Supporting information for

Aggregation induced colour change for phosphorescent iridium(III) complex-based anionic surfactants

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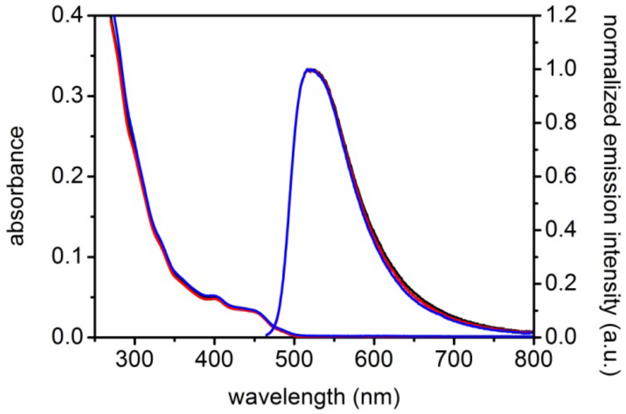

Figure S1. UV-Vis and normalized emission spectra for complexes **2** (black trace), **3** (red trace) and **4** (blue trace) in *N*,*N*-dimethylformamide at concentration of 1.0×10^{-5} M in degassed condition. All the samples were excited at λ = 400 nm.

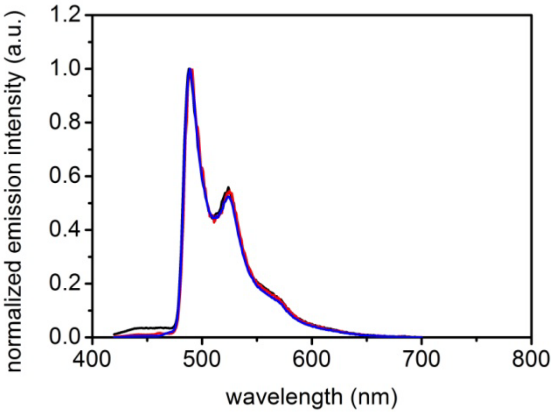

Figure S2. Emission spectra for complexes **2** (black trace), **3** (red trace) and **4** (blue trace) in BuCN glassy matrix at 77K. The samples were excited at λ = 400 nm.

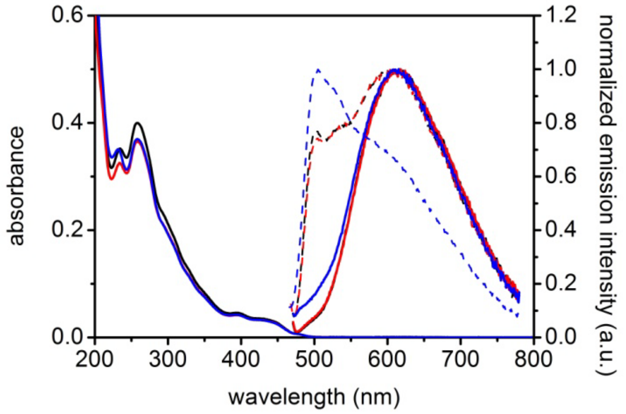

Figure S3. Absorption and emission spectra for complexes **2** (black lines), **3** (red lines) and **4** (blue lines) at concentration of 1.0×10^{-5} M in air-equilibrated (solid traces) and degassed (dashed traces) MeOH. The samples were excited at $\lambda = 400$ nm.

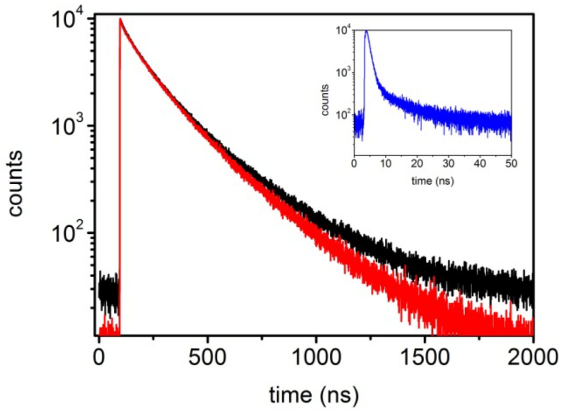

Figure S4. Excited-state emission decay for samples of complex **5** at different concentrations in air-equilibrated bi-distilled H_2O: black trace: 1.8×10^{-3} M; red trace: 4×10^{-4} M. Inset: concentration 1.0×10^{-5} M. The samples were excited at $\lambda = 375$ nm.

