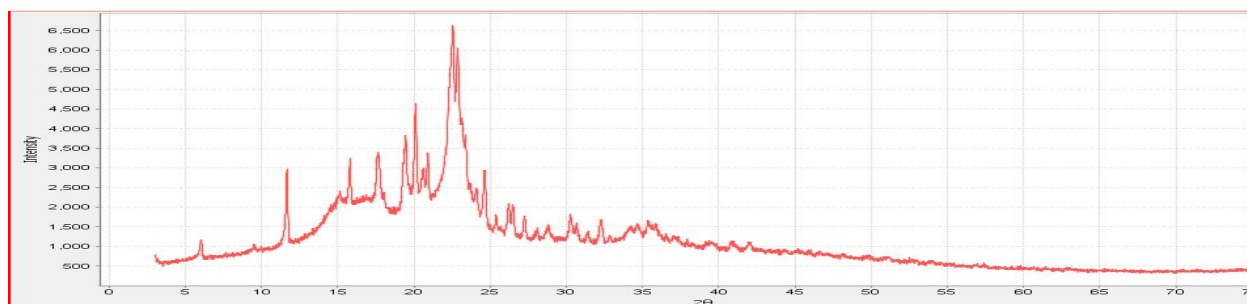


SUCCESSFUL MATERIAL IDENTIFICATION

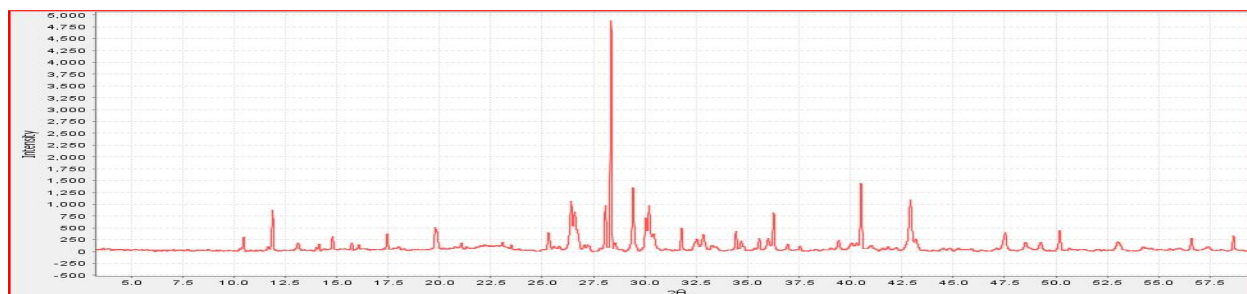
T. G. Fawcett, F. Needham, C. E. Crowder, S. N. Kabekkodu
International Centre for Diffraction Data

In 2009, the ICDD surveyed the global the community of diffractionists about the methods and tools that they use in phase identification analysis. The survey included a question on how successful the analysts were in solving unknown identification problems. This generated a profile of the “successful” material scientist /analytical chemist based on their problem-solving attributes. The profile of successful analysts shows that they tend to be older, use a broad range of diffraction methods, and tend to use both newer software and analysis databases than the norm. These attributes should not be surprising since it demonstrates the common sense expectation that experience combined with capability can lead to better results. A year earlier ICDD conducted a survey of users in the pharmaceutical industry who use PDF-4/Organics. This provided a profile of the types of problems being analyzed in the field.

In this presentation the authors will demonstrate the solutions to several pharmaceutical material identification problems, with a focus on the various methods used, and the experience gained. Examples will include polymorphic blends, identification of low concentration of active ingredients, very complex multi-component mixtures and the identification of crystalline/non-crystalline mixtures. For example in the two data sets shown below routine analysis will often identify only half the materials that can be extracted from the pattern.



Data from a formulated tablet containing polymorphic mixtures and both nanocrystalline and crystalline materials.



Data from a complex formulation where there are several crystalline phases below 5 weight % composition.