PRODUCT DEVELOPMENTS FOR ICDD® 2019 POWDER DIFFRACTION FILE™ SOFTWARE

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International Centre for Diffraction Data® (ICDD) data mining software has the ability to search through the entire Powder Diffraction FileTM (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 2019 product release. Composition diagram lists can be generated using the periodic table. Pressure of data collection can now be searched, as well as displayed, in the search results and PDF card. The size of peak marker symbols can be customized by the user. OEM 2D diffraction patterns can be imported into ring pattern simulations for visual comparison. The user can now drag and drop files into SIeve/SIeve+ for immediate importing. SIeve/SIeve+ can import many new file types such as Rigaku *.raw, DECTRIS Eiger *.h5, and greyscale *.TIFF. The SIeve/SIeve+ user interface has been redesigned to be more powerful, and the matches filter has been redesigned to include more common criteria. The Microanalysis search can import *.csv files and the Microanalysis matches table can be customized using display field preferences. These are just some of the many value-added developments designed to make the ICDD products more functional and powerful for 2019.