Investigation of the orientational phase transition in buckyball (C_{60}) using NCNR Disk Chopper Spectrometer

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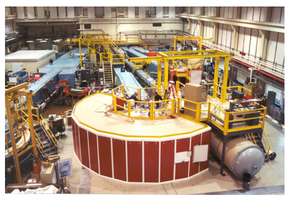
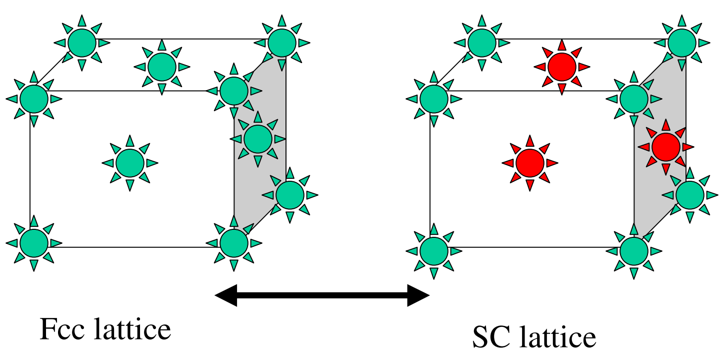


NIST (NCNR)

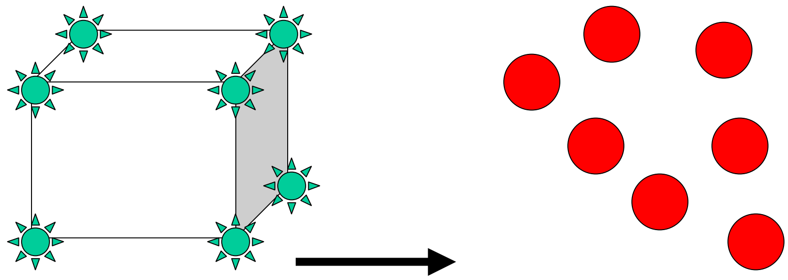
Gaithersburg, MD.

June 21, 2005

First-order phase transition in buckyball



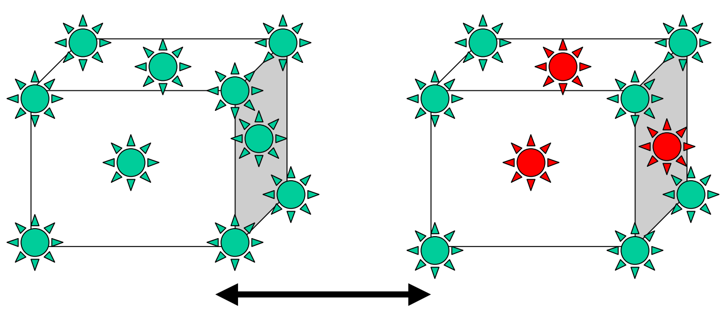
Goal: We want to investigate how this occurs.



Real space
(bravais lattice)

Phase space
(“Ideal” gas)

- Isomorphic to diffusion by Fick’s diffusion law.

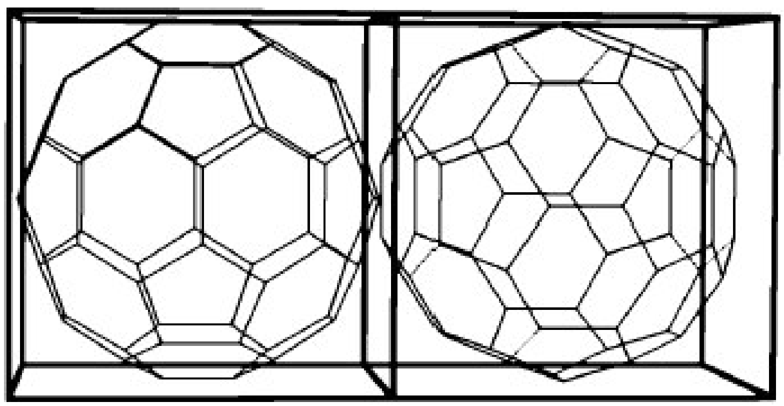


Fcc lattice

SC lattice

- Melting of orientation at ~ 261 K
- Centers of buckyballs are still fcc, but just different orientations.

