The samples are mainly of ancient Egyptian, with some comparative samples from the Near Eastern regions. The analysis yielded interesting results; a marked difference in pattern of elemental composition from one king's reign to another was observed; use of different mineral as colorant was confirmed; a tendency to increase the amount of lead toward the end of the dynastic period was attested, and so on. The above results clearly indicates that procurement of ingredient minerals for the production of ancient vitreous materials changed over the course of time. From the analysis result, we are now able to draw a possible map of ancient trade network for the viterous materials, especially during the middle of the New Kingdom period. The interdisciplinary collaboration between science and archaeology is now able to offer some historical interpretations which had not been possible before.

Keywords: archaeology, ancient Egypt, synchrotron

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Salt corrosion of lead-based pigments: Laboratory experiments and analysis of ancient frescoes

Eva Kotulanova[1], Petr Bezdicka[1], Janka Hradilova[2]
[1]Institute of Inorganic Chemistry AS CR, v.v.i., C.P. 1001, Husinec-Rez, Bohemia, 25068, Czech Republic, [2]Academy of Fine Arts in Prague, ALMA Laboratory, U Akademie 4, 170 22 Praha 7, Czech Republic, E-mail：evulekotule@iic.cas.cz

Salts are one of the most dangerous degradation agents of wall paintings. Salts cause not only mechanical changes by crystallization pressure, but also chemical and mineralogical alteration of colour layer. Although they were not recommended for using in wall paintings, lead-based pigments (lead white, masicot, red lead) were used since antiquity due to their bright colours. Interactions of selected pigments (lead white, masicot, red lead) with different salt solutions were performed within long-term laboratory experiments. We used salts which are part of the environment (Na_2SO_4, $MgSO_4$, $CaSO_4$, NaCl, $NaNO_3$, $Ca(NO_3)_2$, Na_2CO_3, urea) and salts which can be applied on fresco by restorer during fresco cleaning ($NaHCO_3$, $(NH_4)_2CO_3$, NH_4HCO_3). The phase analyses of reaction products were carried out using X-ray powder diffractometer. These analyses allowed us to conclude that minium has tendency to darken irrespective to the character of salt due to the formation of plattnerite. Massicot also reacts irrespective to the character of salt to form hydrocerussite which then transforms to cerrusite. By contrast lead white reacts with suphates to form sussanite, with NaCl to form laurionate. Markedly damaged 11th century frescoes from the small church of St. George in Kostolany pod Tribecom are probably the oldest preserved wall paintings in Slovakia. Samples taken from the dark brown parts of the wall paintings were analysed using X-ray powder microdiffraction. Microdiffraction revealed the presence of several different lead phases: hydrocerussite, cerussite, plattnerite and lead magnesium carbonate. The results of laboratory experiments allowed us to clarify presence of the lead phases as degradation products of red lead. The project was supported by GA AV CR KJB400320602.

Keywords: pigments, microdiffraction, corrosion

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Structural investigations of archaeological hybrid materials

E. Dooryhée, P. Martinetto, C. Dejoie
Neel Institut, CNRS & Joseph Fourier University, Grenoble, France

Organic-inorganic hybrid materials have emerged in various archaeological contexts, long before they captured one's interest owing to their mechanical, thermal, electronic, optical or catalytic properties, and their potential commercial applications. Many examples of hybrid organic-inorganic materials are described in old texts[1]: African patinas[2], body-care oils, mummification[3], tattooing, easel paintings (e.g. acetates, resinates), cosmetics or pharmaceutical products. Some hybrid materials are also found to form after degradation with time (e.g. in reaction with organic binders such as lead soaps[4] in lead paints, bio-mineralised textile fibres and bones, ...). Several examples are discussed. The search for stable dyes, resisting heat and moisture in murals, artefacts and clothing, led artists and craftsmen to substitute vegetal colours with artificial hybrids. Lacquer pigments were developed in Europe in the Greek-Roman periods and the Middle Ages. They consist of plant colouring matter and animal extracts, fixed on an inert mineral host. A blue pigment, formed by heating a mixture of a fibre clay and indigofera leaves, was extensively used in Mesoamerica (300-1500 AD), on frescoes, potteries, sculptures and ritual objects. These materials may be considered as the first artificial organic-inorganic hybrids, associating properties of the mineral substrate (chemical resistance, thermal and mechanical stability) and the colour of the organic dye[5]. The understanding of such complexes and the implementation of the relevant chemical and physical methods (synthesis, characterisation and modelling) lead to the description of historical hybrid materials in their archaeological contexts (use and properties). The open archaeological question is to identify the know-how of the ancient societies, by reproducing the conditions of synthesis and past practices, while monitoring the properties of the materials, their durability and their behaviour. Crystal structure solving of these archaeological composite materials and understanding the nature of the interactions between the guest molecule and its matrix are thus essential.

