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SUPPLEMENTARY MATERIAL TO

Solvent, substituents and pH effects towards the spectral shifts of some highly colored indicators

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The chemical structures and the corresponding abbreviations of the six studied indicators are given in Fig. S-1.

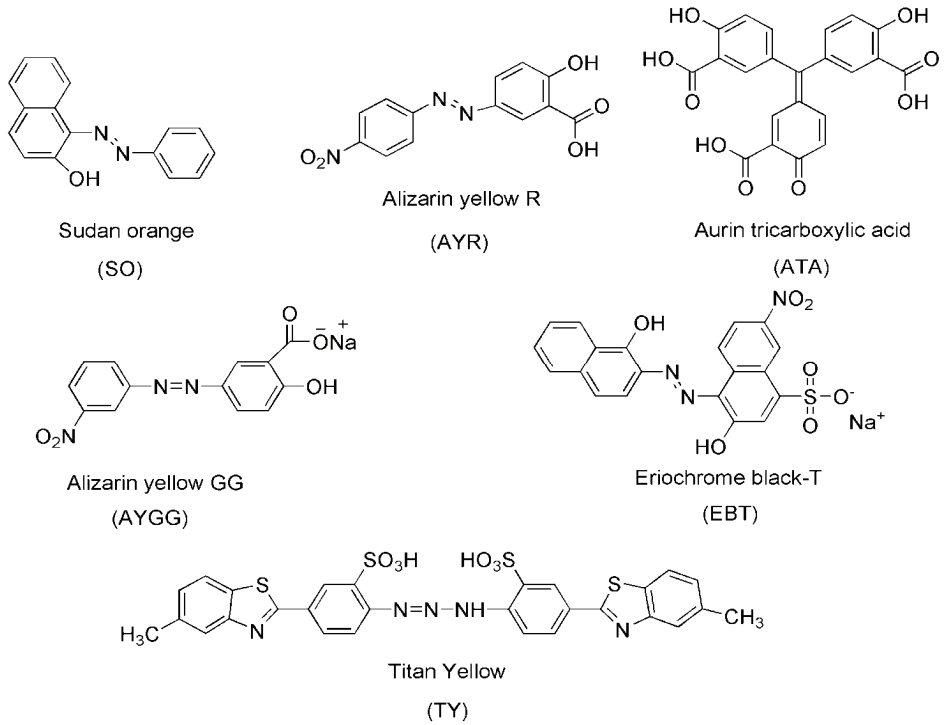

Fig. S-1. Structure of the investigated indicators and their abbreviations.

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The pH effect on the absorption spectra

A representative example for the effect of pH on the absorption spectra of AYGG is given Fig. S-2.

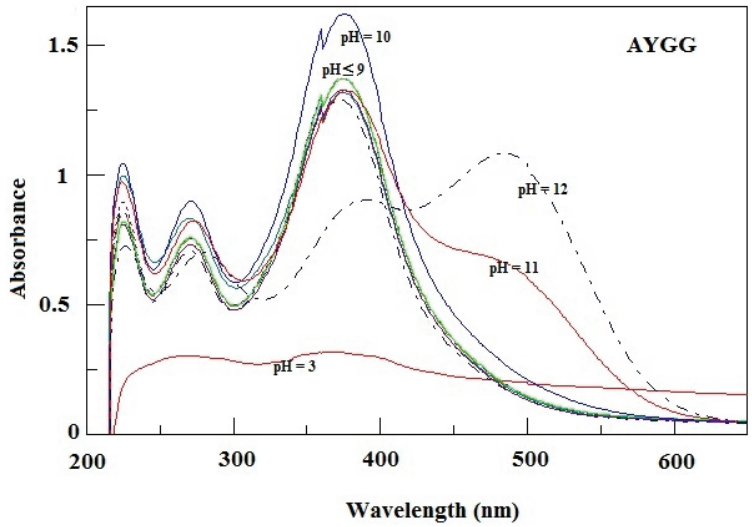

Fig. S-2. Effect of pH on the electronic absorption spectra of 1×10^{-4} M of AYGG.

