Electronic supplementary information (ESI)

Complexes of In(III) with 8-hydroxyquinoline-5-sulfonate in solution: Structural studies and the effect of cationic surfactants on the photophysical behaviour

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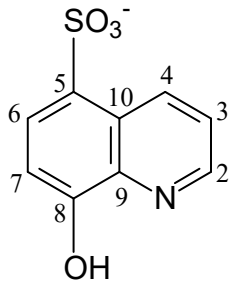
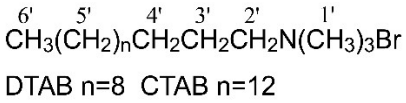


8-HQS



DTAB / CTAB

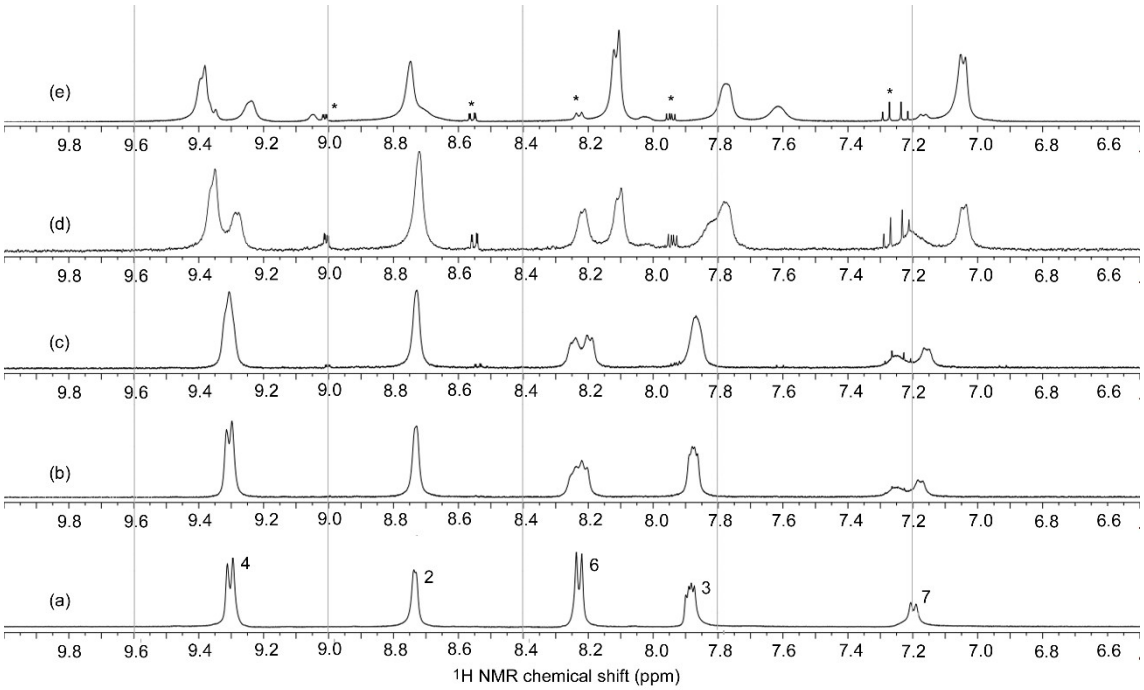


Fig. S1. Expansion 6.5-10 ppm of the ^{1}H NMR spectra of D_2O solutions of (a) In^{3+}/8-HQS 2.5 : 7.5 mmol dm^{-3}, pH 4.25, (b) In^{3+}/8-HQS/CTAB 2.5 : 7.5 : 0.5 mmol dm^{-3}, (c) In^{3+}/8-HQS/CTAB 2.5 : 7.5 : 1.0 mmol dm^{-3} (d) In^{3+}/8-HQS/CTAB 2.5 : 7.5 : 5.0 mmol dm^{-3} (e) In^{3+}/8-HQS/CTAB 2.5 : 7.5 : 10 mmol dm^{-3}, temp. 298 K. *8-HQS ligand signals.

