_0	-995.1534984	-998.3867959	-998.3867959	2.35
	S_1	-995.1518966	-998.3742033	-998.3742033	

[a] Average energy of S_1 and S_0, relative to the energy of the seam minimum (φ=90°).

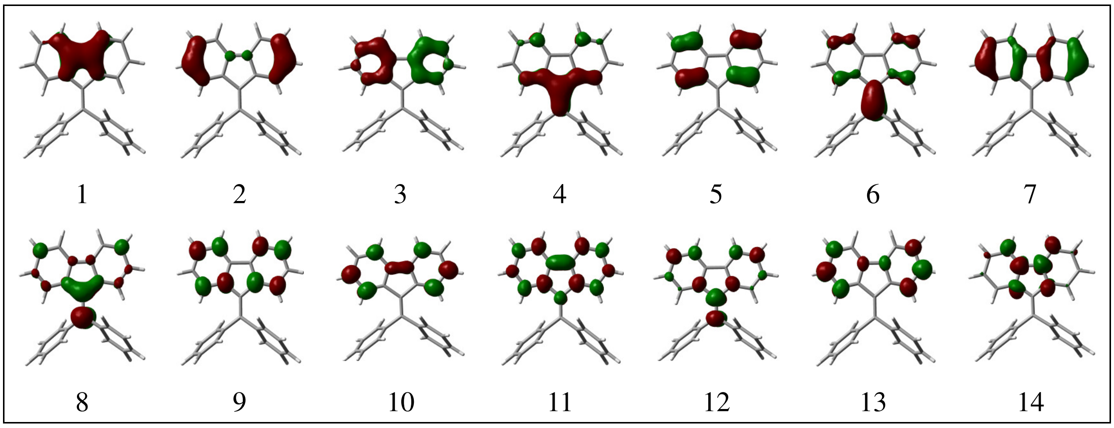
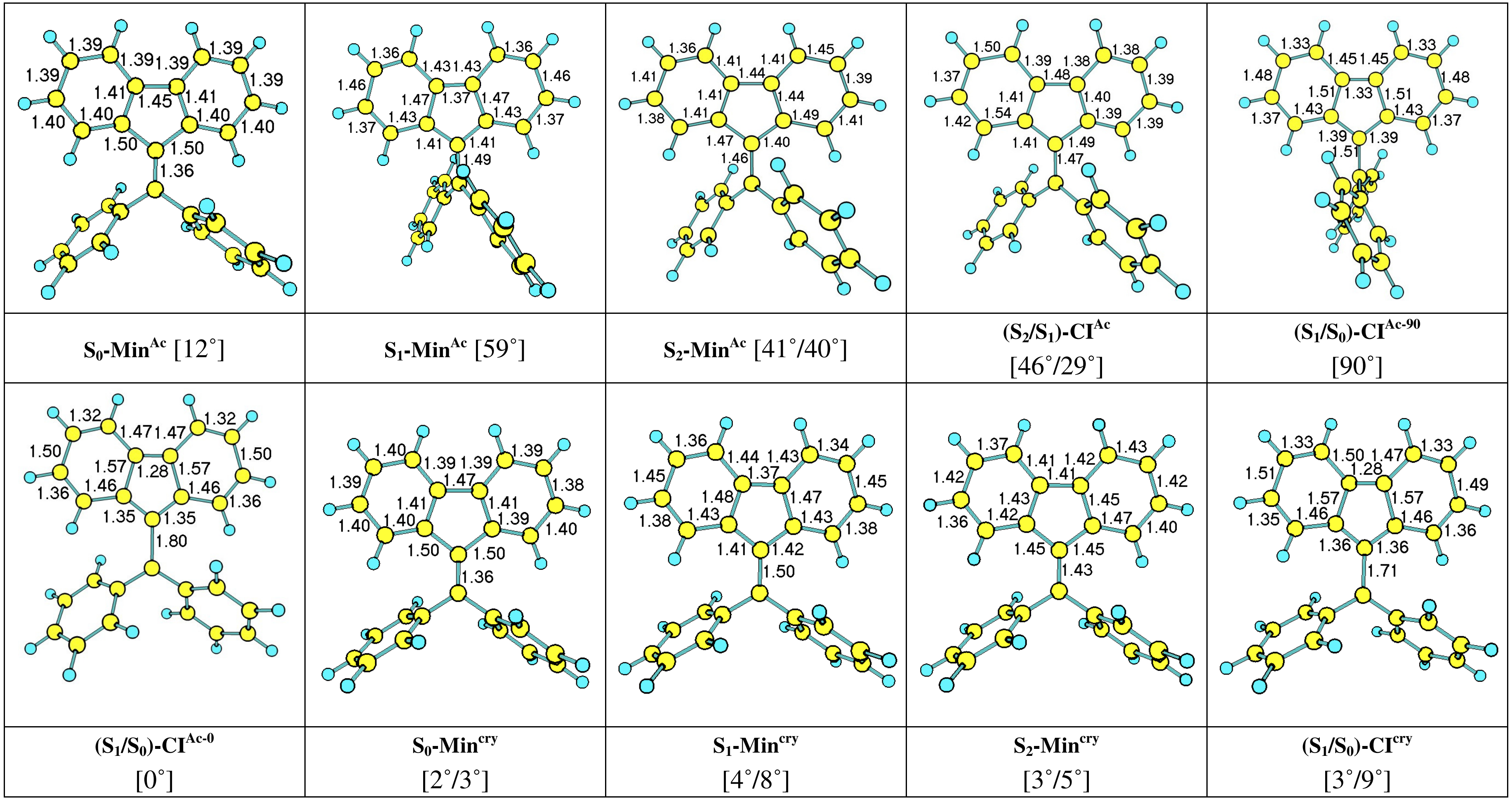


