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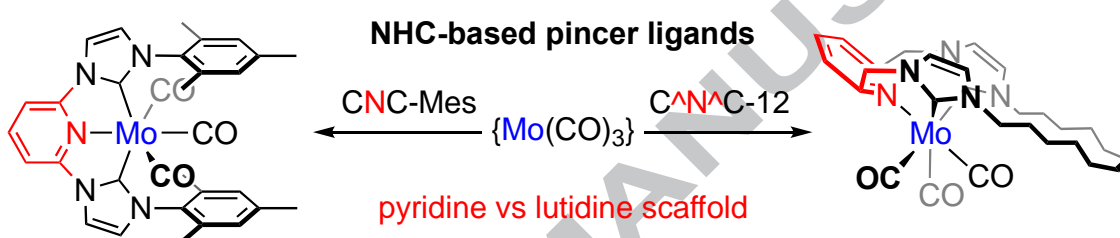


# Divergent stereoisomers of molybdenum carbonyl complexes of NHC-based pincer ligands

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## TOC graphic:



**Keywords:** Molybdenum, NHC, pincer ligands, coordination geometry

## Abstract

The first molybdenum complexes of widely used NHC-based CNC and C<sup>N</sup>^C pincer ligands are described, viz.  $[Mo(L)(CO)_3]$  ( $L = 2,6$ -bis(mesityl-imidazolylidene)pyridine  $\equiv$  CNC-Mes, **1**;  $\alpha, \alpha'$ -(diimidazolylidene-dodecamethylene)lutidine  $\equiv$  C<sup>N</sup>^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<sup>N</sup>^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<sup>-1</sup>) and C<sup>N</sup>^C ( $\Delta\Delta G = +20.0$  kJ·mol<sup>-1</sup>) scaffolds this conformation is significantly destabilised relative to the *mer*-alternative.

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