QUANTUM ROTATIONS IN METHYL IODIDE:

A Study Using HFBS and FANS

Group C

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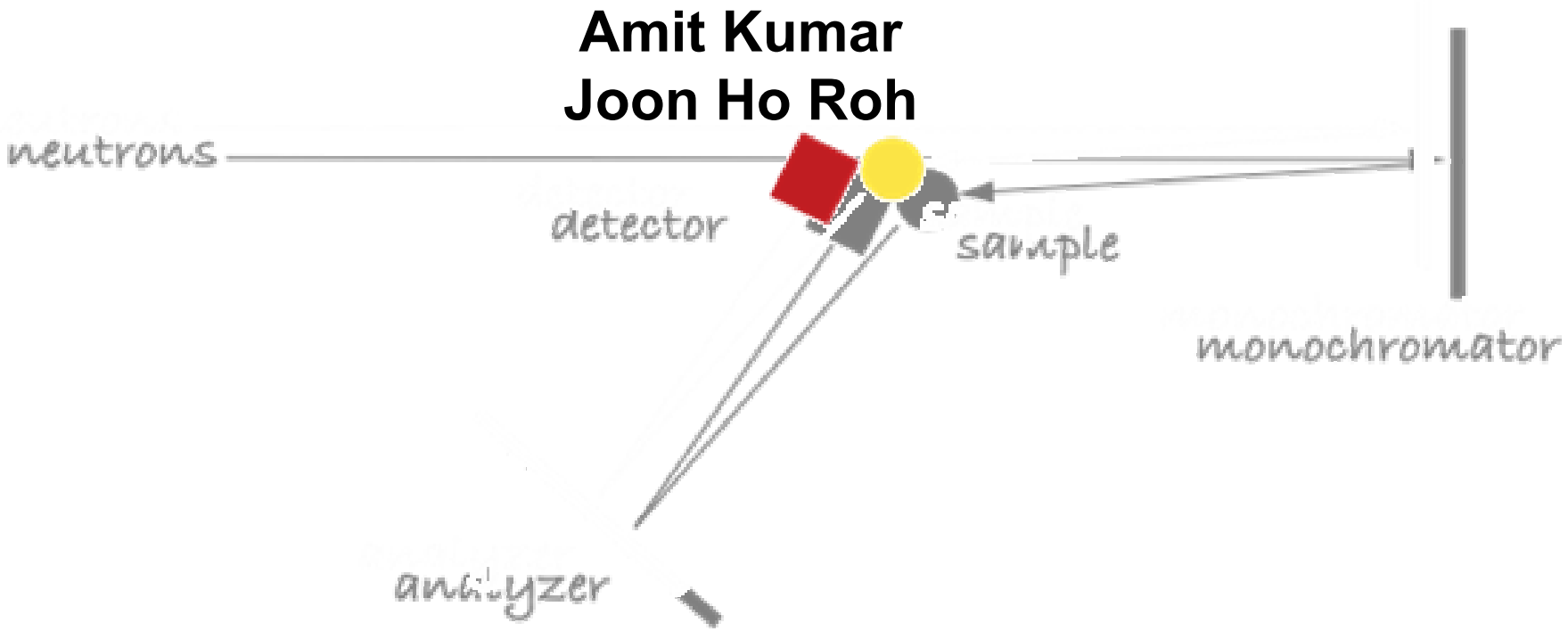
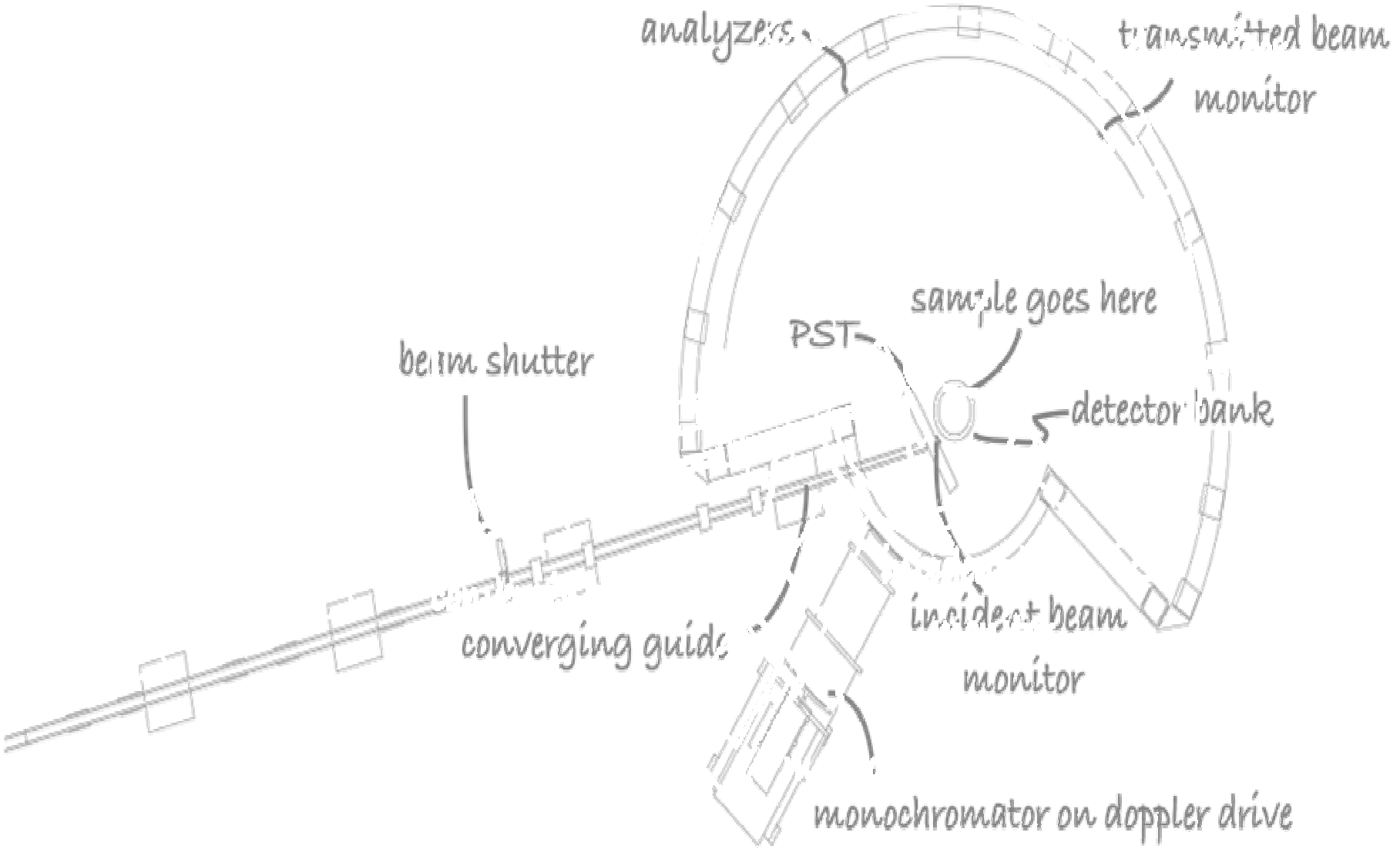


