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Powder Diffraction

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On the Cover: Neutron powder diffraction has long been a powerful tool for characterization of crystalline materials due to several factors including that the neutron scattering factor changes from element to element leading to enhanced sensitivity to light elements, neighboring elements and isotopes as well as the reduced drop off in intensity with increasing Q. Neutron powder diffraction is now more widely available due to the construction of several powerful spallation neutron facilities around the world. In this *PDJ* issue the paper "Calculation of Full-Pattern Neutron Time-of-Flight (TOF) Powder Diffraction Patterns", by John Faber, shows that the release of the Powder Diffraction File (PDF4+) now includes capabilities to calculate the neutron powder pattern including the estimated background. The left box shows the calculation of the pattern with background for La¹¹B₆ (SRM660b) where approximately thirty diffraction lines are clearly seen. The right box shows the impact of inelastic scattering contributing to the background by comparing to the patterns for a deuterated and hydrogenated samples Nd₂Ni₂InD_{7.52} and Nd₂Ni₂InH_{7.52}.

These tools will assist scientists in planning experiments at neutron sources as well as interpreting data collected. In addition, it is now possible to create a Search/Match database of nearly 300,000 inorganic phases for a given neutron instrument. With this, scientists using neutron facilities can now rapidly analyze mixtures of phases.

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