

Experimental and theoretical characterization of Ru(II) complexes with polypyridine and phosphine ligands

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The synthesis and the experimental and theoretical characterization of ruthenium hydride complexes containing phosphorus and polypyridine ligands $[\text{RuH}(\text{CO})(\text{N-N})(\text{PPh}_3)_2]^+$ with N-N = dppz 1, dppz-CH₃ 2 (2.1 isomer), dppz-Cl 3 (3.1 isomer), ppl 4, and 2,2'-biquinoline 5, (where dppz = dipyrido[3,2-a:2',3'-c]phenazine), are presented. ¹H NMR, ³¹P NMR, ¹³C NMR, IR-FT, UV-Vis and elemental analysis are used to characterize the complexes. Optimized molecular geometries in the gas phase at the B3LYP/LACVP(d,p) level showed a distorted octahedral structure for ruthenium, the phosphine ligands are localized in a trans position, while the polypyridine ligand, which in all the cases is planar except in 5, adopt a trans position relative to the carbon monoxide and hydride ligands. The theoretical absorption spectra (one hundred excited states) were calculated for the seven complexes by the time dependent density functional theory (TD-DFT) in the gas phase. They predicted very well the UV-Vis spectra