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Novel mixed-metal cubane-type $\{\text{Mo}_3\text{NiS}_4\}$ and $\{\text{Mo}_3\text{PdS}_4\}$ clusters coordinated with 2,2'-bipyridine type ligands

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Abstract

New cuboidal cluster complexes of general formula $[\text{Mo}_3\text{S}_4(\text{M}'\text{X})\text{Cl}_3\text{L}_3]^{0/+}$ ($\text{M}' = \text{Ni}^0, \text{Pd}^0$; $\text{L} = \text{dnbpy} - 4,4'$ -dinonyl-2,2'-bipyridine or $\text{dbbpy} - 4,4'$ -di-*tert*-butyl-2,2'-bipyridine; $\text{X} = \text{tu}, \text{Cl}$) were synthesized by reactions of trinuclear precursors $[\text{Mo}_3\text{S}_4\text{Cl}_3\text{L}_3]^+$ with $\text{Ni}(\text{COD})_2$ ($\text{COD} = 1,5$ -cyclooctadiene) or $\text{Pd}_2(\text{dba})_3 \cdot \text{CHCl}_3$ ($\text{dba} = \text{dibenzylideneacetone}$) in the presence of thiourea (tu) in good yields. The complexes were characterized by elemental analysis, IR, ^1H NMR and ESI-MS techniques. Crystal structures of $[\text{Mo}_3\text{S}_4(\text{Nitu})\text{Cl}_3(\text{dbbpy})_3]\text{Cl} \cdot \text{tu}$ (**1a**), $[\text{Mo}_3\text{S}_4(\text{Nitu})\text{Cl}_3(\text{dbbpy})_3]\text{Cl}$ (**1b**) and $[\text{Mo}_3\text{S}_4(\text{Pd}'\text{X})\text{Cl}_3(\text{dbbpy})_3]\text{Cl}$ (**2**) were determined by X-ray analysis. The DFT calculations of the electronic structure of $[\text{Mo}_3\text{S}_4(\text{Pd}'\text{X})\text{Cl}_3(\text{bpy})_3]^{0/+}$ ($\text{X} = \text{Cl}$ or tu) were carried out.

Highlights (80 symbols per highlight)

- First examples of $\{\text{Mo}_3\text{S}_4\text{Ni}\}^{4+}$ and $\{\text{Mo}_3\text{S}_4\text{Pd}\}^{4+}$ clusters bearing bipyridine ligands;
- Crystal structure and spectroscopic data discussed;
- The electronic structure investigated.

Keywords: trinuclear sulphide cluster, cubane-type clusters, molybdenum, palladium, nickel, 2,2'-bipyridine, crystal structure, quantum chemical calculations.

1. Introduction

Incomplete cuboidal $\{\text{M}_3\text{Q}_4\}^{4+}$ ($\text{M} = \text{Mo}, \text{W}$; $\text{Q} = \text{S}, \text{Se}$) clusters represent a large and well-studied family of transition metals clusters with diverse catalytic properties [1–6]. One of the most interesting features of these clusters is their ability to act as metalloligands towards a second transition metal (M') in low oxidation state (zero to two) to complete the cuboidal structure with the formation of $\{\text{M}_3\text{M}'\text{Q}_4\}^{n+}$ clusters [4,6]. The success of the incorporation is greatly affected by the affinity of M' for the bridging chalcogen atoms and its reducing ability. Such cuboidal clusters share similarities with some biological catalytic active sites and show specific reactivity and catalytic activity based on the heteroatoms [6–11].

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