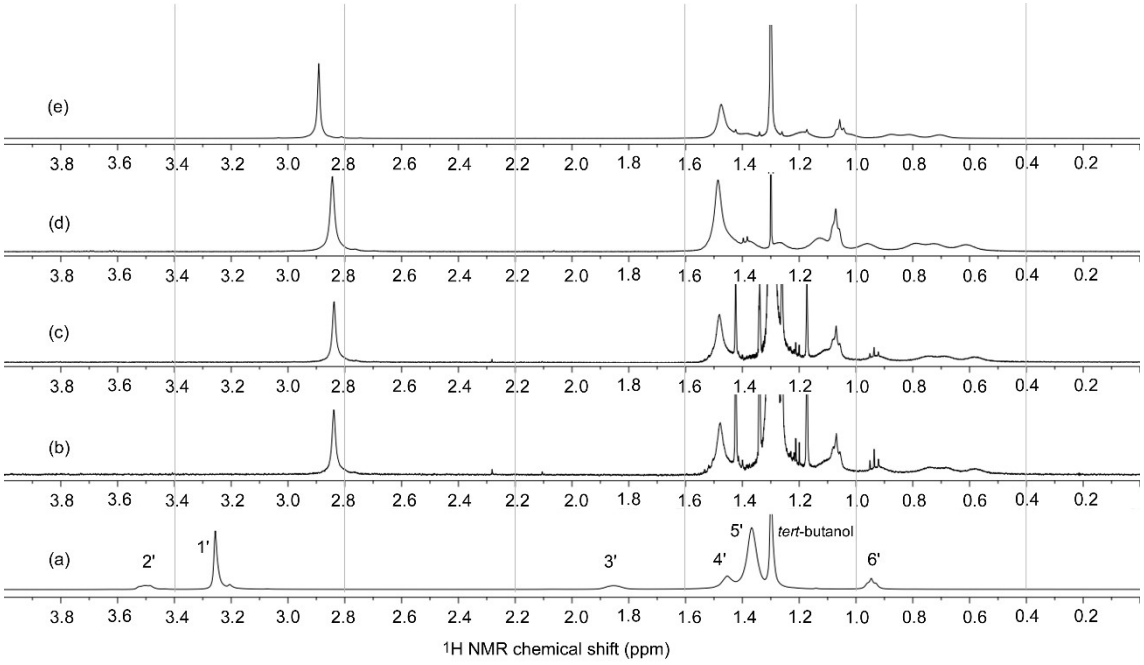


Fig. S2. Expansion 0-4 ppm of the ^{1}H NMR spectra of D_2O solutions of (a) CTAB 10 mmol dm^{-3}, pH* 6.87, (b) In^{3+}/8-HQS/CTAB 2.5:7.5:0.5 mmol dm-3, (c) In^{3+}/8-HQS/CTAB 2.5:7.5:1 mmol dm^{-3}, (d) In^{3+}/8-HQS/CTAB 2.5:7.5:5 mmol dm-3 and (e) In^{3+}/8-HQS/CTAB 2.5:7.5:10 mmol dm-3, temp. 298 K.

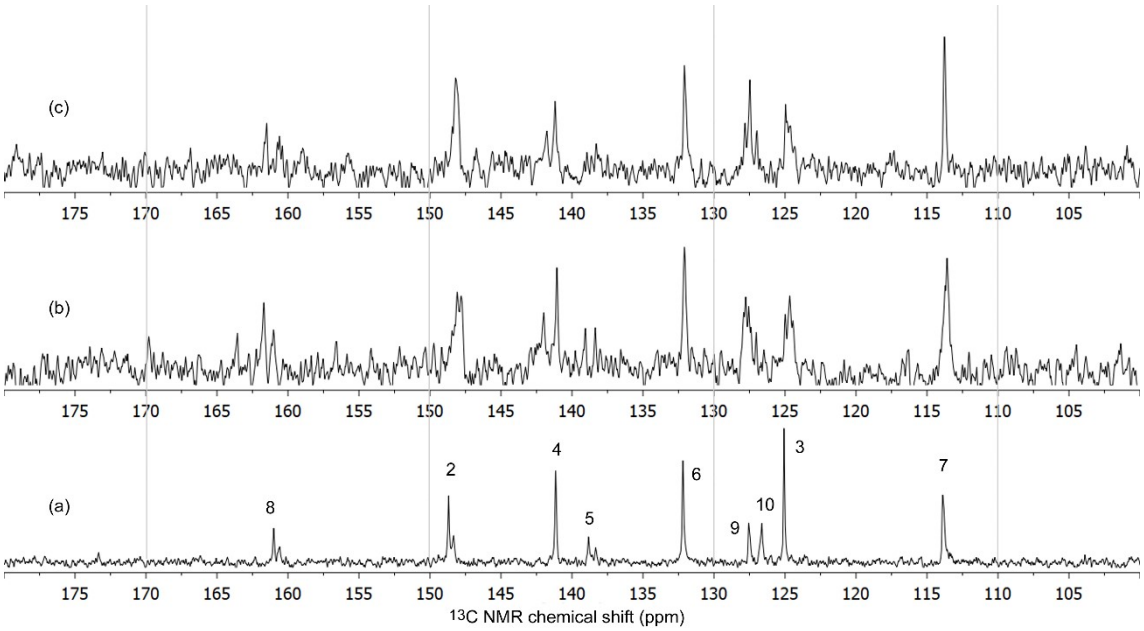


Fig. S3. Expansion 100-180 ppm of the ^{13}C NMR spectra of D_2O solutions of (a) In^{3+}/8-HQS 2.5: 7.5 mmol dm^{-3}, pH 4.25, (b) In^{3+}/8-HQS/DTAB 2.5 : 7.5 : 2.0 mmol dm^{-3}, (c) In^{3+}/8-HQS/DTAB 2.5 : 7.5 : 20 mmol dm^{-3}, temp. 298 K.