Figure SI1 Molecular orbitals included in the (14,14) active space of the MS-CASPT2/ANO-S calcualtion at the FC geometry of DPDBF.



S_0-Min^{Ac} [12°]

S_1-Min^{Ac} [59°]

S_2-Min^{Ac} [41°/40°]

(S_2/S_1)-CI^{Ac} [46°/29°]

(S_1/S_0)-CI$^{Ac\text{-}90}$ [90°]

(S_1/S_0)-CI$^{Ac\text{-}0}$ [0°]

S_0-Min^{cry} [2°/3°]

S_1-Min^{cry} [4°/8°]

S_2-Min^{cry} [3°/5°]

(S_1/S_0)-CI^{cry} [3°/9°]

Figure SI2. Structures of key critical points, including bond lengths in Å and the torsion angle φ. For structures of C_2 symmetry only one value of φ is given; for C_1 structures the two angles C_2-C_1-C_6-C_{15} and C_5-C_1-C_6-C_{21} are given.

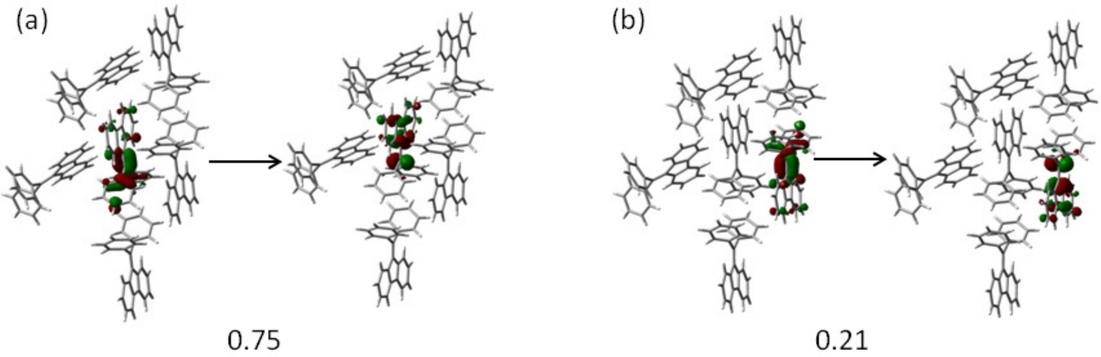


Figure SI3. Natural transition orbitals for S_7 of a DPDBF hexamer, calculated with ωB97XD/6-31G*. The numbers show the participation of each excitation pair in the transition.

