

A spectroscopy approach for the study of the interactions of bioactive vanadium species with bovine serum albumin

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Different spectroscopic methods were applied to study the effects of the interaction of vanadyl (VO^{2+}) and vanadate (VO_3^-) species with bovine serum albumin (BSA), considered as the most abundant plasma protein. UV-vis, Fourier transform infrared (FTIR) and FT-Raman spectroscopies were used to investigate changes in secondary and tertiary structures of BSA induced by the binding of vanadium species. Correlations between the metal ion binding mode, protein conformational transitions, and structural variations were established.

Vanadium detoxification: On the interaction of oxovanadium (IV) and other vanadium species with 2,3-dimercapto-1-propanesulfonate

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The interaction of the VO^{2+} cation with the sodium salt of 2,3-dimercapto-1-propanesulfonic acid (DMPS) was investigated by electronic absorption spectroscopy in aqueous solution, in the pH range between 4 and 12. The spectral behavior point to the generation of a $[\text{VO}(\text{DMPS})_2]^{4-}$ complex in which the oxocation interacts with two pairs of deprotonated $-\text{SH}$ groups of the ligand. By spectrophotometric monitoring it was found that DMPS rapidly reduces vanadates(V) to VO^{2+} which may be chelated by an excess of the acid. DMPS produces also the slow reduction of a V_2O_5 suspension at pH 7.1. The results of this study suggest that DMPS may be a potentially useful detoxification agent for vanadium.

Vibrational spectra of polaprezinc, a polymeric Zn(II) complex of carnosine

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Journal of Raman Spectroscopy 39, 474-477 (2008).

Polaprezinc, the Zn(II) complex of the dipeptide carnosine (β -alanyl histidine) presents an interesting biological and pharmacological activity, specially as an anti-ulcer agent. The IR and Raman spectra of this compound were recorded and briefly discussed. Some comparisons were made with related complexes and with free carnosine. The results confirm the coordination environment of the Zn(II) cation, constituted by the terminal amino N-atom, the deprotonated amide N-atom and one carboxylate oxygen of one dipeptide molecule and the N-atom of the imidazole moiety of a second carnosine molecule.

Vibrational spectra of copper(II) complexes of L-proline

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Latin American Journal of Pharmacy 27, 197-202 (2008).

The infrared and Raman spectra of the Cu(II) complexes of L-proline (L-pro) [Cu(L-pro)₂].5H₂O and [Cu(L-pro)(H₂O)Cl] were recorded and analyzed in relation to its structural peculiarities and by comparison with the spectra of the free amino acid. The electronic spectra of both complexes are also briefly discussed.

Experimental and theoretical studies of calcium fructoborate

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Biological Trace Element Research 122, 64-72 (2008).

Calcium fructoborate simples of composition $\text{Ca}(\text{C}_6\text{H}_{10}\text{O}_6\text{BO})_2 \cdot 3.5\text{H}_2\text{O}$ were characterized by chemical analysis, infrared and Raman spectroscopy, and thermoanalytical (thermogravimetric and differential thermal analysis) data. Theoretical studies, using density functional theory, were made for seven different structural models of the fructoborate moiety, and the most stable structure could be derived from these calculations. The results of the theoretical study also allow improving the assignment of the vibrational spectra of the compound.

Structural and IR-spectroscopic characterization of some new $\text{Sr}_2\text{LnSbO}_6$ perovskites

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Journal of Alloys and Compounds 460, 152-154 (2008).

A series of ternary perovskite-oxides of composition $\text{Sr}_2\text{LnSbO}_6$ (with Ln = La, Nd, Sm, Gd, Dy, Er, Yb, Y), have been prepared and their unit cell parameters determined by X-ray powder diffractometry. The infrared spectra of these materials were also recorded and briefly discussed on the basis of their structural peculiarities and by comparison with those of related oxides.

A new supramolecular assembly obtained by reaction between thiosaccharin and pyridine

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Zeitschrift für Naturforschung, 63b, 877-879 (2008).

The crystal structure of pyridinium thiosaccharinate thiosaccharin $[\text{HNC}_5\text{H}_5]^+[(\text{tsac})(\text{Htsac})]^-$ ($\text{Htsac} = \text{C}_7\text{H}_5\text{NO}_2\text{S}_2$, the thiosaccharin molecule), was determined by single-crystal X-ray diffraction. Both, the thiosaccharinate anion, the corresponding neutral molecule and the pyridinium cation are nearly planar and arranged in the solid state in an almost parallel fashion, hence giving rise to a supramolecular structure. The anion shows small but significant modifications in the bonding of the thioamide group as compared with the neutral molecule. The crystal is further stabilized by an extensive H-bonding network. The FTIR spectrum of the compound is briefly commented.

Spectroscopic investigation of the VO^{2+} /chitosan interaction

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Carbohydrate Polymers 74, 704-706 (2008).

