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Non-Radiative Decay Paths in Rhodamines: New Theoretical Insights

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Supplementary Information

Tables 1, 2, 3: Ground state optimized cartesian cordinates for 5TMR, RhodB, Rhod101.

Tables 4, 5, 6, 7, 8: Excited state optimized cartesian cordinates for 5TMR$_{asym}$, 5TMR, RhodB, RhodB$_{asym}$, Rhod101.

Figure 1 : Energy levels (eV) for 5TMR and 5TMR$_{asym}$ computed at the TD-B3LYP-D/6-31G+(d,p)/CPCM level of theory.

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Table 1: 5TMR cartesian cordinate of S_0 minimum energy, optimization has been performed at B3LYP-D/6-31+g(d,p)/CPCM level of theory

Atom	X	Y	Z
C	0.792010	-3.652065	-0.157569
C	0.049684	-2.499758	-0.134932
C	0.660320	-1.214241	-0.135139
C	2.082603	-1.186262	-0.157766
C	2.856765	-2.330906	-0.182008
C	2.229821	-3.603949	-0.182014
C	-0.054833	-0.000124	-0.084958
C	2.081866	1.187352	-0.157784
C	0.659571	1.214443	-0.135095
C	0.048131	2.499575	-0.134845
H	-1.034520	2.557765	-0.112073
C	0.789737	3.652344	-0.157542
C	2.227572	3.605126	-0.182135
C	2.855317	2.332477	-0.182102
H	0.282918	-4.606488	-0.155074
H	-1.032932	-2.558621	-0.112233
H	3.932773	-2.224913	-0.200440
H	0.280049	4.606449	-0.155004
H	3.931392	2.227160	-0.200550
N	2.961965	-4.743815	-0.205999
O	2.755073	0.000751	-0.156844
N	2.958986	4.745460	-0.206291
C	-1.541733	-0.000555	-0.183533
C	-2.380792	-0.000510	0.945973
C	-3.474688	-0.001286	-1.655636
C	-3.764616	-0.000812	0.750791
C	-4.319921	-0.001208	-0.534254
H	-4.411068	-0.000747	1.620366
C	-2.094070	-0.000946	-1.474052
C	2.301145	6.053613	-0.202230
H	1.695518	6.184630	0.702520
H	3.062547	6.832527	-0.228173
H	1.652498	6.167902	-1.078894
C	4.419645	4.676357	-0.229016
H	4.769006	4.136925	-1.118223
H	4.825433	5.687177	-0.249655
H	4.798699	4.161106	0.662466
C	4.422584	-4.673772	-0.228470
H	4.801099	-4.157883	0.662868
H	4.829033	-5.684338	-0.248566
H	4.771787	-4.134498	-1.117838
C	2.304972	-6.052395	-0.202126
H	1.699228	-6.183832	0.702484
H	1.656601	-6.167084	-1.078940
H	3.066891	-6.830809	-0.227917
C	-1.804676	-0.000229	2.366494
O	-0.542784	-0.000189	2.445911
O	-2.627262	-0.000078	3.321546
H	-1.435358	-0.000974	-2.337023
H	-3.891233	-0.001595	-2.656078
C	-5.801294	-0.001531	-0.663726
O	-6.580963	-0.001314	0.277026
O	-6.225278	-0.002110	-1.947602
H	-7.198003	-0.002269	-1.946237

Table 2: RhodB cartesian cordinate of S_0 minimum energy, optimization has been performed at B3LYP-D/6-31+g(d,p)/CPCM level of theory

