

Accuracy in Powder Diffraction Measurements

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As X-ray powder diffraction becomes more and more commonly used in the analysis of pharmaceuticals with very low absorptivities a review of the fundamentals of diffractometer design, aberrations and calibration is warranted. This talk will describe the fundamentals of diffractometry and the principal sources of error. Techniques for evaluation, calibration and elimination of these errors will be shown. Parallel beam methods using modern X-ray optics will also be shown. Details of the peak fining and smoothing algorithms as well as profile fitting techniques will also be examined.