Application of the Powder Diffraction File™ in Pharmaceutical Analysis

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Diffraction techniques used in the analysis of both crystalline and noncrystalline solids have been utilized in materials science for almost a century. The nondestructive nature and uniqueness in characterizing the solid state makes the diffraction technique a seminal analysis tool. The pharmaceutical industry has embraced this technique for analyzing formulations, polymorphs and in quality control, to name a few applications. The paramount advantage of the diffraction technique is in multiphase analysis, even when the components are present in trace amounts. The success of such detailed analysis depends on both the experimental methods adopted and the quality and content of the database used.

International Centre for Diffraction Data's (ICDD®) Powder Diffraction File (PDF®) is a powerful database for materials identification and has been used extensively by the scientific community for more than seven decades. The Powder Diffraction File in relational database format contains extensive chemical, physical, bibliographic and crystallographic data including atomic coordinates enabling qualitative and quantitative phase analysis. The current PDF release has more than 890,000 diffraction patterns and 330,000 crystal structures, enabling exhaustive qualitative and quantitative phase identification. The database is classified into various categories called subfiles such as minerals, pharmaceuticals, forensic, bioactive, etc. These subfiles are continuously reviewed by scientists with specific field expertise to maintain quality. Subfiles play an important role in minimizing false positives and optimizing the search/match process. The PDF uses many more classifications based on quality, structural similarity, physical properties, etc. Structural classifications play an important role in controlling the quality of the published structure or powder diffraction patterns, as it is an excellent tool to identify similar phases that are otherwise not easily recognizable. Case studies involving analysis of complex pharmaceutical formulations illustrating the comprehensive nature and quality of the database augmented by digital simulations will be presented.

Recent developments in the Powder Diffraction File and its applications in pharmaceutical analysis will be discussed in this presentation