Atom	X	Y	Z
C	3.651492	0.262039	-0.353632
C	2.500562	1.005496	-0.393346
C	1.212937	0.403193	-0.343245
C	1.186456	-1.013241	-0.238791
C	2.330998	-1.788862	-0.196701
C	3.610122	-1.175743	-0.268107
C	0.000015	1.124339	-0.354080
C	-1.186336	-1.013292	-0.238797
C	-1.212878	0.403140	-0.343245
C	-2.500528	1.005387	-0.393361
H	-2.562414	2.086506	-0.451994
C	-3.651426	0.261878	-0.353665
C	-3.609994	-1.175901	-0.268148
C	-2.330844	-1.788965	-0.196727
H	4.598528	0.782445	-0.373021
H	2.562401	2.086618	-0.451982
H	2.209725	-2.859362	-0.115210
H	-4.598486	0.782242	-0.373066
H	-2.209523	-2.859459	-0.115240
N	4.748035	-1.922730	-0.258068
O	0.000075	-1.684395	-0.173410
N	-4.747879	-1.922932	-0.258134
C	-0.000024	2.596044	-0.588019
C	0.000109	3.031476	-1.921967
C	-0.000297	4.899811	0.142403
C	0.000037	4.395675	-2.222064
H	0.000264	2.297169	-2.722539
C	-0.000171	5.334558	-1.184329
H	-0.000450	5.609663	0.962860
H	0.000142	4.720022	-3.258524
H	-0.000231	6.397207	-1.409532
C	-0.000320	3.080396	1.921398
O	-0.000061	1.828339	2.109794
O	-0.000606	3.976751	2.809339
C	-0.000222	3.533928	0.460410
C	-6.069459	-1.280983	-0.218242
H	-6.078903	-0.448631	-0.925844
H	-6.802166	-1.995330	-0.590553
C	-6.454568	-0.814185	1.189073
H	-6.488124	-1.665868	1.877260
H	-5.727865	-0.090011	1.572079
H	-7.443194	-0.341710	1.170450
C	-4.629886	-3.377104	-0.012582
H	-3.984300	-3.798698	-0.791656
H	-4.117022	-3.525596	0.947553
C	-5.945195	-4.149816	-0.005079
H	-6.453514	-4.099157	-0.973293
H	-5.710894	-5.199160	0.199692
H	-6.627715	-3.796006	0.773833
C	6.069594	-1.280738	-0.218157
H	6.802331	-1.995067	-0.590441
H	6.079030	-0.448395	-0.925771
C	6.454658	-0.813908	1.189161
H	5.727924	-0.089749	1.572139
H	6.488222	-1.665580	1.877361
H	7.443271	-0.341405	1.170553
C	4.630087	-3.376903	-0.012506
H	4.117224	-3.525403	0.947627
H	3.984517	-3.798523	-0.791580
C	5.945421	-4.149573	-0.004991
H	6.627927	-3.795736	0.773920
H	5.711153	-5.198923	0.199786
H	6.453742	-4.098905	-0.973204

Table 3: Rhod101 cartesian cordinate of S_0 minimum energy, optimization has been performed at B3LYP-D/6-31+g(d,p)/CPCM level of theory

