

Influence of the N–N Coligand: C–C Coupling Instead of Formation of Imidazol-2-yl Complexes at {Mo(η^3 -allyl)(CO)₂} Fragments. Theoretical and Experimental Studies

New N-methylimidazole (N-Melm) complexes of the {Mo(η^3 -allyl)(CO)₂(N–N)} fragment have been prepared, in which the N,N-bidentate chelate ligand is a 2-pyridylimine. The addition of a strong base to the new compounds deprotonates the central CH group of the imidazole ligand and subsequently forms the C–C coupling product that results from the nucleophilic attack to the imine C atom. This reactivity contrasts with that previously found for the analogous 2,2'-bipyridine compounds [Mo(η^3 -allyl)(CO)₂-(bipy)(N-RIm)]OTf [N-RIm = N-Melm, N-mesitylimidazole (N-MesIm, Mes=2,4,6-trimethylphenyl); OTf = trifluoromethanesulfonate] which afforded imidazol-2-yl complexes upon deprotonation. Density Functional Theory (DFT) computations uncover that the reactivity of the imine C atom along with its ability to delocalize electron density are responsible for the new reactivity pattern found for the kind of molybdenum complexes reported herein.

Fuente de la publicación:

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[Estudios computacionales en Reacciones Multicomponentes](#) [1]

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