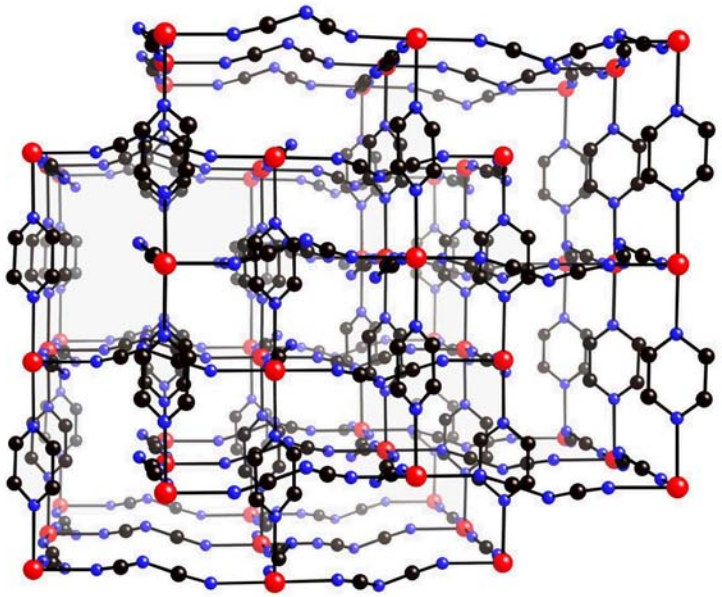
Rotational Ligand Dynamics in $Mn[N(CN)_2]_2$.pyrazine

Group C

Jun Tian, Wei Zhou, Greg Hura, Vicky Garcia Sakai,
Chris Kitchens, Joon Ho Roh, Amit Kumar, Yifu Ding

$Mn[N(CN)_2]_2$.pyrazine

- material consisting of transition metal ions linked by polydentate organic ligands
- forms different structures at low and high temperatures
  - at 1.3K 3D antiferromagnetic order, monoclinic lattice
  - ~ 200K orthorhombic structure
  - ~ 408K DSC shows additional phase transition ?



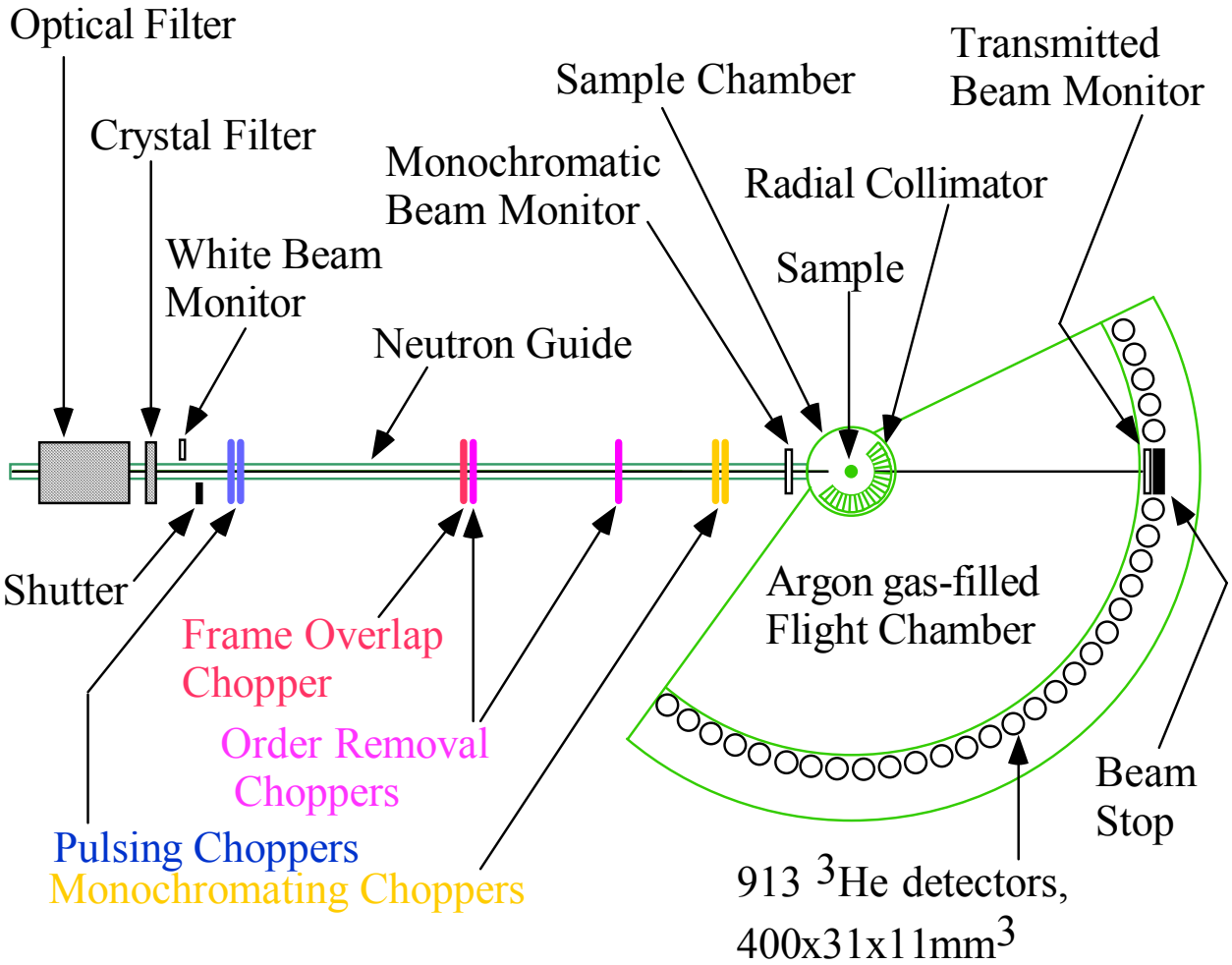
Why use neutron scattering?