Atom	X	Y	Z
C	-0.654109	3.444179	0.498089
C	-0.063295	2.614988	-0.478254
C	0.399346	3.172082	-1.681734
C	0.288001	4.543018	-1.923976
C	-0.300157	5.369265	-0.960497
C	-0.772729	4.815834	0.232109
C	0.033201	1.141245	-0.310875
C	1.289778	0.507670	-0.241484
C	1.353567	-0.912170	-0.134780
O	0.205626	-1.648556	-0.098633
C	-1.024504	-1.061651	-0.175334
C	-1.136529	0.349612	-0.304116
C	2.533402	1.200708	-0.230491
C	3.736578	0.550155	-0.151732
C	3.762287	-0.890418	-0.037408
C	2.539672	-1.622167	-0.040264
C	5.042595	1.306666	-0.167488
C	6.063022	0.593858	0.724084
C	6.236083	-0.839735	0.236239
N	4.951043	-1.537368	0.080245
C	2.552659	-3.130276	0.059761
C	3.852681	-3.674029	-0.539583
C	5.049212	-3.002315	0.122045
C	-2.453960	0.870261	-0.418341
C	-3.567816	0.070320	-0.391876
C	-3.417733	-1.355539	-0.218693
C	-2.113373	-1.919277	-0.118163
N	-4.521158	-2.154978	-0.144862
C	-5.876966	-1.629083	-0.346609
C	-5.997444	-0.190544	0.143261
C	-4.946968	0.666864	-0.564000
C	-4.392088	-3.615869	-0.165621
C	-3.166361	-4.067453	0.620742
C	-1.909955	-3.410428	0.045704
C	-1.123657	2.901408	1.850605
O	-0.444573	1.958000	2.345703
O	-2.136987	3.457844	2.361325
H	-2.580824	1.940647	-0.537005
H	2.523268	2.283412	-0.288516
H	-1.240347	5.443444	0.983827
H	0.654174	4.958726	-2.858041
H	-5.304854	-4.032182	0.269190
H	-4.326288	-3.965175	-1.207754
H	-3.086092	-5.157688	0.573270
H	-3.291538	-3.781259	1.671900
H	-1.672706	-3.859565	-0.928944
H	-1.048052	-3.598063	0.692901
H	2.476068	-3.438926	1.112178
H	1.683810	-3.547357	-0.456482
H	3.873043	-3.473965	-1.617723
H	3.926369	-4.755934	-0.394388
H	5.977033	-3.280361	-0.389582
H	5.139534	-3.321956	1.170532
H	-6.139817	-1.688669	-1.414210
H	-6.562774	-2.282103	0.201134
H	-5.840979	-0.161290	1.228451
H	-7.006954	0.176276	-0.065660
H	-4.951318	1.695077	-0.188048
H	-5.192998	0.713886	-1.634543
H	5.436022	1.345774	-1.193698
H	4.876413	2.338818	0.156566
H	5.710711	0.590253	1.762757
H	7.033960	1.097533	0.695794
H	6.833001	-1.418088	0.950113
H	6.765485	-0.854406	-0.727347
H	0.839012	2.520975	-2.431717
H	-0.390727	6.437208	-1.137713

Table 4: 5TMR$_{asym}$ cartesian cordinate of S_1 minimum energy, optimization has been performed at TD-B3LYP-D/6-31+g(d,p)/CPCM level of theory

Atom	X	Y	Z
C	-3.553094	-1.152168	-0.468073
C	-2.192334	-1.284897	-0.263033
C	-1.324121	-0.169670	-0.121913
C	-1.945283	1.101524	-0.254087
C	-3.304470	1.265822	-0.455644
C	-4.158121	0.134610	-0.548475
C	0.093491	-0.248805	0.061003
C	0.161051	2.210648	-0.069673
C	0.840545	0.971891	0.079724
C	2.238211	1.076769	0.307681
H	2.808401	0.172873	0.487290
C	2.902711	2.290920	0.325902
C	2.204344	3.515139	0.122564
C	0.799862	3.439522	-0.051940
H	-4.154026	-2.046504	-0.568912
H	-1.769255	-2.281993	-0.214728
H	-3.685970	2.273988	-0.551128
H	3.968695	2.294161	0.512150
H	0.191882	4.327228	-0.166248
N	-5.509871	0.281614	-0.715015
O	-1.206870	2.259637	-0.217741
N	2.860686	4.723271	0.100787
C	0.769568	-1.543941	0.218956
C	1.786999	-1.873491	-0.694055
C	1.133788	-3.739630	1.255857
C	2.446296	-3.103272	-0.660667
H	2.047547	-1.161393	-1.468600
C	2.110922	-4.054617	0.321998
H	0.880461	-4.455668	2.030876
H	2.610472	-5.015124	0.350990
C	-0.462929	-2.248351	2.357389
O	-1.263258	-1.262674	2.448533
O	-0.512611	-2.990609	3.376003
C	0.464314	-2.502332	1.226381
C	4.266381	4.787640	0.487723
H	4.872310	4.136340	-0.151864
H	4.621528	5.811566	0.363210
C	2.086651	5.959515	0.096084
H	1.424332	5.995365	-0.776372
H	1.469476	6.060016	1.002262
C	-6.344434	-0.891296	-0.952590
H	-7.386102	-0.577681	-1.027976
H	-6.062268	-1.408177	-1.881555
C	-6.077836	1.609822	-0.917289
H	-5.837970	2.265667	-0.071778
H	-5.695701	2.078383	-1.836310
H	-6.257802	-1.603263	-0.123093
H	-7.162703	1.526810	-0.990214
H	2.770116	6.807751	0.039268
H	4.419023	4.483632	1.534660
C	3.488657	-3.363661	-1.691089
O	3.810316	-2.574886	-2.566991
O	4.066270	-4.577881	-1.565128
H	4.734050	-4.673018	-2.266142