Cartesian coordinates of structures

S_0-Min^{Ac}

6	-0.002862	2.980538	-3.599551
6	0.000000	3.447312	-2.285322
6	-0.012848	2.558372	-1.206516
6	-0.040853	1.184700	-1.453934
6	-0.015905	0.726771	-2.782846
6	-0.004306	1.608786	-3.852053
1	0.006074	3.677639	-4.418335
1	0.014981	4.505561	-2.094410
1	0.001885	2.949813	-0.210956
1	0.012432	1.245671	-4.864128
6	0.040853	-1.184700	-1.453934
6	0.012848	-2.558372	-1.206516
6	0.000000	-3.447312	-2.285322
6	0.002862	-2.980538	-3.599551
6	0.004306	-1.608786	-3.852053
6	0.015905	-0.726771	-2.782846
1	-0.001885	-2.949813	-0.210956
1	-0.014981	-4.505561	-2.094410
1	-0.006074	-3.677639	-4.418335
1	-0.012432	-1.245671	-4.864128
6	0.000000	0.000000	-0.538297
6	0.000000	0.000000	0.821906
6	0.307657	-1.216291	1.645045
6	-0.658500	-1.787271	2.467939
6	1.589609	-1.755439	1.647716
6	-0.357674	-2.888350	3.251270
1	-1.649223	-1.369885	2.492543
6	1.895525	-2.850761	2.439948
1	2.346100	-1.322114	1.018137
6	0.921370	-3.423614	3.240179
1	-1.118963	-3.324863	3.873041
1	2.891974	-3.255387	2.428963
1	1.156227	-4.275480	3.853068
6	-0.307657	1.216291	1.645045
6	-1.589609	1.755439	1.647716
6	0.658500	1.787271	2.467939
6	-1.895525	2.850761	2.439948
1	-2.346100	1.322114	1.018137
6	0.357674	2.888350	3.251270
1	1.649223	1.369885	2.492543
6	-0.921370	3.423614	3.240179
1	-2.891974	3.255387	2.428963
1	1.118963	3.324863	3.873041
1	-1.156227	4.275480	3.853068

S_1-Min

6	0.487618	2.934967	-3.508725
6	0.548380	3.369066	-2.119648
6	0.398262	2.489863	-1.077154
6	0.173233	1.109021	-1.362060
6	0.109596	0.674322	-2.767505
6	0.274877	1.629772	-3.822651
1	0.615428	3.667394	-4.284337
1	0.715731	4.412681	-1.915901
1	0.442902	2.832864	-0.060330
1	0.232511	1.311774	-4.849022
6	-0.173217	-1.109003	-1.362055
6	-0.398261	-2.489844	-1.077139
6	-0.548394	-3.369050	-2.119625
6	-0.487632	-2.934957	-3.508703
6	-0.274874	-1.629765	-3.822633
6	-0.109580	-0.674318	-2.767499
1	-0.442900	-2.832838	-0.060313
1	-0.715757	-4.412662	-1.915872
1	-0.615459	-3.667383	-4.284312
1	-0.232514	-1.311772	-4.849006
6	0.000016	0.000006	-0.515365
6	0.000008	0.000000	0.972965
6	0.984299	-0.832568	1.693981
6	0.677740	-1.448136	2.911230
6	2.256324	-1.046631	1.158277
6	1.607867	-2.234232	3.567954
1	-0.298368	-1.316565	3.339309
6	3.187965	-1.828375	1.818362
1	2.515780	-0.589666	0.221919
6	2.869360	-2.425622	3.026968
1	1.344684	-2.700979	4.500506
1	4.163415	-1.969026	1.388005
1	3.592825	-3.033904	3.539350
6	-0.984291	0.832556	1.693980
6	-2.256301	1.046643	1.158252
6	-0.677750	1.448100	2.911245
6	-3.187948	1.828386	1.818331
1	-2.515739	0.589701	0.221878
6	-1.607884	2.234192	3.567965
1	0.298349	1.316516	3.339341
6	-2.869363	2.425605	3.026956
1	-4.163385	1.969060	1.387953
1	-1.344715	2.700920	4.500531
1	-3.592833	3.033887	3.539333

