

Pd(thiosaccharinato)₂.H₂O, the first thiosaccharinato complex of a platinum-group metal

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Journal of Coordination Chemistry 59, 101-106 (2006).

A Pd(II) complex of the thiosaccharinato (tsac) anion, of stoichiometry Pd(tsac)₂.H₂O was prepared by interaction of Na₂PdCl₄ with thiosaccharin in methanol and characterized by infrared and ¹H and ¹³C NMR spectroscopy. These spectral studies confirmed interaction of the metal center with the thiosaccharinate acting as a bidentate ligand through its thiol group and the N-atom. NMR measurements also confirmed that in solution thiosaccharin is mainly present in its thiolate tautomeric form.

Structural and spectroscopic characterization of ammonium thiosaccharinate monohydrate

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Zeitschrift für Anorganische und Allgemeine Chemie 632, 437-440 (2006).

The crystal structure of NH₄(tsac).H₂O (tsac=anion of the thiosaccharin molecule) has been determined by single crystal X-ray diffractometry. It crystallizes in the orthorhombic space group Pbc_a with Z=8. The IR spectrum of the compound was recorded and its most important features discussed on the basis of its structural peculiarities.

Spectroscopic behavior and SOD-like activity of the copper(II) complex of hippuric acid

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Acta Farmacéutica Bonaerense 25, 71-75 (2006).

The dimeric copper (II) complex of hippuric acid (Hhipp), of stoichiometry $[\text{Cu}_2(\text{hipp})_4(\text{H}_2\text{O})_4] \cdot 2\text{H}_2\text{O}$, has been thoroughly characterized by means of its infrared, Raman and electronic spectra, which could be interpreted on the basis of the known structural data. The superoxide dismutase-like activity of the complex was investigated using the nitrobluetetrazolium/superoxide reduction assay and compared with that obtained for the native Cu_2Zn_2 -SOD enzyme, tested under the same experimental conditions. The results show a very important SOD-like activity, suggesting that these type of complexes may be interesting for the future search of new SOD-mimetic drugs.

New saccharinato/ammonia complexes of nickel(II) and zinc(II). A structural and spectroscopic study.

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Zeitschrift für Anorganische und Allgemeine Chemie 632, 619-623 (2006).

Two new saccharinate/ NH_3 complexes of composition $[\text{Ni}(\text{sac})_2(\text{NH}_3)_4]$ and $[\text{Zn}(\text{sac})_2(\text{NH}_3)_2]$ were obtained and their crystal structures determined by single crystal X-ray diffractometry. The elongated octahedral Ni^{II} complex crystallizes in the monoclinic $\text{P}2_1/c$ space group with $Z=2$ whereas the tetrahedral Zn^{II} complex is triclinic (space group $\text{P}\bar{1}$ and $Z=2$). For the $[\text{Ni}(\text{sac})_2(\text{NH}_3)_4]$ complex the magnetic moment and electron absorption spectrum were obtained and discussed. The infrared spectra of both complexes were also recorded and briefly discussed.

On the interaction of vanadium species with meso-2,3-dimercapto- succinic acid

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Biological Trace Element Research 109, 189-194 (2006).

The interaction of the VO^{2+} cation with meso-2,3-dimercaptosuccinic acid (DMSA) was investigated by electron absorption spectroscopy in aqueous solution at different pH-values. The spectral behavior, complemented with a photometric titration, shows the generation of a $[\text{VO}(\text{DMSA})_2]^{2-}$ complex in which the oxocation interacts with two pairs of deprotonated $-\text{SH}$ groups of the acid. It was also found that DMSA rapidly reduces VO_3^- to VO^{2+} , which might be chelated by an excess of

the acid. DMSA can also produce the partial reduction of a V_2O_5 suspension at pH=5.2. The results of this study suggest that DMSA might be a potentially useful detoxification agent for vanadium.

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

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Carbohydrate Research 431, 717-724 (2006).

Oxovanadium(IV) complexes of the polyalcohols sorbitol, galactitol, and mannitol of stoichiometry $Na_2[VO(L)_2] \cdot H_2O$, were obtained from aqueous alkaline solutions. They were characterized by elemental analysis, IR and UV-vis spectroscopies, thermoanalytical (TG and DTA) data and magnetic susceptibility measurements. The biological activity of the complexes on the proliferation, differentiation and glucose consumption were tested on osteoblast-like cells (MC3T3E1 osteoblastic mouse calvaria-derived cells and UMR106 rat osteosarcoma-derived cells) in culture. The three complexes exerted a biphasic effect on cell proliferation, being slight stimulating agents at low concentrations and inhibitory in the range of 25-100 mM. All the complexes inhibited cell differentiation in tumor osteoblasts. Their effects on glucose consumption were also discussed. The free ligands did not show any effect on the studied biological parameters.

Mean amplitudes of vibration of XeO_3F_2

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Physical Chemistry, An Indian Journal 1, 80-82 (2006).

