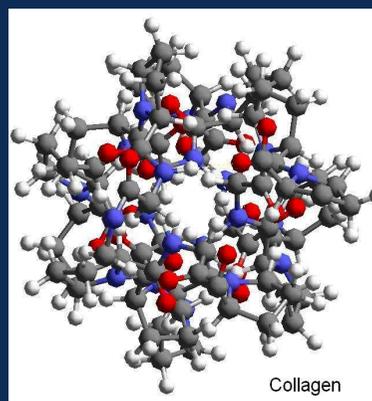


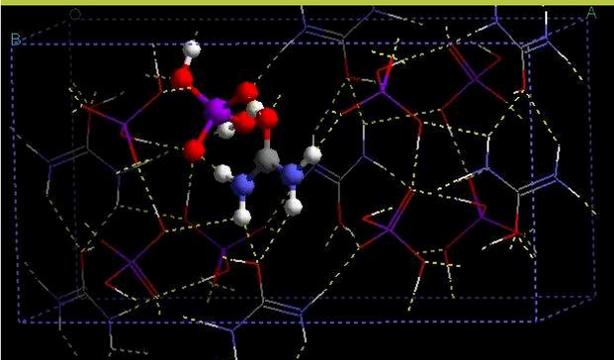
‘Structure and dynamics of oligopeptides and DNA’

by Fabien Fontaine-Vive

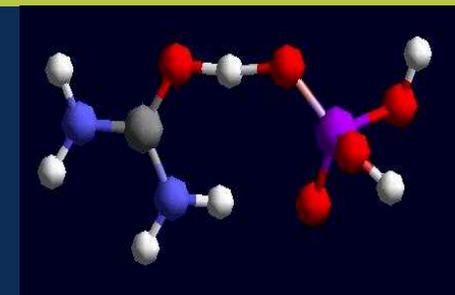
Thesis supervisors:

- * **Mark Johnson**, Computing for Science, Institut Laue-Langevin
- * **Gordon Kearley**, IRI, Delft University of Technology, The Netherlands





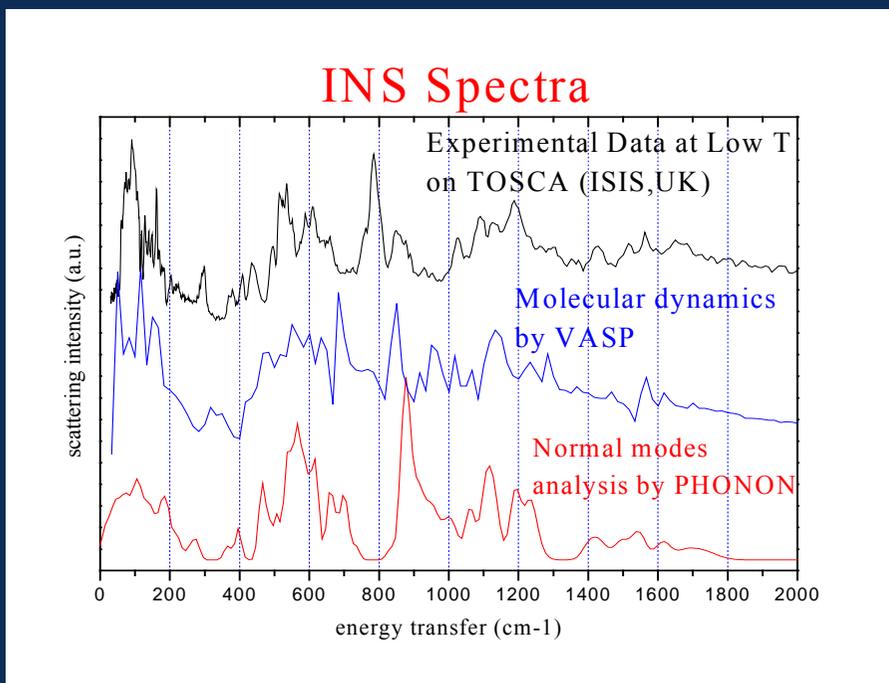
A model for strong hydrogen bond network :
Urea-Phosphoric Acid