S_2-Min

C	0.730215	2.972927	-3.467214
C	0.845159	3.384671	-2.141160
C	0.624578	2.497353	-1.070459
C	0.242823	1.087493	-1.360118
C	0.159464	0.671434	-2.740352
C	0.388097	1.596964	-3.783449
C	-0.263528	-1.152630	-1.404173
C	-0.625366	-2.483388	-1.124611
C	-0.855253	-3.351432	-2.177546
C	-0.737615	-2.916385	-3.518170
C	-0.403650	-1.625647	-3.803032
C	-0.167071	-0.728711	-2.746356
C	-0.002692	-0.012105	-0.522025
C	0.016749	-0.003972	0.935387
C	0.612708	-1.133262	1.687747
C	0.023979	-1.617344	2.858081
C	1.786356	-1.743411	1.242030
C	0.586042	-2.674303	3.552731
C	2.351065	-2.796041	1.940620
C	1.753242	-3.267184	3.098498
C	-0.592769	1.126116	1.674568
C	-1.775083	1.715774	1.222751
C	-0.007186	1.635642	2.836292
C	-2.348850	2.775152	1.904426
C	-0.577943	2.699146	3.513056
C	-1.751908	3.273409	3.050824
H	0.902219	3.667997	-4.266749
H	1.114401	4.402402	-1.925768
H	0.736378	2.830496	-0.058105
H	0.314656	1.291648	-4.812487
H	-0.723206	-2.829309	-0.114212
H	-1.129630	-4.370410	-1.977356
H	-0.920763	-3.614911	-4.314137
H	-0.325171	-1.297535	-4.824210
H	-0.883425	-1.169451	3.219259
H	2.257179	-1.388869	0.343522
H	0.109594	-3.036383	4.446535
H	3.258149	-3.247579	1.579976
H	2.190682	-4.087182	3.639583
H	-2.250405	1.333049	0.338345
H	0.903522	1.200291	3.204934
H	-3.264199	3.207757	1.541161
H	-0.104681	3.080198	4.400683
H	-2.196861	4.097522	3.579529

(S_2/S_1)-CI

C	0.463780	3.013529	-3.483526
C	0.666745	3.421614	-2.175054
C	0.742037	2.482098	-1.147191
C	0.310957	1.189584	-1.413385
C	0.126995	0.786013	-2.737992
C	0.086729	1.715125	-3.758212
C	-0.118791	-1.104768	-1.364645
C	-0.435778	-2.582141	-1.083220
C	-0.691864	-3.442863	-2.180571
C	-0.684338	-2.989127	-3.471042
C	-0.415863	-1.546183	-3.756150
C	-0.146030	-0.670219	-2.709338
C	0.168483	-0.001689	-0.536033
C	0.212544	0.035867	0.928404
C	0.700853	-1.120775	1.717627
C	-0.054548	-1.626606	2.782544
C	1.892840	-1.765363	1.396989
C	0.358203	-2.750309	3.477224
C	2.302766	-2.893785	2.092104
C	1.536484	-3.393365	3.130618
C	-0.455909	1.158107	1.646106
C	-1.621951	1.747431	1.152832
C	0.077810	1.672062	2.833427
C	-2.233404	2.795173	1.829262
C	-0.533912	2.717498	3.504577
C	-1.695273	3.284873	3.006223
H	0.498202	3.745526	-4.264771
H	0.893323	4.446904	-1.978427
H	0.984707	2.802212	-0.156475
H	-0.137075	1.421163	-4.763864
H	-0.472601	-2.960674	-0.081654
H	-0.901712	-4.479833	-1.996607
H	-0.884219	-3.676490	-4.272780
H	-0.421866	-1.179290	-4.768273
H	-0.975909	-1.146368	3.059021
H	2.502530	-1.394135	0.591476
H	-0.244934	-3.128773	4.284527
H	3.224748	-3.379232	1.822283
H	1.853961	-4.270838	3.666676
H	-2.059183	1.398971	0.234754
H	0.980457	1.249355	3.236654
H	-3.132199	3.228556	1.426319
H	-0.097102	3.092753	4.413521
H	-2.170695	4.098411	3.524895

(S_1/S_0)-CI^{ac} (φ=90°)