The mean amplitudes of vibration of the trigonal bipyramidal XeO_3F_2 molecule, were calculated from its spectroscopic data in the temperature range between 0 and 1000 K. The results are compared with those of related species and the bond peculiarities of this interesting species are also briefly discussed.

IR-spectroscopic characterization of $NaLn^{III}TiO_4$ and $AgLn^{III}TiO_4$ oxides related to the K_2NiF_4 structural type

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Journal of Alloys and Compounds 419, 334-336 (2006).

A series of ternary oxides of the type NaLnTiO_4 (with $\text{Ln}=\text{La, Nd, Sm, Eu, Gd, Dy, Y}$) and AgLnTiO_4 (with $\text{Ln}=\text{La, Nd}$), have been prepared and their structures confirmed by X-ray powder diffractometry. They are related to the K_2NiF_4 structural type, with the monovalent and trivalent cations distributed in an ordered way on the K sublattice. The infrared spectra of these materials were recorded and briefly discussed on the basis of their structural peculiarities and by comparison with those of related oxides.

Crystal structure and characterization of mercury(II) dichromate(VI)

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Monatshefte für Chemie, 137, 987-996 (2006).

Dark-red single crystals of HgCr_2O_7 were grown by reacting HgO and CrO_3 in excess at 200 °C for four days. The crystal structure was determined by single crystal X-ray diffractometry. It consists of nearly linear HgO_2 units and dichromate moieties linked into infinite $\text{O}_3\text{Cr-O-CrO}_3\text{-Hg-O}_3\text{Cr-O-CrO}_3$ chains running parallel to the *c*-axis. The dichromate anion exhibits a staggered conformation with a bent Cr-O-Cr bridging angle of 140.7(6)°. Upon heating above 300 °C, HgCr_2O_7 decomposes in a two-step mechanism to Cr_2O_3 . The compound was additionally characterized by vibrational spectroscopy.

Copper complexes with heterocyclic sulfonamides: Synthesis, spectroscopic characterization, microbiological and SOD-like activities. Crystal structure of $[\text{Cu}(\text{sulfisoxazole})_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$

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Journal of Inorganic Biochemistry 10, 1167-1175 (2006).

The synthesis, characterization and comparative biological study of a series of antibacterial copper complexes with heterocyclic sulfonamides were reported. Two kinds of complexes were obtained with the stoichiometries $[\text{Cu}(\text{L})_2]\cdot\text{H}_2\text{O}$ and $[\text{Cu}(\text{L})_2(\text{H}_2\text{O})_4]\cdot n\text{H}_2\text{O}$. They were characterized by IR and electronic spectroscopies and the crystal structure of $[\text{Cu}(\text{sulfisoxazole})_2(\text{H}_2\text{O})_4]\cdot 2\text{H}_2\text{O}$ was determined by single crystal X-ray diffraction. It crystallizes in the monoclinic $\text{C}2/c$ space group with $Z=8$ and Cu(II) is in a slightly distorted CuO_4N_2 environment. The antimicrobial activity was evaluated for all the prepared complexes and ligands using the agar dilution test. The results

showed that the complexes with five-membered heterocyclic rings were more active than the free sulfonamides while the pyrimidine, pyridine and pyridazine complexes had similar or less activity than the free ligands. In order to find an explanation for this behavior lipophilicity and superoxide dismutase-like activity were tested, showing that the $[\text{Cu}(\text{sulfamethoxazol})_2(\text{H}_2\text{O})_4] \cdot 3\text{H}_2\text{O}$ presented the highest antimicrobial potency and a SOD-like activity comparable with pharmacological active compounds.

Peculiarities of I-F and I-O bonds in different hypervalent species of iodine

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Journal of the Argentine Chemical Society 93, 23-27 (2005) (publicado en 2006)

On the basis of mean amplitudes of vibration a comparative analysis of the properties of I-F and I-O bonds of a wide series of hypervalent iodine compounds is presented. The mean amplitudes of the vibration of the I-O bonds are significantly characteristic, whereas those related to the I-F bonds are strongly dependent on the molecular geometry and the oxidation state of iodine, generating important differences between them. The discussion is also extended to some isoelectronic species containing tellurium or xenon.

Spectroscopic and magnetic properties of $\text{Fe}_3^{II}\text{Fe}_4^{III}(\text{AsO}_4)_6$

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Journal of Physics and Chemistry of Solids 67, 1781-1785 (2006).

The Infrared (IR) and ^{57}Fe -Mössbauer spectra of $\text{Fe}_3^{II}\text{Fe}_4^{III}(\text{AsO}_4)_6$ were recorded and analyzed on the basis of its structural characteristics. The IR spectrum presents a high complexity, showing an important number of bands and splittings, as a consequence of the presence of three structurally independent AsO_4^{3-} groups. The analysis of the four quadrupole signals shown by the Mössbauer spectrum allowed to attain a detailed insight into the cation distribution over the available crystallographic sites. The alternating current susceptibility measurements indicate a paramagnetic to ferromagnetic transition in the material at about 59 K.

Structural characterization of a series of new Cu-dipeptide complexes in solid state and in solution

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Polyhedron 25, 2597-2604 (2006).