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Keywords: hydride compounds, archaeological materials, diffraction

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CIF and a new DDL − What it can do; How it is done

Nick Spadaccini, Syd Hall, Ian Castleden
The University of Western Australia, School of Computer Science and

Software Engineering, MBDP M002, 35 Stirling Highway, Crawley, Western Australia, 6009, Australia, E-mail：Nick.Spadaccini@uwa.edu.au

Data items contained within a CIF file are currently defined in domain dictionaries using a data definition language (DDL1 or DDL2). The increasing complexity of data and the need for seamless integration across different sources creates demands that cannot be readily met by current definition capabilities. *DDLm* is an evolution of DDL1 and DDL2 that uses the same syntax but expands the attribute set so as to enrich the semantics of the data and class definitions. It maintains backward compatibility to existing CIF archives. The CIF syntax has been extended to describe more complex data structures, while maintaining the simple tag-value construct. *DDLm* supports a wider range of data types, including container classes such as lists, arrays, tuples and tables. Definitions for a domain, such as that of structural science, can now be modularised into separate dictionaries; each maintained by the relevant sub-discipline. *DDLm* provides for the real-time merging of modules, including the recognition of namespaces, and the resolution of namespace clashes. *DDLm* provides facilities for relating derivative data items via method expressions that are symbolic, easy to read as text, but are computer interpretable and executable [2]. Additionally user-defined processes can be used for data evaluation. The paper will describe the major features of *DDLm* highlighting its simplicity and importance for the more comprehensive definition of data items used in the discipline. The specification details are currently available for examination and comment by members of the crystallographic community [3].

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[2] Spadaccini N, Hall SR, & Castleden IR (2000) *JCICS* 40 1289-1301.
[3] www.iucr.org/iucr-top/cif/ddlm/

Keywords: CIF, data representation, ontology

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CIF software in a DDLm world

James R Hester
Bragg Institute, PMB 1, Menai, NSW, 2234, Australia, E-mail：jamesrhester@gmail.com

Although CIF dictionaries store crystallographic knowledge in a machine-readable form, there has been relatively limited run-time use of DDL1/2 dictionaries in CIF software. This is attributable to the small added value of the primarily descriptive DDL1/2 attributes compared to the cost of implementing a dictionary-aware system. In other words, CIF syntax and DDL1/2 attributes are simple enough for software creators to produce (with occasional errors) and read conformant CIF data files simply by referring to the dictionaries at program creation time. The new DDLm standard enhances DDL1/2 descriptive capabilities while also introducing dictionary-based synthesis of derived data values by including dREL algorithms in data item definitions. While algorithms are usually also implemented as part of program creation, several orders of magnitude more time is involved in developing a correct algorithm compared to a typical DDL1/2 task of specifying a dataitem name and type. A DDLm dictionary gains considerable practical value for this reason. This value is potentially compromised by the work involved in making a DDLm algorithm available to the software. Two practical paths exist: (i) communication with a separate dictionary processing package, or (ii) automatic rewriting of the dREL algorithm into the language of choice. Both approaches are amenable to provision by the IUCr of openly-available tools, which coupled with the clear added value of having tested, standard algorithms will help overcome the implementation barrier experienced by the DDL1/2 standards, a barrier which is even higher for the more complex DDLm standard.

Keywords: crystallographic software development, CIF, data definition language

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Transition to object-oriented data representations: Interconversion between CIF and other formats

Herbert J. Bernstein
Dowling College, Dept. of Mathematics and Computer Science, 150 Idle Hour Blvd KSC 121, Oakdale, NY, 11769-1999, USA, E-mail：yaya@bernstein-plus-sons.com

The Crystallographic Information Framework [1] (CIF) has been very effective in codifying the vocabulary of crystallography, with two Dictionary Definition Languages, DDL1 for small molecules and DDL2 for macromolecules. The more than three-decade old PDB format and the new, remediated PDB format are critical to information management in macromolecular crystallography. There are many alternate representations, ASN.1, NeXus, CML, XML, etc. that convey much the same information with more or less structure, some more convenient for software or databases or for handling by humans, but, in most cases, these formats have focused on the nouns of our vocabulary. The work on a new DDL, DDLm [2], and related work on SBEVSL [3] have increased awareness of the need to deal with the verbs of our vocabulary, the actions that transform information, such as cell edge vectors into cell volumes, as well as the nouns, and raise the prospect of making CIF object-oriented.

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[3] C. Westin, B. Hanson, H. J. Bernstein, I. Awuah Asiamah, D. Boycheva, G. Darakev, N. Darakev, J. Jemilawon, N. Jia, P. Kamburov, G. Todorov, P. A. Craig, S. Mottarella, “SBEVSL: Communicating scripts between molecular visualization programs,” Abstract E003, ACA 2007, Salt Lake City, UT, July 2007
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The bilbao crystallographic server

Mois I. Aroyo, J. Manuel Perez-Mato, G. Madariaga, D. Orobengoa
Universidad del Pais Vasco, Fisica de la Materia Condensada, Apartado 644, Bilbao, Vizcaya, E-48080, Spain, E-mail：mois.aroyo@ehu.es

The Bilbao Crystallographic Server is a free web site with crystallographic databases and programs available at http://www.cryst.ehu.es [1]. The server is built on a core of databases that include data from International Tables for Crystallography, Vol. A: Space-group symmetry and Vol. A1: Symmetry Relations between Space Groups. There is an access to the crystallographic data for