D3 at the ILL:

Structural studies of hydrogenous liquid and amorphous systems using polarised neutrons

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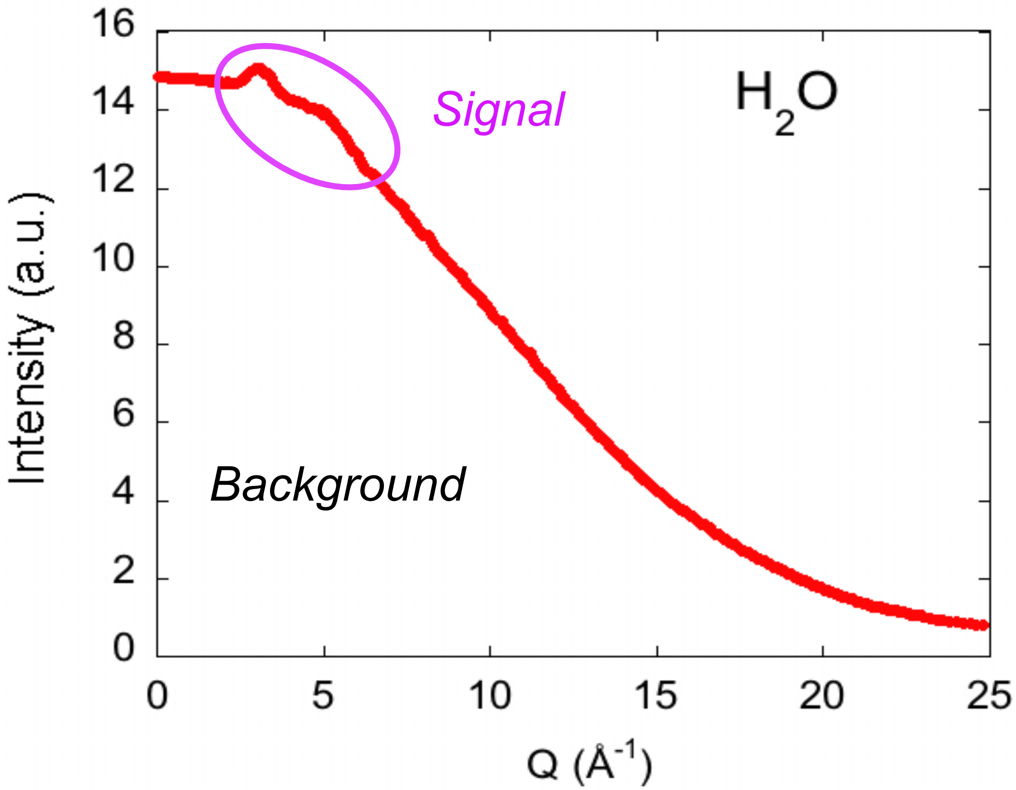
What for: Hydrogen

Isotope	coherent σ (barn)	spin-incoh. σ (barn)	coherent b (10^{-12} cm)
^{1}H	1.7583	80.27	-0.3739
^{2}H (D)	5.592	2.05	0.6671



Incoherent background from Hydrogen

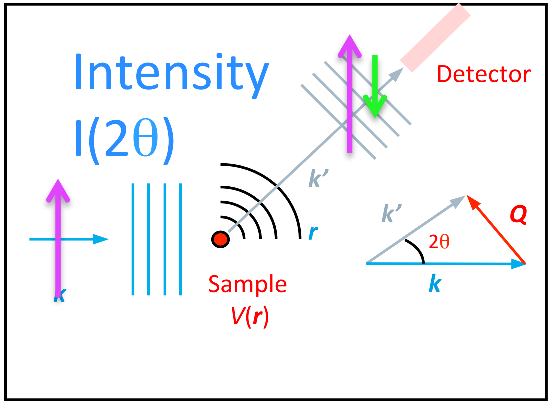
Why bother?

Neutrons DO see the hydrogen (very well!)

Hydrogen bond
Isotopic substitution (partial distributions)
No deuteration
- difficult to impossible
- industrial applications
- geological studies

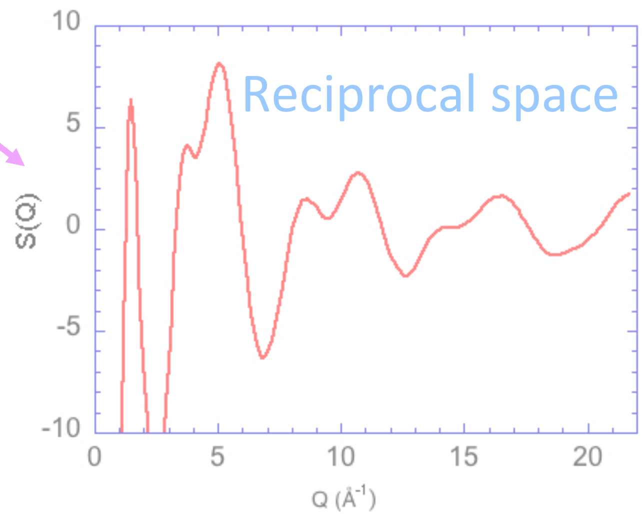
Scope

What for ?
Why polarised neutrons?
How?
Some results
What next?



$$Q = \frac{4\pi}{\lambda}\sin\theta$$

+ corrections



FT

Why: nuclear spin

Nuclear spin: I (^{1}H: $I = ½$)

Nucleus + neutron spin:

$I + ½$: $2(I + ½)+1 = 2I+2$ states , scattering length b^+

$I - ½$: $2(I - ½)+1 = 2I$ states , scattering length b^-

Unpolarised beam scattering probabilities
(randomly oriented nuclear spins)

$$f_+ = \frac{I+1}{2I+1} \qquad f_- = \frac{I}{2I+1}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{nuclear-spin-incoherent} = \frac{\left(b^+ - b^-\right)^2 I\left(I+1\right)}{\left(2I+1\right)^2}$$

