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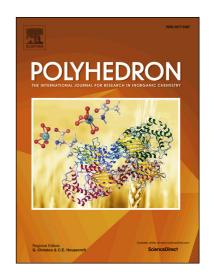
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Visible Light-Induced *cis/trans* Isomerization of Dicarbonyl Fe(II) PNP Pincer Complexes

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Abstract

The synthesis and characterization of dicarbonyl Fe(II) PNP pincer complexes of the type *cis*- $[Fe(PNP-iPr)(CO)_2(X)]^+$ (X = Br, CI) is described. These complexes are slowly formed when solutions of complexes *trans*- $[Fe(PNP-iPr)(CO)_2(X)]^+$ are kept in the dark for 18 h (X = Br) and 3 days (X = CI). 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

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