Two different ways of orienting C_{60} in a cube.



Local min. of Free Energy   Global min. of Free Energy

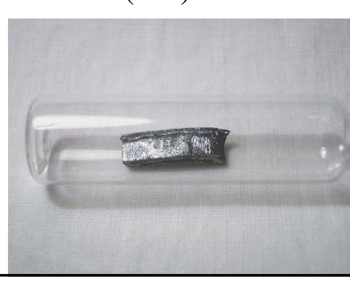
Low T (< 90 K) picture

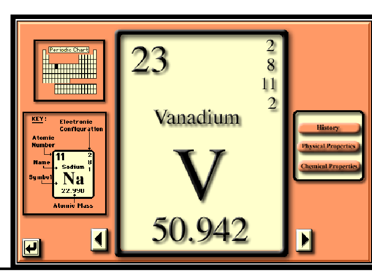
Setting up the experiment:

I. Sample:

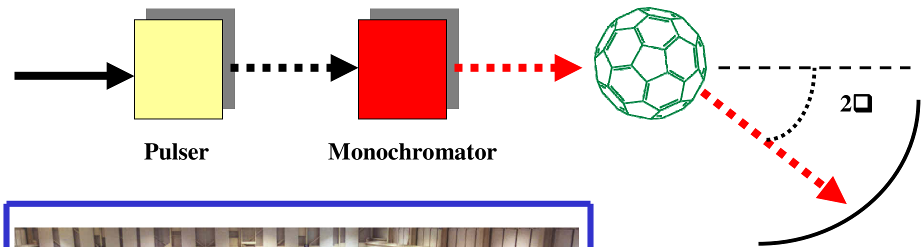
• ~ 15 grams of C_{60} in a 10 cm tall, 1.3 cm diameter Al cell, press sealed with indium wire.

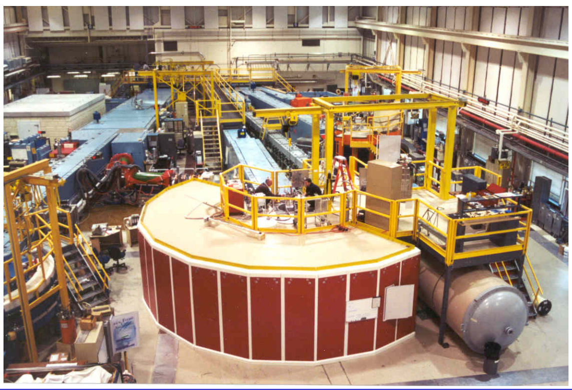
• Data reduction: Use Vanadium to normalize data from different detectors. ♦(coh)=0.02 barns/atom; ♦(inc)=5.19 barns/atom





DCS: Disk Chopper Spectrometer

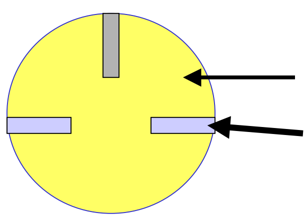




DCS is a "Direct geometry time-of-flight spectrometer".

(from the "DCS Poster", NIST,2002)

Using chopper to create pulses with a certain bandwidth:

