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

Support information for

The absorption and fluorescence spectra interpreted by Franck–Condon simulation for 4-(3-methoxybenzylidene)-2-methyl-oxazalone in various pH solvent environments

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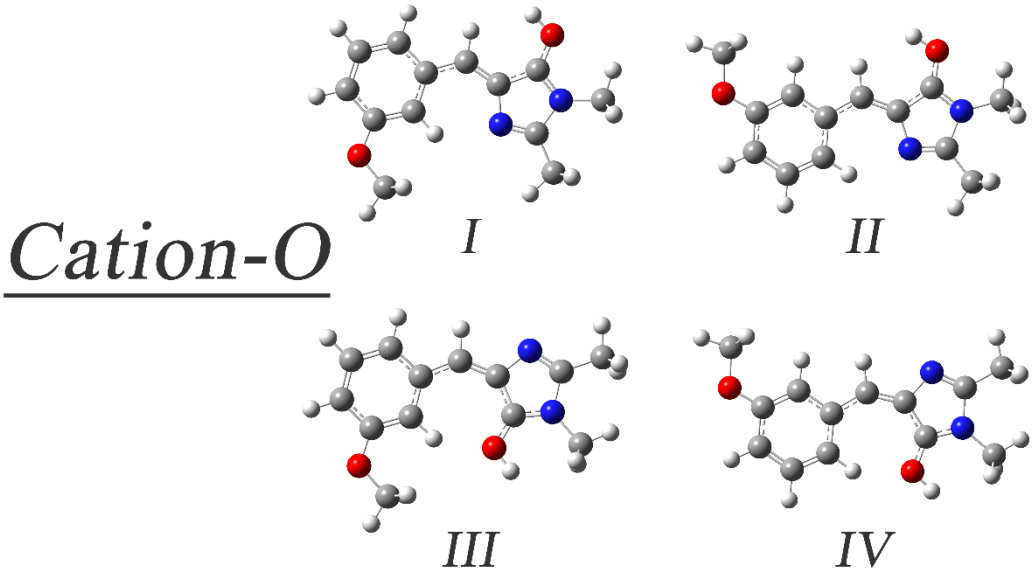

Fig. S1 Optimized geometric structures of the Cation-O form of *m*-MeOBDI in the ground state.

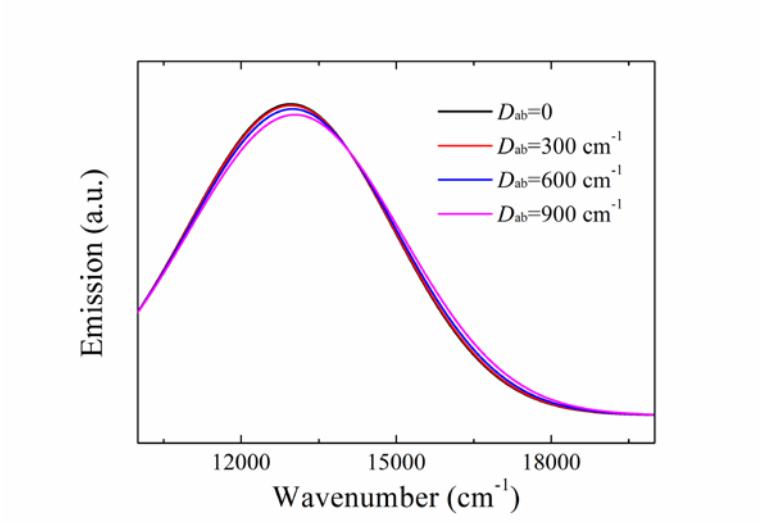

Fig. S2 Simulated emission spectra of the DC-IV* by using different inhomogeneous broadening parameter D_{ab}.