The solvent parameters

TABLE S-I. The Physical parameters for the solvents

Solvent	Dioxane	Ethanol	DMF	DMSO	Acetone	Acetonitrile	H_2O
n	1.422	1.361	1.427	1.478	1.359	1.344	1.333
D	2.2	24.3	36.7	48.9	20.7	37.5	78.5
K	0.223	0.470	0.480	0.485	0.465	0.48	0.491
M	0.203	0.181	0.204	0.221	0.180	0.175	0.171
N	0.031	0.665	0.666	0.658	0.648	0.712	0.757
E	36.0	51.9	43.8	45.0	42.2	46.0	63.1
J	0.286	0.886	0.922	0.941	0.868	0.924	0.963
H	0.254	0.221	0.257	0.283	0.220	0.212	0.206
β	0.37	0.77	0.69	0.76	0.48	0.31	0.47
α	0.00	0.83	0.00	0.00	0.08	0.19	1.17
π^*	0.55	0.54	0.87	1.00	0.71	0.75	1.09

The regression data for the indicator

TABLE S-II. Regression analysis data for Y_1 and Y_2 bands for SO indicator

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
			Y_1				
K	314.092	–10.037				0.281	0.358
M	292.304	89.085				0.585	0.132
N	312.171	–4.339				0.334	0.307
E	323.149	–0.300				0.621	0.113
K,M	297.235	–7.851	81.069			0.752	0.248
K,N	287.678	115.606	–49.984			0.614	0.386
K,E	325.008	6.196	–0.401			0.657	0.343
M,N	296.353	77.102	–3.104			0.745	0.255
M,E	307.574	58.557	–0.208			0.816	0.184
N,E	325.651	1.880	–0.379			0.640	0.360
K,M,N	338.248	–411.615	297.965	162.954		0.925	0.345
K,M,E	307.498	–9.85E–02	58.732	–0.206		0.816	0.529
K,N,E	304.406	85.937	–33.453	–0.294		0.780	0.575
M,N,E	307.699	58.381	5.84E–02	–0.211		0.816	0.529
			Y_2				
K	416.508	–9.860				0.009	0.844
M	317.234	498.397				0.787	0.008
N	416.989	–8.196				0.039	0.672
E	451.818	–0.847				0.490	0.080
K,M	303.480	18.850	526.797			0.816	0.034
K,N	227.867	882.599	–349.177			0.896	0.011
K,E	444.992	52.666	–1.199			0.649	0.123
M,N	306.622	533.118	6.765			0.810	0.036
M,E	351.369	405.771	–0.352			0.845	0.024
N,E	457.490	18.886	–1.206			0.609	0.153
K,M,N	243.283	639.102	177.567	–250.122		0.916	0.040
K,M,E	349.573	47.246	388.287	–0.689		0.943	0.008
K,N,E	269.565	741.252	–286.940	–0.340		0.919	0.038
M,N,E	356.298	409.369	19.379	–0.716		0.969	0.009
K,M,N,E	329.412	187.900	325.422	–58.246	–0.597	0.974	0.051

TABLE S-III. Regression analysis data for Y_1 and Y_2 bands for AYR indicator

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
			Y_1				
K	278.210	52.012				0.640	0.056
M	291.506	49.406				0.020	0.790
N	289.814	19.237				0.582	0.078
E	294.136	0.144				0.037	0.716
K,M	249.686	58.602	133.406			0.774	0.107
K,N	242.474	221.207	–66.036			0.724	0.145
K,E	287.856	75.086	–0.415			0.818	0.078
M,N	254.429	170.495	23.745			0.786	0.099

TABLE S-III. Continued

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
			Y_1				
M,E	250.198	168.840	0.385			0.166	0.761
N,E	307.157	31.277	–0.511			0.815	0.079
K,M,N	288.769	–397.975	415.403	183.635		0.825	0.251
K,M,E	273.621	72.229	55.620	–0.314		0.831	0.243
K,N,E	294.849	48.010	11.358	–0.451		0.819	0.259
M,N,E	282.135	94.008	29.937	–0.349		0.854	0.211
K,M,N,E	370.372	–802.391	535.333	356.551	–0.588	0.977	0.225
			Y_2				
K	379.351	28.895				0.398	0.129
M	415.873	–124.617				0.268	0.234
N	384.916	12.222				0.471	0.089
E	379.131	0.278				0.287	0.215
K,M	398.304	24.081	–88.336			0.522	0.229
K,N	424.896	–186.579	84.305			0.680	0.103
K,E	376.264	22.118	0.130			0.158	0.315
M,N	399.884	–72.301	10.193			0.548	0.204
M,E	397.919	–75.898	0.185			0.354	0.417
N,E	382.270	10.453	7.880			0.484	0.266
K,M,N	436.429	–368.745	132.843	158.411		0.741	0.205
K,M,E	397.034	23.298	–84.520	1.899		0.044	0.472
K,N,E	458.156	–299.326	133.949	–0.271		0.760	0.184
M,N,E	400.555	–73.974	10.364	–9.684E–03		0.548	0.438
K,M,N,E	503.883	–722.116	248.640	308.684	–0.468	0.934	0.128

