

Diarylethene-Dihydroazulene Multimode Photochromes: a theoretical spectroscopic investigation.

Supporting Information

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1. Cartesian coordinates for Do-DHA

6	0.79351	0.10015	0.23239
6	-0.22794	-0.78552	0.09987
6	-1.64313	-0.55081	-0.16098
6	-2.11734	0.29364	-1.14041
6	-2.70141	-1.211	0.55031
16	-3.84421	0.2873	-1.15533
6	-3.9486	-0.85794	0.14154
1	-2.53702	-1.90814	1.36319
6	0.69077	1.5619	0.27174
6	-0.16838	2.26203	1.08315
6	1.51049	2.41846	-0.53416
16	0.02784	3.96226	0.83619
6	1.26737	3.74499	-0.35702
1	2.243	2.04495	-1.24048
6	2.06984	-0.58757	0.3633
6	0.30969	-2.22736	0.23774
6	1.87042	-2.06696	0.19282
6	-1.16202	1.75614	2.07196
1	-0.84379	0.78878	2.467
1	-1.27623	2.44634	2.9112
1	-2.14533	1.61191	1.61152
6	-1.36795	1.11406	-2.13226
1	-1.91222	1.18591	-3.077
1	-1.18826	2.12924	-1.76333
1	-0.3932	0.66437	-2.33351
6	-5.26486	-1.32375	0.66364
1	-5.85648	-1.81658	-0.11385
1	-5.10594	-2.04148	1.47094
1	-5.86129	-0.49634	1.06001
6	1.91054	4.90907	-1.03122
1	2.66226	4.55408	-1.73936
1	1.18392	5.51104	-1.58539
1	2.40848	5.56926	-0.31445
6	-0.07373	-2.78551	1.54159
7	-0.35137	-3.19008	2.58406
6	-0.21737	-3.09833	-0.81607
7	-0.61197	-3.76876	-1.66499
6	3.28071	-0.06529	0.66631
1	3.3359	0.98806	0.92869
6	2.55355	-2.45537	-1.08312
1	1.96169	-2.7905	-1.92986
6	4.5078	-0.8071	0.63891
1	5.33074	-0.4044	1.22418
6	4.78321	-1.86437	-0.17522
1	5.80555	-2.23371	-0.17998
6	3.89572	-2.41596	-1.1661
1	4.3611	-2.81522	-2.06441
1	2.32707	-2.61428	1.0251

2. Cartesian coordinates for Dc-DHA

6	0.7617	0.58905	0.22629
6	0.42129	-0.82537	0.14479
6	-0.8263	-1.27055	-0.11529
6	-1.86621	-0.2177	-0.49834
6	-1.37615	-2.59328	-0.12948
16	-3.49587	-1.05918	-0.25542
6	-2.72617	-2.63688	-0.19066
1	-0.77813	-3.49337	-0.05608
6	-0.23712	1.52195	0.22783
6	-1.67072	1.01476	0.39173
6	-0.18593	2.94322	0.13421
16	-2.74303	2.44218	-0.09118
6	-1.38719	3.54873	-0.03807
1	0.7329	3.51464	0.13086
6	2.20271	0.726	0.28949
6	1.68149	-1.64728	0.40995
6	2.84657	-0.63114	0.14674
6	-1.91077	0.7424	1.88562
1	-2.94545	0.45201	2.07197
1	-1.25338	-0.05763	2.23611
1	-1.6907	1.64831	2.45347
6	-1.70984	0.0722	-1.99857
1	-1.79346	-0.86372	-2.55425
1	-2.47945	0.76057	-2.34925
1	-0.72766	0.51039	-2.19642
6	-3.58335	-3.85128	-0.19216
1	-4.16836	-3.9134	-1.11556
1	-2.9722	-4.75108	-0.10503
1	-4.29381	-3.83058	0.64058
6	-1.63932	5.00473	-0.19838
1	-0.69893	5.55854	-0.19905
1	-2.16658	5.21182	-1.13532
1	-2.26631	5.38378	0.61548
6	1.70174	-2.04922	1.82405
7	1.69976	-2.33201	2.94084
6	1.79034	-2.84737	-0.42087
7	1.87833	-3.78386	-1.08528
6	2.99578	1.81208	0.49405
1	2.54368	2.7507	0.79712
6	3.4468	-0.65701	-1.2211
1	2.99917	-1.26668	-2.0008
6	4.41208	1.81522	0.31181
1	4.95948	2.61601	0.80324
6	5.11846	1.0349	-0.56326
1	6.1702	1.27458	-0.69723
6	4.55785	0.06857	-1.46292
1	5.05899	-0.05966	-2.41958
1	3.63934	-0.76258	0.89163

