Uses of X-Ray Powder Diffraction In the Pharmaceutical Industry

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1 INTRODUCTION

Among the many experimental techniques available for the identification of solid forms, including polymorphs, solvates, salts, cocrystals and amorphous forms, X-ray powder diffraction (XRPD) stands out as a generally accepted "gold standard." While this does not mean that XRPD should be used to the exclusion of other experimental techniques when studying solid forms, X-ray diffraction (XRD) has applications throughout the drug development and manufacturing process, ranging from discovery studies to lot release. The utility of X-ray diffraction becomes evident when one considers the direct relationship between the measured X-ray diffraction pattern and the structural order and/or disorder of the solid. XRPD provides information about the structure of the underlying material, whether it exhibits long-range order as in crystalline materials, or short-range order as in glassy or amorphous materials. This information is unique to each structure—whether crystalline or amorphous—and encoded in the uniqueness of the XRPD pattern collected on a well-prepared sample of the material being analyzed.

One must draw a distinction between crystalline materials, which give rise to XRPD patterns with numerous well-defined sharp diffraction peaks, and glassy or amorphous

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