Supporting information

Analysis of Charge Transfer Transitions in Stacked π-Donor-Acceptor Complexes

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Table S1. Electron affinity (EA) and ionization potential (IP) of acceptor and donor in the dimers, respectively, and intermolecular Coulomb interaction (CE) energies based on NPA charges computed at the PBE0-D3/cc-pVDZ level. All energies are in eV.

Complexes	EA/IP	IP - EA	Coulomb int.
PDI/DAN	1.62/6.76	5.14	-3.24
pClA/TMPD	2.42/5.90	3.48	-2.44
TCNB/Bpe	2.33/8.94	6.61	-0.21

Table S2. Vertical excitation energies ΔEexc (eV) for the PDI/DAN complex, oscillator strengths and charge transfer (q(CT) in *e*) using the SOS/ADC(2)/cc-pVDZ method.

State	Δ*E*exc	f	CT
PBE0-D3/cc-pVDZ geometries			
S_1	3.00	0.07	0.95
S_2	3.85	0.01	0.95
S_3	3.92	0.00	0.62
S_4	4.02	0.09	0.30
S_5	4.23	0.00	0.03
S_6	4.33	0.00	0.04
S_7	4.37	0.12	0.06
S_8	4.52	0.00	0.96
SOS-MP2/cc-pVDZ geometry			
S_1	3.16	0.07	0.96
S_2	3.96	0.01	0.95
S_3	3.98	0.01	0.35
S_4	4.04	0.06	0.35
S_5	4.20	0.00	0.03
S_6	4.30	0.00	0.03
S_7	4.42	0.12	0.06
S_8	4.49	0.00	0.97

Table S3. Vertical excitation energies Δ*E*exc (eV) for the pClA/TMPD complex, oscillator strengths and charge transfer (*q*(CT) in *e* units) using the SOS-ADC(2)/cc-pVDZ.

State	Δ*E*exc	f	CT
PBE0-D3/cc-pVDZ geometries			
S_1	1.18	0.08	0.86
S_2	3.21	0.05	0.89
S_3	3.25	0.06	0.62
S_4	3.44	0.00	0.08
S_5	3.52	0.00	0.27
S_6	3.61	0.00	0.47
S_7	4.28	0.12	0.61
S_8	4.29	0.02	0.34
SOS-MP2/cc-pVDZ geometry			
S_1	1.77	0.08	0.92
S_2	3.44	0.00	0.06
S_3	3.48	0.01	0.24
S_4	3.71	0.03	0.71
S_5	3.76	0.05	0.45
S_6	3.89	0.00	0.70
S_7	4.29	0.00	0.29
S_8	4.44	0.00	0.58

Table S4. Vertical excitation energies Δ*E*exc (eV) for the TCNB/Bpe complex, oscillator strengths and charge transfer (*q*(CT) in *e* units) using the SOS/ADC(2)/cc-pVDZ.

State	Δ*E*exc	f	CT
	PBE0-D3/cc-pVDZ geometries		
S_1	4.06	0.04	0.71
S_2	4.48	0.05	0.30
S_3	4.66	0.10	0.24
S_4	4.68	0.01	0.11
S_5	4.78	0.41	0.16
S_6	4.85	0.00	0.02
S_7	4.89	0.00	0.10
S_8	4.93	0.29	0.65
	SOS-MP2/cc-pVDZ geometry		
S_1	4.09	0.03	0.61
S_2	4.39	0.04	0.43
S_3	4.59	0.04	0.07
S_4	4.60	0.00	0.25
S_5	4.76	0.14	0.38
S_6	4.86	0.63	0.43
S_7	4.88	0.01	0.02
S_8	4.92	0.01	0.11

Table S5. Basis set dependence of the vertical excitation energies ΔE_{exc} (eV), oscillator strengths (*f*) and charge transfer values *q*(CT) for the two lowest states of the three complexes investigated.[a]

Methods	States	ΔE_{exc}	*q*(CT)	*f*
PDI/DAN				
SOS-ADC(2)/cc-pVDZ	S_1	3.00	0.95	0.07
	S_2	3.85	0.95	0.01
SOS-ADC(2)/aug-cc-pVDZ	S_1	2.95	0.98	0.06
	S_2	3.73	0.10	0.01
pClA/TMPD				
SOS-ADC(2)/cc-pVDZ	S_1	1.18	0.86	0.08
	S_2	3.21	0.89	0.05
SOS-ADC(2)/aug-cc-pVDZ	S_1	1.10	0.85	0.07
	S_2	3.11	0.60	0.06
TCNB/Bpe				
SOS-ADC(2)/cc-pVDZ	S_1	4.06	0.71	0.04
	S_2	4.48	0.30	0.05
SOS-ADC(2)/aug-cc-pVDZ	S_1	3.97	0.74	0.04
	S_2	4.41	0.20	0.08

[a] gas phase calculations using the PBE0-D3 geometry.

