Supporting Information

On the Role of Zwitterions in Kindling Fluorescent Protein Photochemistry

Vladimir A. Mironov, [†] *Ksenia B. Bravaya,* [‡] *Alexander V. Nemukhin* *[†,§]

[†] Department of Chemistry, M.V. Lomonosov Moscow State University, Leninskie Gory 1/3, Moscow, 119991, Russian Federation

[‡] Department of Chemistry, Boston University, Boston, MA 02215, USA

[§] N.M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Kosygina 4, Moscow, 119334, Russian Federation

Tables containing all computed bond lengths and bond orders (Table S1, S2) and atomic charges (Table S3). Numbering of atoms (different from that used in Fig.1 of the main text) is clarified in Fig. S1.

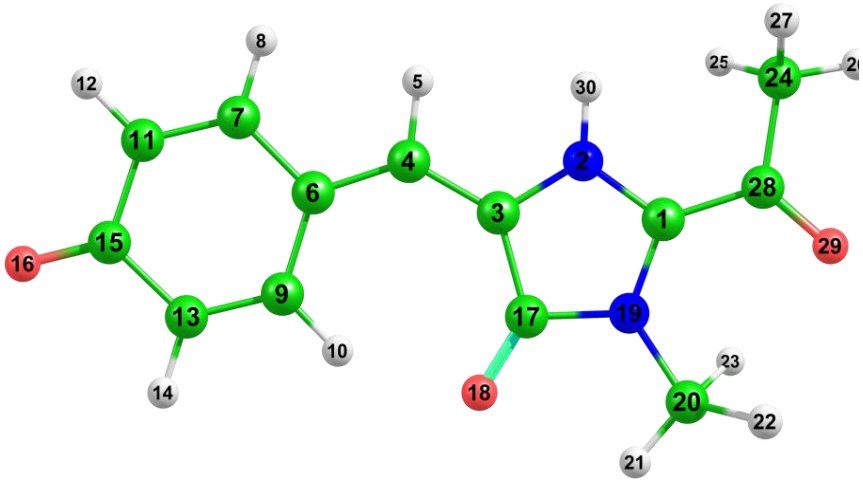

Figure S1. Numbering of atoms used in Tables S1-S3.

Table S1. Bond parameters of the equilibrium structures computed in the XMCQDPT2 approach.

Atom 1	Atom 2	Anion, optimized on S_0			Anion, optimized on S_1			Zwitterion, optimized on S_0			Zwitterion, optimized on S_1		
		length, Å	bond order		length, Å	bond order		length, Å	Bond order		length, Å	bond order	
			S_0	S_1		S_0	S_1		S_0	S_1		S_0	S_1
1	2	1.342	1.489	1.353	1.356	1.465	1.359	1.368	1.205	1.075	1.403	1.141	1.070
1	19	1.386	1.047	1.053	1.390	1.036	1.035	1.372	1.113	1.070	1.376	1.190	1.130
1	28	1.456	1.057	1.086	1.456	1.064	1.095	1.450	1.040	1.127	1.455	1.026	1.078
2	3	1.381	1.310	1.332	1.398	1.287	1.261	1.370	1.164	1.032	1.457	1.061	0.975
2	30	-	-	-	-	-	-	1.017	0.946	0.951	1.027	0.927	0.936
3	4	1.415	1.339	1.248	1.406	1.374	1.356	1.427	1.171	1.403	1.403	1.285	1.485
3	17	1.476	1.068	1.018	1.496	1.043	0.996	1.476	1.082	1.032	1.457	1.102	1.065
4	5	1.101	0.941	0.943	1.099	0.942	0.943	1.101	0.944	0.944	1.100	0.948	0.947
4	6	1.402	1.429	1.194	1.462	1.362	1.091	1.390	1.516	1.113	1.456	1.391	1.145
6	7	1.445	1.175	1.243	1.448	1.175	1.265	1.456	1.157	1.248	1.431	1.193	1.257
6	9	1.445	1.211	1.249	1.411	1.275	1.340	1.454	1.184	1.274	1.427	1.224	1.286
7	8	1.098	0.971	0.972	1.099	0.973	0.973	1.097	0.974	0.974	1.097	0.975	0.975
7	11	1.374	1.608	1.496	1.390	1.595	1.475	1.365	1.740	1.639	1.386	1.694	1.623
9	10	1.094	0.943	0.943	1.093	0.944	0.944	1.093	0.942	0.943	1.092	0.948	0.949
9	13	1.375	1.702	1.666	1.402	1.638	1.576	1.367	1.741	1.642	1.389	1.696	1.626
11	12	1.096	0.971	0.972	1.098	0.972	0.972	1.094	0.970	0.970	1.096	0.971	0.971
11	15	1.468	1.096	1.137	1.467	1.101	1.143	1.477	1.080	1.141	1.463	1.105	1.157
13	14	1.096	0.972	0.971	1.098	0.972	0.972	1.095	0.970	0.970	1.096	0.971	0.971
13	15	1.468	1.107	1.120	1.457	1.132	1.157	1.476	1.078	1.138	1.463	1.102	1.154
15	16	1.248	1.835	1.778	1.271	1.787	1.717	1.237	1.830	1.663	1.266	1.753	1.615
17	18	1.242	1.820	1.812	1.241	1.833	1.834	1.230	1.861	1.899	1.235	1.861	1.897
17	19	1.410	1.118	1.123	1.408	1.123	1.128	1.420	1.111	1.080	1.445	1.048	1.005
19	20	1.448	0.962	0.963	1.451	0.956	0.957	1.459	0.926	0.928	1.457	0.917	0.920
20	21	1.101	0.972	0.972	1.102	0.972	0.972	1.099	0.972	0.972	1.100	0.970	0.970
20	22	1.100	0.983	0.982	1.100	0.983	0.982	1.098	0.982	0.982	1.099	0.979	0.980
20	23	1.100	0.983	0.982	1.100	0.983	0.982	1.098	0.981	0.982	1.100	0.978	0.979
24	25	1.101	0.967	0.967	1.099	0.969	0.969	1.103	0.970	0.970	1.106	0.968	0.967
24	26	1.100	0.976	0.976	1.105	0.969	0.969	1.098	0.973	0.972	1.100	0.972	0.972
24	27	1.101	0.967	0.967	1.106	0.968	0.968	1.103	0.970	0.970	1.103	0.969	0.968
24	28	1.522	1.042	1.042	1.523	1.039	1.040	1.521	1.038	1.038	1.518	1.041	1.042
28	29	1.241	1.983	1.953	1.252	1.961	1.930	1.238	1.885	1.768	1.252	1.861	1.789

