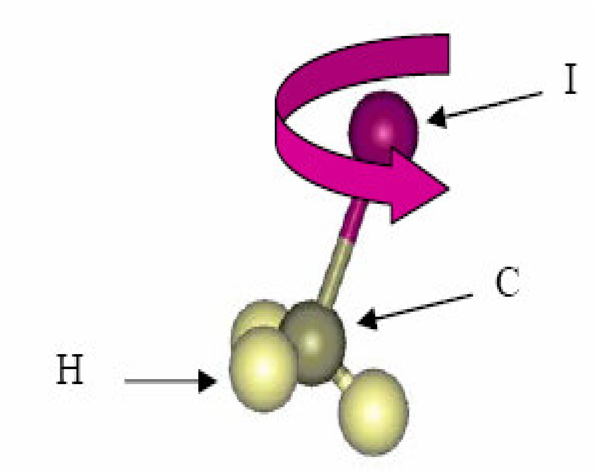
Methyl iodide quantum rotations studied by HFBS and FANS



Group C

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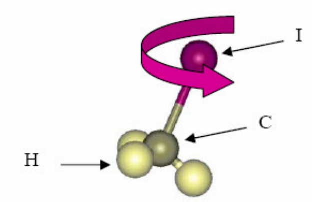
Summer school, June 29th, 2007

Introduction

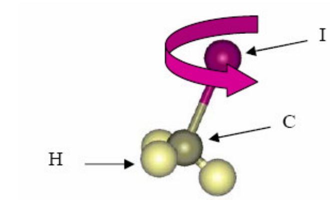


➢ Methyl iodide is a 1D quantum rigid rotor

➢ HRNS can observe tunneling of hydrogen

➢ Data can be easily interpreted – single particle interaction

Goals



- Validate the low temperature dynamics model for the potential energy

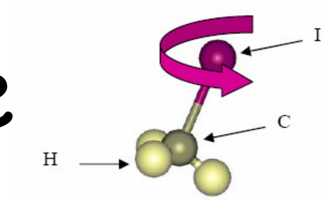
$$H = -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\phi^2} + \frac{V_3}{2}(1-\cos 3\phi)$$ [1]

V_3 is the barrier height

- Transition from quantum to classical behavior with increasing temperature

1 R. M. Dimeo* and D. A. Neumann PHYSICAL REVIEW B, VOLUME 63, 014301

Dynamics of Methyl Iodide

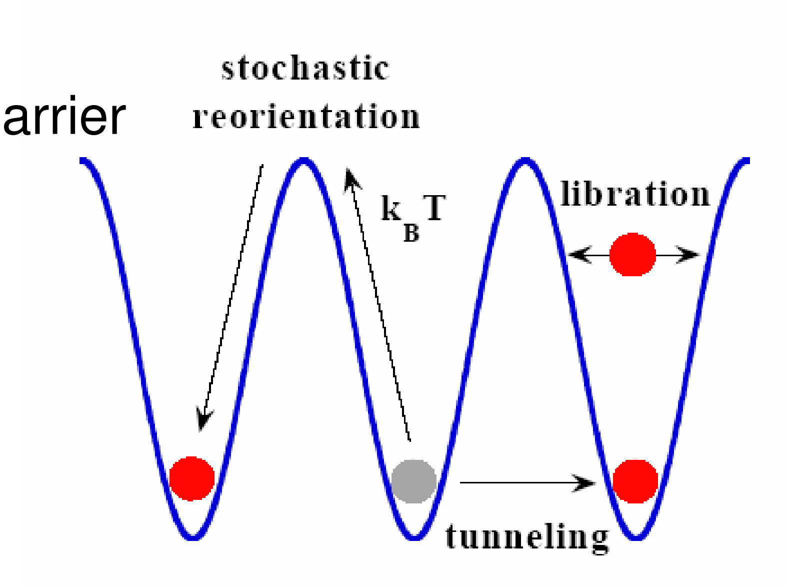


Three independent motions

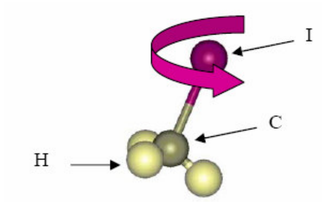
1. Hydrogen tunneling through the potential barrier

2. Librations of the methyl group

3. Stochastic reorientation or jump diffusion



Experiments



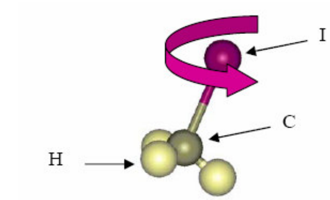
➢ Low energy motion – tunneling – HFBS

- incident neutron energy varied by Doppler shifting of neutrons about a λ = 6.271 Å
- only neutrons with a fixed final energy received in the detectors
- energy resolution of 0.8 μeV
- energy range $\pm$ 11 μeV
- temperature range 5.2 K to 55.2 K