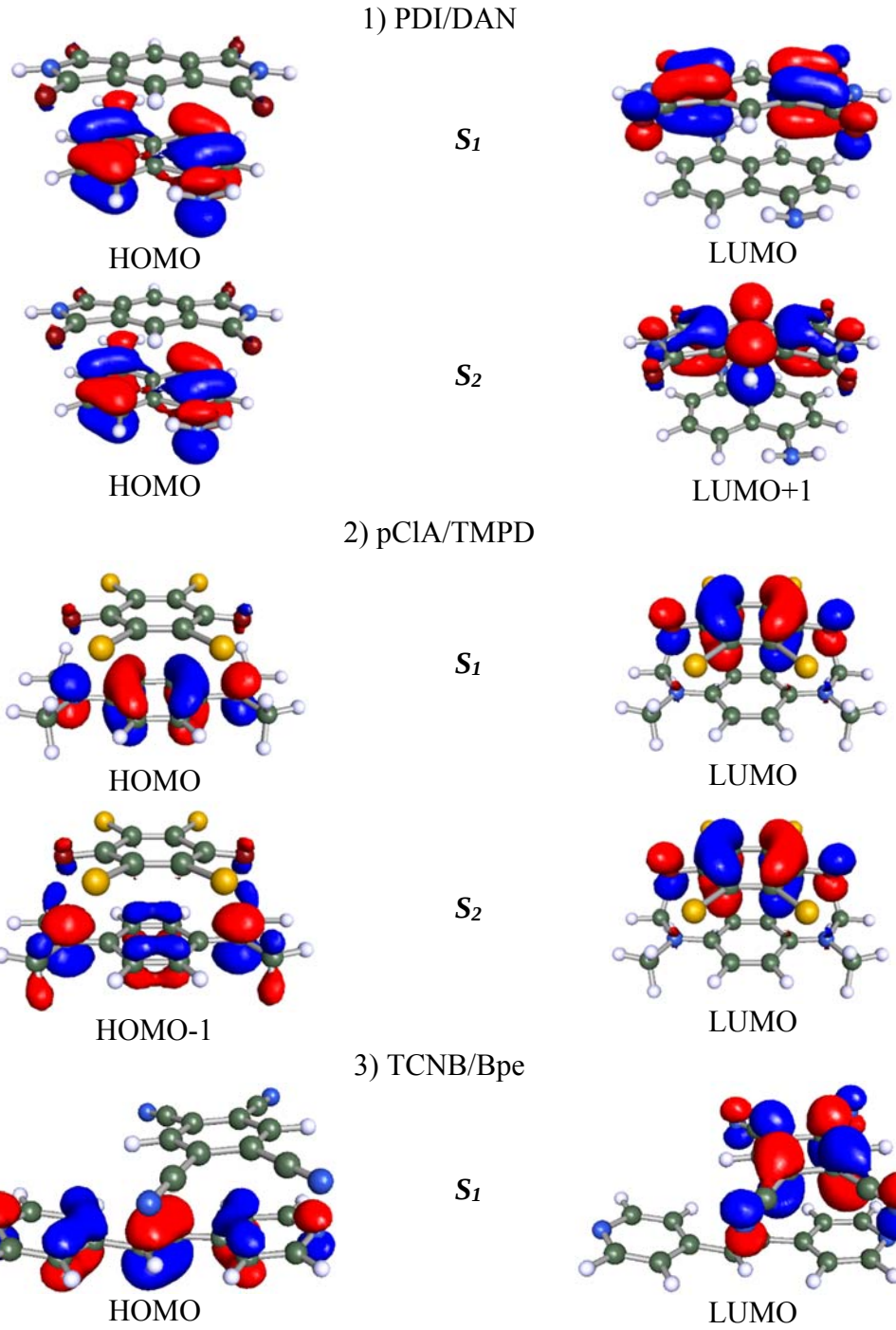

Figure S1. Molecular orbitals obtained at the PBE0-D3/cc-pVDZ level, and the lowest charge-transfer transition are illustrated.

