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A Relational Database Approach to Report Generation
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As the throughput of X-ray diffraction laboratories increases and the groups of users diversify, the need for an automatic report generation system becomes more apparent. Although the type of report varies depending on the user's objectives, the data in the report is always based on information gathered throughout the experiment.

We present a relational database approach to report generation. For each step of the structure determination the relevant pieces of information are recorded, such as the type of operation, input and output data, software version, user name, date and time. Furthermore, by linking the input of an operation to the output of the preceding steps, each piece of information is put into context as and when it becomes available. From the emerging tree structure it is possible to create a report from the beginning of the experiment to any step in the experiment. Wrong paths that did not lead to the final result are preserved too.

Reports come in different shapes and sizes: various formats (e.g. CIF, mmCIF, HTML, and proprietary formats), various purposes (e.g. publication, archiving, or visualization), and varying degrees of detail. In order to serve this wide spectrum of needs we have developed a template language that describes which data is extracted from the database and how it is formatted.

Keywords: report generation, databases, CIF

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Structure Integration with Function, Taxonomy and Sequences (SIFTS)
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One of the major obstacles to the improved integration of structural databases such as MSD (http://www.ebi.ac.uk/msd) and sequence databases like UniProt is the absence of up to date and well maintained mapping between corresponding entries. MSD and UniProt have worked closely to clean up the taxonomy and sequence cross-reference, a vital step in integrating sequence family databases such as Pfam and Interpro with structure-oriented databases (SCOP and CATH). This information has been made available to the eFamily group (http://www.efamily.org.uk/), and now forms the basis of the regular interchange of information between the member databases (MSD, Uniprot, Pfam, Interpro, SCOP and CATH). This work was carried out under the SIFTS initiative (http://www.ebi.ac.uk/msd-srv/docs/sifts/). As well as the domain boundary definitions, the schema also allows any associated sequence or structural alignments to be encapsulated in XML. Since the *e*Family schema is complex, an API has been developed for easy integration into BioPerl. For example, the API allows a Pfam alignment wrapped up in the *e*Family XML to be returned as a BioPerl alignment object and *vice versa*. The use of such API's in the development of production quality webservices will also be discussed.

Keywords: data integration, webservices, data exchange

MS87 REACTIONS IN MOLECULAR SOLIDS
Chairpersons: Leonard Richard MacGillivray, Fumio Toda

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Mechanically Induced Reactivity of Molecular Crystals: Chemistry (almost) without Solvents
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Reactions between solids, such as those activated by mechanical co-grinding of different solid materials, or those between a solid and a gas, are attracting the interest of scientists engaged in the quest for sustainable chemical processes. In Bologna we have been actively involved in the exploration of solvent-free mechanochemical reactions as a means to prepare novel mixed molecular crystals. The basic idea is that molecular diffusion by contact between two molecular crystals can lead to formation of supramolecular bonds and co-crystals or adducts without solvent participation. Under this point of view solvent-free reactions between or within molecular crystals can be regarded as a *green way* to crystal engineering.[1]

In this contribution we report that co-grinding of silver acetate with *trans*-1,4-diaminocyclohexane [$H_2NC_6H_{10}NH_2$] in 1:1 ratio generates novel one- and two-dimensional coordination networks based on Ag--[$H_2NC_6H_{10}NH_2$] coordination bond and on hydrogen bonds between the acetate anions and the bis-amine ligand. The bis-amine [$H_2NC_6H_{10}NH_2$] has been little exploited in crystal engineering experiments and only few examples are known of its use for the construction of hydrogen bonded adducts or coordination networks.

[1] Braga D., Grepioni F., *Angew. Chem. Int. Ed.*, 2004, **43**, 4002.
Keywords: crystal engineering, hydrogen bonding, supramolecular mechanochemistry

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Solid-Solid Reactions of Xanthenols with Unsaturated Hydrocarbons
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The structures of the inclusion compounds of the host H = 9-(4-methoxyphenyl)-9H-xanthen-9-ol with a series of aromatic guests: naphthalene, anthracene, phenanthrene, pyrene and α-naphthol have been elucidated. The structures are similar, crystallise in the space group P(-1), and are characterised by pairs of hydrogen-bonded host molecules, with the guests located at centres of inversion.

The kinetics of the solid-solid reactions between the host, H, and naphthalene and α-naphthol were monitored by X-Ray powder diffraction at 25°C and their rate constants established.

Linear relationships were derived for unit cell volumes versus the number of guest atoms in this series as well as from the structures containing benzene, toluene and the isomers of xylene as guests.

Lattice energy calculations for the naphthalene and α-naphthol structures were reconciled with the results of thermal analysis obtained by DSC.

Keywords: solid-solid reaction, clathrate, kinetics

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Structural and Thermochemical Studies of Lattice Inclusion Hosts
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Lattice inclusion hosts are molecules that form cage or channel type frameworks in the solid-state having Å to nanometer-sized voids [1]. Recent crystal engineering strategies for the design of open-framework solids, inclusion of small guest/solvent molecules in the voids, and thermo-chemical behavior of host-guest complexes will be discussed. Significant structural and functional differences in channel and cage type host structures are due to differences in hydrogen bonding / intermolecular interactions, van der Waals close packing, and the strength of host lattice in trapping guest species. Structural control of the cage/channel lattice and modification of pore size/shape through functional group and guest selection is illustrated in robust organic host systems. Certain volatile guests are tightly enclathrated in the host framework as measured by high T_{onset} values in DSC measurements. Selective guest inclusion is monitored by TG-IR and explained through hydrogen bonding in X-ray crystal structures. Some