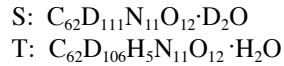


W0302

Combining Neutron Diffraction with Isomorphous Replacement. Herbert A. Hauptman, David A. Langa, Hongliang Xu, Hauptman-Woodward Medical Research Inst. and Dept. of Structural Biology, SUNY at Buffalo, 73 High St., Buffalo, NY 14203.

If one replaces a specified number of hydrogen atoms in a structure S by deuterium atoms (or vice versa), one obtains the isomorphous pair of structures, S, T. Refer to Hauptman *et al* (*Acta Cryst.* **A32**, 877-882 (1976); *Acta Cryst.* **A38**, 289-294 (1982), *Acta Cryst.* **A38**, 294-300 (1982); *Acta Cryst.* **A59**, 250-254 (2003)) for the extension of direct methods to neutron diffraction and to isomorphous replacement.

Application is made to the isomorphous pair of cyclosporine structures S, T where



With error free neutron diffraction data alone, to a resolution of 2.27Å, the values of the 300 phases corresponding to the largest values of |E| are found with an initial average phase error of 38°. At this resolution the total number of phases is 407.

In view of these results we believe that the same approach will succeed with macromolecules provided that suitable H/D derivatives can be prepared.

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