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Transient absorption, femtosecond dynamics, vibrational coherence and molecular modelling of the photoisomerization of N-salicylidene-o-aminophenol in solution

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(Electronic Supplementary Information)

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Table S1: Relative energy (ΔE) of the ground state of each conformer of the keto-tautomer calculated with respect to the lowest value, the respective Boltzmann weight and the corresponding absorption transition energy (E)

Transition $S_0 \rightarrow S_1$			
Conformer	ΔE, kcal/mol	Boltzmann weight	E, eV
1	1.373	0.074	2.773
2[#]	0.000	0.748	2.708
3	0.855	0.177	2.752
4	3.626	0.002	2.855
		Averaged E, eV	**2.721**
Transition $S_0 \rightarrow S_2$			
1	1.373	0.074	2.854
2	0.000	0.748	2.673
3	0.855	0.177	2.761
4	3.626	0.002	2.722
		Averaged E, eV	**2.702**
Transition $S_0 \rightarrow S_3$			
1	1.373	0.074	3.104
2	0.000	0.748	3.113
3	0.855	0.177	3.238
4	3.626	0.002	3.106
		Averaged E, eV	**3.135**

[#]Ground state energy of conformer 2: -707.058700 a. u.

Table S2: Relative energy (ΔE) of the excited state of each conformer of the keto-tautomer calculated with respect to the lowest value, the respective Boltzmann weight and the corresponding emission transition energy (E)

Transition $S_1 \rightarrow S_0$			
Conformer	ΔE, kcal/mol	Boltzmann weight	E, eV
1	3.008	0.006	2.336
2[#]	0.000	0.983	2.346
3	2.690	0.011	2.387
4	5.212	0	2.325
		Averaged E, eV	**2.346**
Transition $S_2 \rightarrow S_0$			
1	0.002	0.497	2.411
2[#]	0.000	0.499	2.411
3	2.889	0.004	2.464
4	4.909	0	20450
		Averaged E, eV	**2.411**

[#]Excited state energy of conformer 2: (S_1) -706.965941 a. u.; (S_2) -706.950928 a. u.

Table S3: Relative energy (ΔE) of the ground state of each conformer of the enol-tautomer calculated with respect to the lowest value, the respective Boltzmann weight and the corresponding absorption transition energy (E)

Transition $S_0 \rightarrow S_1$			
Conformer	ΔE, kcal/mol	Boltzmann weight	E, eV
1	4.764	0.000	2.888
2	6.911	0.000	2.867
3[#]	0.000	0.859	2.893
4	3.448	0.003	2.863
5	1.289	0.097	3.030
6	6.288	0.000	2.980
7	1.800	0.041	3.141
		Averaged E, eV	**2.916**
Transition $S_0 \rightarrow S_2$			
1	4.764	0.000	3.334
2	6.911	0.000	3.291
3	0.000	0.859	3.299
4	3.448	0.003	3.350
5	1.289	0.097	3.295
6	6.288	0.000	3.411
7	1.800	0.041	3.365
		Averaged E, eV	**3.302**
Transition $S_0 \rightarrow S_3$			
1	4.764	0.000	3.625
2	6.911	0.000	3.600
3	0.000	0.859	3.625
4	3.448	0.003	3.541
5	1.289	0.097	3.693
6	6.288	0.000	3.597
7	1.800	0.041	3.720
		Averaged E, eV	**3.635**

[#]Ground state energy of conformer 3: -707.063924 a. u.

Table S4: Relative energy (ΔE) of the excited state of each conformer of the enol-tautomer calculated with respect to the lowest value, the respective Boltzmann weight and the corresponding emission transition energy (E)

Transition $S_1 \rightarrow S_0$			
Conformer	ΔE, kcal/mol	Boltzmann weight	E, eV
7[#]	0.000	1	0.079
		'Averaged' E, eV	**0.079**
Transition $S_2 \rightarrow S_0$			
1	7.041	0.000	3.019
3[#]	0.000	0.911	2.873
5	1.374	0.090	2.861
6	9.888	0.000	3.118
		Averaged E, eV	**2.872**

[#] S_1 energy of conformer 7: -706.969153 a. u.; S_2 energy of conformer 3: -706.937523 a. u.