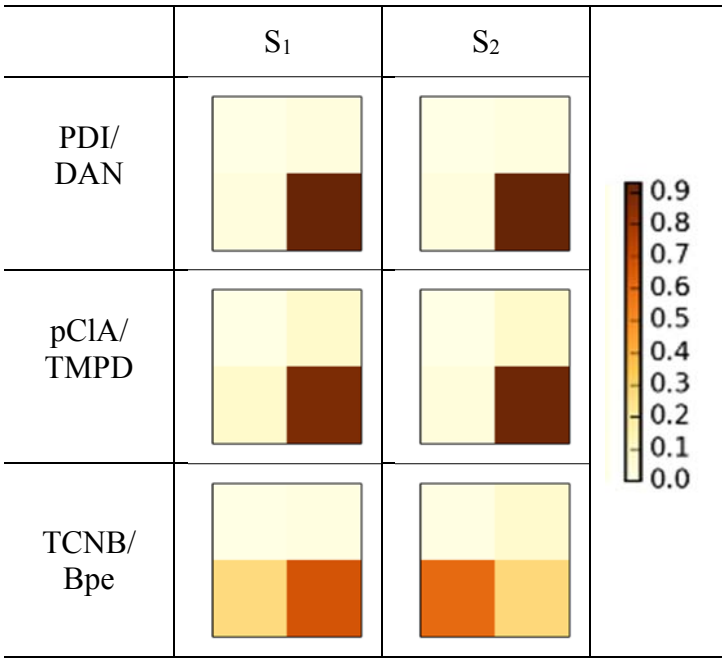

Figure S2. Ω_{AB}^{n} plots for the first two excited states of the three complexes investigated using the SOS-ADC(2)/cc-pVDZ level. The two segments in the plots represent the two monomers in the complex.

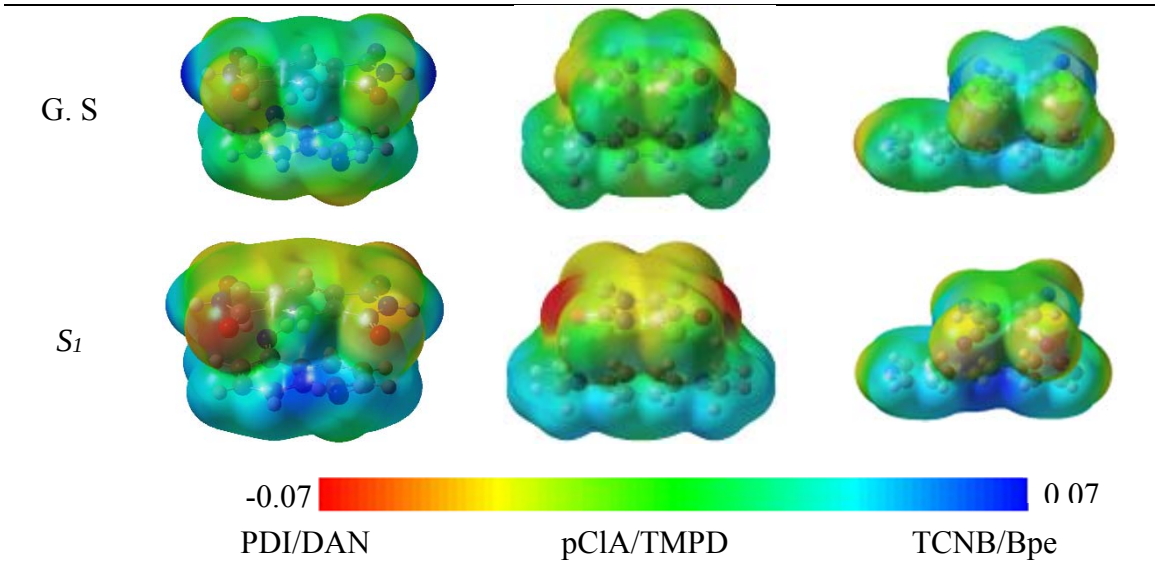

Figure S3. Projection of the electrostatic potential on the molecular van der Waals surface using the SOS-MP2(G.S.) and SOS-ADC(2) (S_1) methods with the cc-pVDZ basis for the gas phase. Geometries have been optimized for the respective state in gas phase. The vdW surface is defined by the 0.001e/bohr^3 contour of the electronic density.

Table S6. Coordinates for the ground states.