6	-0.011705	2.959209	-3.516564
6	-0.020137	3.398301	-2.103911
6	-0.012062	2.510690	-1.065365
6	0.000000	1.103385	-1.341825
6	0.000000	0.664141	-2.784682
6	0.000000	1.664193	-3.840053
1	-0.014238	3.701450	-4.295801
1	-0.033407	4.458414	-1.891988
1	-0.024059	2.855047	-0.044103
1	0.005795	1.345174	-4.867319
6	0.000000	-1.103385	-1.341825
6	0.012062	-2.510690	-1.065365
6	0.020137	-3.398301	-2.103911
6	0.011705	-2.959209	-3.516564
6	0.000000	-1.664193	-3.840053
6	0.000000	-0.664141	-2.784682
1	0.024059	-2.855047	-0.044103
1	0.033407	-4.458414	-1.891988
1	0.014238	-3.701450	-4.295801
1	-0.005795	-1.345174	-4.867319
6	0.000000	0.000000	-0.495512
6	0.000000	0.000000	1.011505
6	1.294807	-0.000001	1.714037
6	1.472394	-0.639212	2.937387
6	2.404525	0.624080	1.132685
6	2.705145	-0.638565	3.566886
1	0.642461	-1.145750	3.392243
6	3.629195	0.637602	1.762685
1	2.290147	1.098774	0.179320
6	3.785740	0.004385	2.987053
1	2.820191	-1.143892	4.508645
1	4.462054	1.134641	1.299959
1	4.740331	0.008681	3.481070
6	-1.294807	0.000001	1.714037
6	-2.404525	-0.624080	1.132685
6	-1.472394	0.639212	2.937387
6	-3.629195	-0.637602	1.762685
1	-2.290147	-1.098774	0.179320
6	-2.705145	0.638565	3.566886
1	-0.642461	1.145750	3.392243
6	-3.785740	-0.004385	2.987053
1	-4.462054	-1.134641	1.299959
1	-2.820191	1.143892	4.508645
1	-4.740331	-0.008681	3.481070

(S_1/S_0)-CI^{ac} (φ=0°)

6	0.044895	2.941300	-3.839556
6	0.133398	3.371867	-2.405024
6	0.105452	2.511231	-1.357952
6	0.000000	1.065704	-1.570511
6	-0.000001	0.641506	-3.082586
6	-0.000001	1.654192	-4.150914
1	0.033594	3.682033	-4.622819
1	0.230554	4.432552	-2.188112
1	0.232651	2.900548	-0.363850
1	-0.046116	1.316647	-5.172334
6	0.000000	-1.065704	-1.570511
6	-0.105452	-2.511231	-1.357952
6	-0.133398	-3.371867	-2.405024
6	-0.044895	-2.941300	-3.839556
6	0.000001	-1.654192	-4.150914
6	0.000001	-0.641506	-3.082586
1	-0.232651	-2.900548	-0.363850
1	-0.230554	-4.432552	-2.188112
1	-0.033594	-3.682033	-4.622819
1	0.046116	-1.316647	-5.172334
6	0.000000	0.000000	-0.734406
6	0.000000	0.000000	1.068810
6	0.000000	-1.255276	1.839894
6	-0.922066	-1.425546	2.867299
6	0.969324	-2.217445	1.638659
6	-0.901299	-2.558995	3.647690
1	-1.648272	-0.654788	3.031413
6	1.010026	-3.351929	2.429456
1	1.708695	-2.053641	0.881975
6	0.068773	-3.527513	3.429408
1	-1.624104	-2.684642	4.430941
1	1.779719	-4.084474	2.277515
1	0.100101	-4.404992	4.046878
6	0.000000	1.255276	1.839894
6	-0.969324	2.217445	1.638659
6	0.922066	1.425546	2.867299
6	-1.010026	3.351929	2.429456
1	-1.708695	2.053641	0.881975
6	0.901299	2.558995	3.647690
1	1.648272	0.654788	3.031413
6	-0.068773	3.527513	3.429408
1	-1.779719	4.084474	2.277515
1	1.624104	2.684642	4.430941
1	-0.100101	4.404992	4.046878