^{1}H: $b^+ = 1.04 \times 10^{-12}$ cm, $b^- = 4.744 \times 10^{-12}$ cm

Polarised neutron scattering from randomly oriented nuclear spins

Intensity	Incoming Neutron spin	Scattered Neutron spin	
I^{++}	↑	↑	Non-Spin-Flip, NSF
I^{--}	↓	↓	
I^{+-}	↑	↓	Spin-Flip, SF
I^{-+}	↓	↑	

Coherent cross section:

$$\left(\frac{d\sigma}{d\Omega}\right)^{++}_{coh} = \left(\frac{d\sigma}{d\Omega}\right)^{--}_{coh} = \frac{\sigma_{coh}}{4\pi} \qquad \left(\frac{d\sigma}{d\Omega}\right)^{+-} = \left(\frac{d\sigma}{d\Omega}\right)^{-+} = 0$$

NSF

Spin-incoherent cross section:

$$\left(\frac{d\sigma}{d\Omega}\right)^{++}_{inc} = \left(\frac{d\sigma}{d\Omega}\right)^{--}_{inc} = \frac{1}{3}\frac{\sigma_{inc}}{4\pi} \qquad \left(\frac{d\sigma}{d\Omega}\right)^{+-}_{inc} = \left(\frac{d\sigma}{d\Omega}\right)^{-+}_{inc} = \frac{2}{3}\frac{\sigma_{inc}}{4\pi}$$

1/3 NSF

2/3 SF

W.G. Williams, Polarized Neutrons, Clarendon, 1988

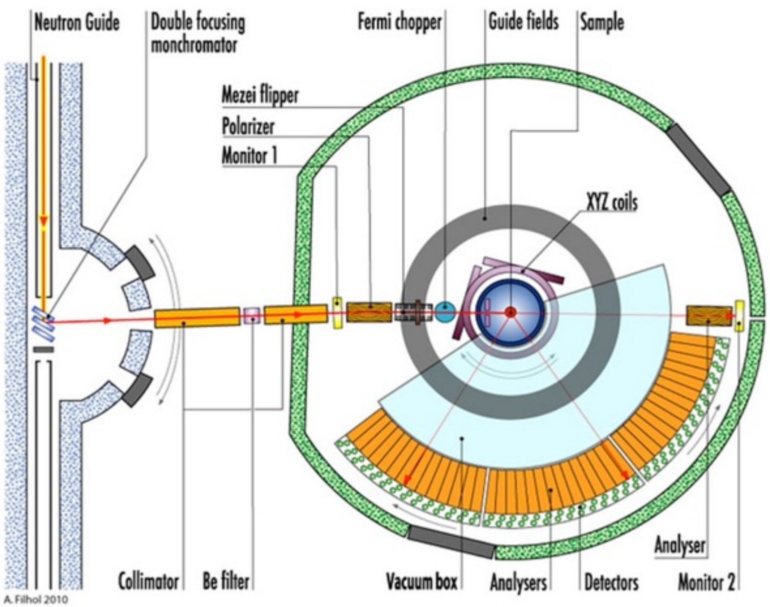
Polarised neutron scattering from randomly oriented nuclear spins

$$I_{spin-incoherent}(Q): 1/3\ non-spin-flip$$
$$2/3\ spin-flip$$
$$I_{coherent}(Q) \quad \text{or} \quad I_{isotope-incoherent}(Q): non-spin-flip$$

$$I_{coh}(Q) + I_{isotope-incoh}(Q) = I^{NSF}(Q) - \frac{1}{2} I^{SF}(Q)$$
$$I_{spin-incoh}(Q) = \frac{3}{2} I^{SF}(Q)$$

Directly remove spin-incoherent background

Why now?



The technique is far from new

D7 at ILL

Cold neutrons

λ_{min} = 3.12 Å, Q_{max} = 3.91 $Å^{-1}$

Wider Q-range: hot neutrons

D3 at ILL: λ_{min} = 0.4 Å, Q_{max}= 25 $Å^{-1}$

Polarisation?