High Flux Backscattering Spectrometer



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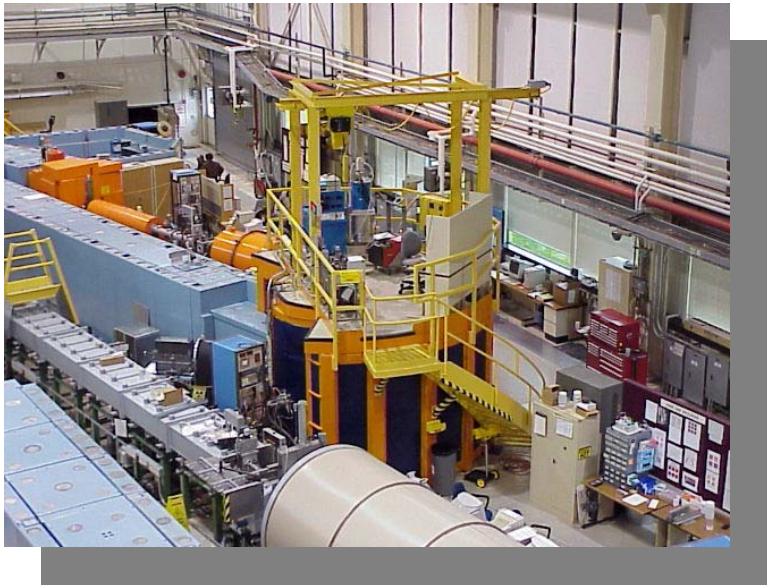
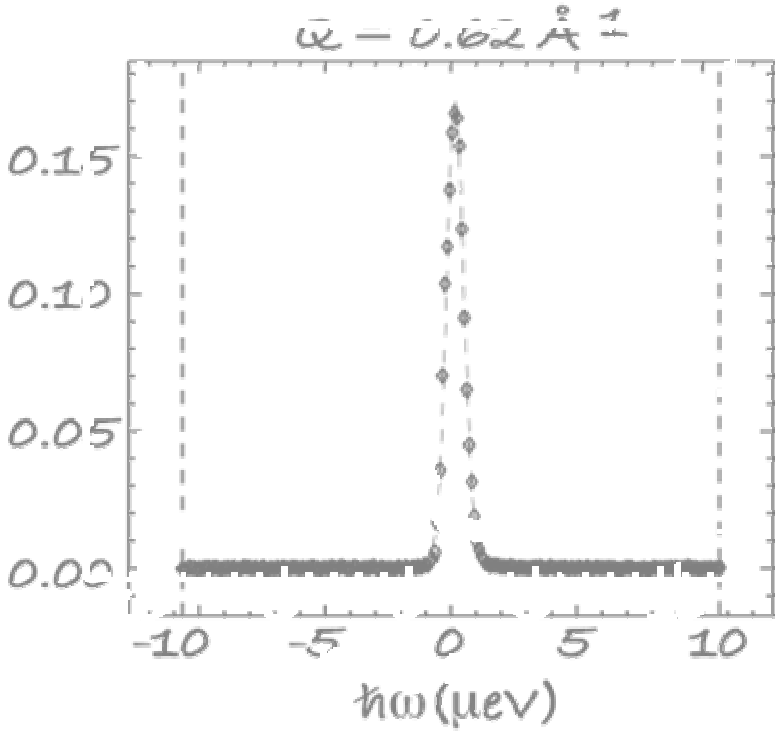
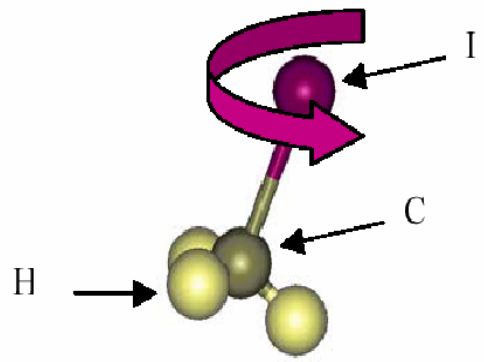