3. Cartesian coordinates for Dc-VHF

C	0.8731690677	0.8062611486	0.0364669174
C	0.5339067014	-0.6201666583	0.2083964192
C	-0.7643548014	-1.0142239839	0.0737881378
C	-1.8099148807	0.0077466839	-0.3613805948
C	-1.3454177855	-2.296548957	0.3402014491
S	-3.4401152614	-0.7516816317	0.0718119413
C	-2.6950991927	-2.3189609378	0.3737753483
H	-0.753128885	-3.183838622	0.5275628759
C	-0.1156438978	1.7549203095	0.0572542676
C	-1.5275331704	1.3045645411	0.4143397874
C	-0.066298034	3.1336733883	-0.303174661
S	-2.6334448543	2.700140419	-0.0838708732
C	-1.2749536273	3.7421629513	-0.4135689685
H	0.8512024122	3.659926681	-0.5353234524
C	-1.6287401915	1.1573169212	1.9396001759
H	-2.6414530179	0.8765779662	2.23265676
H	-0.935486241	0.3907181285	2.2923658921
H	-1.3738418353	2.1072256924	2.4134288378
C	-1.7684396891	0.1767363731	-1.8853954959
H	-1.9006444254	-0.7998278614	-2.3545027542
H	-2.5605988584	0.8420356884	-2.2333565241
H	-0.8023500937	0.5827431702	-2.1978643369
C	-3.5730881173	-3.4879397957	0.6413660012
H	-4.2331932165	-3.6854710556	-0.2097953081
H	-2.9712571817	-4.3787106333	0.8285289865
H	-4.2124864927	-3.3099809826	1.512323999
C	-1.5237704198	5.1586553506	-0.7894282982
H	-0.5840977102	5.6726700298	-0.997213308
H	-2.1613160722	5.2213349119	-1.6767119918
H	-2.0410376497	5.687630948	0.0174086121
C	1.6532804058	-1.5157177682	0.513770908
C	2.5492854079	-1.1698608901	1.539306487
C	1.7366716663	-2.8058402514	-0.0316066454
N	3.2859603008	-0.8282110187	2.3716633317
N	1.804916232	-3.8601588058	-0.5175699328
C	2.2767112425	1.0846412457	-0.2505298954
C	2.9156305379	2.1470327027	0.3762698565
C	2.8961131455	0.1275896824	-1.1126938591
C	4.2592539106	2.5385395816	0.342693035
H	2.280679912	2.7472095326	1.0213230626
H	2.2170838563	-0.4943325797	-1.6821452335
C	4.2469046967	-0.0295803242	-1.4054139214
H	4.4895800786	3.4394860658	0.9039213823
C	5.3403670473	1.8958220168	-0.2322815929
H	4.4768134245	-0.857553866	-2.0704217928
C	5.3376558996	0.7197572564	-0.9854332161
H	6.3108338803	2.3556698104	-0.0710049002
H	6.3076196969	0.3767606259	-1.3330540646

4. Cartesian coordinates for Do-VHFcis

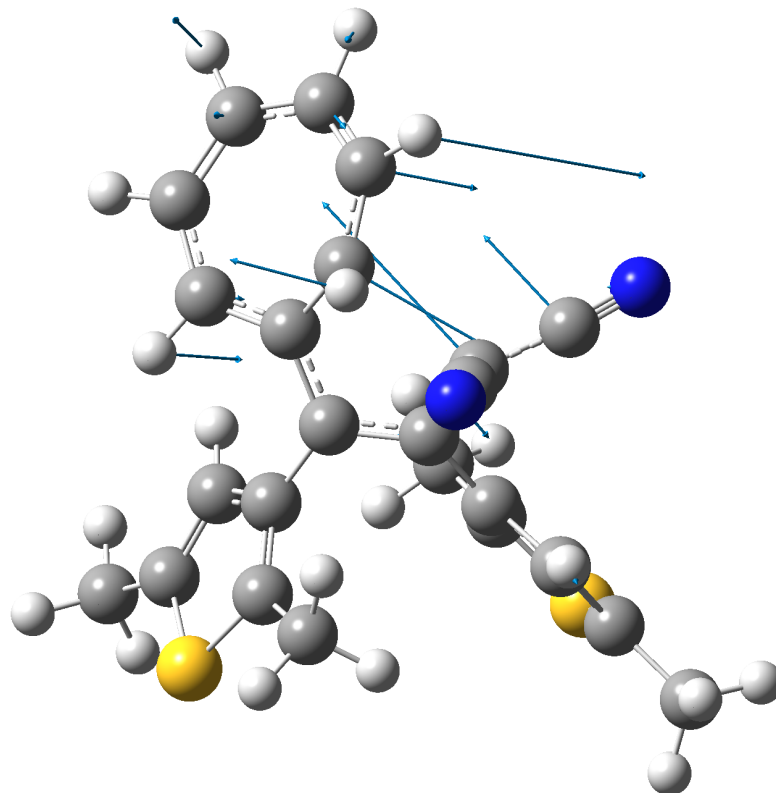
C	0.79075	-0.07202	0.10605
C	-0.1992	-1.12519	0.11298
C	-1.56263	-0.83344	-0.36043
C	-1.85644	-0.26692	-1.57987
C	-2.73775	-1.12467	0.40705
S	-3.56311	-0.09187	-1.76273
C	-3.89865	-0.77007	-0.20118
H	-2.70753	-1.57229	1.3932
C	0.2883	1.29511	0.38888
C	-0.36003	1.64935	1.54568
C	0.41947	2.398	-0.51877
S	-0.82163	3.31703	1.49956
C	-0.13162	3.55842	-0.07305
H	0.90972	2.31707	-1.48255
C	2.15463	-0.26922	-0.15951
C	0.0448	-2.38565	0.64908
C	3.07131	0.79511	0.17429
C	-0.67619	0.8138	2.73912
H	-0.04197	-0.07498	2.75496
H	-0.50629	1.36308	3.66898
H	-1.72081	0.48474	2.73312
C	-0.95054	0.11616	-2.69998
H	-1.19519	-0.43767	-3.61156
H	-1.02593	1.18365	-2.92704
H	0.08636	-0.10051	-2.44051
C	-5.29499	-0.89822	0.30381
H	-5.90697	-1.52249	-0.3543
H	-5.28624	-1.36221	1.29215
H	-5.787	0.07539	0.39098
C	-0.1954	4.88349	-0.75377
H	0.31709	4.82789	-1.71662
H	-1.22805	5.19478	-0.93962
H	0.28447	5.66897	-0.16183
C	1.205	-2.68829	1.40683
N	2.13793	-2.95846	2.03617
C	-0.86164	-3.46985	0.49833
N	-1.55763	-4.38726	0.38655
C	2.60431	-1.46206	-0.83374
H	1.806	-2.13378	-1.13322
C	4.42473	0.87986	0.06567
H	4.85532	1.80126	0.44989
C	3.84925	-1.87746	-1.18935
H	3.8801	-2.83017	-1.71146
C	5.12294	-1.26771	-0.99089
H	5.97733	-1.84398	-1.33433
C	5.37678	-0.05313	-0.4407
H	6.41659	0.25467	-0.37742
H	2.59549	1.65673	0.63081

