

## **X-RAY POWDER DIFFRACTION DATABASE TOOLS FOR THE PHARMACEUTICAL SCIENTIST: NEW CAPABILITIES**

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As the PDF-4+/Organics database continues to grow in size (now over 400,000 entries), the tools available for accessing, searching, and utilizing this database continue to be enhanced. The database itself has undergone some upgrades to facilitate matching of X-ray powder diffraction (XRPD) patterns and, coupled with the enhanced tools, provides a more powerful arsenal for solving pharmaceutical problems with XRPD. Database enhancements include eight new subfile designations for improved database screening; inclusion of National Institute of Science & Technology (NIST) standard materials for proper identification of standard peaks in specimens with internal standards; and d-I listings to  $60^\circ 2\theta$  (Cu  $K\alpha_1$  radiation) for all Cambridge Structural Database (CSD)-derived entries so that higher-angle peaks belonging to identified phases can be properly accounted for. Additionally, selected experimentally-derived entries have full raw pattern data included for direct comparison to raw patterns collected by the user.

Associated software now provides data mining capabilities via 53 different search criteria with a total of 85 different specifiable fields for results display. This enables mining for polymorphic forms, hydrates and solvates, derivatives with specific functional groups, common excipients, and so on. New tools allow displays of simulated XRPD patterns that mimic the user's instrument configuration as well as the specimen crystallite size. Additionally, displays of interactive electron diffraction spot patterns with simulated kinematic intensities are also possible.

The talk will illustrate the practical applications of many of these enhancements using examples from the pharmaceutical domain.