Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPLEMENTARY INFORMATION

The effect of chemical substituents on the functionality of a molecular switch system: a theoretical study of several quinoline compounds

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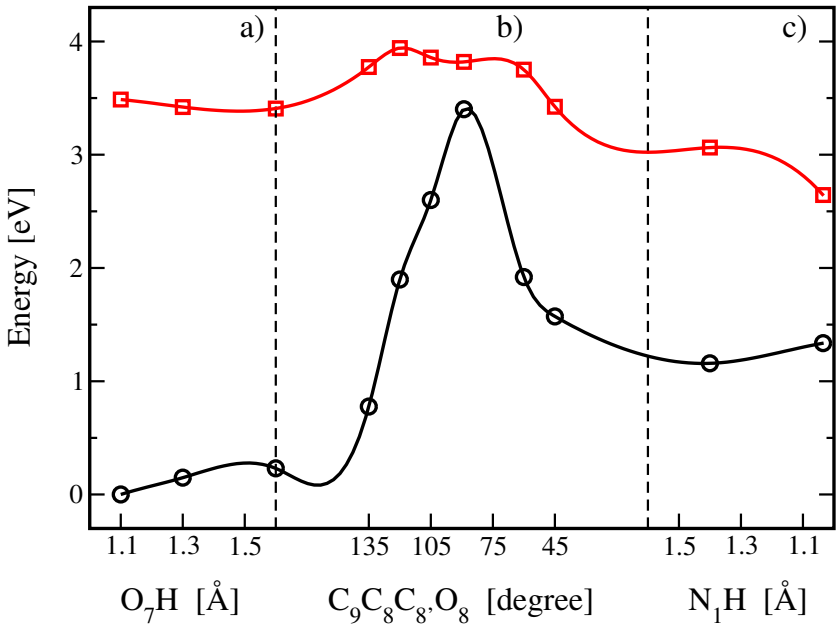

Figure 1: Potential energy profiles of the 4A7HQ8CA molecule in the ground (circle) and first excited states (square) calculated at the CC2/cc-pVDZ level of theory. The geometries along the reaction path have been optimized in the first excited state with the CC2/def-SV(P) method.

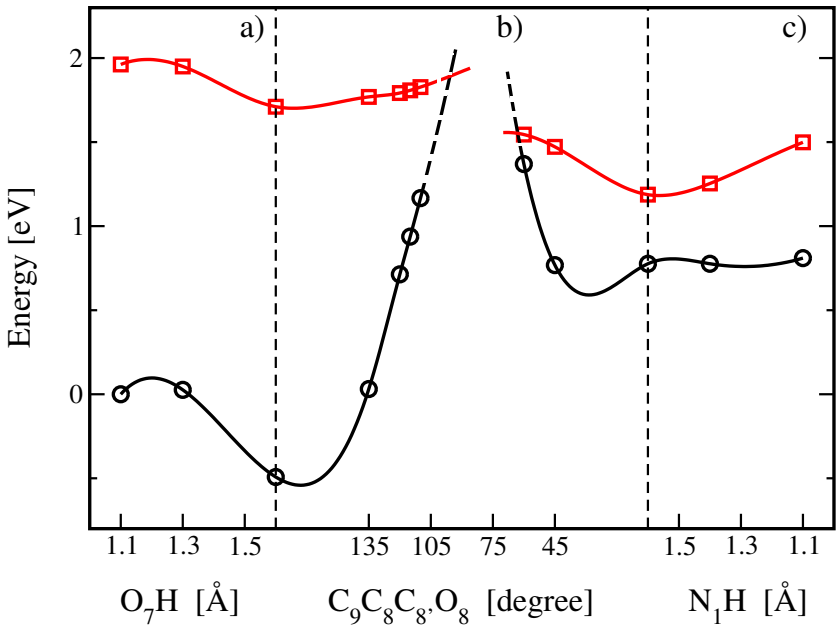

Figure 2: Same as in Fig.1 but for the 4A7HQ8CB molecule.

