Supporting Information for

Photo-deactivation pathways of a double H-bonded photochromic Schiff base investigated by combined theoretical calculations and experimental time-resolved studies

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Geometries and Energies of the Structures

In what follows the geometries of the structures discussed in the paper are presented. Each geometry is presented framed in a table as a list of lines, each specifying the atomic number and the (*x*,*y*,*z*)-coordinates in Ångstrom. We note that the atom sequence is not the same in each structure, but the order in which the corresponding program selected to present the structure.

Each table has a heading identifying the chemical structure by the abbreviation given in the text, and the program under which it renders this energy (GAUSSIAN or TURBOMOLE). As usual, an asterisk denotes a structure in the excited state. At the bottom, the absolute energy obtained is reproduced to 8 decimal figures.

When a single structure is given and two energies are reported this means:

1. If it is a CI candidate, the reported TDDFT energies of ground and excited states at that point, which ideally should be equal.
2. Otherwise, the structure has been optimized in the ground state with the program indicated in the header of the Table, and a point calculation has been done for the excited state (that is, this is a Franck-Condon excitation).

Energies in the paper for the ground state use as energy origin the minimum in S_0 obtained with Gaussian03. The energies appearing in the paper for the excited state structures are computed with Turbomole, using as energy origin the minimum in S_0 obtained with Turbomole to have a coherent set of data.

Stable Structures (Ground State):

E Optimized GAUSSIAN				MK Optimized GAUSSIAN			
6	7.035922	0.864888	-0.419105	6	-6.928077	1.221692	0.109977
6	5.637698	0.745952	-0.387905	6	-5.508018	0.964739	0.107522
6	5.045147	-0.348616	0.305044	6	-5.105934	-0.436031	-0.083041
6	5.883186	-1.283625	0.946158	6	-6.095148	-1.454086	-0.247208
6	7.262362	-1.158365	0.910169	6	-7.428639	-1.149265	-0.235008
6	7.831761	-0.075609	0.221039	6	-7.834443	0.208243	-0.053971
1	7.466464	1.705326	-0.952873	1	-7.239770	2.251788	0.248227
1	5.422965	-2.115556	1.474161	1	-5.764396	-2.481826	-0.384153
1	7.894450	-1.886552	1.407173	1	-8.176843	-1.924532	-0.360997
1	8.912210	0.031894	0.186448	1	-8.897231	0.438275	-0.046432
8	4.898355	1.671884	-1.012558	8	-4.656995	1.890450	0.261684
1	3.941790	1.424287	-0.875704	6	-3.748311	-0.767292	-0.098870
6	3.607871	-0.510602	0.359938	7	-2.797753	0.154129	0.054561
7	2.796848	0.326404	-0.203313	1	-3.446130	-1.803583	-0.232403
1	3.233117	-1.377176	0.919579	6	-1.407417	-0.017071	0.046526
6	1.406636	0.126319	-0.190679	6	-0.614386	1.090164	0.388564
6	0.582627	1.263662	-0.220638	6	0.770283	0.992718	0.400976
6	-0.800675	1.143744	-0.211057	6	1.406824	-0.216151	0.067115
6	-1.406654	-0.126035	-0.190636	6	0.605510	-1.326291	-0.248428
6	-0.582602	-1.263396	-0.220811	6	-0.778870	-1.231057	-0.275417
6	0.800665	-1.143485	-0.211268	1	-1.096621	2.023802	0.662926
1	1.050560	2.242543	-0.250233	1	1.359664	1.851275	0.706122
1	-1.415361	2.036913	-0.261184	1	1.093054	-2.263846	-0.495217
1	-1.050593	-2.242248	-0.250546	1	-1.360952	-2.103063	-0.552662
1	1.415374	-2.036626	-0.261574	7	2.799180	-0.393629	0.068880
7	-2.796825	-0.326189	-0.203238	6	3.607433	0.577444	-0.215567
6	-3.607949	0.510699	0.360074	6	5.045274	0.427479	-0.159206
6	-5.045189	0.348622	0.305025	6	5.878671	1.515999	-0.489258
6	-5.883376	1.283550	0.946081	6	7.258648	1.405722	-0.444191
6	-7.262526	1.158104	0.910068	6	7.833771	0.182573	-0.063487
6	-7.831778	0.075230	0.220991	6	7.042945	-0.910112	0.265541
6	-7.035803	-0.865179	-0.419102	6	5.643799	-0.807389	0.223451
6	-5.637592	-0.746034	-0.387915	1	5.413895	2.454687	-0.781602
1	-5.423278	2.115573	1.474046	1	7.887274	2.252128	-0.699442
1	-7.894721	1.886224	1.407037	1	8.915061	0.085517	-0.025098
1	-8.912214	-0.032413	0.186405	1	7.478300	-1.859014	0.559832
1	-7.466207	-1.705709	-0.952837	1	3.229311	1.558911	-0.528952
1	-3.233266	1.377277	0.919754	8	4.909139	-1.880588	0.544309
8	-4.898134	-1.671883	-1.012559	1	3.951583	-1.618843	0.451428
1	-3.941593	-1.424217	-0.875688	1	-3.236825	1.103748	0.190281
$E(S_0)$	$-1031.75257505\ E_h$			$E(S_0)$	$-1031.74456498\ E_h$		

DK Optimized GAUSSIAN				ER Optimized GAUSSIAN			
6	6.952356	1.153466	-0.003544	6	6.198565	0.704171	1.054777
6	5.527245	0.928986	-0.003703	6	4.854131	0.321923	0.926041
6	5.094043	-0.475422	0.002231	6	4.278003	0.221977	-0.372743
6	6.060960	-1.527749	0.007285	6	5.076076	0.514988	-1.497237
6	7.400944	-1.252699	0.006885	6	6.402385	0.891310	-1.360912
6	7.836526	0.107631	0.001421	6	6.957005	0.982778	-0.074351
1	7.286363	2.185807	-0.007616	1	6.618031	0.773352	2.052713
1	5.707965	-2.557195	0.011481	1	4.627830	0.437633	-2.485053
1	8.132229	-2.053871	0.010624	1	7.004751	1.112390	-2.235605
1	8.904267	0.313297	0.001277	1	7.996091	1.276836	0.043903
8	4.695964	1.885603	-0.008074	8	4.149131	0.062684	2.035184
6	3.729109	-0.774820	0.003213	1	3.227140	-0.183766	1.746039
7	2.801551	0.182837	-0.001376	6	2.897067	-0.173643	-0.551372
1	3.403318	-1.812598	0.008046	7	2.120904	-0.444630	0.448326
6	1.408416	0.051508	-0.001456	1	2.529964	-0.220705	-1.584677
6	0.644402	1.230219	-0.001546	6	0.801975	-0.886841	0.252991
6	-0.742210	1.184247	-0.001635	6	-0.155258	-0.548672	1.224768
6	-1.408424	-0.051505	-0.001418	6	-1.479476	-0.941932	1.092770
6	-0.644409	-1.230215	-0.001746	6	-1.887058	-1.723700	-0.008017
6	0.742204	-1.184244	-0.001868	6	-0.913982	-2.118937	-0.946673
1	1.151226	2.190494	-0.001585	6	0.404074	-1.690246	-0.830013
1	-1.294772	2.117020	-0.002274	1	0.158578	0.045854	2.076905
1	-1.151234	-2.190490	-0.001943	1	-2.208595	-0.665387	1.846902
1	1.294764	-2.117016	-0.002687	1	-1.211455	-2.775188	-1.758350
7	-2.801557	-0.182833	-0.001319	1	1.139631	-2.024031	-1.555182
6	-3.729111	0.774827	0.003360	7	-3.184274	-2.245119	-0.121508
6	-5.094045	0.475426	0.002460	6	-4.261624	-1.553593	-0.057219
6	-6.060969	1.527747	0.007277	6	-4.537061	-0.098574	-0.016021
6	-7.400952	1.252687	0.006776	6	-5.702958	0.279716	0.684201
6	-7.836522	-0.107646	0.001339	6	-6.114950	1.600011	0.780961
6	-6.952343	-1.153475	-0.003322	6	-5.369947	2.590780	0.130737
6	-5.527236	-0.928984	-0.002987	6	-4.237638	2.250717	-0.596085
1	-5.707982	2.557196	0.011303	6	-3.809967	0.917553	-0.684273
1	-8.132243	2.053854	0.010286	1	-6.282932	-0.502009	1.168622
1	-8.904262	-0.313320	0.001004	1	-7.007456	1.856629	1.341912
1	-7.286341	-2.185819	-0.007381	1	-5.679755	3.630383	0.183080
1	-3.403321	1.812606	0.008151	1	-3.656542	3.000277	-1.122608
8	-4.695941	-1.885591	-0.007447	1	-5.177390	-2.152796	-0.017626
1	3.267769	1.131068	-0.004802	8	-2.733295	0.706869	-1.479992
1	-3.267786	-1.131068	-0.004988	1	-2.357160	-0.176381	-1.344228
$E(S_0)$	-1031.73607915 E_h			$E(S_0)$	-1031.72711410 E_h		

