

Powder diffraction – pragmatic, precise, or both?

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Powder diffraction fulfils a number of roles within industry; phase identification, phase quantification, structure determination, structure stability as a function of time, crystallite size and strain, to name but a few. Each role has its own particular requirements for accuracy and precision of the PXRD data and the associated derived quantities. Often, the industrial imperatives do not necessarily match those that are of a more academic nature. For example, the time and effort that an academic can afford to spend on a particular material may be prohibitive for an industrial researcher who is working to a particular deadline. Similarly, equipment availability frequently determines the level to which a particular problem can be studied.

This presentation will expand upon the themes above, using examples taken from the pharmaceutical, drug development and foodstuffs industries. In particular, using examples of crystal structure solution and quantitative phase analysis, we will show how precision and pragmatism can sometimes be achieved, to the satisfaction of academic and industrialist alike.