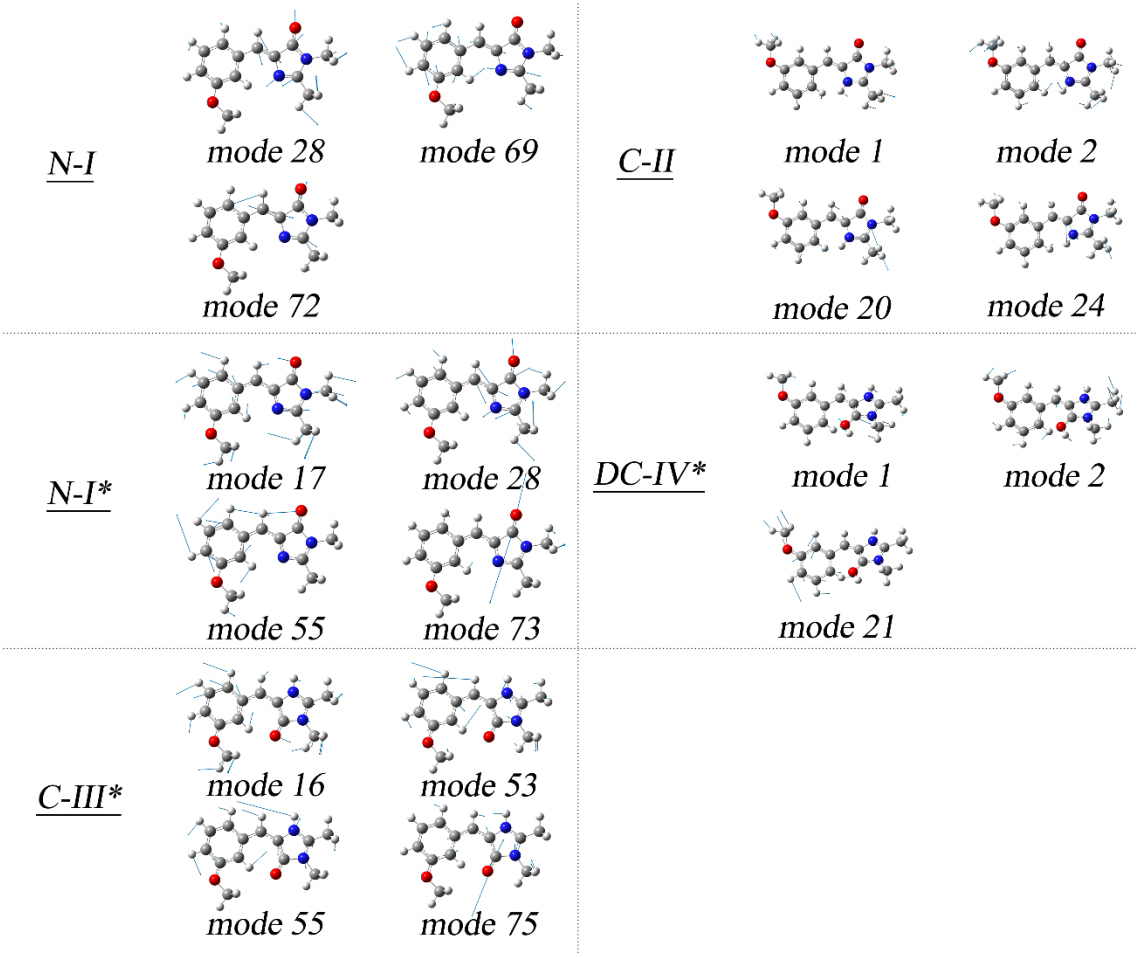

Fig. S3 The dominating vibrational modes in the simulated absorption and emission spectra.

Table S1 Calculated energies of the Cation-N (the cation form of *m*-MeOBDI with protonation of the–N– group) and Cation-O (the cation form of *m*-MeOBDI with protonation of the C=O group) structures in both S_0 and S_1 states by using B3LYP and cam-B3LYP functionals.

		Cation-N				Cation-O			
		I	II	III	IV	I	II	III	IV
B3LYP	S_0	-764.478	-764.479	-764.478	-764.477	-764.453	-764.452	-764.444	-764.444
	S_1	---	-764.383	-764.385	-764.384	-764.365	-764.366	---	-764.336
cam-B3LYP	S_0	-764.088	-764.088	-764.087	-764.086	-764.061	-764.060	-764.052	-764.052
	S_1	-763.972	-763.972	-763.974	-763.973	-763.954	-763.954	-763.946	-763.948

Table S2 Calculated Electronic Excitation Energy (EEE), and corresponding Oscillator Strength (OS) of the low-lying electronically excited states for N-I and C-II species, as well as Orbital Transition (OT) contributions to the electronic excited states.

