Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information

The ultrafast reactions in the photochromic cycle of water-soluble fulgimide photoswitches

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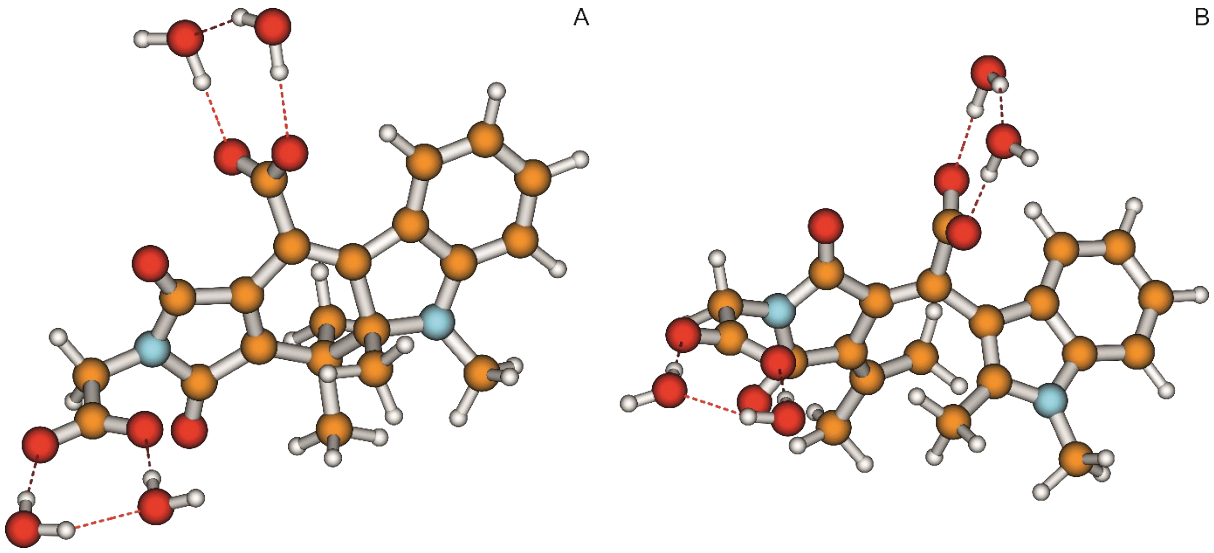

Figure S1. Geometry optimized molecular structures of the investigate C- (A) and Z-form (B) of WF including four explicit molecules. These structure were used for the theoretical calculations.

