

Solvent, coordination and hydrogen-bond effects on the chromic luminescence of the cationic complex [(phen)(H₂O)Re(CO)₃]⁺

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This journal is © The Royal Society of Chemistry and the Centre National de la Recherche Scientifique 2016. The [(phen)(H₂O)Re(CO)₃]⁺(CF₃SO₃)⁻ salt, 1⁺(CF₃SO₃)⁻, has been crystallized in the form of two new solvates, [(phen)(H₂O)Re(CO)₃]⁺(CF₃SO₃)⁻·(C₄H₈O)_{0.5} and [(phen)(H₂O)Re(CO)₃]⁺(CF₃SO₃)⁻·CH₂Cl₂. The structures, as determined by single-crystal X-ray diffraction, show intense hydrogen bonding between the coordinated water molecule on 1⁺ and the triflate oxygen atoms, with O_{water}···O_{triflate} in the range from 2.608(13) to 2.972(13) Å. This feature, to the best of our knowledge, is preserved for each solvate of 1⁺(CF₃SO₃)⁻. The spectroscopic characterization of 1⁺(CF₃SO₃)⁻ in solution together with DFT and TD-DFT results suggest that its photophysical behavior depends on the solvent polarity, as normally found for MLCT, but additionally, on the coordinating and hydrogen bonding ability of the solvent. The results suggest that in low-polarity, non-coordinating and non-hydrogen bonding