

Non-Radiative Decay Paths in Rhodamines: New Theoretical Insights

Marika Savarese,^{a,b} Umberto Raucci,^a Carlo Adamo,^{c,d} Paolo A. Netti,^e Ilaria
Ciofini,^c Nadia Rega^{a,b*}

^a *Dipartimento di Scienze Chimiche, Università di Napoli 'Federico II', Complesso Universitario
di M.S.Angelo, via Cintia, I-80126 Napoli, Italy*

^b *Italian Institute of Technology, IIT@CRIB Center for Advanced Biomaterials for Healthcare,
Largo Barsanti e Matteucci, I-80125 Napoli, Italy*

^c *Laboratoire d'Electrochimie, Chimie des Interfaces et Modelisation pour l'Energie, CNRS
UMR-7575, Ecole Nationale Supérieure de Chimie de Paris, Chimie ParisTech, 11 rue P. et M.
Curie, F-75231 Paris Cedex 05, France*

^d *Institut Universitaire de France, 103 Bd Saint-Michel, F-75005 Paris, France*

^e *Center for Advanced Biomaterials for Health Care@CRIB, Istituto Italiano di Tecnologia,
Largo Barsanti e Matteucci n, 53 80125 Napoli*

E-mail: nadia.rega@unina.it, phone: +39-081674207

*To whom correspondence should be addressed

Supplementary Information

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

Tables 4, 5, 6, 7, 8: Excited state optimized cartesian coordinates 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 coordinate 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	H	3.066891	-6.830809	-0.227917
C	0.049684	-2.499758	-0.134932	C	-1.804676	-0.000229	2.366494
C	0.660320	-1.214241	-0.135139	O	-0.542784	-0.000189	2.445911
C	2.082603	-1.186262	-0.157766	O	-2.627262	-0.000078	3.321546
C	2.856765	-2.330906	-0.182008	H	-1.435358	-0.000974	-2.337023
C	2.229821	-3.603949	-0.182014	H	-3.891233	-0.001595	-2.656078
C	-0.054833	-0.000124	-0.084958	C	-5.801294	-0.001531	-0.663726
C	2.081866	1.187352	-0.157784	O	-6.580963	-0.001314	0.277026
C	0.659571	1.214443	-0.135095	O	-6.225278	-0.002110	-1.947602
C	0.048131	2.499575	-0.134845	H	-7.198003	-0.002269	-1.946237
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				

Table 2: RhodB cartesian coordinate 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	H	-4.117022	-3.525596	0.947553
C	2.500562	1.005496	-0.393346	C	-5.945195	-4.149816	-0.005079
C	1.212937	0.403193	-0.343245	H	-6.453514	-4.099157	-0.973293
C	1.186456	-1.013241	-0.238791	H	-5.710894	-5.199160	0.199692
C	2.330998	-1.788862	-0.196701	H	-6.627715	-3.796006	0.773833
C	3.610122	-1.175743	-0.268107	C	6.069594	-1.280738	-0.218157
C	0.000015	1.124339	-0.354080	H	6.802331	-1.995067	-0.590441
C	-1.186336	-1.013292	-0.238797	H	6.079030	-0.448395	-0.925771
C	-1.212878	0.403140	-0.343245	C	6.454658	-0.813908	1.189161
C	-2.500528	1.005387	-0.393361	H	5.727924	-0.089749	1.572139
H	-2.562414	2.086506	-0.451994	H	6.488222	-1.665580	1.877361
C	-3.651426	0.261878	-0.353665	H	7.443271	-0.341405	1.170553
C	-3.609994	-1.175901	-0.268148	C	4.630087	-3.376903	-0.012506
C	-2.330844	-1.788965	-0.196727	H	4.117224	-3.525403	0.947627
H	4.598528	0.782445	-0.373021	H	3.984517	-3.798523	-0.791580
H	2.562401	2.086618	-0.451982	C	5.945421	-4.149573	-0.004991
H	2.209725	-2.859362	-0.115210	H	6.627927	-3.795736	0.773920
H	-4.598486	0.782242	-0.373066	H	5.711153	-5.198923	0.199786
H	-2.209523	-2.859459	-0.115240	H	6.453742	-4.098905	-0.973204
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				

