

PRODUCT DEVELOPMENTS FOR ICDD® 2020 POWDER DIFFRACTION FILE™ SOFTWARE

J. Blanton, R. Vithayathil, D. Sagnella, S. Kabekkodu, T. Blanton, S. Gates-Rector
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, neutron diffraction data, and electron diffraction data to patterns in the PDF® database.

To enhance the value of the PDF® software, ICDD has incorporated many new developments for the 2020 product release. Data mining searches can be cancelled at any time by clicking the Cancel button or by pressing the ESC key. New searches and display fields have been added for zeolite names and molecular weights. Composition diagram lists now support five component systems (quinary sorting). A new composition graph can be plotted that allows the user to graph binary and ternary systems on a color-coded, triangular graph. Preferred orientation settings now dynamically change the graph, allowing the user to estimate the PMD value when comparing to experimental data. SAED, EBSD, and ring patterns can be exported to image files. SIEve/SIEve+ can import diffraction patterns from Proto Manufacturing (*.xml) and Shimadzu (*.raw) diffractometers. The decimal places of d-spacings throughout the program now more accurately reflect experimental data and are no longer fixed to six decimal places. The font size can be increased for all components in the program. These are just some of the many value-added developments designed to make the ICDD products more functional and powerful for 2020.