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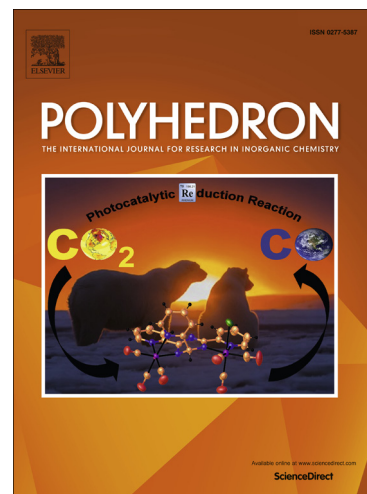
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Synthesis, Structure, and Conformational Dynamics of Rhodium and Iridium Complexes of Dimethylbis(2-pyridyl)borate†

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Keywords

Rhodium, Iridium, Inversion Recovery, Back Bonding, Ring Flip

Abstract

Rhodium(I) and Iridium(I) borate complexes of the structure $[\text{Me}_2\text{B}(2\text{-py})_2]\text{ML}_2$ ($\text{L}_2 = (\text{tBuNC})_2, (\text{CO})_2, (\text{C}_2\text{H}_4)_2, \text{cod}, \text{dppe}$) were prepared and structurally characterized ($\text{cod} = 1,5\text{-cyclooctadiene}$; $\text{dppe} = 1,2\text{-diphenylphosphinoethane}$). Each contains a boat-configured chelate ring that participates in a boat-to-boat ring flip. Computational evidence shows that the ring flip proceeds through a transition state that is near planarity about the chelate ring.

We observe an empirical, quantitative correlation between the barrier of this ring flip and the π acceptor ability of the ancillary ligand groups on the metal. The ring flip barrier correlates weakly to the Tolman and Lever ligand parameterization schemes, apparently

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