

Processing of New Entries Using “DataQUACkER”

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The literature publication of traditional d-spacing-intensity (d-I) lists has decreased in recent years with the steadily increasing use of full profile refinement techniques to analyze powder diffraction data. However, authors are also submitting raw powder diffraction patterns more frequently as supplemental information. “DataQUACkER” was created to help, not only the grantees with their submission of data to the Powder Diffraction File™, but also with processing supplemental data which is usually in Crystallographic Information File (CIF) format from the literature. In 2009, we added approximately 125 entries to the editorial process using “DataQUACkER” and we expect that number to increase significantly this year with the grantees submitting new data primarily as CIF’s generated from the “DataQUACkER”. This poster discusses how the abstracted data from powder CIF’s and grantees is ultimately abstracted and inserted into the Powder Diffraction File™.