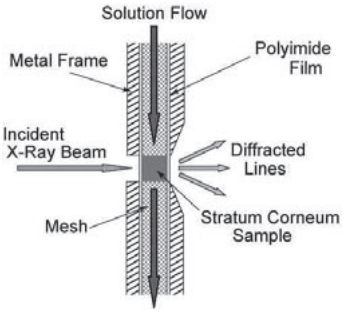
application of the chemical agents and furthermore the problem of the individual difference of stratum corneum might be overcome since not the degree but the behavior of the structural changes seems to be less affected by the individuals. The performance of the present method was demonstrated in the extraction process of lipids from stratum corneum, the deterioration of barrier properties and the penetration mechanism in stratum corneum by ethanol application and the effect of a penetration enhancer of d-limonene to stratum corneum. Based upon these studies, we can propose that in the study of function in stratum corneum this method enables the molecular-level evaluation of the effects of cosmetics, drugs, etc.



Keywords: lipids, SAXD/WAXD, stratum corneum

P25.10.13

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XRPD lab instrument measurements and crystallographic analysis on insulin and insulin derivatives

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A successful first structure refinement of lysozyme [1] already proved the value of standard XRPD laboratory instruments for protein structure research. In this contribution we will present new measurements and crystallographic analysis results of insulin and insulin derivatives performed on data from a PANalytical X'Pert Pro diffractometer (equipped with a capillary spinner, a focusing mirror and an X'Celerator detector). We additionally demonstrate that even fast measurements on a 96 well plate as used for polymorph screening purposes, result in high quality data, which is suitable for automatic crystallographic analyses like indexing [2] and LeBail [3] fitting.
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[2] A.Boultif and D. Louër, Powder pattern indexing with the dichotomy method, J. Appl. Cryst. (2004), 37, 724 - 731.
[3] A. Le Bail, H. Duroy & J.F. Fourquet, Ab-initio structure determination of LiSbWO6 by x-ray powder diffraction, Mat. Res. Bull. (1988), 23, 447 - 452.

Keywords: X-ray diffractometry of polycrystal compounds, polymorphism, protein structure analysis

P26.05.01

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Teaching crystallography on-line by the Bilbao Crystallographic Server

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The Bilbao Crystallographic Server (www.cryst.ehu.es) is a web site with crystallographic databases and programs [1]. It can be used free of charge from any computer with a web browser via Internet. The on-line accessible databases and variety of applications convert the server in an excellent web tool for studying and teaching basic and applied crystallography. The server is built on a core of databases and the different applications are classified in shells. The innermost one is formed by simple retrieval tools accessing data from International Tables for Crystallography, Vol. A (Space-group Symmetry), Vol. A1 (Symmetry Relations between Space Groups) and Vol. E (Subperiodic Groups). The next shells contain applications that are essential for problems involving group-subgroup relations between space groups or representation theory of space and point groups. There are a number of applications related to problems of solid-state physics, crystal chemistry and theoretical crystallography: structural phase transitions, pseudosymmetry search, infrared and Raman selection rules, phonon extinction rules, etc. The programs on the Bilbao Crystallographic server have user-friendly interfaces with an on-line help. Some applications are linked to visualization applets. One of the important advantages of the server is that the different programs can communicate with each other and in this way the Bilbao Crystallographic Server has turned into a web-interactive environment with the appropriate tools for teaching theoretical and material crystallography.
[1] M. I. Aroyo, J. M. Perez-Mato, C. Capillas, E. Kroumova, S. Ivantchev, G. Madariaga, A. Kirov & H. Wondratschek. Z. Kristallog. (2006), 221, 1, 15-27.

Keywords: Bilbao Crystallographic Server, computer-aided crystallographic teaching, web resources

P26.06.02

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Cambridge Crystallographic Database System utilization in undergraduate chemistry teaching

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Many aspects of chemistry education, particularly when teaching undergraduate students, rely heavily upon 3-D molecular visualization. Currently there is widespread interest in e-learning and efforts to prepare computer based teaching materials for molecular visualization are ubiquitous. Most are based on theoretical structures, which is often sufficient. Nonetheless, with the Cambridge Structural Database (CSD) containing rapidly approaching 500,000 entries of crystallographically determined atomic coordinate for organic containing small molecules, there exists a vast resource for teaching molecular visualization as well as examining molecular bonding in general. The CSD and its associated programs, known as the Cambridge Crystallographic Database System (CSDS) are predominantly used as research tools. This poster explores some of the potential teaching uses of the CSDS. Through funding from the National Science Foundation Discovery Corps Fellowship (NSF-DCF) program, the author has been providing CSDS access

to approximately 30 Primarily Undergraduate Institutions (PUIs); offering training workshops, focusing upon utilization of the CSDS in chemistry education, to faculty at these PUIs; collaborating with the Cambridge Crystallographic Data Centre (CCDC) to build teaching modules making effective use of the CSDS; and encouraging faculty to prepare their own teaching modules. Details regarding the NSF-DCF project and examples of CSDS related chemistry teaching modules will be presented.