~~Supermirror~~ Critical angle

~~Crystal (Heusler)~~ Size/distance

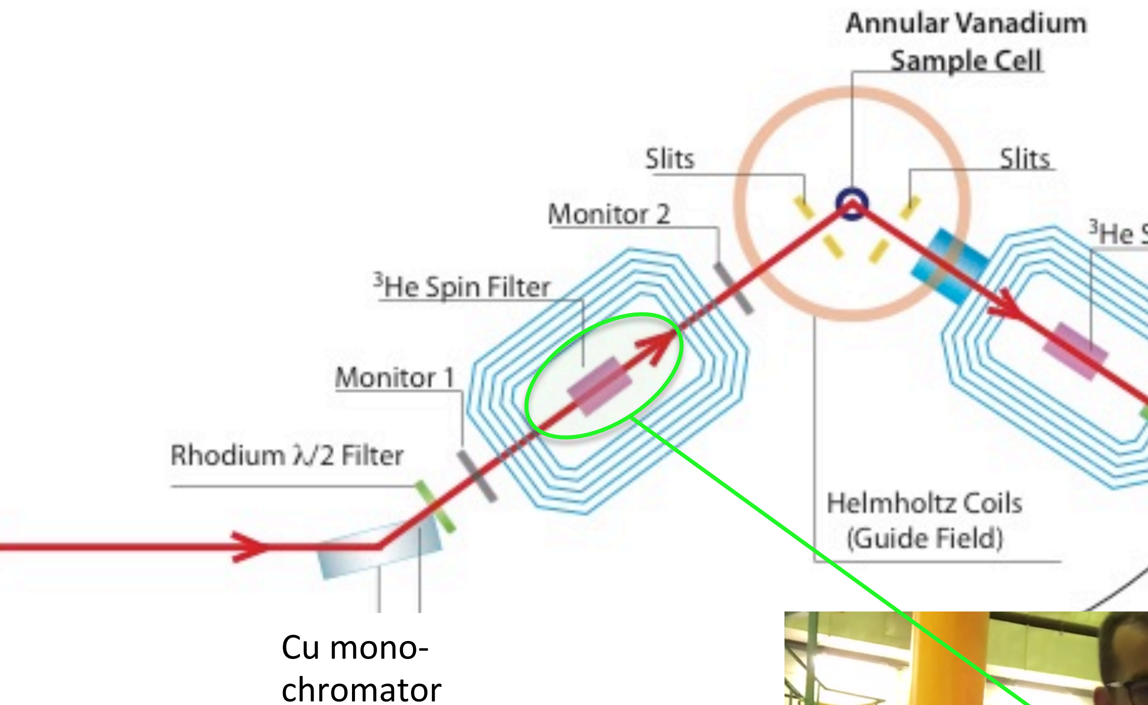
^{3}He spin filter

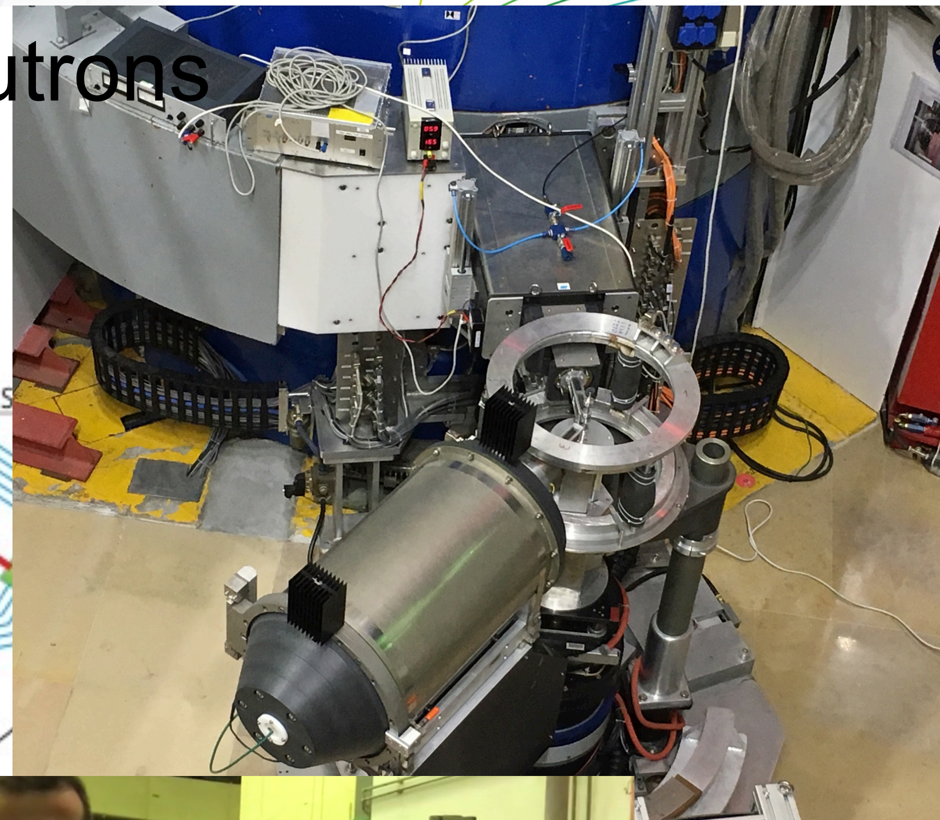
$$T^{\pm} = e^{-O(\lambda)(1 \pm P_{He})}$$

