Macromolecular Neutron Crystallography Experiments Featured by ACA

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- **Growing interest in neutron crystallography paralleling development of dedicated beamlines, new detectors, and new software tools to handle multi-wavelength data**
- **Neutron diffraction unsurpassed as method for accurately locating positions of hydrogen atoms**
- **Next generation of neutron sources, such as SNS, will benefit the crystallographic community from an increase of several orders of magnitude in neutron flux**

Macromolecular Neutron Crystallography Experiments Featured by ACS (continued)

Reflected on the cover of the Winter 2002 issue of the *American Crystallographic Association Newsletter* are images from recent macromolecular neutron crystallography experiments. The growing interest in neutron crystallography is paralleling the development of dedicated beamlines, new detectors, and new software tools to handle multi-wavelength data. At moderate resolution, neutron diffraction data can provide strong support for the orientation of hydrogen atoms in water molecules, and can elucidate the ionization states of amino acids. Neutron diffraction is unsurpassed as a method for accurately locating the positions of hydrogen atoms, especially the mobile hydrogens needed for determining enzymatic mechanisms, hydrogen bonding patterns, and solvation of macromolecules in enzymes and other macromolecules. (On the bottom right, neutron density of a tryptophan residue from rubredoxin, clearly shows the difference between H atoms [red contours] and D atoms [blue contours] [kindly provided by Robert Bau]). The new LANSCE macromolecular neutron beamline at Los Alamos has been commissioned (upper right), providing an opportunity to collect diffraction data from larger proteins such as D-xylose isomerase (middle right, left side), from large crystals grown in hardware developed by NASA for microgravity studies (bottom middle). Topics ranging from structures to new beamlines and proposed new sources will be discussed in this year's Transactions Symposium at ACA 2003. When the next generation of neutron sources such as the Spallation Neutron Source (SNS) become operational in several years, the crystallographic community will benefit from an increase of several orders of magnitude in neutron flux. Neutron scattering and diffraction will soon become powerful and more widely available tools for macromolecular crystallography.