Mean amplitudes of vibration of the $VO_2F_2^-$ and $VO_2Cl_2^-$ anions

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Physical Chemistry, An Indian Journal 12, 1-5 (2017).

The mean amplitudes of vibration of the $VO_2F_2^-$ and $VO_2Cl_2^-$ anions, derived from vanadium(V), were calculated from known spectroscopic and structural data, in the temperature range between 0 and 1000 K. The results are discussed and compared with those of the isoelectronic chromium(VI) species CrO_2F_2 and CrO_2Cl_2 and with those of other simple vanadium compounds.

Three new thiosaccharin derivatives generated in a complex reaction mixture

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Journal of the Argentine Chemical Society 104, 1-10 (2017).

The reaction between thiosaccharin and ethylamine showed to be relatively complex. The main product of this reaction is 3-ethylamino-1,2-benzisothiazole 1,1-dioxide (**1**), which could be clearly identified by NMR and IR spectroscopies. Ethylammonium thiosaccharinate (**2**) and 3-vinylamino-1,2-benzisothiazole 1,1 dioxide (**3**) were generated as minor by products during this reaction and their

structures were determined by X-ray diffraction methods. The (**2**) salt crystallizes in the monoclinic $P2_1/c$ space group with a=13.1367(5), b=9.9721(4), c=8.8217(3) Å, β=99.125(4)°, and Z=4, whereas compound (**3**) belongs to the $P2_1/m$ space group with a=7.1572(5), b=7.0242(7), c=9.5503(8) Å, β=95.008(7)°, and Z=2.

Decoding the anticancer activity of VO-clioquinol compound: the mechanism, of action and cell death pathway in human osteosarcoma cells

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Metallomics 9, 891-901 (2017).

Vanadium compounds were studied in recent years by considering them as representatives of a new class of non-platinum metal anticancer drugs. This research deals with the alterations in the intracellular signaling pathways promoted by an oxovanadium(IV) complex with clioquinol (5-chloro-7-iodo-8-quinolinol), $VO(CQ)_2$, on an osteosarcoma cell line (MG-63). Herein are reported, for the first time the antitumor properties of $VO(CQ)_2$ and the relative abundance of 224 proteins (which are involved in most of the most common intracellular pathways) to identify novel targets of the studied complex. Besides, full length human recombinant AKT1 kinase was produced by using an IVTT system to evaluate the variation of relative tyrosin-phosphorylation levels caused by this compound. The results of the differential protein expression levels reveal several up-regulated proteins and down-regulated ones. Moreover, cell signaling pathways invoñved in several altered pathways related to the PKC and AP2 family have been identified in both treatments (2.5 and 10 μM) suggesting the crucial antitumoral role of $VO(CQ)_2$. Finally, it has been

demosnstarted that this compound (10 μM, 6h) triggers a decrease of 2-fold in *in situ* AKT1 expression.

Structural and IR-spectroscopic characterization of cadmium and lead(II) acesulfamates

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Zeitschrift für Naturforschung 72b, 739-745 (2017).

Cadmium and lead(II) acesulfamate, $Cd(C_4H_4NO_4S)_2{\cdot}2H_2O$ and $Pb(C_4H_4NO_4S)_2$, were prepared by the reaction of acesulfamic acid and the respective metal carbonates in aqueous solution, and characterized by elemental analysis. Their crystal structures were determined by single crystal X-ray diffraction methods. The Cd(II) compound crystallizes in the monoclinic space group $P2_1/c$ with $Z = 4$ and the corresponding Pb(II) salt in the triclinic space group $P\bar{1}$ with $Z = 2$. In both salts, acesulfamate acts both as a bi-dentate ligand through its nitrogen and carbonyl oxygen atoms and also as a mono-dentate ligand through this same oxygen atom, giving rise to polymeric structures; in the Pb(II) salt the ligand also binds the cation through its sulfoxido oxygen atoms. The FTIR spectra of the compounds were recorded and are briefly discussed. Some comparisons with other related acesulfamate and saccharinate complexes are made.

Structural and IR-Spectroscopic Characterization of Aqua Lithium Acesulfamate, an Outlier of the M(ace), M: Na^+, K^+, Rb^+, Cs^+, Isomorphic Series

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Journal of Chemical Crystallography 47, 226-232 (2017).

The crystal structure of aqua lithium 6-methytl-1,2,3,-oxathiazine-4(3H)-one, 2.2-dioxide, for short Li(ace)H_2O, was determined by X-ray diffraction methods. It crystallizes in the triclinic $P\bar{1}$ space group with *a* = 6.1750(9) Å, *b* = 7.3969(9) Å, *c* = 9.016(1) Å, *α* = 105.88(1)°, *β* = 94.59(1)°, *γ* = 97.80(1)°, and *Z* = 2 molecules per unit cell. The crystal structure of Li(ace)H_2O sharply departs from the other heavier alkaline-metal acesulfamates, namely the monoclinic isotypic M-ace (M from Na^+ to Cs^+) family of salts. Lithium is in a distorted LiO_4 tetrahedral coordination with acesulfamate carbonyl, sulfoxide and water oxygen atoms. The FTIR spectrum of the new compound was also recorded and is briefly discussed. Some comparisons with other simple acesulfamate salts are also made.

Vanadio: Un Nuevo elemento estratégico?

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Anales de la Academia Nacional de Ciencias Exactas, Físicas y Naturales 69, 84-114 (2017).

Se presentan los aspectos más importantes de la química del vanadio, comenzando con una breve introducción histórica y con un análisis de los

depósitos de vanadio en nuestro país así como de su presencia en sistemas biológicos. A continuación se discute la obtención y principales propiedades del metal, presentando luego sus compuestos más importantes, incluyendo sus complejos de coordinación y compuestos organometálicos. Luego se analizan sus aplicaciones y usos más importantes, enfatizando especialmente su utilización en las nuevas baterias redox y discutiendo la eventual importancia que el elemento pueda tener en su desarrollo e implementación a amplia escala en un futuro próximo.

Terapia por Captura de Neutrones

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Revista ADEQ 2, 12-16 (2017).

La terapia por captura de neutrones es una metodología radioterapeútica basada en las reacciones de captura y fisión que tienen lugar cuando el ^{10}B, constituyente no radiactivo del boro elemental natural, es irradiado con neutrones térmicos de baja energía, generando partículas alfa y núcleos de ^{7}Li de alta energía. Si el ^{10}B está acumulado en un tejido tumoral, esta energía liberada es capaz de destruir selectivamente el tumor, sin afectar el tejido sano circundante. El interés clínico de esta terapia se ha centrado fundamentalmente en el tratamiento de tumores cerebrales (gliomas). En este artículo se analizan en detalle, los aspectos químicos, físicos y biológicos de estas terapias.

La Química Bioinorgánica en el Contexto de un Curso Moderno de Química Inorgánica

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Industria & Química 368, 31-35 (2017).

Se analiza la manera en que la temática de la Química Bioinorgánica puede insertarse en un curso moderno y actualizado de Química Inorgánica y la potencialidad didáctica que esta temática ofrece.

Nickel and its Role in Plant Physiology

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Advances in Plant Physiology (H. Hemantaranjan, Editor), vol. 17, pp. 291-313 (2017). Scientific Publishers, Johdpur.

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Plant purple acid phosphatases: Structure and functions

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Advances in Plant Physiology (H. Hemantaranjan, Editor), vol. 17, pp. 331-359 (2017). Scientific Publishers, Johdpur.

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