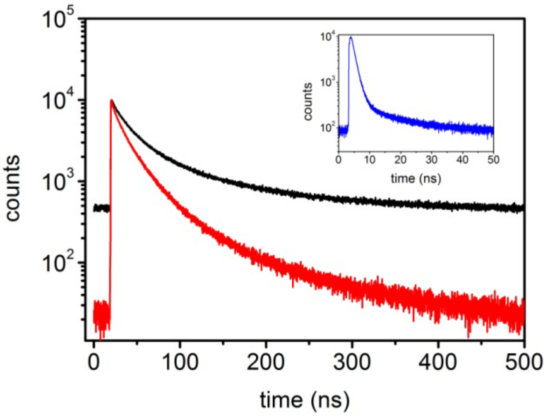

Figure S5. Excited-state emission decay for samples of complex **6** at different concentrations in air-equilibrated bi-distilled H_2O: black trace: 1.9 $\times 10^{-3}$ M; red trace: 4×10^{-4} M. Inset: concentration 1.0 x10^{-5} M. The samples were excited at $\lambda = 375$ nm.

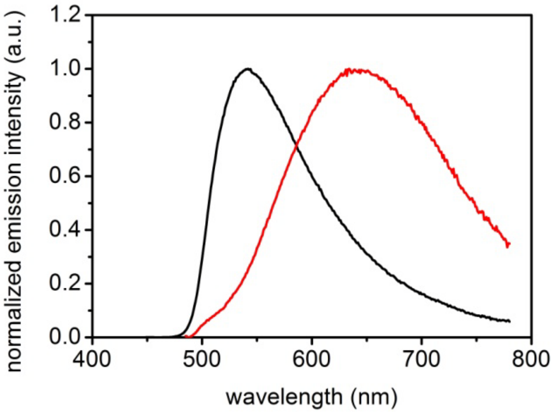

Figure S6. Normalized emission spectra of complex **6** at concentration 1.9×10^{-3} M (black trace) and 1.0×10^{-5} M (red trace) in air-equilibrated H_2O, showing the blue shift upon aggregation at higher concentration.

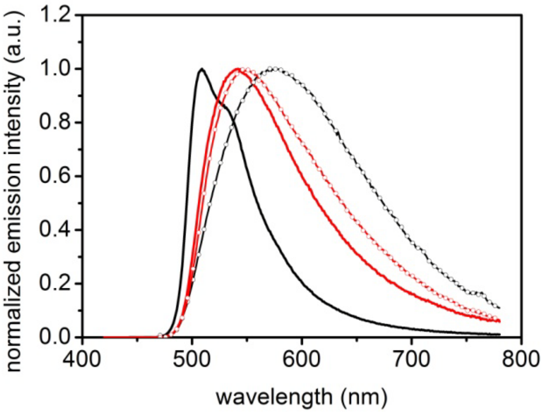

Figure S7. Comparison between emission of aggregates in solutions and solid state samples for complexes **5**–**6**. Black curves: complex **5** at concentration 1.8×10^{-3} M in air-equilibrated H_2O (solid line) and solid state sample (empty circles); red curves: complex **6** at concentration 1.9×10^{-3} M (solid line) and solid state sample (empty circles). The samples were excited at $\lambda = 400$ nm.

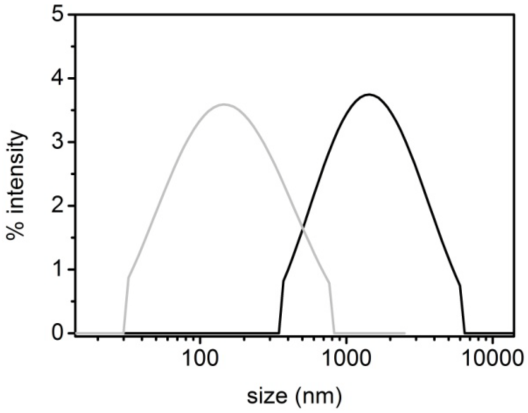

Figure S8. Size distribution at concentration of *ca.* 2×10^{-3}M for aggregated complex **5** (black trace) and **6** (gray trace) in bi-distilled H_2O, as obtained by DLS analysis.