Table 3: Rhod101 cartesian coordinate 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	H	-3.291538	-3.781259	1.671900
C	-0.063295	2.614988	-0.478254	H	-1.672706	-3.859565	-0.928944
C	0.399346	3.172082	-1.681734	H	-1.048052	-3.598063	0.692901
C	0.288001	4.543018	-1.923976	H	2.476068	-3.438926	1.112178
C	-0.300157	5.369265	-0.960497	H	1.683810	-3.547357	-0.456482
C	-0.772729	4.815834	0.232109	H	3.873043	-3.473965	-1.617723
C	0.033201	1.141245	-0.310875	H	3.926369	-4.755934	-0.394388
C	1.289778	0.507670	-0.241484	H	5.977033	-3.280361	-0.389582
C	1.353567	-0.912170	-0.134780	H	5.139534	-3.321956	1.170532
O	0.205626	-1.648556	-0.098633	H	-6.139817	-1.688669	-1.414210
C	-1.024504	-1.061651	-0.175334	H	-6.562774	-2.282103	0.201134
C	-1.136529	0.349612	-0.304116	H	-5.840979	-0.161290	1.228451
C	2.533402	1.200708	-0.230491	H	-7.006954	0.176276	-0.065660
C	3.736578	0.550155	-0.151732	H	-4.951318	1.695077	-0.188048
C	3.762287	-0.890418	-0.037408	H	-5.192998	0.713886	-1.634543
C	2.539672	-1.622167	-0.040264	H	5.436022	1.345774	-1.193698
C	5.042595	1.306666	-0.167488	H	4.876413	2.338818	0.156566
C	6.063022	0.593858	0.724084	H	5.710711	0.590253	1.762757
C	6.236083	-0.839735	0.236239	H	7.033960	1.097533	0.695794
N	4.951043	-1.537368	0.080245	H	6.833001	-1.418088	0.950113
C	2.552659	-3.130276	0.059761	H	6.765485	-0.854406	-0.727347
C	3.852681	-3.674029	-0.539583	H	0.839012	2.520975	-2.431717
C	5.049212	-3.002315	0.122045	H	-0.390727	6.437208	-1.137713
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				

Table 4: 5TMR_{asym} cartesian coordinate of S₁ 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	H	-5.837970	2.265667	-0.071778
C	-2.192334	-1.284897	-0.263033	H	-5.695701	2.078383	-1.836310
C	-1.324121	-0.169670	-0.121913	H	-6.257802	-1.603263	-0.123093
C	-1.945283	1.101524	-0.254087	H	-7.162703	1.526810	-0.990214
C	-3.304470	1.265822	-0.455644	H	2.770116	6.807751	0.039268
C	-4.158121	0.134610	-0.548475	H	4.419023	4.483632	1.534660
C	0.093491	-0.248805	0.061003	C	3.488657	-3.363661	-1.691089
C	0.161051	2.210648	-0.069673	O	3.810316	-2.574886	-2.566991
C	0.840545	0.971891	0.079724	O	4.066270	-4.577881	-1.565128
C	2.238211	1.076769	0.307681	H	4.734050	-4.673018	-2.266142
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				

Table 5: 5TMR cartesian coordinate of S₁ 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	H	-3.061683	6.852179	-0.212401
C	-0.039907	2.504367	-0.171822	C	1.814128	-0.014998	2.355146
C	-0.650041	1.217790	-0.168366	O	0.559460	0.087416	2.459369
C	-2.073648	1.198083	-0.173652	O	2.653881	0.075671	3.295189
C	-2.839967	2.346791	-0.185382	H	1.495552	-0.024450	-2.369703
C	-2.209084	3.623142	-0.190456	H	3.956790	-0.044181	-2.655284
C	0.076493	-0.007687	-0.148654	C	5.832524	-0.053613	-0.628849
C	-2.091856	-1.180542	-0.167523	O	6.598444	-0.054200	0.323949
C	-0.668743	-1.222019	-0.161994	O	6.280173	-0.056816	-1.905780
C	-0.078356	-2.517757	-0.158839	H	7.252571	-0.061935	-1.884918
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				

