P.30.01.1 Poster Session: 30 August, Board: 191
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Surface: A Micro Instrument for *in situ* XRD-XRF and Optical Measurements
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The "SURFACE MONITOR" instrument is an innovative and integrated portable XRD-XRF apparatus combined with a reflectance spectro-photometrical system. The instrument was designed by ISMN-CNR and Assing in the frawork of an European project (EUREKA-Eurocare) “Surface Monitor”, aimed to develop a portable system of multispectral analysis for the not destructive and not invasive characterisation of archaeological artefacts. Concerning the XRD analysis, the innovative design of the SURFACE MONITOR equipments allows to carry out the characterisation by using a Theta-Theta configuration from –10 to 140° 2 Θ. XRD analysis can be also carried out in angular scan and in energy scan modality. The data collected by the detector are elaborated in an innovative 3D mode, indeed, for each step, the XRF spectrum is first stored and then all the fluorescence spectra are represented in a three-dimensional mode, by plotting the energy on the abscissas, the scan angle on ordinates in a horizontal plane and the measured intensity in the vertical plane (Z co-ordinates). By plotting the results in this mode, the user can friendly decide "to cut" the XRD spectrum to the wavelength of more interest, within the used energetic range in the experiment and to filter the scattering that reduces the signal-to-noise ratio. According to this new approach, the XRD spectrum is obtained not to as a single window of energy, but using all the available energies and therefore it turns out extremely more resolved, also using lowest powers. In order to validate this new instrument a large scale characterisation of metal archaeological artefacts has been carried out also for gaining deep insight into the micro-chemical structure of the stratified corrosion layers and of the bulk metallurgical features. This innovative apparatus and approach has evidenced that SURFACE MONITOR with its optical, XRD and XRD facilities have significant potential in studies of the corrosion products of archaeological silver and copper objects for their stabilisation and conservation.

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Crystal Structures of Uricase Complexed with its Real Substrate and Product
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Uricase is a copper-containing enzyme that catalyzes the conversion of uric acid to allantoin during the breakdown of purines in some mammalian species, as well as in amphibians and most fishes. Uricase from small organisms, however, does not require any metal ion or cofactor for its catalytic activity. Since humans do not produce uricase, this enzyme may be useful as a drug to prevent uric acid accumulation.

To clarify the reaction mechanism, three X-ray structures of uricase from a prokaryote *Arthrobacter globiformis*, and of complexes with its substrate uric acid and with a product allantoin have been solved at 2.0, 1.9 and 1.9 Å resolutions, respectively. In every structure, the two subunits are associated to form a ring-shaped dimer, and the two dimers are stacked on each other to complete a cylinder-like tetramer with a long tunnel at the center. The site of uric acid and allantoin binding to the protein are the same, located at interface between two subunits of the ring.

Keywords: X-ray structure, uricase, *Arthobacter globiformis*

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Antimony Oxides: the Pyrochlore-type Structure Revisited
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Antimony oxides display a variety of structural arrangements with different stoichiometries resulting from two stable speciations for Sb ions. They commonly occur as minerals with well known crystal structure, but there are still questions regarding stibiconite - a very rare yellow mineral with pyrochlore-type structure and approximate formula $Sb_3O_6(OH)$ [1]. Great interest has been focused on synthetics because of antimony speciation in relation to color and crystal structure [2], and important ion exchange properties of Sb-pyrochlores were recently pointed out [3].

When studying yellow glazes from majolica-type tiles using X-ray absorption spectroscopy at the Sb K-edge [4], the possibility of an Sb-pyrochlore being the final responsible for the actual coloring was advanced, despite antimony being added during the manufacture process as bindheimite, $Sb_2Pb_2O_7$ (*giallo di Napoli*).

An analysis is presented on the two possible crystallographic descriptions for a pyrochlore-type array under the usual cubic space group that could account for an anomalous intensification of 111 reflection for Sb-pyrochlore within the glaze and simulataneously correlate with XANES data.

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Enzyme Ribonucleotide Reductase. The Paradigm of Enzyme Inhibition by Furanone Derivatives
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Ribonucleotide Reductase (RNR) is the enzyme responsible for the physiological reduction of all four ribonucleotides to 2’-deoxyribonucleotides. The activity of this enzyme is therefore essential for the stability and survival of the cell, since it is directly involved in DNA synthesis and repair. This key role makes it an attractive target for anti-tumor, anti-viral and anti-bacterial therapies, having been largely studied for the past few years[1-4]. Several 2'-substituted-2'-deoxyribonucleotides are potent inactivators of the enzyme ribonucleotide reductase (RNR), that destroy the essential tyrosil radical located in subunit R2 or/and add covalently to subunit R1. In the absence of reductors the inactivation of the former is related with the alquilation of a furanone derivative that is detected in solution by UV spectroscopy. The furanone is a degradation product of a keto-deoxyribonucleotide that is an intermediate of the inhibitory mechanism of a wide group of 2'-substituted inhibitors. Interestingly the same keto-deoxyribonucleotide is also a proposed intermediate of the natural substrate during the reduction mechanism but, by some reason it does not dissociates from the active site and does not inactivate the enzyme [5]. This study was dedicated to this paradigm and allowed to evaluate the interaction between the enzyme and this keto-deoxyribonucleotide. A model containing a complete R1 subunit was used to model the desire minimums and to deal with such a big system a QM/MM method was employed. The results allowed to conclude that the release of the keto-deoxyribonucleotide is dependent on the charged/neutral nature of the atoms/group that is/are attached to carbon C-2’ of the deoxyribonucleotide and their tendency to dissociate through solution.

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