Supporting Information

Coupled-Cluster Studies of the Lowest Excited States of the 11-*cis*-Retinal Chromophore

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Table I: The Cartesian coordinates (in Å) for the atoms of the protonated 11-*cis*-retinal chromophore optimized at the MP2/TZVP level.

C	4.277582	-0.510163	0.609030	H	3.177516	-2.187531	1.492036
C	5.240085	0.551888	1.144748	H	4.616834	-1.695793	2.383560
C	5.545442	1.620921	0.112658	H	5.828351	-1.950629	0.165235
C	4.264358	2.362511	-0.230878	H	4.349701	-2.222728	-0.748322
C	3.097703	1.451050	-0.504297	H	5.425478	-0.903505	-1.205631
C	3.097533	0.148931	-0.102790	H	2.408122	2.731650	-2.062072
C	3.768985	-1.324571	1.803825	H	1.310470	1.385407	-1.743450
C	5.011376	-1.447754	-0.357000	H	1.393868	2.758812	-0.632899
C	1.984682	2.101534	-1.278629	H	2.243798	-1.760266	-0.648377
C	1.985539	-0.746237	-0.358368	H	0.406599	0.529929	0.207227
C	0.668621	-0.449451	-0.179182	H	0.406632	-2.658750	-1.908807
C	-0.407360	-1.359582	-0.422230	H	0.568718	-3.251345	-0.259197
C	-0.100292	-2.730849	-0.945812	H	-0.984899	-3.343434	-1.085589
C	-1.687237	-0.912215	-0.143283	H	-1.761295	0.101701	0.223251
C	-2.859131	-1.679044	-0.273259	H	-2.727122	-2.740079	-0.453020
C	-4.178506	-1.290504	-0.115281	H	-4.895400	-2.103980	-0.077909
C	-4.736138	0.002664	-0.037129	H	-4.536162	2.077110	-0.604429
C	-3.919842	1.231283	-0.313306	H	-3.350547	1.520834	0.572138
C	-6.091125	0.082059	0.290911	H	-6.623226	-0.847053	0.468030
C	-6.808653	1.258855	0.414462	H	-6.341764	2.221476	0.254241
N	-8.090300	1.312842	0.749784	H	-8.570063	2.194343	0.835392
H	6.154259	0.056341	1.482490	H	-8.624442	0.474641	0.926336
H	4.789915	1.028837	2.022265	H	4.418144	3.009100	-1.098389
H	5.960423	1.168497	-0.790335	H	3.990217	3.029874	0.596651
H	6.293083	2.319661	0.491096	H	-3.216407	1.045569	-1.122841
H	3.151608	-0.705136	2.457836				

Table II: The Cartesian coordinates (in Å) for the atoms of the ground-state of the protonated 11-*cis*-retinal model chromophore optimized at the MP2/TZVP level.

C	4.740764	-0.874351	-0.571245	C	-5.732993	0.095617	-0.003319
C	6.029951	-0.170279	-0.162385	C	-6.176092	1.395099	-0.202436
C	5.900204	1.329192	-0.401487	N	-7.444641	1.771302	-0.221610
C	4.817654	1.905660	0.505064	H	6.872091	-0.584999	-0.718547
C	3.585019	1.059214	0.521432	H	6.218572	-0.350547	0.900671
C	3.519144	-0.190184	-0.000592	H	5.631043	1.503261	-1.447994
H	4.750144	-1.915252	-0.234388	H	6.848803	1.836991	-0.220880
H	4.661106	-0.901576	-1.663417	H	2.384980	-2.034199	0.008234
H	2.708301	1.469224	1.017343	H	0.869250	0.637579	-0.033440
C	2.287667	-0.948961	0.028057	H	-1.597199	0.233094	0.160017
C	1.020850	-0.436185	0.022585	H	-2.210651	-2.798551	0.240897
C	-0.113777	-1.279481	0.093894	H	-4.530127	-2.292904	0.259494
H	0.061695	-2.354019	0.105868	H	-6.453462	-0.699984	0.155724
C	-1.412952	-0.836256	0.159052	H	-5.452900	2.188388	-0.362582
C	-2.483564	-1.747797	0.175871	H	-7.700333	2.736355	-0.358906
C	-3.839585	-1.460748	0.176004	H	-8.193002	1.108251	-0.079307
C	-4.376604	-0.187042	-0.020654	H	4.545912	2.919031	0.193027
H	-3.696464	0.646126	-0.184439	H	5.195288	2.001132	1.530810

Table III: The Cartesian coordinates (in Å) for the atoms of the first excited-state of the protonated 11-*cis*-retinal model chromophore optimized at the CC2/TZVP level.

C	4.782219	-0.797983	-0.528684	C	-5.602816	0.224417	0.000296
C	5.992662	0.001092	-0.057177	C	-6.020875	1.540924	-0.176125
C	5.777568	1.481832	-0.346268	N	-7.308434	1.930294	-0.192812
C	4.597466	1.997669	0.471171	H	6.892598	-0.368283	-0.551666
C	3.437036	1.070844	0.464312	H	6.127869	-0.144190	1.019756
C	3.480105	-0.217222	-0.034180	H	5.570937	1.616058	-1.412832
H	4.845983	-1.839081	-0.198569	H	6.671632	2.061580	-0.111633
H	4.753388	-0.820515	-1.625096	H	2.494299	-2.121326	-0.233670
H	2.513619	1.429975	0.915493	H	0.798675	0.425314	0.149423
C	2.323558	-1.060247	-0.055399	H	-1.548393	-0.007151	0.283962
C	1.012081	-0.636543	0.039504	H	-2.361918	-3.012394	0.323478
C	-0.103388	-1.521685	0.005566	H	-4.632718	-2.245178	0.219293
H	0.086453	-2.586348	-0.115798	H	-6.356798	-0.540002	0.177158
C	-1.389770	-1.079036	0.178449	H	-5.293197	2.328051	-0.349899
C	-2.544090	-1.946255	0.224486	H	-7.552058	2.907898	-0.240153
C	-3.843380	-1.501648	0.139531	H	-8.051179	1.277411	0.015538
C	-4.264851	-0.152654	-0.070948	H	4.259642	2.981842	0.123537
H	-3.520566	0.617906	-0.261021	H	4.896894	2.155472	1.518923