Four new Cu(II)-dipeptide complexes were studied in solid state and in solution. They were synthesized and characterized by IR, electronic and EPR spectroscopic techniques. The crystal structures of [Cu(gly-val)].1/2H₂O, [Cu(val-phe)] and [Cu(phe-phe)] was determined by X-ray diffraction methods. In all the complexes the Cu(II) ion is in a pyramidal square-based environment, equatorially coordinated to a terminal NH₂ group, the deprotonated amide group and one of the oxygen atoms of the carboxylate group. The fourth equatorial ligand is a carboxylate oxygen of a second dipeptide molecule and the fifth coordination position is occupied by the oxygen of an amide group belonging to a third dipeptide molecule. The structural study of the complexes in solution by EPR and electronic spectroscopy suggests that in the frozen solutions the complexes exist mostly as polymeric species while the monomer moiety becomes significant at the lowest concentrations studied. It can also be concluded that, at room temperature, the solutions mainly contain monomeric species.

Metal complexes of saccharin

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Coordination Chemistry Reviews 250, 1980-1999 (2006).

Metal complexes of the saccharinate anion, obtained by deprotonation of the N-H moiety of saccharin (o-sulfobenzimide) are reviewed. A wide variety of metal species based on mononuclear, binuclear, polynuclear complexes and extended coordination polymers are discussed in relation to the coordination modes of the anion, i.e., monodentate (through the N- or the carbonylic O-atom), bidentate, tridentate or bridging forming. The most important physicochemical properties, such as vibrational and electronic spectra, thermal, magnetic and redox properties as well as quantum-chemical theoretical studies of these compounds are briefly described. With regard to saccharin in food and its health effects, the biological properties of saccharin and its complexes are also summarized. Finally, for comparative purposes, a brief overview on the so far characterized metallic complexes of thiosaccharin is given. This survey demonstrates that saccharinate is a very versatile and polyfunctional ligand in coordination chemistry.

Structural and spectroscopic characterization of bis(thiosaccharinato) bis(benzimidazole)cadmium(II)

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Journal of Molecular Structure 797, 56-60 (2006).

The crystal structure of $[\text{Cd}(\text{tsac})_2(\text{bzim})_2] \cdot \text{CH}_3\text{OH}$ (tsac, anion of thiosaccharine; bzim, benzimidazole) has been determined by single crystal X-ray diffractometry. It crystallizes in the triclinic space group $P\bar{1}$ with $Z=2$. The Cd(II) cation is in a distorted tetrahedral CdS_2N_4 environment coordinated to two thiosaccharinate anions and two benzimidazole molecules. The FTIR spectrum of the complex is recorded and briefly discussed. Some comparisons with related complexes are made.

Raman spectrum of thiosaccharin

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Journal of Raman Spectroscopy 37, 948-950 (2006).

The Raman spectrum of crystalline thiosaccharin was recorded and assigned by comparison with known IR spectroscopic data derived from experimental as well as theoretical studies.

X-ray Diffraction and IR Spectroscopic Characterization of $\text{AgLn}^{\text{III}}\text{TiO}_4$ Oxides Related to the K_2NiF_4 Structural Type

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Journal of the Brazilian Chemical Society 17, 1436-1439 (2006).

Ternary oxides of the type $\text{AgLn}^{\text{III}}\text{TiO}_4$ (with Ln=La, Nd, Sm, Eu, Gd, Dy, Y) have been prepared and their unit cell parameters determined by X-ray powder diffractometry. They are related to the K_2NiF_4 structural type with Ag^{I} and Ln^{III} cations distributed in an ordered way on the K-sub lattice.

The infrared spectra of these materials were recorded and discussed on the basis of their structural peculiarities and by comparison with those of related oxides. They show a close relationship with the parent $\text{NaN}^{\text{III}}\text{TiO}_4$ materials.

Vibrational spectra of three new diarsenates containing scandium(III)

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Journal of Raman Spectroscopy 37, 1335-1340 (2006).

The powder FTIR IR and Raman spectra of the new isotypic diarsenates $\text{RbScAs}_2\text{O}_7$, $\text{TlScAs}_2\text{O}_7$ and $(\text{NH}_4)\text{ScAs}_2\text{O}_7$ are discussed with a factor group analysis, on the basis of their known structural characteristics. The spectroscopic behavior clearly reflects all the structural peculiarities and also confirms the rotational quenching of the NH_4^+ cation in $(\text{NH}_4)\text{ScAs}_2\text{O}_7$. The crystal structure of $\text{TlScAs}_2\text{O}_7$ is also reported for the first time and is briefly discussed.

Vibrational spectra of $\text{ScAsO}_4 \cdot \text{H}_2\text{O}$

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Journal of Raman Spectroscopy 37, 1453-1455 (2006).

The powder FTIR and Raman spectra of $\text{ScAsO}_4 \cdot \text{H}_2\text{O}$ were recorded and are discussed with a factor group analysis based on its known structural characteristics.