

The Methylene Blue Self-aggregation in Water/Organic Solvent Mixtures: Relationship Between Solvatochromic Properties and Singlet Oxygen Production

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Supporting Information

Table S1. Photophysical properties of MB, concentration of 3.13×10^{-4} mol L⁻¹, in water/acetonitrile, water/ethanol, water/glycerol and water/dioxane mixtures.

	λ_A (nm)	ν (cm ⁻¹)	Abs	ϵ (Lmol ⁻¹ cm ⁻¹)	λ_F (nm)	ν (cm ⁻¹)	$\nu_A - \nu_F$ (cm ⁻¹)
EtOH %							
0	667	14993	0.08	80450	685	14600	393
10	668	14967	0.09	88660	685	14600	367
20	669	14949	0.10	96720	685	14600	349
30	669	14949	0.09	94710	685	14595	354
40	671	14906	0.11	105810	686	14575	331
50	668	14967	0.08	84980	688	14536	431
60	667	14993	0.09	90270	684	14610	383
70	668	14967	0.10	97540	685	14605	362
80	662	15107	0.10	104320	684	14625	482
90	661	15124	0.10	96770	680	14700	424
100	659	15178	0.11	112200	677	14771	407
ACN %							
0	668	14973	0.05	39050	685	14599	374
10	669	14949	0.05	40260	683	14640	309
20	668	14973	0.05	25540	687	14558	415

30	667	14989	0.05	32410	684	14622	367
40	666	15013	0.05	28650	686	14576	437
50	666	15013	0.06	36940	683	14640	373
60	666	15021	0.06	50470	684	14626	395
70	664	15070	0.06	39120	682	14672	398
80	663	15078	0.06	39310	680	14709	369
90	661	15127	0.06	44970	677	14770	357
100	658	15198	0.06	65970	674	14837	361
Diox %							
0	670	14934	0.04	39050	685	14594	340
10	669	14942	0.04	40260	685	14594	348
20	667	14986	0.03	25540	687	14564	422
30	668	14968	0.03	32410	688	14534	434
40	668	14968	0.03	28650	687	14554	414
50	668	14960	0.04	36940	684	14618	341
60	667	14994	0.05	50470	684	14624	371
70	668	14977	0.04	39120	685	14599	378
80	667	14994	0.04	39310	683	14638	356
90	666	15012	0.04	44970	681	14678	333
100	652	15342	0.07	65970	663	15075	268
Gly %							
0	664	15060	0.04	39050	688	14535	525
10	666	15015	0.04	40260	692	14451	564
20	667	14993	0.03	25540	693	14430	562
30	669	14948	0.03	32410	693	14430	518
40	670	14925	0.03	28650	695	14388	537
50	669	14948	0.04	36940	696	14368	580
60	669	14948	0.05	50470	698	14327	621
70	667	14993	0.04	39120	699	14306	686
80	666	15015	0.04	39310	700	14286	729
90	666	15015	0.04	44970	700	14286	729
100	662	15106	0.07	65970	700	14286	820

λ_A : wavelength of maximum absorption. λ_F : wavelength of maximum emission. ε : molar absorptivity coefficient. ν_A - ν_F : Stokes shift. ABS: absorbance.