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ACCEPTED MANUSCRIPT

Chalcogenolato-Bridged Dinuclear Half Sandwich Complexes of Ruthenium and Iridium

Benson Joseph^a, Koushik Saha^a, Rini Prakash^a, Chandan Nandi^a, Thierry Roisnel^b and Sundargopal Ghosh^{*a}

^aDepartment of Chemistry, Indian Institute of Technology Madras, Chennai 600036, India. Phone: (+91) 44 2257 4230, Fax: (+91) 44 2257 4202

E-mail: sghosh@iitm.ac.in

*For Correspondence

^bInstitut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Ecole Nationale Supérieure de Chimie de Rennes-Université de Rennes 1, F-35042 Rennes Cedex, France.

E-mail: Thierry.Roisnel@univ-rennes1.fr

Abstract:

In an effort to synthesize metallaheteroborane complexes of ruthenium, we carried out the reaction of ruthenium methanedithiolate complex, $[(Cp*Ru)_2(B_3H_8)(CS_2H)]$, $(Cp* = \eta^5 - C_5Me_5)$ **1** with $[BH_3SPh]Li$ at elevated temperature that yielded a dinuclear bridged thiolate complex $[Cp*Ru(\mu-SPh)_2(\mu-\eta^1-S_2)RuCp*]$, **2**. In a similar fashion, reaction of $[Cp*IrCl_2]_2$ with $[BH_3TePh]Li$ yielded tellurolato-bridged diiridium half sandwich complex $[Cp*IrH(\mu-TePh)_2HIrCp*]$, **5**. All the compounds have been characterized by various spectroscopic techniques and the structures were unequivocally established by crystallographic analysis. Further, the density functional theory (DFT) calculations were performed to investigate the bonding and electronic properties of **2'** and **5'** (Cp analogues of **2** and **5**).

Keywords: Ruthenium, Iridium, Chalcogenolato-Bridge, Boron.

1. Introduction

Transition metal complexes with chalcogen ligands are well established. They not only exhibit unique reactivities toward small molecules such as alkynes, hydrogen gas and carbon monoxide [1-6], but also are active catalysts in several C-C and C-heteroatom bond-forming reactions [7-9]. These complexes are promising anticancer agents and thus, demand more attention in biological studies [10-12]. Recently, Therrien and co-workers have shown that the thiolato-bridged dinuclear arene-ruthenium complexes of the type $[(\eta^6-p-\text{MeC}_6\text{H}_4^i\text{Pr})_2\text{Ru}_2(\mu-$

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