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XRPD Measurements on Single Crystal Diffractometers. Kingsley L. Smith, Scott K. Goodwin, R. Curtis Haltiwanger, Bob B. He, Bruker AXS Inc. 5465 East Cheryl Parkway, Madison, WI 53711 USA.

Few crystallographers have used their single crystal diffractometer for powder diffraction to confirm their structure is representative of the bulk sample. We will compare measured and calculated powder diffraction data from various single crystal diffractometers using PILOT and SHELXTL software. Several compounds previously used for single crystal structure determination, are re-examined using powder diffraction. Powder samples can be in filled capillaries and loops, or spread on small reflection mount (SEM "T" disks), depending upon the amount of material available. PILOT software optimizes the powder diffraction data collection strategy for each type of sample mount. Resulting powder spectrums are compared to the calculated pattern from SHELXTL using the single crystal data set.