(S$_0$)-Min^{cry}

C	-0.470034	2.935063	-3.612925
C	-0.408915	3.418514	-2.322791
C	-0.240196	2.563210	-1.232227
C	-0.122583	1.191875	-1.453976
C	-0.133427	0.717267	-2.778418
C	-0.325677	1.571624	-3.853451
C	0.136543	-1.170086	-1.427182
C	0.296343	-2.534179	-1.165588
C	0.442832	-3.423864	-2.233550
C	0.416321	-2.974442	-3.552797
C	0.210347	-1.622051	-3.828843
C	0.067145	-0.736371	-2.765050
C	0.016824	0.022001	-0.524418
C	0.012264	0.030124	0.833949
C	0.197220	-1.213491	1.654903
C	-0.895459	-1.842765	2.241444
C	1.464286	-1.744123	1.859991
C	-0.730026	-3.000121	2.984391
C	1.632712	-2.894960	2.611170
C	0.536542	-3.531809	3.167493
C	-0.179121	1.264899	1.666607
C	-1.437202	1.834669	1.824502
C	0.897995	1.821960	2.348896
C	-1.609755	2.953963	2.622736
C	0.727409	2.938196	3.149330
C	-0.527189	3.511278	3.282043
H	-0.621532	3.611974	-4.435109
H	-0.487824	4.475662	-2.146765
H	-0.200949	2.981984	-0.248715
H	-0.364890	1.184178	-4.854382
H	0.318949	-2.916299	-0.169008
H	0.592660	-4.469336	-2.033042
H	0.564354	-3.674598	-4.351459
H	0.177521	-1.272917	-4.845136
H	-1.879974	-1.432949	2.103480
H	2.312982	-1.272332	1.399384
H	-1.587643	-3.486471	3.414197
H	2.615278	-3.305816	2.745266
H	0.671935	-4.433445	3.734889
H	-2.280306	1.413407	1.307246
H	1.872292	1.378766	2.252991
H	-2.587424	3.390365	2.725649
H	1.569951	3.359216	3.668133
H	-0.660579	4.382230	3.894980

(S$_1$)-Min^{cry}

C	-0.419838	2.904584	-3.648605
C	-0.328116	3.387467	-2.288759
C	-0.166504	2.548020	-1.210407
C	-0.086440	1.136159	-1.424767
C	-0.107047	0.675876	-2.824673
C	-0.298835	1.593474	-3.906951
C	0.102801	-1.116271	-1.403472
C	0.218372	-2.519279	-1.158219
C	0.358850	-3.388478	-2.217836
C	0.364862	-2.947893	-3.594995
C	0.187315	-1.632718	-3.892927
C	0.046724	-0.684896	-2.815656
C	0.022916	0.017060	-0.563477
C	0.045541	0.030325	0.935676
C	0.259126	-1.219629	1.718438
C	-0.813056	-1.840236	2.355633
C	1.518793	-1.796659	1.828410
C	-0.637873	-3.021635	3.056383
C	1.698820	-2.971862	2.538679
C	0.621383	-3.593407	3.146506
C	-0.208801	1.264786	1.729804
C	-1.467970	1.854641	1.784921
C	0.825415	1.841205	2.464730
C	-1.681833	3.001994	2.531222
C	0.615509	2.987800	3.211090
C	-0.639296	3.575436	3.239874
H	-0.579111	3.611553	-4.442668
H	-0.376237	4.448749	-2.118678
H	-0.096042	2.967127	-0.228994
H	-0.359375	1.210175	-4.908126
H	0.210647	-2.910229	-0.164444
H	0.475624	-4.439720	-2.020090
H	0.514837	-3.675960	-4.366826
H	0.178274	-1.289493	-4.911767
H	-1.792074	-1.400695	2.287811
H	2.351003	-1.335449	1.328891
H	-1.481973	-3.494878	3.525470
H	2.674974	-3.413528	2.601198
H	0.764272	-4.513768	3.681228
H	-2.279761	1.422370	1.229288
H	1.799991	1.387688	2.447155
H	-2.660137	3.448402	2.554785
H	1.428762	3.421023	3.765824
H	-0.804494	4.470766	3.808162