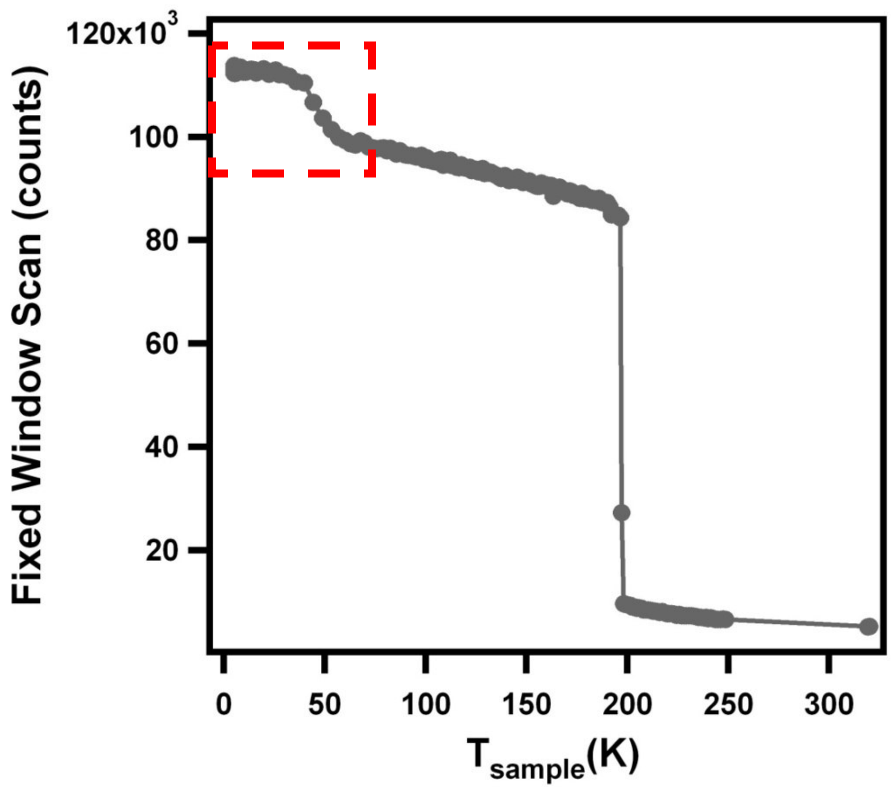
➢ Intermediate energy – librations – FANS

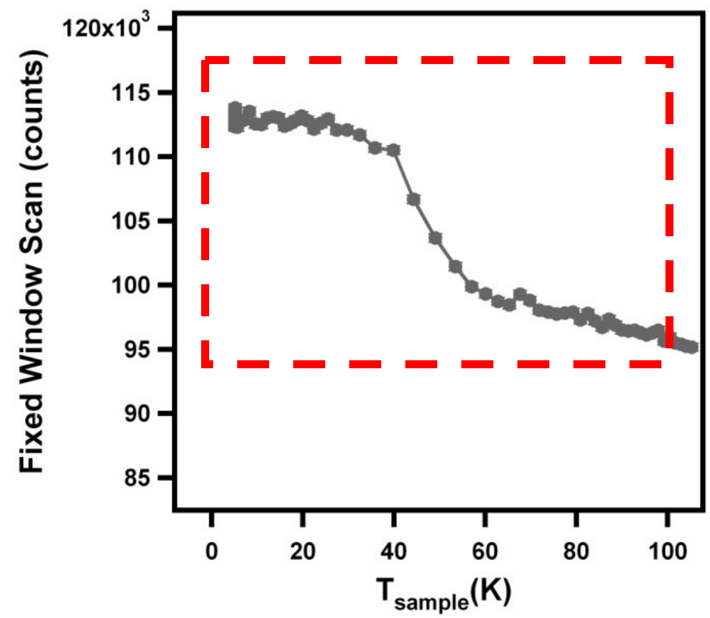
- incident neutrons monochromated via a PG
- only neutrons with final energies < 1.8 meV are counted
- energy resolution 1 meV
- temperature 5 K only