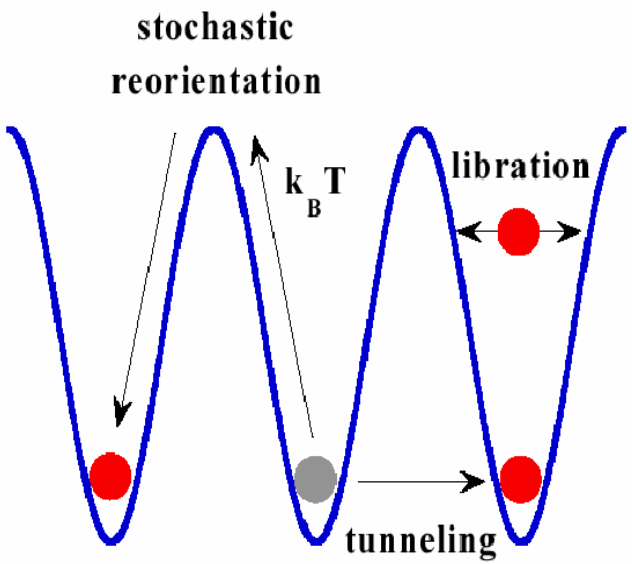




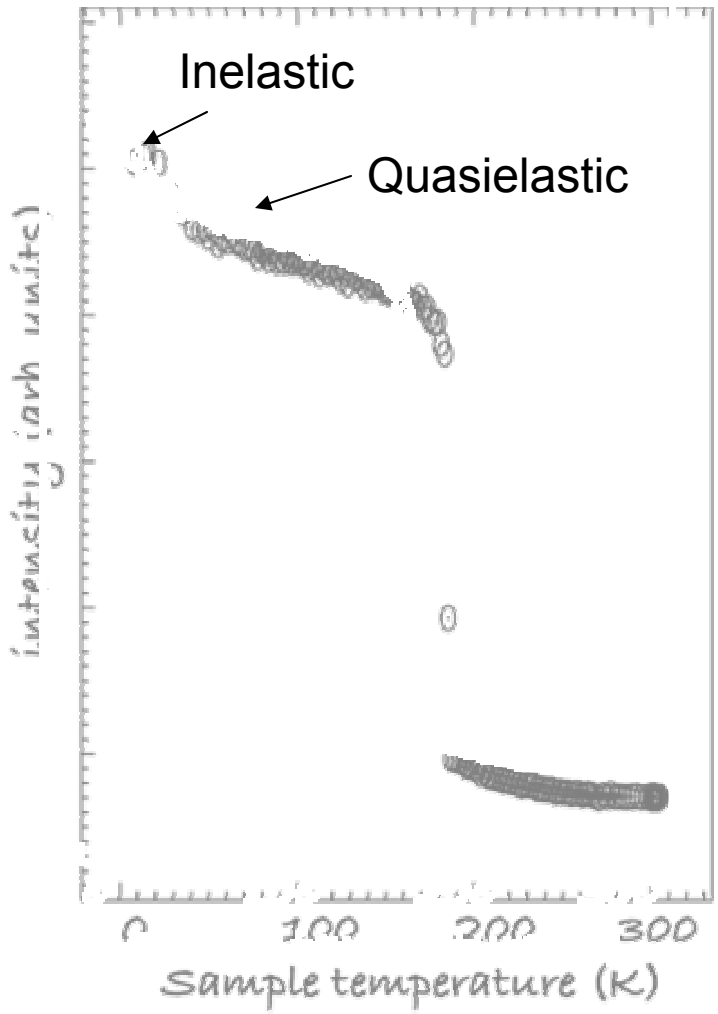
- resolution ~ 1 μeV
- energy transfers upto ±50 μeV
- motions on ns timescales
- momentum transfers from 0.25 $Å^{-1}$ to 1.75 $Å^{-1}$

