METHYL IODIDE ROTATIONS: A Study Using HFBS and FANS

Group D

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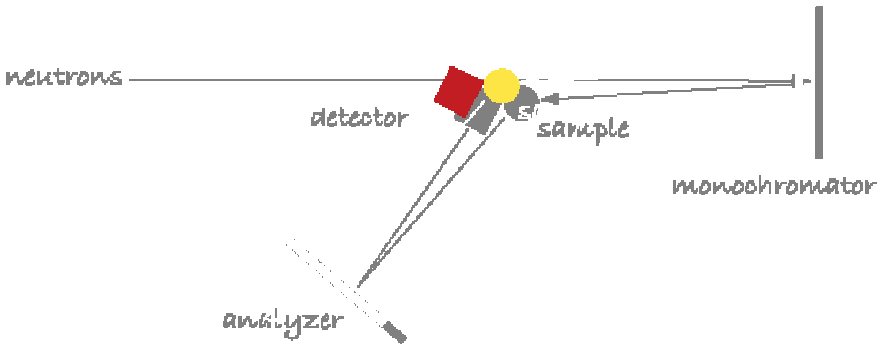
1

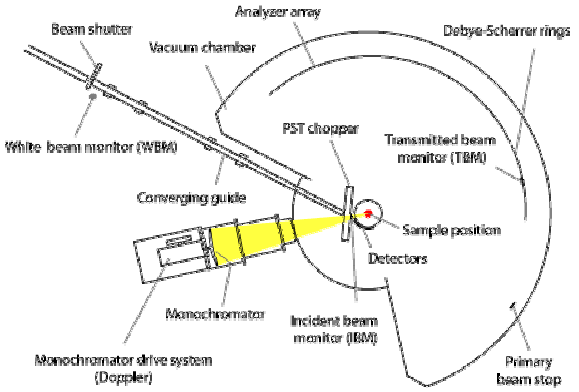
Backscattering: A High Resolution, Fixed Configuration Triple –Axis Spectrometer



$$\frac{\delta\lambda}{\lambda} = \frac{\delta d}{d} + \frac{\delta\theta}{\tan\theta}$$

2

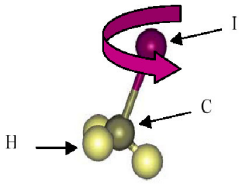
High Flux Backscattering Spectrometer

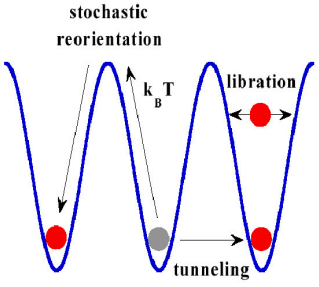


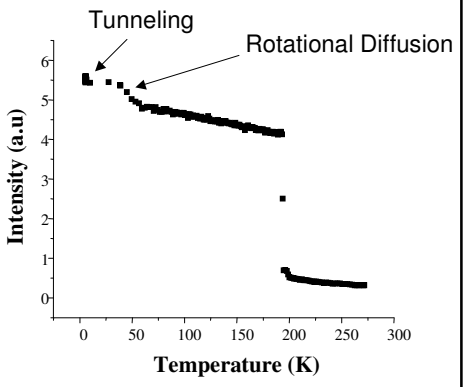
Instrument Characteristics	
Final Energy	2.08 meV (6.27 Å)
Fixed Scattering Angles	$0.25Å^{-1}<Q_{EL}<1.75Å^{-1}$
Dynamic Range	$-50\mu eV<\Delta E<50\mu eV$
Resolution	$\delta e<1\mu eV$ $\delta Q\approx 0.1Å^{-1}$

3

Methyl Iodide Dynamics





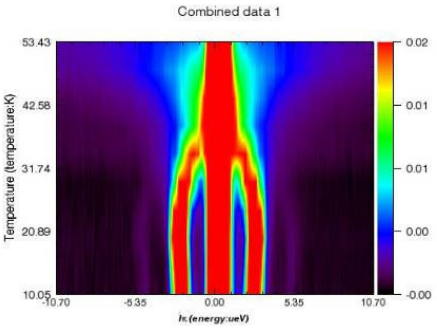


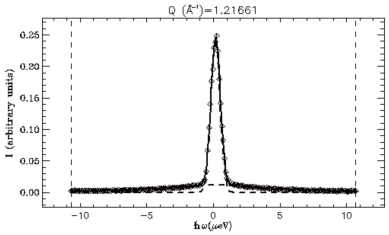
Use 3-fold symmetric potential

$$V(\theta)=\frac{V_3}{2}(1-\cos 3\theta)$$

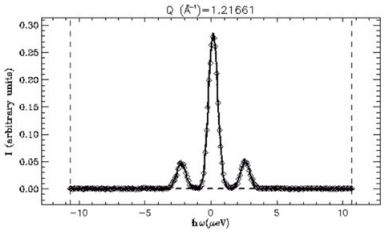
4

Data analysis (DAVE)





