

## Experimental and theoretical studies of the ancillary ligand

### (E)-2-((3-amino-pyridin-4-ylimino)-methyl)-4,6-di-tert-butylphenol in the rhenium(i) core

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The fac-[Re(CO)<sub>3</sub>(deeb)L]<sup>+</sup> complex (C2) where L is the

(E)-2-((3-amino-pyridin-4-ylimino)-methyl)-4,6-di-tert-butylphenol ancillary ligand, which presents an intramolecular hydrogen bond, has been synthesized and characterized using UV-vis, <sup>1</sup>H-NMR, FT-IR, cyclic voltammetry and DFT calculations. The UV-vis absorption and emission properties have been studied at room temperature and the results were compared with TDDFT calculations including spin-orbit effects. We report an alternative synthesis route for the fac-Re(CO)<sub>3</sub>(deeb)Br (C1) complex where deeb = (4,4'-diethanoate)-2,2'-bpy. Besides, we have found that the C1 shows a red shift in the emission spectrum due to the nature of the ancillary electron donating ligand, while the C2 complex shows a blue shift in the emission spectrum suggesting that the ancillary ligand L has electron withdrawing ability and the importance of the intramolecular hydrogen bond. The calculations suggest that an experimental mixed absorption band at 361 nm could be

assigned to MLCT and LLCT transitions. The electron withdrawing nature of the ancillary ligand in C2 explains the electrochemical behavior, which shows the oxidation of ReI at 1.83 V and the reduction of deeb at -0.77 V. © 2015 The Royal Society of Chemistry and the Centre National de la Recherche Scientifique.