TABLE S-IV. Regression analysis data for Y_1 and Y_2 bands for ATA indicator

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
			Y_1				
K	277.052	58.079				0.767	0.022
M	307.047	–23.663				0.004	0.901
N	289.746	21.932				0.727	0.031
E	290.565	0.251				0.107	0.528
K,M	263.341	61.247	64.127			0.797	0.092
K,N	256.988	153.074	–37.076			0.792	0.095
K,E	284.264	75.332	–0.310			0.862	0.051
M,N	268.593	101.924	24.627			0.797	0.091
M,E	265.345	96.912	0.389			0.148	0.787
N,E	303.739	31.646	–0.412			0.873	0.045
K,M,N	267.393	13.901	93.369	19.042		0.797	0.288
K,M,E	290.157	76.514	–23.026	–0.352		0.864	0.196
K,N,E	306.314	–10.043	35.813	4.000		0.873	0.184
M,N,E	298.825	18.463	31.383	–0.380		0.874	0.182
K,M,N,E	333.112	–311.794	189.954	158.299	–0.473	0.892	0.475

TABLE S-IV. Continued

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
			Y_2				
K	395.774	–2.715				0.004	0.888
M	381.445	68.929				0.102	0.486
N	395.625	–1.782				0.012	0.812
E	409.108	–0.310				0.445	0.102
K,M	380.618	1.135	70.639			0.102	0.806
K,N	364.235	146.492	–58.378			0.172	0.686
K,E	406.428	20.673	–0.448			0.610	0.152
M,N	381.167	69.841	0.178			0.102	0.807
M,E	413.732	–18.680	–0.333			0.450	0.303
N,E	411.825	9.050	–0.482			0.628	0.138
K,M,N	359.967	213.910	–49.164	–85.804		0.183	0.875
K,M,E	412.932	21.042	–26.467	–0.483		0.620	0.349
K,N,E	438.568	–105.482	52.570	–0.606		0.671	0.287
M,N,E	416.029	–17.003	9.030	–0.503		0.633	0.333
K,M,N,E	461.618	–318.611	125.339	140.654	–0.705	0.726	0.473

TABLE S-V. Regression analysis data for Y_1 and Y_2 bands for AYGG indicator

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
			Y_1				
K	262.225	–0.893				0.000	0.969
M	232.235	154.026				0.444	0.149
N	262.764	–1.600				0.009	0.856
E	270.978	–0.192				0.149	0.449
K,M	227.077	7.227	164.386			0.470	0.386
K,N	207.004	260.556	–102.042			0.463	0.394
K,E	269.581	16.704	–0.316			0.238	0.665
M,N	227.773	168.598	2.857			0.469	0.387
M,E	226.827	169.662	5.045			0.449	0.409
N,E	273.380	5.769	–0.313			0.210	0.702
K,M,N	218.124	111.824	99.783	–42.069		0.476	0.672
K,M,E	229.644	8.689	156.042	–3.368		0.471	0.676
K,N,E	204.243	269.686	–106.121	2.378		0.463	0.685
M,N,E	230.533	160.977	3.474	–3.474		0.471	0.677
K,M,N,E	218.371	110.600	100.146	–41.545	–1.780	0.476	0.896
			Y_2				
K	374.040	–39.781				0.159	0.376
M	388.693	–169.431				0.104	0.481
N	364.214	–13.167				0.115	0.457
E	360.080	–7.793				0.005	0.883
K,M	427.655	–53.400	–249.885			0.366	0.402
K,N	468.745	–487.830	175.300			0.414	0.343
K,E	367.186	–54.827	0.288			0.201	0.639
M,N	421.536	–276.889	–20.937			0.353	0.419
M,E	429.300	–279.617	–0.419			0.197	0.645

TABLE S-V. Continued

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
				Y_2			
N,E	354.093	–19.934	0.301			0.156	0.713
K,M,N	466.733	–456.053	–23.173	162.373		0.415	0.608
K,M,E	431.245	–260.674	–51.188	–5.367		0.367	0.667
K,N,E	532.935	–705.420	271.109	–0.523		0.477	0.529
M,N,E	424.142	–283.381	–20.275	–3.759		0.353	0.684
K,M,N,E	557.250	–930.240	132.215	364.024	–0.628	0.488	0.762

