J Nanomed Nanotechnol 2013, 4:6
http://dx.doi.org/10.4172/2157-7439.S1.015

OMICS Group Conferences
Accelerating Scientific Discovery

3rd International Conference on
Nanotek & Expo

December 02-04, 2013 Hampton Inn Tropicana, Las Vegas, NV, USA

Advanced structural characterization of chromium (iii) coordination species with bis(3,5 dimethylpyrazol-1-yl)acetic acid

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The synthesis of the coordination compounds with the polydentate ligand bis(3,5-dimethylpyrazol-1 yl)acetic acid (HL = $C1_2H_{16}N_4O_2$) has been described extensively in the last decade. This may well be related to the enzymatic mimicking potential of the polypirazolyl-carboxylate family, to which this ligand belongs. At first glance, chromium may not be a convenient choice of a metal for the biocatalytic material. Nevertheless, it can be drawn into a focus due to its relation to the other first row transition metals as with molybdenum and tungsten from the same sixth side group of the periodic table. Thus, it is not a surprise only two chromium compounds with the polypirazolyl-carboxylate type of ligands were described so far. Herein, we present a chromium compound $[Cr(HL)Cl_3]$, where the corresponding crystal structure has been determined combining powder XRD and DFT geometry optimization. This is a method of a choice, due to the crystallization difficulties or other challenges resulting in luck of a single crystal. The chromium +3 oxidation state and the neutral form of the coordinated ligand in (1) remain as in the starting compounds. Typically, HL would dehydronate upon coordination, as usually observed in the compounds with this ligand. On the contrary to (1), the related [ML2] species with MN_4O_2 chromophores are more stable, but due to such stable closed coordination sphere, they are not catalytically promising.

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Optically stimulated luminescence for external and retrospective dosimetry: Description of devices developed at SCK•CEN and applications

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For more than thirty years, the expert group of radiation dosimetry and calibration of the Belgian nuclear research centre (SCK•CEN) is using thermoluminescence dosemeters (TLD) for routine measurements and for R&D investigations. In 2002, an experimental device based on the optically stimulated luminescence (OSL) technique is developed and used for research only. This device is working with AL2O3:C detectors (TLD-500 &Luxel®) stimulated by a green line (501.7 nm) or by a blue line (488 nm) generated by a 150 mW ionized Argon laser. In 2008, the development of a modular device has been initiated to extend the OSL measurements to other materials. It uses light emitting diodes (LED) working with the reflection or the transmission mode. The presentation describes the set-up of the different OSL readers and their characteristics (detections limits, linearity and sensitivity) and their applications. Four types of detectors can be used with the modular system: mono-crystalline AL2O3:C, powdered AL2O3:C, sintered BeO and natural quartz. The modular device, developed to obtain a versatile tool, presents different advantages in terms of measurement possibilities: a small number of modules allows the use of different detectors and different filters accordingly to the measurement method (TL, CWOSL). The modules are controlled by a personal computer through a microcontroller array or through a USB card. This choice allows an easy control of all the important parameters of each module. The modular device can measure thermolumuinescence also. The whole set is characterized by a low price. The device is also able to measure a wide range of doses by changing the number of blue LEDs (emitting at 465 nm) according to the level of the measured dose. It is designed to make in situ measurements. Different applications of these techniques in space dosimetry, medical and retrospective dosimetry are described as well as the R&D works initiated in these fields.

The possible future trends will be commented as well as other applications they will allow to develop. The reading filter can be removed to measure doses in special detectors (SrS:Ce,Sm etc.) which are required for special applications. In this case, infrared LEDs are used. In the measurement by transparency, only one LED is used but the light output can be controlled. The choice of type and concentration of the doping materials used in the detector are crucial in these detectors and the applications of the nano-sciences in crucial for optimum results. The presentation also will comment some improvements in the general OSL techniques and a method to quantify ultraviolet doses with a special arrangement of the modules. Several applications of these measurement devices will be presented.

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