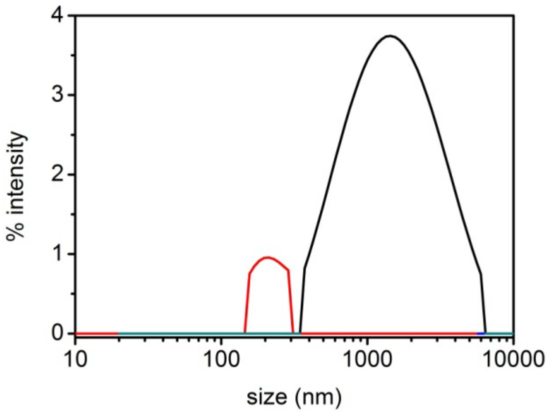

Figure S9. Effect on the particle size distributions for complex **5** at concentration of 1.8×10^{-3} M in air-equilibrated bi-distilled H_2O upon titration with SDS, as obtained by DLS analysis. Titration with 0.1 M SDS solution, upon adding 0 eq. of SDS (black trace); 1/24 eq. of SDS (red trace); 1/12 eq. of SDS (blue trace); 1/6 eq. of SDS (green trace).

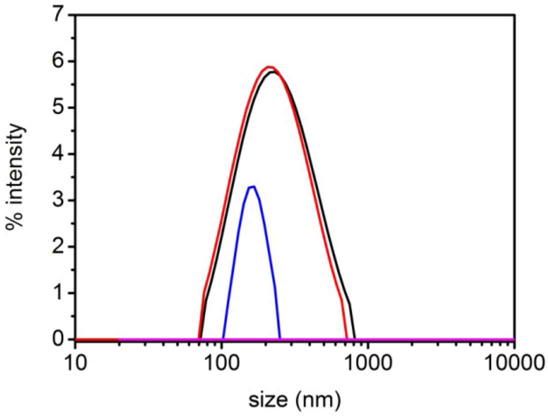

Figure S10. Effect on the particle size distributions for of complexes **6** at concentration of 4×10^{-4} M in air-equilibrated bi-distilled H_2O upon titration with SDS, as obtained by DLS analysis. Titration with 0.1 M SDS solution, upon adding 0 eq. of SDS (black trace); 1/24 eq. of SDS (red trace); 1/12 eq. of SDS (blue trace); 1/6 eq. of SDS (magenta trace).

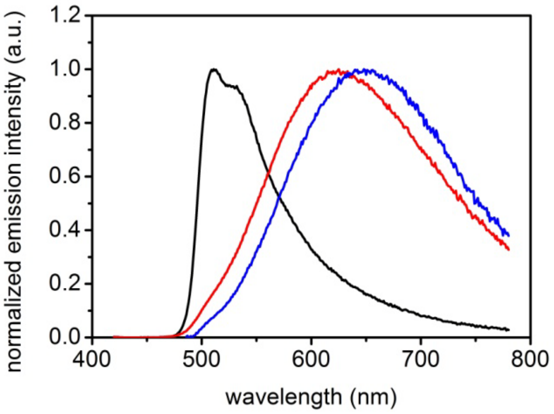

Figure S11. Comparison between emission spectra of complex **5** in air-equilibrated H_2O: aggregated species at concentration 1.8×10^{-3} M (black trace); upon addition of 1/6 eq. of SDS (red trace); sample at concentration 1.0×10^{-5} M (blue curve). The samples were excited at $\lambda = 400$ nm.

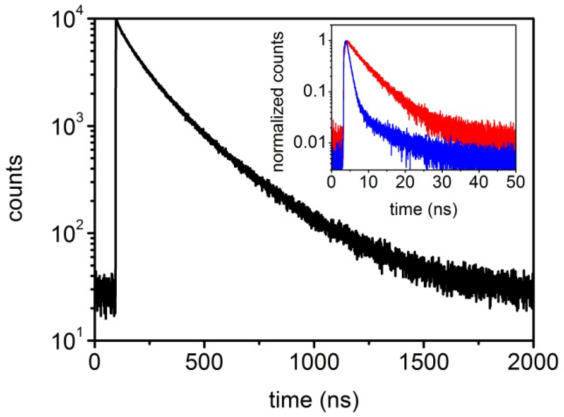

Figure S12. Time resolved emission decays of complex **5** in air-equilibrated H_2O: aggregated species at concentration 1.8×10^{-3} M (black trace). Inset: decay upon addition of 1/6 eq. of SDS (red trace); sample at concentration 1.0×10^{-5} M (blue curve). The samples were excited at $\lambda = 400$ nm.

