

“Glass and Liquid Diffraction at IPNS and APS”

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Argonne National Laboratory

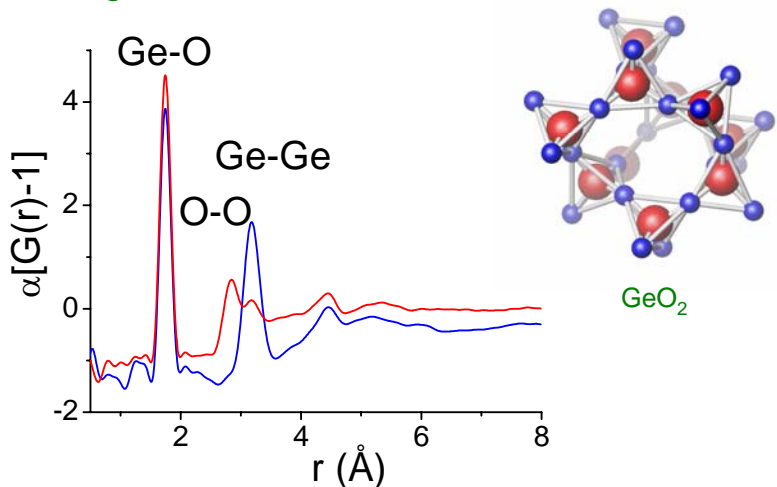


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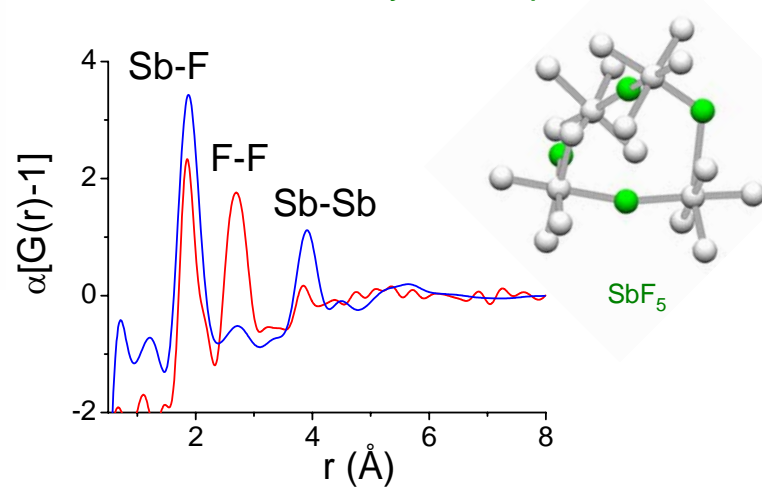


Total Scattering technique

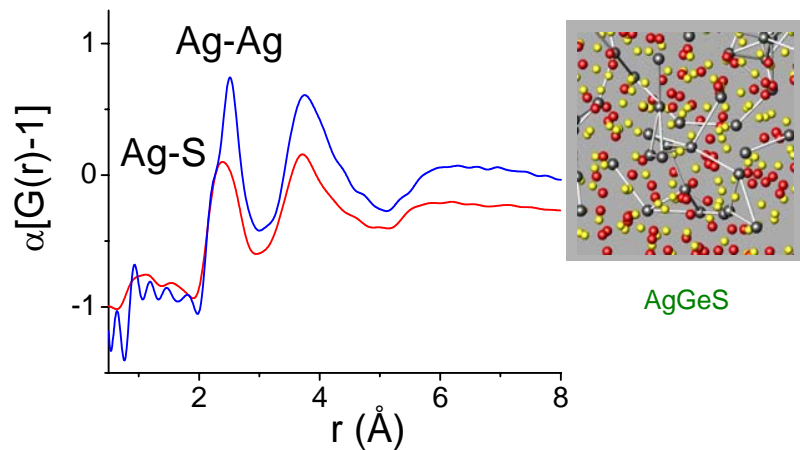
Oxide glasses: Minerals and laser materials