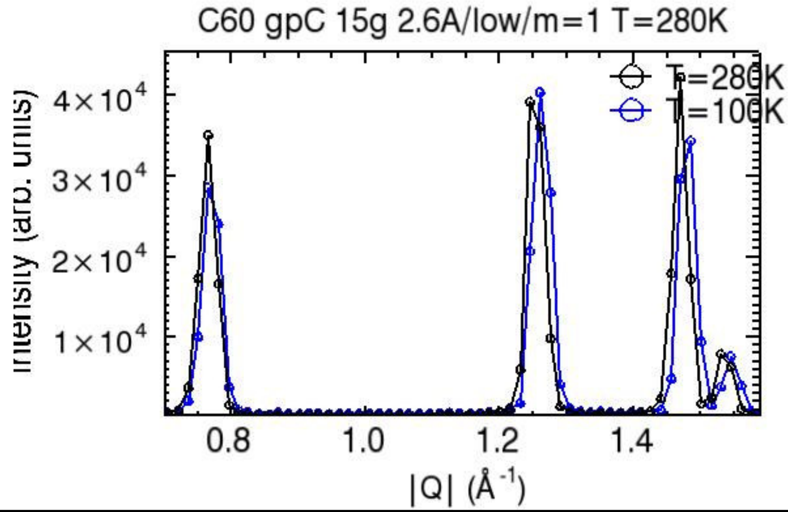


Back view of chopper disk

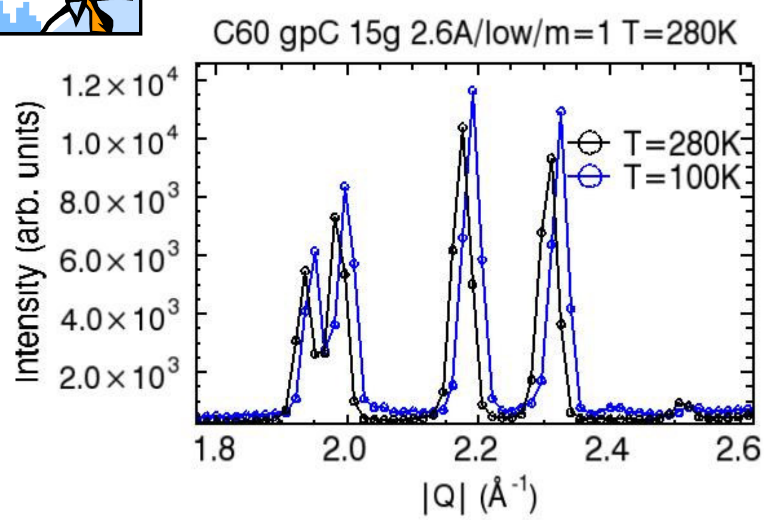
- DCS has 7 disk choppers: Their rotation axis is aligned with the beam. By setting the rotation frequency of each of the disks in series, can admit monochromatic pulses of neutrons.

- With 7 disk choppers, can cut out neutrons that are commensurate in velocity, thus removes frame overlapping. (*Analogy: Think of stroboscopes…*)

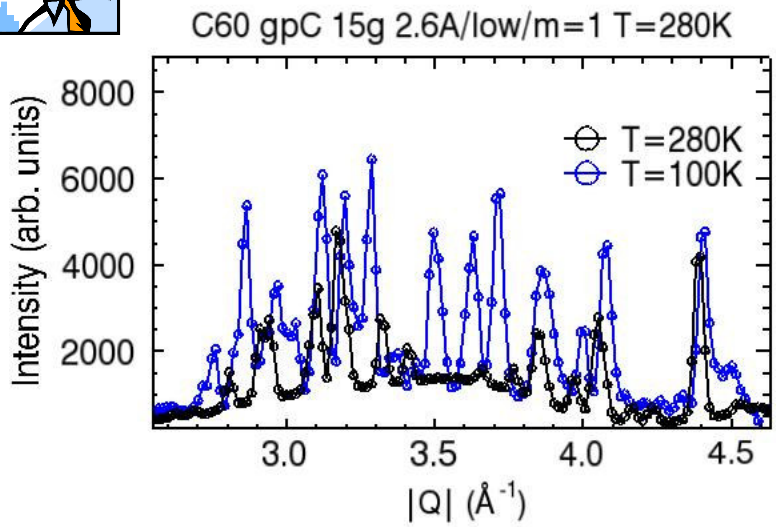
DAVE: Data Analysis and Visualization Environment (Reduction, visualization, analysis of data from DCS)



Shift of diffraction peaks:



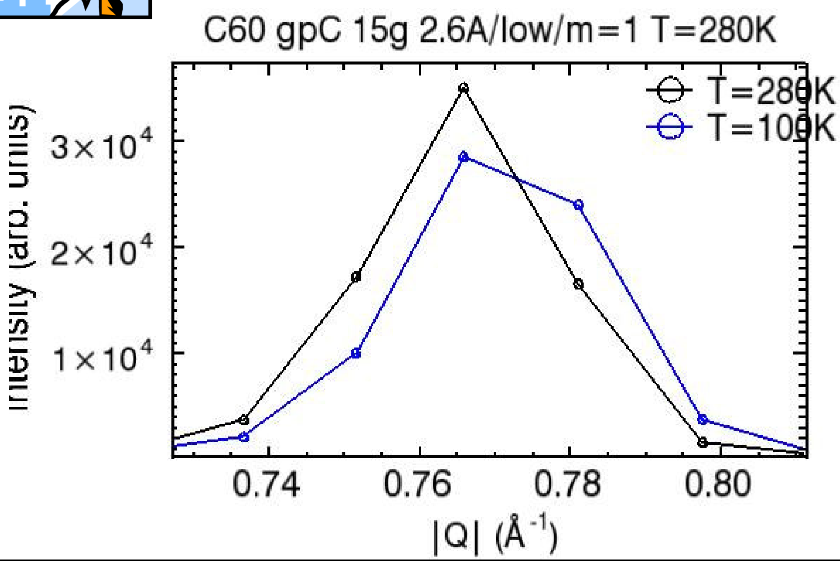
New peaks appear after the phase transition