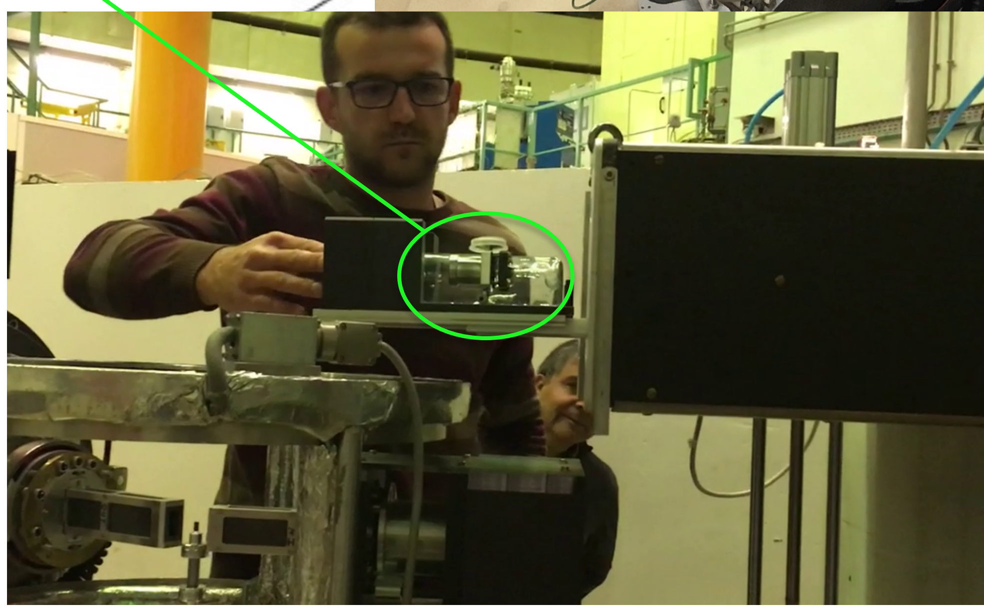
$$P_{He} = P^0_{He} e^{-t/T_1}$$

$$O(\lambda) = 0.0732\ p[\text{bar}]\ L[\text{cm}]\ \lambda[\text{Å}]$$

D3 at ILL: polarised hot neutrons







^{3}He spin filter

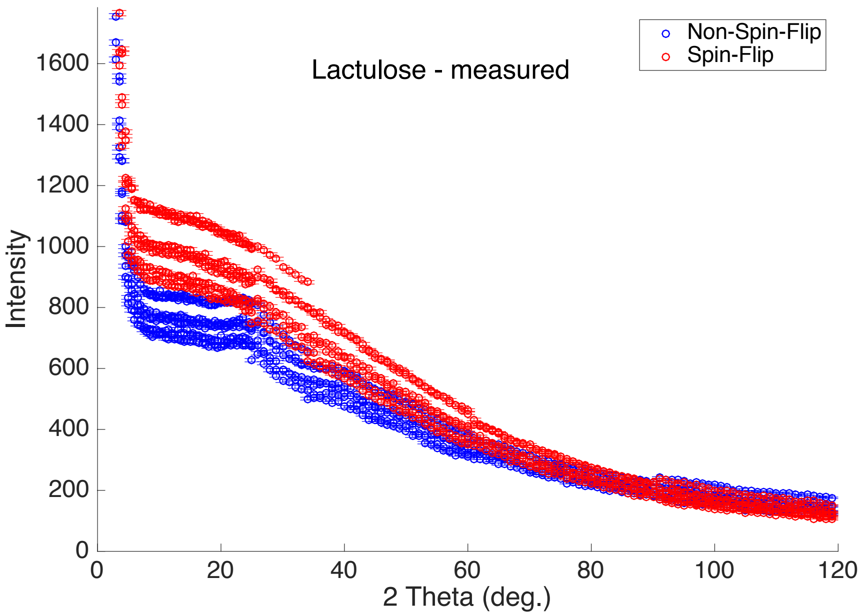
Sample container

Si crystal:
calibration of the polarisation

Double walled Vanadium sample cell

Sample volume
In beam: 0.4 cm^3

Measurement



Lactulose:

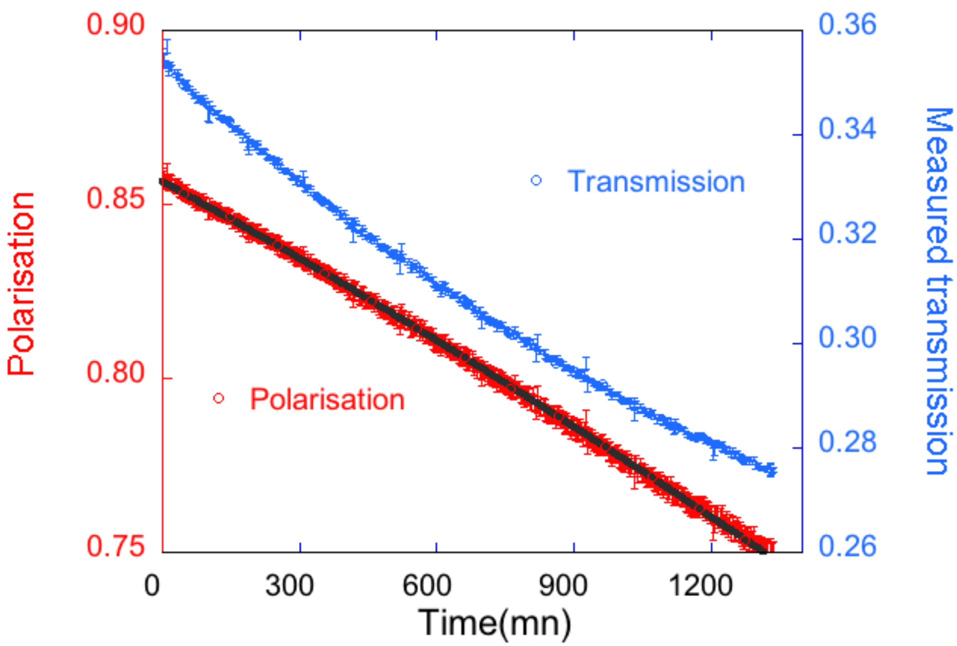
(F. Ngono, ILL thesis, F. Affouard, Univ. Lille, G. Cuello, M. Jimenez Ruiz, ILL)

Possible excipient
Pharmaceutical industry

Scan, scan, scan….

Data reduction: spin filters

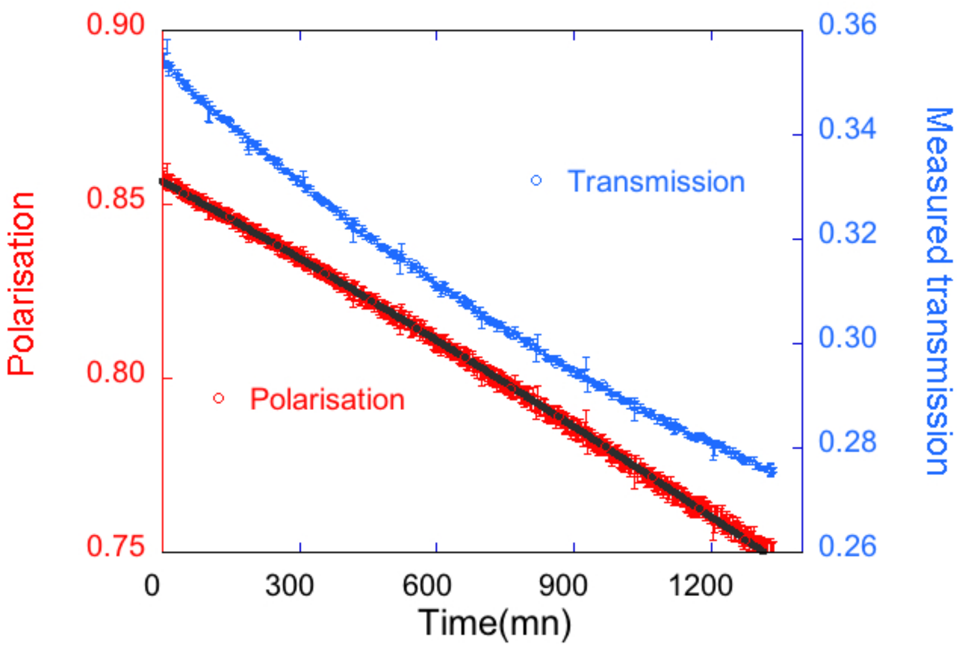
Filter 1: Transmission (monitors)