MKR1 Optimized GAUSSIAN				MKR2 Optimized GAUSSIAN			
6	5.975409	-1.527579	-0.702757	6	7.401811	0.832312	0.251579
6	4.641668	-0.979090	-0.651347	6	5.966866	1.116308	0.278123
6	4.427038	0.106319	0.315906	6	5.079572	-0.055613	0.021115
6	5.502086	0.560490	1.140335	6	5.652432	-1.350673	-0.228178
6	6.746866	0.000856	1.046496	6	7.001771	-1.533147	-0.235660
6	6.970913	-1.053829	0.109756	6	7.879167	-0.417745	0.008982
1	6.148856	-2.329441	-1.412900	1	8.062319	1.673405	0.436141
1	5.309771	1.365487	1.847046	1	5.003775	-2.205394	-0.415756
1	7.561061	0.348802	1.673187	1	7.426140	-2.513770	-0.424945
1	7.964584	-1.490647	0.044035	1	8.952577	-0.591991	-0.003092
8	3.709175	-1.407723	-1.394300	8	5.521190	2.251564	0.498850
6	3.161878	0.689962	0.426800	6	3.728959	0.219727	0.045122
7	2.135588	0.290447	-0.323346	7	2.718694	-0.652653	-0.153106
1	2.996294	1.488765	1.146270	1	3.461890	1.252162	0.246548
6	0.822599	0.778523	-0.338593	6	1.336831	-0.393417	-0.136010
6	-0.110954	0.107678	-1.146154	6	0.462589	-1.463263	-0.381097
6	-1.431901	0.527375	-1.204919	6	-0.912902	-1.272739	-0.378341
6	-1.864711	1.643449	-0.460487	6	-1.458338	-0.001924	-0.126317
6	-0.913444	2.334773	0.315201	6	-0.574379	1.068486	0.088065
6	0.404549	1.900495	0.393819	6	0.801342	0.883163	0.097382
1	0.210324	-0.753108	-1.725297	1	0.866672	-2.450975	-0.590464
1	-2.138535	0.000926	-1.837247	1	-1.564704	-2.109649	-0.607072
1	-1.229590	3.222797	0.852863	1	-0.988879	2.055783	0.263668
1	1.104607	2.459354	1.005121	1	1.446455	1.734425	0.279109
7	-3.155408	2.179409	-0.573280	7	-2.835114	0.272091	-0.121522
6	-4.245273	1.510698	-0.473568	6	-3.702421	-0.614391	0.250379
6	-4.554658	0.119840	-0.070835	6	-5.127696	-0.369902	0.202306
6	-5.697074	-0.449671	-0.674053	6	-6.026583	-1.368405	0.630526
6	-6.135157	-1.729619	-0.371030	6	-7.396565	-1.167575	0.594853
6	-5.443412	-2.471441	0.593888	6	-7.894795	0.057805	0.123653
6	-4.337405	-1.929253	1.233224	6	-7.038156	1.063476	-0.303214
6	-3.883707	-0.639748	0.919089	6	-5.648534	0.868627	-0.271000
1	-6.235746	0.144294	-1.408278	1	-5.620966	-2.310338	0.992403
1	-7.007376	-2.142568	-0.866705	1	-8.075996	-1.945489	0.926451
1	-5.774886	-3.472068	0.855135	1	-8.967546	0.225845	0.091778
1	-3.798610	-2.479413	1.997246	1	-7.413618	2.013566	-0.667785
1	-5.142886	2.075955	-0.745264	1	-3.386872	-1.592788	0.635198
8	-2.838370	-0.197084	1.660022	8	-4.849984	1.860149	-0.687416
1	-2.447983	0.604064	1.279775	1	-3.910530	1.543892	-0.585742
1	2.440542	-0.495112	-0.958999	1	2.968738	-1.615116	-0.339112
$E(S_0)$	$-1031.71881902\ E_h$			$E(S_0)$	$-1031.72653511\ E_h$		

DKR1 Optimized GAUSSIAN				DKR2 Optimized GAUSSIAN			
6	-6.912668	1.334625	0.007502	6	-7.499612	-0.739260	-0.018782
6	-5.507005	1.009571	0.005524	6	-6.078116	-1.084247	-0.036909
6	-5.174924	-0.421958	-0.012719	6	-5.139399	0.075597	-0.003147
6	-6.213913	-1.402901	-0.031214	6	-5.654392	1.417376	0.045931
6	-7.530957	-1.033597	-0.028892	6	-6.994830	1.655235	0.059289
6	-7.868735	0.354247	-0.008820	6	-7.921086	0.552919	0.025065
1	-7.172718	2.387919	0.022064	1	-8.197109	-1.570303	-0.043333
1	-5.934828	-2.454717	-0.046173	1	-4.968026	2.262499	0.078226
1	-8.317349	-1.780645	-0.041867	1	-7.375785	2.670516	0.098112
1	-8.919154	0.635305	-0.006895	1	-8.986144	0.772327	0.036584
8	-4.609484	1.904006	0.017052	8	-5.682108	-2.258070	-0.078162
6	-3.834499	-0.816498	-0.016870	6	-3.802425	-0.257230	-0.021671
7	-2.841054	0.072242	-0.003710	7	-2.752033	0.590962	-0.016529
1	-3.582304	-1.874489	-0.039074	1	-3.581676	-1.319603	-0.051757
6	-1.461053	-0.163526	0.007969	6	-1.384718	0.264446	-0.004345
6	-0.606564	0.941997	-0.131301	6	-0.450831	1.300667	-0.151088
6	0.772868	0.789537	-0.133606	6	0.914413	1.047761	-0.150230
6	1.339272	-0.486077	0.012323	6	1.384718	-0.264443	0.004400
6	0.486920	-1.591649	0.154091	6	0.450830	-1.300664	0.151144
6	-0.892670	-1.438025	0.154322	6	-0.914413	-1.047758	0.150286
1	-1.035163	1.932403	-0.250405	1	-0.797117	2.323004	-0.279572
1	1.396808	1.666016	-0.260943	1	1.600178	1.875924	-0.282195
1	0.910424	-2.585214	0.277657	1	0.797116	-2.323001	0.279627
1	-1.515521	-2.316044	0.283434	1	-1.600179	-1.875921	0.282253
7	2.726298	-0.710691	0.019818	7	2.752032	-0.590960	0.016583
6	3.713283	0.210912	0.032796	6	3.802426	0.257231	0.021715
6	5.069869	-0.028458	0.001123	6	5.139399	-0.075599	0.003200
6	5.675132	-1.330629	-0.079595	6	5.654391	-1.417380	-0.045848
6	7.028476	-1.475913	-0.107403	6	6.994828	-1.655240	-0.059251
6	7.877912	-0.313833	-0.055978	6	7.921085	-0.552922	-0.025151
6	7.369647	0.945156	0.018244	6	7.499612	0.739259	0.018663
6	5.927872	1.191837	0.053494	6	6.078118	1.084242	0.036972
1	5.047991	-2.220092	-0.126779	1	4.968023	-2.262503	-0.078099
1	7.477509	-2.461700	-0.171435	1	7.375781	-2.670522	-0.098064
1	8.955304	-0.459727	-0.079503	1	8.986142	-0.772327	-0.036756
1	8.008866	1.821346	0.055743	1	8.197111	1.570305	0.043082
1	3.417680	1.254193	0.081980	1	3.581679	1.319604	0.051792
8	5.453443	2.334443	0.122714	8	5.682111	2.258076	0.077938
1	-3.238109	1.051926	0.000647	1	-2.955131	1.581833	-0.033175
1	3.002611	-1.683822	0.024729	1	2.955130	-1.581831	0.033239
$E(S_0)$	-1031.71767403 E_h			$E(S_0)$	-1031.70011001 E_h		

Stable Structures (Excited State):

E Optimized TURBOMOLE				E* Optimized TURBOMOLE			
6	7.037615	0.864544	-0.509497	6	6.947338	1.158574	-0.318179
6	5.638589	0.746567	-0.475750	6	5.564150	0.923417	-0.239281
6	5.046679	-0.347647	0.219335	6	5.061415	-0.430556	-0.253380
6	5.885183	-1.283452	0.859977	6	6.001248	-1.484034	-0.349769
6	7.265073	-1.159288	0.821120	6	7.362405	-1.234081	-0.429496
6	7.834230	-0.076894	0.129755	6	7.834865	0.094430	-0.414451
1	7.468111	1.704556	-1.044921	1	7.289469	2.188435	-0.304121
1	5.424966	-2.115034	1.389519	1	5.632162	-2.506880	-0.360062
1	7.897962	-1.887903	1.317516	1	8.064293	-2.059413	-0.501882
1	8.915208	0.029242	0.092365	1	8.901858	0.289046	-0.477364
8	4.897793	1.672039	-1.099473	8	4.736349	1.962423	-0.149575
1	3.941307	1.423238	-0.960524	1	3.799379	1.578314	-0.091834
6	3.608800	-0.508500	0.275465	6	3.659045	-0.702439	-0.170047
7	2.797685	0.328645	-0.288851	7	2.777348	0.285507	-0.066390
1	3.233262	-1.374135	0.836819	1	3.352929	-1.751341	-0.171947
6	1.407235	0.127728	-0.276467	6	1.423811	0.097743	-0.060307
6	0.581498	1.264708	-0.306321	6	0.609148	1.232084	0.226770
6	-0.802295	1.143172	-0.296888	6	-0.762069	1.148913	0.276436
6	-1.407235	-0.127728	-0.276467	6	-1.425779	-0.096349	0.029481
6	-0.581498	-1.264708	-0.306321	6	-0.612832	-1.222002	-0.294870
6	0.802295	-1.143172	-0.296888	6	0.758724	-1.140670	-0.336570
1	1.048727	2.244468	-0.335796	1	1.111056	2.177575	0.412077
1	-1.418010	2.036247	-0.347382	1	-1.340108	2.043426	0.482188
1	-1.048727	-2.244468	-0.335796	1	-1.115981	-2.161441	-0.505838
1	1.418010	-2.036247	-0.347382	1	1.333594	-2.021002	-0.603157
7	-2.797685	-0.328645	-0.288851	7	-2.778004	-0.289418	0.061213
6	-3.608800	0.508500	0.275465	6	-3.642504	0.619357	0.498948
6	-5.046679	0.347647	0.219335	6	-5.052666	0.389911	0.422592
6	-5.885183	1.283452	0.859977	6	-5.972717	1.352071	0.902918
6	-7.265073	1.159288	0.821120	6	-7.341022	1.141158	0.835373
6	-7.834230	0.076894	0.129755	6	-7.841154	-0.054448	0.279820
6	-7.037615	-0.864544	-0.509497	6	-6.973667	-1.027299	-0.200331
6	-5.638589	-0.746567	-0.475750	6	-5.583895	-0.828667	-0.142817
1	-5.424966	2.115034	1.389519	1	-5.582226	2.272002	1.331779
1	-7.897962	1.887903	1.317516	1	-8.027399	1.894075	1.210906
1	-8.915208	-0.029242	0.092365	1	-8.913856	-0.218154	0.227194
1	-7.468111	-1.704556	-1.044921	1	-7.337370	-1.954948	-0.630587
1	-3.233262	1.374135	0.836819	1	-3.312878	1.557307	0.952898
8	-4.897793	-1.672039	-1.099473	6	-4.775742	-1.777184	-0.612484
1	-3.941307	-1.423238	-0.960524	1	-3.828714	-1.445443	-0.465857
E(S_0) E(S_1)	-1031.11748921 E_h -1031.00104426 E_h			E(S_1)	-1031.01120014 E_h		