- Have wavelengths comparable to interatomic distances and energies comparable to phonon and intermolecular interaction energies

  $\therefore$ obtain information on geometry and time-scale of motions simultaneously

- Interact differently with H and D
- Have a magnetic moment
- Interact directly with the nucleus

Disc-Chopper Spectrometer



Experimental runs

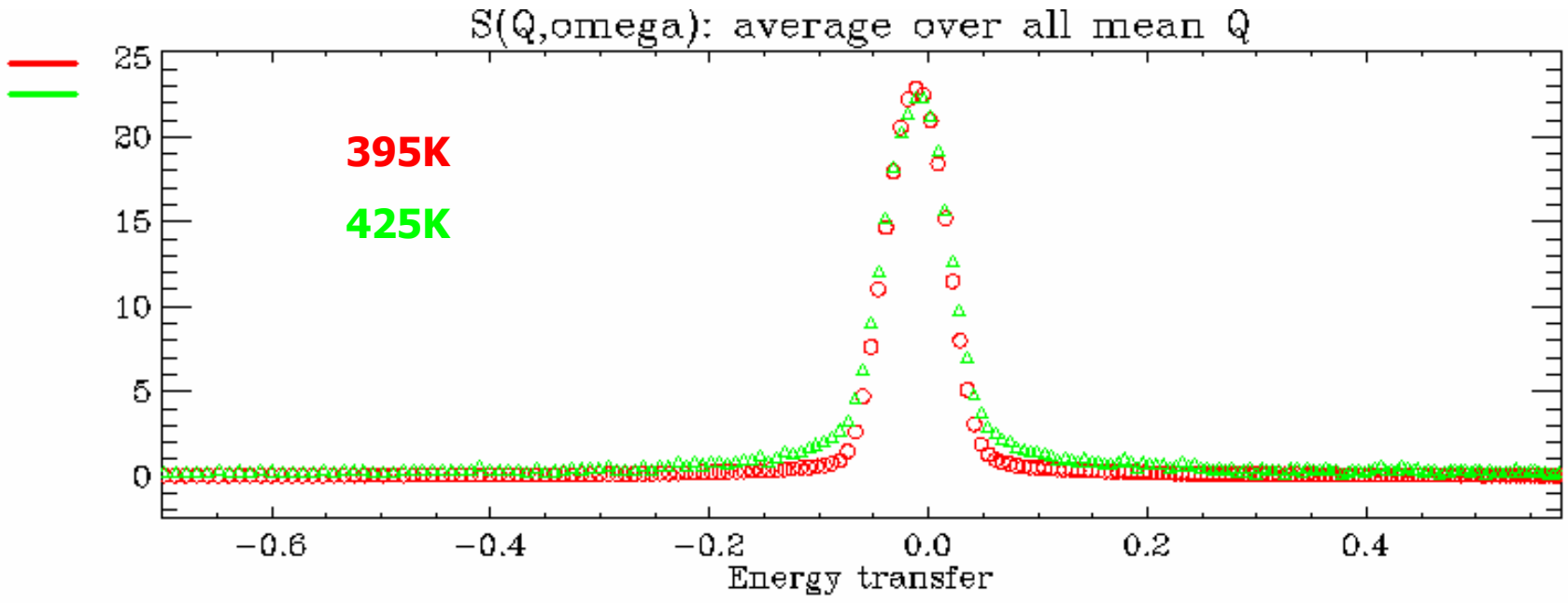
- protonated (T=395, 405, 415, 425K)
- deuterated (T=300, 390, 400K)
- vanadium
- background

