

Use of a Single Crystal Diffractometer and CCD Area Detector for Phase Identification

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CCD-based single crystal X-ray diffractometers are widely used in the fields of chemistry, materials science, biology and mineralogy for crystal structure determination. However, CCD detectors have not yet been widely utilized in the field of powder diffraction.

A new Phase Identification option has now been integrated into the Bruker APEX2 software suite, so that the same hardware and software may be used for both structure determination and powder diffraction measurements. This module will be offered as an optional add-on feature for the small molecule single crystal instruments using the APEX2 (Version 2.0) software suite. For more specialized applications, data may also be exported to the Bruker DIFFRAC^{plus} (EVA & TOPAS) programs.

The powder diffraction option is intended to supplement the primary use of a single-crystal diffractometer to verify that the sample is a single phase or polymorph and that the analyzed single crystal specimen is representative of the bulk sample.

Various examples of powder diffraction patterns collected on Bruker Kappa APEX II and SMART APEX II instruments equipped with Cu- or Mo-wavelength X-ray sources will be presented.

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