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Tailoring the Schiff Base Photoswitching – non-adiabatic molecular dynamics study of substituent effect on Excited State Proton Transfer

Joanna Jankowska,[*,†,‡] Mario Barbatti,[¶] Joanna Sadlej,[‡] and Andrzej L. Sobolewski[†]

Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland, Faculty of Chemistry, University of Warsaw, 02-093 Warsaw, Poland, and Aix Marseille Univ, CNRS, ICR, Marseille, France

E-mail: jjankows@usc.edu

[*]To whom correspondence should be addressed
[†]Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland
[‡]Faculty of Chemistry, University of Warsaw, 02-093 Warsaw, Poland
[¶]Aix Marseille Univ, CNRS, ICR, Marseille, France

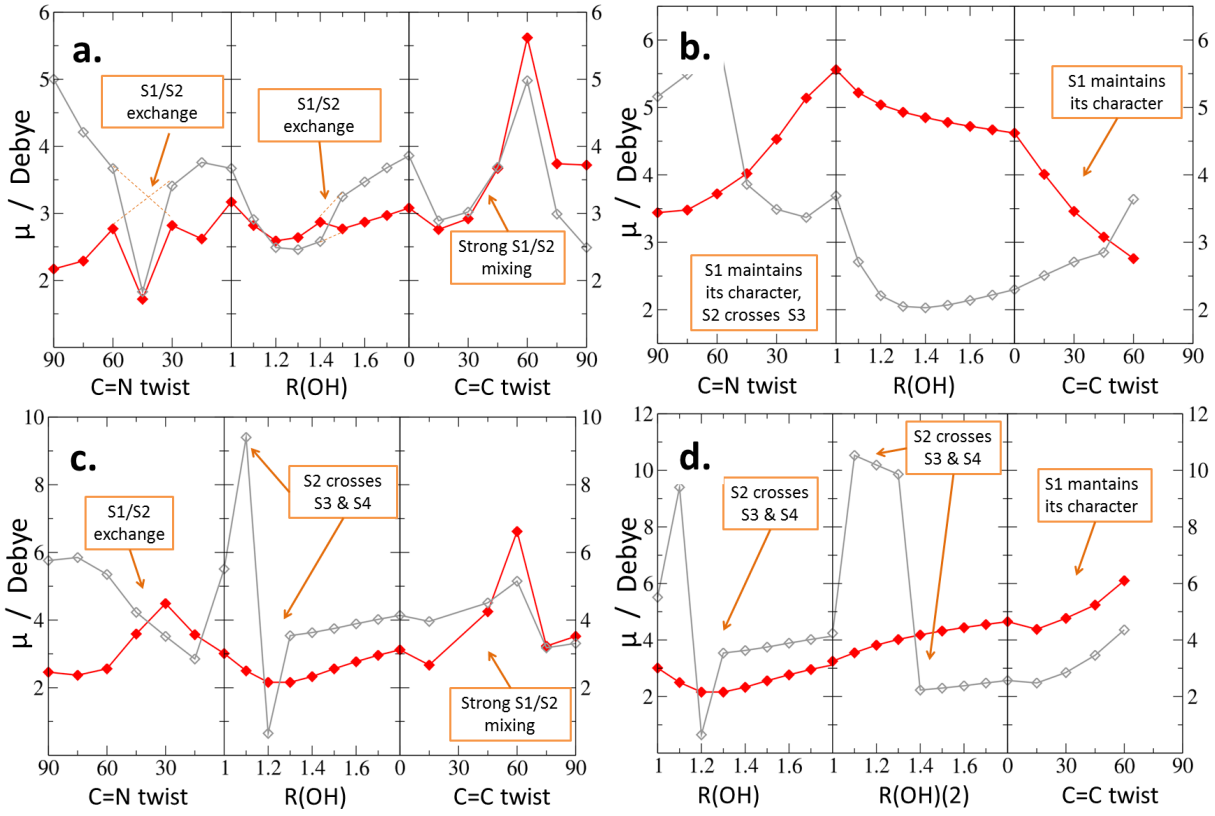

Figure S1: S_1 (full red diamonds) and S_2 (empty gray diamonds) dipole moment profiles along photophysically relevant reaction coordinates for SMA (a.), 6-CN-SMA (b.), and 3-OH-SMA (c., d.) systems. All values have been calculated on S_1 structures optimized at TD-DFT-TDA(B3LYP)/aug-cc-pVDZ level of theory.

