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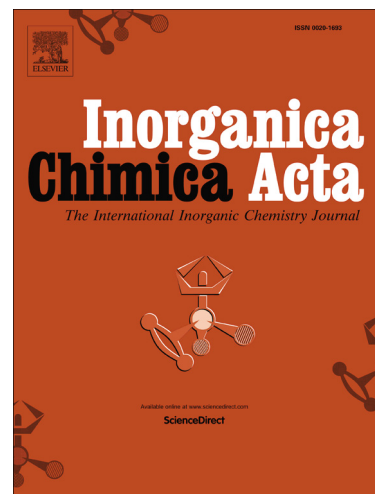
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Synthesis, Structure, Theoretical Studies and Electrochemistry of Ru(II)-N Heterocyclic Carbenes

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Abstract

Synthesis, structure, electrochemistry and theoretical studies of Ru(II) complexes, 1-(2-Pyrimidyl)-3-(methyl)imidazoline-2-ylidene tetraacetoneitrileruthenium(II)hexafluorophosphate, **2** and 1-(2-Pyrimidyl)-3-(methyl)benzimidazoline-2-ylidene tetraacetoneitrileruthenium(II)hexafluorophosphate, **4** bearing pyrimidine functionalized C,N donor N-heterocyclic carbene proligands 1-(2-Pyrimidyl)-3-(methyl)imidazolium hexafluorophosphate; **1-H(PF₆)** and 1-(2-Pyrimidyl)-3-(methyl)benzimidazolium hexafluorophosphate; **3-H(PF₆)** have been reported. The compounds were fully characterized by elemental analysis, NMR, UV-Vis spectroscopy and finally the solid state structure of **2** is confirmed by X-ray diffraction studies. Theoretically geometry of complex **4** is optimized using B3LYP-D3/def2-TZVP. Natural Bond Orbital (NBO) analysis of complexes **2** and **4** support the π -back bonding $\text{Ru} \rightarrow \text{N}=\text{C}_{\text{carbene}}$. Cyclic voltammetry studies revealed Ru(II)/Ru(III) reversible oxidation couple at 0.50 and 0.52 eV respectively for complexes **2** and **4**; the higher oxidation potential of **4** compared to **2** is assigned due to π -acid character of benzimidazole.

Keywords: N-heterocyclic carbene; Pyrimidine; Electrochemistry; Ruthenium-NHC; X-ray structure

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