$$P_0 = \sqrt{1 - \left(\frac{e^{-O(\lambda)}}{Trans}\right)^2}$$

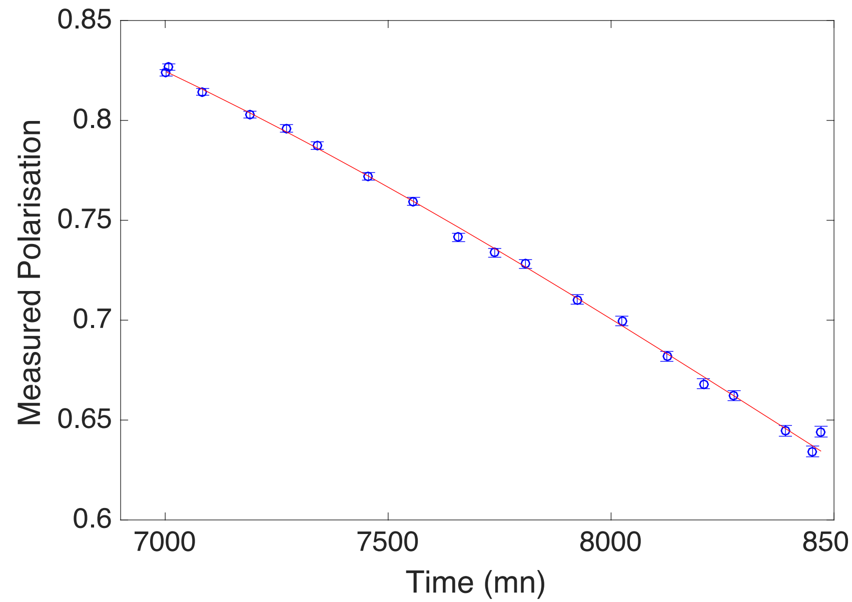
Data reduction: spin filters

Filter 1: Transmission (monitors)



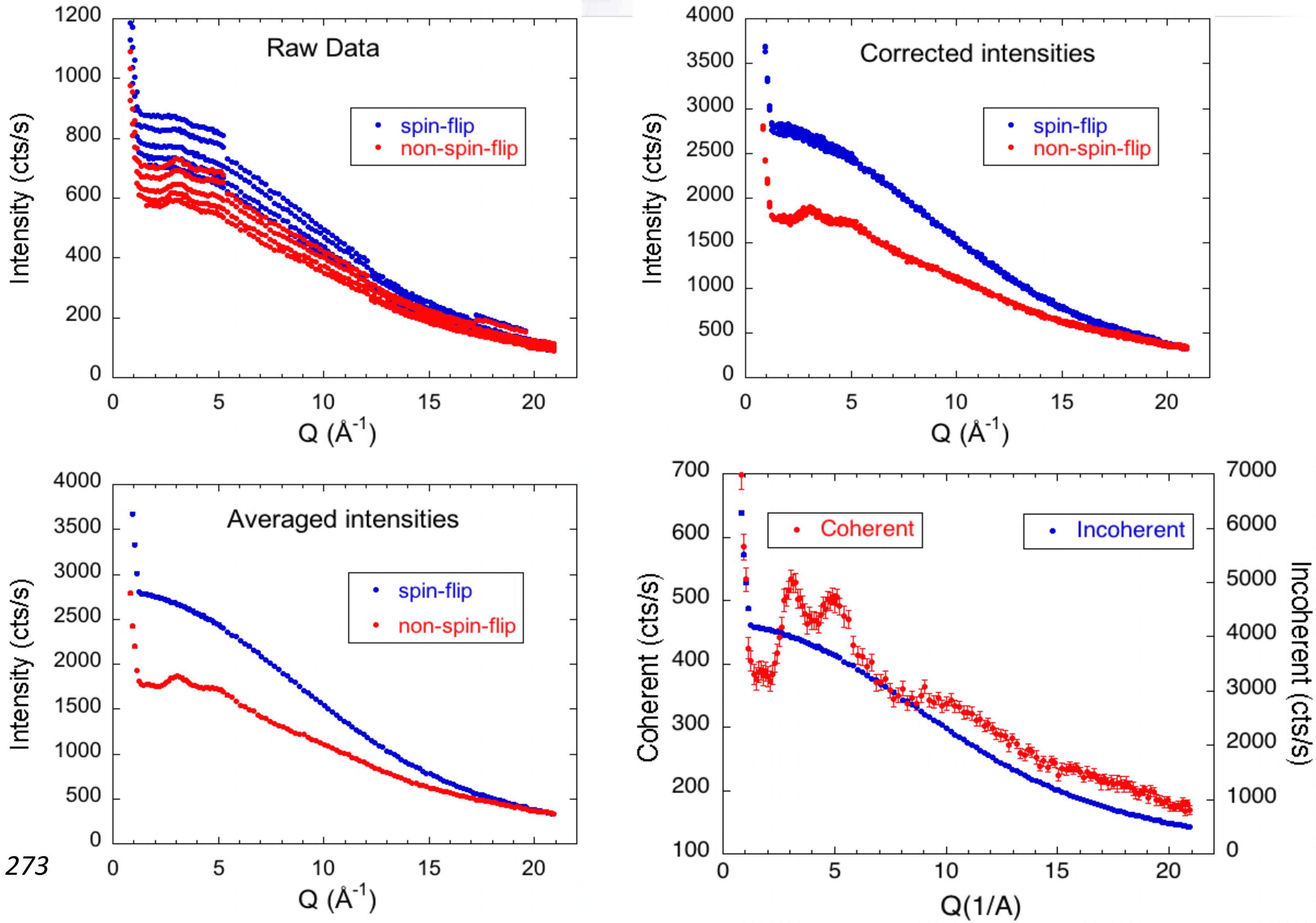
$$P_0 = \sqrt{1 - \left(\frac{e^{-O(\lambda)}}{Trans}\right)^2}$$

