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Synthesis of new dithiocarbazate V(V) and Mo(VI) complexes: A crystallography perspective

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ABSTRACT

Metal complexes bearing dithiocarbazates exhibit structures with variety of physical and chemical properties. Among transition and non-transition metals, complexes of molybdenum and vanadium have still retained the attention of coordination inorganic chemists, especially because of the numerous oxidation states. The new complexes $[MoO_2(sedtc)MeOH]$ (**1**) and $[VO(sedtc)OCH_3.MeOH]$ (**2**) (sedtc: *S*-ethyl-3-(2-hydroxy-phenyl)methylenedithiocarbazate)) are crystallized in the space group $P2_1/c$ and $P\bar{1}$ respectively and characterized by ^{1}H-, ^{13}C-NMR and IR spectroscopies, mass spectrometry and X-ray diffraction analysis. The X-ray diffraction data show that both complexes have distorted octahedral structure where the sedtc tridentate ONS ligand is coordinated to metallic ion *via* phenolic oxygen, imine nitrogen, and thioenolate sulfur donor atoms accompanied by an oxido-oxygen atom in **1** or a methoxy fragment in **2** in equatorial positions, while the other two axial positions in **1** and **2** are similarly occupied by an oxido-oxygen atom and a methanol molecule. Crystal structure investigation of the Mo complex illustrates the molecules are linked *via* O4-H4A···N2^i (*i*: 1-*x*,1-*y*,1-*z*) hydrogen bonds to form dimers and afterwards expand through H4-C4···S1^i (*i*: x,1+y,z) hydrogen bonds into one dimensional arrangement along the *a* axis. This dimer arrangement includes the $R_2^2(10)$ graph set. Similarly, adjacent molecules in crystal structure of the V(V) complex makes dimmers *via* O4-H4A···N2^i pairs of hydrogen bonds with alike graph set. In the ^{1}H-NMR study, O-H and N-H signals are found to disappear in complexes which verifies ligands are coordinated to the central atoms in their deprotonated forms.

Keywords: dithiocatrbazate, dioxomolybdenum(VI) complex, oxovanadium(V) complex

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