ICDD PDF-4 PRODUCT DEVELOPMENTS FOR RELEASE 2017

J. Blanton, R. Vithayathil, C. Karumuhinzi, S. Kabekkodu, T. Blanton, J. Faber
International Centre for Diffraction Data
Newtown Square, PA

International Centre for Diffraction Data® (ICDD) data mining software has the ability to search through the entire Powder Diffraction File™ (PDF®) database using numerous permutations of search criteria. Once the desired search entries are obtained, the software can view extensive experimental data, crystallographic data, physical properties, classifications, bibliographic data, and more. In addition, these entries can generate 2D chemical structures, 3D molecular structures, ring pattern simulations, and electron diffraction pattern simulations. The power of the data mining software can be greatly extended with SIeve/SIeve+, ICDD's phase identification software. Using highly optimized algorithms, SIeve/SIeve+ can rapidly match user's experimental X-ray diffraction data, electron diffraction data, and neutron diffraction data to patterns in the PDF® database.

To enhance the value of the PDF® software, ICDD has incorporated many new developments for the 2017 product release. Patterns in a temperature series can be vertically offset using the temperature of data collection as the intensity baseline. Unique symbols can be displayed at the top of each peak position in simulated diffraction patterns. Isotopic substitution of deuterium for simulated neutron diffraction patterns can be done on a global basis. The matches table in SIeve/SIeve+ can be customized to use any of 80+ display fields. SIeve+ can import time-of-flight neutron diffraction patterns and DECTRIS® 2D X-ray diffraction patterns for phase identification. The SIeve/SIeve+ d-spacing correction algorithms can use Standard Reference Materials (SRM) from NIST (National Institute of Standards and Technology) as the data source. These are just some of the many value-added developments designed to make the ICDD products more functional and powerful for 2017.