

PDF-4/ORGANICS 2006 REFERENCE POWDER PATTERNS AND THEIR PHARMACEUTICAL APPLICATION

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The importance of X-ray powder diffraction (XRPD) patterns for pharmaceutical substances, either active ingredients of diagnostic/therapeutic drugs or excipients for corresponding formulation, cannot be over-emphasized. There are 286,000 XRPD reference patterns in the PDF-4/Organics 2006 database. Among them, 28,000 patterns are data collected from XRPD experiments and 258,000 patterns are data calculated from single crystal data. A majority of them are substances related to life sciences.

Examples are used to illustrate the properties presented in the PDF-4/Organics database. Some of these properties are described here. The non-ambient XRPD collection temperatures for the 64,000 patterns in the PDF-4 database will shed some light on the stability of the substances in question. The crystallinities of the organic/organometallic materials in the database are readily observed from the quality marks of both experimental and calculated reference patterns. Many materials are known for their bioactivity, such as antibacterial, antineoplastic and other pharmaceutical applications. A wide variety of excipients including both organic and inorganic compounds in the database exhibit their polymorphic solid state information. Representative cases for the aforementioned properties will be presented.