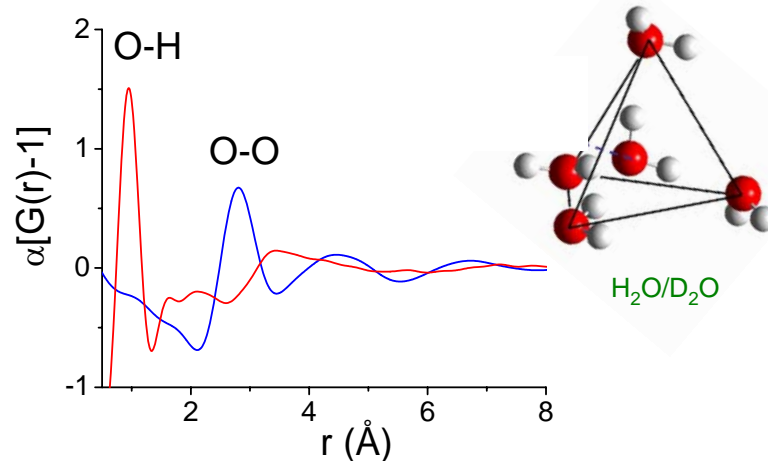
Fluorine chemistry and superacids



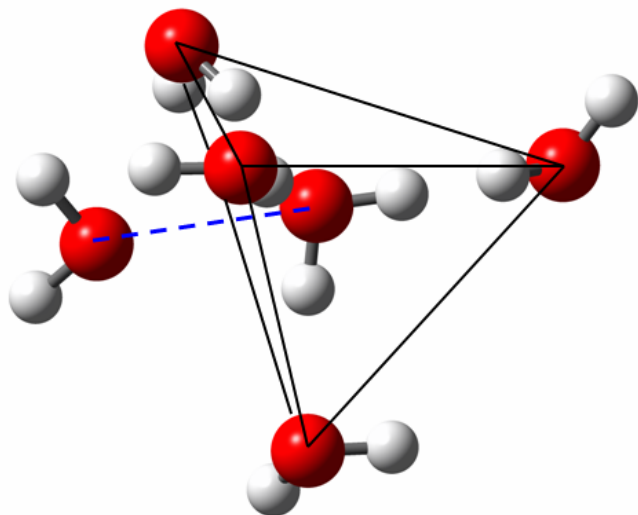
Fast ion conducting and optical chalcogenide glasses



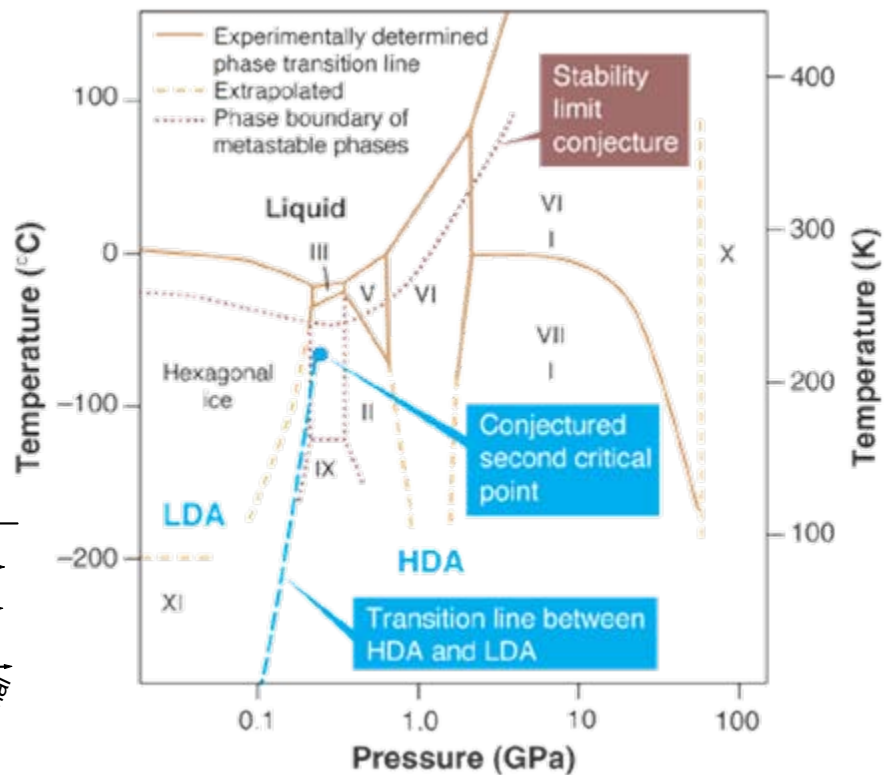
Hydrogenous molecular liquids



Water and amorphous ice



Water and Ice. A. K. Soper *Science* 2002 (297) 1288.