Filter 2: Polarisation (crystal)



$$P_n = \frac{I^+ - I^-}{I^+ + I^-} = \tanh\left[O(\lambda)\ P_{He}^0\ e^{-\frac{t}{T_1}}\right]$$

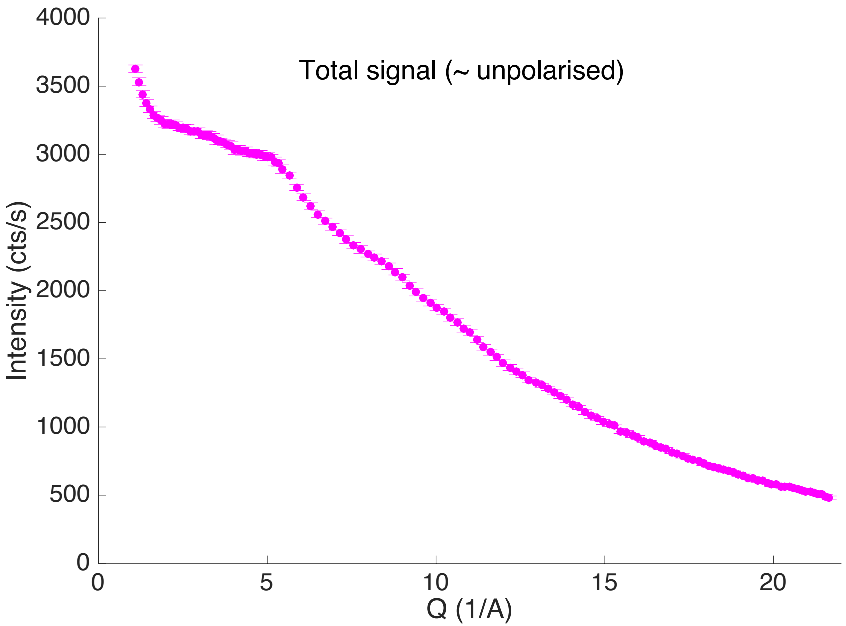
Water, analysis

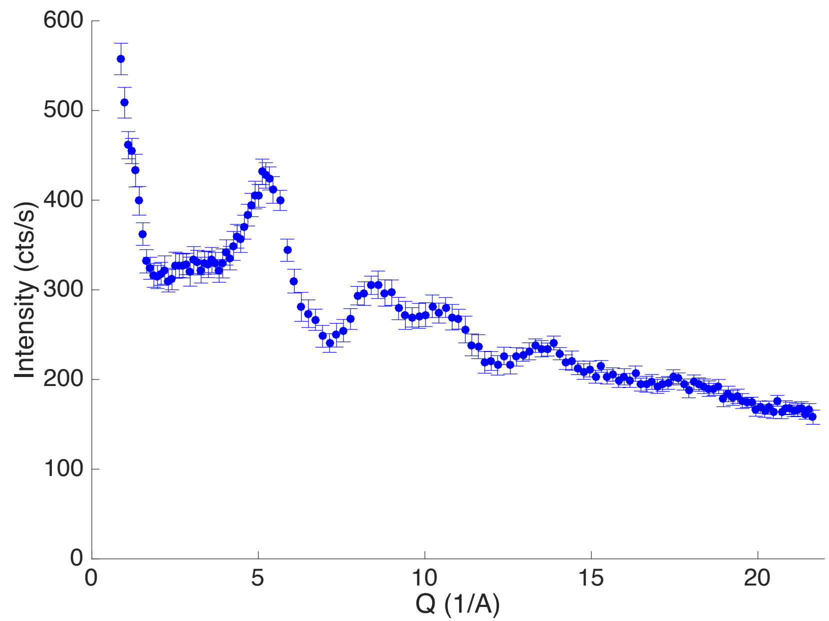


