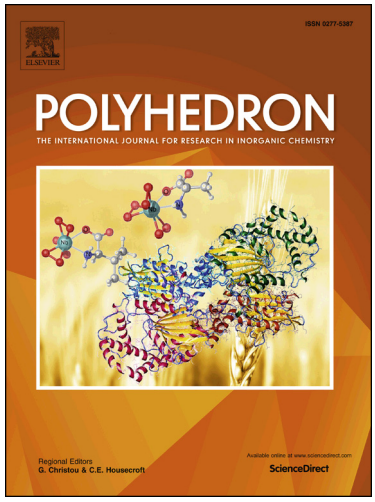

Examining the Effects of Variations in Ligand Framework and Pnictogen Substitution on the Geometry and Electronic Structure of Metal Complexes of *N*-Heterocyclic Phosphido Ligands Incorporated into a Diphosphine Pincer Ligand Framework

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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,