5. Cartesian coordinates for Do-VHFtrans

6	0.49931	0.28688	-0.18395
6	-0.33365	-0.88709	-0.36559
6	-1.72479	-0.86197	0.107
6	-2.81759	-1.35007	-0.58048
6	-2.08437	-0.26942	1.36222
16	-4.25932	-1.07629	0.32635
6	-3.41237	-0.31917	1.63879
1	-1.35566	0.16018	2.0391
6	1.90541	0.04563	0.19896
6	2.99715	0.56741	-0.4536
6	2.27988	-0.79568	1.2985
16	4.46129	0.03673	0.29384
6	3.62109	-0.8984	1.48975
1	1.5583	-1.3048	1.92784
6	-0.00143	1.59342	-0.27444
6	0.18583	-2.07878	-0.85124
6	-1.23162	1.85047	-0.98802
6	3.0363	1.42494	-1.67033
1	2.0893	1.34745	-2.20874
1	3.19452	2.48188	-1.4243
1	3.83565	1.11476	-2.34776
6	-2.91284	-1.9667	-1.93428
1	-2.97088	-3.05796	-1.86659
1	-3.79702	-1.61012	-2.46874
1	-2.0304	-1.72548	-2.53142
6	-4.1328	0.15785	2.85317
1	-4.61612	-0.66613	3.38692
1	-3.42568	0.63283	3.5362
1	-4.90613	0.89095	2.60445
6	4.35999	-1.67071	2.52898
1	3.64939	-2.19416	3.17209
1	5.02173	-2.41836	2.08116
1	4.97324	-1.02138	3.16157
6	-0.4829	-3.32076	-0.68847
7	-0.98865	-4.35456	-0.56747
6	1.41983	-2.17027	-1.55359
7	2.38104	-2.30505	-2.18244
6	0.76085	2.66731	0.31795
1	1.66377	2.33403	0.81973
6	-1.91187	3.00454	-1.21796
1	-2.81382	2.89076	-1.81398
6	0.52256	4.00418	0.39363
1	1.26542	4.56883	0.95159
6	-0.55216	4.78852	-0.12445
1	-0.49481	5.85471	0.07588
6	-1.62391	4.34835	-0.82992
1	-2.34497	5.09432	-1.1521
1	-1.66954	0.9751	-1.45231

