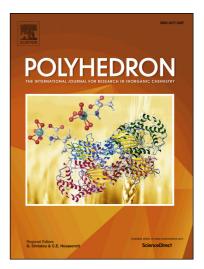
Accepted Manuscript

Examining the Effects of Variations in Ligand Framework and Pnictogen Substitution on the Geometry and Electronic Structure of Metal Complexes of *N*-Heterocyclic Phosphido Ligands Incorporated into a Diphosphine Pincer Ligand Framework

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PII:	S0277-5387(17)30715-5
DOI:	https://doi.org/10.1016/j.poly.2017.11.015
Reference:	POLY 12917
To appear in:	Polyhedron
Received Date:	7 July 2017
Accepted Date:	9 November 2017



Please cite this article as: C.M. Thomas, G.P. Hatzis, M.J. Pepi, Examining the Effects of Variations in Ligand Framework and Pnictogen Substitution on the Geometry and Electronic Structure of Metal Complexes of *N*-Heterocyclic Phosphido Ligands Incorporated into a Diphosphine Pincer Ligand Framework, *Polyhedron* (2017), doi: https://doi.org/10.1016/j.poly.2017.11.015

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Examining the Effects of Variations in Ligand Framework and Pnictogen Substitution on the Geometry and Electronic Structure of Metal Complexes of *N*-Heterocyclic Phosphido Ligands Incorporated into a Diphosphine Pincer Ligand Framework

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ABSTRACT. A series of compounds comprised of *N*-heterocyclic phosphido-containing ligands bound to a $Co(CO)_2$ fragment are explored computationally using density functional theory (DFT). Computational methods are used to identify expected changes in the electronic structure and bonding in these molecules as a function of substituent and backbone modifications, with the ultimate goal of identifying the most intriguing targets for further experimental studies. A series of N, As, and Sb derivatives are also explored through computational studies to better understand the geometric and electronic effects of varying the central pnictogen atom.

KEYWORDS: pincer ligands, N-heterocyclic phosphido, cobalt, metal carbonyl

Introduction

Tridentate ligands that coordinate in a meridional fashion, or "pincer" ligands, have proven to be exceptionally versatile scaffolds in transition metal and organometallic chemistry, Download English Version:

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