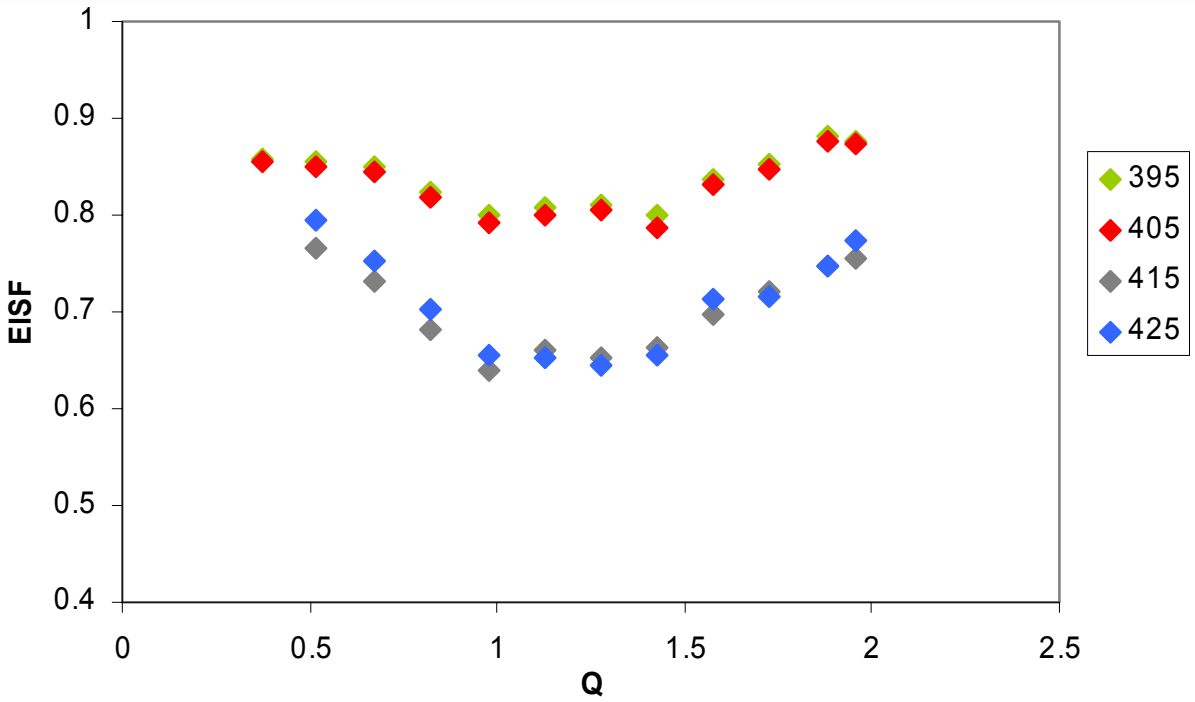
Measured Scattering

- Incoherent scattering dominated by protons
- $S_{inc}(Q,\omega)$ is the space and time FT of the self-correlation function..probability of finding a particle at time t in position r given that it was at the origin at time t=0
- Fit using model such as diffusional motion of protons among equivalent sites

$$S_{inc}(Q,\omega) = \frac{1}{2}\left(1+\frac{\sin[QR]}{QR}\right)\delta(\omega) + \frac{1}{2}\left(1-\frac{\sin[QR]}{QR}\right)\frac{1}{\pi}\left(\frac{2\tau}{4+\tau^2\omega^2}\right)$$

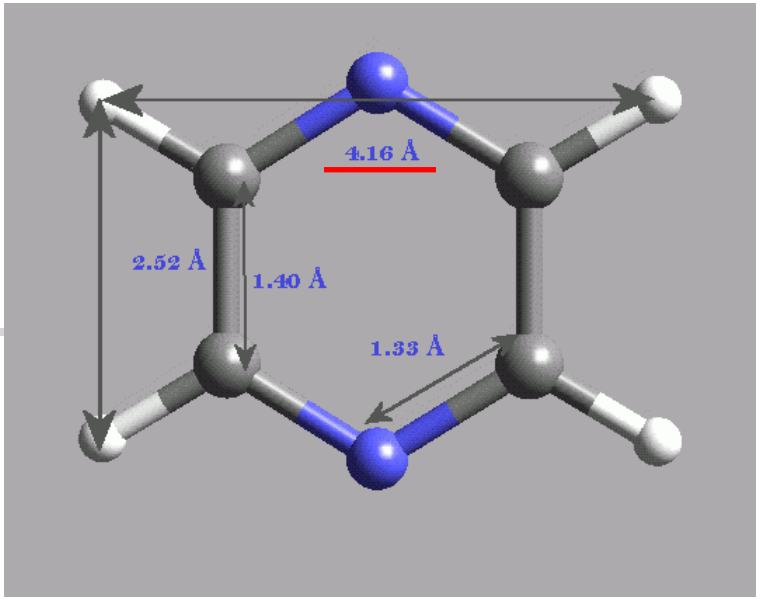
Elastic contribution **Inelastic contribution**