6. Transition state TSA

6.1 Representation of the imaginary vibrational mode (264i cm⁻¹)



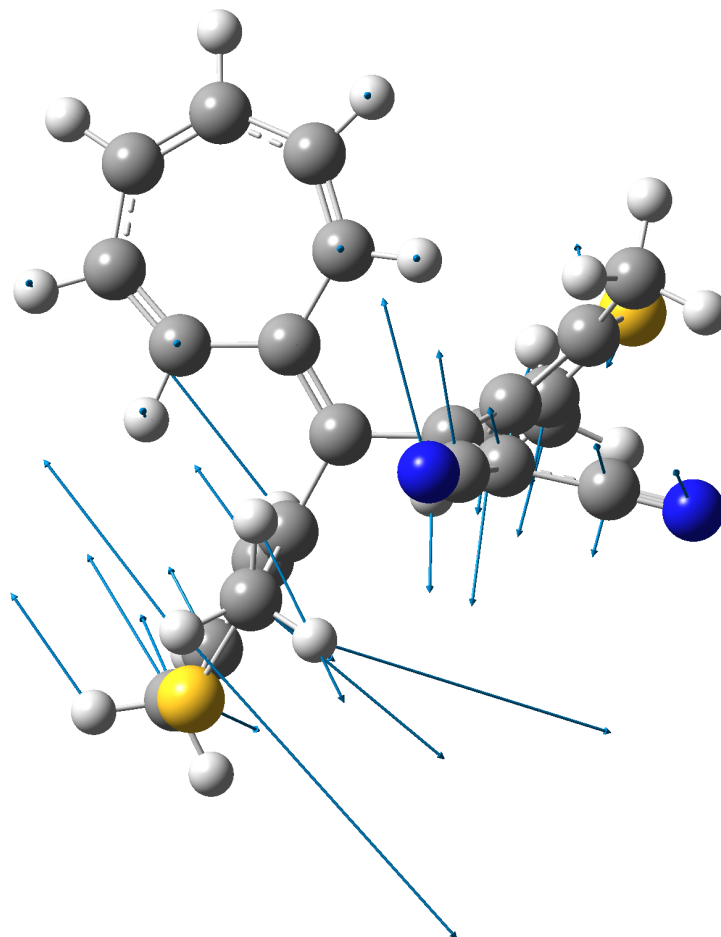
6.2 Cartesian coordinates

C	0.0838022352	-0.1583494338	-0.0762360456
C	0.1594414766	-0.2538307084	1.3086715763
C	1.4577479863	-0.0189349164	1.8716912082
C	1.6156180317	0.4137168085	3.18335942
H	0.8023382595	0.164290293	3.8600852495
C	2.6148630416	1.2342565417	3.7190195446
H	2.4998895533	1.4760911339	4.771943921
C	3.6386946405	1.8843306878	3.0542217563
H	4.2002697149	2.6123235882	3.6330147417
C	4.0831448248	1.6698750067	1.743576381
H	4.9349670517	2.2641951711	1.4251105717
C	3.7070414721	0.6434070529	0.8980737787
H	4.3724884083	0.4482587226	0.05909375
C	2.6213621019	-0.2357529612	1.0108114782
H	2.8036995507	-1.2584072144	0.704414633
C	1.2879089123	-0.3728349439	-0.8731389009
C	1.7301447667	-1.7030369718	-1.0855031718
N	2.0951498194	-2.7959268864	-1.2113691663
C	1.5730067395	0.5373525708	-1.9297404935
N	1.8715077441	1.3138577811	-2.7345194797

C	-1.1238736619	0.2397526578	-0.8082149299
C	-1.8992966717	1.3491350661	-0.5558561088
C	-1.7232666301	2.4224779551	0.4612194135
H	-0.7031775812	2.4058361271	0.8501061875
H	-2.4059812706	2.2892385096	1.3058293435
H	-1.9047527796	3.4093988924	0.0276838976
S	-3.1828851381	1.456543733	-1.7039329305
C	-2.6896321942	0.0184014545	-2.5407658775
C	-3.4453887098	-0.4903176048	-3.7204556387
H	-2.9539338326	-1.3827301996	-4.113200185
H	-4.4741952168	-0.7579786409	-3.4604342307
H	-3.4880918391	0.2514149757	-4.5237865952
C	-1.5749528656	-0.4929910562	-1.9574475226
H	-1.081984446	-1.389217419	-2.317076724
C	-1.0560114483	-0.3705090267	2.1409818369
C	-1.9119855566	-1.4384709568	2.0123834736
C	-1.8443039875	-2.5946763397	1.0731056436
H	-0.8101109161	-2.7952845838	0.7849402741
H	-2.2518197247	-3.5018664075	1.525833649
H	-2.4095746199	-2.3903645114	0.1572887424
S	-3.2236029917	-1.3053173787	3.128362242
C	-2.6419680841	0.1887195366	3.781216785
C	-3.3775524638	0.9075807629	4.8609852925
H	-2.8450831737	1.8246721878	5.1224107573
H	-4.389668093	1.1836530661	4.5495874421
H	-3.4653410944	0.300256325	5.7671655957
C	-1.4870315815	0.5475133047	3.1562364614
H	-0.9716538058	1.471508225	3.3896119036

