The M1 site is an antiprism sharing faces with two AO_6 octahedra. The M2 site is a large cage bounded by 8 oxygens.

MS33 P01

Atomic resolution structure of HEWL in complex with tris-dipicolinate lanthanide Guillaume Pompidor[a], Olivier Maury[b], Jean Vicat[a], Richard Kahn[a], [a]*Institut de Biologie Structurale, CEA-CNRS-UJF, UMR 5075, Grenoble, France.* [b]*Laboratoire de Chimie, UMR 5182, ENS-Lyon, France.*
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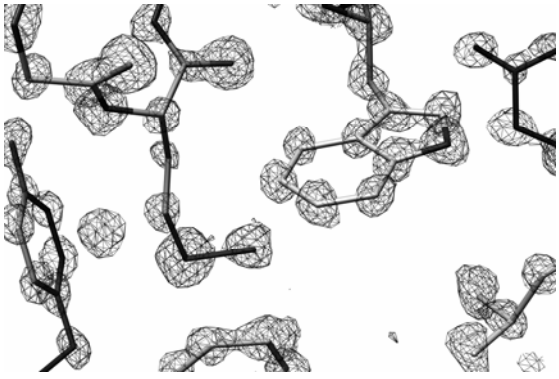
Keywords: macromolecular phase determination, atomic resolution crystallography, lanthanide

Tris-dipicolinate lanthanide complex, $Na_3.[Ln(DPA)_3]$, where DPA stands for pyridine-2,6 dicarboxylate, was used to obtain derivative crystals of hen egg-white lysozyme (HEWL). Derivative crystals were prepared by co-crystallization using conditions close to those leading to the native tetragonal HEWL crystals by adding in the crystallization drops solutions of Ce or Lu complexes to a final concentration of 50-100 mM. The crystals, belonging to a new monoclinic form of lysozyme, space group C2, were diffracting to a resolution never achieved with lysozyme crystals. Diffraction data for the Ce and Lu derivative crystals were recorded to resolutions of 0.80 and 0.85 Å, respectively. Taking advantage of the anomalous signal of Lu ($f'' = 7.8\ e^-$ at $\lambda = 0.85$ Å), experimental phases were determined by the SAD method using the program *SHARP* [1]. Most of the atoms in the structure could be individually observed in the experimental electron-density map, similar in quality to the final 2Fo-Fc map.



Experimental electron-density map of lysozyme at 0.85 Å resolution (contours at 2.0 σ)

The structures were refined against anomalous diffraction data using the program *SHELX* [2]. Among 5 sites found for the lanthanide complexes, 2 sites turned out to be almost fully occupied. The tris-dipicolinate lanthanide complexes, located at the interface between protein molecules are involved in the crystal packing. Strong interactions between each lanthanide complex and different lysozyme molecules strengthen the packing thus enhancing the diffracting power of the crystals.

[1] La Fortelle, E. de, Bricogne, G., *Methods Enzymol.*, 1997, 276, 472. [2] Sheldrick, G., Schneider, T. *Methods Enzymol.*, 1997, 277, 319.

MS35 P06

A comparative study of natural and synthetic calcium sulphates F. Karim[a], M. Waqif[a] and L. Saadi[a], [a] *Laboratory of Condensed Matter and Nanostructures, Team of Study and Valorization of Mineral Resources and Synthetic Materials Evar-mimas, Department of Chemistry, Faculty of Science and Technology Guéliz, Marrakech, Morocco.*
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Keywords : Gypsum, calcium sulphate, medical plasters, mineralogy , chemistry.

In the past, plaster obtained by calcination of gypsum, has been used as biomaterial. However, there has been limited research on the Moroccan gypsum, although the Moroccan gypsum reserves are very significant.
Our study respectively refers to a physicochemical characterization of gypsum samples from three different areas of Morocco: Midelte (GMB), Immentanoute (GIB) and Safi (GRST). These samples were compared with medical plaster (PMC).
The mineralogy and chemistry of all samples were studied by X-ray Diffraction (XRD), IR X-ray fluorescence,. DTA and TGA. The morphology of gypsum was studied by Scanning Electron Microscopy (SEM).
The chemical analyses revealed that the three natural gypsum samples GMB, GIB, GRST and PMC, are made up mainly by calcium sulphate and calcium oxide . These natural samples are characterized by a high purity comparable to sample PMC. SiO_2, Al_2O_3 and MgO, are present in very small abundances, in miuneral impurities such as traces of clays and carbonates as was confirmed by XRD on bulk samples.
From thermal behavior point of view, samples GMB, GIB, GRST and PMC show almost the same thermal phenomena with increasing temperature. Using XRD it was possible to assign modifications in gypsum during calcination to the following gradual dehydration reactions:

$$CaSO_4, 2H_2O \leftrightarrows CaSO_4, 1/2H_2O \leftrightarrows CaSO_4.$$

In conclusion the Moroccan natural samples studied consist mainly of gypsum associated with traces of clay and carbonates. They raw materials are characterized by high purity and their mineralogy and chemistry are comparable to those of the medical plaster.

MS41 P28

Crystal structures of the $K_{1,125}Rb_{1,875}La(VO_4)_2$ and $Rb_{1,435}Cs_{1,565}La(VO_4)_2$ vanadates . L. Rghioui[a,b], L. Benarafa[a] , S. Zaydoun[a] and L. El Ammari[c]. [a]Laboratoire de Spectroscopie infrarouge, Département de Chimie, Faculté des Sciences, B.P. 1014, Rabat, Maroc.[b] Equipe Phisico-chimie de la matière condensée, Département de Chimie, Faculté des Sciences, B.P. 4010 Beni M'hamed, Meknès, Maroc. . [c]Laboratoire de Chimie du Solide Appliquée, Département de Chimie, Faculté des Sciences, B.P. 1014, Rabat, Maroc
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Keywords : analysis of disordered structures, infrared spectroscopy, single-crystal structure

The new vanadates $K_{1,125}Rb_{1,875}La(VO_4)_2$ and $Rb_{1,435}Cs_{1,565}La(VO_4)_2$ have been synthesized by the reactive flux method. Their crystal structures were determined by single crystal X-ray diffraction. Both