



## *Cicle de conferències de química\**

### **Iridium Complexes with Binucleating Nitrogen Ligands: From Organometallic Processes to Catalysis**

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The reactivity of diiridium(I) complexes with binucleating nitrogen donor ligands of formula  $[\text{Ir}_2(\mu\text{-pz})_2(\text{CO})_2(\text{PPr}_3)_2]$  or  $[\text{Ir}_2(\mu\text{-1,8-(NH)}_2\text{-naphth})(\text{CO})_2(\text{PPr}_3)_2]$  (Hpz = pyrazole, 1,8-(NH<sub>2</sub>)<sub>2</sub>naphth = 1,8-diamino-naphthalene) with hydrogen and halocarbons shows remarkable differences, that can be rationalized in mechanistic terms, since hydrogen and halocarbons undergo oxidative addition through different mechanisms. The related neutral tetrahydrido diiridium(III) complex  $[\text{Ir}_2(\mu\text{-pz})_2(\mu\text{-H})(\text{H})_3(\text{PPr}_3)_2(\text{NCCH}_3)]$  presents a remarkable capability for the activation of H-H, C-H and C-Cl bonds and acts as hydrogenation catalyst. The experimental observations on the mechanism followed by the hydrogenations of diphenylacetylene and ethylene catalyzed by the tetrahydrido diiridium complex  $[\text{Ir}_2(\mu\text{-pz})_2(\mu\text{-H})(\text{H})_3(\text{PPr}_3)_2(\text{NCCH}_3)]$  indicate that these hydrogenations involve a dinuclear mechanism, in which both metals participate in a concerted way. This is possible through processes of vacancy migrations between metals, which are the consequence of the high mobility of hydrides combined with the transmission of *trans* effects within the dinuclear frames.

Interestingly, the dinuclear cationic species generated from the compound  $[\text{Ir}_2(\mu\text{-pz})_2(\mu\text{-H})(\text{H})_3(\text{NCCH}_3)(\text{PPr}_3)_2]$  after treatment with acids have been found to be efficient catalysts for the homogeneous hydrogenation, under mild conditions, of imines such as N-benzylidenaniline, following an ionic outer sphere mechanism. The NMR spectroscopic observations on these catalytic reactions and their likely elementary steps, the kinetic evidence, and theoretical calculations suggest that the hydrogenation cycle consists of fast elementary steps of H<sup>+</sup> transfer to the imine and H<sup>-</sup> transfer to the iminium cation, followed by a slow amine by dihydrogen substitution

**Dijous 18 de febrer**

**12:00h**

**Sala d'Actes, Facultat de Ciències i Biociències**

*\*Aquesta conferència forma part de les activitats formatives programades pel seguiment del progrés del doctorand*