Keywords: education, database, e-learning

P28.01.01

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X-ray diffraction applied to calcium determination in Mexican clays for Talavera production

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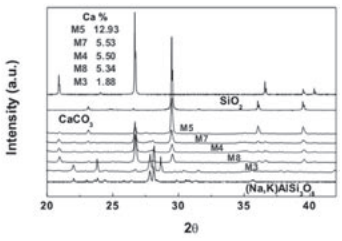
Eight types of clays used by the craftsmen of Tlaxcala Mexico, in the elaboration of the recognized world-wide level Mexican Talavera ceramic, were analyzed (M1-M8). The presence of calcium, iron and feldspars, in the samples, gives to the clay, malleability in its handling and hardness. EDX spectra of analyzed clays, showed the presence of: calcite ($CaCO_3$), quartz (SiO_2) and the feldspar ((Na,K) $AlSi_3O_8$). EDX results, in atomic percentage, showed that only a half of the samples had Ca and Na (M4, M5, M7 and M8). And M3 is the sample with the higher feldspar concentration. The sample M5 was the only one that showed to have the best relation between these three components ($CaCO_3$, SiO_2, (Na, K) $AlSi_3O_8$). The clay samples were also analyzed by infrared spectroscopy in diffuse reflectance mode (RD-IR), in which several absorption bands associated to Ca-O bonds were observed. In particular, a band located at 1795 cm^{-1} increase in intensity in proportional form with the calcium content. This result is in agreement with EDX results. From these results, a correlation function between EDX and RD-IR was obtained, to evaluate in a practical form the calcium content.



Keywords: X-ray diffracction, clays, infrared spectroscopy

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X-ray characterization of the early Islamic reddish luster painted pottery

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'Luster' refers to iridescent decoration on glazed pottery, produced by metal pigments on white glaze, creating a metallic copper or gold sheen. A characteristic of luster decoration is the presence of several colors (red, olive green or brown). In this study, chemical composition of glaze and luster pigment was analyzed by XRF analysis and chemical states of the metallic elements were by XAFS. We focused on the luster pottery with reddish colored decoration which was made in Iraq, especially 9th-10th centuries. Portable XRF spectrometer, OURSTEX100FAII was taken to Egypt. A total of 3,165 luster painted potteries made in Iraq were excavated in Raya till 2005, where is an archeological site in Sinai Peninsula, Egypt (Director, Dr. M. Kawatoko). Of these, 214 pieces were accompanied with reddish-colored luster. A classification of the glaze on these 214 pieces was performed by their chemical composition. Moreover, 79 pieces, which are stored in a museum in Japan, were also studied as well. In addition, XAFS analysis was carried out using synchrotron radiation at Photon Factory, Tsukuba, Japan. The white glaze of Iraq luster pottery can be classified into alkali-lime glaze and alkali-lead lime glaze.1) Our XRF analysis showed that 67% of the Iraq luster painted pottery with reddish color excavated in Raya was alkali-lime glaze. This proportion is much higher than that of other colored luster potteries. XAFS analysis of the museum specimens revealed the relationship between the chemical state of copper and their color. An existence of metallic copper was found only in the luster painted pottery with reddish color, among various colored decorations. As a result, it can be said that strong reducing condition was necessary for the production of the reddish luster decoration.

Keywords: archaeology, EXAFS, ceramics

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Building of three dimensional Escher patterns by Layer-manufacturing

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Three-Dimensional Escher Patterns (3DES) are built by Layer-manufacturing. Two types of solid model are presented, whose original data are designed using CADPAC2 software. In the preparation of the model building an icosahedron is considered as a basic unit of modeling, which is an isotropic regular polyhedron with the maximum facet in the five regular-polyhedrons. Several inscribed cubes in the icosahedrons can be arranged such that they form cubic lattice decorated by set of icosahedrons. Assembled icosahedrons are formed to be 3D periodic structure with overlapped region of the icosahedrons inside and icosahedrons facet outside of the assembly (Icosahedrons assembly). Externals of icosahedron-assembly are much available for creating the object of motif such as a body of animal that has mirror symmetry. Model building of 3DES begins with the