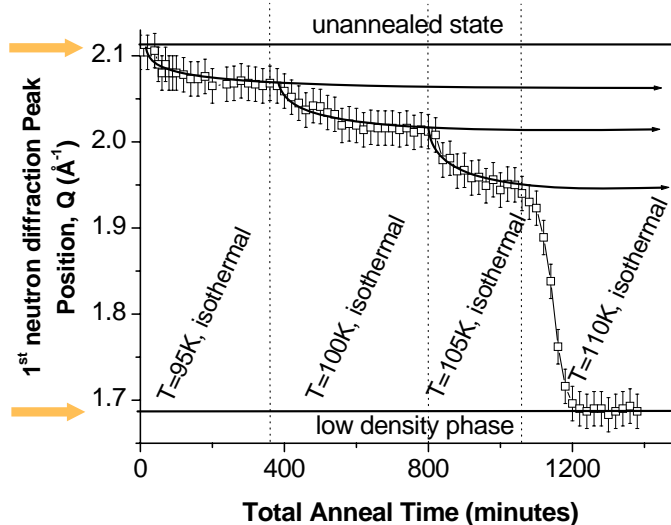
Structural studies of several distinct metastable forms of amorphous ice
C.A. Tulk *et al. Science* 297, 1320-1323 (2002)



HDA

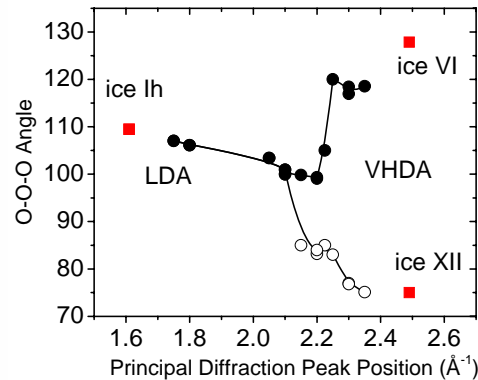
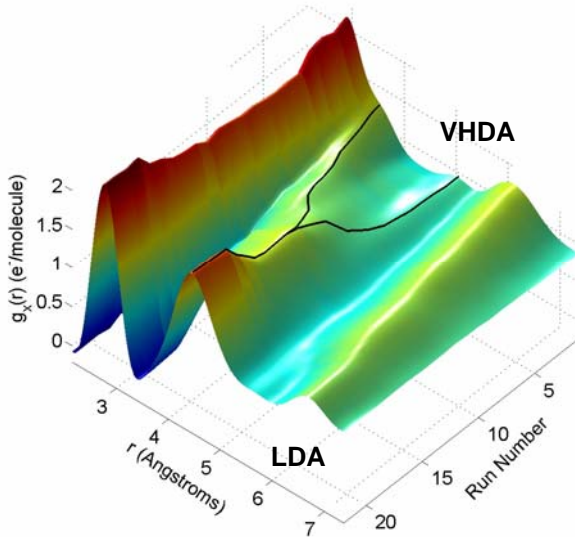
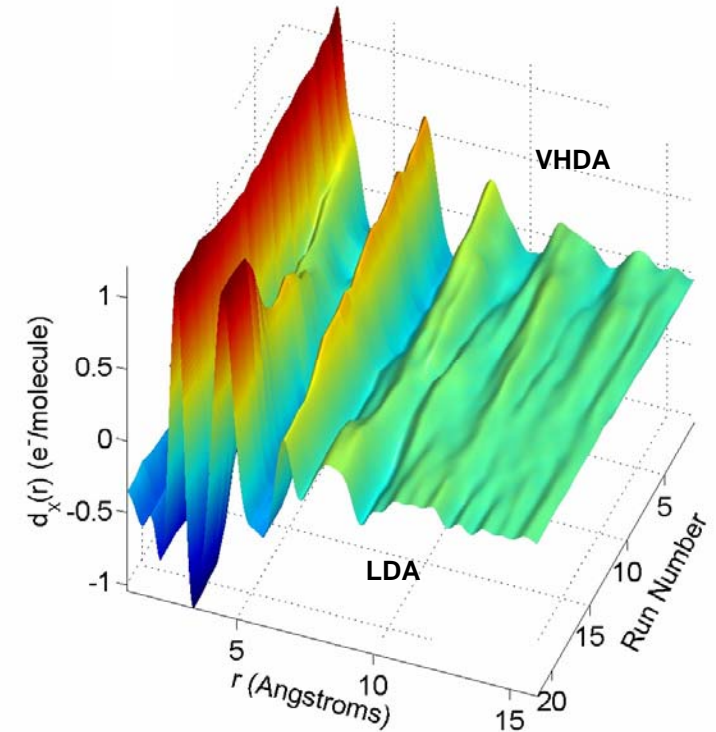
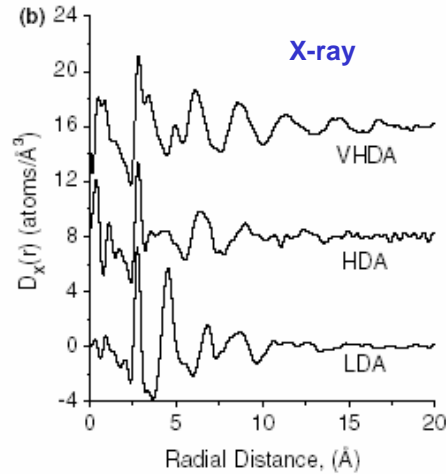
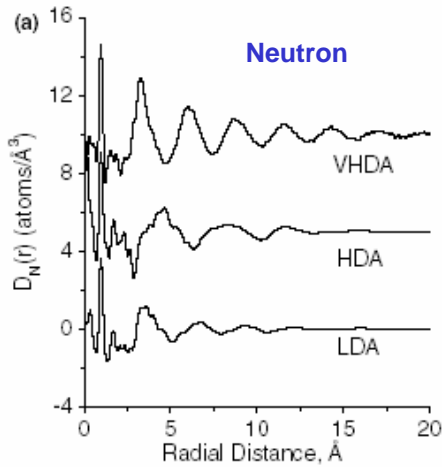


