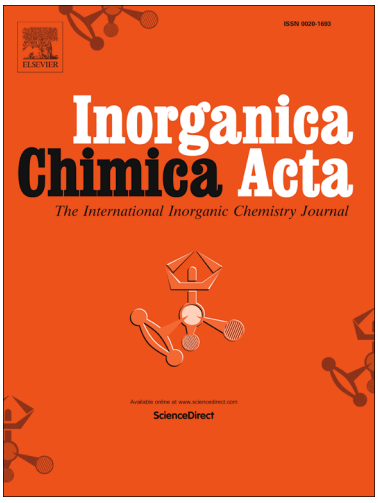

Research paper

Transfer hydrogenation of ketones catalyzed by a trinuclear Ni(II) complex of a Schiff base functionalized *N*-heterocyclic carbene ligand

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Transfer hydrogenation of ketones catalyzed by a trinuclear Ni(II) complex of a Schiff base functionalized *N*-heterocyclic carbene ligand

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Abstract

A new Schiff base-functionalized *N*-heterocyclic carbene ligand precursor 3-benzyl-1-[2-((2-hydroxy-benzylidene)-amino]-ethyl-3*H*-imidazol-1-ium bromide (**3**), and its trinuclear Ni(II) complex [LNiL-Ni-LNiL].2Br (**4**) where L = 2-[2-(3-benzylimidazol-1-yl) ethyliminomethyl]phenol, were synthesized via the solventless and free carbene routes respectively. Both compounds were characterized by spectroscopic and X-ray diffraction techniques. Single crystal XRD analysis of **4** showed that it is composed of a central square planar Ni(II) ion symmetrically linked to two distorted square planar Ni(II) ions via two bridging ligands. The central Ni(II) ion is only bound to the Schiff base moieties of the bridging ligands via the phenolate oxygen donor (O1) and imine nitrogen donor (N1) atoms in a trans [N^O^(Ni^{2+})^N^O] mode, whilst the carbene moieties of each bridging ligand and a tridentate L are coordinated in a distorted square planar C_{NHC}-(Ni^{2+})^N^O^C_{NHC} mode to stabilise each of the terminal Ni(II) ions. Complex **4** showed significant activity as a catalyst in the transfer hydrogenation of a range of aliphatic and aromatic ketones, at a catalyst concentration of 0.1 mol%. An excellent conversion up to 100% was achieved for aromatic ketones after 4 h.

Keywords: Trinuclear Ni(II); Solventless synthesis; *N*-heterocyclic carbene; Schiff base; Bifunctional ligand; Transfer hydrogenation.

1. Introduction

The successful isolation and full characterization of stable *N*-heterocyclic carbenes (NHCs) has revolutionized the field of organometallic chemistry and homogeneous catalysis.[1] This is because NHCs have proven to be good stabilizing ligands to a wide range of metal ions and have over the last few decades been accepted as credible alternatives to traditional ligands like the amines and phosphines.[2] Added to this is the ease of preparation and relatively long shelf lives of their precursor salts. Monodentate NHCs have been widely studied and complexed to a range of transition metals, usually applied as catalysts in a variety of small molecule activation studies that include reduction of ketones, C-N and C-C coupling reactions.[3] However, there is a limitation to the range and scope of reactivity and structural variations obtainable from monodentate carbene ligands, hence one of the current challenges in this field is the development of new multi-functional or polydentate NHC ligands by the

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