WHIPPET –A New Sheriff in Town

Diane E. Sagnella
Senior Scientific Programmer
International Centre for Diffraction Data, Newtown Square, PA 19073 USA

The program SQLAIDS (previously NBS*AIDS83) is the cornerstone of the editorial work performed at the International Centre for Diffraction Data (ICDD®). The program is used to ensure consistency and quality in each of the patterns published in the Powder Diffraction File™ (PDF®). Among the functions of SQLAIDS are to check indexed reflections, formulas, names and densities, and improve cell parameters. The key to running the AIDS program is the creation of an AIDS input file. This file has a strictly defined structure based on the concept of "PDF cards", which places strict limits on the number of reflections, the magnitude of intensities, the length of names, etc. For many years, these limits were more than adequate for processing of diffraction data for the PDF. However, with the ever increasing capabilities of radiation sources and detectors, more complex materials systems, and more supporting data, it is clear that the needs of the scientific community have been changing and the editorial process for reviewing diffraction data must also change. As a result, the current limits of SQLAIDS now serve more as restrictions. We have created a solution to these woes called WHIPPET. This poster will show what WHIPPET can do and how it is already being used to enhance data and facilitate the editorial process at ICDD.