

## Accurate Charge Densities in under a Day with a Home X-ray Source

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The assembly and evaluation of a new in-lab facility for the rapid collection of charge density quality diffraction data will be presented. The system uses an 18 kW Mo rotating anode generator, graphite monochromator, large curved image plate, and an open flow helium cryostat. The rationale for the choice and operating conditions of each of the components will be discussed. The need and application of a flood field correction will be demonstrated. Data integration with the program *VIIPP* [1] was shown to be superior to any other program available to us. Proof of principle experiments have been carried out in under a day. The quality of the diffraction data obtained at 15 K to  $(\sin\theta/\lambda)_{\max} = 1.32 \text{ \AA}^{-1}$  has been evaluated from the statistics provided by SORTAV [2], and by the quality of the multipole refinements [3] as judged by final R factors, residual maps, deformation density maps, etc. Although not as fast as a synchrotron experiment, a home source is always available, is more stable than most synchrotrons, and has no travel overhead associated with its use.

[1] Zhurova E.A., Zhurov V.V., Tanaka K., *Acta Cryst.*, 1999, **B55**, 917. [2] Blessing R.H., *Cryst. Rev.*, 1987, **1**, 3. [3] Koritsanszky T., Howard S., Mallison P.R., Su Z., Ritcher T., Hansen N.K., *XD. A computer Program Package for Multipole Refinement and Analysis of Electron Densities from Diffraction Data. User's Manual*, University of Berlin, Germany, 1995.

**Keywords:** charge density, home x-ray source, rapid collection