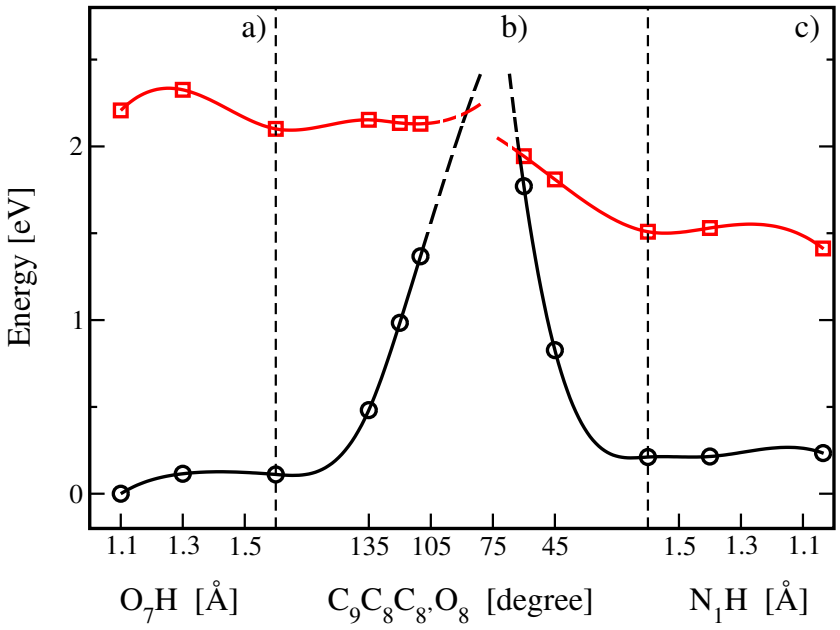

Figure 3: Same as in Fig.1 but for the 4A7HQ8CC molecule.

Table I: Geometry coordinates (in Ångstrom) of the 7HQ8CA molecule at the S_0-S_1 conical intersection determined with the CASSCF(6/5)/6-31G* method.

Atom	X	Y	Z
N	-1.462236	-0.001709	0.983105
C	-0.195789	-0.006947	0.564282
C	0.889973	0.006255	1.454771
C	0.610003	0.049624	2.814779
C	-0.701235	0.073617	3.237988
C	-1.701380	0.041107	2.272066
C	0.044509	-0.060704	-0.864215
C	1.418438	-0.053964	-1.379677
C	2.512100	-0.081176	-0.384998
C	2.257659	-0.038527	0.936259
C	-1.062153	-0.061096	-1.836184
O	-1.647609	1.141037	-2.121294
O	1.650594	0.008306	-2.561282
N	-1.914422	-1.156358	-1.859200
H	-2.736865	0.047424	2.563602
H	-0.953318	0.109150	4.281059
H	1.415827	0.062952	3.527577
H	-0.992919	1.731969	-2.470944
H	3.510900	-0.111205	-0.777441
H	3.063189	-0.039068	1.649041
H	-2.649867	-1.022374	-2.523516
H	-2.306080	-1.359155	-0.957619

Table II: Same as in Table I. but for the 4A7HQ8CA molecule.

Atom	X	Y	Z
C	-1.948148	-0.103424	-1.056494
C	-0.514367	-0.015459	-1.296517
C	0.362917	-0.022904	-0.212465
C	-0.158271	-0.060953	1.130049
C	-1.606137	-0.056086	1.360970
C	-2.465303	-0.131777	0.170220
C	0.038206	0.051091	-2.599930
C	1.415785	0.050009	-2.718454
C	2.194664	-0.004660	-1.550062
N	1.707104	-0.030163	-0.350252
N	-0.780613	0.064932	-3.722759
C	0.727184	-0.040191	2.309104
N	1.562719	-1.128184	2.520476
O	-2.068262	0.033545	2.473949
O	1.234607	1.173138	2.686336
H	3.267993	-0.016113	-1.634189
H	1.890992	0.091020	-3.681466
H	0.517009	1.756601	2.897949
H	-3.522389	-0.202788	0.344503
H	-2.603853	-0.175305	-1.904186
H	2.138767	-0.983978	3.325151
H	2.138498	-1.329885	1.723411
H	-0.300625	0.267341	-4.573160
H	-1.606148	0.617770	-3.644773

Table III: Same as in Table I. but for the 7HQ8CB molecule.

