Influence of the N−N Coligand: C−C Coupling Instead of Formation of Imidazol-2-yl Complexes at {Mo(η3-allyl)(CO)2} Fragments. Theoretical and Experimental Studies

New N-methylimidazole (N-MeIm) complexes of the {Mo(η3-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(η3-allyl)(CO)2-(bipy)(N-RIm)]OTf [N-RIm = N-MeIm, 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.

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Proyectos relacionado:
Estudios computacionales en Reacciónes Multicomponentes [1]

URL de origem:https://www.cenits.es/pt-pt/enlaces/publicaciones/influence-nn-coligand-cc-coupling-instead-formation-imidazol-2-yl-complexes

Ligações
[1] http://www.cenits.es/proyectos/estudios-computacionales-reacciones-multicomponentes-0