MK Optimized TURBOMOLE				MK* Optimized TURBOMOLE			
6	-6.927566	1.223234	0.144415	6	-6.969390	1.205612	0.093754
6	-5.507373	0.963550	0.139566	6	-5.552277	0.948064	0.083474
6	-5.107850	-0.437907	-0.053499	6	-5.145669	-0.447398	-0.010167
6	-6.099146	-1.454418	-0.218615	6	-6.100818	-1.443244	-0.081597
6	-7.432864	-1.147199	-0.204264	6	-7.496051	-1.149777	-0.067561
6	-7.836504	0.211341	-0.020185	6	-7.911018	0.173520	0.019701
1	-7.237114	2.254104	0.284956	1	-7.273949	2.244965	0.162511
1	-5.770248	-2.482940	-0.357635	1	-5.785412	-2.482535	-0.150724
1	-8.182905	-1.921380	-0.330555	1	-8.214794	-1.959734	-0.125284
1	-8.899379	0.443240	-0.010742	1	-8.970728	0.411264	0.030898
8	-4.654022	1.887726	0.294089	8	-4.703487	1.891524	0.152785
6	-3.749827	-0.770739	-0.069225	6	-3.732819	-0.805655	-0.030079
7	-2.799150	0.150942	0.085786	7	-2.798916	0.102476	0.036039
1	-3.447778	-1.807301	-0.203757	1	-3.447743	-1.851650	-0.101981
6	-1.408399	-0.019982	0.081722	6	-1.395844	-0.032887	0.026728
6	-0.616526	1.088972	0.423755	6	-0.630186	1.139339	0.137202
6	0.768815	0.992571	0.439661	6	0.752749	1.085402	0.132582
6	1.407427	-0.217091	0.109581	6	1.435949	-0.160076	0.008901
6	0.607146	-1.329017	-0.205469	6	0.633357	-1.331956	-0.087010
6	-0.777932	-1.234991	-0.235578	6	-0.745108	-1.280740	-0.082589
1	-1.100208	2.023358	0.694643	1	-1.134034	2.098689	0.235067
1	1.357040	1.852869	0.743973	1	1.311086	2.007608	0.245129
1	1.096158	-2.267040	-0.449657	1	1.144417	-2.285753	-0.174084
1	-1.358970	-2.108673	-0.511465	1	-1.309441	-2.204841	-0.166779
6	2.800377	-0.392995	0.111019	6	2.796022	-0.331178	-0.012538
6	3.607882	0.579229	-0.174153	6	3.652258	0.681655	-0.092588
6	5.046530	0.429324	-0.122447	6	5.066268	0.476131	-0.058125
6	5.879664	1.518037	-0.455232	6	5.958118	1.574896	-0.156049
6	7.260403	1.406559	-0.415291	6	7.332017	1.401509	-0.123260
6	7.836373	0.182198	-0.036846	6	7.864047	0.107722	0.009430
6	7.045570	-0.910476	0.295001	6	7.020203	-0.997349	0.106655
6	5.645584	-0.806815	0.257598	6	5.629911	-0.837241	0.074904
1	5.414418	2.457722	-0.745320	1	5.535684	2.572495	-0.257839
1	7.889124	2.252883	-0.672564	1	7.993144	2.259868	-0.199146
1	8.918222	0.084197	-0.002939	1	8.940762	-0.036867	0.036000
1	7.481405	-1.860239	0.587505	1	7.414499	-2.003817	0.208434
1	3.228338	1.560950	-0.486043	1	3.310644	1.714192	-0.212157
8	4.910473	-1.879222	0.579918	8	4.846323	-1.924016	0.167743
1	3.952822	-1.615873	0.487894	1	3.899487	-1.593203	0.119078
1	-3.240010	1.101290	0.220397	1	-3.219263	1.062984	0.102543
E(S_0)	-1031.10941466 E_h						
E(S_1)	-1031.00802837 E_h			E(S_1)	-1031.01727473 E_h		

DK* Optimized TURBOMOLE				ER Optimized TURBOMOLE			
6	6.989175	1.160213	0.019326	6	6.206425	0.631281	1.093855
6	5.564855	0.930288	0.012772	6	4.864672	0.236959	0.965073
6	5.127706	-0.461465	-0.005741	6	4.286167	0.143135	-0.333826
6	6.061875	-1.482222	-0.016941	6	5.078140	0.454796	-1.458293
6	7.456208	-1.213920	-0.010757	6	6.401324	0.844120	-1.321638
6	7.901827	0.107634	0.007486	6	6.958970	0.928887	-0.035116
1	7.314639	2.195190	0.033454	1	6.628136	0.695351	2.091748
1	5.725183	-2.516649	-0.030634	1	4.627628	0.382910	-2.445982
1	8.160870	-2.038063	-0.020126	1	6.998940	1.081112	-2.195988
1	8.967115	0.318673	0.012600	1	7.995855	1.232512	0.082930
8	4.736998	1.890765	0.022517	8	4.164049	-0.038656	2.072910
6	3.710257	-0.787653	-0.011611	1	3.242233	-0.286448	1.782309
7	2.793733	0.134443	0.001475	6	2.906734	-0.260392	-0.510653
1	3.405908	-1.830884	-0.027039	7	2.135097	-0.540001	0.490825
6	1.382198	0.019244	0.001645	1	2.535246	-0.303276	-1.543037
6	0.636535	1.205354	-0.005426	6	0.815354	-0.981879	0.297734
6	-0.748507	1.175561	-0.007169	6	-0.141991	-0.636884	1.268120
6	-1.440140	-0.066783	-0.001151	6	-1.468255	-1.025280	1.135567
6	-0.663038	-1.260520	0.007463	6	-1.877763	-1.809834	0.036624
6	0.714730	-1.222522	0.008886	6	-0.904610	-2.212722	-0.899738
1	1.151931	2.163276	-0.010447	6	0.415505	-1.788034	-0.783407
1	-1.296698	2.109603	-0.012491	1	0.173132	-0.039641	2.118415
1	-1.179733	-2.215514	0.014136	1	-2.197935	-0.742179	1.887292
1	1.264123	-2.159288	0.018156	1	-1.204002	-2.870634	-1.709924
6	-2.795227	-0.180091	-0.001956	1	1.150892	-2.126910	-1.507037
6	-3.736834	0.819268	-0.008746	7	-3.177539	-2.324726	-0.078069
6	-5.096535	0.503497	-0.004762	6	-4.252390	-1.628283	-0.016617
6	-6.083343	1.537965	-0.011738	6	-4.520515	-0.171294	0.021881
6	-7.428491	1.249058	-0.007106	6	-5.685435	0.214134	0.721085
6	-7.856819	-0.105250	0.004765	6	-6.090263	1.537502	0.816514
6	-6.945922	-1.142049	0.011572	6	-5.338589	2.524105	0.165981
6	-5.531971	-0.909033	0.007118	6	-4.206982	2.176654	-0.559618
1	-5.744447	2.572874	-0.020708	6	-3.786340	0.840378	-0.646580
1	-8.162094	2.050243	-0.012397	1	-6.270214	-0.564286	1.206031
1	-8.922018	-0.325623	0.008514	1	-6.982212	1.799716	1.376694
1	-7.266818	-2.179627	0.020601	1	-5.642550	3.565995	0.217400
1	-3.404021	1.851938	-0.017433	1	-3.620767	2.922737	-1.086371
8	-4.689562	-1.870760	0.013160	1	-5.171498	-2.223244	0.022607
1	3.223207	1.090459	0.013364	8	-2.709673	0.622708	-1.440562
1	-3.296855	-1.117630	0.005367	1	-2.334978	-0.260387	-1.299139

