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## Visible Light-Induced *cis/trans* Isomerization of Dicarbonyl Fe(II) PNP Pincer Complexes

Jan Pecak,<sup>a</sup> Mathias Glatz,<sup>a</sup> Berthold Stöger,<sup>b</sup> Roland Bittner,<sup>a</sup> Helmuth Hoffmann,<sup>a</sup> Andrew Atkins,<sup>c</sup> Leticia González,<sup>c</sup> and Karl Kirchner<sup>a,\*</sup>

<sup>a</sup> Institute of Applied Synthetic Chemistry, Vienna University of Technology, Getreidemarkt 9, A-1060 Vienna, AUSTRIA

<sup>b</sup> X-ray Centre, Vienna University of Technology, Getreidemarkt 9, A-1060 Vienna, AUSTRIA

<sup>c</sup> 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)<sub>2</sub>(X)]<sup>+</sup> (X = Br, Cl) is described. These complexes are slowly formed when solutions of complexes *trans*-[Fe(PNP-*i*Pr)(CO)<sub>2</sub>(X)]<sup>+</sup> 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 several 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)

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