Different oxovanadium(IV) complexes were prepared by interaction of aqueous $\text{VOSO}_4 \cdot 5\text{H}_2\text{O}$ solutions with chitosan solutions in diluted acetic acid, or by direct interaction of the vanadyl salt with chitosan suspensions in water. A detailed analysis of the IR spectra of pure chitosan and its VO^{2+} complex is presented. On the basis of this analysis, it is suggested that VO^{2+} /chitosan interactions involves only N-donors of the biopolymer.

Vanadium detoxification: Chemical and biochemical aspects

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Chemistry and Biodiversity 5, 1475-1484 (2008).

A brief review on vanadium toxicity and detoxification. In particular, different aspects of biological detoxification routes are discussed on the basis of the metabolic pattern of vanadium in the higher forms of life. Chemical detoxification, using different chelating, reducing and/or reducing/chelating agents is also discussed. Emphasis is given on recently developed chelating agents.

Spectroscopic study of $\text{YBa}_3\text{B}_9\text{O}_{18}$, an interesting material containing a six-membered borate ring

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Zeitschrift für Anorganische und Allgemeine Chemie 634, 2127-2129 (2008).

The IR and Raman spectra of $\text{YBa}_3\text{B}_9\text{O}_{18}$ were recorded and interpreted on the basis of the D_{3h} local symmetry of the six membered planar B_3O_6 rings present in its structure. For comparative purposes also the IR spectra of $\text{NdBa}_3\text{B}_9\text{O}_{18}$, $\text{GdBa}_3\text{B}_9\text{O}_{18}$, and $\text{YbBa}_3\text{B}_9\text{O}_{18}$ were recorded and analyzed.

Mean amplitudes of vibration of molecules and ions with interhalogen bonds and related species

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Journal of Fluorine Chemistry 129, 1060-1072 (2008).

Mean amplitudes of vibration of molecules and ions containing interhalogen bonds are reviewed and critically analyzed. The presented information comprises pure interhalogen compounds as well as oxohalides. Correlations between mean amplitude values and structural and bond properties are discussed. Comparisons with data of related –specially isoelectronic- species are also performed. Characteristic ranges for the mean amplitudes of vibration for halogen-halogen- and halogen-oxygen bonds could be established. The presented and discussed results are also of central importance for the analysis and interpretation of electron diffraction studies.

Structural and spectroscopic characterization of 2,2'-methylenedi-8-quinolinol dihydrochloride dihydrate

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Journal of Molecular Structure 892, 216-219 (2008).

The crystal structure of the title compound, a promising ligand for chelatotherapies in the treatment of Alzheimer's disease, has been determined by single crystal X-ray diffractometry. It crystallized in the monoclinic space group C2/c with Z = 4. The dimeric 8-quinolinol molecule is sited on a crystallographic two-fold axis passing through the CH₂ carbon atom that links the symmetry related molecular halves, giving rise to a two-bladed propeller-like conformation. The ¹H- and ¹³C-NMR- as well as the FTIR and Raman spectra of the compound were also recorded and are briefly discussed. Some comparisons with spectra of related species are made.

Study of the $[\text{Zn}(\text{H}_2\text{O})_4\text{CuEDTA}]\cdot 2\text{H}_2\text{O}$ complex, a potential trace-metal supplier: synthesis, crystal structure, spectroscopic behavior and metal release

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Ethylenediaminetetraacetic acid (H_4EDTA) is widely used in the pharmaceutical and bromatological industries and as a drug in chelation therapies. Besides, coordinated with metal ions it is used for the supplementation of essential trace elements. In this work the synthesis, crystallographic, and spectroscopic studies (EPR, IR, UV/Vis) of $[\text{Zn}(\text{H}_2\text{O})_4\text{CuEDTA}]\cdot 2\text{H}_2\text{O}$ are reported. The release of the metal cations at gastric pH was also investigated.

Mean amplitudes of vibration of the IF_8^- Anion

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The mean amplitudes of vibration of the interesting IF_8^- anion (D_{4d} symmetry), containing iodine(VII), were calculated from known spectroscopic and structural data in the temperature-range between 0 and 1000 K. The results are discussed in comparison with those of related species.

La nueva farmacoterapia inorgánica. XIX. Compuestos de galio.

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Se presentan las características relevantes de la química del galio(III) y su relación con la del hierro(III), que parece ser fundamental para su actividad biológica y farmacológica. Luego se discuten los efectos farmacológicos del nitrato de galio y sus limitaciones prácticas y se analizan las características y posibilidades de algunos nuevos complejos de coordinación del Ga(III) con ligandos orgánicos. Finalmente, se consideran las potencialidades de los radiofármacos de galio.

Easy synthesis of CaB_2O_4 via pyrolysis of calcium fructoborate

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Materials Research 11, 493-494 (2008).

The investigation of the thermal behavior of calcium fructoborate samples of composition $\text{Ca}(\text{C}_6\text{H}_{10}\text{O}_6\text{BO})_2 \cdot 3.5\text{H}_2\text{O}$ showed that CaB_2O_4 is generated as the final pyrolysis residue. On the basis of these observations a new, very easy, synthetic procedure for the preparation of this calcium borate is proposed. The material was characterized by X-ray powder diffractometry and IR spectroscopy.