DK*		ER	
		$E(S_0)$	$-1031.09195084\ E_h$
$E(S_1)$	$-1031.01158215\ E_h$	$E(S_1)$	$-1030.92083027\ E_h$

MKR1
Optimized TURBOMOLE

6	5.971685	-1.503617	-0.743236
6	4.638816	-0.951370	-0.692927
6	4.424216	0.129435	0.280130
6	5.498320	0.576636	1.110671
6	6.742752	0.014332	1.016953
6	6.966826	-1.036530	0.074781
1	6.144940	-2.302754	-1.457095
1	5.305841	1.378367	1.821519
1	7.556595	0.357096	1.647755
1	7.960026	-1.475663	0.009431
8	3.706886	-1.373093	-1.441379
6	3.159095	0.715139	0.390181
7	2.134957	0.321453	-0.367088
1	2.991798	1.510119	1.113876
6	0.822112	0.811105	-0.383112
6	-0.111791	0.143482	-1.194081
6	-1.433094	0.564096	-1.251769
6	-1.865339	1.678873	-0.504262
6	-0.913630	2.367981	0.273809
6	0.404578	1.932053	0.352040
1	0.209440	-0.716041	-1.776051
1	-2.140695	0.039589	-1.885502
1	-1.229526	3.255214	0.813942
1	1.104875	2.488776	0.965867
6	-3.157272	2.212914	-0.613600
6	-4.245648	1.541580	-0.510421
6	-4.547175	0.148668	-0.106181
6	-5.683187	-0.431535	-0.712743
6	-6.110870	-1.715743	-0.409200
6	-5.416055	-2.449979	0.560394
6	-4.316613	-1.896604	1.203190
6	-3.872115	-0.603551	0.887652
1	-6.224765	0.156888	-1.449820
1	-6.977530	-2.137905	-0.907827
1	-5.739883	-3.453367	0.822568
1	-3.775912	-2.440443	1.970891
1	-5.146559	2.104271	-0.779270
8	-2.832397	-0.150091	1.630119
1	-2.446607	0.651521	1.246586
1	2.442904	-0.461303	-1.006789

E(S_0)	-1031.08357418 E_h
E(S_1)	-1030.97936330 E_h

MKR2 Optimized TURBOMOLE				MKR2* Optimized TURBOMOLE			
6	7.443967	1.009556	0.250304	6	-7.327862	-0.688889	1.253024
6	6.008776	1.297219	0.252821	6	-5.878049	-0.781504	1.306695
6	5.122064	0.121981	0.006456	6	-5.129940	-0.149656	0.207604
6	5.695192	-1.178844	-0.213761	6	-5.810391	0.491826	-0.817486
6	7.044733	-1.364171	-0.201351	6	-7.215725	0.551439	-0.821829
6	7.921972	-0.246005	0.035511	6	-7.962492	-0.039786	0.215300
1	8.104090	1.852851	0.428709	1	-7.875163	-1.154043	2.065101
1	5.046531	-2.035783	-0.393615	1	-5.276874	0.959089	-1.640358
1	7.469480	-2.349161	-0.368362	1	-7.723792	1.057893	-1.634435
1	8.995523	-0.422829	0.040726	1	-9.045817	0.019350	0.190835
8	5.562614	2.437499	0.446576	8	-5.292465	-1.367702	2.238866
6	3.771143	0.399498	0.014233	6	-3.687144	-0.265536	0.300710
7	2.761070	-0.475392	-0.178900	7	-2.818600	0.223488	-0.512810
1	3.503786	1.435895	0.196840	1	-3.298103	-0.823476	1.149473
6	1.378673	-0.216505	-0.165279	6	-1.367313	0.074417	-0.390729
6	0.505000	-1.286906	-0.413964	6	-0.623544	1.063117	0.257704
6	-0.871290	-1.097849	-0.410475	6	0.757713	0.966127	0.310259
6	-1.418393	0.172186	-0.154454	6	1.459905	-0.124675	-0.307872
6	-0.534824	1.243545	0.061529	6	0.647603	-1.093848	-0.980019
6	0.841745	1.059675	0.070279	6	-0.727422	-1.001287	-1.032859
1	0.910228	-2.274001	-0.626093	1	-1.124225	1.908553	0.725143
1	-1.522147	-1.935512	-0.641386	1	1.310369	1.745520	0.820690
1	-0.950524	2.230150	0.240800	1	1.154509	-1.928106	-1.454799
1	1.486070	1.911403	0.255359	1	-1.307325	-1.756751	-1.557351
7	-2.795731	0.444560	-0.141950	7	2.799827	-0.305293	-0.321168
6	-3.661516	-0.446257	0.225376	6	3.657929	0.501109	0.347853
6	-5.087257	-0.199343	0.191227	6	5.064998	0.328938	0.255883
6	-5.985189	-1.202402	0.612711	6	5.958068	1.171638	0.973366
6	-7.355467	-0.996856	0.592745	6	7.334684	1.023898	0.891560
6	-7.854576	0.237713	0.144732	6	7.881961	0.017680	0.081519
6	-6.998591	1.247652	-0.275481	6	7.037124	-0.833326	-0.638752
6	-5.608601	1.048248	-0.259294	6	5.649933	-0.698633	-0.566809
1	-5.578923	-2.151317	0.956520	1	5.531019	1.952331	1.600397
1	-8.034686	-1.777985	0.918737	1	7.985924	1.687547	1.454543
1	-8.927570	0.409441	0.126109	1	8.959144	-0.104933	0.010925
1	-7.374830	2.204701	-0.621907	1	7.436451	-1.621061	-1.271075
1	-3.343769	-1.429547	0.596698	1	3.300756	1.298205	1.004090
8	-4.809850	2.042812	-0.667740	8	4.870073	-1.542180	-1.274636
1	-3.870612	1.720371	-0.577938	1	3.920097	-1.272586	-1.071744
1	3.011688	-1.440294	-0.353046	1	-3.163553	0.753735	-1.312910
$E(S_0)$ $E(S_1)$	-1031.09134748 E_h -1030.99046611 E_h			$E(S_1)$	-1031.00610148 E_h		

DKR1 Optimized TURBOMOLE				DKR2 Optimized TURBOMOLE			
6	-6.872557	1.520565	-0.004393	6	-7.502842	-0.740202	-0.020468
6	-5.467309	1.190777	-0.002290	6	-6.080518	-1.084712	-0.035912
6	-5.139546	-0.242263	0.005039	6	-5.142352	0.076214	-0.001382
6	-6.181693	-1.220792	0.007120	6	-5.658107	1.418376	0.046061
6	-7.498340	-0.847099	0.004854	6	-6.999355	1.655703	0.057234
6	-7.832215	0.542595	-0.000697	6	-7.925537	0.552326	0.022163
1	-7.129161	2.575180	-0.009227	1	-8.199953	-1.572097	-0.046209
1	-5.905868	-2.274092	0.011443	1	-4.971850	2.264190	0.078737
1	-8.287458	-1.592131	0.007235	1	-7.381124	2.671193	0.094673
1	-8.882255	0.826693	-0.002287	1	-8.991199	0.771277	0.031884
8	-4.566307	2.082610	-0.008026	8	-5.683746	-2.258666	-0.075752
6	-3.799244	-0.640047	0.005233	6	-3.804680	-0.256860	-0.017889
7	-2.804526	0.248168	0.000511	7	-2.753522	0.591648	-0.011965
1	-3.549358	-1.699186	0.003029	1	-3.584904	-1.320005	-0.046585
6	-1.424346	0.011450	0.007609	6	-1.385646	0.264871	-0.001288
6	-0.569423	1.118770	-0.121132	6	-0.451446	1.302414	-0.143138
6	0.810636	0.966364	-0.127367	6	0.914607	1.050070	-0.143515
6	1.377400	-0.311213	0.003857	6	1.385643	-0.263423	0.003888
6	0.524687	-1.418880	0.133479	6	0.451444	-1.300928	0.145985
6	-0.855540	-1.265341	0.137284	6	-0.914601	-1.048567	0.146550
1	-0.998437	2.110816	-0.227801	1	-0.797930	2.325750	-0.266350
1	1.434347	1.844795	-0.245640	1	1.600145	1.879876	-0.270125
1	0.948775	-2.414268	0.243402	1	0.797922	-2.324291	0.269008
1	-1.478011	-2.145913	0.253626	1	-1.600149	-1.878280	0.273758
7	2.765006	-0.535820	0.008746	7	2.753447	-0.590460	0.013764
6	3.751291	0.387268	0.034279	6	3.804966	0.257603	0.016406
6	5.109118	0.151051	0.007227	6	5.142446	-0.076241	-0.000138
6	5.718624	-1.149231	-0.079263	6	5.657399	-1.418861	-0.043199
6	7.073205	-1.290458	-0.099621	6	6.998501	-1.657028	-0.054121
6	7.919517	-0.125899	-0.035054	6	7.925350	-0.554088	-0.022991
6	7.406787	1.131546	0.044825	6	7.503430	0.738831	0.015312
6	5.963433	1.373923	0.073563	6	6.081310	1.084250	0.029792
1	5.094195	-2.040525	-0.135804	1	4.970635	-2.264390	-0.072441
1	7.525770	-2.274945	-0.167368	1	7.379651	-2.672861	-0.088493
1	8.997931	-0.268882	-0.052964	1	8.990880	-0.773707	-0.032237
1	8.043193	2.009804	0.092167	1	8.201044	1.570392	0.038012
1	3.453921	1.430074	0.091359	1	3.585762	1.320935	0.041976
8	5.485249	2.514869	0.148822	8	5.685260	2.258586	0.065215
1	-3.202825	1.228900	-0.010091	1	-2.956605	1.582888	-0.027730
1	3.041334	-1.509228	0.004320	1	2.956224	-1.581727	0.031511
$E(S_0)$	-1031.08243072 E_h			$E(S_0)$	-1031.06480619 E_h		
$E(S_1)$	-1031.13341903 E_h			$E(S_1)$	-1031.11714720 E_h		