*Physica B **551**, 273*

A. Stunault, ADD20

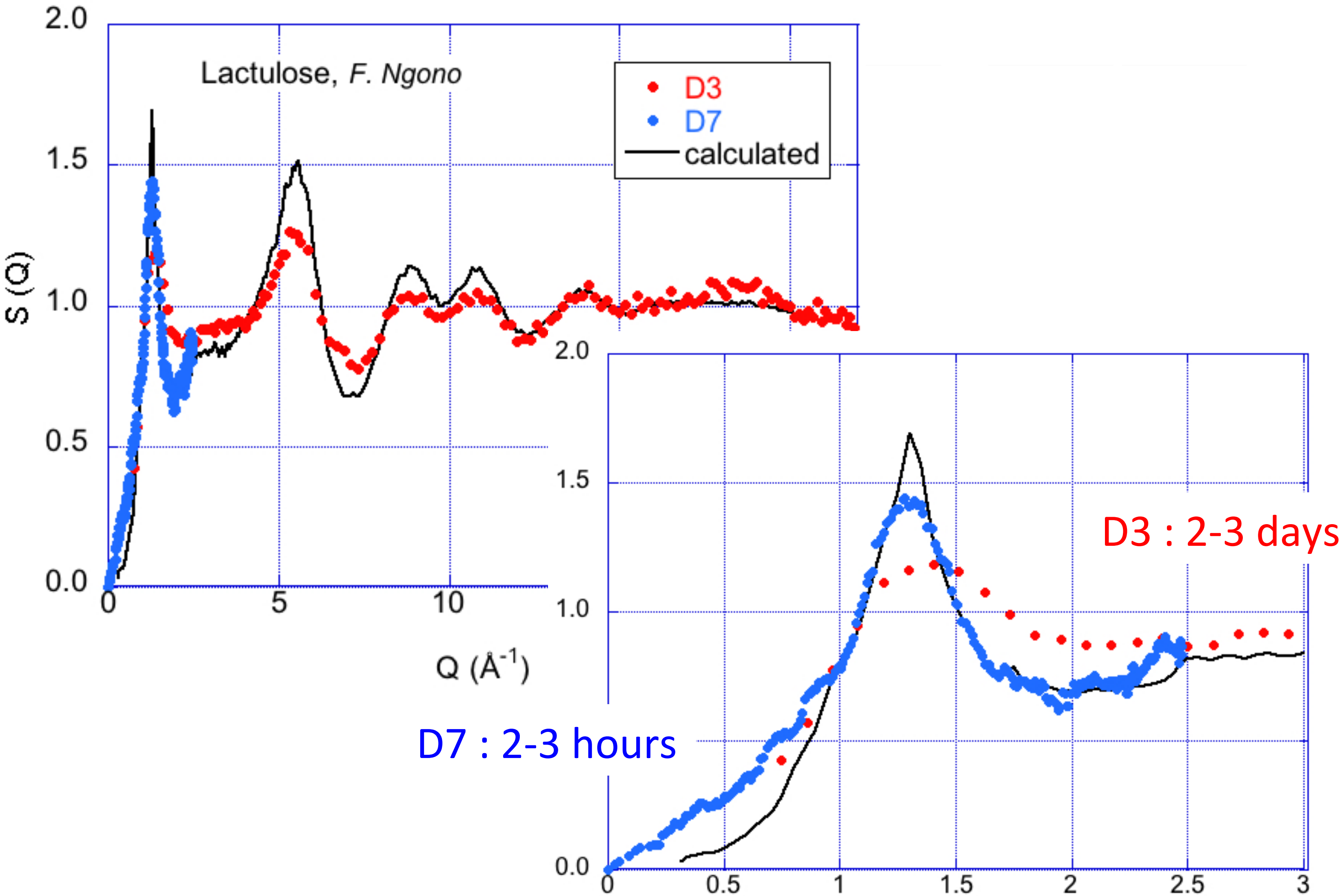
Lactulose: polarised *vs* unpolarised





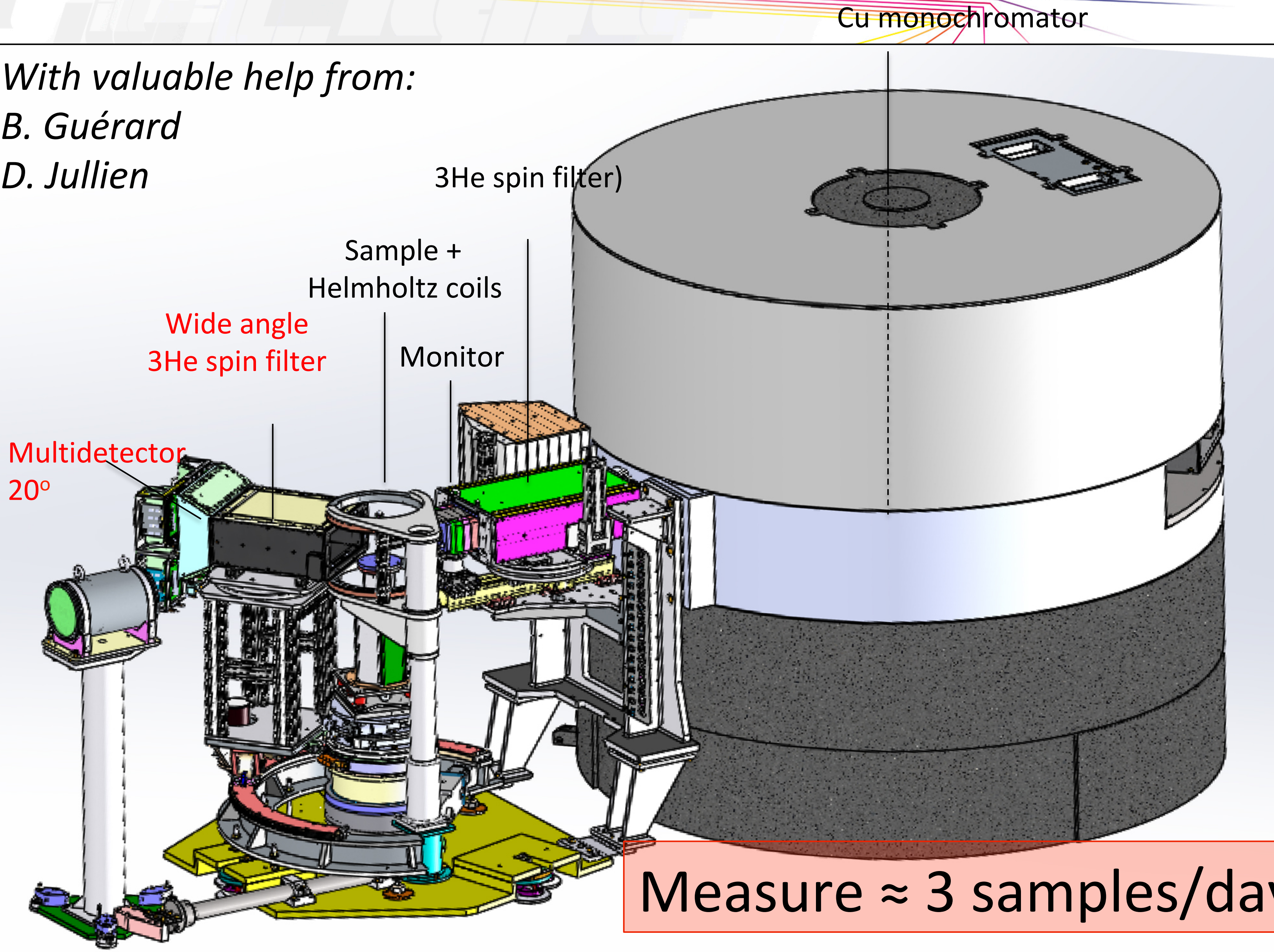
F. Ngono, thesis

Complementarity with D7 (cold neutrons)