BULK CH_3I DYNAMICS



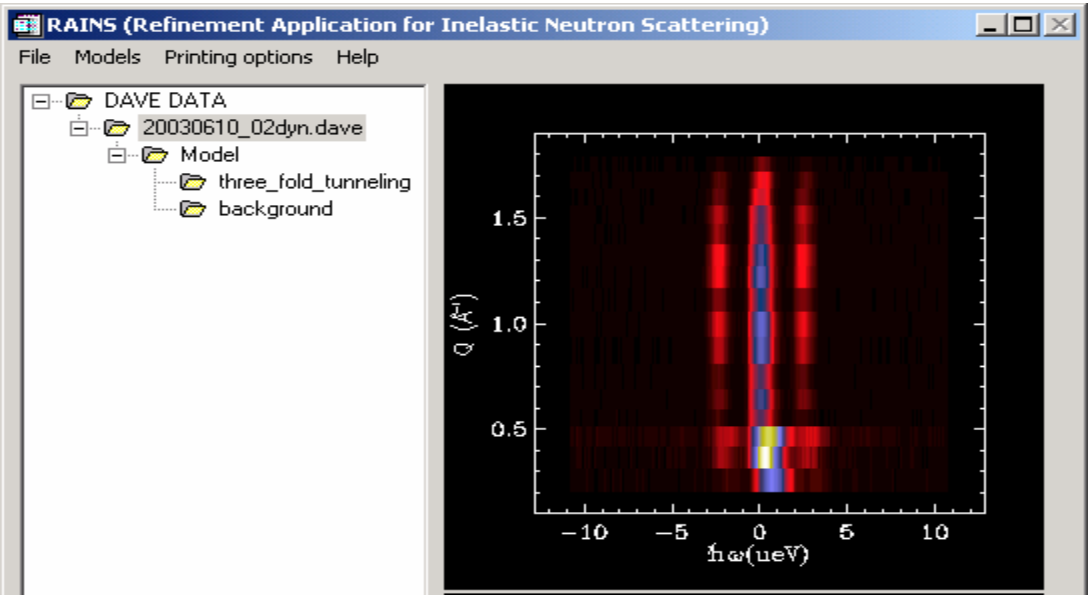


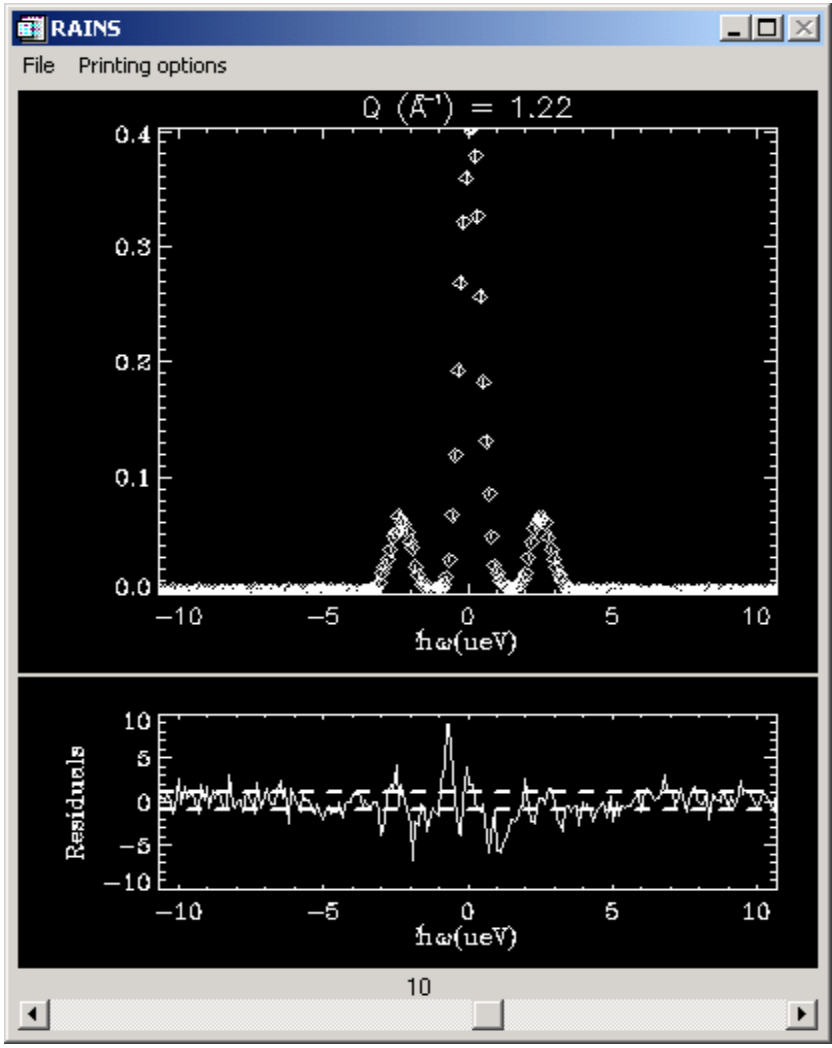
Use 3-fold symmetric potential



