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Vibrational spectra of Hg₃TeO₆ and Hg₂TeO₅

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The infrared and Raman spectra of the crystalline hexaoxotellurates Hg₃TeO₆ and Hg₂TeO₅ were recorded and discussed on the basis of a site symmetry analysis derived from known structural data. Approximate values for the Te-O bond force constants are reported and some comparisons with related species are made.

Vanadium (V) complexes with salicylaldehyde semicarbazone derivatives bearing in vitro anti-tumor activity toward kidney tumor cells (TK-10): crystal structure of [V^{VO}₂(5-bromosalicylaldehyde semicarbazone)]

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Journal of Inorganic Biochemistry 99, 443-451 (2005).

As a contribution to the development of novel vanadium complexes with pharmacologically interesting moieties, new dioxovanadium(V) semicarbazone complexes with the formula *cis*-VO₂L, where L=5-bromosalicylaldehyde semicarbazone and 2-hydroxynaphtalen-I-carboxaldehyde semicarbazone have been synthesized and characterized by ¹H and ¹³C NMR, Raman and FTIR spectroscopies. Results were compared with those previously reported for other three analogous complexes of this series. The five complexes were tested in three different human tumor cell lines for bioactivity as potent anti-tumor agents, showing selective cytotoxicity on TK-10 cell line. Results showed that structural modifications on the semicarbazone moiety could have a significant

effect on the anti-tumor activity of the vanadium complexes. In addition, the electrochemical behavior of all the complexes was studied. No apparent correlation could be demonstrated between reduction potentials of the complexes and their anti-tumor activities. The molecular structure of the novel $[V^VO_2(5\text{-bromosalicylaldehyde semicarbazone})]$ complex was solved by X-ray diffraction methods.

Evidence of formation of glushinskite as a biomineral in a Cactaceae species

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Phytochemistry 66, 611-614 (2005)

The X-ray diffractometric and infrared spectroscopic investigation of crystalline material isolated from the Cactaceae species *Opuntia ellisiana* shows the presence of a very complex mineral composition, including whewellite (monohydrated calcium oxalate), opal (SiO_2), calcite ($CaCO_3$) and glushinskite (dihydrated magnesium oxalate). This is the first report of the presence of magnesium oxalate in plants.

The saccharinate anion: a versatile and fascinating ligand in coordination chemistry

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Química Nova 28, 326-328 (2005)

The saccharinate anion, obtained by deprotonation of the N-H moiety of saccharin (o-sulfobenzimide) is a very versatile and polyfunctional ligand in coordination chemistry. In this review the different forms of metal-to-ligand interactions involving this anion and some other coordination peculiarities are briefly discussed on the basis of some selected examples.

Transition metal promoted addition of methanol to cyanoguanidine. Molecular structure and properties of the generated copper(II) and nickel(II) complexes

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Zeitschrift für Anorganische und Allgemeine Chemie 631, 1502-1506 (2005).

The reaction of Cu(II) and Ni(II) complexes of saccharin with dicyandiamide (cyanoguanidine, cnge) in methanol produces the addition of methanol to the nitrile moiety of this molecule. Furthermore, the product of the reaction coordinates to the metal centers generating two new complexes containing saccharinate as the counter anion. The crystal structures of $[Cu(cnge-OCH_3)_2](\text{sac})_2$ and $[Ni(cnge-OCH_3)_2](\text{sac})_2 \cdot 2H_2O$ (cnge-OCH₃=1-amidino-O-methylurea) were

solved by single crystal X-ray diffractometry. The complexes were characterized by means of electronic and infrared spectroscopy and also their magnetic and thermal behavior was investigated.

Structural and spectroscopic characterization of aqua-diargininate-copper(II)-carbonate monohydrate

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Journal of Inorganic Biochemistry 99, 1250-1254 (2005).