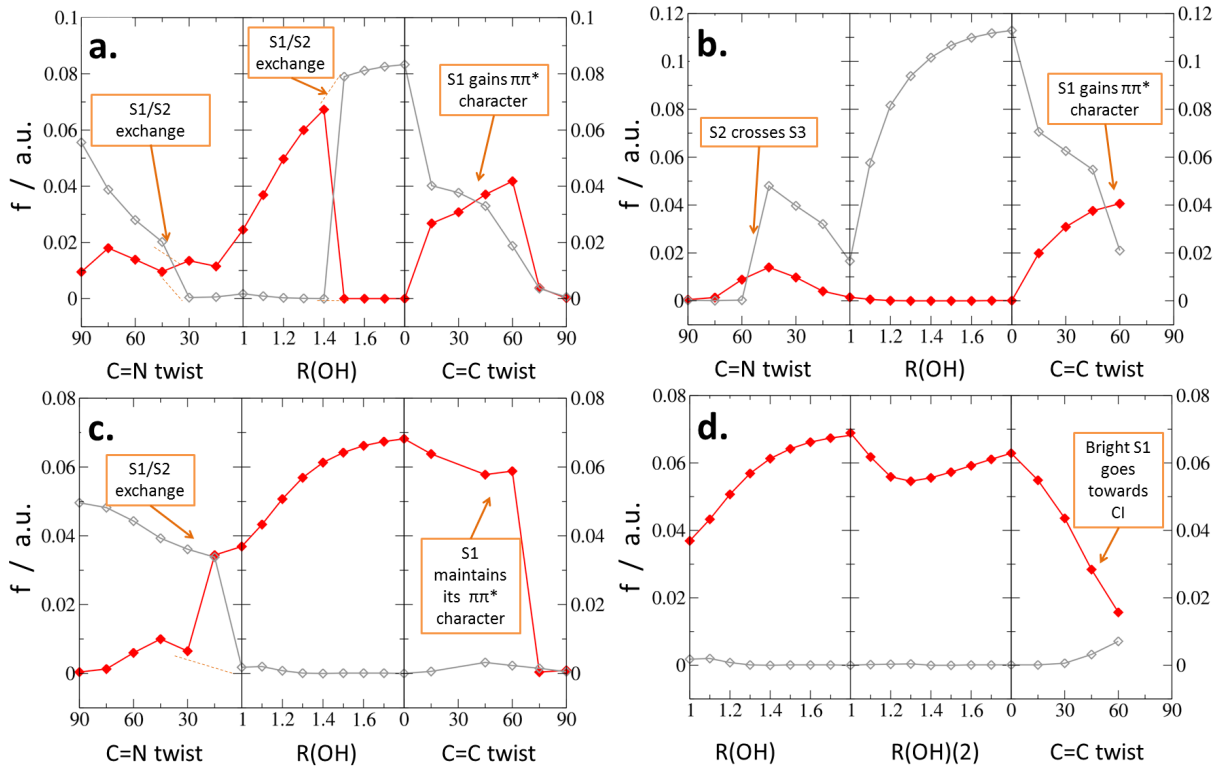

Figure S2: S_1 (full red diamonds) and S_2 (empty gray diamonds) oscillator strength profiles along photophysically relevant reaction coordinates for SMA (a.), 6-CN-SMA (b.), and 3-OH-SMA (c., d.) systems. All values have been calculated on S_1 structures optimized at TD-DFT-TDA(B3LYP)/aug-cc-pVDZ level of theory.

