

PHARMACEUTICAL REFERENCE APPLICATIONS OF PDF-4/ORGANICS 2008

E. Needham, C. Crowder, J. Faber, T. Fawcett
International Centre for Diffraction Data

PDF-4/Organics 2008 is ICDD's collection of standard reference X-ray powder diffraction (XRPD) patterns for organic compounds. It includes 29,653 experimental patterns and 311,887 patterns derived from single crystal data. Most of the derived patterns are based on data from the Cambridge Structural Database (CSD) through an agreement between ICDD and CCDC (Cambridge Crystallographic Data Centre). This database contains XRPD patterns for more than half of the USP (United States Pharmacopeia) APIs (active pharmaceutical ingredients) and their polymorphs. Additionally, it contains a large number of patterns for inorganic and organic excipients typically found in pharmaceutical formulation.

Since the solid state of a pharmaceutical substance can affect its pharmacological action, the polymorph study is a must for any API, which can exist in more than one solid state. PDF-4/Organics 2008 contains many substances with polymorphs and has many physical and chemical properties associated with polymorphism. These include habit, space group, cell parameters, cell volume, crystal system, density, and melting point. There is also standardized cell data as well as author-reported raw data in the database. The standardization assures data uniformity. It provides not only the swift and easy means for data comparison, but also the accuracy of data representation. The population distribution for these properties and their applications were studied, compared, and will be presented.

Many phase identification processes have been widely researched and reported. These processes generally utilize techniques involving data reduction, peak finding, modeling, and refinement. Illustrations of this traditional process, for pharmaceutical materials, using PDF-4/Organics 2008 for the pattern matching between experimental data and reference patterns will be given.