Electronic supplementary information (ESI)

Synthesis, structure, spectral and electrochemical properties of chromium(III) *tris*-(8-hydroxyquinolinate)

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Assignment of bands in FTIR spectra

Table S1. FT-IR spectral data obtained using ATR for Crq_3 solid

Band/cm^{-1}	Tentative assignment[a]
525	In-plane ring deformation
572	In-plane ring deformation
635	Out-of-plane ring deformation
743	Out-of-plane C-H bend
781	Out-of-plane C-H bend
822	Out-of-plane C-H bend
873	In-plane C-H bend
1053	In-plane ring deformation
1107	In-plane C-H bend, C-O stretch
1166	In-plane C-H bend
1216	Ring stretching; In-plane C-H bend
1274	In plane C-H bend
1316	Ring stretching
1371	Ring stretching
1459[b]	C-O stretch
1492	Ring stretching
1571	C=C stretch
1595	C=N stretch
2866[b]	C-H stretch
2960[b]	
2964[b]	
3053	
3325	O-H stretch

a. Using assignments from references 1 and 2.

b. Bands attributed to methanol from spectral data in reference 3.

Use of Crq_3 as an NMR Relaxation Agent

The Cr(III) metal complex can act through pseudocontact interactions as a good relaxation agent of non-complexed molecules in solution, as shown in Figures S1 and S2. Here the ^{1}H NMR signals of unbound 8-Hq molecules (outer-sphere) are observed to be increasingly broadened with the addition of the Crq_3 complex with no significant change in the chemical shifts.

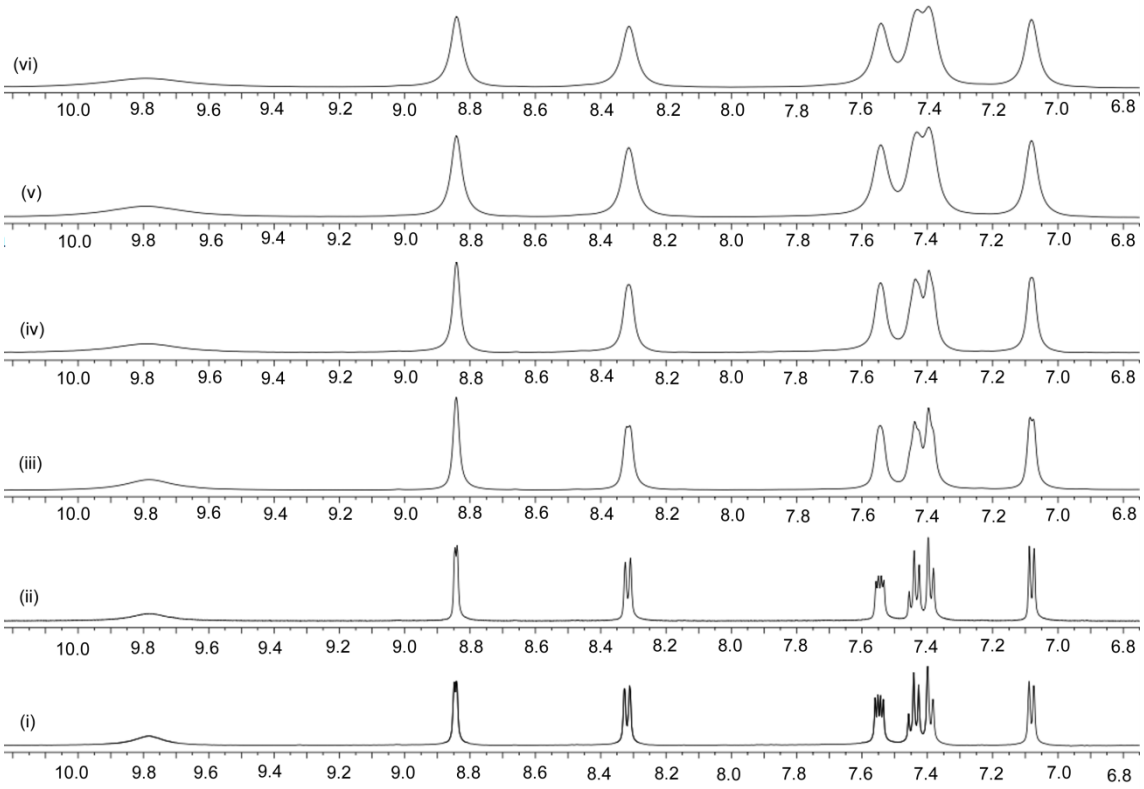

Fig. S1. Expansions from 6 to 11 ppm (8-Hq signals) of ^{1}H NMR spectra (499.824 MHz) of DMSO-d_6 solutions of (i) 8-Hq 10 mmol dm^{-3}, (ii) Crq_3:8-Hq 2:10 mmol dm^{-3}, (iii) Crq_3:8-Hq 4:10 mmol dm^{-3}, (iv) Crq_3:8-Hq 6:10 mmol dm^{-3}, (v) Crq_3:8-Hq 8:10 mmol dm^{-3}, and (vi) Crq_3:8-Hq 10:10 mmol dm^{-3}, 298 K.