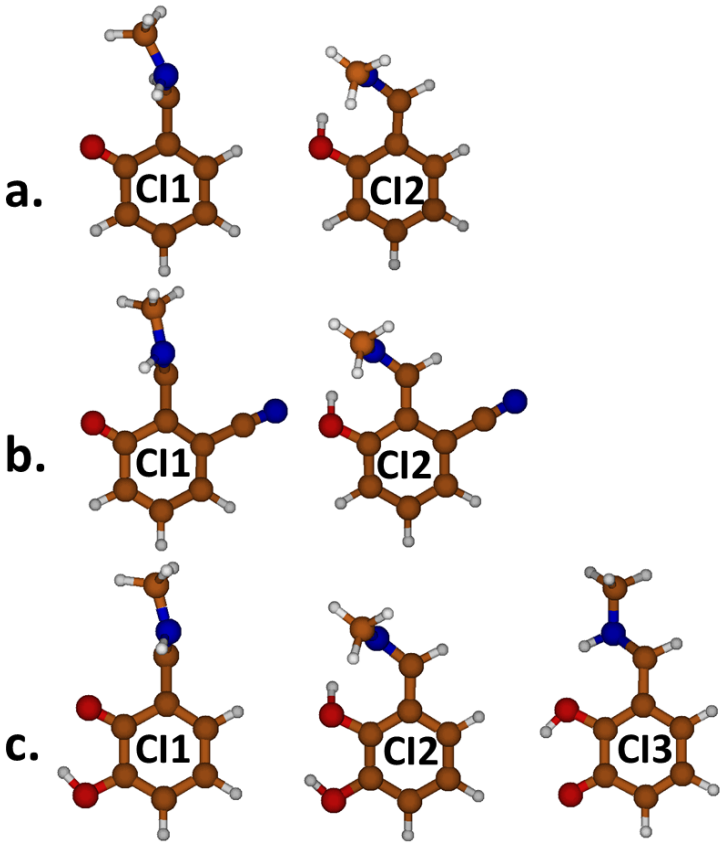

Figure S3: Conical intersection structures for SMA (a.), 6-CN-SMA (b.), and 3-OH-SMA (c.), optimized at the CASSCF(6,6)/cc-pVDZ level of theory.

Table S1: Cartesian coordinates of the SMA CI1 and CI2 conical intersection structures optimized at the CASSCF(6,6)/cc-pVDZ level of theory (Å).

CI1		x	y	z
	C	-1.499916	2.172230	0.043497
	C	-0.187680	2.749457	0.241632
	C	0.916809	1.994306	0.187272
	C	0.844281	0.543636	-0.068451
	C	-0.514146	-0.026659	-0.295297
	C	-1.631285	0.807799	-0.219195
	O	1.827544	-0.150346	-0.083494
	C	-0.610951	-1.462030	-0.580242
	N	-0.590578	-2.368414	0.472557
	C	-0.031137	-3.679112	0.222806
	H	-2.613897	0.384132	-0.373409
	H	-2.373701	2.805247	0.095806
	H	-0.113758	3.811639	0.437031
	H	1.906274	2.404214	0.334820
	H	-0.279590	-1.830172	-1.544437
	H	-0.163427	-4.301506	1.107667
	H	-0.568410	-4.155645	-0.598651
	H	1.034862	-3.651383	-0.031219
	H	-0.268107	-1.965412	1.331230
CI2		x	y	z
	C	-0.307138	0.905754	0.054771
	C	0.575123	2.032635	-0.058167
	C	1.972251	1.760674	-0.111478
	C	2.467636	0.469433	0.005651
	C	1.580293	-0.599163	0.157616
	C	0.194483	-0.359132	0.165052
	C	0.127561	3.371501	-0.134590
	N	-1.177491	3.790967	-0.046440
	C	-1.623454	4.099312	1.297053
	O	-1.652324	1.058001	0.066828
	H	2.653880	2.593438	-0.223821
	H	3.534777	0.296205	-0.020821
	H	1.948723	-1.611006	0.250439
	H	0.854510	4.144582	-0.368728
	H	-1.901736	1.857464	-0.377699
	H	-1.527256	3.223773	1.945832
	H	-2.663385	4.419956	1.271183
	H	-1.011559	4.899424	1.726855
	H	-0.506731	-1.177805	0.248238

Table S2: Cartesian coordinates of the 6-CN-SMA CI1 and CI2 conical intersection structures optimized at the CASSCF(6,6)/cc-pVDZ level of theory (Å).