Broad Range Scan

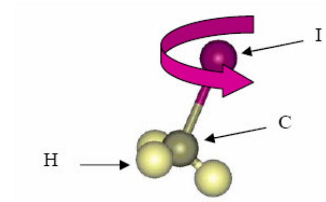


- Fixed Window Scan

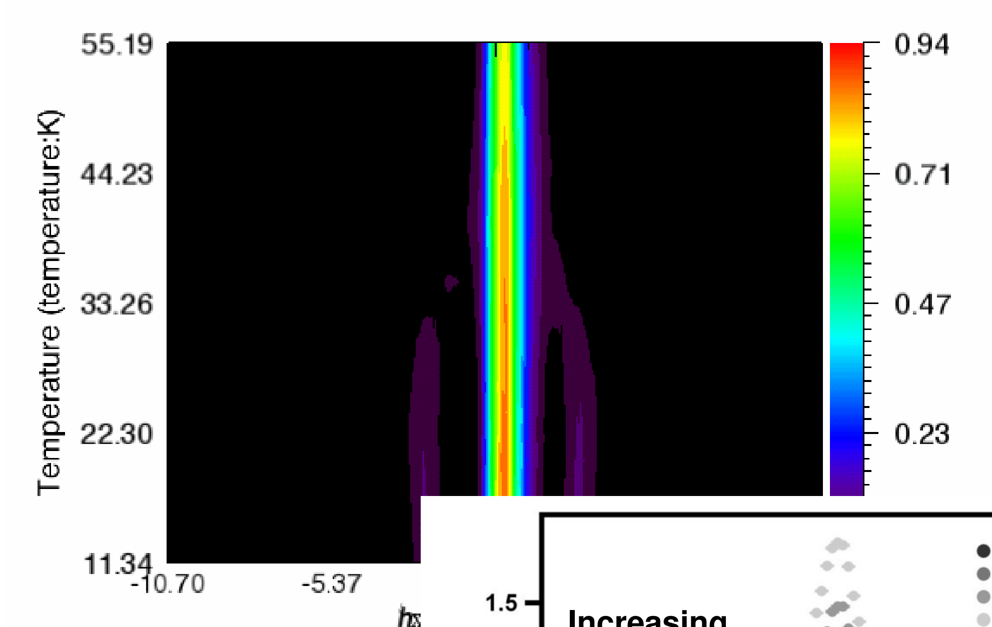


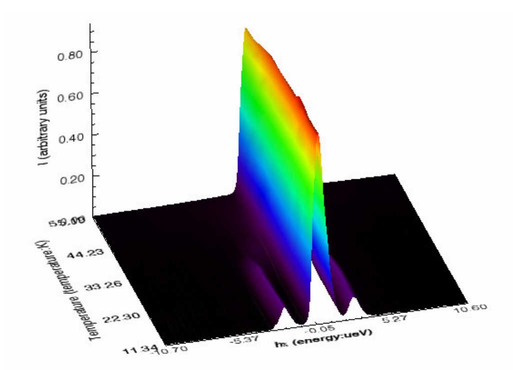


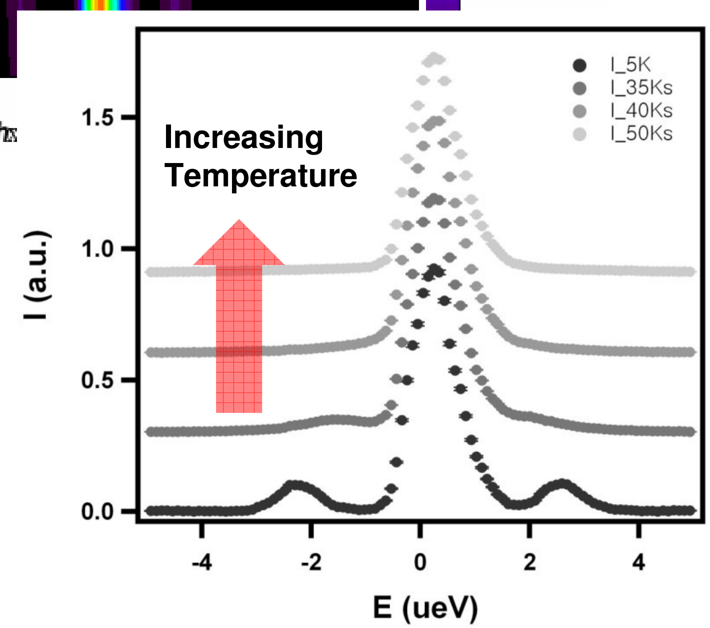
Temperature Dependence



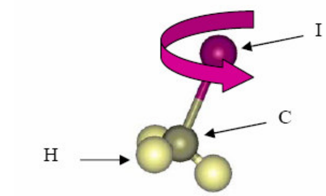
- Transition from inelastic scattering to quasielastic scattering as resulted from increasing temperature
- Transition from Gaussian to Lorentzian

