

at 800°C) was established by the Lacorre et al [1]. There is no such a compound in the Nd_2O_3 - MoO_3 system, but there is one with the fluorite-like structure near the Nd_2MoO_6 [2], [3], [4]. Chemical composition and crystal structure of the $\text{Nd}_5\text{Mo}_3\text{O}_{16}$ compound were studied before on polycrystals [4] as well as similar structure of $\text{Pr}_5\text{Mo}_3\text{O}_{16}$ [5]. It was found that the $\text{Pr}_5\text{Mo}_3\text{O}_{16}$ crystals have a fluorite-like superstructure in Pn-3n sp. gr. There are Pr1 at 12e position, Pr2 at 8c, Mo at 16f, and two kinds of oxygen atoms O1 at 48i and O2 at 16f. Overrated thermal parameters are given in [5] for the Pr2 ($B_{\text{eq}}=1.32(16) \text{ \AA}^2$) and Mo ($B_{\text{eq}}=0.98(7) \text{ \AA}^2$) atoms, while $B_{\text{eq}}=0.71(4) \text{ \AA}^2$ for the O2 atom.

Single-crystal structure refinement of $\text{Nd}_5\text{Mo}_3\text{O}_{16}$ and study of the physical properties have been performed. Dark-violet cubical $\text{Nd}_5\text{Mo}_3\text{O}_{16}$ single crystals were grown by spontaneous flux crystallization. The conductivity of the compound is hypothetically anionic and reaches approximately 10^{-2} S/cm at 800°C.

The structure of $\text{Nd}_5\text{Mo}_3\text{O}_{16}$ single crystal was studied by the X-ray techniques (XCalibur S CCD-diffractometer, $T=293 \text{ K}$). The unit cell was found to be cubic with $a=11.028(1) \text{ \AA}$, which relates to that of fluorite CaF_2 as $a \approx 2a_f$. The structure was solved using the Pn-3n symmetry group. It was found that the Nd1 and Mo atoms are shifted from their positions on the 4-fold axis with the formation of 4 positions (0.25 occupation) around it. The Nd2 atoms are not disordered; they are located on the 3-fold axis and are surrounded by oxygens with 6 Nd2-O2 distances equal to 2.597 Å and 2 distances Nd2-O1 equal to 2.294 Å (coordination polyhedron of Nd2 – slightly distorted cube). Inclusion of Mo atoms into $\text{Nd}_5\text{Mo}_3\text{O}_{16}$ structure, which are surrounded by O2 atoms (Mo-O2 distances from 1.695 to 1.892 Å) lead to the strong distortion of the Nd1 – polyhedron and to the deviation of the structure framework from the fluorite-like. Some shift of the Nd1 and Mo atoms from the axis appears as a result, which was established in the present work ($R=3.6\%$, $R_w=3.27\%$, $S=1.99$, $B_{\text{eq}}=0.24(1) \text{ \AA}^2$ for the Pr2 atom).

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Synthesis and structure of new vanadium(IV) complex based on isonicotinic hydrazide

Maria Cocu,^a Sergiu Shova,^b Victoria Gutium,^a Ion Bulhac,^a ^a*Institute of Chemistry of ASM, Republic of Moldova*. ^b*Institute of Applied Physics of the ASM, Republic of Moldova*. E-mail: mariacocu@gmail.com

Although the biological significance of vanadium was recognized long ago, the coordination chemistry of this element continues to attract the attention of researchers, not least because of the discovery that vanadium is present at the active site of several enzymes, such as some peroxidases, as models for bromoperoxidase, nitrogenases and other biological systems.

The crystalline coordination compound $\text{VO}_2\text{L}\cdot 2\text{H}_2\text{O}$ has been obtained as the result of interaction of 2,4-pentanedione isonicotinic hydrazone (HL) with $\text{VOSO}_4\cdot 3\text{H}_2\text{O}$. This compound is soluble in

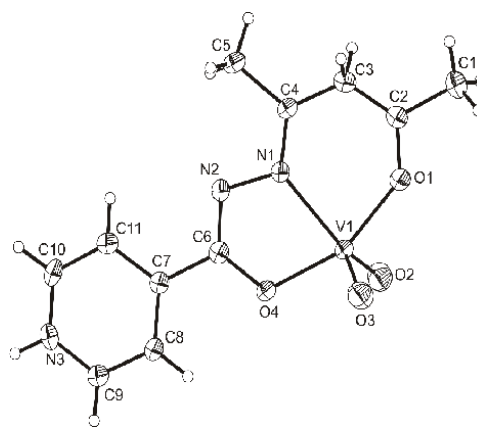
chloroform, dimethylformamide, less soluble in EtOH and MeOH.

The product $\text{VO}_2\text{L}\cdot 2\text{H}_2\text{O}$ is characterized using IR spectroscopy, elemental analysis and X-ray method.

The disappearance of the band at 1624 cm^{-1} ($\nu(\text{C}=\text{O})$) and the absence of oscillations bands of N-H, as well as the appearance of absorbance in the regions $2700\text{-}2500$ and $2250\text{-}2000 \text{ cm}^{-1}$ attributed to vibrations of $=\text{C}=\text{NH}^+$ in the spectrum of $\text{VO}_2\text{L}\cdot 2\text{H}_2\text{O}$ as compared to that of the uncoordinated ligand, indicates upon the coordination L in enolic form with proton migration (from NH) to the heterocyclic nitrogen. The presence of a narrow band of moderate intensity at 1636 cm^{-1} confirms the formation $=\text{C}=\text{N}-\text{N}=\text{C}$. The new band at 1520 cm^{-1} may be attributed to the oscillations of coordinated $\nu(\text{C}=\text{O})_{\text{acac}}$.

The crystallization water molecules are associated ($\nu(\text{OH})=3215 \text{ cm}^{-1}$), forming three hydrogen bonds. The oscillations $\nu(\text{V}=\text{O})$ are manifested at 908 cm^{-1} and is the most intensive band in the spectrum.

According to the x-ray single crystal study, the isolated compound $\text{VO}_2\text{L}\cdot 2\text{H}_2\text{O}$ has a molecular structure composed by neutral $[\text{VO}_2\text{L}]$ complexes and solvate water molecules in 1:2 ration. Vanadium atom adopts a NO_4 trigonal-bipyramidal environment, being coordinated by two oxygen atoms and one tridentate Schiff-base ligand L.



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X-Ray studies in a manganese lawsonate coordination polymer

Marcos M. P. Silva, Mauricio Lanznaster, Jackson A.L.C Resende, Francisco L. S. Bustamante, *Departament of Inorganic Chemistry, Federal University Fluminense, Niterói, (Brazil)*. E-mail: jresende@vm.uff.br

Lawsonate (2-hydroxy-1,4-naphthoquinone) is a natural spin carrier in metal complexes molecules. The redox properties of quinones and their complexes have been explored for applications such as the development of new drugs for cancer [1] and switches for molecular electronics [2]. Here, we describe the synthesis and the characterization of $[\text{Mn}(\text{C}_{10}\text{H}_5\text{O}_3)_2]_n$ by infrared and ultraviolet spectroscopy, thermogravimetric analysis and single-crystal X-ray diffraction. X-ray data shows the formation of a coordination polymer with the manganese atom in a center of a fully distorted octahedron (C2/c). The carbonyl and the phenoxy oxygens (O1 and O2, respectively) chelate to the manganese, and the other carbonyl oxygen (O3) bridges to another metal center forming a 2D arrangement. Temperature dependent X-ray studies (225K and 110K) shows a significantly variation in bond distances around the metal center, which indicates change in the bond