

DATA QUACKER: A New Program to Filter and Funnel Data into the ICDD

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Abstract:

Experimental data for publication in the Powder Diffraction File™ (PDF) are acquired through contributions from individual scientists, corporate laboratories, literature surveys, and a Grant-in-Aid (GiA) program. While each of these contributions is critical to the PDF, there has been a steady decrease in high quality experimental patterns found there over the past several years, making submissions from sources such as the GiA program even more vital.

Multiple data files, containing raw data, D-I lists, atomic coordinates and details concerning the sample preparation & experimental conditions, are typically submitted separately. To make matters more challenging, the format of these data files is as varied as the contributors themselves. As a result, extracting the appropriate data is a labor intensive effort. Therefore, the goal of the ICDD was to develop an easy-to-use, unified data entry program that can read a variety of data formats for the various input files and produce a single data file containing all the data required by the ICDD.

This presentation will describe a prototype for a newly developed, easy-to-use, unified data entry program that can read various input file formats for a variety of data, graphically display the data and produce a single CIF file containing all data required by the ICDD. This program, called Data QUACKER, [Data QUALity Control & Entry Resource], is the next step in helping both the submitters and the ICDD place experimental data into the PDF!