Vibrational spectra of the Cu(II) complex of L-asparagine and L-glutamine

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The infrared and Raman spectra of the copper (II) complexes $[Cu(L\text{-}asn)_2]$ and $[Cu(L\text{-}gln)_2]$ (L-asn = L-asparagine; L-gln = L-glutamine), were recorded and analyzed in relation to its structural peculiarities. Some comparisons between the spectra of these complexes and with those of related systems are made. The characteristics of the carboxylate and amide groups of the bonded ligands are discussed in detail.

Single-crystal growth and characterization of disilver (I) monoflurophosphate (V), Ag_2PO_3F: Crystal structure, thermal behavior, vibrational spectroscopy, and solid-state ^{19}F, ^{31}P, and ^{109}Ag MAS NMR spectroscopy

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Inorganic Chemistry 46, 801-808 (2007).

Single crystals of Ag_2PO_3F were obtained by slow evaporation of a diluted aqueous solution. It adopts a new structure type and crystallizes in the monoclinic space group C2/c with Z = 8. The nmonofluorophosphate anion deviates slightly from C_{3v} symmetry and exhibits the characteristic differences in bond lengths, with a mean of 1.510 Å for the P.O bonds and one considerable longer P-F bond of 1.575(2) Å. The compound was further characterized by vibrational (IR and Raman) spectroscopy and solid state ^{17}F, ^{31}P and ^{107}Ag MAS NMR spectroscopy. Thermal analysis (TG, DSC) revealed a reversible phase transition at 308 ⌗C, which is very close to the decomposition range of Ag_2PO_3F. Under release of POF_3, $Ag_4P_2O_7$ and Ag_3PO_4 are the thermal decomposition products at temperatures above 450 ⌗C.

Vibrational spectra of clioquinol and its Cu(II) complex

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Journal of Raman Spectroscopy 38, 373-376 (2007).

The infrared and Raman spectra of 5-chloro-7-iodo-8-hydroxyquinoline (clioquinol, CQ) and that of its Cu(II) complex of stoichiometry $[Cu(CQ)_2]$ were recorded and briefly discussed. Some comparisons were made with related complexes. The interest of the investigated systems in relation to Alzheimer's disease is briefly commented.

X-ray structure and EPR behavior of a new dimeric copper(II) complex with 4-amino-N-(5-methoxy-2-pyrimidinyl)benzenesulfonamide

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Polyhedron 26, 3277-3285 (2007).

A new complex, $[Cu_2(sulfameter)_4]_3.2.5H_2O$ (sulfameter = 4-amino-N-(5-methoxy-2-pyrimidinyl)benzenesulfonamide), has been synthesized. Its structure has been determined by single-crystal X-ray diffraction and its spectroscopic properties (EPR, IR, Raman, UV-Vis) have been analyzed. The structure presented three different dimeric units in the unit cell and the EPR spectra, characteristic of antiferromagnetically coupled dimmers, revealed two magnetically different dimeric environments.

Mean amplitudes of vibration of the $BrO_3F_2^-$ anion

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Journal of the Argentine Chemical Society 94, 1-4 (2006).

The mean amplitudes of vibration of the recently characterized $BrO_3F_2^-$ anion, containing Br(VII), were calculated from its 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 peculiarities of the new anion are also briefly discussed.

Mean amplitudes of vibration of OsO_3F_2

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Physical Chemistry, An Indian Journal 2, 101-103 (2007).

The mean amplitudes of vibration of OsO_3F_2, one of the rare examples of an EO_3F_2 molecule possessing a trigonal bipyramidal structure, 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 peculiarities of the molecule are also briefly discussed.

La nueva farmacoterapia inorgánica. XVIII. Compuestos de lantánidos

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Latin American Journal of Pharmacy 26, 626-634 (2007).

Se presentan las características relevantes de la química de los lantánidos y su posible impacto en sistemas biológicos. Luego se discuten diversos aspectos relacionados con la actividad farmacológica de algunos elementos de este grupo, en particular su actividad antiemética, antimicrobiana y antitumoral. Asimismo, se analiza el impacto del carbonato de lantano para el tratamiento de hiperfosfatemias y de los nuevos complejos de gadolinio que se utilizan como agentes de contraste en estudios de resonancia magnética nuclear. También se analiza el potencial de algunos radiofármacos conteniendo metales de este grupo. Finalmente, se hacen breves comentarios sobre la toxicidad de estos elementos.

Spectroscopic caharacterization of a VO^{2+} complex of oxodiacetic acid and its bioactivity on osteoblast-like cells in culture

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Biological Trace Element Research 118, 159-166 (2007).

The oxovanadium(IV) complex of oxodiacetic acid (H_2oda) of stoichiometry [VO(oda)(H_2O)$_2$], which presents an unprecedented tridentate OOO coordination, was thoroughly characterized by infrared, Raman, electronic, and EPR spectroscopies. The biological activity of the complex on the cell proliferation and differentiation were tested on osteoblast-like cells (MC3T3E1 osteoblastic mouse calvaria-derived cells and UMR106 rat osteosarcoma-derived cells) in culture. The complex caused inhibition of cellular proliferation in both osteoblast-like cells in culture, but the cytotoxicity was stronger in the normal (MC3T3E1) than in the tumoral (UMR106) osteoblasts. The effect of the complex in cell differentiation was tested through the specific activity of alkaline phosphatase of the UMR106 cells since they expressed a high activity of this enzyme. As occurs with other vanadium compounds [VO(oda)(H_2O)$_2$] is an inhibitory agent of osteoblast differentiation.

Vibrational spectra of palladium 5-nitrofuryl thiosemicarbazone complexes: Experimental and theoretical study

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Spectrochimica Acta 68A, 341-348 (2007).

The vibrational spectroscopic behavior of a series of 16 Pd(II) complexes with 8 bioactive nitrofuran containing thiosemicarbazones as ligands has been studied in the solid state. Experimental spectra were satisfactorily described by density functional theory (DFT) calculations. A characteristic vibrational spectroscopic pattern could be defined for this type of complexes.

Vibrational and electronic spectra of synthetic moolooite

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Spectrochimica Acta 68A, 424-426 (2007).

The infrared and Raman spectra of synthetic moolooite, $Cu(C_2O_4).nH_2O$, were recorded and analyzed on the basis of its structural characteristics and by comparison with related species. The thermogravimetric analysis of the investigated samples show that the water content n, was equal to 0.2. The electronic (reflectance) spectrum of the complex was also recorded and briefly discussed.

A new supramolecular assembly obtained by reaction between thiosaccharin and hexamethylenediamine

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Zeitschrift für Naturforschung, 62b, 1530-1534 (2007).

The crystal structure of hexamethylenediammonium bis(thiosaccharinate) dihydrate, $[H_3N\text{-}(CH_2)_6\text{-}NH_3](tsac)_2.2H_2O$ (tsac = $C_7H_4NO_2S_2$, the anion of thiosaccharin), was solved by single-crystal X-ray diffraction methods. It crystallizes in the monoclinic space group $P2_1/a$ with Z = 4. The thiosaccharinate moiety is planar and shows small but significant modifications in the bonding of the thioamide functional group as compared with the protonated neutral molecule. The ionic crystal is further stabilized by an extensive H-bonding network, which links the anions and cations into an infinite three-dimensional supramolecular assembly. The FTIR spectrum of the compound is briefly discussed in comparison with those of the neutral constituent molecules.