LDA

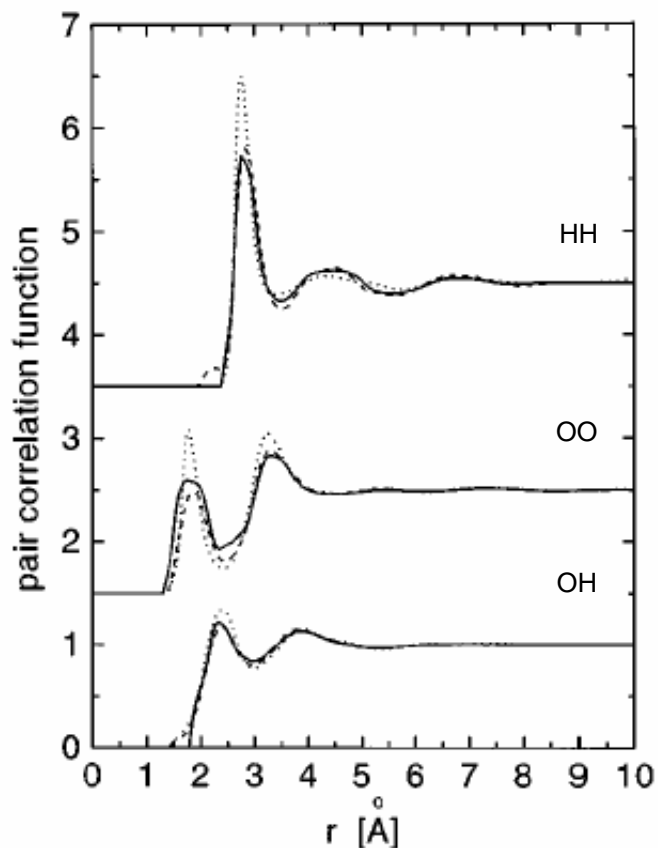


Low, high and very high density amorphous ice

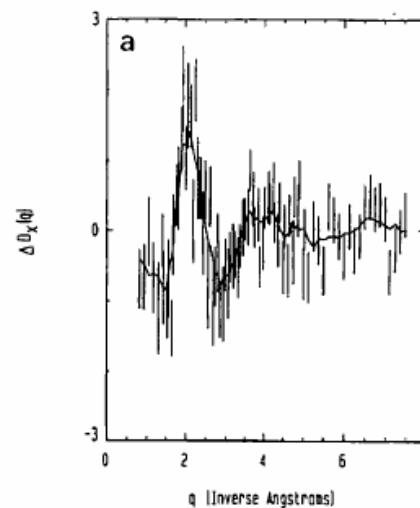
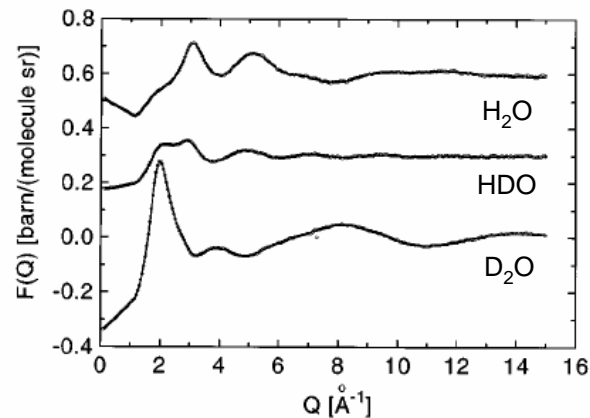
A structural study of very high-density amorphous ice. M. Guthrie *et al.*
Chem. Phys. Lett., 397 (2004) 335



