

## X-Ray Structure Determination

**( Change the highlighted values with the values from your own experiment)**

A deep-red rectangular shaped crystal of (XYZ), approximate dimensions .30mm x .25mm x .32mm, was mounted in a thin-walled glass capillary tube under an inert atmosphere for data collection. The X-ray intensity data were measured at room temperature on a Bruker SMART 1000 CCD-based X-ray diffractometer system equipped with a Mo-K $\alpha$  radiation ( $\lambda = 0.71073 \text{ \AA}$ ). The detector was placed at a distance of 4.986 cm from the crystal.

A total of 1800 frames were collected with a scan width of  $0.3^\circ$  in  $\omega$ , with an exposure time of 10 sec./frame. The total data collection time was 16.6 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame integration algorithm. The integration of the data using a triclinic unit cell yielded a total of 15000 reflections to a maximum  $2\theta$  angle of  $56.26^\circ$ , of which 7500 were independent (redundancy 2.00,  $R_{\text{int}} = 1.7\%$ ,  $R_{\text{sig}} = 2.2\%$ ) and 6760 (90%) were greater than  $4\sigma$  (F). The final cell constants of  $a = 10.394(17) \text{ \AA}$ ,  $b = 10.480(16) \text{ \AA}$ ,  $c = 9.909(3) \text{ \AA}$ ,  $\alpha = 107.86(3)^\circ$ ,  $\beta = 6.56(2)^\circ$ ,  $\gamma = 111.25(2)^\circ$ ,  $V = 926.2(5) \text{ \AA}^3$ , are based upon the refinement of the XYZ centroids of 3200 reflections above  $20\sigma(I)$ . Analysis of the data showed negligible decay during data collection.

The positions of the four copper atoms were obtained from the Patterson map and the remaining structure was obtained from difference Fourier map. The structure was refined using the Bruker SHELXTL (Version 6.12) Software Package, in the space group P1(No.1), with  $Z = 1$  for the formula unit xyz. The final anisotropic full-matrix least-squares refinement on  $F^2$  converged at  $R1 = 3.44\%$ ,  $wR2 = 6.57\%$  and a goodness-of-fit of 0.944. The largest peak on the final difference map was  $1.510 \text{ e/ \AA}^3$  close to one of the Cu atoms. The calculated density for XYZ is  $1.466 \text{ g/cm}^3$ .