

**W0038**

**Structural Determination of a Partial Hemihedral Twinned Actin Crystal.** Robbie Reutzler, Lakshmanan Govindasamy, Mavis Agbandje-McKenna, Robert McKenna, Dept. of Biochemistry & Molecular Biology, McKnight Brain Institute, Univ. of Florida College of Medicine, Gainesville, FL 32610.

An orthorhombic actin crystal (space group  $P2_12_12_1$  with unit cell dimensions  $a = 101.56$ ,  $b = 103.03$ ,  $c = 126.96$  Å) was converted to a partial hemihedral twinned tetragonal crystal (space group  $P4_3$  with unit cell dimensions  $a = b = 101.50$ ,  $c = 104.2$  Å) by induced condensation. Diffraction data for the twinned tetragonal crystal were collected at 100 K to 3.0 Å resolution (completeness 99.8 % with  $R_{\text{sym}}$  of 8.1 %) using synchrotron radiation. The hemihedral twinning of the data was observed by self-rotation function analysis and was determined to have a partial twin fraction of 0.376 from intensity statistics. The structure, with two actin molecules in the crystallographic asymmetric unit, was determined by molecular replacement methods and refined to an  $R_{\text{factor}}$  of 0.193. As a consequence of the crystal lattice transformation from the orthorhombic  $P2_12_12_1$  to the tetragonal  $P4_3$  space group, actin-actin contacts were rearranged and an inter-actin dimer disulphide bond (cys-374) observed in the orthorhombic crystal form was broken in the tetragonal crystal form.