CH_3I melting point = 206 K

HFBS DATA FOR CH_3I at T = 8 K





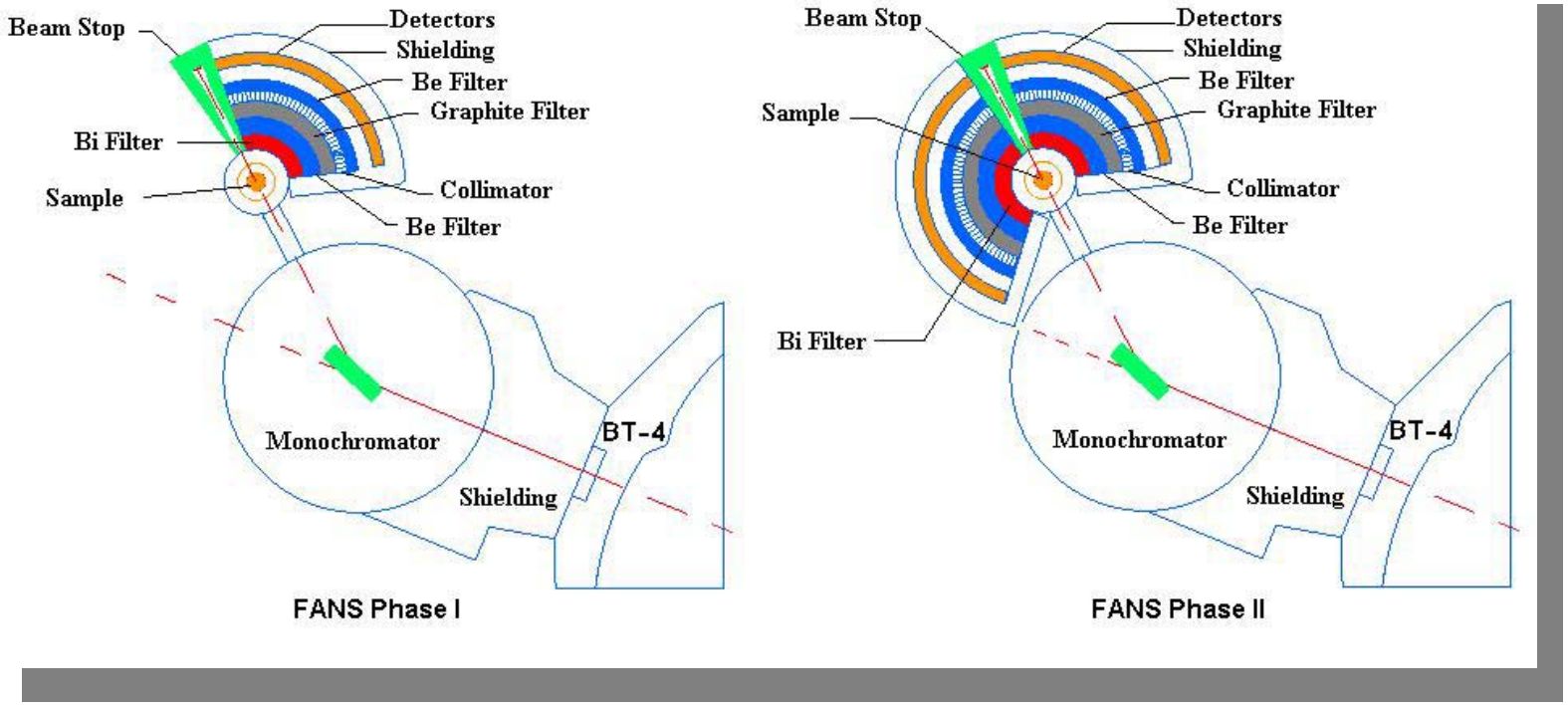
E_t = 2.3 μeV ⟹ V_3 = 42 meV

⇓

E ~ 7.5 meV ?