H/D substitution in neutron diffraction



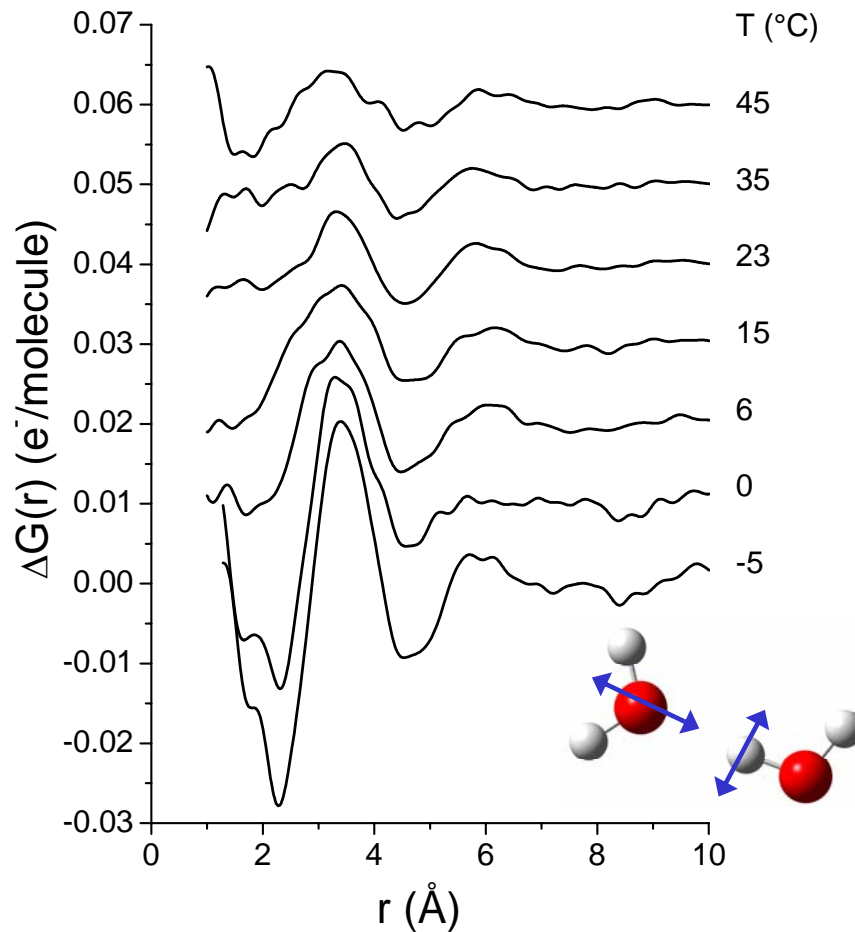
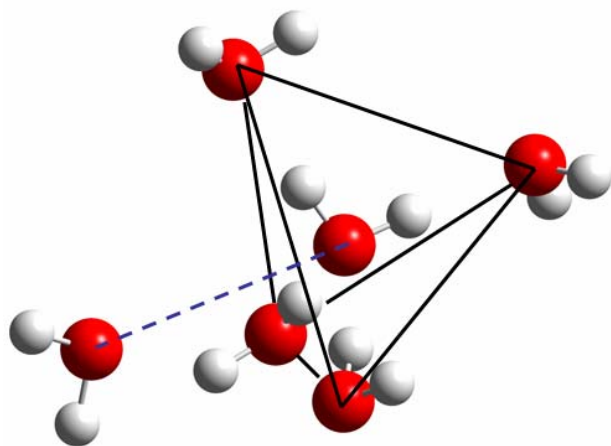
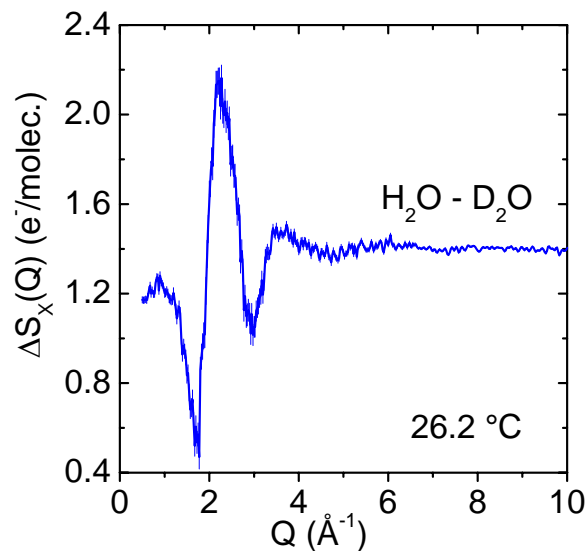
Site-Site pair correlation functions of water
A.K. Soper *et al.* *J. Chem. Phys.* 106, 247 (1997)