Table 6: RhodB cartesian coordinate 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	H	-4.117660	-3.526535	0.965601
C	2.509124	0.994663	-0.383601	C	-5.954015	-4.165297	0.036137
C	1.215354	0.402637	-0.344726	H	-6.464918	-4.137479	-0.931376
C	1.184896	-1.015517	-0.241935	H	-5.713423	-5.208858	0.261390
C	2.326752	-1.792882	-0.199511	H	-6.634564	-3.798357	0.810355
C	3.614063	-1.185484	-0.263863	C	6.073581	-1.323872	-0.259488
C	-0.001660	1.141738	-0.386957	H	6.791576	-2.049894	-0.638117
C	-1.193773	-1.012237	-0.241864	H	6.064524	-0.498011	-0.975085
C	-1.220089	0.406200	-0.345711	C	6.501803	-0.838019	1.133424
C	-2.512450	1.001747	-0.383724	H	5.788152	-0.105823	1.524264
H	-2.576670	2.082963	-0.438005	H	6.554963	-1.679529	1.831986
C	-3.671112	0.253925	-0.341570	H	7.490764	-0.370346	1.071332
C	-3.623434	-1.175304	-0.260892	C	4.626309	-3.402679	0.001802
C	-2.337739	-1.786229	-0.197614	H	4.103648	-3.539738	0.958976
H	4.614506	0.762053	-0.354849	H	3.980656	-3.825271	-0.777848
H	2.576169	2.075735	-0.437264	C	5.936723	-4.182543	0.025785
H	2.201813	-2.863961	-0.124383	H	6.619639	-3.818364	0.799224
H	-4.618314	0.775054	-0.352285	H	5.693509	-5.225635	0.250366
H	-2.215771	-2.857576	-0.121428	H	6.446002	-4.155205	-0.942590
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				

Table 7: RhodB_{asym} cartesian coordinate of S₁ 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	H	-4.422501	-3.282628	1.085305
C	2.448359	0.878926	-0.589786	C	-6.218472	-3.897448	0.054126
C	1.125647	0.380175	-0.464861	H	-6.717668	-3.768981	-0.912753
C	1.025628	-1.029832	-0.340244	H	-6.009324	-4.962934	0.194291
C	2.124606	-1.871905	-0.313131	H	-6.902466	-3.580429	0.847772
C	3.442103	-1.353105	-0.435536	C	5.881720	-1.619026	-0.271601
C	-0.060149	1.175791	-0.490028	H	6.612409	-2.359585	-0.596965
C	-1.360756	-0.905761	-0.305644	H	5.996262	-0.773246	-0.953901
C	-1.321908	0.507423	-0.423166	C	6.166521	-1.196124	1.174270
C	-2.590262	1.142665	-0.401008	H	5.442654	-0.443854	1.505546
H	-2.630624	2.225189	-0.442150	H	6.096941	-2.060895	1.844200
C	-3.778806	0.436979	-0.316233	H	7.174461	-0.772982	1.256418
C	-3.797305	-0.985109	-0.244997	C	4.331557	-3.602070	-0.070106
C	-2.536979	-1.634210	-0.215031	H	3.895554	-3.653553	0.940105
H	4.534992	0.526037	-0.647641	H	3.592586	-4.025371	-0.758666
H	2.591171	1.948282	-0.697827	C	5.580394	-4.478588	-0.127790
H	1.933502	-2.930053	-0.200760	H	6.332750	-4.176262	0.607538
H	-4.699258	1.004221	-0.291936	H	5.281681	-5.507728	0.096206
H	-2.445064	-2.706596	-0.113051	H	6.035003	-4.462204	-1.124340
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				

Table 8: Rhod101 cartesian coordinate 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	H	-3.245880	-3.818536	1.673214
C	-0.062830	2.643034	-0.449110	H	-1.585227	-3.863521	-0.903795
C	0.552220	3.256394	-1.559997	H	-0.986656	-3.590342	0.725511
C	0.459217	4.631323	-1.776896	H	2.525150	-3.414755	1.103844
C	-0.272196	5.424279	-0.884174	H	1.722028	-3.514867	-0.459420
C	-0.899216	4.826359	0.212078	H	3.908423	-3.426744	-1.634967
C	0.042342	1.179679	-0.303793	H	3.964300	-4.722103	-0.425337
C	1.313968	0.532251	-0.222308	H	6.021084	-3.250393	-0.406730
C	1.385913	-0.886486	-0.118949	H	5.182824	-3.309498	1.151998
O	0.244577	-1.647380	-0.075923	H	-6.065040	-1.777340	-1.473546
C	-0.993464	-1.060272	-0.156619	H	-6.524013	-2.391809	0.124993
C	-1.125862	0.348057	-0.288707	H	-5.852832	-0.256071	1.182028
C	2.558935	1.222732	-0.186859	H	-7.003402	0.060919	-0.131107
C	3.773463	0.575546	-0.106848	H	-4.968471	1.619177	-0.204873
C	3.803442	-0.858674	-0.023315	H	-5.179658	0.653587	-1.666488
C	2.576849	-1.593633	-0.033372	H	5.462452	1.440847	-1.109730
C	5.070530	1.345098	-0.086185	H	4.892871	2.358571	0.287695
C	6.101029	0.604637	0.771201	H	5.759215	0.563703	1.812546
C	6.275267	-0.812355	0.235495	H	7.070630	1.111102	0.750381
N	4.996376	-1.515278	0.086453	H	6.897082	-1.410549	0.910893
C	2.594704	-3.100553	0.051952	H	6.778862	-0.790709	-0.743652
C	3.891366	-3.638798	-0.559107	H	1.096515	2.634172	-2.264839
C	5.091755	-2.977296	0.105577	H	-0.355184	6.495951	-1.042214
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				

