

Vibrational spectra of Zn(II) complexes of the amino acids with hydrophobic residues

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The infrared and Raman spectra of the bis-chelated Zn(II) complexes of the amino acids glycine, alanine, valine, leucine, isoleucine and phenylalanine were recorded and analyzed in relation to its structural peculiarities. Some comparisons between the recorded spectra are also presented and the characteristics of the carboxylate motions as well as those of the metal-to-ligand vibrations are discussed in detail.

Synthesis and spectroscopic characterization of hydroxylamido/amino acid complexes of oxovanadium(V)

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A series of mixed ligand oxovanadium(V) complexes of the type $[\text{VO}(\text{NH}_2\text{O})_2(\text{aa})]$, containing the hydroxylamido ligand and simple amino acids, were prepared and characterized. Seven of these complexes, with aa = valine, leucine, isoleucine, phenylalanine, tryptophan, cysteine and methionine were described for the first time. Their infrared and Raman spectra, together with those of the previously investigated similar species with aa = glycine, serine, threonine and alanine, and those of the related $[\text{VO}(\text{NH}_2\text{O})_2(\text{imidazole})_2]\text{Cl}$ complex, were recorded and assigned. The spectroscopic behavior of the new complexes is similar to that of the other five, whose structures has been determined by X-ray crystallography, suggesting an identical structure for the full series of complexes. The spectroscopic results also allow to obtain a better characterization of the vibrational behavior of the interesting O-N- “side-on” bonded hydroxylamido ligand.

Oxovanadium(IV) complexes of carbohydrates: A brief overview

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In this brief review the most recent studies and the most relevant aspects of the complexes generated by interaction of carbohydrates and related molecules with the oxovanadium (IV) cation, VO^{2+} , are presented and discussed. The survey includes complexes of mono-, di- and polysaccharides, and of other molecules related to simple sugars. First studies with conduritols and related molecules are also described. Moreover, complexes of ascorbic and quinic acids and of some peculiar flavonoids are also included. Some comments on the general physicochemical properties of these complexes are made and their biological activities and effects are also briefly discussed.

Mean amplitudes of vibration of the ClF_6^- , BrF_6^- and IF_6^- anions

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Journal of Fluorine Chemistry 130, 534-536 (2009).

Mean amplitudes of vibration for the title hexafluoroanions were calculated on the basis of its vibrational-spectroscopic and structural data in the temperature range between 0 and 1000 K. The results are briefly discussed in comparison with those of other related species.

Spectroscopic investigations of iron(II) and iron(III) oxalates

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Journal of the Brazilian Chemical Society 20, 445-450 (2009).

In an attempt to contribute to a better characterization of Fe^{II} and Fe^{III} oxalate complexes an investigation of its vibrational (infrared and Raman) and ⁵⁷Fe-Mössbauer spectra was performed. It is shown that the two polymorphs, α and β , of FeC₂O₄·2H₂O cannot be accurately differentiated with any of these spectroscopic methods, demonstrating the very close structural similarity of these two crystalline forms. Partially deuterated samples of β -FeC₂O₄·2H₂O were also investigated to improve the vibrational-spectroscopic analysis. In the case of Fe₂(C₂O₄)₃·4H₂O, a structural model, derived from results of combined vibrational and Mössbauer data, could be proposed. The 298 K Mössbauer spectrum for this complex is discussed in detail, for the first time.

Vibrational spectroscopic investigation of the hydrates of manganese(II) oxalate

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Journal of Raman Spectroscopy 40, 915-920 (2009).

The three known hydrates of manganese(II) oxalate, α - $\text{MnC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$, γ - $\text{MnC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ and $\text{MnC}_2\text{O}_4 \cdot 3\text{H}_2\text{O}$ were synthesized by known procedures and characterized by X-ray powder diffractometry. Their infrared and Raman spectra were recorded and discussed on the basis of its structural peculiarities allowing to establish some interesting relations between them and with other, previously investigated, oxalate complexes. The IR spectra of partially deuterated samples of α - $\text{MnC}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ were also discussed, reinforcing some of the performed assignments.

Two new supramolecular assemblies obtained by reaction between saccharin and long-chain diamines

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Zeitschrift für Naturforschung 64b, 1041-1045 (2009).

