

Experimental and Theoretical Studies of the ancillary ligand (E)-2-((3-amino-pyridin-4-ylimino)-methyl)-4,6-di-tert-butylphenol in Rhenium(I) core

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Abstract

The *fac*-[Re(CO)₃(**deeb**)**L**]⁺ 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, ¹H-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)₃(**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 Re^I at 1.83 V and the reduction of **deeb** at -0.77 V.