Check with FANS

Filter Analyzer Neutron Spectrometer

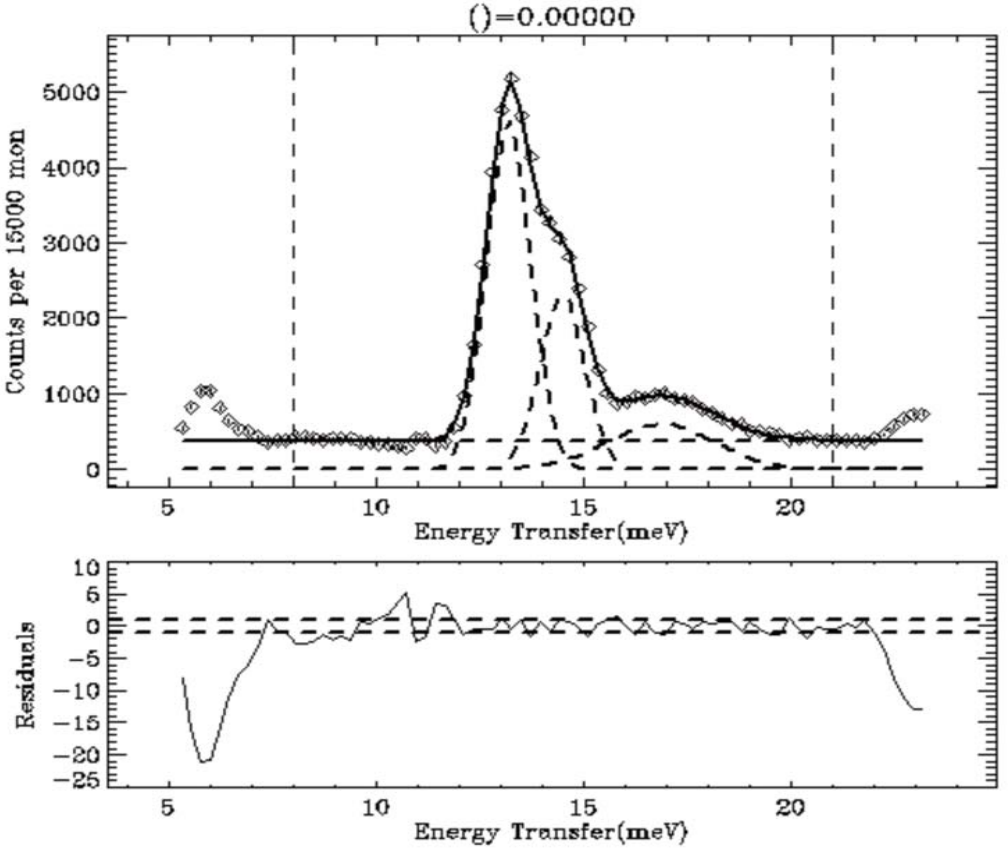


- measures vibrational motion
- energy transfers of order 10 to 100 meV
- resolution about 1 meV

