

ICDD PRODUCT DATABASES

R. Vithayathil

International Centre for Diffraction Data, Newtown Square, PA 19073, USA

The ICDD Database department collects and edits data annually to build the database snapshot. Each year the Engineering & Design department receives PDF-4+, Minerals, PDF-2 and WebPDF-4+ data in February and PDF-4 Organics data in May. The first database snapshot consists of experimental, ICSD, NIST, LPF and modulated datasets and the second snapshot consists of the organics database which includes Cambridge and in-house organic datasets. The Engineering & Design department builds custom databases using SQL Server using different tools such as store procedures, queries, and Java programs in order to build the tables for our product databases. After remotely transferring the data into Sybase SQL Anywhere, actual product databases are built for each product. Each year in this database, ICDD adds new data and updates existing data for each product to improve the quality and add new features.

Main features of database:

- Atomic coordinates
- X-ray, Electron, Neutron (constant wavelength and time-of-flight) diffraction patterns
- Reference – Digital Object Identifier
- Subfiles – Large collection of minerals, ceramics, metals & alloys, polymers and pharmaceuticals
- 2D diagrams
- Physical property sheets

As a result, the ICDD product database release each year benefits many educational labs, OEM companies, and different scientific groups in their specific research needs. These benefits include data mining, phase identification and quantitative analysis of inorganic materials, and phase identification combining both single crystal and powder diffraction data for organics.

This poster illustrates the process of building the product database. Internal, external editors, Database Department, and J. Blanton contributed to build the database.