7. Transition state TSB

7.1 Representation of the imaginary vibrational mode (121i cm⁻¹)



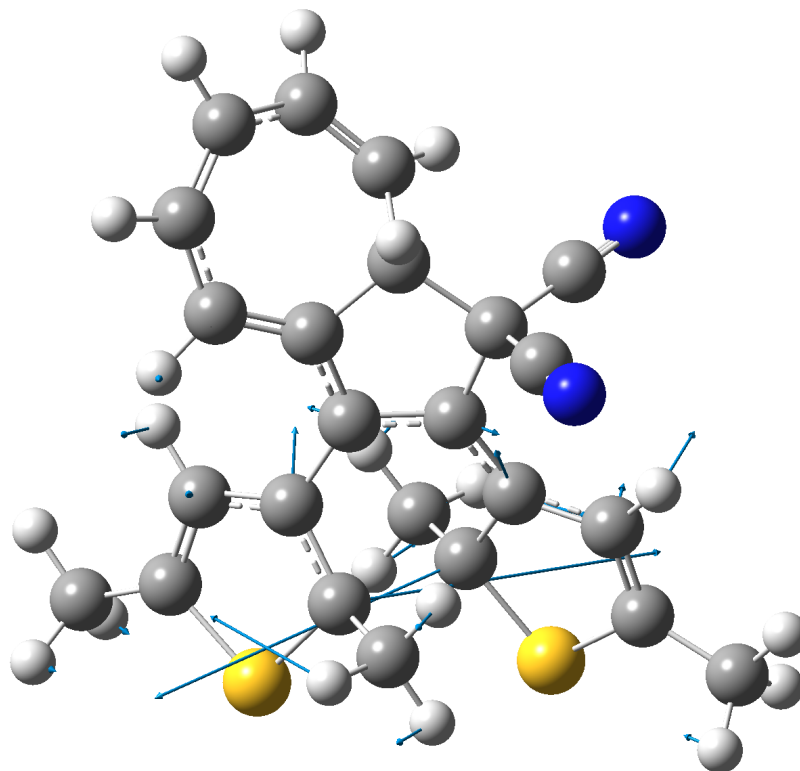
7.2 Cartesian coordinates

C	-0.0105936748	-0.0379590809	-0.0002074223
C	-0.0147007781	-0.0377698991	1.4938323239
C	1.1640268581	0.0120394594	2.193150228
C	1.1241089804	0.0731578723	3.6467304034
H	0.1389182936	-0.1104511651	4.0689466452
C	2.1029511281	0.3457578875	4.5408747014
H	1.7871889559	0.356467174	5.5827268198
C	3.4911523582	0.648207487	4.3346833421
H	4.0405360639	0.95223171	5.2232514501
C	4.1893479661	0.554563039	3.1795211204
H	5.251332732	0.7871532104	3.2191252962
C	3.6975964348	0.1252004567	1.9011924217
H	4.46757876	-0.023291158	1.1458548304

C	2.4319863584	-0.1168375513	1.4888754152
H	2.3439475667	-0.4622811162	0.4623347249
C	-0.3251620071	-1.1527729309	-0.7338368551
C	-0.6120138071	-1.0935545545	-2.1296999016
N	-0.8734177028	-1.0901613853	-3.2550783765
C	-0.3358319333	-2.4712828572	-0.1965614868
N	-0.2842845579	-3.5696725579	0.1572810058
C	0.3522589383	1.1961502391	-0.702184872
C	1.2852950296	1.2607065417	-1.7238305817
C	2.1177024448	0.2024421981	-2.3637567654
H	2.1651611803	-0.6958424046	-1.7425121002
H	3.1382758936	0.5572121969	-2.534258276
H	1.6944098095	-0.0959092303	-3.3302516081
S	1.5039416475	2.8953670264	-2.2264884201
C	0.3330910355	3.5055319017	-1.0992926329
C	-0.0140069949	4.9540703549	-1.0520173265
H	-0.74329204	5.1306140605	-0.2574970519
H	0.8658715062	5.5742384725	-0.8500129725
H	-0.4517822236	5.2951307084	-1.9963132953
C	-0.1668104629	2.4869802925	-0.355191759
H	-0.9408397588	2.6354061692	0.3872609314
C	-1.3274993175	0.1387339848	2.1871048274
C	-2.1847844668	-0.8469710298	2.6122447674
C	-2.0764828736	-2.3326911257	2.5446437391
H	-1.0300630751	-2.6365994063	2.4854673891
H	-2.5151689072	-2.7931740203	3.4348177591
H	-2.5909132345	-2.7453207945	1.6708821513
S	-3.5560418993	-0.1555737922	3.4173619423
C	-2.9780472774	1.4642317509	3.2242937611
C	-3.7382788637	2.6345107765	3.7499246861
H	-3.1745945242	3.552638002	3.5649294716
H	-4.7149481186	2.7338723338	3.2637633908
H	-3.9122438524	2.5552427946	4.8283995193
C	-1.7886802495	1.4472296375	2.5643562066
H	-1.2155570956	2.3509521274	2.3806299837