Table S2. Bond parameters of the equilibrium structures computed in the CASSCF approach.

Atom 1	Atom 2	Anion, optimized on S_0			Anion, optimized on S_1			Zwitterion, optimized on S_0			Zwitterion, optimized on S_1		
		length, Å	bond order		length, Å	bond order		length, Å	Bond order		length, Å	bond order	
			S_0	S_1		S_0	S_1		S_0	S_1		S_0	S_1
1	2	1.305	1.547	-	1.346	-	1.301	1.334	1.259	-	1.372	-	1.142
1	19	1.388	1.040	-	1.383	-	1.046	1.360	1.129	-	1.346	-	1.196
1	28	1.458	1.027	-	1.439	-	1.110	1.463	1.011	-	1.463	-	1.030
2	3	1.374	1.279	-	1.349	-	1.400	1.367	1.167	-	1.457	-	0.944
2	30	-	-	-	-	-	-	0.998	0.947	-	1.004	-	0.939
3	4	1.420	1.307	-	1.444	-	1.198	1.440	1.147	-	1.370	-	1.552
3	17	1.452	1.107	-	1.484	-	0.999	1.449	1.120	-	1.454	-	1.065
4	5	1.085	0.935	-	1.082	-	0.945	1.086	0.935	-	1.085	-	0.937
4	6	1.382	1.495	-	1.434	-	1.208	1.369	1.611	-	1.447	-	1.187
6	7	1.454	1.147	-	1.431	-	1.252	1.469	1.093	-	1.425	-	1.259
6	9	1.455	1.169	-	1.442	-	1.213	1.467	1.119	-	1.424	-	1.278
7	8	1.084	0.970	-	1.085	-	0.971	1.083	0.972	-	1.084	-	0.972
7	11	1.356	1.644	-	1.381	-	1.482	1.332	1.819	-	1.355	-	1.638
9	10	1.079	0.942	-	1.077	-	0.951	1.078	0.946	-	1.077	-	0.956
9	13	1.344	1.752	-	1.351	-	1.705	1.334	1.817	-	1.356	-	1.651
11	12	1.083	0.972	-	1.083	-	0.970	1.081	0.970	-	1.081	-	0.970
11	15	1.471	1.079	-	1.450	-	1.157	1.478	1.059	-	1.452	-	1.142
13	14	1.083	0.971	-	1.084	-	0.969	1.081	0.970	-	1.081	-	0.969
13	15	1.468	1.087	-	1.462	-	1.113	1.477	1.058	-	1.453	-	1.134
15	16	1.221	1.881	-	1.236	-	1.792	1.213	1.908	-	1.236	-	1.733
17	18	1.221	1.852	-	1.215	-	1.854	1.211	1.893	-	1.201	-	1.933
17	19	1.389	1.125	-	1.376	-	1.152	1.396	1.117	-	1.421	-	0.997
19	20	1.442	0.974	-	1.446	-	0.959	1.457	0.926	-	1.457	-	0.921
20	21	1.087	0.973	-	1.086	-	0.974	1.084	0.972	-	1.084	-	0.972
20	22	1.090	0.983	-	1.088	-	0.982	1.086	0.983	-	1.086	-	0.980
20	23	1.090	0.983	-	1.088	-	0.983	1.087	0.983	-	1.086	-	0.979
24	25	1.084	0.969	-	1.085	-	0.970	1.092	0.969	-	1.094	-	0.965
24	26	1.092	0.969	-	1.092	-	0.968	1.087	0.970	-	1.087	-	0.970
24	27	1.092	0.968	-	1.093	-	0.967	1.092	0.969	-	1.091	-	0.967
24	28	1.516	1.043	-	1.515	-	1.048	1.514	1.041	-	1.509	-	1.050
28	29	1.205	2.032	-	1.215	-	1.960	1.210	1.942	-	1.220	-	1.853

