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New Rhenium(V) Nitrofuryl Semicarbazone Complexes. Crystal Structure of [ReOCl₂(PPh₃)(3-(5-Nitrofuryl)acroleine semicarbazone)]

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The synthesis and characterization of the first two Re complexes with semicarbazone ligands is presented. Selected ligands are 5-Nitro-2-furaldehyde semicarbazone (Nitrofurazone) (L1) and its derivative 3-(5-Nitrofuryl)acroleine semicarbazone (L2). Complexes of general formula [ReVOCl₂(PPh₃)L], where L=L1 and L2, were prepared in good yields and high purity by reaction of [ReVOCl₃(PPh₃)₂] with L in ethanol or methanol solutions. The complexes formula and molecular structures were supported by elemental analyses and electronic, FTIR, ¹H, ¹³C and ³¹P NMR spectroscopies. In addition, the crystal and molecular structure of [ReVOCl₂(PPh₃)L₂] was determined by X-ray diffraction methods. [ReOCl₂(PPh₃)(3-(5-Nitrofuryl)acroleine semicarbazone)] crystallizes in the space group P-1 with a=11.2334(2), b=11.3040(2), c=12.5040(2) Å, α=81.861(1), β=63.555(1), γ=83.626(1)°, and Z=2. The Re(V) ion is in a distorted octahedral environment, equatorially coordinated to a deprotonated semicarbazone molecule acting as a bidentate ligand through its carbonylic oxygen and azomethynic nitrogen atoms, to an oxo ligand and a chlorine atom. The six-fold coordination is completed by another chlorine atom and a triphenylphosphine ligand at the axial positions.

Synthesis and characterization of new ruthenium complexes with active ligands against Chagas' disease

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Chagas' disease, considered incurable, is a major third world parasitosis that affects millions of people in Latin America. Previous work has shown that ruthenium clotrimazole complexes are more active against *Trypanosoma cruzi*, causative agent of Chagas' disease, than the corresponding free ligand. In this work, the synthesis and characterization of a series of new Ru(II) complexes with different anti-trypanosomal active compounds is presented. Complexes of general formulae $[RuICl(dmsO)_2L]$, where dmsO=dimethylsulfoxide and L=5-nitro-2-furaldehyde semicarbazone (L1), N4-n-butyl-5-nitro-2-furaldehyde semicarbazone (L2) or 3-(5-nitrofuryl) acroleine semicarbazone (L3), were prepared in good yields by reaction of $[RuICl_2(dmsO)_4]$ with L in ethanol or toluene solutions. Complexes were characterized by elemental analyses and electronic, FTIR, 1H and $^{13}CNMR$ spectroscopies. Crystal and molecular structures of $[RuCl_2(dmsO)_2L1]$ and $[RuCl_2(dmsO)_2L2]$ were determined by X-ray diffraction methods. In both crystals the ruthenium metal atom is in a quite similar elongated octahedral environment, equatorially coordinated to the semicarbazone molecule, acting as a bidentate ligand through its azomethynic nitrogen and carbonylic oxygen atoms. The six fold coordination is completed with the sulphur atoms of two dimethylsulfoxide ligands at cis-positions and two chlorine ions at the axial positions. The proposed formula for L3 complex was supported by FTIR, NMR and theoretical studies. NOE-NMR experiments allowed to assign L3 spatial distribution in the complex.

A Crystallographic and Vibrational Study of $Cs_4[Na_2(H_2O)_{10}](V_{10}O_{28})$

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The title compound crystallizes in the triclinic space group P-1, with $a=8.6161(4)$, $b=10.591(1)$, $c=11.406(1)$ Å, $\alpha=67.9770(1)$, $\beta=86.8750(1)$, $\gamma=67.7910(1)$, and $Z=1$. The structure was refined to $R_1=0.0413$. The decavanadate anion, $V_{10}O_{28}^{6-}$, and the $[Na_2(H_2O)_{10}]^{2+}$ bridged cation are located at inversion centers. Partial deuteration of the substance indicates that the coordinated water molecules are strongly asymmetric, forming weak hydrogen bonds with acceptor oxygen atoms from the decavanadate anion. The infrared and Raman spectra are dominated by the water and decavanadate anion bands.
