USE OF X-RAY POWDER DIFFRACTOMETRY IN DRUG DISCOVERY, PREFORMULATION AND DRUG PRODUCT CHARACTERIZATION

Raj Suryanarayanan, College of Pharmacy, University of Minnesota, Minneapolis, MN 55455, USA

Conventionally, X-ray powder diffractometry (XRD) has found widespread use for the identification of crystalline solid phases. Recent advances in instrumentation and software have extensively extended the utility of the technique. For example, high throughput X-ray diffractometry, requiring the preparation and rapid analyses of a large number of samples, is becoming a routine technique. When there is screening of the physical form of the active pharmaceutical ingredient, including polymorph screening, XRD is often coupled with thermal and spectroscopic techniques. XRD is particularly well-suited to monitor processing-induced phase transformations. The XRD patterns of solid dosage forms can be complex with numerous overlapping X-ray lines. Using pattern subtraction techniques, the contribution of the excipients can be selectively subtracted. This enables not only the detection, but also the quantification of phase transitions during processing. Though XRD has limited utility in the characterization of amorphous phases, it is a sensitive technique, not only in providing the first evidence of crystallization but also to characterize the extent of disorder in partially ordered lattices.