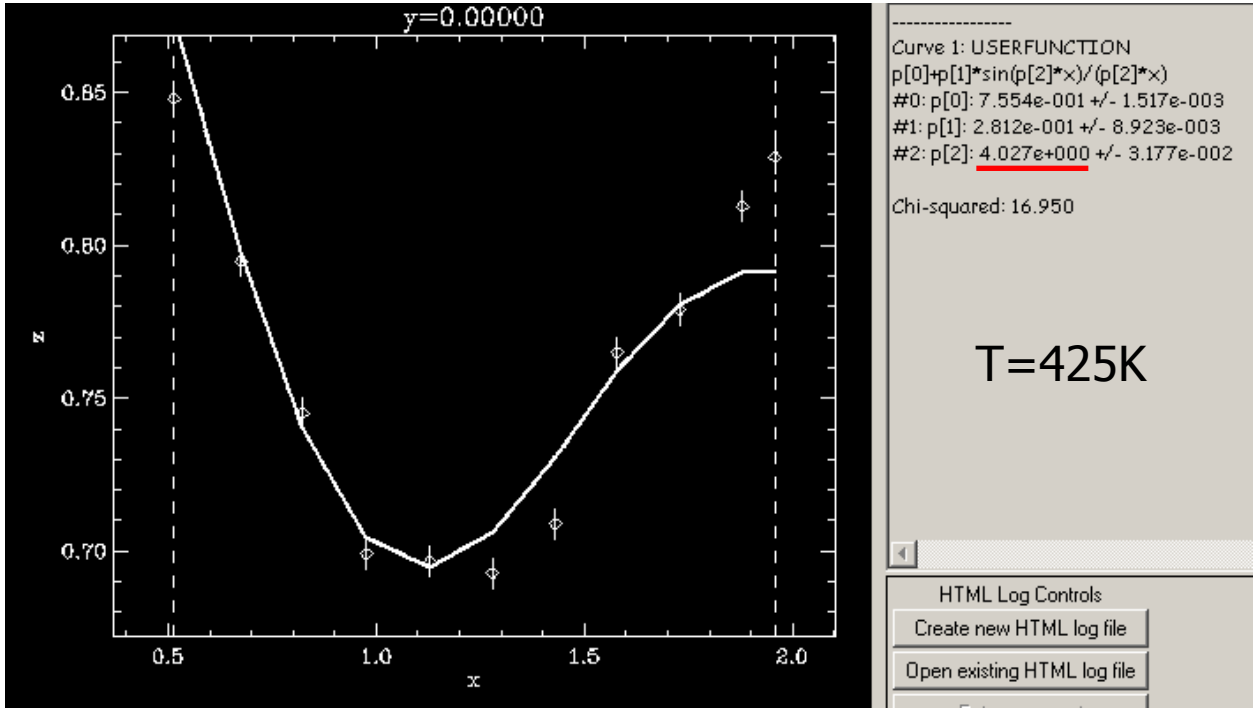

S(Q,omega): average over all mean Q
395K
425K
25
20
15
10
5
0
−0.6
−0.4
−0.2
0.0
0.2
0.4
Energy transfer


1
0.9
0.8
0.7
0.6
0.5
0.4
EISF
0
0.5
1
1.5
2
2.5
Q
395
405
415
425

Results

$$EISF = \frac{I_{elastic}}{I_{total}} = \frac{G_p}{G_p + L_p - \left(m_p / m_d\right) L_d}$$





Curve 1: USERFUNCTION
p[0]+p[1]*sin(p[2]*x)/(p[2]*x)
#0: p[0]: 7.554e-001 +/- 1.517e-003
#1: p[1]: 2.812e-001 +/- 8.923e-003
#2: p[2]: 4.027e+000 +/- 3.177e-002

Chi-squared: 16.950

T=425K

HTML Log Controls
Create new HTML log file
Open existing HTML log file

Conclusion

A thermally activated 2-fold jump motion about the coordinating nitrogen axis takes place which actually starts at 200K. At 408K more pyrazine rings perform this motion and a more open framework structure forms.

Thanks to the organizers!