

W0505

New Possibilities for the Determination of Macromolecular Structures from Selected H/D Derivative Crystals Utilizing Neutron Data Alone. Herbert A. Hauptman, David A. Langa, Hongliang Xu, Hauptman-Woodward Medical Research Inst., 700 Ellicott Street, Buffalo, NY.

The impending development of higher flux neutron spallation facilities has generated a renewed interest in the possibilities for structure determination using neutron beams. Much of the interest in biological circles stems from being able to use the differences in scattering between H and D to answer important questions concerning macromolecules. For the most part these investigations rely on the structural results from previous X-ray studies to seed their investigations. In this presentation we would like to call attention to some interesting possibilities that neutron diffraction offers toward the actual structure determination of macromolecules by exploiting perdeuterated proteins that have been selectively hydrogenated for specific amino acid residues. It is our contention that such structures can be solved *ab initio* by direct methods procedures if suitable H/D derivatives can be synthesized.

Research support from NIH grant GM-46733 is gratefully acknowledged.