Table S3. Mulliken atom charges at the equilibrium structures.

Atom	Anion				Zwitterion			
	S_0 optimized		S_1 optimized		S_0 optimized		S_1 optimized	
	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1
1	0.240	0.225	0.243	0.219	0.296	0.369	0.321	0.358
2	-0.300	-0.318	-0.305	-0.333	-0.211	-0.324	-0.271	-0.337
3	-0.203	-0.001	-0.170	-0.005	-0.023	-0.012	-0.066	-0.095
4	0.128	0.038	0.104	0.045	0.056	0.105	0.044	0.118
5	0.006	0.005	0.013	0.012	0.026	0.026	0.035	0.034
6	-0.185	-0.137	-0.175	-0.143	-0.128	-0.119	-0.111	-0.134
7	0.051	0.015	0.038	0.013	0.033	0.018	0.026	0.019
8	-0.012	-0.013	-0.008	-0.008	0.022	0.022	0.023	0.023
9	0.025	-0.002	0.022	-0.005	0.008	-0.001	0.006	0.003
10	0.059	0.059	0.058	0.058	0.081	0.081	0.071	0.071
11	-0.090	-0.104	-0.082	-0.085	-0.073	-0.054	-0.063	-0.057
12	-0.010	-0.010	-0.005	-0.005	0.040	0.040	0.040	0.040
13	-0.115	-0.106	-0.119	-0.107	-0.065	-0.044	-0.058	-0.047
14	-0.004	-0.004	-0.001	-0.001	0.042	0.042	0.043	0.043
15	0.213	0.175	0.206	0.177	0.208	0.162	0.195	0.166
16	-0.379	-0.409	-0.401	-0.418	-0.297	-0.248	-0.316	-0.276
17	0.382	0.373	0.389	0.389	0.385	0.427	0.395	0.445
18	-0.422	-0.368	-0.410	-0.367	-0.380	-0.315	-0.375	-0.300
19	-0.490	-0.483	-0.489	-0.486	-0.464	-0.516	-0.437	-0.499
20	0.134	0.134	0.137	0.137	0.119	0.118	0.117	0.116
21	0.054	0.054	0.054	0.054	0.082	0.082	0.089	0.089
22	0.035	0.035	0.038	0.038	0.062	0.061	0.069	0.066
23	0.036	0.036	0.038	0.038	0.063	0.061	0.071	0.068
24	-0.008	-0.008	-0.025	-0.026	-0.050	-0.051	-0.044	-0.045
25	0.054	0.053	0.066	0.066	0.058	0.056	0.059	0.058
26	0.030	0.030	0.038	0.038	0.074	0.074	0.075	0.075
27	0.053	0.053	0.041	0.040	0.058	0.057	0.072	0.071
28	0.126	0.101	0.135	0.108	0.113	0.026	0.103	0.052
29	-0.410	-0.423	-0.429	-0.441	-0.278	-0.283	-0.276	-0.280
30	-	-	-	-	0.141	0.139	0.164	0.155