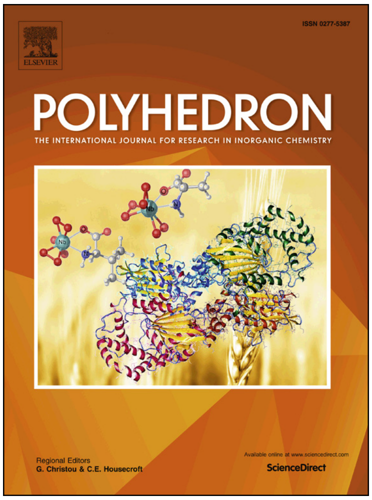

Divergent stereoisomers of molybdenum carbonyl complexes of NHC-based pincer ligands

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Divergent stereoisomers of molybdenum carbonyl complexes of NHC-based pincer ligands

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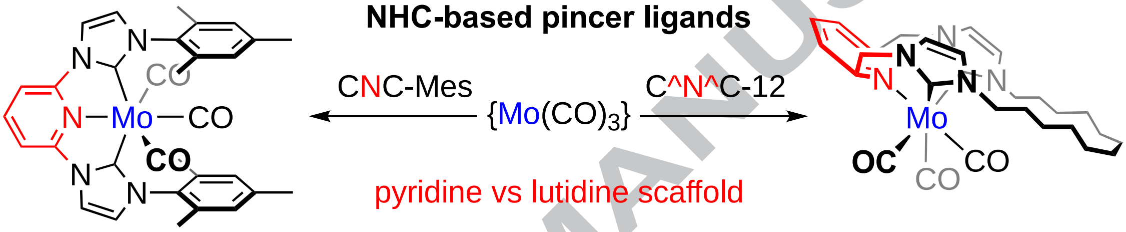

Keywords: Molybdenum, NHC, pincer ligands, coordination geometry

Abstract

The first molybdenum complexes of widely used NHC-based CNC and C^N^C pincer ligands are described, *viz.* [Mo(L)(CO)$_3$] (L = 2,6-bis(mesityl-imidazolylidene)pyridine ≡ CNC-Mes, **1**; α,α'-(diimidazolylidene-dodecamethylene)lutidine ≡ C^N^C-12, **2**). These complexes have been thoroughly characterised in solution and the solid-state, revealing different stereochemical preferences of the tridentate ligands depending on the nature of the scaffold. In the case of flexible C^N^C-12 an uncommon *fac*-coordination geometry is observed, whilst the complex of rigid CNC-Mes adopts the expected *mer*-configuration. For the combination of donors associated with the ligands, DFT calculations establish preferential *fac*-coordination, however, within the CNC ($\Delta\Delta G$ = +63.1 kJ·mol^{-1}) and C^N^C ($\Delta\Delta G$ = +20.0 kJ·mol^{-1}) scaffolds this conformation is significantly destabilised relative to the *mer*-alternative.