TABLE S-VI. Regression analysis data for Y_1 and Y_2 bands for EBT indicator

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
				Y_1			
K	292.604	–24.960				0.277	0.283
M	277.336	22.536				0.008	0.868
N	287.216	–9.543				0.269	0.291
E	293.709	–0.253				0.213	0.357
K,M	295.651	–25.664	–14.251			0.280	0.611
K,N	296.073	–41.386	6.411			0.279	0.612
K,E	295.264	–18.596	–0.114			0.303	0.582
M,N	293.484	–30.201	–10.342			0.282	0.609
M,E	319.778	–100.179	–0.396			0.298	0.588
N,E	290.760	–7.083	–0.104			0.288	0.601
K,M,N	289.698	43.877	–57.202	–27.970		0.282	0.850
K,M,E	315.035	–14.628	–77.250	–0.254		0.350	0.793
K,N,E	330.868	–156.449	57.827	–0.300		0.358	0.786
M,N,E	313.523	–85.523	–5.863	–0.252		0.358	0.795
K,M,N,E	331.456	–163.070	4.168	60.514	–0.301	0.358	0.945
				Y_2			
K	406.647	–16.443				0.254	0.308
M	398.778	3.728				0.000	0.970
N	403.180	–6.528				0.254	0.308
E	425.142	–0.581				0.789	0.018
K,M	410.305	–17.088	–17.440			0.262	0.634
K,N	404.526	–6.353	–4.017			0.254	0.644
K,E	428.191	12.975	–0.778			0.857	0.054
M,N	408.474	–25.851	–7.038			0.271	0.622
M,E	441.902	–67.092	–0.666			0.898	0.032
N,E	432.249	6.086	–0.819			0.877	0.043
K,M,N	387.182	181.010	–109.178	–80.219		0.319	0.820
K,M,E	447.011	14.899	–73.530	–0.900		0.986	0.021
K,N,E	458.665	–109.310	50.698	–0.911		0.951	0.072
M,N,E	448.921	–66.859	6.059	–0.903		0.985	0.022
K,M,N,E	444.832	31.449	–80.942	–6.781	–0.895	0.986	0.174

TABLE S-VII. Regression analysis data for Y_1 and Y_2 bands for TY indicator

Parameter	a_0	a_1	a_2	a_3	a_4	*MCC*	*P*
			Y_1				
K	441.698	–249.581				0.423	0.235
M	315.416	32.548				0.054	0.708
N	352.286	–44.369				0.402	0.251
E	322.126	–1.052				0.001	0.964
K,M	437.571	–256.181	38.442			0.497	0.503
K,N	416.697	–160.021	–26.165			0.508	0.492
K,E	457.720	–293.802	0.105			0.489	0.511
M,N	385.178	–73.920	–71.621			0.527	0.473
M,E	307.423	53.033	8.209			0.081	0.919
N,E	374.626	–108.172	0.436			0.946	0.054
K,M,N	–1108.976	7002.622	–3050.621	–1965.685		0.920	0.356
K,M,E	491.609	–458.300	151.594	0.435		0.993	0.109
K,N,E	415.892	–105.074	–93.282	0.416		0.991	0.120
M,N,E	393.261	–44.800	–120.976	0.411		0.991	0.123
			Y_2				
K	280.821	266.019				0.094	0.555
M	355.899	278.413				0.558	0.088
N	437.009	–41.882				0.058	0.645
E	403.565	9.798				0.011	0.841
K,M	280.611	161.641	266.772			0.591	0.261
K,N	125.796	811.188	–155.246			0.502	0.351
K,E	266.602	303.183	–7.385			0.098	0.856
M,N	311.567	338.076	48.338			0.610	0.244
M,E	303.972	399.963	0.597			0.870	0.047
N,E	483.512	–168.709	0.829			0.331	0.548
K,M,N	670.455	–1444.981	864.913	390.868		0.679	0.441
K,M,E	465.715	–415.608	504.412	0.962		0.975	0.038
K,N,E	153.963	873.589	–306.078	0.929		0.841	0.229
M,N,E	355.892	358.552	–87.805	0.925		0.947	0.079
K,M,N,E	670.285	–1269.805	821.065	216.230	0.905	1.000	0.011