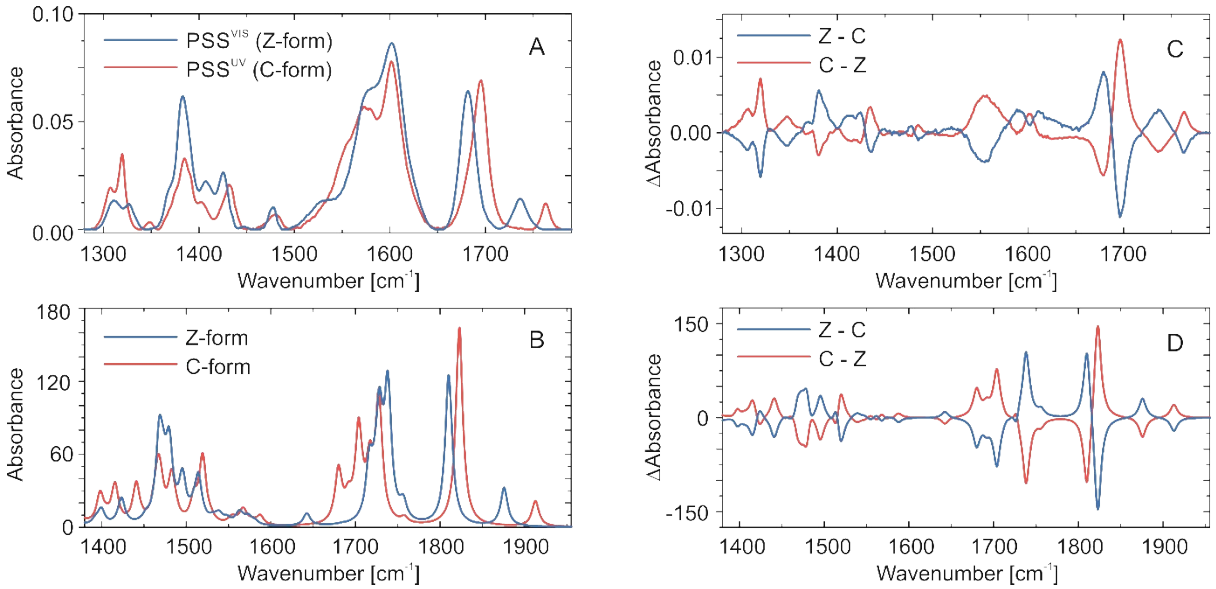

Figure S2. A) Experimental IR absorption spectra of the WF C- and Z-forms dissolved in sodium phosphate buffer (pD 7.4); B) Theoretical IR spectra of the WF C- and Z-forms obtained as described in the manuscript; C) Experimental IR absorption difference spectra resulting from the ring-opening and the ring-closing reaction of WF: D) Theoretical infrared absorption difference spectra of the WF C- and Z-forms obtained as described in the manuscript.

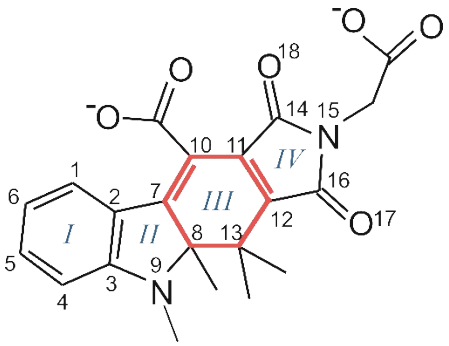

Figure S3. Chemical structure of the C-form of the water-soluble indolylfulgimide (WF).

Table S1. Comparison of the electrostatic properties of the C-form of WF in the relaxed ground (S_0) and excited (S_1) states. The atoms with largest change in their partial charge are highlighted.

Atom number	Atom	S_0 charge	S_1 charge	Difference
1	C	-0.41244	-0.34648	0.065961
2	C	0.3678	0.347493	-0.02031
3	C	0.064401	0.164811	0.10041
4	C	-0.24851	-0.33023	-0.08173
5	C	-0.14721	-0.08828	0.058937
6	C	-0.17398	-0.17822	-0.00424
7	C	-0.55271	-0.58271	-0.03
8	C	0.577424	0.429617	-0.14781
9	N	-0.25711	-0.06717	0.189941
10	C	0.124498	0.280976	0.156478
11	C	-0.2202	-0.35377	-0.13357
12	C	-0.36889	-0.35301	0.015877
13	C	0.600031	0.591127	-0.0089
14	C	0.711282	0.630331	-0.08095
15	N	-0.34023	-0.20671	0.133524
16	C	0.715441	0.573793	-0.14165
17	O	-0.55174	-0.61514	-0.0634
18	O	-0.55172	-0.60744	-0.05573
19	C	-0.33337	-0.35269	-0.01932
20	C	0.831012	0.843655	0.012643
21	O	-0.79125	-0.79503	-0.00378
22	C	-0.50658	-0.50107	0.005515
23	C	-0.58139	-0.50995	0.071447
24	C	-0.53775	-0.42611	0.111643
25	C	0.757263	0.737248	-0.02002
26	O	-0.74354	-0.74693	-0.00339
27	C	-0.30207	-0.36359	-0.06152
28	O	-0.78034	-0.76232	0.018023
29	O	-0.71013	-0.72008	-0.00995
30	H	0.117031	0.114243	-0.00279
31	H	0.114078	0.123853	0.009775
32	H	0.123085	0.108392	-0.01469
33	H	0.129038	0.109457	-0.01958
34	H	0.117583	0.102411	-0.01517
35	H	0.155468	0.141155	-0.01431
36	H	0.176044	0.19803	0.021986
37	H	0.161238	0.158458	-0.00278

38	H	0.281199	0.238026	-0.04317
39	H	0.123369	0.158316	0.034947
40	H	0.136942	0.149951	0.013009
41	H	0.113836	0.148129	0.034293
42	H	0.123472	0.112258	-0.01121
43	H	0.129923	0.113309	-0.01661
44	H	0.159484	0.128032	-0.03145
45	H	0.155931	0.148377	-0.00755
46	H	0.151937	0.141816	-0.01012
47	H	0.147575	0.159634	0.012059
48	H	0.474104	0.467454	-0.00665
49	O	-1.0476	-1.02483	0.022765
50	H	0.500617	0.48804	-0.01258
51	H	0.467635	0.469703	0.002068
52	O	-0.97072	-0.96608	0.004646
53	H	0.456057	0.458473	0.002416
54	H	0.512393	0.506947	-0.00545
55	O	-1.07657	-1.07352	0.003046
56	H	0.490676	0.488202	-0.00247
57	H	0.43141	0.436449	0.005039
58	O	-0.95106	-0.9524	-0.00133
59	H	0.457813	0.455575	-0.00224