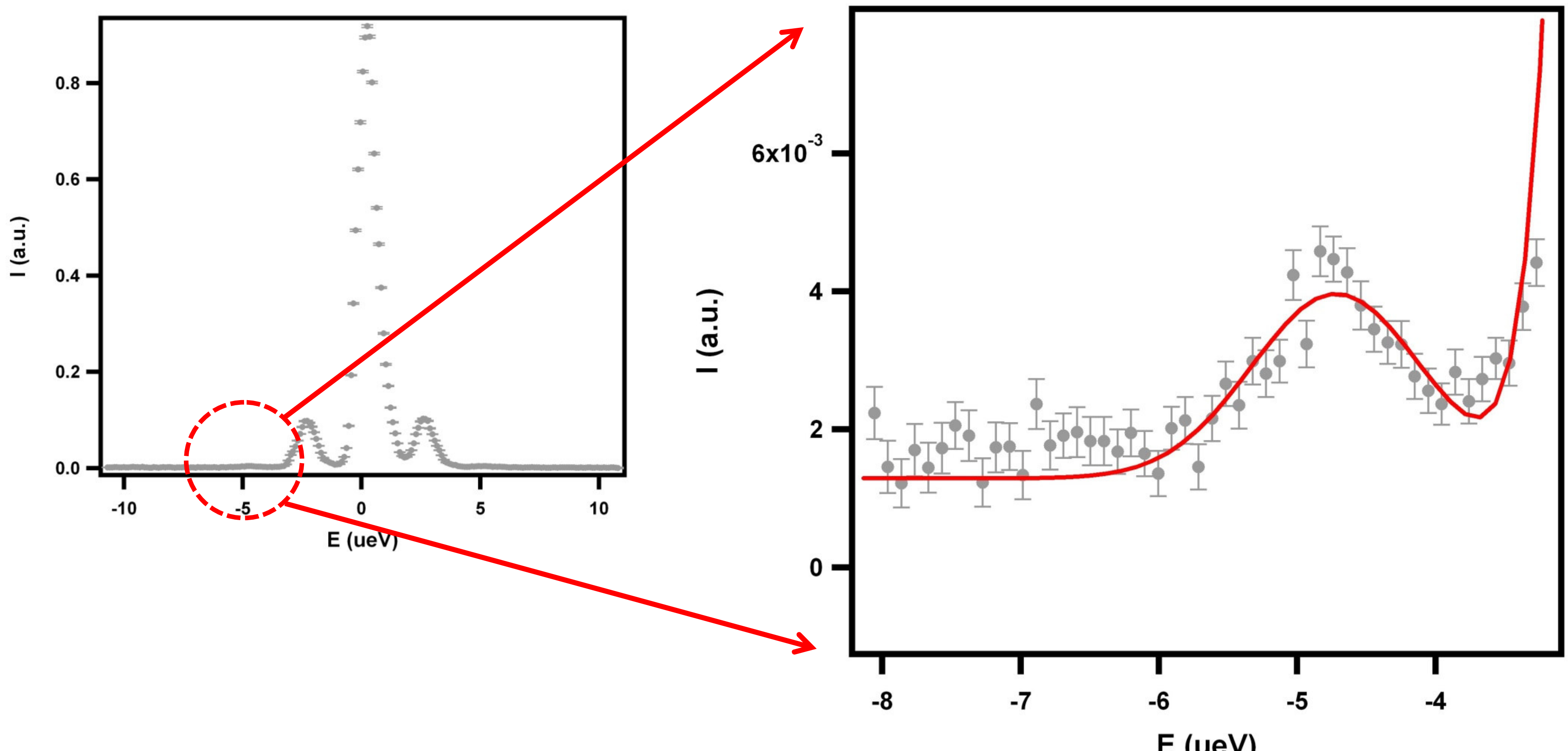






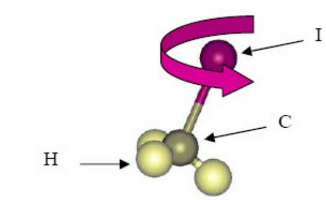
Multiple Scattering



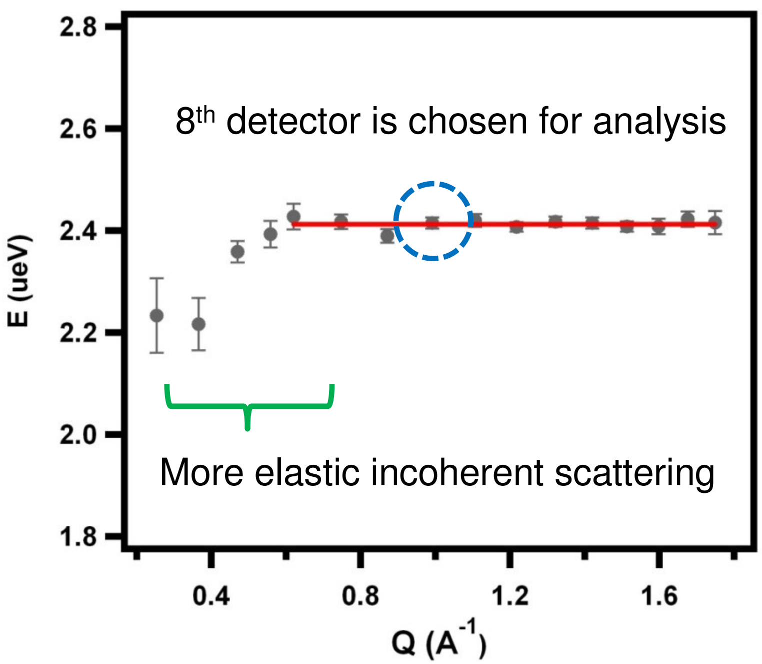


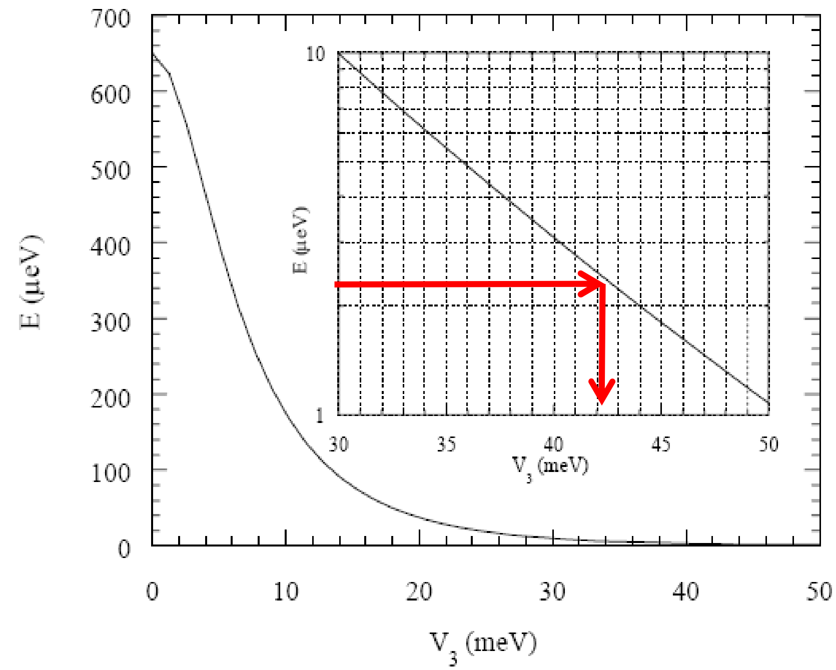
With good statistics (summed data from 5K to 26K including 16 detectors), satellite peaks are observed at 4.8 ueV indicating multiple scattering from the sample. (note that Et = 2.4 ueV)