PBE0				SOS-MP2			
1) PDI/DAN							
O	3.0775293	2.1883464	1.4113142	O	3.1060366	-2.2125177	1.4974760
O	2.9388954	2.3930894	1.6571914	O	2.9620318	2.4116781	1.6713660
N	3.3467579	0.1088441	1.6140178	N	3.3768849	0.1070253	1.6633344
C	2.6195972	-1.0745027	1.5367457	C	2.6468766	-1.0890509	1.5874699
C	2.5469789	1.2521363	1.6383546	C	2.5716405	1.2621134	1.6590907
C	1.1926792	-0.6586373	1.6193512	C	1.2038180	-0.6656435	1.6338566
C	1.1468632	0.7401417	1.6448635	C	1.1580616	0.7442682	1.6512251
C	-0.0475423	1.4459526	1.6472323	C	-0.0472409	1.4590643	1.6595833
H	-0.0824359	2.5356308	1.6503829	H	-0.0808035	2.5535047	1.6784027
O	-3.0775252	2.1882074	1.4112812	O	-3.1060456	2.2124982	1.4974554
O	-2.9388260	-2.3931142	1.6572637	O	-2.9620195	-2.4116910	1.6713916
N	-3.3467370	-0.1088731	1.6140369	N	-3.3768879	-0.1070372	1.6633328
C	-2.6195807	1.0743599	1.5367604	C	-2.6468846	1.0890410	1.5874630
C	-2.5469578	-1.2522053	1.6383944	C	-2.5716217	-1.2621189	1.6591084
C	-1.1927957	0.6586736	1.6193625	C	-1.2038064	0.6656569	1.6338608
C	-1.1469252	-0.7400853	1.6448642	C	-1.1580907	-0.7442527	1.6512210
C	0.0473688	-1.4458948	1.6472097	C	0.0472478	-1.4591018	1.6595820
H	0.0825342	-2.5354885	1.6502809	H	0.0808016	-2.5534944	1.6783916
N	-1.4818056	2.6850354	-1.3839994	N	-1.4772686	2.7286842	-1.4577370
N	1.4819712	-2.6850546	-1.3839102	N	1.4772342	-2.7286863	-1.4577215
C	-1.3527035	1.3121552	-1.4951379	C	-1.3622913	1.3230197	-1.5079743
C	-0.0505454	0.7123589	-1.5828892	C	-0.0517216	0.7169241	-1.5779808
C	1.1258088	1.4996313	-1.6180331	C	1.1379722	1.5138221	-1.6339415
H	1.0634547	2.5863561	-1.6761918	H	1.0696773	2.6035503	-1.7121925
C	2.3640258	0.8937454	-1.6237461	C	2.3839627	0.9003705	-1.6494308
H	3.2675237	1.5051139	-1.6639733	H	3.2928576	1.5112195	-1.7132042
C	2.4808608	-0.5015191	-1.5410078	C	2.4990862	-0.5138858	-1.5625750
H	3.4686325	-0.9658868	-1.4937233	H	3.4917532	-0.9816151	-1.5363957
C	1.3526942	-1.3121311	-1.4951660	C	1.3622589	-1.3230128	-1.5079719
C	0.0505192	-0.7122933	-1.5828955	C	0.0517137	-0.7169276	-1.5779778
C	-1.1259015	-1.4996411	-1.6180148	C	-1.1379830	-1.5137782	-1.6339315
H	-1.0634799	-2.5862537	-1.6761953	H	-1.0696714	-2.6035624	-1.7121867
C	-2.3639517	-0.8936737	-1.6236586	C	-2.3839441	-0.9003503	-1.6494134
H	-3.2674470	-1.5051652	-1.6638711	H	-3.2928619	-1.5112192	-1.7131843
C	-2.4808039	0.5014972	-1.5409357	C	-2.4990351	0.5138698	-1.5625642
H	-3.4685979	0.9658956	-1.4936514	H	-3.4917695	0.9816276	-1.5363756
H	-2.3500593	2.9709329	-0.9408156	H	-2.3870676	3.0095971	-1.0887650
H	-0.6972489	3.1454886	-0.9370739	H	-0.7611361	3.1484889	-0.8639620
H	0.6971828	-3.1454322	-0.9370722	H	0.7611444	-3.1484619	-0.8639499
H	2.3500064	-2.9709417	-0.9406930	H	2.3870857	-3.0095977	-1.0887448
H	4.3554851	0.1440117	1.5369034	H	4.3908077	0.1413882	1.6022869
H	-4.3554989	-0.1441181	1.5368442	H	-4.3908021	-0.1414069	1.6022823
2) pClA/TMPD							
H	0.9755271	50.2576503	12.3981289	H	1.1330806	50.2200475	12.3742849
H	3.6038051	50.2485242	9.7717471	H	3.9164186	49.6590517	9.4261953
H	-0.9754198	50.2577285	5.2238309	H	-0.8158147	49.7580075	4.9712576
H	-3.6038367	50.2486325	7.8503449	H	-3.5665810	50.3615391	7.9477546
H	-1.0952635	48.4676019	5.1301504	H	-1.4482869	48.1256860	5.3855234
H	-3.6776142	48.4570735	7.7452564	H	-3.5599571	48.5871046	7.6402645
H	1.0952319	48.4677060	12.4919276	H	1.3908798	48.4396958	12.2902816
H	3.6776894	48.4571410	9.8767222	H	3.5184031	48.0105106	10.0257082