State	N-I			C-II		
	EEE (nm)	OS	OT	EEE (nm)	OS	OT
S_1	332.07	0.7361	H→L	340.44	0.3928	H→L
S_2	296.55	0.0005	H-3→L+1	305.25	0.4285	H-1→L
S_3	288.95	0.0229	H-1→L	268.43	0.0007	H-3→L
S_4	256.38	0.1411	H-2→L	244.85	0.0101	H-2→L
S_5	219.32	0.0003	H-5→L	223.24	0.1073	H→L+1
S_6	215.57	0.0745	H→L+1	208.71	0.2125	H→L+2

Table S3 Huang–Rhys factors of the dominating normal modes for the $S_0 \rightarrow S_1$ absorption of N-I, $S_1 \rightarrow S_0$ emissions of N-I* and C-III*.

Absorption ($S_0 \rightarrow S_1$) of N-I			*vs*	Emission ($S_1 \rightarrow S_0$) of N-I*			*vs*	Emission ($S_1 \rightarrow S_0$) of C-III*		
modes	ω	S		modes	ω	S		modes	ω	S
17	355.1082	0.1353		17	349.7936	0.1135		4	82.6303	0.1057
28	724.8818	0.2480		28	729.1128	0.1338		16	318.8042	0.1525
52	1306.6538	0.1208		55	1386.7916	0.1228		20	435.7734	0.1020
69	1652.398	0.1915		73	1699.0021	0.1011		34	799.0847	0.1136
70	1659.0341	0.1170						53	1279.4718	0.1343
72	1729.3395	0.2569						55	1350.3739	0.1264
								75	1698.7643	0.1321

Table S4 Large and unusable Huang–Rhys factors of the high-frequency normal modes for the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ absorptions of C-II, $S_1 \rightarrow S_0$ emissions of DC-IV*, which have been removed in the following FC simulations.

Absorption ($S_0 \rightarrow S_1$) of C-II			*vs*	Absorption ($S_0 \rightarrow S_2$) of C-II			*vs*	Emission ($S_1 \rightarrow S_0$) of DC-IV*		
modes	ω	S		modes	ω	S		modes	ω	S
33	824.8164	1.0903		37	963.8058	1.7565		33	756.8862	12.9309
37	963.8058	4.7416		43	1073.2531	1.1707		47	1163.8785	10.3757
38	980.4851	3.0418		79	3118.0606	3.6545		82	3180.8083	14.6977
46	1164.8073	2.0607		80	3149.0593	2.9396		84	3183.6513	22.5716
79	3118.0606	2.1326						85	3215.9174	11.6185
81	3178.6701	4.0055								

Table S5 Huang–Rhys factors of the low-frequency normal modes for the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ absorptions of C-II, $S_1 \rightarrow S_0$ emissions of DC-IV*, which are involved in the following FC simulations.

Absorption ($S_0 \rightarrow S_1$) of C-II			*vs*	Absorption ($S_0 \rightarrow S_2$) of C-II			*vs*	Emission ($S_1 \rightarrow S_0$) of DC-IV*		
modes	ω	S		modes	ω	S		modes	ω	S
1	29.3958	1.1333		1	29.3958	2.8618		2	49.6738	6.5675
2	55.5958	5.1811		7	136.8322	0.1694		3	71.079	5.5221
3	68.9975	0.1880		13	269.3266	0.1882		5	126.212	2.4656
4	100.8659	0.1106		14	282.3839	0.3677		6	140.6789	1.2246
7	136.8322	0.1305		20	498.9786	1.0812		12	234.369	2.0150
10	211.7405	0.1892		21	557.9497	0.6141		13	263.8674	1.4738
11	221.9794	0.2410		22	583.5515	0.3167		17	338.9507	2.4474
12	252.5548	0.3915		23	594.0724	0.1087		19	372.505	1.2110
13	269.3266	0.2664		24	597.6835	0.1963		21	465.0474	4.1829
14	282.3839	0.5537		27	666.0833	0.2210				
16	328.3478	0.4046		31	773.3502	0.3290				
17	354.7018	0.1526		32	802.706	0.5083				
19	462.3081	0.1140		34	885.0354	0.2864				
20	498.9786	1.7425		35	927.2171	0.2518				
21	557.9497	0.2243		36	929.3747	0.2381				
22	583.5515	0.2349								
23	594.0724	0.1666								
24	597.6835	2.7904								
27	666.0833	0.4062								
28	674.7309	1.5607								