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Cu(II) Complex with $L(CH_3CH_2)$ (L=1-thiocarboxamide-3-Methyl-4-ethanol-3-pyrazolin -5-one). Z. K. Jacimovic[a], Z. D. Tomic[b] G. Giester[c], A. Galani[d], V. Dokorou[d], D. Kovala Demertzi[d]. [a]*Faculty of Metallurgy and Technology, University of Montenegro, Montenegro.* [b]*'Vinča' Institute of Nuclear Sciences Serbia.* [c]*Institut für Mineralogie und Kristallographie, Universität Wien, Austria,* [d]*University of Ioannina, Greece.*
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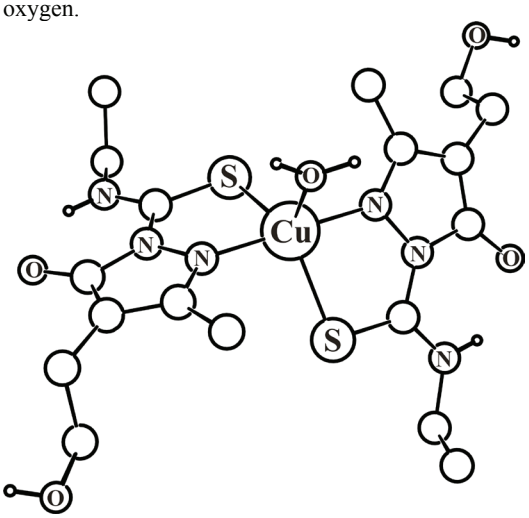
In the reaction of $Cu(CH_3COO)_2$ and the 1-thiocarboxamide-3-Methyl-4-ethanol-3-pyrazolin-5-one the title complex was obtained. One H atom in thiocarboxamide fragment of the uncoordinated molecule is substituted with the CH_3CH_2 fragment.(Fig.). Copper(II) is five-coordinate by the two ligands of and one water molecule. Ligand is bidentately coordinated through the deprotonated pyrazole nitrogen and thiocarboxamide sulfur.The asymmetric unit consists of half of the $Cu[(L(CH_3CH_2))_2(H_2O)]$ complex located on a 2-fold rotational axis, and one solvent water molecule. The Addison distortion index τ (τ=0 for a square pyramid and τ =1 for a trigonal bipyramid) is 0.91. This suggest that the coordination polyhedron around copper could be best described as a slightly distorted trigonal bipyramid. There is no significant changes in the ligand geometry comparing to the non-coordinated molecule of L. The most significant difference in the bond distances is lenghtening of the C-S bond of 0.03Å. The mean planes of the thiocarboxamide fragment and of the pyrazole ring form dihedral angle of 3.6(1)° which is comparable to the value of 4.0(2)° observed in the noncoordinated molecule. Both observations are in accordance with the supposed 'softness' of the S atom (in the context of Hard-Soft-Acid-Base principle). Association of complex molecules in the crystal is determined by hydrogen bonds formed between the coordinated water molecules and pyrazolon oxygen, leading to the formation of the molecular chains. This arrangement is additionally stabilized by the stacking interactions between the pyrazole rings (distance between the ring centroids is 3.48Å), and the hydrogen bonds involving solvent water and pyrazolon oxygen.



Keywords: pyrazolon; Cu-complex; X-ray structure

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Structural Characterization of Drug/Hydrotalcite Nanocomposites. D. Viterbo[a], G. Croce[a], F. Carniato[a], E. Conterosito[a], M. Milanesio[a], L. Palin[a], V. Ambrogi[b], L. Perioli[b]. [a]*DISTA, Università del Piemonte Orientale, Viale Michel 11, 15100 Alessandria, Italy.* [b]*Dipartimento di Chimica e Tecnologia del Farmaco, Università di Perugina, 06123, Perugia, Italy.*
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Hydrotalcites are inorganic layered hydroxides containing exchangeable anions, in which the lamellar plane is constituted by bivalent and trivalent metals octahedrally coordinated to six hydroxyl groups The increasing interest for these materials is due to their numerous applications in particular in catalysis and in pharmaceutical formulations. In the last case an improvement of the dissolution rate of poorly water soluble drugs and prolonged drug release may be achieved. The use of hydrotalcites for intercalating anionic sunscreens was also proposed, with the purpose of improving the sunscreen photostability.
The comprehension of the structural features of these hybrid organic-inorganic materials and the transformations induced by external stimuli is fundamental to understand the stability of the materials and to identify the optimal modifications to produce improved materials and/or formulations.
An hydrotalcite sample was exchanged with the anionic form of 2-phenylbenzimidazol-5-sulphonic acid (EUS), used as sun screen and the obtained nanocomposite showed interesting pharmacological properties. To elucidate the exchange and release mechanisms at the molecular level, these host-guest materials have been studied by X-ray powder diffraction also at in situ conditions, exploring the differences in the structural features of the hosting framework after the drug encapsulation and the features of the organic molecule in a confined context. The extent of the different intermolecular forces acting on the drug molecules constrained in a confined space have been investigated by Raman spectroscopy.

Keywords: composite layered materials; drug formulation; raman/XRPD