Atom	X	Y	Z
N	-1.500711	0.008432	1.028129
C	-0.235894	0.014080	0.586250
C	0.872167	-0.004714	1.456055
C	0.617306	-0.029803	2.819371
C	-0.687333	-0.039599	3.271505
C	-1.705725	-0.021443	2.324404
C	-0.014826	0.047239	-0.823932
C	1.302537	0.005309	-1.405346
C	2.425515	0.005843	-0.447261
C	2.214902	-0.001997	0.886901
C	-1.136866	-0.017255	-1.748244
O	-1.684494	1.088329	-2.152581
O	1.475215	-0.028740	-2.610403
B	-1.720612	-1.349658	-2.367631
H	-2.734797	-0.028935	2.640092
H	-0.918873	-0.060471	4.319607
H	1.436917	-0.043997	3.516980
H	-1.268298	1.844826	-1.744589
H	3.413688	-0.000922	-0.868038
H	3.048627	-0.010639	1.567205
H	-2.466246	-1.273386	-3.284345
H	-1.397376	-2.383476	-1.894958

Table IV: Same as in Table I. but for the 4A7HQ8CB molecule.

Atom	X	Y	Z
C	-1.945062	-0.060802	-0.950098
C	-0.533759	0.002565	-1.278668
C	0.396749	0.019496	-0.221929
C	-0.077980	0.037798	1.119648
C	-1.477136	-0.027702	1.452323
C	-2.395079	-0.078667	0.308438
C	-0.028229	0.015265	-2.591324
C	1.352090	0.006531	-2.760683
C	2.163466	-0.004036	-1.638037
N	1.729144	0.011623	-0.400522
N	-0.861661	-0.008313	-3.688324
C	0.881376	-0.008932	2.210979
B	1.570628	-1.331400	2.728566
O	-1.871574	-0.033184	2.619099
O	1.228186	1.093350	2.799551
H	3.233084	-0.017635	-1.763097
H	1.786087	0.003800	-3.743834
H	0.762394	1.837974	2.423541
H	-3.444094	-0.144355	0.531398
H	-2.659860	-0.125279	-1.750727
H	2.647829	-1.261912	3.215934
H	0.996177	-2.356784	2.601900
H	-0.430289	0.224151	-4.555538
H	-1.754522	0.418274	-3.586616

Table V: Same as in Table I. but for the 7HQ8CC molecule.

Atom	X	Y	Z
C	-2.085389	-0.293864	-1.493786
C	-0.662178	-0.144018	-1.786856
C	0.233158	0.099350	-0.731596
C	-0.275655	0.194123	0.606731
C	-1.688666	0.055760	0.916668
C	-2.572162	-0.200903	-0.238641
C	-0.132208	-0.231717	-3.067086
C	1.226270	-0.079408	-3.254293
C	2.019216	0.162090	-2.136635
N	1.547591	0.253102	-0.915303
C	0.634066	0.381429	1.713952
C	1.219683	-0.718482	2.417141
N	1.666844	-1.623227	2.941007
O	-2.109809	0.155839	2.047124
O	0.976651	1.552087	2.171396
H	-0.781688	-0.419029	-3.904341
H	3.082262	0.287517	-2.244444
H	1.668390	-0.143467	-4.230405
H	0.548283	2.240845	1.670571
H	-3.617878	-0.311169	-0.021450
H	-2.749167	-0.482648	-2.318989

Table VI: Same as in Table I. but for the 4A7HQ8CC molecule.

Atom	X	Y	Z
N	-1.687542	0.260064	0.423647
C	-0.337655	0.128182	0.399550
C	0.446758	-0.063616	1.537892
C	-0.208462	-0.102044	2.794559
C	-1.581598	0.016543	2.806001
C	-2.263842	0.188980	1.598283
C	0.292827	0.192671	-0.879258
C	1.735580	0.072441	-1.045413
C	2.489444	-0.169251	0.189915
C	1.880715	-0.234261	1.376784
C	-0.507571	0.351788	-2.077486
O	-0.805900	1.520344	-2.590535
O	2.260419	0.169080	-2.133122
N	0.501385	-0.299953	3.962786
C	-1.006261	-0.765349	-2.812274
N	-1.390527	-1.683705	-3.362655
H	-3.335459	0.285757	1.607818
H	-2.129698	-0.015993	3.729827
H	-0.432350	2.219309	-2.063437
H	3.549592	-0.304443	0.086005
H	2.473087	-0.443538	2.248351
H	-0.015744	-0.139064	4.799394
H	1.408393	0.107681	4.008109