8. Transition state TSC

8.1 Representation of the imaginary vibrational mode (741i cm⁻¹)



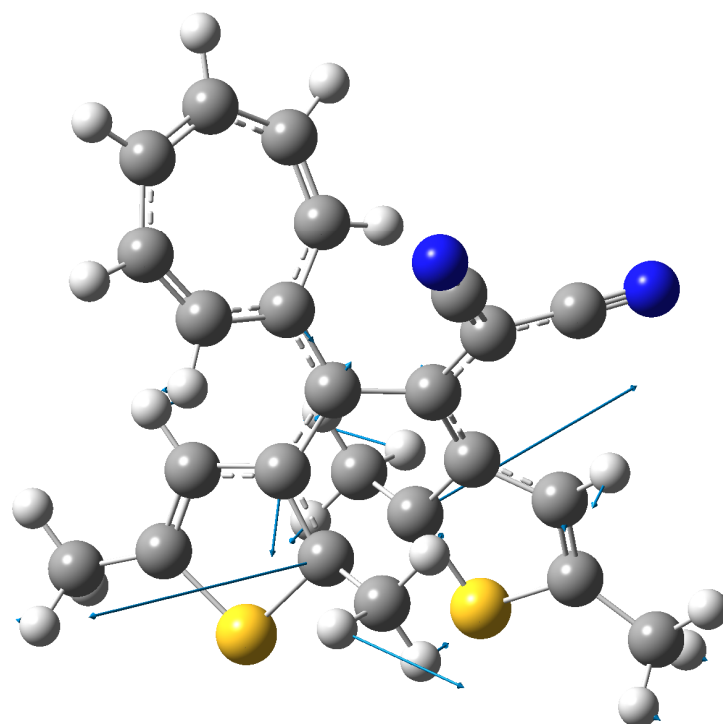
8.2 Cartesian coordinates

C	0.0198588243	0.0116302772	0.0362230927
C	0.0228337251	-0.0701435096	1.4230147503
C	1.3584821663	-0.1281010368	1.9324405007
C	1.7832147937	-0.3512874234	3.2100854474
H	1.0426553842	-0.6330681738	3.9539808157
C	3.1371812319	-0.2284553613	3.6437828688
H	3.3919702577	-0.7296149077	4.5744483492
C	4.0936361453	0.5836524094	3.1003336677
H	5.0362396432	0.661010661	3.6359592984
C	3.9067360376	1.4899800394	1.9988326764
H	4.4947151029	2.4048671497	2.0211909014
C	3.0562620632	1.3154256003	0.9700290358
H	2.9026006429	2.1109781919	0.2467528237
C	2.343144738	0.0092127119	0.7986955029
H	3.0772691243	-0.8037043272	0.835774715
C	1.4491321922	-0.1437972483	-0.4893309923
C	1.630937638	-1.4935133855	-1.0440809522
N	1.7515121066	-2.5665539202	-1.4462838756

C	1.7584263931	0.8340159739	-1.5362227316
N	1.9976022553	1.6162335548	-2.3467188189
C	-1.1539791263	0.0962773689	-0.7611259418
C	-2.3844565482	0.5810749239	-0.1541763478
C	-2.4585098965	1.9717112208	0.424473719
H	-1.6076871724	2.1657160951	1.0781378178
H	-3.3781862019	2.1136864634	0.9984290044
H	-2.4415992259	2.7081908314	-0.383734122
S	-3.7124472886	0.2202334955	-1.2810636906
C	-2.6515958759	-0.522875842	-2.450916834
C	-3.2002688668	-1.149412218	-3.6826393104
H	-2.3880786591	-1.5450846246	-4.2955729004
H	-3.8800420998	-1.9740994797	-3.4425446763
H	-3.7626800349	-0.4285924234	-4.2850633071
C	-1.3486656736	-0.4817849616	-2.0378324041
H	-0.5542415799	-0.9343269435	-2.6210478657
C	-1.2208630652	-0.0900875527	2.1694765904
C	-2.4105772316	-0.6163330214	1.5401596987
C	-2.4625344251	-1.9971658371	0.9381607402
H	-1.6023763394	-2.1696982734	0.2898221267
H	-2.447353023	-2.7493862808	1.7315733844
H	-3.3723779438	-2.1363196812	0.3484770419
S	-3.783755675	-0.2343912376	2.5961658807
C	-2.8027306319	0.6645654786	3.7218564244
C	-3.4175701341	1.392851857	4.8631597615
H	-2.6404415802	1.8645178334	5.4681516446
H	-3.9918247424	0.7221911	5.5108814057
H	-4.1017708411	2.1759604167	4.518147132
C	-1.4804073526	0.6270816492	3.3509193956
H	-0.7135013106	1.1656861878	3.8969330769