Table 5: 5TMR cartesian cordinate of S_1 minimum energy, optimization has been performed at TD-B3LYP-D/6-31+g(d,p)/CPCM level of theory

Atom	X	Y	Z
C	-0.780401	3.669484	-0.183182
C	-0.039907	2.504367	-0.171822
C	-0.650041	1.217790	-0.168366
C	-2.073648	1.198083	-0.173652
C	-2.839967	2.346791	-0.185382
C	-2.209084	3.623142	-0.190456
C	0.076493	-0.007687	-0.148654
C	-2.091856	-1.180542	-0.167523
C	-0.668743	-1.222019	-0.161994
C	-0.078356	-2.517757	-0.158839
H	1.003760	-2.589167	-0.148875
C	-0.836575	-3.671461	-0.164381
C	-2.264373	-3.603301	-0.172084
C	-2.875670	-2.317441	-0.173518
H	-0.264356	4.620582	-0.182580
H	1.043178	2.559277	-0.162250
H	-3.916970	2.244857	-0.188628
H	-0.335142	-4.630330	-0.158913
H	-3.950986	-2.199060	-0.177436
N	-2.955931	4.766790	-0.200004
O	-2.771234	0.014053	-0.165413
N	-3.028595	-4.735449	-0.176034
C	1.557366	-0.019260	-0.217631
C	2.383772	-0.022752	0.926828
C	3.524568	-0.038243	-1.661288
C	3.771657	-0.033813	0.749286
C	4.350538	-0.041739	-0.525697
H	4.405729	-0.036479	1.627523
C	2.142120	-0.027151	-1.497047
C	-2.394883	-6.050202	-0.171979
H	-1.771080	-6.177668	0.722435
H	-3.166079	-6.819033	-0.178042
H	-1.758212	-6.176655	-1.057338
C	-4.485075	-4.641845	-0.179251
H	-4.836876	-4.103184	-1.068890
H	-4.907986	-5.645318	-0.182736
H	-4.841138	-4.107506	0.711386
C	-4.413669	4.695360	-0.202571
H	-4.777651	4.170940	0.690758
H	-4.821258	5.705128	-0.210997
H	-4.773818	4.157700	-1.089472
C	-2.302269	6.071746	-0.202523
H	-1.676509	6.194187	0.691228
H	-1.663846	6.184098	-1.088521
H	-3.061683	6.852179	-0.212401
C	1.814128	-0.014998	2.355146
O	0.559460	0.087416	2.459369
O	2.653881	0.075671	3.295189
H	1.495552	-0.024450	-2.369703
H	3.956790	-0.044181	-2.655284
C	5.832524	-0.053613	-0.628849
O	6.598444	-0.054200	0.323949
O	6.280173	-0.056816	-1.905780
H	7.252571	-0.061935	-1.884918

Table 6: RhodB cartesian cordinate of S_1 minimum energy, optimization has been performed at TD-B3LYP-D/6-31+g(d,p)/CPCM level of theory