The molecular structure of the title complex, $[\text{Cu}(\text{C}_6\text{H}_{14}\text{N}_4\text{O}_2)_2(\text{H}_2\text{O})]\text{CO}_3 \cdot \text{H}_2\text{O}$, was determined by single crystal X-ray diffractometry. It crystallizes in the monoclinic space group $P2_1$, with $Z=2$. The Cu(II) ion is in a square pyramidal environment, trans coordinated at the basis by two arginate groups acting as bidentate ligands through their amino nitrogen and carboxylate oxygen atoms. The coordination around copper is completed by a water molecule at the pyramid apex. The infrared, Raman and electronic spectra are briefly discussed on the basis of the structural peculiarities of the complex.

Spectroscopic and electrochemical behavior of the methyl and ethyl derivatives of bis(acetylacetonato) oxovanadium(IV)

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Zeitschrift für Anorganische und Allgemeine Chemie 631, 1903-1908 (2005).

The infrared, Raman and electronic spectra of the oxovanadium(IV) complexes of 3-methyl and 3-ethyl substituted acetylacetonate were recorded and discussed in detail, in comparison with that of the bis(acetylacetonato) complex and on the basis of the known structural data of these compounds. The electrochemical behavior was investigated by cyclic voltammetry in DMSO solutions, and the mechanism of the involved processes is briefly discussed.

Structural data and vibrational spectra of the copper(II) complex of L-selenomethionine

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Zeitschrift für Naturforschung 60b, 663-666 (2005).

A Cu(II) complex of the amino acid L-selenomethionine of stoichiometry $\text{Cu}(\text{L-SeMet})_2$, has been prepared and characterized. Crystallographic data were obtained by means of X-ray powder diffractometry and showed that the compound is isostructural with the related complex of L-methionine, $\text{Cu}(\text{L-Met})_2$. The structural analogy is also supported by the analysis of the IR and Raman spectra of the complex, which are briefly discussed in comparison with those of free L-selenomethionine.

Vibrational properties of tellurium tetrachloride

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Zeitschrift für Naturforschung 60a, 408-410 (2005).

On the basis of the most recently reported spectroscopic data on vibrational modes and structural parameters of TeCl_4 , an estimation of its main force constants complemented with the calculation of mean amplitudes of vibration, in a wide temperature range, have been performed. Also thermodynamic functions for the ideal gaseous state of the molecule were calculated, using the statistical mechanics approach.

On the interaction of oxovanadium(IV) with homocysteine

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Biological Trace Element Research 105, 53-58 (2005).

The interaction of the VO_2^+ cation with homocysteine was investigated by electron absorption spectroscopy in aqueous solution at different metal-to-ligand ratios. The direct reduction of vanadate(V) solutions with homocysteine was also investigated. The results suggest that the interaction is different from that found in the case of cysteine and occurs through pairs of amino and carboxylate groups of the amino acid. The interaction with VO_2^+ with homocystine, the oxidation product of homocysteine, was also analyzed. The interest of the results in relation to vanadium metabolism and detoxification is briefly discussed.

Mean amplitudes of vibration of phosphine borane and trifluorophosphine borane

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Zeitschrift für Naturforschung 60a, 554-556 (2005).

The mean amplitudes of vibration of PH_3BH_3 and PF_3BH_3 were calculated from known spectroscopic and structural data between 0 and 1000 K and compared with those of related species. Bond peculiarities are also briefly discussed.

Incidence of hypocupremia in cattle in northern Uruguay and its alleviation with an injected Cu-phenylalanine complex

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Livestock Production Science 95, 49-56 (2005).

Serum copper in diary cattle have been studied in eight locations throughout Department of Salto, in Uruguay. The overall incidence of hypocupraemia lies in 30% which is not homogeneously distributed since some farms are almost exempt from hypocupraemial individuals. The Cu(II) complexes Cu(Phe)₂, Cu(Gly)₂·H₂O and Cu(Val)₂ were evaluated as injectable sources of supplemental copper in the most hypocupraemic herd and Cu(Phe)₂ proved to be the best at improving Cu status. The efficacy of this complex was tested in a further hypocupraemic herd, showing that the treated cattle maintained the serum copper level at an adequate level for at least 100 days.

At the same time, analyses of copper, molybdenum, sulphur and phosphorous levels in grass were done along the year. Our result show that the copper content in grass was under adequate levels most part of the year, and the efficiency was more critical in autumn. Although the molybdenum and sulphur levels were low enough not to expect them to interfere in copper absorption, the Mo content may be enhancing the copper deficiency.