Quantum effects in
the structure of water
measured by γ -ray
diffraction

J.H. Root *et al.* *J.*
Chem. Phys. 109, 437
(1986)

Quantum (isotope) effects in water



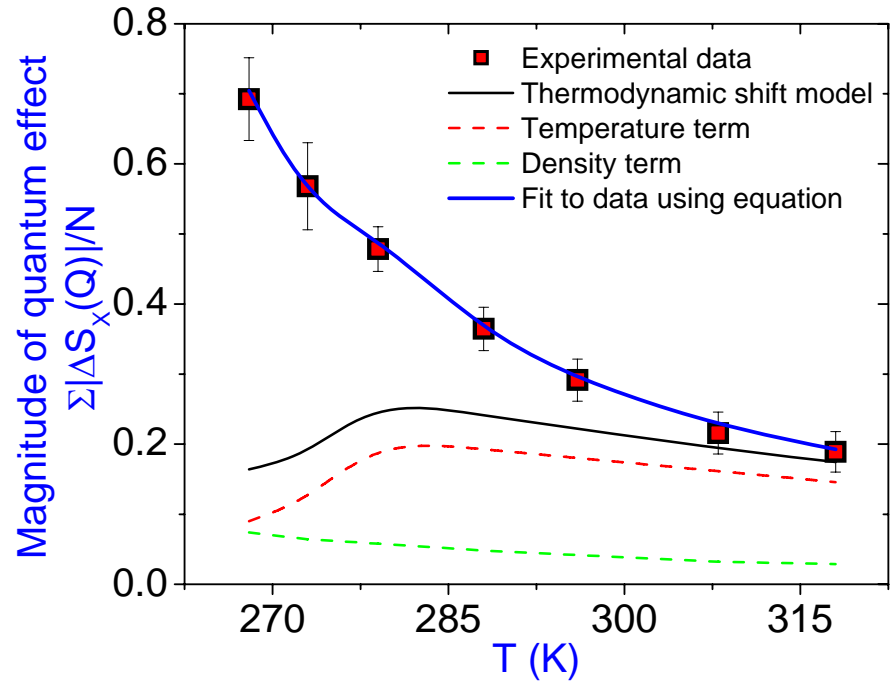
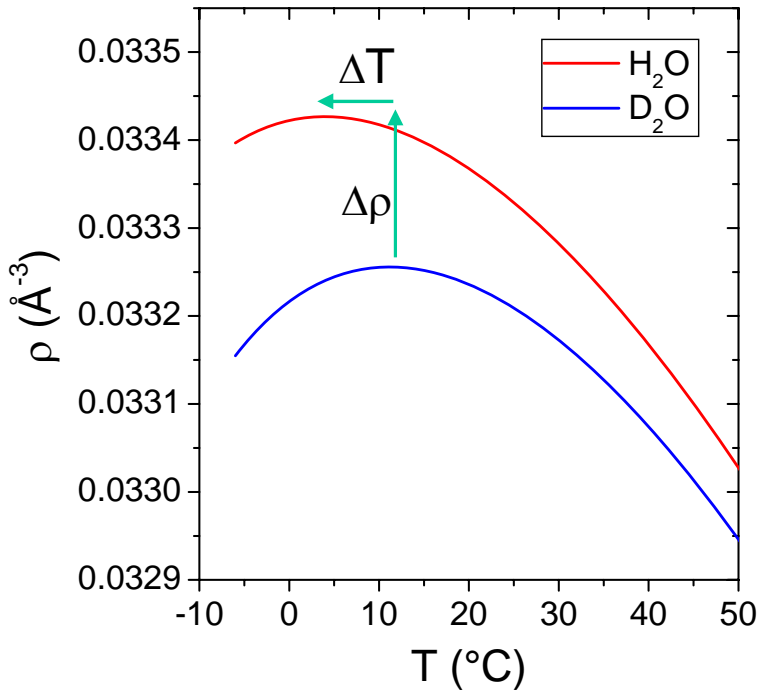
Temperature dependence of isotopic quantum effects in water.

R. T. Hart et al. Phys. Rev. Lett., 94 (2005) 047801.

Also appeared in Virtual J. Biological Phys. Res., 9 (4) 2005.



Same fluid in a different part of phase space ?