Tunneling Energy to V_3



Q independent of tunneling energy

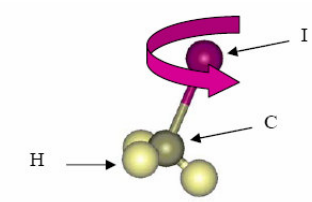


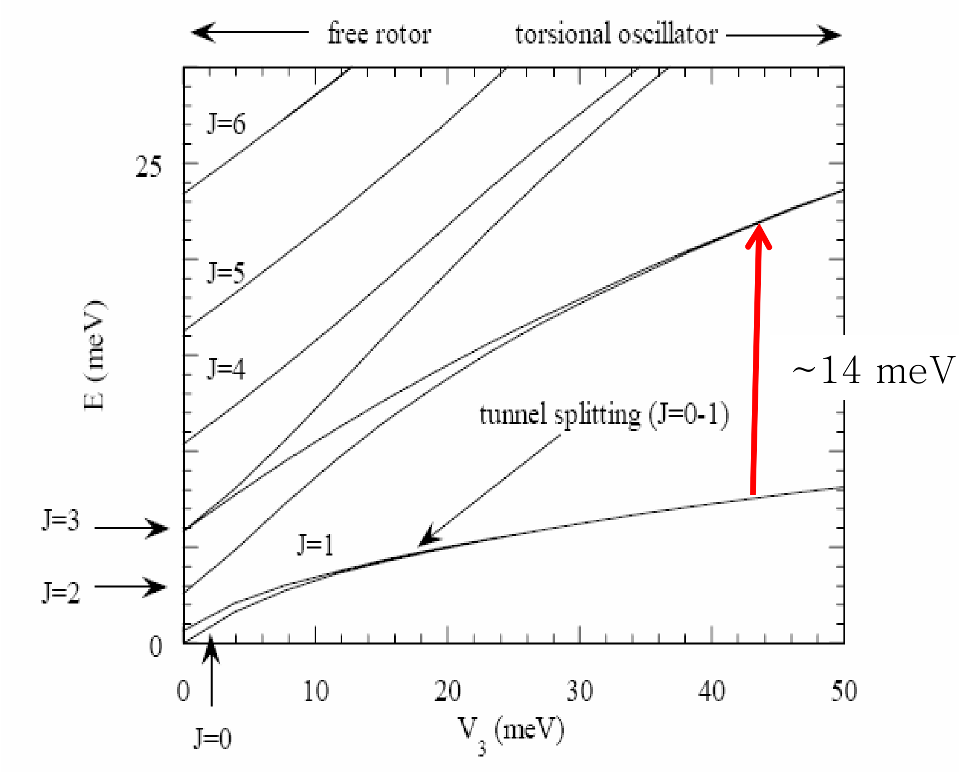


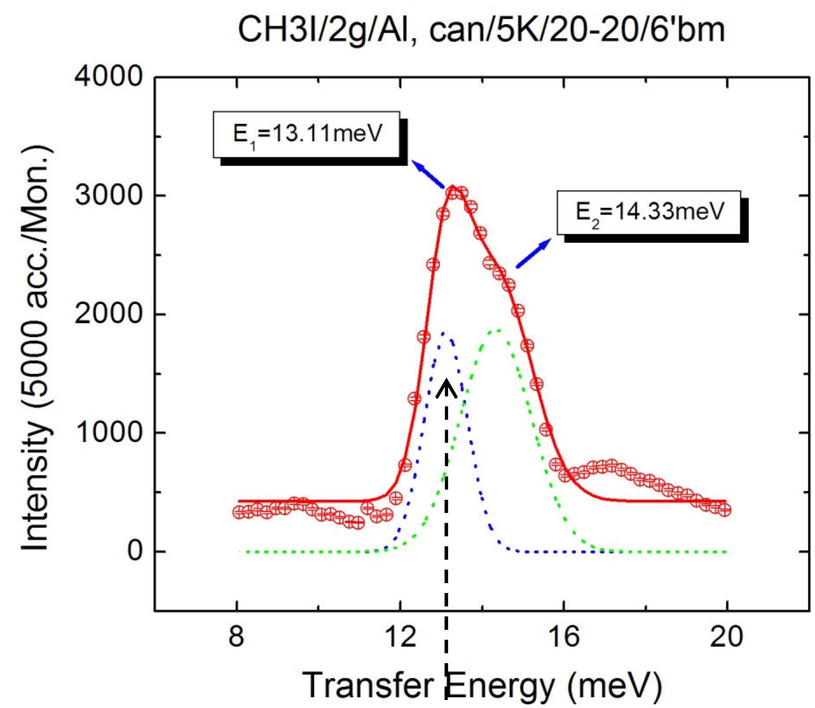
Fitted Value of Tunneling Energy
2.4126 ± 0.0036 ueV

V3= 41.2meV

FANS Verification

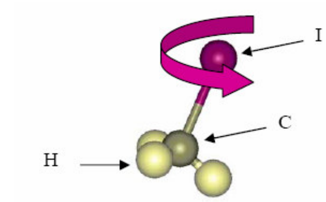






$$3\hbar\sqrt{V_3/2I} \quad \sim 14 \text{ meV}$$

Elastic Incoherent Structure Factor



Tunneling

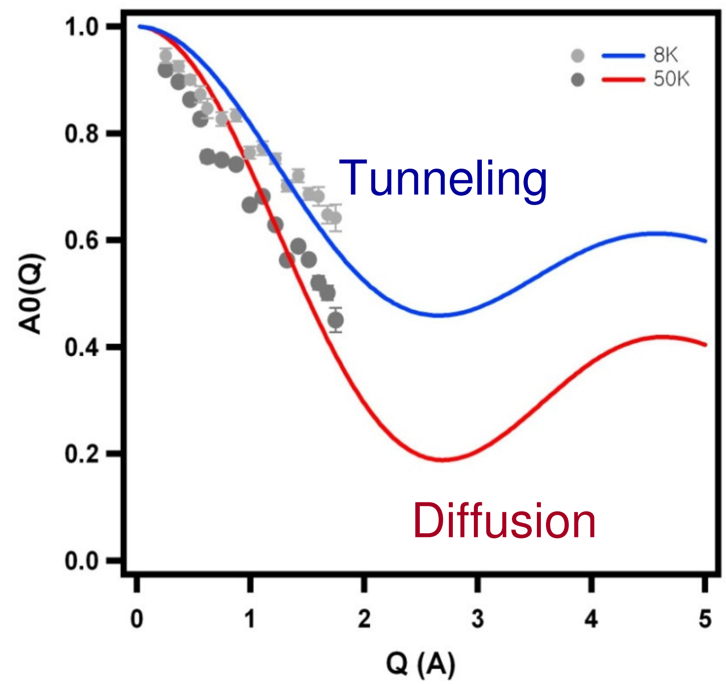
$$S(Q,E) = A_0(Q)\delta(E) + \frac{(1 - A_0(Q))}{2}[\delta(E - E_t) + \delta(E + E_t)]$$

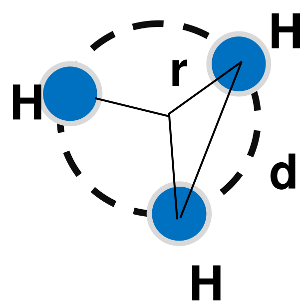
$$A_0(Q) = \frac{5 + 4j_0(Qr\sqrt{3})}{9}$$

