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What Can Be Learned About Biochemical Reactions From Neutron Diffraction Studies? Amy Katz*^{\$}, Xinmin Li^{\$}, B. Leif Hanson[%], Jenny P. Glusker*, H.L. Carrell*, Paul Langan[#], Benno Schoenborn[#], Gerard J. Bunick^{\$}, *Fox Chase Cancer Center, Philadelphia, PA, ^{\$}Univ. of Tennessee/ORNL-GST, Oak Ridge, TN, [%]Univ. of Toledo, Toledo, OH, [#]Biosciences Div., LANL, Los Alamos, NM.

Neutron diffraction provides an excellent experimental method for directly locating hydrogen atoms in proteins. The precise locations of hydrogen atoms are important in the catalytic mechanism of many enzymes. Neutron diffraction also provides a wide range of information on hydrogen bonding networks between water molecules. We have determined the neutron diffraction structure of the enzyme D-xylose isomerase whose mechanism of action has a ring-opening step and an isomerization step. Both of these steps involve hydrogen atoms. We will provide examples from our own work and that of others of hydrogen atom locations on functional groups such as histidine, aspartate, glutamate, lysine, arginine and cysteine that might be involved in catalytic mechanisms. We will also examine hydrogen-bonding networks found at the active sites of enzymes.

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