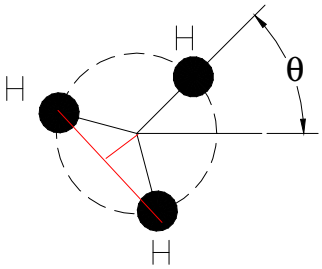
55 K



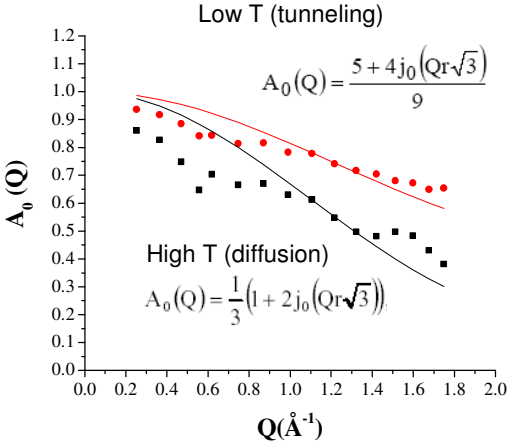
10 K

5

Data Analysis



R_{theor} = 1.03Å
R_{tunnel} = .98Å
R_{diff} = 1.08Å



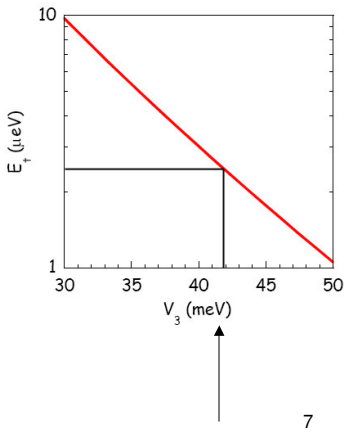
6

Data Analysis

- Average tunneling 2.42 μeV → V_3 = 42 meV
  - Using equation for separation betwee librational levels
    (I = 5.3 e^{-47} kg m^2)

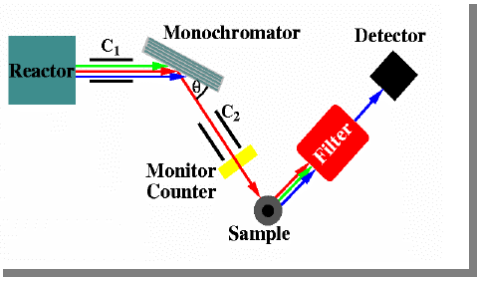
$$E_{lib} = \frac{3h}{2\pi}\sqrt[3]{\frac{V_3}{2I}}$$

  - **E_{lib}= 15.6 meV**
  - *confirm value from FANS…..*



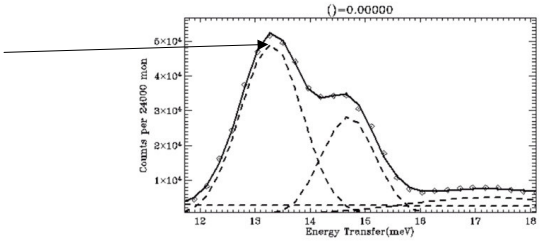
7

Filter Analyzer Neutron Spectrometer (FANS)



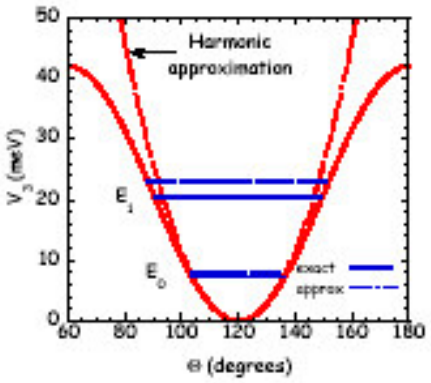
- Density of states
- Vary input energy, filter rejects all but 1.2 meV
- Measures 10's-100's meV

- **E_{lib} = 13.2 meV**
- **(E_{lib}= 15.6 meV HFBS)**



Data Analysis

- $\ln E = \ln E° - 1/T(E_a/R)$
- $E_a = 21.7$ meV
  (42 meV from low T data)



9

SUMMARY

- HFBS was used to study the rotational dynamics of CH_3I from 10-55 K.
- Radius of the methyl group was estimated by fitting the EISF data.
- Tunneling energy determined – estimate V_3 (potential barrier) and calculate $E_{libration}$.
- Data from FANS was used to verify the prediction of the libration transition energy.
- E_a for J 0 → 1 transition was calculated

10

THANK YOU

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11