Possible Degeneracy Points ("Conical Intersections"):

CI E↔ER TURBOMOLE				CI MK↔MKR1 TURBOMOLE			
6	-6.347102	1.134666	1.005702	6	-6.512668	0.586872	-0.404304
6	-5.025080	0.927391	0.579264	6	-5.086919	0.350227	-0.464042
6	-4.639996	-0.359026	0.082013	6	-4.659072	-1.051801	-0.642830
6	-5.604005	-1.396102	0.055150	6	-5.639776	-2.085938	-0.743583
6	-6.897802	-1.182148	0.490389	6	-6.976908	-1.798058	-0.679904
6	-7.264061	0.094565	0.960188	6	-7.406392	-0.443231	-0.508406
1	-6.619195	2.118253	1.373575	1	-6.833312	1.615131	-0.273118
1	-5.306440	-2.371005	-0.323556	1	-5.301227	-3.111557	-0.873834
1	-7.624394	-1.987616	0.471928	1	-7.716508	-2.588557	-0.757837
1	-8.282126	0.270762	1.296288	1	-8.472618	-0.235028	-0.459183
8	-4.153991	1.934693	0.674882	8	-4.248724	1.289604	-0.367677
1	-3.270082	1.588556	0.367210	6	-3.297804	-1.368654	-0.698857
6	-3.318732	-0.597517	-0.421856	7	-2.347179	-0.428458	-0.596413
7	-2.341421	0.258932	-0.222730	1	-2.985214	-2.402331	-0.817201
1	-3.123246	-1.598768	-0.819812	6	-0.975095	-0.568621	-0.626375
6	-1.049313	0.050797	-0.638662	6	-0.184904	0.577790	-0.332881
6	-0.109137	1.075949	-0.312967	6	1.183051	0.507753	-0.298867
6	1.208534	0.981895	-0.661320	6	1.883087	-0.727868	-0.597045
6	1.703422	-0.172078	-1.391535	6	1.046313	-1.875184	-0.901010
6	0.728451	-1.202099	-1.719982	6	-0.319758	-1.796552	-0.920934
6	-0.581257	-1.096127	-1.357475	1	-0.688846	1.516182	-0.115715
1	-0.476394	1.944410	0.225188	1	1.768234	1.392339	-0.078482
1	1.894840	1.773991	-0.391336	1	1.550991	-2.802112	-1.150319
1	1.082971	-2.064138	-2.274605	1	-0.896809	-2.676243	-1.188441
1	-1.264705	-1.893515	-1.629374	7	3.188035	-0.880895	-0.656930
7	2.926486	-0.350014	-1.805479	6	4.118285	0.154600	-0.699993
6	3.946746	0.515696	-1.350956	6	4.792702	0.813710	0.332690
6	4.740683	0.312436	-0.214331	6	5.754341	1.826138	-0.001391
6	5.690071	1.310302	0.185267	6	6.370165	2.586942	0.971089
6	6.458551	1.171305	1.324717	6	6.064066	2.378419	2.327924
6	6.324475	0.026097	2.130474	6	5.155437	1.381004	2.697268
6	5.427140	-0.981486	1.764812	6	4.543325	0.589506	1.733953
6	4.653197	-0.865294	0.614743	1	5.982055	1.987858	-1.052132
1	5.790066	2.196981	-0.435177	1	7.091429	3.348452	0.688534
1	7.165734	1.948596	1.598952	1	6.540070	2.981200	3.094491
1	6.918017	-0.081400	3.033018	1	4.907211	1.202556	3.738409
1	5.321991	-1.884803	2.357367	1	4.347517	0.494055	-1.714365
1	4.202646	1.369284	-1.976571	8	3.679744	-0.380426	2.142307
8	3.876454	-1.926460	0.261793	1	3.378280	-0.875724	1.363545
1	3.446590	-1.720460	-0.588968	1	-2.794604	0.516899	-0.468140
$E(S_0)$	-1031.03501872 E_h			$E(S_0)$	-1031.03413797 E_h		
$E(S_1)$	-1031.03017321 E_h			$E(S_1)$	-1031.02955865 E_h		

CI MK↔MKR2 TURBOMOLE				CI DK↔DKR1 TURBOMOLE			
6	-6.507228	2.782405	1.795878	6	6.777589	-2.157509	1.616635
6	-5.091733	2.474476	1.807022	6	5.528528	-1.422362	1.625385
6	-4.790715	1.055033	1.661638	6	4.340288	-2.291092	1.669740
6	-5.778722	0.079006	1.531207	6	4.433056	-3.691099	1.687767
6	-7.128944	0.443473	1.527763	6	5.671574	-4.327710	1.670076
6	-7.472974	1.803888	1.663486	6	6.838541	-3.536078	1.637355
1	-6.770252	3.832267	1.888362	1	7.679772	-1.552726	1.594487
1	-5.492877	-0.967159	1.434856	1	3.517639	-4.280586	1.717479
1	-7.901758	-0.309214	1.411501	1	5.739217	-5.410820	1.682333
1	-8.524177	2.083289	1.661632	1	7.809061	-4.029044	1.627085
8	-4.176828	3.328615	1.934044	8	5.447617	-0.172011	1.572765
6	-3.365443	0.708588	1.699289	6	3.048008	-1.626029	1.727045
7	-2.649674	0.675264	0.619262	7	2.419418	-1.284021	0.624031
1	-2.852664	0.463502	2.630216	1	2.572206	-1.359278	2.670677
6	-1.268939	0.353330	0.425703	6	1.181060	-0.632628	0.435000
6	-0.740643	0.557337	-0.859680	6	0.756565	-0.401476	-0.881545
6	0.583201	0.254344	-1.124724	6	-0.450393	0.229442	-1.142797
6	1.417316	-0.273004	-0.100392	6	-1.267583	0.648259	-0.076516
6	0.865885	-0.444259	1.197005	6	-0.834432	0.415020	1.242653
6	-0.456377	-0.151981	1.463929	6	0.371845	-0.215643	1.502746
1	-1.371581	0.971816	-1.642922	1	1.382558	-0.719053	-1.711507
1	0.991966	0.451067	-2.109781	1	-0.745293	0.391646	-2.172400
1	1.507944	-0.832672	1.980637	1	-1.453861	0.735646	2.076468
1	-0.848570	-0.314219	2.462028	1	0.672106	-0.372769	2.532413
7	2.757101	-0.589495	-0.281779	7	-2.495727	1.287213	-0.264414
6	3.211407	-1.011344	-1.434766	6	-3.096369	1.604688	-1.438355
6	4.606662	-1.239823	-1.671519	6	-4.308641	2.234993	-1.598710
6	5.022634	-1.707776	-2.933650	6	-5.162644	2.674050	-0.525664
6	6.387806	-1.951440	-3.199673	6	-6.348916	3.291035	-0.782216
6	7.341673	-1.718241	-2.176651	6	-6.768455	3.514626	-2.143678
6	6.968513	-1.260091	-0.927394	6	-6.009543	3.124950	-3.202681
6	5.587443	-1.011548	-0.649609	6	-4.721452	2.455119	-3.019136
1	4.271750	-1.872234	-3.701891	1	-4.863224	2.515011	0.509879
1	6.703822	-2.309524	-4.172820	1	-6.987659	3.619482	0.031741
1	8.394635	-1.900545	-2.376757	1	-7.721228	4.010342	-2.316030
1	7.695163	-1.082332	-0.142201	1	-6.323684	3.292639	-4.228159
1	2.526730	-1.246286	-2.259520	1	-2.576003	1.338886	-2.353121
8	5.256921	-0.583675	0.584386	8	-4.020389	2.094052	-3.974415
1	4.269090	-0.480254	0.598001	1	2.951652	-1.533350	-0.208855
1	-3.177561	0.939413	-0.212116	1	-2.982805	1.538184	0.586440
$E(S_0)$	-1031.03150361 E_h			$E(S_0)$	-1031.00654820 E_h		
$E(S_1)$	-1031.03098295 E_h			$E(S_1)$	-1031.00469789 E_h		

CI DKR1↔DKR2 TURBOMOLE			
6	-7.438535	-0.999500	0.019078
6	-6.008867	-1.304540	-0.041893
6	-5.103738	-0.114825	-0.010096
6	-5.652123	1.212198	0.072261
6	-6.998015	1.409463	0.121783
6	-7.894413	0.281227	0.094461
1	-8.115121	-1.848132	0.000590
1	-4.986622	2.074929	0.100960
1	-7.405505	2.413643	0.185130
1	-8.965200	0.468406	0.136408
8	-5.579287	-2.470128	-0.116694
6	-3.761352	-0.393022	-0.064322
7	-2.766235	0.525744	-0.079720
1	-3.482141	-1.441473	-0.104553
6	-1.389159	0.293195	-0.092503
6	-0.528937	1.397017	-0.244675
6	0.847796	1.238069	-0.264683
6	1.400640	-0.045388	-0.143541
6	0.550976	-1.148539	0.014460
6	-0.826977	-0.990088	0.040260
1	-0.951025	2.391708	-0.359960
1	1.478299	2.113357	-0.374570
1	0.972736	-2.143014	0.136884
1	-1.451714	-1.864341	0.174628
7	2.793344	-0.282202	-0.160651
6	3.802233	0.570087	-0.195368
6	5.175898	0.135276	-0.076062
6	5.987560	-0.095201	-1.199759
6	7.323592	-0.434141	-1.048292
6	7.851420	-0.576947	0.261011
6	7.070253	-0.403992	1.378735
6	5.673896	-0.013262	1.303482
1	5.560115	-0.015168	-2.198933
1	7.962923	-0.555927	-1.916530
1	8.907325	-0.812492	0.377616
1	7.459937	-0.569211	2.379884
1	3.544463	1.626517	-0.191819
8	4.940636	0.131312	2.305778
1	-3.067728	1.500914	-0.103683
1	3.068652	-1.261527	-0.115101
$E(S_0)$ $E(S_1)$	-1031.00573372 E_h -1031.00325583 E_h		