9. Transition state TSD

9.1 Representation of the imaginary vibrational mode (691i cm⁻¹)



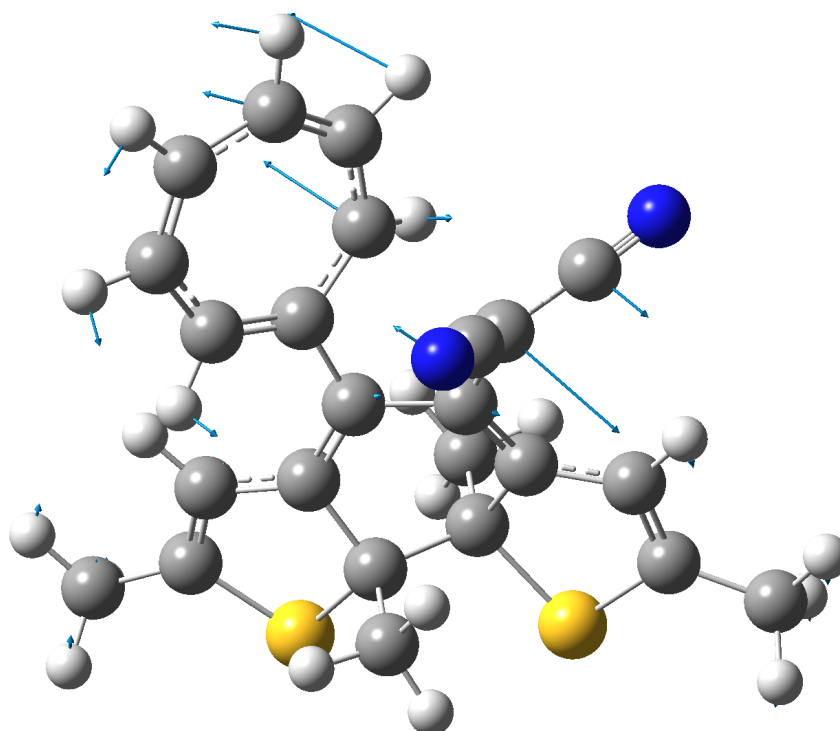
9.2 Cartesian coordinates

C	-0.0017765717	0.2830393233	0.1010240795
C	0.0033234451	-0.0254570277	1.5538610167
C	1.233141851	-0.0389461542	2.260979562
C	2.4440229365	0.493928389	1.6585894172
C	1.5217262663	-0.8978603587	3.3707168673
S	3.8320132824	-0.0602995634	2.6162720463
C	2.8321818676	-1.0337639791	3.6802466065
H	0.7605948422	-1.4674889069	3.8944713157
C	1.2575309051	0.1718877601	-0.5994692404
C	2.3835148822	-0.5404039519	-0.0562415879
C	1.6264611057	0.9902786608	-1.6967722068
S	3.81690679	-0.1746753578	-1.042907134
C	2.9475420182	0.9277116378	-2.0475358635
H	0.9455231539	1.6873351807	-2.1767008706
C	2.3104719618	-1.9912569358	0.3466533977
H	3.1912710903	-2.2851827972	0.925957132
H	1.4147038044	-2.1894026159	0.9362122415
H	2.2674224651	-2.6142886217	-0.5518597159
C	2.5642401674	1.9440902017	1.2599176396
H	2.6554111659	2.5427389734	2.1709620431

H	3.4516569846	2.1232121724	0.6454355829
H	1.6779927197	2.2828539998	0.7224274019
C	3.4583519168	-1.9036834022	4.7103623786
H	4.0717905791	-1.3241734075	5.4100382442
H	2.6813058448	-2.4154427696	5.2836677649
H	4.1082623561	-2.6614988781	4.25609882
C	3.643783144	1.7398754507	-3.0802480891
H	4.3927093374	2.3980504002	-2.6247004569
H	4.166714505	1.1025271229	-3.8017185025
H	2.9241875973	2.357667757	-3.6222444316
C	-1.19526965	-0.4241100728	2.1743390154
C	-2.2882430453	-0.9678935463	1.4563295677
C	-1.3932413605	-0.3514954239	3.5724055648
N	-3.1944901558	-1.4580639615	0.9260627708
N	-1.5967590881	-0.2740933609	4.7109531176
C	-1.1390573443	0.8030344543	-0.5477576266
C	-1.3318003077	0.4948103161	-1.9428734499
C	-2.0639242732	1.6391998048	0.1824974686
C	-2.309796574	0.8527610325	-2.8177763026
H	-0.5927832341	-0.1927166158	-2.3482869599
H	-1.7790634222	1.8298465342	1.2135221851
C	-3.1917457095	2.282930348	-0.2172859196
H	-2.217842824	0.4217706261	-3.8128967675
C	-3.462256674	1.6796009488	-2.6282063602
H	-3.6682970953	2.8909196379	0.5492507029
C	-3.8479146576	2.3061950542	-1.4897109377
H	-4.0981066581	1.804730857	-3.5020614564
H	-4.7582084268	2.9000688171	-1.5354754724

10. Transition state TSE

10.1 Representation of the imaginary vibrational mode (118i cm⁻¹)



10.2 Cartesian coordinates

C	0.0120163305	0.025586211	-0.0193004068
C	0.0069776631	0.028255679	1.453093792
C	1.179689968	0.006635385	2.1374824853
C	2.4865441756	0.1275712661	1.3576341354
C	1.4048882999	-0.1306314627	3.5462253572
S	3.795858689	-0.4531392035	2.5291597524
C	2.6870966239	-0.3716036476	3.8951543304
H	0.6075249546	-0.0810714996	4.2826443096
C	1.1626074884	-0.2554180881	-0.7022984628
C	2.3662251338	-0.7436773334	0.0987427082
C	1.4616461352	-0.1103934017	-2.090015876
S	3.8118591288	-0.5753832093	-1.0436842605
C	2.7732230499	-0.2451504925	-2.409681785
H	0.7200013661	0.1489146907	-2.8397822031
C	2.1774141403	-2.2401223112	0.3895869509
H	3.0468462235	-2.6482784042	0.9087650928
H	1.2905976139	-2.3958419472	1.0104165677