Complete Reference 45

M. J. Frisch and G. W. Trucks and H. B. Schlegel and G. E. Scuseria and M. A. Robb and J. R. Cheeseman and G. Scalmani and V. Barone and B. Mennucci and G. A. Petersson and H. Nakatsuji and M. Caricato and X. Li and H. P. Hratchian and A. F. Izmaylov and J. Bloino and G. Zheng and J. L. Sonnenberg and M. Hada and M. Ehara and K. Toyota and R. Fukuda and J. Hasegawa and M. Ishida and T. Nakajima and Y. Honda and O. Kitao and H. Nakai and T. Vreven and Montgomery, Jr., J. A. and J. E. Peralta and F. Ogliaro and M. Bearpark and J. J. Heyd and E. Brothers and K. N. Kudin and V. N. Staroverov and R. Kobayashi and J. Normand and K. Raghavachari and A. Rendell and J. C. Burant and S. S. Iyengar and J. Tomasi and M. Cossi and N. Rega and J. M. Millam and M. Klene and J. E. Knox and J. B. Cross and V. Bakken and C. Adamo and J. Jaramillo and R. Gomperts and R. E. Stratmann and O. Yazyev and A. J. Austin and R. Cammi and C. Pomelli and J. W. Ochterski and R. L. Martin and K. Morokuma and V. G. Zakrzewski and G. A. Voth and P. Salvador and J. J. Dannenberg and S. Dapprich and A. D. Daniels and ĀŰ. Farkas and J. B. Foresman and J. V. Ortiz and J. Cioslowski and D. J. Fox, Gaussian 09 Revision A.2. Gaussian Inc. Wallingford CT 2009

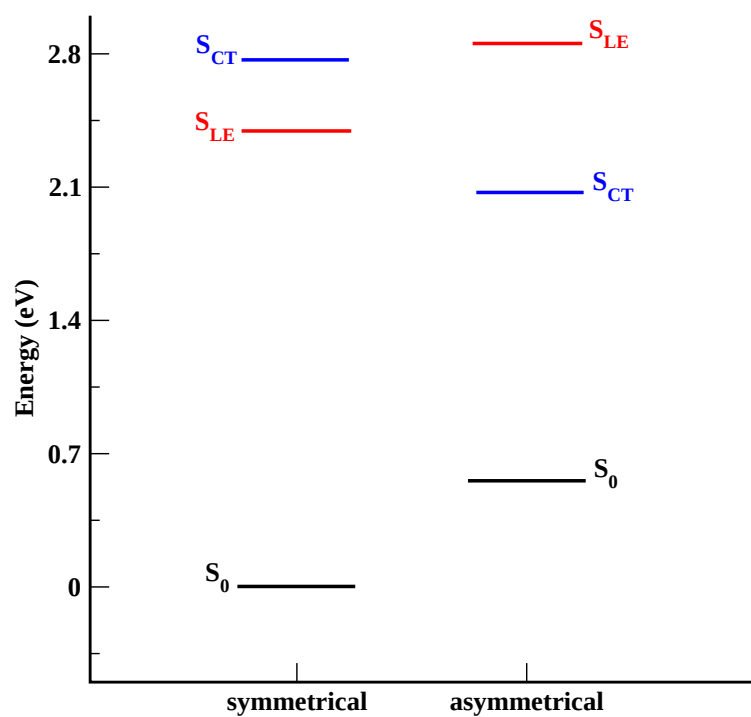


Figure 1: Energy levels (eV) of 5TMR and 5TMR_{asy} in ACN calculated at the TD-B3LYP-D/6-31G+(d,p)/CPCM level of theory.