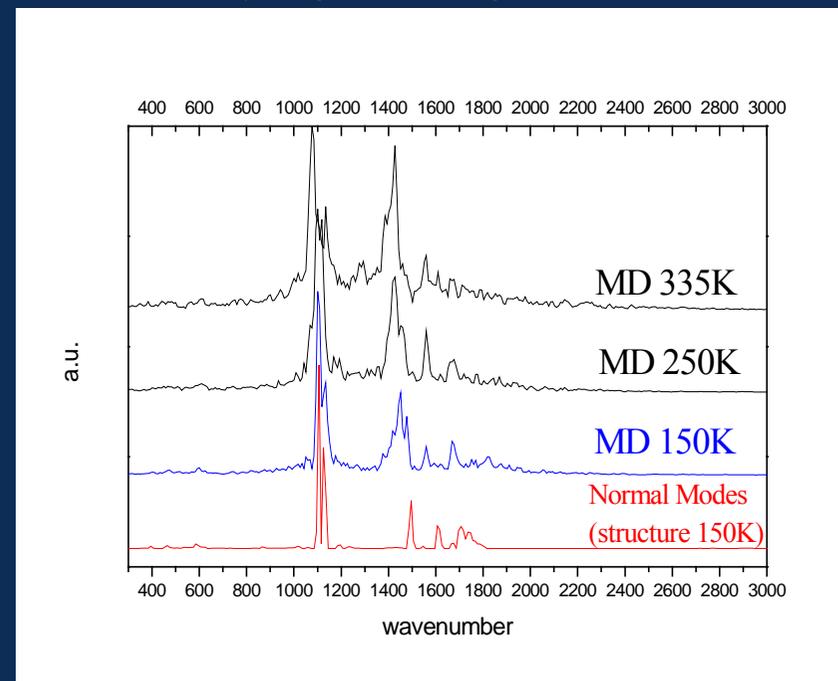
Vibrational properties of :

Urea-Phosphoric Acid

Hydrogen in strong H-bond



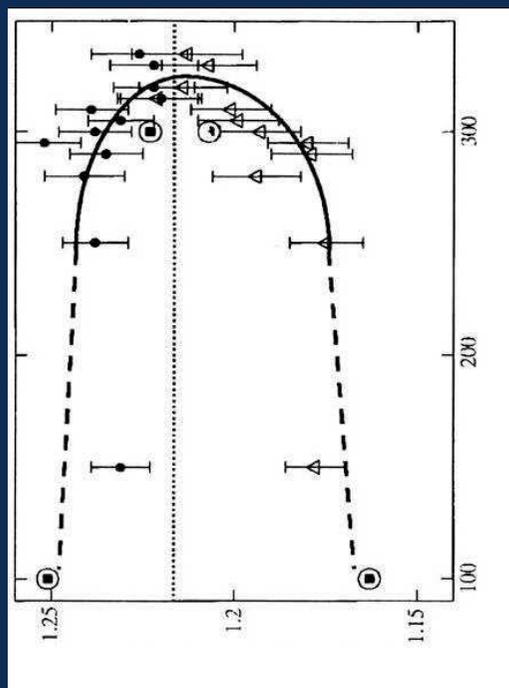
Inelastic Neutron Scattering



Vibrational density of states of H in strong hydrogen bond

Structural properties of U-PA:

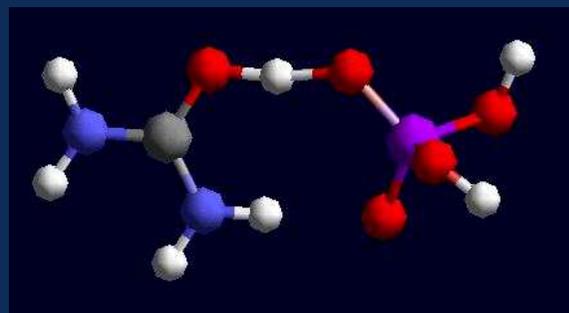
Neutron diffraction data:
(Wilson, Acta.Cryst.B, 2001)



H-bond distance

● : Filled circle: H...PA distance

△: Open triangle: Urea...H distance



T ↗

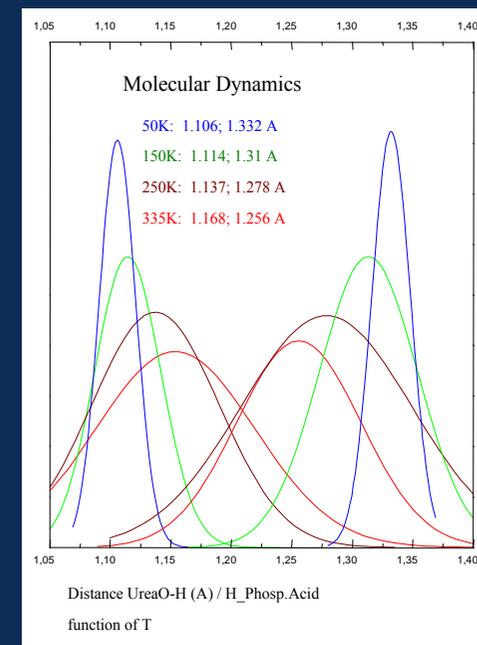
Hydrogen migration process:

Low temperature:
Urea-O-H...O-Phos.Acide

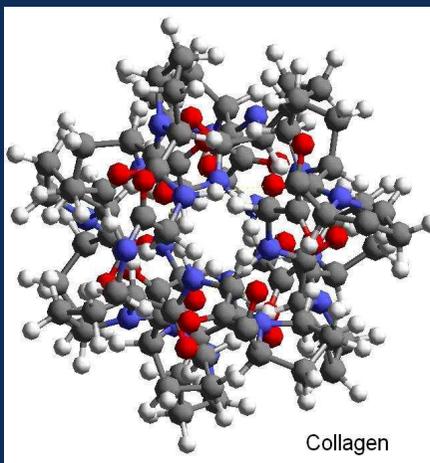
Room temperature :
Urea-O...H...O-Phos.Acide

*Activated by thermal motion
of molecules*

DFT Molecular dynamics



Histogram of distribution of :
H...PA distance // Urea...H distance



* Following work on Kevlar fibers... (polymer with amide linkages giving Beta-sheet structure)

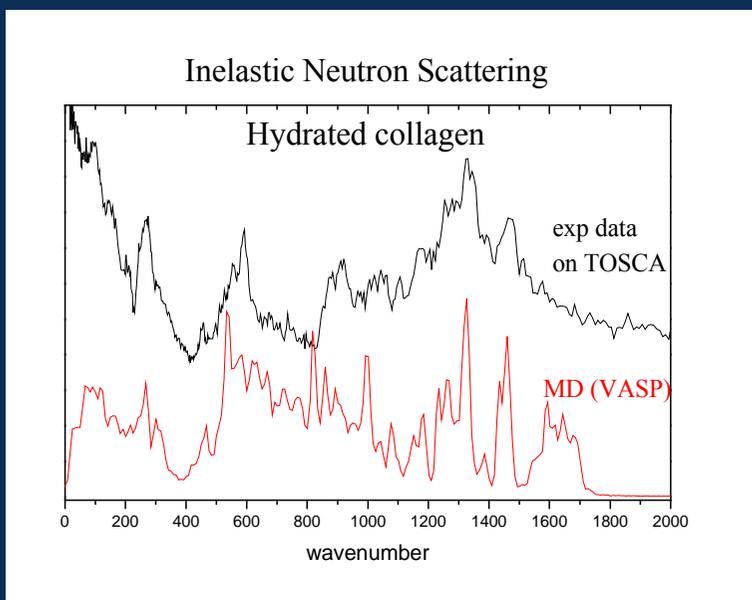
* Collagen is the fibrous protein constituent skin, cartilage, bone, and other connective tissue.

* It is constituted by three chains of amino acids of proline and glycine wound together in a tight triple helix.

* Identify characteristic low frequency collective dynamics of helices

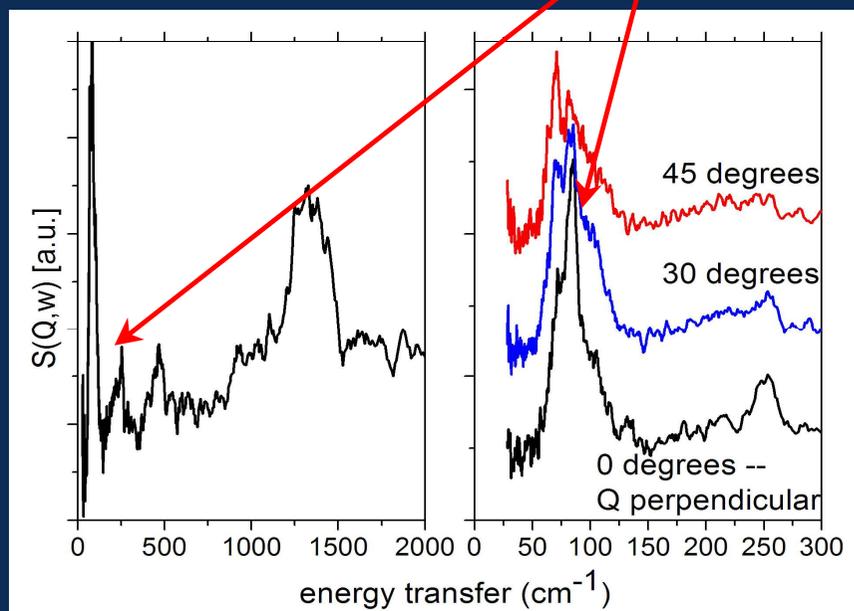
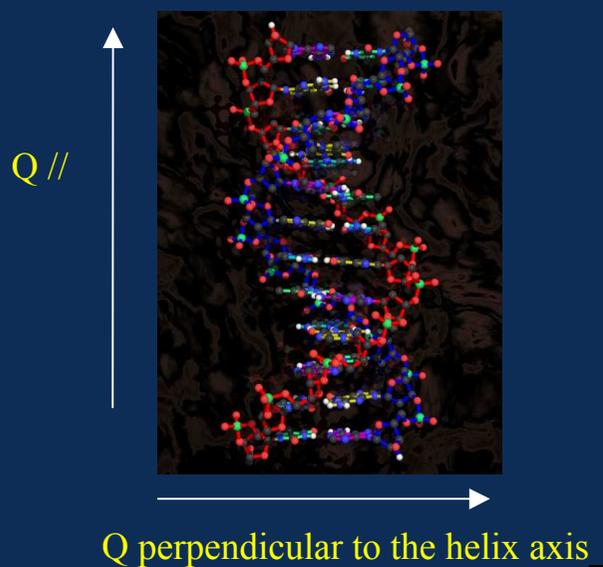
* Influence of water content on protein / water dynamics ?