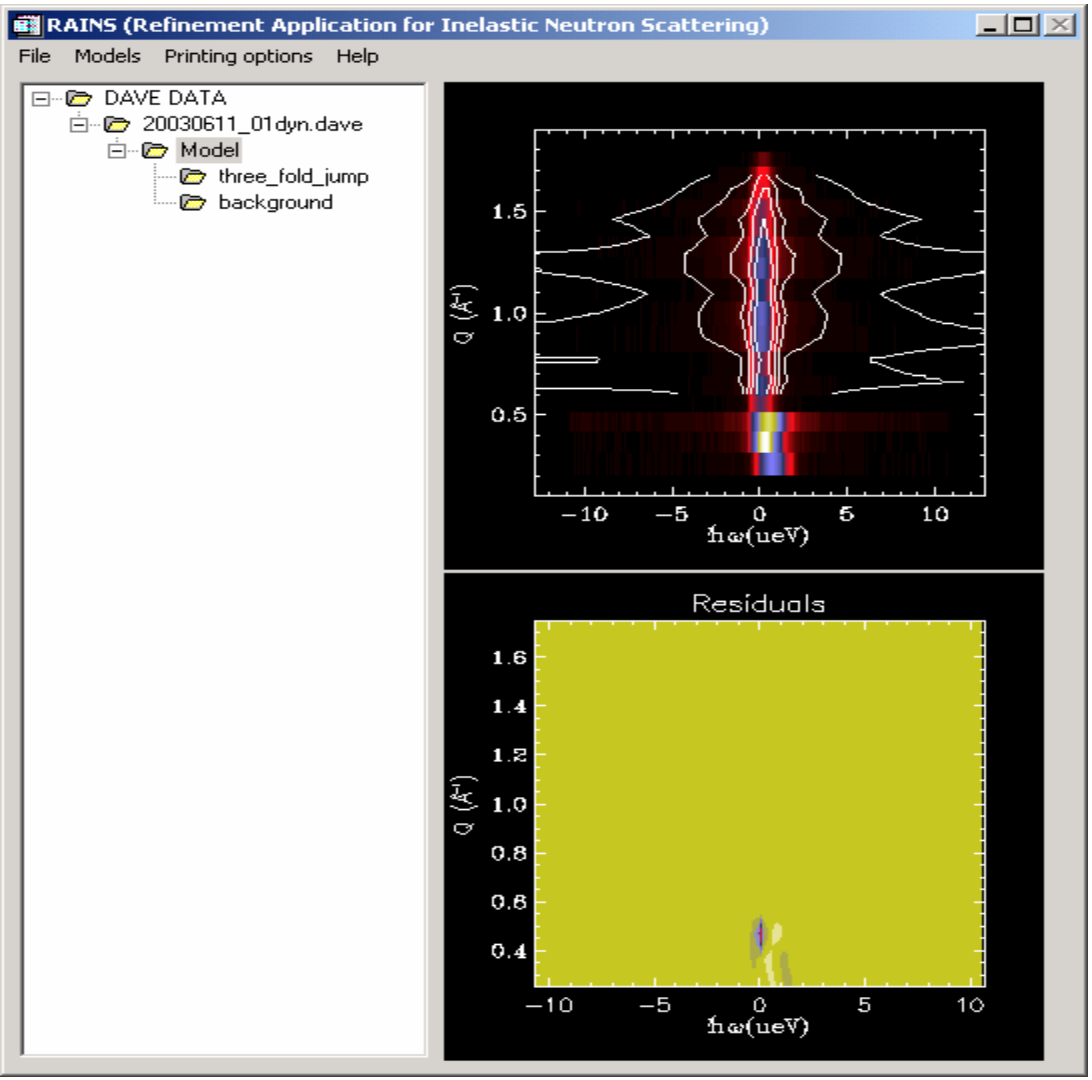
FANS DATA at T = 12 K

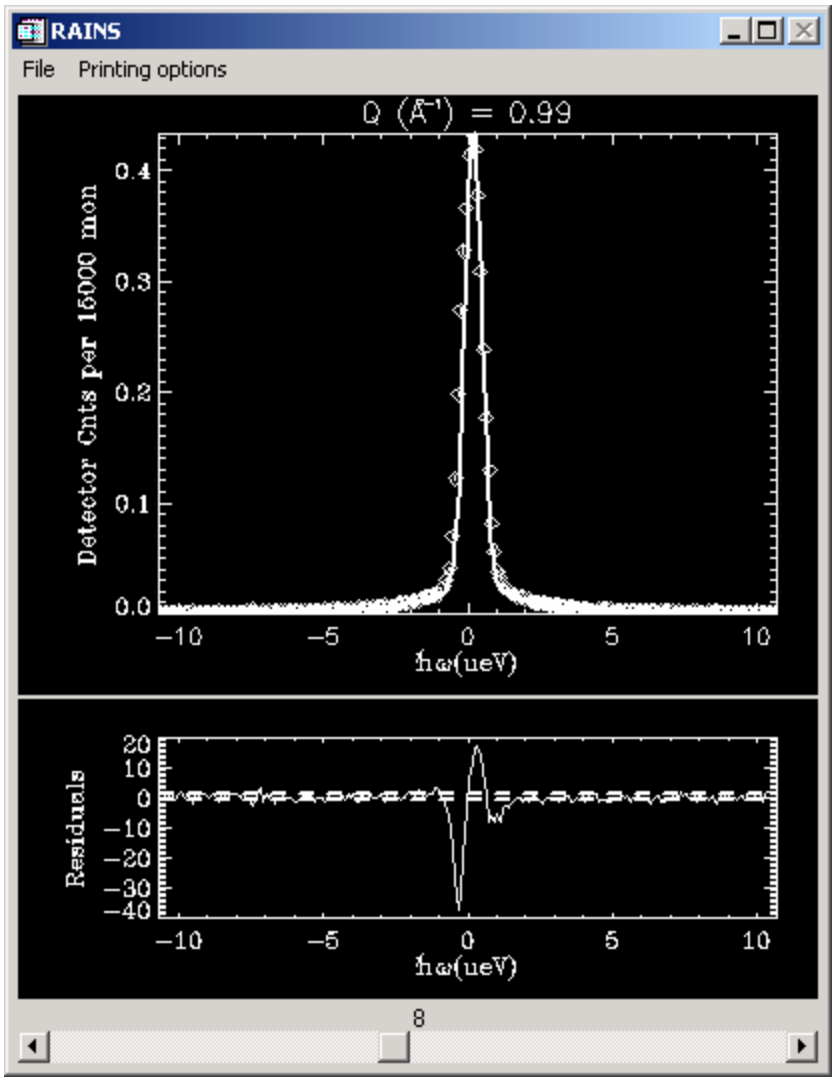
Fit Results :

