

GEOMETRY AND CONFIGURATION OF XRD SYSTEMS FOR PHARMACEUTICAL

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Application of X-ray diffraction for pharmaceutical research and discovery has dramatically increased in recent years. The geometry and configuration of an X-ray diffractometer is an important consideration in terms of samples preparation, data quality, productivity, and easy of operation. For instance, the conventional Bragg-Brentano parafocusing geometry may be suitable for a sample prepared with large quantity of powder, but most pharmaceutical samples have limited quantity or special form not suitable for making a conventional powder sample. In this case, a parallel point focus beam geometry with linear or area detector is more suitable. In combinatorial screening process for polymorphism study, many samples are packed in a well plate and typical 2θ measuring range of pharmaceutical compound is from 2 to 60° . In this case, transmission geometry may be the best choice to avoid the defocusing effect and cross contamination associated with reflection mode diffraction.

Fueled by recent technological advances in detectors, X-ray sources, optics, and software, numerous choices are available for a pharmaceutical X-ray diffractometer. This presentation covers some basics and recent development in geometry and configuration of XRD systems for pharmaceutical study. Comparisons between various X-ray sources, optics and detectors are also given with application examples in pharmaceutical powder diffraction.