H	2.0448966124	-2.7766416757	-0.5531094966
C	2.7534289348	1.6099097362	1.0629440862
H	2.7358674734	2.1679117454	2.0022445868
H	3.7266983278	1.7510115098	0.5883329093
H	1.9769324127	2.0118928059	0.4047451171
C	3.225230763	-0.5807777559	5.2646258066
H	3.97429979	0.180991128	5.5102076967
H	2.4198192057	-0.5294871454	6.0008152626
H	3.7157301369	-1.5574249605	5.3492728638
C	3.3776314735	-0.124194422	-3.7622247026
H	2.6131083624	0.1171148017	-4.504030894
H	4.1438701031	0.6591999466	-3.7793477833
H	3.8668017727	-1.0609262675	-4.0535154862
C	-1.3370042187	0.0783537115	2.0676036897
C	-2.2242380616	-0.9945298812	1.8429162606
C	-1.5960105231	0.9126358341	3.1716696722
N	-2.9513090546	-1.8626582567	1.5882480464
N	-1.8134976975	1.6466739566	4.0447422865
C	-1.281274941	0.3791999317	-0.5962529186
C	-1.7864503549	-0.3025592526	-1.6822745537
C	-1.9755345493	1.3560882599	0.2036275404
C	-3.059531524	-0.2328677451	-2.2851707903
H	-1.1121994205	-1.0342500238	-2.1224763643
H	-1.3385606807	2.0532679024	0.739693758
C	-3.3325062101	1.7197984104	0.1272676918
H	-3.1805738741	-0.8481269352	-3.1744694125
C	-4.1804996183	0.4356589651	-1.857860784
H	-3.6437645162	2.4653533511	0.8574404456
C	-4.3086941819	1.2822690471	-0.7387339417
H	-5.0820422293	0.2942733819	-2.4497025228
H	-5.3005191237	1.7011139217	-0.5802600426

Table S1. Computed dipole moments (D) and Merz-Kollman (MK) charges for the fragments of **DHA**, **VHFcis** and **VHFtrans**. All values are computed at the PCM(toluenes)-CAM-B3LYP/6-311+G(2d,p)//PCM-PBE0/6-311G(d,p) level and reported for both the ground (S_0) and first excited (S_1) states.

Form	State	MK charges				Dipole moment
		I	II	III	IV	
DHA	S_0	0.17	-0.15	-0.12	0.10	5.5
	S_1	0.27	-0.28	-0.12	0.13	6.0
VHFcis	S_0	0.61	-0.12	-0.57	0.08	10.0
	S_1	0.61	-0.08	-0.58	0.04	10.0
VHFtrans	S_0	0.54	-0.07	-0.58	0.11	13.6
	S_1	0.48	-0.01	-0.60	0.13	15.1

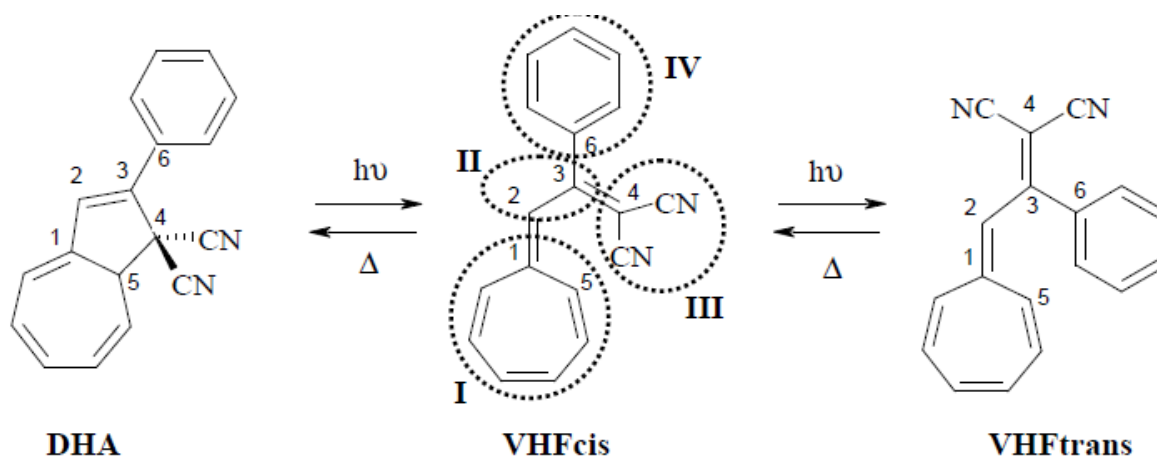


Table S2. Computed dipole moments (D) and Merz-Kollman (MK) charges for the different fragments of the hybrid system. Values are computed at the PCM(toluene)-CAM-B3LYP/6-311+G(2d, p)//PCM-PBE0/6-311G(d,p) level for the ground state S_0 as well as for the vertical S_1 state.

Form	State	MK charges				Dipole moment
		I	II	III	IV	
Do-DHA	S_0	0.21	0.76	-0.73	-0.25	5.9
	S_1	0.23	0.49	-0.69	-0.03	6.3
Dc-DHA	S_0	0.12	-0.01	-0.32	0.21	6.1
	S_1	0.04	0.07	-0.33	0.21	6.6
Do-VHFcis	S_0	0.68	0.00	-0.67	0.00	9.3
	S_1	0.65	0.08	-0.73	0.00	11.0
Do-VHFtrans	S_0	0.18	0.01	0.32	-0.51	12.2
	S_1	0.20	0.17	0.34	-0.70	14.0
Dc-VHF	S_0	0.64	0.09	-0.86	0.13	13.3
	S_1	0.37	0.08	-0.63	0.18	7.4