Atom	X	Y	Z
C	3.665836	0.243627	-0.343300
C	2.509124	0.994663	-0.383601
C	1.215354	0.402637	-0.344726
C	1.184896	-1.015517	-0.241935
C	2.326752	-1.792882	-0.199511
C	3.614063	-1.185484	-0.263863
C	-0.001660	1.141738	-0.386957
C	-1.193773	-1.012237	-0.241864
C	-1.220089	0.406200	-0.345711
C	-2.512450	1.001747	-0.383724
H	-2.576670	2.082963	-0.438005
C	-3.671112	0.253925	-0.341570
C	-3.623434	-1.175304	-0.260892
C	-2.337739	-1.786229	-0.197614
H	4.614506	0.762053	-0.354849
H	2.576169	2.075735	-0.437264
H	2.201813	-2.863961	-0.124383
H	-4.618314	0.775054	-0.352285
H	-2.215771	-2.857576	-0.121428
N	4.750610	-1.952810	-0.247725
O	-0.005353	-1.700429	-0.181491
N	-4.762175	-1.939261	-0.242186
C	0.000714	2.610793	-0.597050
C	-0.011812	3.066896	-1.926952
C	0.019499	4.916022	0.143366
C	-0.008507	4.431772	-2.223564
H	-0.023804	2.336269	-2.731333
C	0.007658	5.362491	-1.179426
H	0.031460	5.623134	0.965849
H	-0.018122	4.762394	-3.258360
H	0.010628	6.427470	-1.394618
C	0.027628	3.122040	1.934164
O	0.021747	1.880610	2.175313
O	0.041332	4.048974	2.794615
C	0.016088	3.547411	0.459094
C	-6.083361	-1.306473	-0.251274
H	-6.073663	-0.481233	-0.967586
H	-6.804328	-2.030673	-0.627762
C	-6.507106	-0.818300	1.142162
H	-6.561120	-1.659115	1.841514
H	-5.790470	-0.087894	1.530911
H	-7.494848	-0.347779	1.082064
C	-4.641456	-3.389117	0.009083
H	-3.998272	-3.814593	-0.771038
H	-4.117660	-3.526535	0.965601
C	-5.954015	-4.165297	0.036137
H	-6.464918	-4.137479	-0.931376
H	-5.713423	-5.208858	0.261390
H	-6.634564	-3.798357	0.810355
C	6.073581	-1.323872	-0.259488
H	6.791576	-2.049894	-0.638117
H	6.064524	-0.498011	-0.975085
C	6.501803	-0.838019	1.133424
H	5.788152	-0.105823	1.524264
H	6.554963	-1.679529	1.831986
H	7.490764	-0.370346	1.071332
C	4.626309	-3.402679	0.001802
H	4.103648	-3.539738	0.958976
H	3.980656	-3.825271	-0.777848
C	5.936723	-4.182543	0.025785
H	6.619639	-3.818364	0.799224
H	5.693509	-5.225635	0.250366
H	6.446002	-4.155205	-0.942590

Table 7: RhodB$_{asym}$ cartesian cordinate of S_1 minimum energy, optimization has been performed at TD-B3LYP-D/6-31+g(d,p)/CPCM level of theory