C	-0.3604467	49.2398503	10.1524758	C	-0.1949891	49.6148475	10.0794255
C	1.0186755	49.2769710	9.8229686	C	1.1728125	49.5081902	9.7172428
C	-1.3393639	49.2401619	9.1801710	C	-1.2187076	49.6439014	9.1159537
C	1.6164386	49.3905545	12.1795346	C	1.8407025	49.4325444	12.0685686
C	3.3788592	49.3790258	10.4073755	C	3.5198814	49.0921068	10.2843781
H	-0.6737985	49.2408935	11.1950120	H	-0.4908142	49.6777718	11.1302836
H	-2.3797452	49.2434690	9.5006002	H	-2.2474775	49.7276623	9.4768939
H	2.5252872	49.4904479	12.7825537	H	2.7493372	49.5551770	12.6787567
H	3.9883450	49.4636842	11.3135476	H	4.2085472	49.2514418	11.1290753
N	1.9836520	49.3539498	10.7824167	N	2.2009966	49.5945415	10.6618117
C	0.3604584	49.2398530	7.4695213	C	0.4223090	49.3588555	7.3699571
C	-1.0185985	49.2770143	7.7990069	C	-0.9432331	49.5674925	7.7262025
C	1.3393675	49.2401495	8.4419436	C	1.4396561	49.3304267	8.3270539
C	-1.6164166	49.3906241	5.4423792	C	-1.6676037	49.2155729	5.4131810
C	-3.3789128	49.3791074	7.2146444	C	-3.3321580	49.5841657	7.2028468
H	0.6737473	49.2408790	6.4269603	H	0.7088814	49.2278226	6.3233152
H	2.3797372	49.2434681	8.1213549	H	2.4626197	49.1785439	7.9730476
H	-2.5253823	49.4905375	4.8394258	H	-2.5467647	49.4145552	4.7801845
H	-3.9883638	49.4637846	6.3083675	H	-3.9922800	49.7513955	6.3371284
N	-1.9836595	49.3540871	6.8395836	N	-1.9452661	49.7101864	6.7598212
Cl	-0.7969069	52.4582174	11.8474762	Cl	-0.8851544	52.7756995	12.2636991
Cl	-3.0421079	52.4670591	9.5843461	Cl	-3.2488420	52.8403728	10.0529994
C	-0.4092586	52.3828653	10.1733841	C	-0.5765965	52.7129791	10.5605908
C	1.0329425	52.2910263	9.8517132	C	0.8734837	52.6114086	10.1714480
C	-1.3652101	52.3851487	9.2099238	C	-1.5726257	52.7402618	9.6289772
O	1.8895650	52.1695378	10.7138754	O	1.7663871	52.5960458	11.0062526
Cl	0.7969460	52.4582590	5.7745282	Cl	0.4754758	52.6118413	6.0627175
Cl	3.0420811	52.4670183	8.0377462	Cl	2.8408570	52.5484624	8.2747480
C	0.4092611	52.3828641	7.4486400	C	0.1648317	52.5942938	7.7653396
C	-1.0328947	52.2909792	7.7703965	C	-1.2835831	52.6713660	8.1537582
C	1.3652279	52.3851219	8.4120764	C	1.1626840	52.5673227	8.6986911
O	-1.8896447	52.1693323	6.9081019	O	-2.1756602	52.7075384	7.3187302
3) TCNB/Bpe							
N	4.0448009	0.6287084	1.7846232	N	4.0292749	0.7144292	1.7443522
C	3.6627020	1.7113671	1.1027048	C	3.6278043	1.7982809	1.0465168
C	2.6873185	1.7008315	0.1085630	C	2.6262885	1.7748544	0.0594431
H	2.4100752	2.6307297	-0.3941590	H	2.3501874	2.7022686	-0.4582541
C	2.0410894	0.4983250	-0.2142249	C	1.9721657	0.5601137	-0.2443481
C	2.4723134	-0.6481691	0.4737322	C	2.4161120	-0.5865852	0.4565705
C	3.4591072	-0.5260496	1.4453999	C	3.4259362	-0.4539267	1.4221829
C	0.9269591	0.5162126	-1.1587475	C	0.8659103	0.5507506	-1.2268007
N	-1.5678167	-2.6241459	1.4117051	N	-1.7156129	-2.6562416	1.6924679
N	-1.3944825	4.0070183	-0.0665897	N	-1.3813635	4.0812238	0.1550182
C	-1.1896074	-1.5711140	1.7245376	C	-1.2586943	-1.5966652	1.9530911
C	-0.7022082	-0.2639654	2.0365008	C	-0.6871397	-0.2894882	2.2101276
C	-1.1817817	0.8250643	1.3089565	C	-1.1681221	0.8213765	1.4914543
H	-1.9495646	0.6756440	0.5502415	H	-1.9885317	0.6978901	0.7776852
C	-0.6368827	2.0937268	1.5072418	C	-0.5713144	2.0837824	1.6654060
C	-1.0617774	3.1671976	0.6640512	C	-1.0214529	3.1965147	0.8528677
H	3.7873054	-1.4109214	1.9998729	H	3.7713102	-1.3384665	1.9737407
H	0.2831532	-1.4809895	-0.9390286	H	0.0581377	-1.3586985	-0.7543693
N	-3.5623450	-0.4351466	-3.6543830	N	-3.4984692	-0.5354757	-3.9931629
C	-3.0736416	-1.5547653	-3.1184324	C	-3.0676776	-1.6214580	-3.3194530
C	-1.8875986	-1.6176944	-2.3911708	C	-1.9553379	-1.6285758	-2.4594414
H	-1.5553794	-2.5661977	-1.9634985	H	-1.6714531	-2.5511445	-1.9383425
C	-1.1342120	-0.4509060	-2.2015765	C	-1.2133423	-0.4421444	-2.2732042
C	-1.6502423	0.7307365	-2.7581443	C	-1.6667608	0.7056191	-2.9657236
C	-2.8471269	0.6785913	-3.4628554	C	-2.7903996	0.6009635	-3.7985598
C	0.0897232	-0.5098532	-1.4055626	C	-0.0465828	-0.4496857	-1.3629301

