

## **BASICS OF POWDER X-RAY DIFFRACTION AND ITS APPLICATION FOR PHARMACEUTICAL ANALYSIS USING THE PDF-4/ORGANICS DATABASE**

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One of the challenges of an analytical scientist is to use a nondestructive technique that can handle mixtures and can differentiate the various components in the sample. Powder X-ray diffraction (PXRD) is a nondestructive method that identifies and characterizes polycrystalline materials. The scattering of X-rays produce a diffraction pattern that contains information about the atomic arrangement within a crystal. Each phase has a unique diffraction pattern like a fingerprint, which can be used for phase identification of a pure substance or complex mixtures like pharmaceuticals. PXRD has applications in patent law, quality control, counterfeit detection, pharmaceutical engineering, and drug identification. When using PXRD for pharmaceutical analysis, one can not only identify the crystalline phases, but also gain information about the amorphous components commonly used in excipients by using a full profile fit using the PDF-4/Organics database. The organics database consists of over 535,600 total entries, including 21,927 bioactive entries, 1,729 polymers, 11,818 pharmaceutical and excipient entries, and 1,243 pigments and dyes; all of which are of use during pharmaceutical analysis.