Maxima on the Proton-Transfer Coordinates:

Transition State Structure E→MK Optimized GAUSSIAN				Transition State Structure E*→MK* Optimized TURBOMOLE			
6	-6.852665	-1.166304	-0.385161	6	6.842840	1.255550	-0.055444
6	-5.460374	-0.865815	-0.308024	6	5.469466	0.890201	-0.080769
6	-5.090766	0.427824	0.237742	6	5.096028	-0.488879	-0.330120
6	-6.092201	1.333773	0.673725	6	6.108622	-1.411784	-0.538354
6	-7.424564	1.006004	0.581616	6	7.471699	-1.031595	-0.509993
6	-7.792070	-0.255610	0.045957	6	7.830887	0.299384	-0.268234
1	-7.137073	-2.130517	-0.793004	1	7.081098	2.296861	0.134796
1	-5.785687	2.295226	1.080673	1	5.850183	-2.450936	-0.727045
1	-8.190246	1.699372	0.912692	1	8.237442	-1.782539	-0.677162
1	-8.846810	-0.509338	-0.024726	1	8.877610	0.585834	-0.246880
8	-4.556097	-1.701179	-0.700995	8	4.544136	1.790613	0.119476
1	-3.437905	-1.067709	-0.459366	1	3.566197	1.209867	0.042226
6	-3.714359	0.743783	0.327467	6	3.684016	-0.855633	-0.350417
7	-2.818008	-0.130491	-0.083520	7	2.793223	0.087848	-0.142282
1	-3.400483	1.700180	0.748196	1	3.411779	-1.894537	-0.533091
6	-1.426604	0.034027	-0.089735	6	1.422771	-0.049758	-0.115584
6	-0.637271	-1.116124	-0.252287	6	0.652676	1.113266	0.135387
6	0.748423	-1.029810	-0.268192	6	-0.724163	1.069420	0.189919
6	1.389232	0.213484	-0.119723	6	-1.423229	-0.160894	-0.003667
6	0.593937	1.366156	-0.000615	6	-0.640424	-1.320594	-0.271846
6	-0.791006	1.282961	0.021009	6	0.734164	-1.278714	-0.324745
1	-1.126671	-2.078104	-0.369874	1	1.173626	2.056125	0.282727
1	1.336025	-1.927997	-0.428581	1	-1.271790	1.988350	0.367983
1	1.086837	2.329853	0.077455	1	-1.168020	-2.256893	-0.428443
1	-1.375068	2.194248	0.095096	1	1.284415	-2.192243	-0.527602
7	2.782765	0.381161	-0.137251	7	-2.783847	-0.323435	0.036797
6	3.582278	-0.536167	0.305684	6	-3.624667	0.636970	0.392738
6	5.021489	-0.404051	0.239633	6	-5.041759	0.433615	0.380502
6	5.845021	-1.430917	0.745232	6	-5.922613	1.472252	0.772129
6	7.225989	-1.336677	0.695153	6	-7.296863	1.297848	0.768981
6	7.812179	-0.192415	0.130481	6	-7.838862	0.062880	0.369676
6	7.031256	0.838747	-0.373975	6	-7.007130	-0.982649	-0.020719
6	5.631115	0.751637	-0.328147	6	-5.614798	-0.820543	-0.023434
1	5.371712	-2.309030	1.178239	1	-5.493266	2.423635	1.079211
1	7.846944	-2.135412	1.086515	1	-7.951814	2.109118	1.072774
1	8.894356	-0.108564	0.086350	1	-8.916131	-0.079943	0.365552
1	7.475153	1.726772	-0.810920	1	-7.408580	-1.942422	-0.330761
1	3.195387	-1.453375	0.767630	1	-3.272611	1.617321	0.727134
8	4.906085	1.764558	-0.820503	8	-4.841854	-1.846368	-0.403261
1	3.946100	1.525636	-0.696036	1	-3.890455	-1.526598	-0.328154
E(S_0)	-1031.74300623 E_h			E(S_1)	-1031.00945537 E_h		

Transition State Structure MK→DK Optimized GAUSSIAN				Transition State Structure MK*→DK* Optimized TURBOMOLE			
6	-6.940209	1.141998	0.057194	6	6.985066	1.142315	0.016528
6	-5.513887	0.923536	0.056068	6	5.560429	0.919981	0.012326
6	-5.074479	-0.475694	-0.044050	6	5.117737	-0.468696	-0.005552
6	-6.036875	-1.528831	-0.130761	6	6.046634	-1.493138	-0.018015
6	-7.377826	-1.259465	-0.124382	6	7.444783	-1.233072	-0.014107
6	-7.819492	0.095781	-0.029086	6	7.895262	0.084674	0.003199
1	-7.278813	2.170289	0.129745	1	7.315982	2.175661	0.030004
1	-5.679296	-2.554171	-0.202636	1	5.704574	-2.525945	-0.031046
1	-8.105585	-2.061127	-0.190571	1	8.144395	-2.061486	-0.024565
1	-8.888110	0.296840	-0.025261	1	8.961250	0.292513	0.006530
8	-4.687354	1.880322	0.136966	8	4.736587	1.885327	0.023435
6	-3.708812	-0.770004	-0.052370	6	3.697492	-0.789090	-0.009911
7	-2.783958	0.187192	0.028650	7	2.786421	0.139305	0.004542
1	-3.379162	-1.804033	-0.123828	1	3.387345	-1.830580	-0.025766
6	-1.390477	0.058915	0.024626	6	1.375196	0.033437	0.005328
6	-0.630359	1.229977	0.182957	6	0.637375	1.225420	-0.000640
6	0.755990	1.183272	0.190845	6	-0.747510	1.203392	-0.002452
6	1.426666	-0.040693	0.029324	6	-1.451423	-0.033884	0.002255
6	0.664196	-1.211422	-0.117125	6	-0.679416	-1.231038	0.010189
6	-0.722781	-1.167388	-0.122985	6	0.699138	-1.204149	0.011651
1	-1.140480	2.179593	0.314127	1	1.160309	2.179411	-0.004734
1	1.311375	2.102105	0.344977	1	-1.288320	2.142249	-0.006694
1	1.176264	-2.160604	-0.239825	1	-1.204723	-2.181146	0.015948
1	-1.274924	-2.091858	-0.249519	1	1.242882	-2.144311	0.020115
7	2.820530	-0.169214	0.021766	7	-2.809000	-0.151445	0.000871
6	3.704492	0.797314	-0.132748	6	-3.714867	0.857309	-0.008438
6	5.084989	0.494527	-0.087153	6	-5.085083	0.536083	-0.005672
6	6.072840	1.499992	-0.255247	6	-6.094120	1.539890	-0.015593
6	7.410262	1.184269	-0.214848	6	-7.433490	1.207853	-0.012374
6	7.797867	-0.164980	-0.005125	6	-7.816131	-0.154127	0.000980
6	6.873013	-1.172299	0.159333	6	-6.868142	-1.165353	0.010775
6	5.475328	-0.888187	0.125634	6	-5.480186	-0.870826	0.007792
1	5.751193	2.527020	-0.415199	1	-5.786082	2.584100	-0.025773
1	8.165363	1.952650	-0.341328	1	-8.191820	1.985535	-0.019988
1	8.856914	-0.408420	0.025725	1	-8.872663	-0.411465	0.003601
1	7.172881	-2.202659	0.318432	1	-7.155368	-2.212473	0.020968
1	3.376825	1.822610	-0.309730	1	-3.392397	1.896477	-0.018592
8	4.584325	-1.811838	0.273514	8	-4.579401	-1.810177	0.016608
1	3.452626	-1.156817	0.168532	1	3.223973	1.092628	0.016307
1	-3.251520	1.131171	0.099008	1	-3.472688	-1.151163	0.009959
$E(S_0)$	-1031.73470056 E_h			$E(S_1)$	-1031.01012824 E_h		

Maxima on the Way to the Conical Intersections:

Maximum on Path to CI: E*↔ER* Optimized TURBOMOLE				Maximum on Path to CI: MK*↔MKR1* Optimized TURBOMOLE			
6	6.847183	1.025810	-1.159018	6	-6.547266	1.118134	2.868515
6	5.510572	0.867546	-0.770196	6	-5.190772	0.864440	2.442578
6	5.022556	-0.433868	-0.380495	6	-4.909966	-0.465915	1.909679
6	5.937467	-1.521824	-0.414545	6	-5.918892	-1.412034	1.833208
6	7.250728	-1.348366	-0.812364	6	-7.235878	-1.121738	2.262060
6	7.706840	-0.068728	-1.187978	6	-7.533327	0.144410	2.775957
1	7.181534	2.019314	-1.440834	1	-6.756086	2.106518	3.264319
1	5.579423	-2.505339	-0.118782	1	-5.698450	-2.400173	1.435064
1	7.930840	-2.194837	-0.830969	1	-8.004582	-1.883030	2.188330
1	8.738521	0.067983	-1.499945	1	-8.543797	0.367517	3.105479
8	4.709062	1.938813	-0.758756	8	-4.292073	1.751879	2.527611
1	3.814108	1.630124	-0.420132	6	-3.572199	-0.809692	1.458772
6	3.677118	-0.623983	0.034276	7	-2.585884	0.029385	1.512301
7	2.806548	0.391938	0.107193	1	-3.388639	-1.805956	1.064148
1	3.375041	-1.632960	0.330814	6	-1.225857	-0.127507	1.120463
6	1.459783	0.216062	0.109910	6	-0.373771	0.965636	1.311797
6	0.637835	1.317352	0.506434	6	0.964056	0.888274	0.953278
6	-0.730889	1.218126	0.550734	6	1.500322	-0.293450	0.363443
6	-1.386876	-0.003079	0.193785	6	0.601589	-1.390593	0.185959
6	-0.573119	-1.089193	-0.235054	6	-0.724918	-1.315030	0.556337
6	0.798227	-0.993054	-0.284077	1	-0.763255	1.881463	1.752351
1	1.136492	2.242882	0.779106	1	1.622707	1.727984	1.144960
1	-1.312490	2.083887	0.849638	1	0.998527	-2.299650	-0.254348
1	-1.071783	-2.010192	-0.524447	1	-1.365091	-2.178860	0.398713
1	1.389337	-1.829779	-0.641510	7	2.797066	-0.451539	-0.008286
7	-2.741096	-0.212664	0.220801	6	3.645025	0.598594	-0.108216
6	-3.619587	0.658201	0.684959	6	4.992187	0.543060	0.313803
6	-5.026040	0.384106	0.633061	6	5.857032	1.669652	0.179253
6	-5.963270	1.317158	1.133669	6	7.171528	1.630153	0.606703
6	-7.324835	1.064706	1.092512	6	7.687411	0.451845	1.177224
6	-7.797662	-0.145438	0.542226	6	6.879188	-0.679688	1.309698
6	-6.912926	-1.089132	0.041027	6	5.548270	-0.658524	0.887062
6	-5.527791	-0.848055	0.074004	1	5.451418	2.576574	-0.264198
1	-5.592148	2.247420	1.557110	1	7.805166	2.506230	0.500212
1	-8.027299	1.794471	1.483029	1	8.719856	0.416366	1.513215
1	-8.865696	-0.341757	0.510768	1	7.261999	-1.600393	1.739388
1	-7.256633	-2.025762	-0.385773	1	3.281350	1.551516	-0.511499
1	-3.315117	1.607617	1.133486	8	4.801137	-1.769061	1.016153
8	-4.701156	-1.768995	-0.413097	1	3.895115	-1.545127	0.641120
1	-3.762799	-1.406508	-0.290571	1	-2.887785	0.947692	1.909145
$E(S_1)$	$-1031.01038856\ E_h$			$E(S_1)$	$-1031.01147311\ E_h$		

Maximum on Path to CI: MK↔MKR2 Optimized TURBOMOLE				Maximum on Path to CI: DK↔DKR1 Optimized TURBOMOLE			
6	-6.856957	1.200733	-0.313568	6	6.947659	1.075287	0.410787
6	-5.486904	0.860423	-0.482509	6	5.550388	0.807804	0.522293
6	-5.123368	-0.526092	-0.207709	6	5.112803	-0.529071	0.131072
6	-6.044059	-1.376439	0.350288	6	5.996658	-1.394960	-0.470390
6	-7.422516	-1.006687	0.494486	6	7.389057	-1.087240	-0.582036
6	-7.810671	0.267125	0.142472	6	7.845949	0.133070	-0.120767
1	-7.158325	2.196393	-0.624830	1	7.296838	2.031859	0.786804
1	-5.734010	-2.369455	0.667257	1	5.639353	-2.348305	-0.853395
1	-8.141400	-1.743414	0.837598	1	8.068832	-1.823626	-0.997093
1	-8.851409	0.568023	0.227147	1	8.901935	0.380794	-0.183793
8	-4.576144	1.707401	-0.803384	8	4.695739	1.682917	0.895871
6	-3.689737	-0.878142	-0.346204	6	3.681162	-0.843404	0.259234
7	-2.819321	0.016521	0.096529	7	2.803679	0.101167	-0.002765
1	-3.331409	-1.716534	-0.940392	1	3.326237	-1.824941	0.560266
6	-1.429741	-0.081507	0.131034	6	1.408466	0.022597	-0.035870
6	-0.667003	1.101955	0.176282	6	0.662806	1.204113	0.133685
6	0.715386	1.044013	0.188121	6	-0.719737	1.173043	0.129846
6	1.388752	-0.200946	0.153903	6	-1.407726	-0.052720	-0.047509
6	0.609807	-1.377013	0.158409	6	-0.648039	-1.231031	-0.238811
6	-0.774298	-1.329395	0.138414	6	0.733181	-1.200943	-0.234649
1	-1.174897	2.063068	0.194602	1	1.182205	2.146893	0.286145
1	1.280264	1.968462	0.253152	1	-1.266339	2.099322	0.265511
1	1.124550	-2.332851	0.173157	1	-1.169089	-2.169809	-0.402889
1	-1.350978	-2.248327	0.168544	1	1.289501	-2.114393	-0.419523
7	2.774046	-0.352962	0.158273	7	-2.782446	-0.163214	-0.057468
6	3.586735	0.594032	-0.213454	6	-3.711308	0.800227	0.089068
6	5.021436	0.441737	-0.151115	6	-5.076818	0.492903	0.050326
6	5.862624	1.493738	-0.574587	6	-6.054493	1.521416	0.207611
6	7.242809	1.377945	-0.527660	6	-7.396746	1.237215	0.174762
6	7.814398	0.186899	-0.049795	6	-7.822815	-0.108185	-0.019639
6	7.016741	-0.869810	0.372973	6	-6.922288	-1.134761	-0.176508
6	5.618053	-0.762221	0.329834	6	-5.503687	-0.900237	-0.151990
1	5.402700	2.408933	-0.941629	1	-5.711327	2.544156	0.355422
1	7.875020	2.196864	-0.855984	1	-8.132346	2.026551	0.295205
1	8.895747	0.086169	-0.009509	1	-8.888762	-0.324072	-0.043997
1	7.447522	-1.794828	0.742561	1	-7.246216	-2.160341	-0.324959
1	3.214475	1.545908	-0.611104	1	-3.383625	1.825558	0.240218
8	4.876610	-1.800092	0.741216	8	-4.660776	-1.844504	-0.296634
1	3.920230	-1.534312	0.628240	1	3.247742	1.046762	0.059621
1	-3.244759	0.974682	0.128941	1	-3.275607	-1.097900	-0.193061
$E(S_1)$	$-1031.01182586\ E_h$			$E(S_1)$	$-1031.00437235\ E_h$		

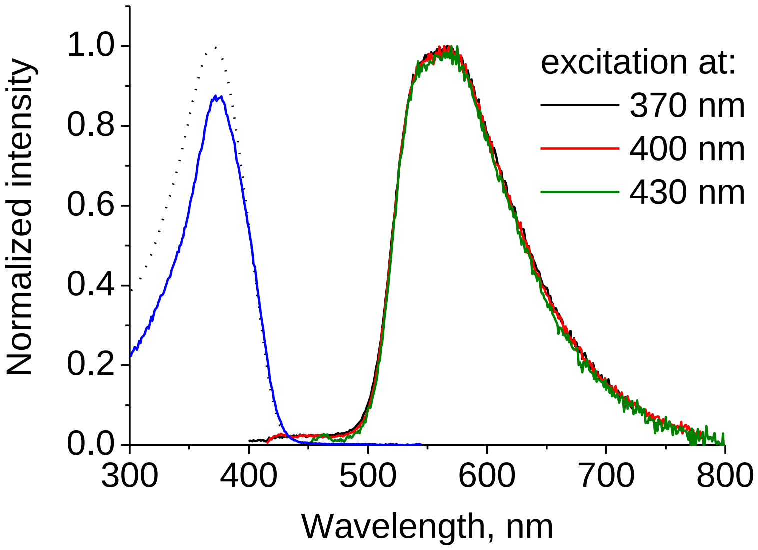

Figure S1. Normalized stationary absorption (1-10^{-A}, where A is absorbance, dotted line) and emission spectra of BSP in DCM upon excitation at indicated wavelength (solid lines). The solid blue line shows the fluorescence excitation spectrum measured for 560 nm observation wavelength and normalized to the absorption spectrum.

Table S1.

Time constants and their fractional amplitudes (in parentheses, normalized to 100 %) obtained from exponential functions fits to the fs-transients (convoluted with an IRF of 210 fs) at the indicated emission wavelengths of BSP in HEX and upon excitation at 370 nm.

Wavelength / nm	τ_1 / fs	τ_2 / ps	τ_3 / ps
455	80 (100%)		
535	130 (68%)		20 (32%)
550	100 (31%)	2.8 (14%)	23 (55%)
600		1.0 (23%)	21 (77%)
650		2.4 (30%)	25 (70%)

Table S2.