H	-3.2605456	1.5940721	-3.8976643	H	-3.1505708	1.4856469	-4.3396262
H	0.7372793	1.4865664	-1.6286473	H	0.7675389	1.4598091	-1.8355013
N	1.4903952	4.5996087	2.7903777	N	1.6738842	4.5804970	2.8777698
N	1.2882982	-2.0919461	4.3034538	N	1.3536958	-2.2077311	4.4246309
C	0.9829767	3.5647595	2.6468001	C	1.1401037	3.5330262	2.7478415
C	0.3811035	2.2804624	2.4663065	C	0.5020861	2.2421517	2.5822270
C	0.8418796	1.1961974	3.2143186	C	0.9698377	1.1355296	3.3164456
C	0.3147040	-0.0774259	2.9965411	C	0.3878981	-0.1328219	3.1246217
C	0.8433288	-1.1912752	3.7205682	C	0.9124605	-1.2767599	3.8435845
H	-1.1434590	1.6897386	-2.6370866	H	-1.1701921	1.6760354	-2.8554930
H	-3.6672159	-2.4613758	-3.2733112	H	-3.6460325	-2.5421366	-3.4721670
H	2.0405258	-1.6299356	0.2713850	H	1.9961574	-1.5781087	0.2527551
H	4.1519233	2.6514896	1.3767746	H	4.1281545	2.7435297	1.2951503
H	1.6446598	1.3360965	3.9368864	H	1.8098405	1.2530888	4.0078863

Table S7. Coordinates for the exited states.

