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The New PDF-4+ 2005: A Relational Database (RDB) with Atomic Structure Information and On-the-fly Total Pattern Analysis Capability

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The ICDD is continuing to develop new RDB database capability for the Powder Diffraction File™ (PDF®) [1,2]. The PDF-4+ 2005 will be released in August, 2005. This database will contain approximately 84,000 new entries with complete atomic coordinate information. Using the structure data, powder patterns will be calculated for electron, neutron and x-ray diffraction; these are calculated on-the-fly (as needed). Scattering contrast studies as a function of probe and wavelength can be used to aid experiment design. In addition to the standard peak intensity listing in the PDF, integrated intensity information will be available for all unique hkl's within each entry. Elemental composition data (available for all entries in the PDF) can be used as filter criteria for effective searches in the RDB. We will show how atomic evironment data can be used to help understand classes of materials properties. One of the aims of these initiatives is to enhance our ability to perform materials design studies. Fully digitized powder patterns are a first step in the realization of this process.

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Keywords: database preparation, powder diffraction analysis, powder patterns

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Carbonyl-Carbonyl Interactions in First-row Transition Metal Complexes

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Carbonyl-carbonyl interactions in organic species have been previously documented [1]. In theory, the strength of carbonyl-carbonyl interactions should be greater when the carbonyls are directly attached to a transition metal since the magnitude of the carbonyl dipole is greater than in purely organic compounds. The Cambridge Structural Database [2] was used to identify first row transition metal carbonyl species in which two carbonyl groups were separated by less than 3.6 Å and could potentially interact. Only two of the three main carbonyl-carbonyl interaction motifs previously identified for organic carbonyl species are possible in transition metal carbonyl compounds; these are illustrated Figure1.

Data analysis suggests that transition metal carbonyl-carbonyl interactions in motifs A and B are more prevalent than organic carbonyl-carbonyl interactions, with around 33% of transition metal carbonyls suitably orientated to interact while only 8% of organic

Figure 1 – *interaction motifs in transition metal carbonyl species.*

carbonyls can potentially interact. A comparison of the geometries of the interaction motifs is provided along with an analysis of accompanying theoretical calculations.
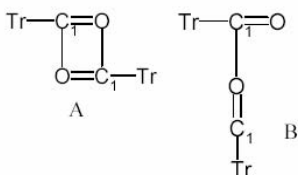
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ISOBASEmm: Isostructurality in the Protein Data Bank

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The ISOQUEST program [1,2], a method for the comparison of crystal structures based on pattern matching techniques [3], has recently been applied to analyse the Cambridge Structural Database (CSD) [4]. A full analysis of all entries in the CSD led to ISOBASE, a database which contains all isostructurality relations in the CSD. Investigation of this ISOBASE shows that many classes of identical or closely related structures can be found, although the chemistry within those classes can vary considerably. This information can be used to extract crystal packing rules that otherwise can not be revealed.

To extend the range of applicability of the ISOQUEST method an analogous approach was chosen to analyse the collection of all macromolecular structures present in the Protein Data Bank (PDB) [5]. This poster presents the resulting macromolecular database ISOBASEmm and examples of structural relations in the PDB that can be extracted from this database.

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Powder Diffraction CIFs: Preparation and Review

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The IUCr now strongly urges authors to submit observed and computed powder diffraction data in CIF format when publishing Rietveld results [1]. This will offer obvious benefits for the archival of data and for the testing of alternative models where structures are in dispute. The most immediate application is likely to be for manuscript review, as the quality of a Rietveld fit is best judged graphically, not from statistical figures of merit, such as profile R-factors or χ^2 values. Figures submitted for publication are seldom sufficient for close examination.

This paper will present some resources for reporting Rietveld results in CIF format, including information on software available for preparation of a CIF from a Rietveld fit. For the review of Rietveld results from a CIF, the pdCIFplot program will also be discussed [2]. This open-source program runs on all common computer platforms (Windows, Macintosh, & Unix) and allows powder diffraction data and fits to be plotted in a variety of formats directly from a CIF.

[1] http://journals.iucr.org/services/cif/powder.html
[2] http://www.ncnr.nist.gov/xtal/software/cif/pdCIFplot.html
Keywords: CIF, powder diffraction, Rietveld analysis

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Automating the Identification of Packing Motifs; dSNAP

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With the explosion in high quality structural determinations in the area of small molecule crystallography, the problem of efficient and meaningful mining of the data in, for example, the Cambridge Structural Database (CSD) [1] is very relevant for structural chemists.

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