Practical Considerations for Neutron Data Collection from Biological Macromolecules

By
B. Leif Hanson and Gerard J. Bunick

The collection of neutron diffraction data from biological macromolecules is not simply the same as X-ray diffraction data experiments with larger crystals and longer data collection times. Our work with D-xylose isomerase has revealed to us several pitfalls in the process of sample preparation, crystal growth, deuterium exchange and crystal mounting. The simplest practice for the neutron crystallographer may be to consider hydrogen as highly communicable pathogen to be avoided at all cost. Thus for biologists, the neutron crystallographer's mindset may be easier to achieve than those without training in universal precautions. Overall, neutron protein crystallography, although demanding care and trade-offs, is not intractable. Among aspects described will be the means we use to grow large crystals, how to evaluate buffers and other solutions for neutron experimentation, how we deuterate our proteins and protein crystals, and how crystals are mounted to assure minimal back-exchange of hydrogen. In the context of the other addresses in this session, the information presented should provide a useful road map for those interested in pursuing neutron diffraction studies with biological macromolecules.