Diffusion

$$S(Q,E) = A_0(Q)\delta(E) + (1 - A_0(Q))\frac{\Gamma}{\pi}\frac{1}{E^2 + \Gamma^2},$$

$$A_0(Q) = \frac{1}{3}\left(1 + 2j_0(Qr\sqrt{3})\right),$$

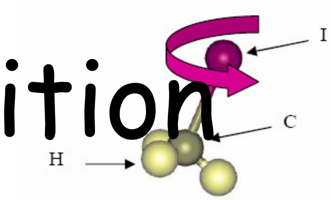


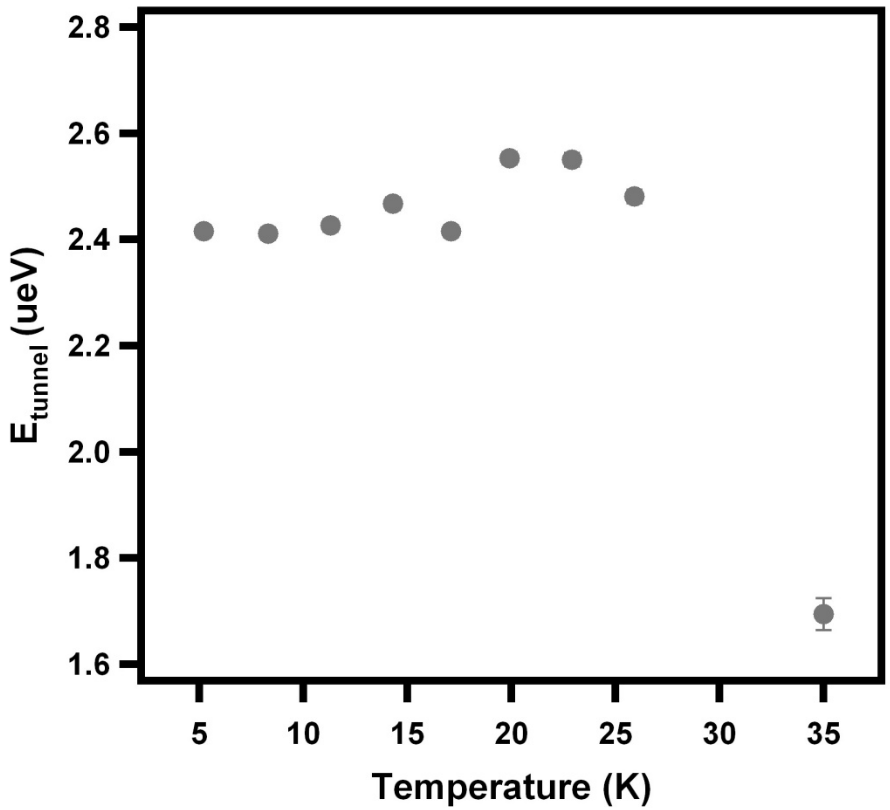


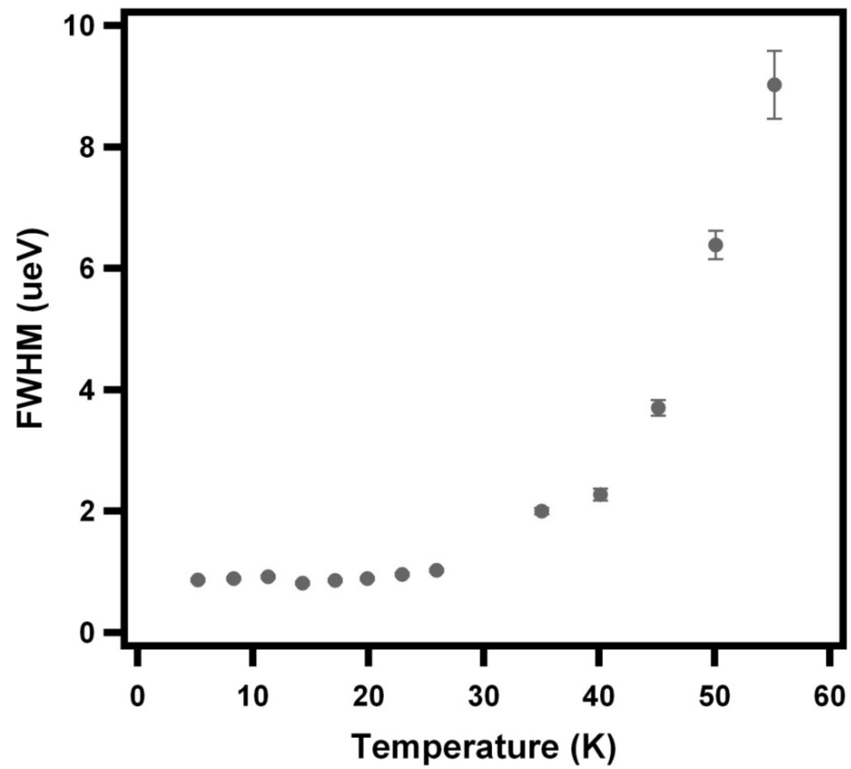
$$r_{experiment} = 0.97 \pm 0.02\,\overset{0}{A}$$