* Influence of temperature ?



First results obtained on hydrated collagen (30% of relative humidity) at low temperature

Modes with perpendicular polarization at 85 cm⁻¹,
related to the base-pair opening in a replication process ?



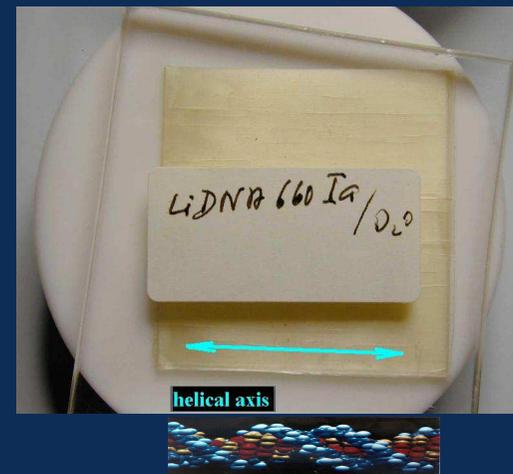
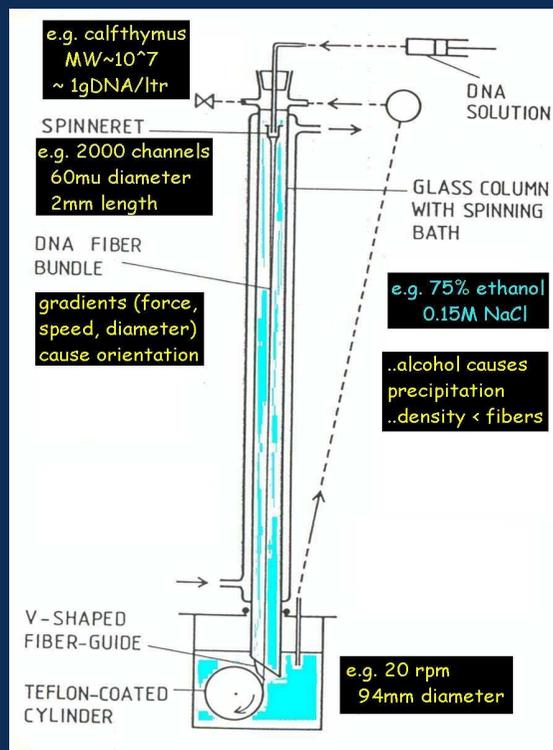
Measurement of the vibrational density-of-states at 10 K
on TOSCA at ISIS using an aligned, oriented sample of Li
B-DNA. Future measurements on IN4 in 2005.

Extend these measurements to higher temperatures and other structural forms of DNA to gain more
detailed insight into the dynamics of this molecule

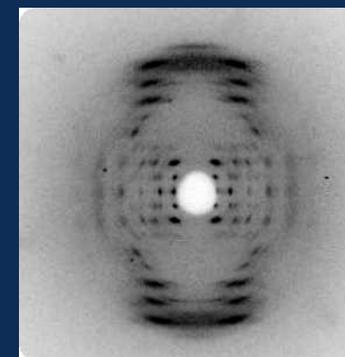
Making oriented fibres of A,B,C-DNA: the wet spinning apparatus



The wet spinning apparatus designed by Allan Rupprecht



Film of oriented fibres of Li-B-DNA



X-ray pattern