

The New Organic Powder Diffraction File, PDF-4/Organic 2002, with Integrated Search and Retrieval Functions

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The PDF has exhibited recent dramatic growth in entry population over the past 5 years. In 1998, the ICDD reached an agreement with the Cambridge Crystallographic Data Center (CCDC) that allows for the calculation of x-ray powder patterns from the structural information in the Cambridge Structural Database (CSD). As a result of this agreement, the organic entry population has risen from 25,000 to 150,000 entries. To house these entries, a successor relational database was developed^{1,3}. Together, these make up the PDF-4/Organic 2002 RDB. To facilitate viewing and extracting information from the PDF-4, a new viewing software package has been integrated into the RDB.

Searching options for the PDF-4/Organics include 31 searchable fields. Cumulative search results are connected using Boolean operators, and display the relevant information for all searchable fields. Subfile operators are used to partition the RDB into scientific or functional fields. For example, these include Drug Activity, Pharmaceutical, Excipients, Forensic, Pigment, Polymer and Explosives.

Most experimental entries are characterized via organic functional group classification. In addition, almost all entries will show 2D structures and exhibit fully digitized powder patterns. In the case of calculated patterns from the CSD, the patterns are calculated from first principles and are rigorously correct. For experimental patterns, several approximations are required since an a-priori knowledge of the instrumental resolution function for each entry is not available.

Several examples involving the application of the PDF-4/Organic 2002 RDB will be presented. The application of data mining techniques will also be discussed².

1. J. Faber and T. Fawcett, *Acta Cryst.* **B58**, 325-332 (2002).
2. S. N. Kabekkodu, J. Faber and T. Fawcett, *Acta Cryst.* **B58**, 333-337 (2002).
3. J. Faber and F. Needham, *Amer. Pharmaceutical Review* **5**, 70-75 (2002).