Dual Emission of a Novel (P,N) Re^I Complex: A Computational and Experimental Study on [P,N-{(C<inf>6</inf>H<inf>5</inf>)<inf>2</inf>(C<inf>5</inf>H<inf>4</inf>N)P}Re(CO)<inf>3</inf>Br]

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 The spectroscopic, electrochemical, and photophysical properties of the new complex [P,N-{(C<inf>6</inf>H<inf>5</inf>)<inf>2</inf>(C<inf>5</inf>H<inf>4</inf>N)P}Re(CO)<inf>3</inf>Br] are reported. The UV-vis spectrum in dichloromethane shows an absorption maximum centered at 315 nm and a shoulder at 350 nm. These absorption bands have been characterized to have MLCT character. Excitation at both wavelengths (maximum and shoulder) leads to an emission band centered at 550 nm. Cyclic voltammetry experiments show two ill-defined irreversible oxidation waves around +1.50 and 1.80 V that are assigned to Re^I/Re^{II} and Re^{II}/Re^{III} couples whereas an irreversible reduction signal centered at -1.80 V is likewise assigned to a ligand reduction process. These results support the proposal of the MLCT nature of the states implied by the emission of the complex. The luminescent decay fits to a biexponential function, where t