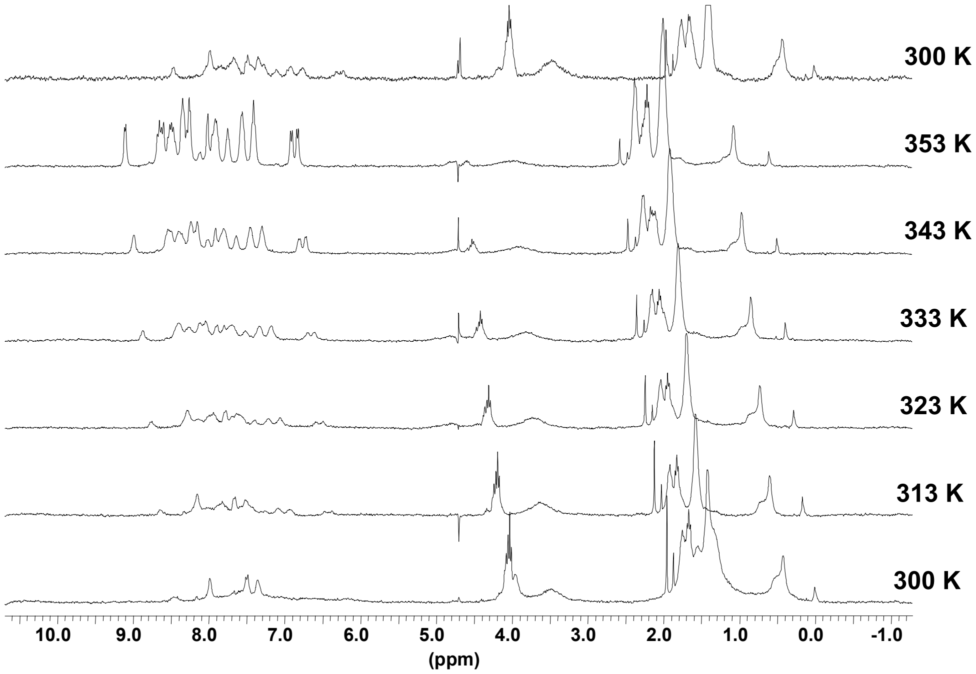

Figure S13. Variable temperature ^{1}H NMR spectra (from the bottom) of a 3.0×10^{-3} M solution of compound **5** in D_2O. The upper trace has been recorded after cooling the sample back to 300 K.

		air-equilibrated			*degassed*		
Complex	abs (ε) [nm, (10^3 M^{-1} cm^{-1})]	λ_{em} [nm]	τ [ns]	PLQY (%)	λ_{em} [nm]	τ [ns]	PLQY (%)
2	233 (35.0), 259 (40.0), 396 (4.6), 437 (3.3), 480 (0.6)	615	6	0.2	502, 527, 615sh	2 (58%) [b] 10 (35%) [b] 339 (5%) [b] 692 (2%) [b] 6 (97%) [c] 33 (3%) [c]	0.3
3	233 (32.4), 259 (36.5), 396 (4.2), 437 (3.1), 480 (0.6)	615	6	0.2	502sh, 615	6 (89%) [b] 20 (5%) [b] 317 (3%) [b] 710 (2%) [b] 6 (99%) [c] 33 (1%) [c]	0.3
4	233 (35.0), 259 (37.0), 396 (4.2), 437 (3.0), 480 (0.6)	615	6	0.2	503, 525, 613 [a]	5 (79%) [b] 26 (9%) [b] 453 (10%) [b] 1080 (2%) [b] 7 (98%) [c] 43 (2%) [c]	0.4
5	233 (28.3), 259 (30.9), 396 (3.7), 437 (2.7), 480 (0.6)	615	7	0.3	502, 525sh, 613	2 (62%) [b] 9 (32%) [b] 502 (5%) [b] 2148 (1%) [b] 7 (97%) [c] 39 (3%) [c]	0.4
6	232 (31.0), 259 (30.7), 396 (3.5), 437 (2.6), 480 (0.5)	615	6	0.3	503, 525sh, 613	6 (96%) [b] 38 (2%) [b] 661 (2%) [b] 7 (99%) [c] 38 (1%) [c]	0.3

Table S1. Most meaningful photophysical data for complexes **2**–**6** at concentration of 1.0×10^{-5} M in both air-equilibrated and degassed MeOH solutions. [a] very broad; [b] measured at 502 nm; [c] measured at 625 nm.