wB97xD				SOS-ADC(2)			
1) PDI/DAN							
O	2.5142510	-2.8605460	1.4741340	O	3.1167998	-2.2200334	1.2930274
O	3.5326860	1.6322550	1.6886620	O	2.9875156	2.4014177	1.4634483
N	3.3152730	-0.6850110	1.6607620	N	3.3551761	0.0900854	1.5827507
C	2.3113150	-1.6602040	1.6357860	C	2.6161795	-1.1099727	1.5353373
C	2.8309320	0.6357190	1.7261070	C	2.5555951	1.2574918	1.5989666
C	1.0621530	-0.9129030	1.7301350	C	1.2175532	-0.7011689	1.6985450
C	1.3773410	0.4884000	1.7760400	C	1.1727593	0.7553450	1.7158100
C	0.3890930	1.4611820	1.7940600	C	-0.0332808	1.4633790	1.7160546
H	0.6349980	2.5240970	1.8258430	H	-0.0481803	2.5612361	1.7229694
O	-2.3694390	2.9729140	1.5519990	O	-3.1168032	2.2199749	1.2930055
O	-3.3907860	-1.5227100	1.4656010	O	-2.9875217	-2.4014456	1.4634882
N	-3.1760820	0.7916610	1.5891650	N	-3.3552092	-0.0901090	1.5827397
C	-2.1715990	1.7658490	1.6514950	C	-2.6161272	1.1099631	1.5353266
C	-2.6923360	-0.5302590	1.5858080	C	-2.5556023	-1.2575102	1.5989802
C	-0.9251380	1.0128370	1.7413030	C	-1.2176519	0.7012263	1.6985316
C	-1.2403030	-0.3870920	1.6911890	C	-1.1727097	-0.7554039	1.7158228
C	-0.2523090	-1.3609680	1.6965750	C	0.0332857	-1.4634862	1.7160665
H	-0.5000470	-2.4232080	1.6571250	H	0.0481661	-2.5612047	1.7229886
N	-2.1707650	2.1442730	-1.3542110	N	-1.5197844	2.6470240	-1.1975050
N	2.0403300	-2.2427640	-1.3694990	N	1.5197814	-2.6470217	-1.1974885
C	-1.7002320	0.8907700	-1.5434800	C	-1.3615338	1.3182336	-1.4405890
C	-0.2828270	0.6337230	-1.5922290	C	-0.0482267	0.7239924	-1.5846151
C	0.6541760	1.6708970	-1.6010510	C	1.1193254	1.5003164	-1.6804048
H	0.3303320	2.7107010	-1.6243920	H	1.0667713	2.5928015	-1.7360614
C	2.0276420	1.3950250	-1.6125030	C	2.3958932	0.8819053	-1.7120142
H	2.7415240	2.2174350	-1.6067590	H	3.2917741	1.5066500	-1.7909377
C	2.4870980	0.0958470	-1.5716170	C	2.5209371	-0.4961008	-1.5861880
H	3.5563680	-0.1081590	-1.5149700	H	3.5079425	-0.9674111	-1.5269057
C	1.5785000	-0.9849530	-1.5212990	C	1.3615732	-1.3182555	-1.4405763
C	0.1615370	-0.7265850	-1.6289460	C	0.0481710	-0.7239533	-1.5846129
C	-0.7691310	-1.7597480	-1.7552950	C	-1.1193290	-1.5002834	-1.6803783
H	-0.4441020	-2.7967520	-1.8354470	H	-1.0667697	-2.5927798	-1.7360231
C	-2.1392240	-1.4791050	-1.8094550	C	-2.3958058	-0.8818190	-1.7119825
H	-2.8531260	-2.2973250	-1.8935170	H	-3.2918165	-1.5066629	-1.7909059
C	-2.6008970	-0.1829280	-1.7047060	C	-2.5209176	0.4960944	-1.5861834
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H	-3.1598680	2.2332930	-1.1565640	H	-2.3842293	2.8897501	-0.7057312
H	-1.6211980	2.7920730	-0.7991330	H	-0.7187843	3.1287769	-0.7955270
H	1.4417110	-2.9231880	-0.9158720	H	0.7188138	-3.1287375	-0.7955355
H	3.0050970	-2.3484470	-1.0780770	H	2.3842177	-2.8897190	-0.7057345
H	4.3021950	-0.9071830	1.6553970	H	4.3589568	0.1180236	1.4294651
H	-4.1625040	1.0151180	1.5725850	H	-4.3589519	-0.1180530	1.4294677
2) pClA/TMPD							
H	2.0069810	50.6391310	12.3157690	H	1.2153112	50.4084867	12.3094421
H	3.4400380	50.5008300	9.8693650	H	3.5044853	50.4266818	10.0390074
H	-1.3126200	50.3382140	5.3092240	H	-1.2153162	50.4084791	5.3125744
H	-3.5290640	50.2368030	7.5580990	H	-3.5044735	50.4266810	7.5830109
H	-0.9384170	48.6024850	4.9788400	H	-0.8855229	48.6328837	5.0984354
H	-3.8159030	48.4696850	7.7987890	H	-3.7176959	48.6602452	7.9577533
H	0.4523140	49.8148160	12.2261440	H	0.8855237	48.6328826	12.5235633
H	3.5412220	48.7120070	9.6405620	H	3.7176839	48.6602432	9.6642500