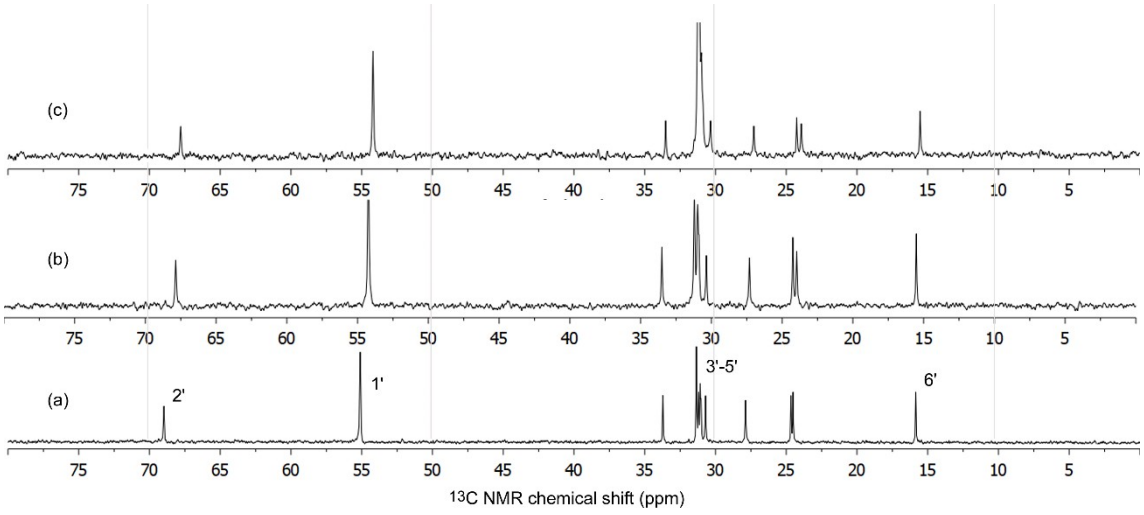


Fig. S4. Expansion 0-80 ppm of the ^{13}C NMR spectra of solutions in D_2O of (a) DTAB 20 mmol dm^{-3}, pH 6.04, (b) In^{3+}/8-HQS/DTAB 2.5 : 7.5 : 2.0 mmol dm^{-3} (c) In^{3+}/8-HQS/DTAB 2.5 : 7.5 : 20 mmol dm^{-3}, temp. 298 K.

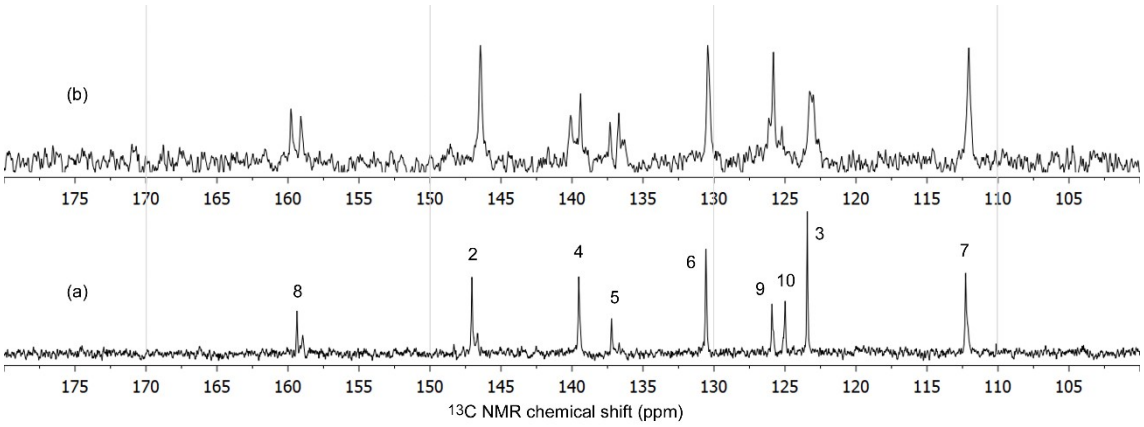


Fig. S5. Expansion 100-180 ppm of the ^{13}C NMR spectra of D_2O solutions of (a) In^{3+}/8-HQS 2.5:7.5 mmol dm-3, pH 4.25 (b) In^{3+}/8-HQS/CTAB 5:10:5.0 mmol dm^{-3}, temp. 298 K.