$$\sum_Q \Delta S(\rho, T) = \sum_Q \left(\frac{\partial S}{\partial T} \right)_{\rho} \Delta T + \sum_Q \left(\frac{\partial S}{\partial \rho} \right)_{T} \Delta \rho + A \exp(c/T)$$

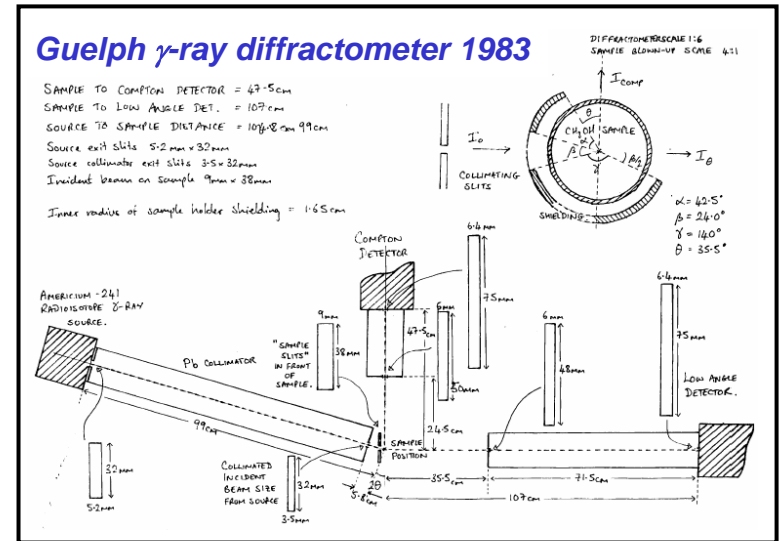
Density shift

Temperature shift

Additional term
required at low T

Summary

- The **Neutron/X-ray** combination is very powerful in the structure determination of disordered materials.
- **High energy x-rays** have been used to help develop the **Neutron Diffraction Isotopic Substitution** technique.



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