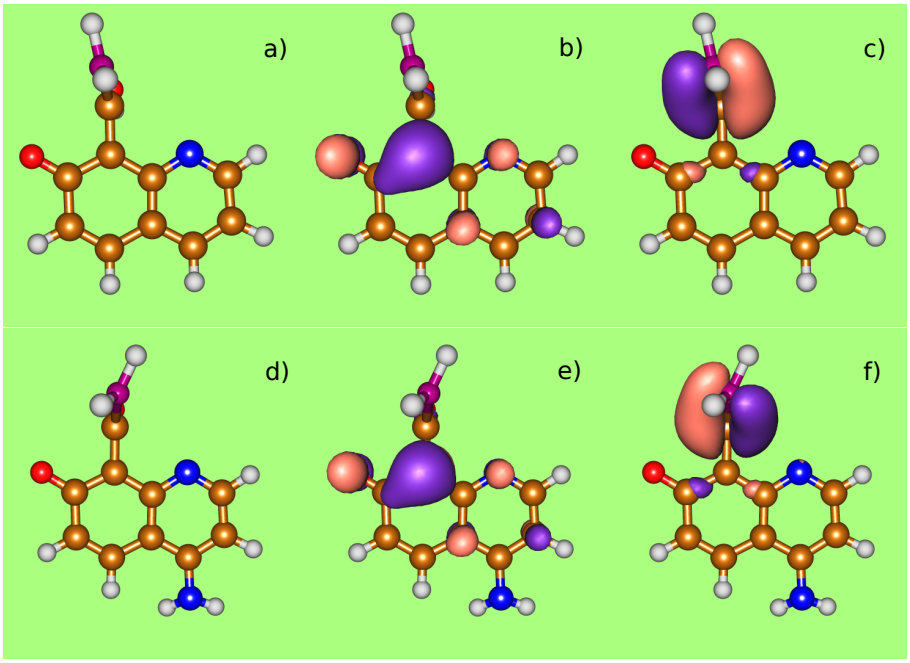

Figure 4: Geometries of the 7HQ8CB and 4A7HQ8CB molecules ((a) and (d))at the S_0-S_1 conical intersections determined at the CASSCF(6/5)/6-31G* level. Panels (b),(e) and (c),(f) present the related HOMO and LUMO orbitals, respectively.

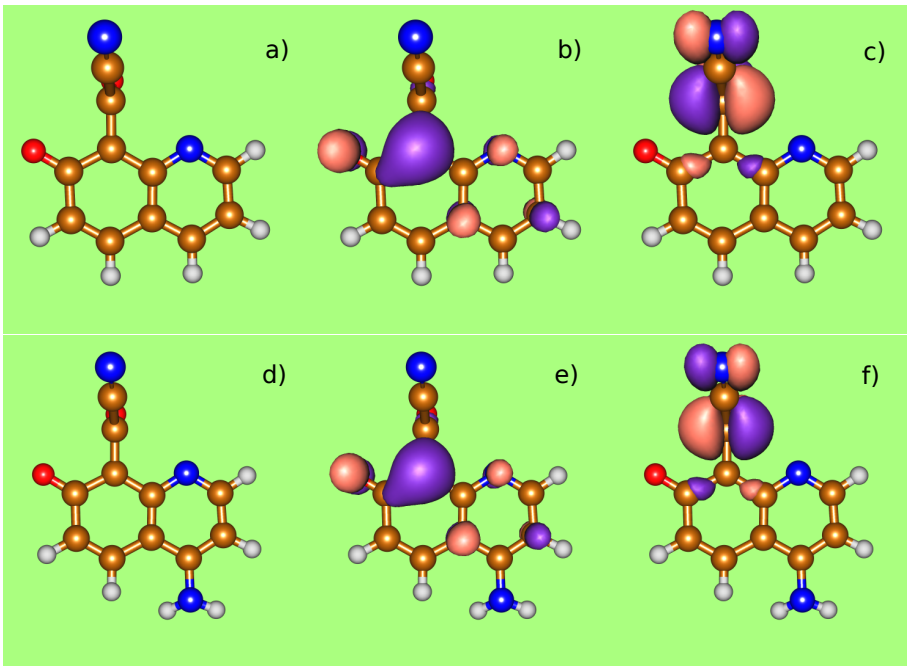

Figure 5: Same as in Fig.4 but for the 7HQ8CC and 4A7HQ8CC molecules.