

Advancing X-ray powder data compilation and crystal structures of pharmaceutical compounds

The International Center for Diffraction Data (ICDD) has long encouraged the entry of quality reference data and structures of crystalline and today even microcrystalline and amorphous compounds through multiple efforts of data abstraction, data collection, and data assessment. This vast data collection is available as the Powder Diffraction File (PDF), which is widely used for phase identification by X-ray, electron, and neutron diffraction methods. Since the inception of the PDF, the file has proven more and more valuable to identify phases in multiphase mixtures. Today, high-quality experimental PXRD data sets are gathered from all accessible sources including the published literature, investigator submissions, ICDD Grant-in-Aid projects, and database organization collaborations such as those between ICDD and the CSD, ICSD, and LPF crystal structure databases. These efforts are steadily expanding the scope and coverage of the pharmaceutical compound library in the PDF. The focus area of pharmaceutical compounds is one that today is of special interest around the world.

One mechanism available to research teams to further expand the collection of PDF entries of pharmaceutical materials is publishing in the journal *Powder Diffraction*. Such submitted and accepted manuscripts contain high-quality PXRD data, and very frequently crystal structure solutions, of current or future pharmaceutical materials. This issue of the journal *Powder Diffraction* contains eight such manuscripts, all of which involve high quality, high-resolution PXRD data collection, both Rietveld and DFT structure solutions, and deposition of both the PXRD pattern data and

crystal structure with ICDD. The methods employed in these eight papers in this issue are extremely comprehensive and aim to assure that the data is of outstanding quality and value to the research community. The manuscripts also often compare the reported data with that found in the patent literature and open scientific literature and, not infrequently, resolve issues or conflicts in the prior literature.

While this issue happens to include a larger number of reports on pharmaceutical materials, the Journal typically includes manuscripts on crystalline inorganic, metal, organic, and polymer phases. The Journal also regularly accepts PXRD-related papers on experimental and computational methods, instrumentation, software, and education. Making the PDF as comprehensive and accurate as possible has a wide and critical impact on furthering the analyses that diffraction scientists are undertaking.

We look forward to receiving your submissions of the manuscript on any of these topics.

To submit your manuscript to PDJ, please see:

Author Notes: <https://www.icdd.com/pdj-authors-notes/>
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For more information and requirements about the ICDD Grant-in-Aid program, please see: <https://www.icdd.com/grant-in-aid/>

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