$$r_{theory} = 1.02\,\overset{o}{A}$$

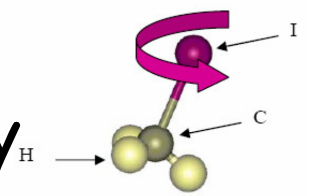
Quantum to Classical Transition

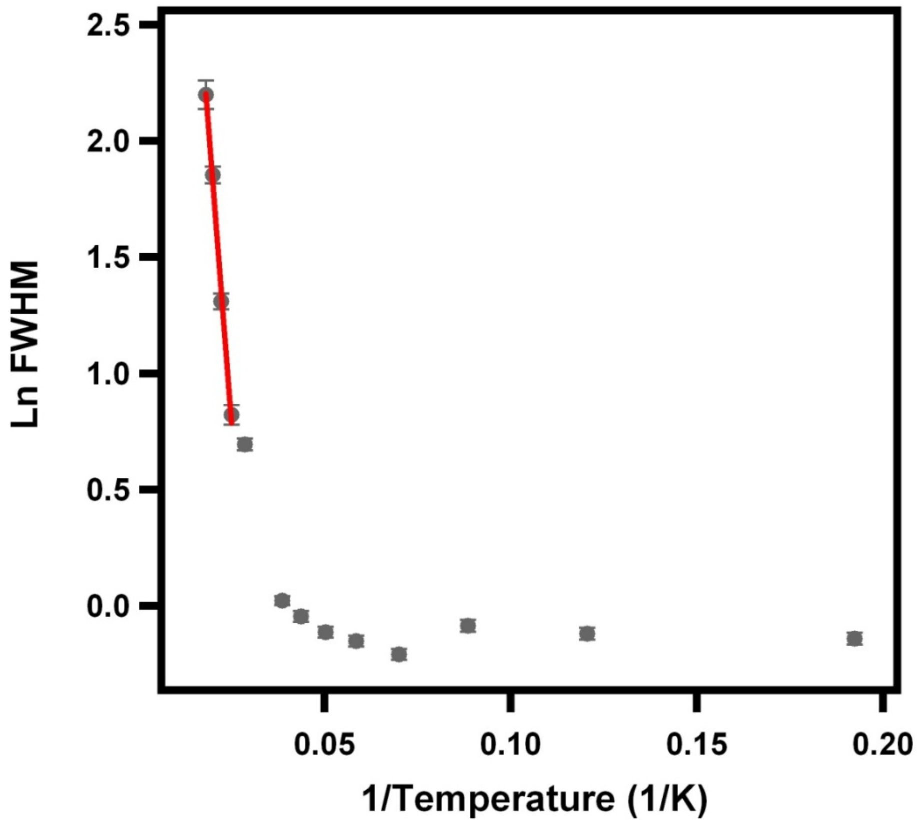






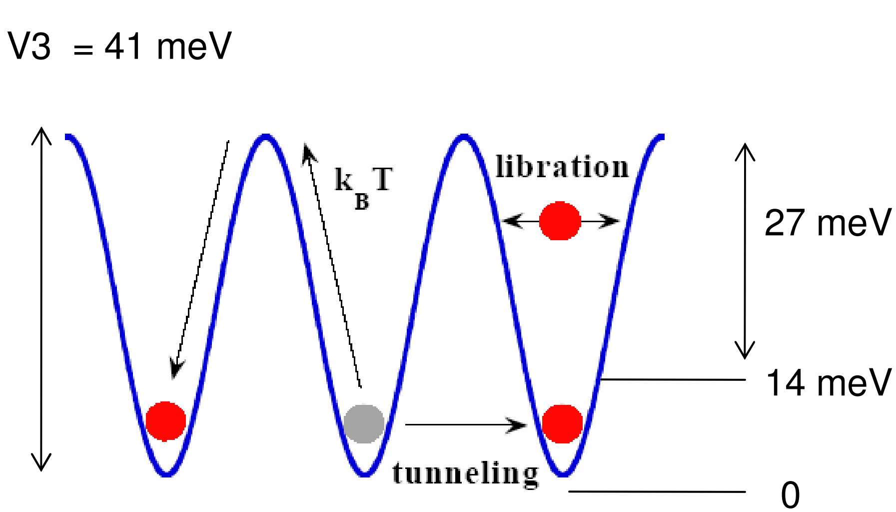
Arrhenius Fit for Activation Energy



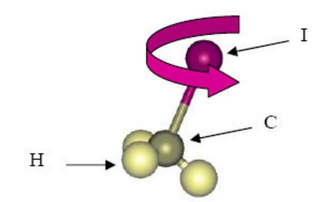


With errors weighted,
-207.85 ± 9.18 slope gives
17.91 ± 0.79 meV

Ln T= mT- (Ea/kT)

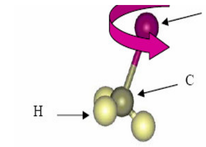


Conclusions



Tunelling Energy
Potential Barrier
Proton-Proton Distance
Activation Energy
Confirming Periodic Potential Model
Quantum to Classical Transition

Acknowledgements



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