Suplementação de elementos-traços

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Quimica Nova na Escola 6, 7-12 (2005).

Some aspects related to the function and essential character of inorganic systems which are fundamental to the correct and balanced development of physiological and metabolic processes in living organisms are discussed. It is well known that deficiencies of essential trace elements cause many physiological disorders and diseases. Hence supplementation of these elements become a subject of increasing importance in modern Pharmacology. Inorganic Medicinal Chemistry proposes a variety of methods and ways to make supplementation more effective and potent. These methods are illustrated with examples involving supplementation of iron, zinc, copper, chromium, magnesium, selenium and some other ultra micro trace elements.

Structural and vibrational properties of vanadium(III) oxofluoride and oxochloride -a theoretical study

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Journal of Molecular Structure (THEOCHEM) 732, 155-159 (2005).

The potential energy surfaces of FVO and CIVO are studied using density functional theory. It is found that the potential energy surface of both molecules is dominated by triplet states. Several singlet states are found close in energy, though. A good agreement is found between experimental and calculated vibrational frequencies except for the V-F stretching mode, which is predicted to be low by the present results. The frequencies corresponding to the O-V-X bending mode are provided as a guide for future experimental studies. An estimation of force constants, mean amplitudes of vibration, and thermodynamic functions is performed, too, in order to get a deeper insight into the bond properties of the title molecules.

Synthesis, characterization and biological activity of oxovanadium(IV) complexes with cyclic polyalcohols

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Oxovanadium (IV) complexes of the cyclic polyalcohols conduritol C (cond) and myo-inositol (inos) of stoichiometry $\text{Na}_2[\text{VO}(\text{cond})_2] \cdot 2\text{H}_2\text{O}$ and $\text{Na}_2[\text{VO}(\text{inos})_2] \cdot \text{H}_2\text{O}$ were obtained in aqueous alkaline solutions. They were characterized by IR and UV-vis spectroscopy's, thermoanalytical (thermogravimetric and differential thermal analysis) data and magnetic susceptibility measurements. The biological activities of the complexes on the proliferation, differentiation and glucose consumption were tested on osteoblast-like cells in culture. Conduritol C and myo-inositol did not produce any effect on these parameters. Normal and tumoral cell proliferation was inhibited about ca. 40-60% by the two oxovanadium(IV) complexes in concentrations as low as 100 M. The complexes were also inhibitory on cell differentiation (ca. 70-80%) while they stimulate glucose consumption. Comparisons of these effects with those of the VO_2^+ cation, under the same experimental conditions, were also performed.

Mean amplitudes of vibration of $[\text{NH}_3\text{F}]^+$ and $[\text{NH}_3\text{Cl}]^+$

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Zeitschrift für Naturforschung 60a, 863-864 (2005).

The mean amplitudes of vibration of $[\text{NH}_3\text{F}]^+$ and $[\text{NH}_3\text{Cl}]^+$ were calculated from known spectroscopic and structural data in the temperature range between 0 and 1000 K. The results are compared with those of related species and the bond properties are also briefly discussed. Mean amplitude values for the NH_4^+ cation, at some selected temperatures, are also reported.

Applications of vibrational spectroscopy to the investigation of plant material

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Advances in Plant Physiology, A. Hemantaranjan (Editor), Scientific Publishers, Jodhpur/India, 2005, Vol. 8, pp. 365-392.

A review devoted to the applications of infrared and Raman spectroscopy and of some special techniques derived from these methodologies (resonance Raman spectroscopy, surface enhanced Raman spectroscopy, infrared and Raman microspectroscopy, attenuated total reflection spectroscopy, etc.) to the investigation of plants and other materials of vegetal origin. The presented and discussed examples include the spectroscopic analysis of woods, conifer needles, essential oils, epicuticular waxes, alkaloids of plants, lichen and mushroom components, plant biominerals as well as studies of lichen biodeterioration processes, plant pigments and metalloproteins. Finally, vibrational spectroscopic studies of foods and other products of vegetal origin are presented and critically discussed.