E_{lib} = 13.2 meV

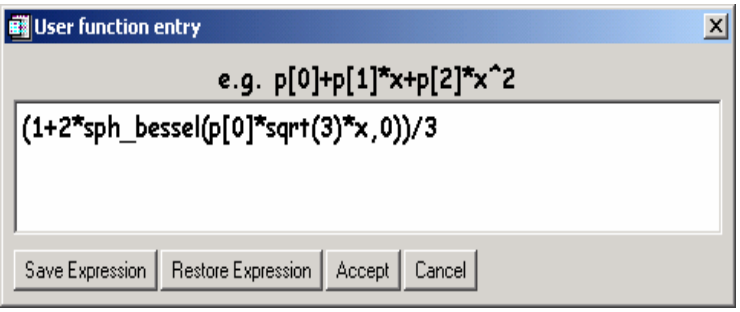


HFBS DATA FOR CH_3I at T = 40 K



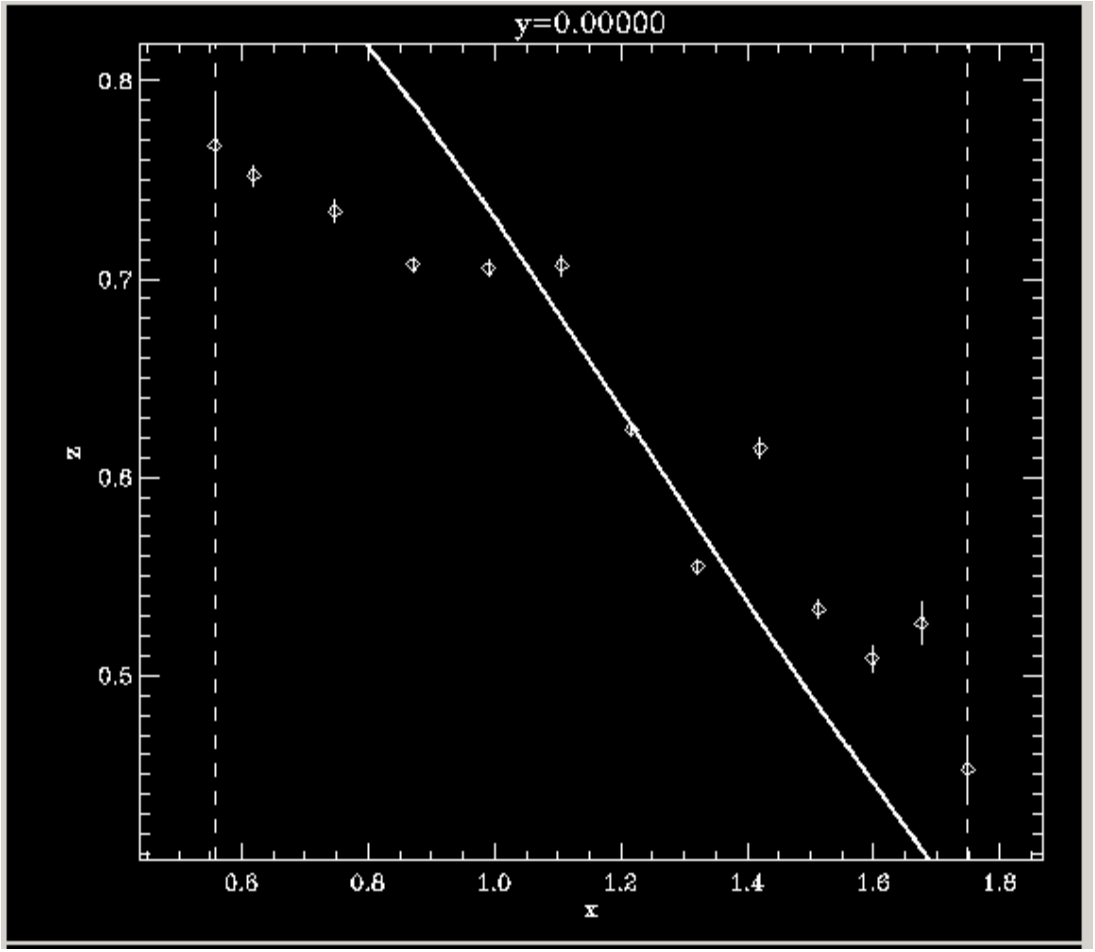


EISF Fitting for T = 40 K data



R_{fit} = 0.965 Å

R_{exp} = 1.03 Å



SUMMARY

- HFBS was used to study the rotational dynamics of CH_3I.
- Tunneling energy was determined using HFBS from which the barrier height and the transition energy for libration was calculated.
- Data from FANS was used to verify the prediction of the libration transition energy.
- Radius of the methyl group was estimated by fitting the EISF data.

ACKNOWLEDGEMENTS

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