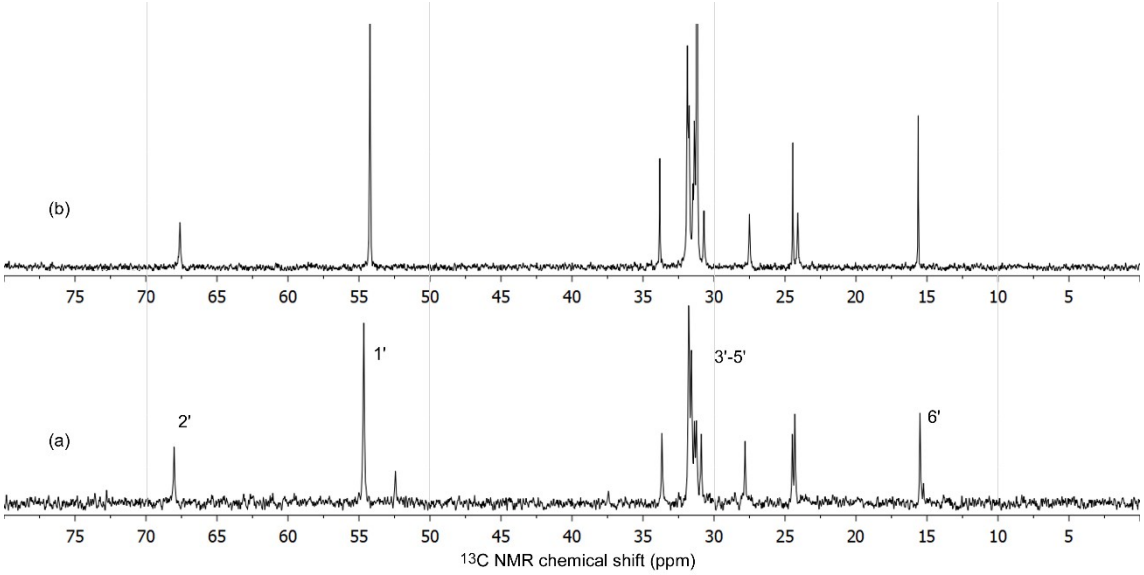
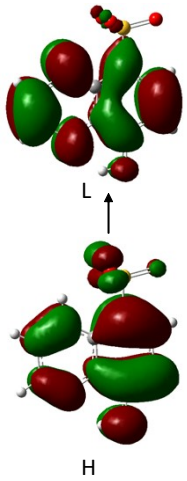


Fig. S6. Expansion 0-80 ppm of the ^{13}C NMR spectra of solutions in D_2O of (a) CTAB 10 mmol dm^{-3}, pH 6.87, (b) In^{3+}/8-HQS/CTAB 2.5 : 7.5 : 10 mmol dm^{-3}, temp. 298 K.



S_1, 8-HQS

Fig. S7. Main excitation contributing to the lowest energy singlet, S_1, electronic excited sates of the ligand **8-HQS** calculated by TD-DFT with the CAM-B3LYP functional.

Table S1. ^{1}H NMR chemical shifts [a)] of CTAB and DTAB as function of their concentrations in solutions of In^{3+}/8-HQS

	H-1'	H-2'	H-3'	H-4'	H-5'	H-6'
CTAB	3.24	3.50	1.86	1.45	1.37	0.95
In^{3+}/8-HQS/CTAB						
2.5:7.5:0.5 mmol dm^{-3}	2.83	- [b)]	- [c)]	1.48	1.07 [c)]	1.07
2.5:7.5:1.0 mmol dm^{-3}	2.84	- [b)]	- [c)]	1.48	1.06 [c)]	1.07
2.5:7.5:5.0 mmol dm^{-3}	2.85	- [b)]	- [c)]	1.49	0.95/0.79/ 0.72/0.62	1.05
2.5:7.5:10 mmol dm^{-3}	2.88	- [b)]	- [c)]	1.47	0.87/0.81/ 0.70	1.06
DTAB	3.24	3.48	1.85	1.45	1.36	0.95
In^{3+}/8-HQS/DTAB						
2.5:7.5:1.0 mmol dm^{-3}	3.12	3.25	1.65	- [d)]	1.11/1.04/ 0.94/0.89	0.85
2.5:7.5:5.0 mmol dm^{-3}	3.02	3.08	1.47	- [d)]		0.97
2.5:7.5:10 mmol dm^{-3}	2.94	2.99	1.44	1.36	1.12/1.00/ 0.89/0.80	1.04
2.5:7.5:20 mmol dm^{-3}	2.93	2.97	1.43	1.36	1.12/0.99/ 0.85/0.78	1.04

a) δ Values, in ppm, in ppm, relative to Me_4Si, using *tert*-butyl alcohol (δ_H=1.3) as internal reference.
b) superimposed with the signal of H-1'.
c) broad.
d) superimposed with the signal of the reference.