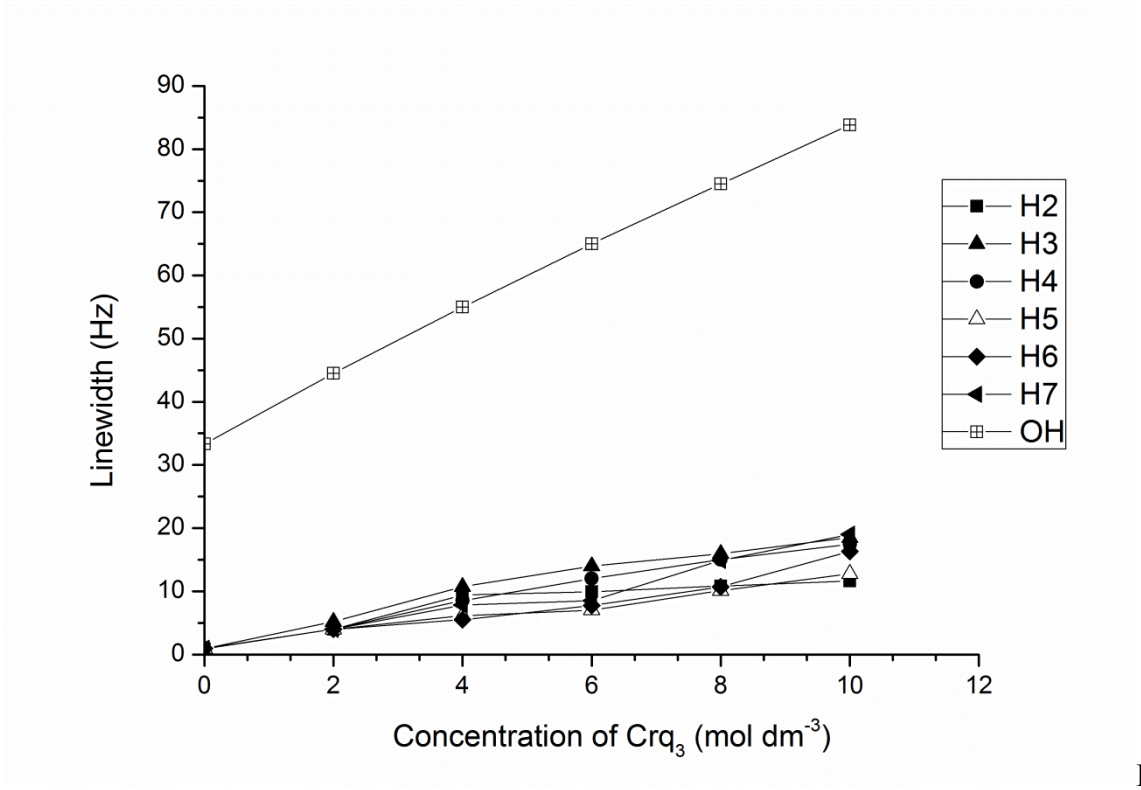

Fig. S2. Line width (Hz) of the ^{1}H NMR signals of 8-Hq 10 mmol dm^{-3}, in DMSO-d_6 solution, as a function of the concentration of Crq_3 added to the solution.

Photoluminescence spectrum

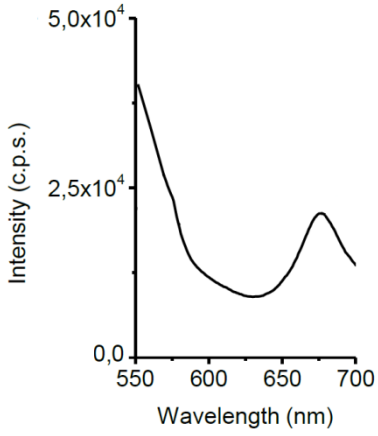

Fig. S3. Luminescence spectrum of Crq_3 in DMSO solution at room temperature ($\lambda_{excitation}$ 430 nm). The apparent emission below 550 nm is due to a Raman band.

References

1. R. Marchon, L. Bokobza, G. Cote, *Spectrochim. Acta A* 1986, **42A**, 537-542.
2. C. C. Wagner, A. C. González-Baró, E. J. Baran, *Spectrochim. Acta Part A*, 2011, **78**, 1762-1765.
3. E. K. Plyler *J. Res. Natl. Bureau Standards* 1952, **48**, 281- 286