The crystal structures of heptamethylenediammonium bis(saccharinate) monohydrate, $[\text{H}_3\text{N}-(\text{CH}_2)_7-\text{NH}_3](\text{sac})_2 \cdot \text{H}_2\text{O}$ (**1**) and octamethylenediammonium bis(saccharinate) hemihydrate, $[\text{H}_3\text{N}-(\text{CH}_2)_8-\text{NH}_3](\text{sac})_2 \cdot 0.5\text{H}_2\text{O}$ (**2**), were determined by single-crystal X-ray diffraction methods. Compound **1** crystallizes in the triclinic space group $P\bar{1}$ with 2 molecules per unit cell and **2** in the monoclinic, space group $P2_1/a$ with $Z = 4$. The saccharinate moiety is planar in both compounds presenting bonding characteristics comparable to those found in other saccharinate salts. The ionic crystals are further stabilized by an extensive H-bonding network, which links the anions and cations into an infinite three-dimensional supramolecular assembly. The FTIR spectra of the adducts are briefly discussed in comparison with those of the constituent molecules.

Vibrational spectra of the physiologically and pharmacologically relevant Cu(L-His)₂ complex

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Latin American Journal of Pharmacy 28, 789-792 (2009).

The infrared spectrum of the Cu(II) complex of L-histidine (L-His) of composition [Cu(L-His)₂].1.5H₂O, generated at physiological conditions, was recorded and analyzed in relation to its structural peculiarities and by comparison with the spectrum of the free amino acid. The electronic spectrum of the complex is also briefly discussed.

⁵⁷Fe-Mössbauer study of a Fe^{II}₄O₄ cubane like-moiety

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An. Acad. Nac. Cs. Ex. Fís. Nat. 60, 109-111 (2008).

The room temperature ⁵⁷Fe-Mössbauer spectrum of [C(NH₂)₃]₈[Fe(cit)₄].8H₂O, a Fe(II)/citrate complex, containing a cubane-like Fe₄O₄ arrangement, has been recorded and analyzed. The obtained hyperfine parameters, coherent with the structural and electronic features of the compound, reveal that the electronic density of the Fe(II) cations is slightly distorted over the metallic sites.

Vibrational spectra of the layered monofluorophosphate(V), $\text{NH}_4\text{Ag}_3(\text{PO}_3\text{F})_2$

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Journal of Raman Spectroscopy 40, 1698-1700 (2009).

The powder Fourier-transform (FT) infrared and Raman spectra of the recently characterized $\text{NH}_4\text{Ag}_3(\text{PO}_3\text{F})_2$ were recorded and are discussed with a site-symmetry analysis based on its known structural data. Some comparisons are made with the solution spectra of the PO_3F^{2-} anion and with those of crystalline $\text{Ag}_2\text{PO}_3\text{F}$.

Spectroscopic behavior and biological activity of $\text{K}_3[\text{VO}(\text{O}_2)_2\text{CO}_3]\cdot\text{H}_2\text{O}$

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Biological Trace Element Research 132, 176-183 (2009).

The potassium salt of the carbonato oxodiperoxovanadate(V) complex, obtained by a known synthetic procedure, was thoroughly characterized by infrared, Raman and electronic spectroscopy. The bioactivity of the complex on the cell proliferation was tested on osteoblast-like cells (MC3T3E1 osteoblastic mouse-calvaria derived cells and UMR106 rat osteosarcoma-derived cells) in culture. At low doses the complex is more toxic for the non-transformed osteoblasts than for the tumoral ones, whereas at higher doses the deleterious effects are similar for both cell lines. This peroxy complex seems to be the most toxic compound that has so far been tested on osteoblast-like cells in culture.

Vibrational spectra of lead(II) oxalate

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Journal of Raman Spectroscopy 40, 2050-2052 (2009).

The infrared and Raman spectra of anhydrous lead oxalate, PbC_2O_4 , were recorded and discussed on the basis of its structural peculiarities. Some comparisons with other previously investigated metallic oxalates were made.

Characterization of calcium oxalate biominerals in *Pereskia* species (Cactaceae)

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Zeitschrift für Naturforschung 64c, 763-766 (2009).

Calcium oxalate druses were isolated from the stems and leaves of six *Pereskioidea* family members and investigated by infrared spectroscopy, showing that in all samples the biomineral was present in the form of whewellite, $\text{CaC}_2\text{O}_4 \cdot \text{H}_2\text{O}$. As *Pereskia* are thought to represent the “ancestral” condition of the leafless stem-succulent cacti, these results suggest that the biomineralization of calcium oxalate in Cactaceae represents a primitive characteristic of the group and also support a close genetic relationship between *Pereskia* and *Opuntia*.