CI1		x	y	z
	C	-0.184404	-2.801526	0.351862
	C	-1.347739	-2.143030	0.301921
	C	-1.396405	-0.692713	0.039089
	C	-0.097178	-0.002322	-0.222475
	C	1.085673	-0.747579	-0.141843
	C	1.071904	-2.120292	0.137033
	O	-2.426849	-0.077444	0.048698
	C	-0.131440	1.429450	-0.533292
	N	-0.282151	2.326402	0.519118
	C	-0.616368	3.688835	0.164292
	C	2.370214	-0.111848	-0.369810
	N	3.395617	0.345345	-0.546778
	H	1.999756	-2.668986	0.182389
	H	-0.161016	-3.863588	0.555348
	H	-2.298278	-2.632010	0.460548
	H	-0.445335	1.736442	-1.526423
	H	-0.875038	1.968106	1.246172
	H	-0.658999	4.294535	1.068824
	H	0.164593	4.101447	-0.475139
	H	-1.575948	3.777597	-0.360367
CI2		x	y	z
	C	0.641977	-2.195428	0.186768
	C	-0.311249	-1.218923	0.185801
	C	0.052632	0.168606	0.083197
	C	1.448912	0.450067	-0.079531
	C	2.409797	-0.559557	-0.073118
	C	2.009024	-1.885077	0.071845
	O	-1.599194	-1.600197	0.288471
	C	-0.889755	1.218309	0.118930
	N	-2.222924	1.076259	0.326757
	C	-2.696529	1.141628	1.695819
	C	1.890830	1.819228	-0.227464
	N	2.239854	2.895973	-0.344425
	H	0.314598	-3.222200	0.265675
	H	3.452927	-0.302091	-0.180725
	H	2.743173	-2.677206	0.078600
	H	-0.553547	2.221062	-0.130056
	H	-2.178978	-0.926283	-0.044343
	H	-2.205613	0.385617	2.315348
	H	-3.772653	0.983413	1.712862
	H	-2.472897	2.123610	2.124156

Table S3: Cartesian coordinates of the 3-OH-SMA CI1, CI2, and CI3 conical intersection structures optimized at the CASSCF(6,6)/cc-pVDZ level of theory (Å).

CI1		x	y	z
	C	0.930319	-2.381919	0.199544
	C	-0.353349	-1.893341	0.175509
	C	-0.635131	-0.474973	-0.077930
	C	0.513367	0.400191	-0.312906
	C	1.800470	-0.137550	-0.279839
	C	2.018354	-1.503232	-0.028375
	O	-1.418978	-2.672941	0.387927
	O	-1.789272	-0.092989	-0.077013
	C	0.245865	1.809572	-0.585868
	N	0.239732	2.729574	0.409705
	C	-0.363593	4.029672	0.221752
	H	2.647187	0.512481	-0.453541
	H	3.027438	-1.889266	-0.007508
	H	1.094696	-3.432392	0.393390
	H	0.050103	2.169295	-1.586142
	H	0.186572	2.355236	1.335715
	H	-0.003031	4.466842	-0.709603
	H	-0.066227	4.686592	1.037897
	H	-1.456479	3.983659	0.184326
	H	-2.185611	-2.111533	0.319993
CI2		x	y	z
	C	-0.359328	0.943824	-0.099513
	C	0.558297	2.031567	-0.163064
	C	1.925009	1.819694	-0.046774
	C	2.426337	0.526401	0.113048
	C	1.536340	-0.563488	0.138343
	C	0.186842	-0.366693	0.037264
	O	2.054670	-1.802842	0.263252
	O	-0.593331	-1.488749	0.086629
	C	-1.744696	1.200360	-0.197272
	N	-2.739552	0.262105	-0.147716
	C	-3.283797	-0.005082	1.168128
	H	0.169838	3.032894	-0.287629
	H	2.606226	2.658695	-0.081594
	H	3.484645	0.330669	0.200372

	H	-2.060256	2.212538	-0.436771
	H	-1.362205	-1.379335	-0.458338
	H	-2.499646	-0.350460	1.847846
	H	-4.060249	-0.764466	1.093407
	H	-3.715801	0.906971	1.593351
	H	1.343833	-2.429597	0.242949
Cl3		x	y	z
	C	0.210051	-0.394166	0.141952
	C	-0.337397	0.874345	-0.098254
	C	0.571546	1.944613	-0.238496
	C	1.975596	1.755228	-0.164983
	C	2.508379	0.531231	0.050475
	C	1.640463	-0.614994	0.217453
	C	-1.778931	1.154387	-0.154525
	N	-2.709699	0.205227	-0.530877
	C	-4.104467	0.516970	-0.318709
	O	2.056868	-1.762296	0.426045
	O	-0.571759	-1.471395	0.322831
	H	0.183368	2.936967	-0.417489
	H	2.620757	2.615131	-0.287185
	H	3.574181	0.363444	0.108123
	H	-2.070476	2.182426	-0.320837
	H	-2.461497	-0.726232	-0.265373
	H	-4.374118	0.609983	0.740302
	H	-4.719359	-0.264148	-0.765422
	H	-4.352465	1.457334	-0.814443
	H	0.002669	-2.217441	0.462745