(S_2)-Min^{cry}

C	-0.475459	2.974106	-3.607986
C	-0.375473	3.457081	-2.279835
C	-0.190758	2.590357	-1.200812
C	-0.103541	1.139285	-1.441613
C	-0.111844	0.674892	-2.817435
C	-0.332401	1.581863	-3.884597
C	0.123412	-1.157563	-1.431412
C	0.264827	-2.542911	-1.173119
C	0.408582	-3.414917	-2.207378
C	0.400164	-2.977846	-3.558224
C	0.211845	-1.649324	-3.853673
C	0.067566	-0.727720	-2.791120
C	0.016060	-0.002344	-0.553935
C	0.019771	0.021027	0.873295
C	0.221244	-1.221487	1.681541
C	-0.860649	-1.845380	2.296350
C	1.486347	-1.774077	1.840817
C	-0.687907	-3.010733	3.024657
C	1.662712	-2.932791	2.577884
C	0.576656	-3.559825	3.164304
C	-0.197015	1.260009	1.682613
C	-1.453191	1.849109	1.787531
C	0.861282	1.820992	2.393694
C	-1.640526	2.984888	2.558558
C	0.676409	2.954255	3.166762
C	-0.575247	3.543768	3.244575
H	-0.645848	3.661829	-4.416633
H	-0.422991	4.512621	-2.098420
H	-0.093980	2.991976	-0.214531
H	-0.401872	1.216353	-4.889709
H	0.267822	-2.918178	-0.173465
H	0.538818	-4.461883	-2.005271
H	0.548906	-3.698085	-4.338830
H	0.194777	-1.310144	-4.873172
H	-1.844409	-1.424243	2.190090
H	2.326452	-1.311968	1.355134
H	-1.538550	-3.490260	3.475453
H	2.643145	-3.358382	2.676365
H	0.717699	-4.468361	3.719186
H	-2.284790	1.424796	1.254407
H	1.833282	1.364640	2.341907
H	-2.616868	3.432099	2.621481
H	1.505896	3.374871	3.707082
H	-0.720357	4.427604	3.836329

(S_1/S_0)-CI^{cry}

6	-0.736178	2.813829	-3.769726
6	-0.616632	3.310114	-2.368428
6	-0.392894	2.499861	-1.304302
6	-0.216561	1.065893	-1.486152
6	-0.252511	0.581021	-2.975125
6	-0.549724	1.532551	-4.053598
6	0.307050	-1.017390	-1.471749
6	0.482333	-2.443064	-1.231181
6	0.589590	-3.317838	-2.257527
6	0.578148	-2.898479	-3.712589
6	0.419380	-1.626275	-4.056174
6	0.247772	-0.592889	-2.977439
6	0.067931	0.038774	-0.644991
6	0.068648	0.048223	1.067589
6	0.207412	-1.215118	1.822916
6	-0.890419	-1.769390	2.465529
6	1.432195	-1.850337	1.902981
6	-0.779228	-2.971868	3.131677
6	1.557562	-3.046745	2.581835
6	0.447997	-3.616865	3.183221
6	-0.143013	1.287845	1.844488
6	-1.325325	1.998153	1.788012
6	0.876859	1.723976	2.687772
6	-1.481000	3.152236	2.537761
6	0.733011	2.872047	3.431824
6	-0.450817	3.591791	3.350449
1	-0.961081	3.510563	-4.560064
1	-0.691599	4.376381	-2.193077
1	-0.274912	2.938299	-0.330455
1	-0.588186	1.140104	-5.053045
1	0.468145	-2.823169	-0.227348
1	0.692124	-4.371977	-2.031407
1	0.700606	-3.641789	-4.474079
1	0.396670	-1.324219	-5.088599
1	-1.828693	-1.250334	2.418985
1	2.274580	-1.401523	1.413225
1	-1.640168	-3.402658	3.607070
1	2.509801	-3.537339	2.628756
1	0.543263	-4.556438	3.690949
1	-2.116323	1.646926	1.154371
1	1.780630	1.147442	2.733469
1	-2.400128	3.705812	2.488574
1	1.526346	3.201980	4.076290
1	-0.572661	4.491882	3.918149