Time constants and their fractional amplitudes (in parentheses, normalized to 100 %) obtained from exponential functions fits to the fs-transients (convoluted with an IRF of 220 fs) at the indicated emission wavelengths of BSP in DCM and upon excitation at 375 nm.

Wavelength / nm	τ_1 / fs	τ_2 / ps	τ_3 / ps
455	50 (100%)		
490	50 (88%)	1.8 (9%)	20 (3%)
550	50 (26%)	0.7 (12 %)	20 (62%)
600	-	1.0 (15%)	19 (85%)
650	-	3.1 (23%)	20 (77%)

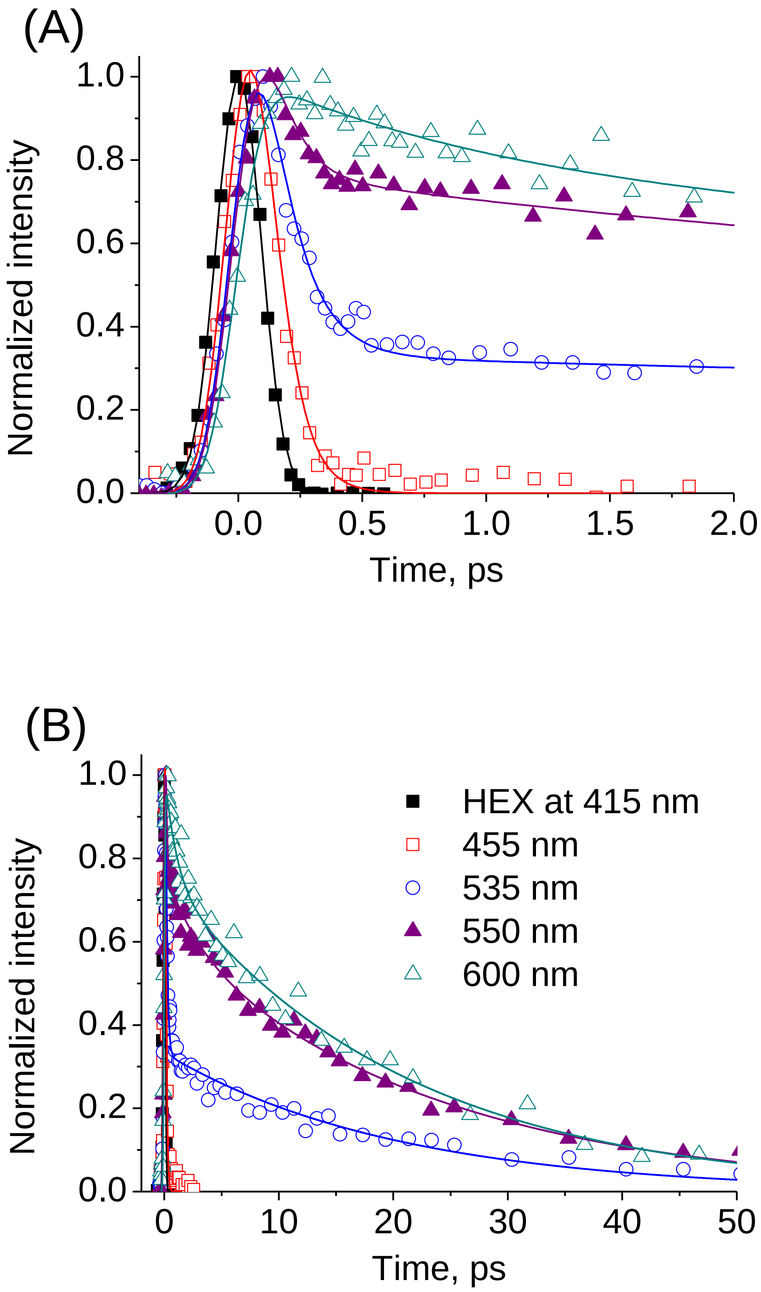

Figure S2. Femtosecond (fs) emission transients of BSP in HEX on shorter (A) and longer (B) time scale at the indicated, representative wavelengths of observation, and upon excitation at 370 nm. The solid lines are from the best fit (see Table S1), and the dotted one is of IRF (FWHM=210 fs) measured at the Raman emission at 415 nm.

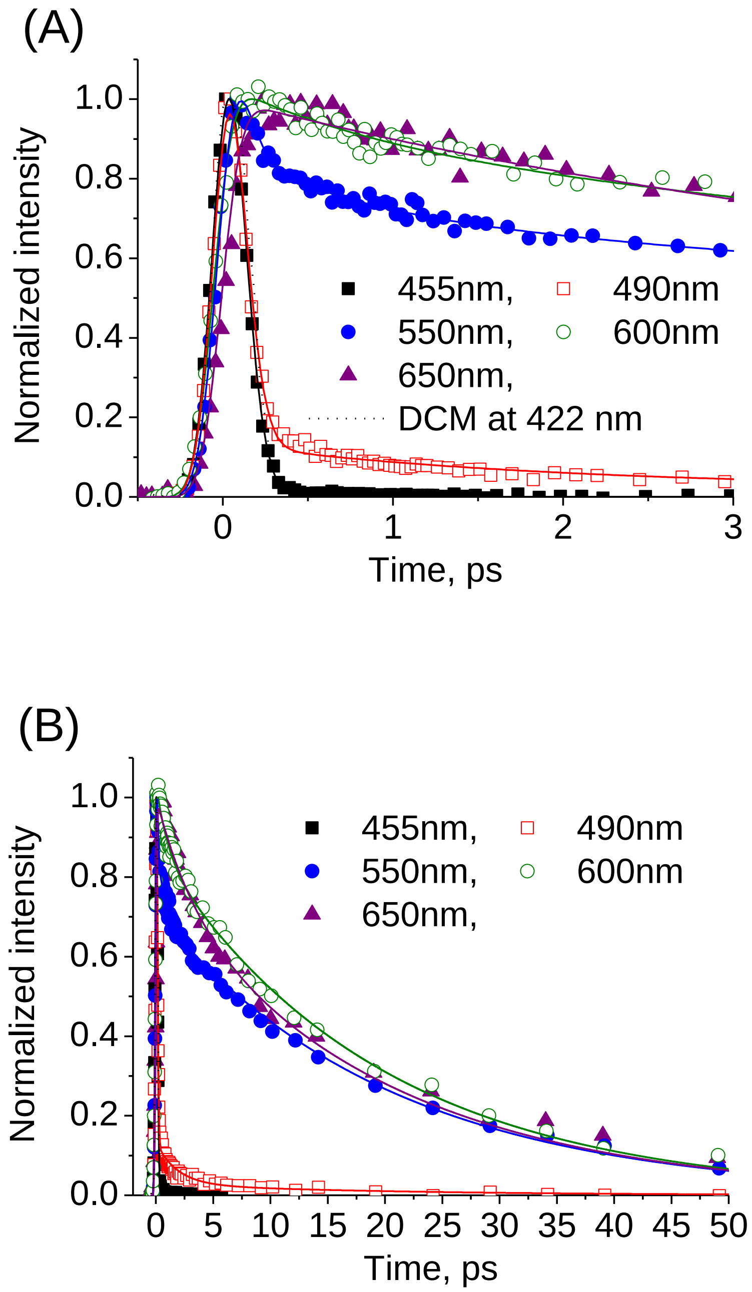

Figure S3. Femtosecond (fs) emission transients of BSP in DCM on shorter (A) and longer (B) time scale at the indicated wavelengths of observation, and upon excitation at 375 nm. The solid lines are from the best fit (see Table 1), and the dotted one is of IRF (FWHM=220 fs) measured at the Raman emission at 422 nm.

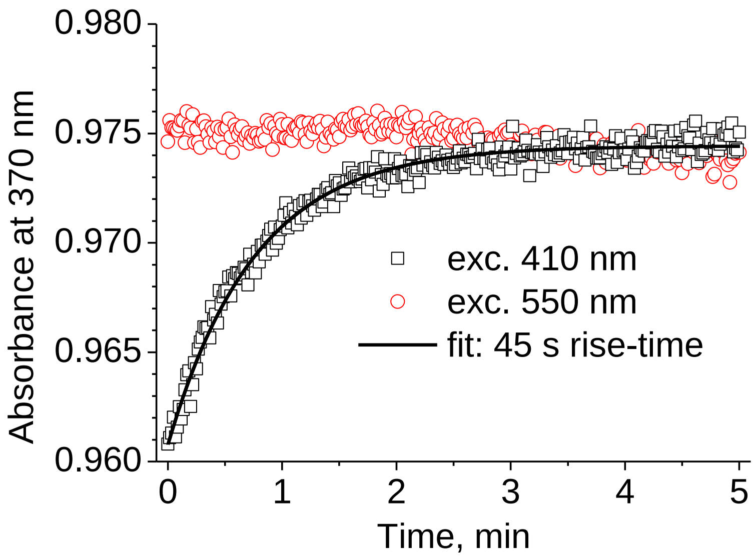

Figure S4. Temporal changes in the absorbance measured at 370 nm at the stationary absorption setup after the irradiation of the BSP/HEX with 410 nm, 3 mJ nanosecond pulses for 4 minutes at 10 Hz (open black squares). The time between the end of the irradiation and the beginning of the kinetics measurements is about 25 s. The solid line shows the fit with 1-exp rise and the characteristic time of 45 s. For the reference, the irradiation experiment with the same conditions was performed, but with the excitation far away from the absorption band of BSP (at 550 nm, open red circles), showing no changes in the absorbance.