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C 0.8843660 49.1818480 9.7234970	C 1.0226423 49.0988173 9.8273716
C -1.4480690 48.8847240 9.0701880	C -1.3561704 49.0783539 9.1968094
C 1.5236210 49.6865430 12.0597780	C 1.6159409 49.3885647 12.1929803
C 3.2327770 49.5187390 10.3177350	C 3.3905252 49.3969976 10.4148284
H -0.8200990 48.9575490 11.0803690	H -0.6907389 49.1332829 11.2135080
H -2.4853240 48.7838500 9.3774520	H -2.3983440 49.1361560 9.5165138
H 1.9037720 48.8772860 12.7024010	H 2.5256067 49.2805634 12.7994007
H 3.8175210 49.4333470 11.2402980	H 4.0017791 49.2651926 11.3182203
N 1.8220400 49.3992220 10.6642540	N 1.9798062 49.1588382 10.7804367
C 0.2764130 49.0295290 7.3630770	C 0.3775846 49.0772167 7.4527650
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C -3.4474710 49.2362050 7.1038150	C -3.3905263 49.3969952 7.2071796
H 0.5973690 49.0791740 6.3264300	H 0.6907390 49.1333009 6.4085009
H 2.2615950 49.2912110 8.0278490	H 2.3983423 49.1361363 8.1055001
H -2.5809530 49.2153610 4.7224810	H -2.5256095 49.2805599 4.8226019
H -4.0690720 49.1962220 6.2033440	H -4.0017855 49.2652074 6.3037903
N -2.0631860 48.9807070 6.7277620	N -1.9798104 49.1588239 6.8415691
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Cl -2.7744560 52.2065830 9.9058820	Cl -3.0594129 52.5108142 9.6058482
C -0.1259630 52.5574670 10.4055770	C -0.3729097 52.5288843 10.1692462
C 1.2930570 52.6047860 10.0669800	C 1.0561993 52.4396465 9.8674311
C -1.1040930 52.3805960 9.4631120	C -1.3584464 52.5284457 9.1835915
O 2.1932630 52.5897030 10.9204770	O 1.9383056 52.2416207 10.7500839
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Cl 3.2403050 52.7402040 8.1841410	Cl 3.0594173 52.5108032 8.0161586
C 0.5851040 52.4419670 7.6925940	C 0.3729162 52.5288838 7.4527595
C -0.8164460 52.2549240 8.0411900	C -1.0561948 52.4396454 7.7545736
C 1.5661080 52.6064090 8.6327790	C 1.3584497 52.5284417 8.4384130
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3) TCNB/Bpe	
N 4.4133400 0.6846120 1.6380120	N 4.4256932 0.9518025 1.5936377
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C 2.8633210 1.8200870 0.2094170	C 2.7123698 1.9839142 0.2202720
H 2.5191860 2.7600030 -0.2220640	H 2.3036639 2.8979632 -0.2263135
C 2.1626300 0.6162800 -0.0309200	C 2.0574116 0.7317700 0.0260106
C 2.6425230 -0.5572000 0.6002210	C 2.6379748 -0.4101261 0.6618631
C 3.7568680 -0.4627080 1.4126560	C 3.8041615 -0.2411610 1.4151734
C 0.9937700 0.6593780 -0.8426300	C 0.8705691 0.6875755 -0.7815360
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C -1.0905730 -0.3363140 1.8381730	C -1.0924037 -0.2549206 1.7156270
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H -2.4063490 0.7086180 0.5102550	H -2.3161485 0.9745167 0.4161179
C -0.9119030 2.0335640 1.2876310	C -0.7110401 2.1526513 1.2842484
C -1.2572820 3.0530410 0.3627750	C -0.9795031 3.2828933 0.4404369
H 4.1342720 -1.3465520 1.9305470	H 4.2665064 -1.1032023 1.9104517
H 0.4230560 -1.3986990 -0.6798760	H 0.3935163 -1.3999543 -0.5047260
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C -2.9489180 -1.5245620 -2.7837250	C -2.8337239 -1.8647234 -2.8710306
C -1.7753880 -1.5689260 -2.0434090	C -1.7081695 -1.7895129 -2.0319452
H -1.4561450 -2.4945980 -1.5650490	H -1.3366572 -2.6852197 -1.5233387
C -1.0320090 -0.3813180 -1.8813320	C -1.0746456 -0.5332539 -1.8409392
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C -2.7219600 0.7226440 -3.1830350	C -2.7623590 0.3996410 -3.3146540

C	0.1665990	-0.4276960	-1.1040580	C	0.0892698	-0.4626110	-0.9850625
H	-3.1441370	1.6193350	-3.6418760	H	-3.2180500	1.2503709	-3.8354561
H	0.7303790	1.6310300	-1.2615030	H	0.5845059	1.6198140	-1.2820527
N	1.5787790	4.3466290	2.3453160	N	1.7192528	4.3537089	2.7860920
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C	0.9329840	3.3807870	2.3115890	C	1.0831149	3.3718575	2.5778436
C	0.2035490	2.1672220	2.2085650	C	0.3586928	2.1659267	2.2813968
C	0.6344140	1.0402720	2.9045960	C	0.7088393	0.9540552	2.9183624
C	0.0570320	-0.2153180	2.7219860	C	0.0480236	-0.2662331	2.6360008
C	0.6690970	-1.3589420	3.2981050	C	0.5568547	-1.4987378	3.1692125
H	-1.0527200	1.7671280	-2.3455430	H	-1.2332671	1.6042099	-2.3832040
H	-3.5478630	-2.4276550	-2.9213050	H	-3.3375482	-2.8258050	-3.0297635
H	2.1438580	-1.5182060	0.4891430	H	2.1971974	-1.4077836	0.5765842
H	4.5087410	2.7185350	1.2697390	H	4.3763202	2.9939407	1.1817569
H	1.4906730	1.1316340	3.5734680	H	1.5324172	0.9557518	3.6428450