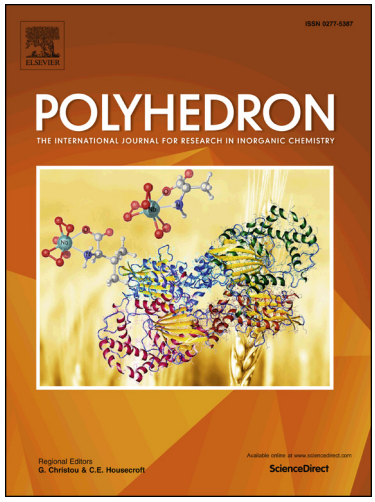

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Jan Pecak,[a] Mathias Glatz,[a] Berthold Stöger,[b] Roland Bittner,[a] Helmuth Hoffmann,[a] Andrew Atkins,[c] Leticia González,[c] and Karl Kirchner[a,*]

[a] Institute of Applied Synthetic Chemistry, Vienna University of Technology, Getreidemarkt 9, A-1060 Vienna, AUSTRIA

[b] X-ray Centre, Vienna University of Technology, Getreidemarkt 9, A-1060 Vienna, AUSTRIA

[c] Institute of Theoretical Chemistry, University of Vienna, Währinger Straße 17. A-1090 Vienna, AUSTRIA.

Abstract

The synthesis and characterization of dicarbonyl Fe(II) PNP pincer complexes of the type *cis*-[Fe(PNP-*i*Pr)$(CO)_2$(X)]$^+$ (X = Br, Cl) is described. These complexes are slowly formed when solutions of complexes *trans*-[Fe(PNP-*i*Pr)$(CO)_2$(X)]$^+$ are kept in the dark for 18 h (X = Br) and 3 days (X = Cl). Upon exposure to visible light these complexes isomerize to the respective *trans*-dicarbonyl complexes within a few hours. The visible-light reaction seems to involve reversible CO dissociation. The isomerization can be repeated serval times. A mechanistic rationale for this isomerization process is established by means of DFT calculations.

Keywords: Iron complexes, PNP pincer ligands, Photochemistry, Carbon monoxide, Isomerization, DFT calculations

* Corresponding author. Tel.: +43 1 58801 163611; Fax.: +43 1 58801 16399
E-mail: karl.kirchner@tuwien.ac.at (K. Kirchner)