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Experimental and DFT characterization of the organic-inorganic monohydrated Co(II) complex with 2,6-diaminopyridine ligand, $(C_5H_8N_3)_2[CoBr_4] \cdot H_2O$

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Single crystals of the new organic-inorganic compound $(C_5H_8N_3)_2[CoBr_4] \cdot H_2O$ were grown by hydrothermal technique and characterized by X-ray diffraction, infrared absorption, Raman spectroscopy scattering, optical absorption and thermal analysis. The title compound belongs to the triclinic space group $P\bar{1}$ and in the crystal structure, the inorganic layers are built from tetrabromidocobaltate anions $[CoBr_4]^{2-}$ and free water molecules, linked together by O-H...Br hydrogen bonds and halogen...halogen interactions. The organic cations are intercalated between the mineral layers via N-H...Br hydrogen bonds and form chains through $\pi\cdots\pi$ interactions. Theoretical calculations were performed using density functional theory with the B3LYP/LanL2DZ level for studying the molecular structure and vibrational spectra of the title compound. Good consistency was found between the calculated results and the experimental structure, IR and Raman spectra. The optical properties were investigated by optical absorption showing ligand-to-metal charge-transfer transitions in the visible region and organic related $\pi\text{-}\pi^*$ transitions in the UV region.

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Synthesis, characterization and reactivity of metal carbonyl complexes containing hemilabile phosphines as ligands

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The hemilability of polydentated hybrid ligands has become an attractive area of study due to their high potential in homogeneous catalytic systems to enhance selectivity or stabilize reactive intermediates. The lability of π -coordinated substituents to metal centers has been taken as an advantage to design potentially hemilabile phosphine ligands. Thus, it has been shown that functionalized phosphines with alkenyl substituents behave as hemilabile ligands in transition metal clusters. We have found that diallylphosphine ligands $RP(CH_2CH=CH_2)_2$, where $R=iPr_2N$, $p\text{-MeOC}_6H_4$ and $o\text{-MeOC}_6H_4$, coordinate to dirhenium and triosmium metal carbonyl, preferably by the phosphorus atom, but also through the allyl fragment. We have observed that complexes with metal-allyl π -bond exist as a mixture of two conformational isomers, and such isomerization can be described as a reorientation of the coordinated double bond with respect to dirhenium or triosmium metal complex. These complexes also display hemilability properties, which are evidenced by reaction with nucleophiles (such as: CO, PPh_3 and allene), leading to cleavage of the allyl π -coordination and its substitution through the corresponding nucleophile. Additionally, these results suggest that the metal-allyl π -interaction is stronger for diallyldiisopropylaminophosphine than diallyl (p -methoxyphenyl) phosphine ligand.

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