Atom	X	Y	Z
C	3.563006	0.059025	-0.568011
C	2.448359	0.878926	-0.589786
C	1.125647	0.380175	-0.464861
C	1.025628	-1.029832	-0.340244
C	2.124606	-1.871905	-0.313131
C	3.442103	-1.353105	-0.435536
C	-0.060149	1.175791	-0.490028
C	-1.360756	-0.905761	-0.305644
C	-1.321908	0.507423	-0.423166
C	-2.590262	1.142665	-0.401008
H	-2.630624	2.225189	-0.442150
C	-3.778806	0.436979	-0.316233
C	-3.797305	-0.985109	-0.244997
C	-2.536979	-1.634210	-0.215031
H	4.534992	0.526037	-0.647641
H	2.591171	1.948282	-0.697827
H	1.933502	-2.930053	-0.200760
H	-4.699258	1.004221	-0.291936
H	-2.445064	-2.706596	-0.113051
N	4.542506	-2.191856	-0.447323
O	-0.200083	-1.648540	-0.247820
N	-4.982684	-1.707922	-0.217711
C	0.011114	2.646928	-0.582628
C	-0.563784	3.277414	-1.702011
C	0.657331	4.873762	0.217506
C	-0.516391	4.660721	-1.874425
H	-1.039457	2.655792	-2.454011
C	0.104755	5.468362	-0.913907
H	1.127363	5.487370	0.979987
H	-0.955284	5.106916	-2.762077
H	0.155138	6.544496	-1.044682
C	1.144260	2.986927	1.691668
O	1.441301	1.780461	1.967397
O	1.333139	3.746147	2.681150
C	0.616368	3.479437	0.395508
C	-6.228634	-1.014518	0.130179
H	-6.313757	-0.112071	-0.479250
H	-7.063272	-1.649121	-0.169166
C	-6.330220	-0.677204	1.622202
H	-6.286029	-1.593237	2.222790
H	-5.504371	-0.025044	1.926682
H	-7.276795	-0.167285	1.835994
C	-4.890892	-3.144243	0.097192
H	-4.223069	-3.602688	-0.639297
H	-4.422501	-3.282628	1.085305
C	-6.218472	-3.897448	0.054126
H	-6.717668	-3.768981	-0.912753
H	-6.009324	-4.962934	0.194291
H	-6.902466	-3.580429	0.847772
C	5.881720	-1.619026	-0.271601
H	6.612409	-2.359585	-0.596965
H	5.996262	-0.773246	-0.953901
C	6.166521	-1.196124	1.174270
H	5.442654	-0.443854	1.505546
H	6.096941	-2.060895	1.844200
H	7.174461	-0.772982	1.256418
C	4.331557	-3.602070	-0.070106
H	3.895554	-3.653553	0.940105
H	3.592586	-4.025371	-0.758666
C	5.580394	-4.478588	-0.127790
H	6.332750	-4.176262	0.607538
H	5.281681	-5.507728	0.096206
H	6.035003	-4.462204	-1.124340

Table 8: Rhod101 cartesian cordinate of S_1 minimum energy, optimization has been performed at TD-B3LYP-D/6-31+g(d,p)/CPCM level of theory

