Publication of new diffraction data in *Powder Diffraction*

Reference powder diffraction data have been used extensively for phase identification of crystalline materials and other powder diffraction applications for decades. In recognition of the importance of new diffraction data for powder diffraction analysis, *Powder Diffraction* welcomes the submission of articles on new diffraction data. New diffraction data have been reported in *Powder Diffraction* since the first issue of the journal in March 1986. About 25% of the technical papers published in *Powder Diffraction* have been new-diffraction-data papers

New diffraction data suitable for publication in *Powder Diffraction* can be data of a newly discovered compound, data of a known compound not in the powder diffraction file (PDF), or data to replace an existing low-quality PDF entry with improvements in new crystal system, space group, *hkl* indices, or significantly higher FoMs. Detailed GiA data with added information on experimental and data-reduction methods are also welcomed.

New diffraction data with values of 2θ, d, and I are normally reported in a diffraction-data table of a short article in the section of new diffraction data. The diffraction-data table should contain both observed and calculated values of 2θ, d, and I. For uniformity, diffraction-data tables must have columns of $2\theta_{obs}$, d_{obs}, I_{obs}, hkl, $2\theta_{cal}$, d_{cal}, I_{cal} (optional), and $\Delta 2\theta$. The procedure for obtaining both the observed and calculated data is as follows:

Values of $2\theta_{obs}$, d_{obs}, and I_{obs} can be obtained directly from an experimental diffraction pattern by first or second derivative method or by peak fitting without using unit-cell and/or crystal-structure information.

Crystal system, values of hkl, and possible space group(s) are then determined by automatic or manual indexing. Lattice parameters a, b, c, α, β, and γ, as well as values of $2\theta_{cal}$ and d_{cal}, are obtained by least-squares refinement. To improve the accuracy of the results, a correction for zero-angle displacement error should be included in the least-squares refinement process if possible. Values of $2\theta_{cal}$, d_{cal}, and I_{cal} can also be obtained from structure-refinement results.

New crystal-structure papers published in the technical-article section may also include diffraction-data tables of $2\theta_{cal}$, d_{cal}, and I_{cal}. Authors are encouraged to include values of $2\theta_{obs}$, d_{obs}, and I_{obs} so that the data tables have similarities to those reported in regular new-diffraction-data articles.

Keep this journal in mind for reporting your new diffraction data to the world.

Ting C. Huang
Editor-in-Chief

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