

W0146

Adventures with Neutron Diffraction: Protonation states of D-xylose Isomerase. Gerard J. Bunick^{*§}, B. Leif Hanson^{*}, Paul Langan[^], Amy Katz[#], H. L. Carrell[#], Benno P. Schoenborn[^], Jenny P. Glusker[#], ^{*}UT/ORNL-GST, Oak Ridge, TN, [^]Bioscience Div., LANL, Los Alamos, NM, [#]Fox Chase Cancer Center, Philadelphia, PA, [§]Life Sciences Division, ORNL, Oak Ridge, TN.

D-xylose isomerase (XI), a metalloenzyme, catalyzes the interconversion of xylose to xylulose. The precise mechanism of the interconversion is under investigation by us. The enzyme is used commercially in the production of fructose from glucose. To ascertain the protonation and solvation state of the enzyme's catalytic site residues, neutron diffraction measurements have been made at the LANSCE protein crystallography station (*Acta Cryst.* D 60, 241-249) from XI crystals with different metal ions. In the past year, data were measured from a crystal containing cobalt as the cofactor. Data are reasonably complete to 1.7 Å with significant data to 1.5 Å. I/σ_1 is 3.2 in the highest resolution shell. The overall Rmerge is 14.5%. These XI neutron data compare well with data from steady state sources, matching or exceeding published neutron data for a similar sized protein. The neutron density maps of the active site region show the position of the metal ions, solvent waters and exchanged protons within the structure. The implications of these observations with the proposed modes of action for enzyme will be discussed.