Atom	X	Y	Z
C	-0.794707	3.449052	0.457460
C	-0.062830	2.643034	-0.449110
C	0.552220	3.256394	-1.559997
C	0.459217	4.631323	-1.776896
C	-0.272196	5.424279	-0.884174
C	-0.899216	4.826359	0.212078
C	0.042342	1.179679	-0.303793
C	1.313968	0.532251	-0.222308
C	1.385913	-0.886486	-0.118949
O	0.244577	-1.647380	-0.075923
C	-0.993464	-1.060272	-0.156619
C	-1.125862	0.348057	-0.288707
C	2.558935	1.222732	-0.186859
C	3.773463	0.575546	-0.106848
C	3.803442	-0.858674	-0.023315
C	2.576849	-1.593633	-0.033372
C	5.070530	1.345098	-0.086185
C	6.101029	0.604637	0.771201
C	6.275267	-0.812355	0.235495
N	4.996376	-1.515278	0.086453
C	2.594704	-3.100553	0.051952
C	3.891366	-3.638798	-0.559107
C	5.091755	-2.977296	0.105577
C	-2.451388	0.837958	-0.433211
C	-3.560963	0.018645	-0.412219
C	-3.388016	-1.395894	-0.230045
C	-2.070208	-1.936126	-0.104690
N	-4.478844	-2.224946	-0.170154
C	-5.835384	-1.720553	-0.396200
C	-5.990132	-0.284700	0.094334
C	-4.944861	0.595786	-0.593301
C	-4.317304	-3.679171	-0.184449
C	-3.096030	-4.102610	0.624818
C	-1.844618	-3.420391	0.068779
C	-1.428728	2.889141	1.733137
O	-0.761396	2.028054	2.373842
O	-2.558932	3.359349	2.052501
H	-2.599100	1.903506	-0.563172
H	2.550588	2.306038	-0.218747
H	-1.475405	5.428198	0.908176
H	0.943562	5.077110	-2.641144
H	-5.231939	-4.116753	0.224103
H	-4.216786	-4.021465	-1.228287
H	-2.993270	-5.190811	0.578341
H	-3.245880	-3.818536	1.673214
H	-1.585227	-3.863521	-0.903795
H	-0.986656	-3.590342	0.725511
H	2.525150	-3.414755	1.103844
H	1.722028	-3.514867	-0.459420
H	3.908423	-3.426744	-1.634967
H	3.964300	-4.722103	-0.425337
H	6.021084	-3.250393	-0.406730
H	5.182824	-3.309498	1.151998
H	-6.065040	-1.777340	-1.473546
H	-6.524013	-2.391809	0.124993
H	-5.852832	-0.256071	1.182028
H	-7.003402	0.060919	-0.131107
H	-4.968471	1.619177	-0.204873
H	-5.179658	0.653587	-1.666488
H	5.462452	1.440847	-1.109730
H	4.892871	2.358571	0.287695
H	5.759215	0.563703	1.812546
H	7.070630	1.111102	0.750381
H	6.897082	-1.410549	0.910893
H	6.778862	-0.790709	-0.743652
H	1.096515	2.634172	-2.264839
H	-0.355184	6.495951	-1.042214

Complete Reference 45

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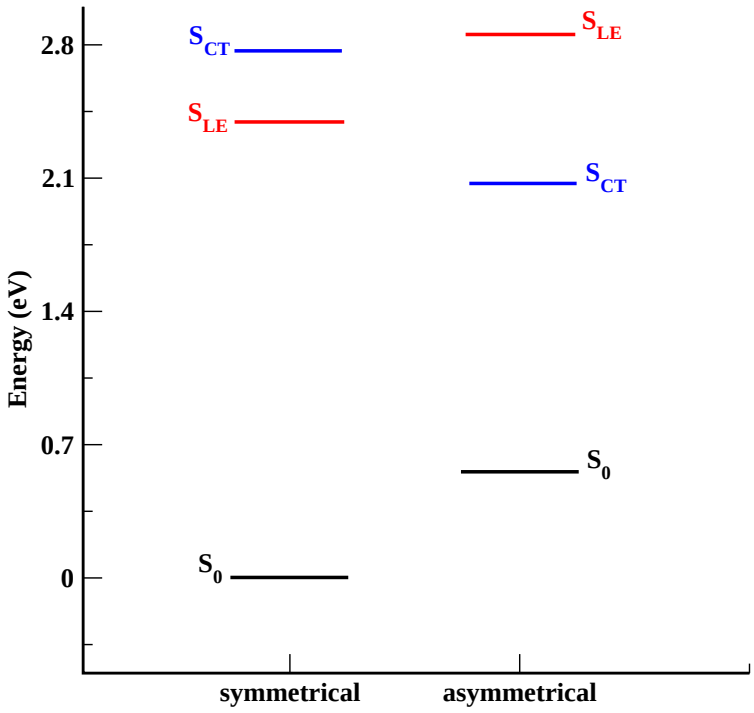

Figure 1: Energy levels (eV) of 5TMR and 5TMR$_{asym}$ in ACN calculated at the TD-B3LYP-D/6-31G+(d,p)/CPCM level of theory.