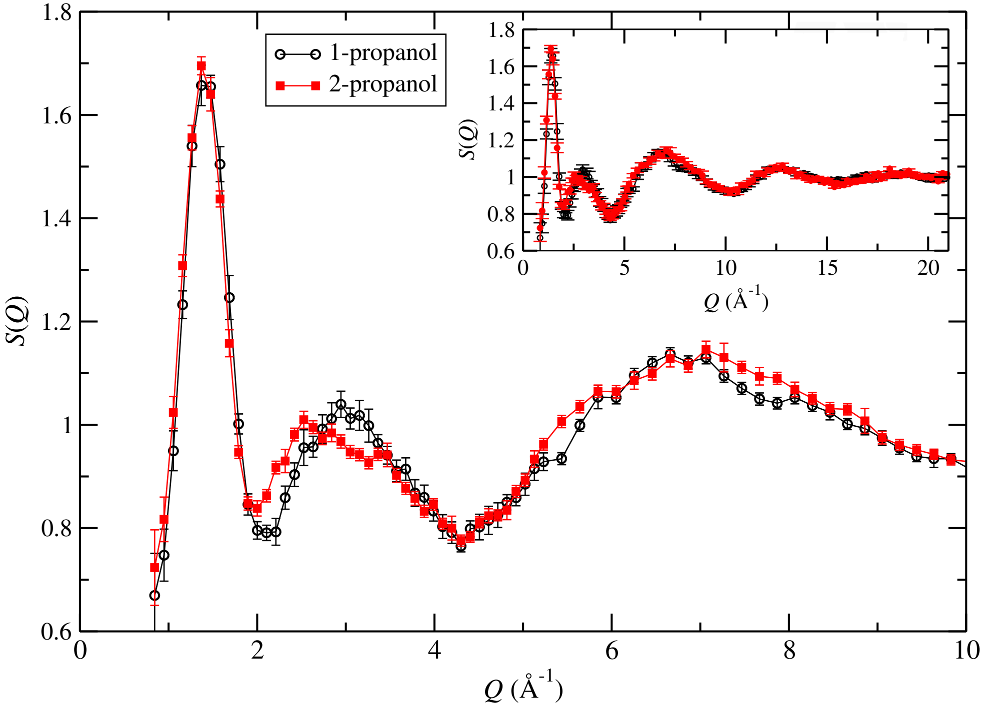
ILL Endurance project → September 2019

With valuable help from:
B. Guérard
D. Jullien



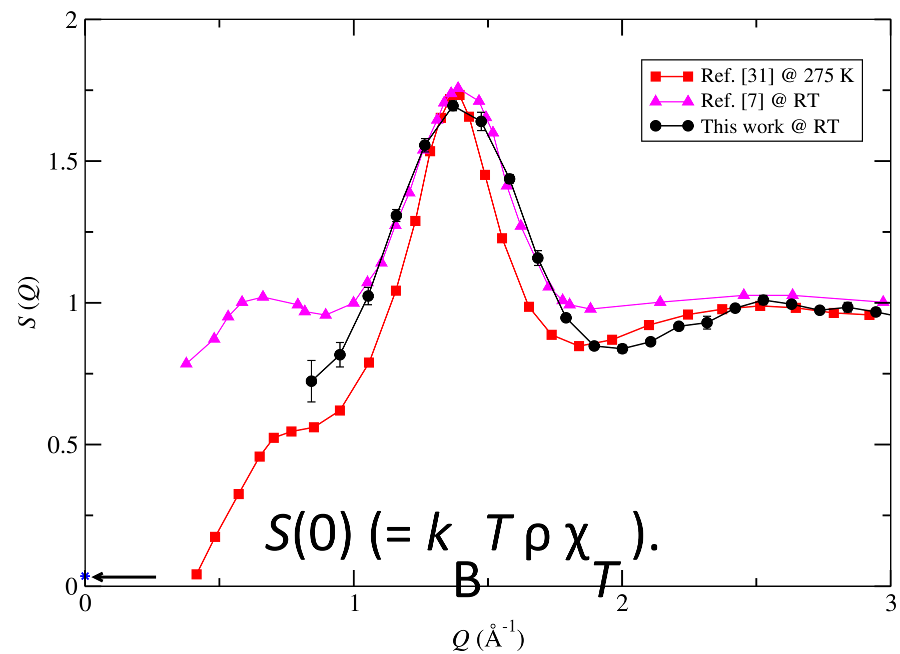
Measure ≈ 3 samples/day

Propanol

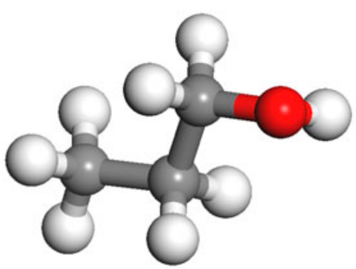


Propanol,
(Rodriguez-Palomino, Dawidowsky, Cuello, Phil. Mag. 2015)

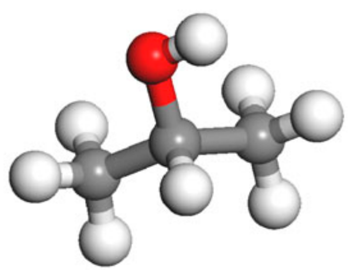
(Monte Carlo,
based on Granada's "synthetic model", PRB 1985)



$S(0)$ $(= k_B T \rho \chi_T)$.



1-propanol



2-propanol

What next

Upgraded instrument: September 2019

Extraction of “clean” S(Q)

from measured I(2θ) and calibration/background measurements

(*cf. G. Cuello’s talk at the school)*

Multiple scattering…

Conclusion

D3: a unique instrument for the study of liquid/amorphous systems with high ^1H contents

Complementary to unpolarised instruments (D4)

Complementary to cold neutron polarised instruments (D7, DNS)

We will soon do even better with a multidetector

Extraction of “clean” S(Q) in progress