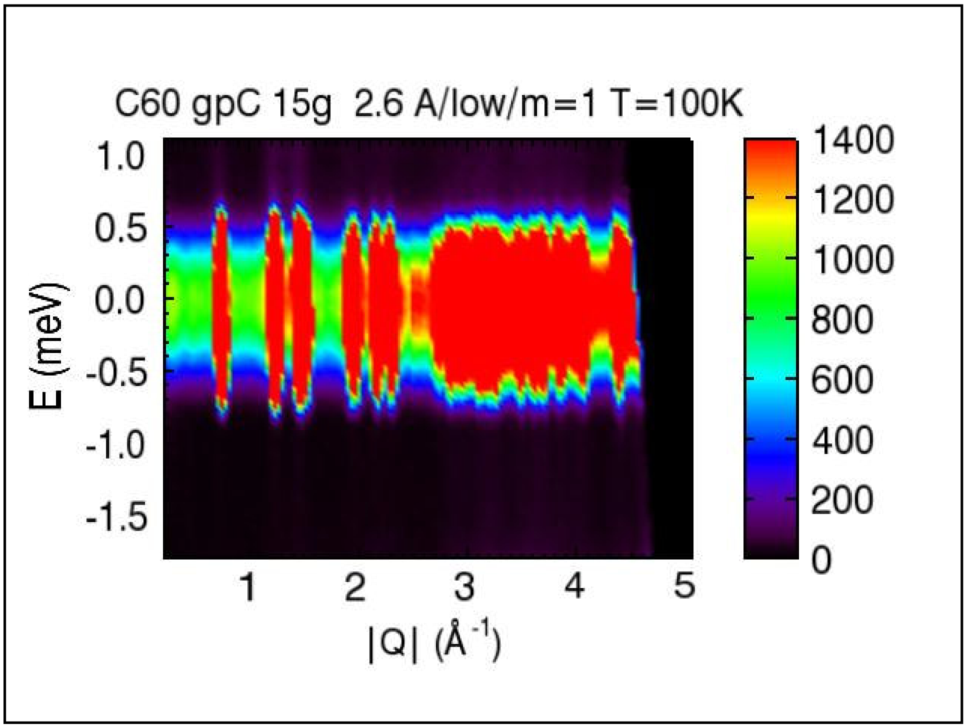


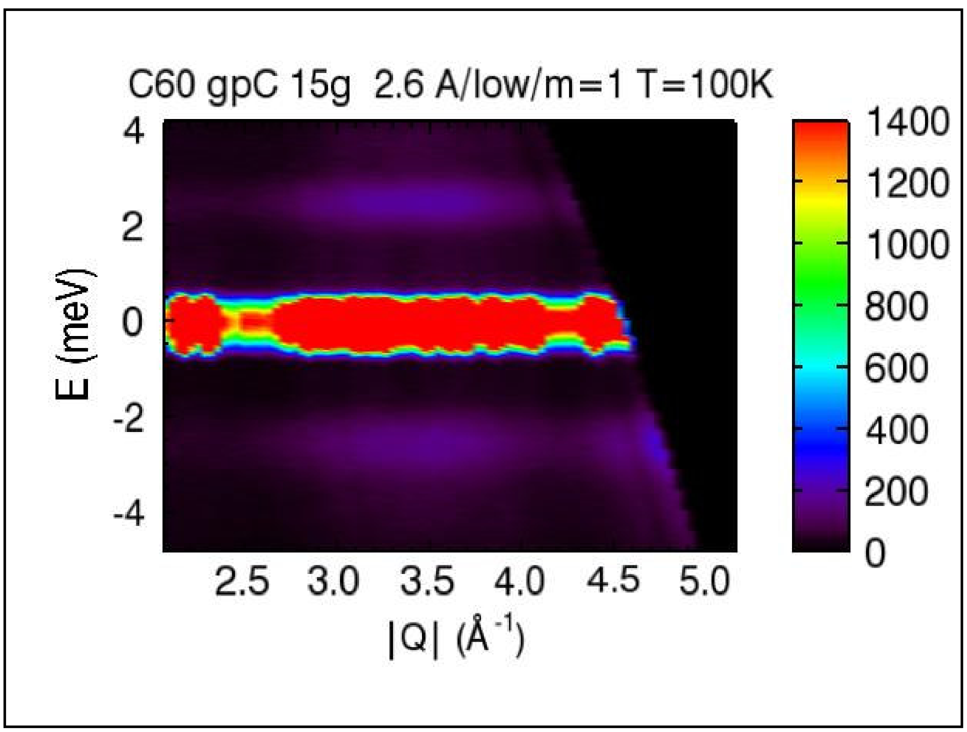
Calculate lattice constant a(T):

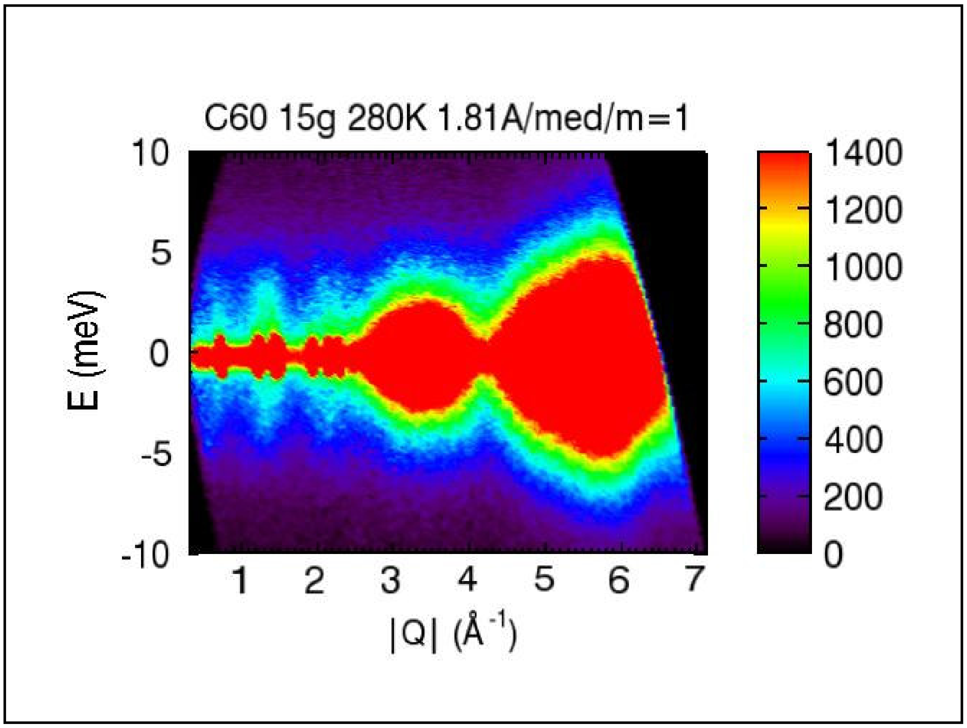
a(T=280K) ~14.2 A; a(T=100K)~14.13A

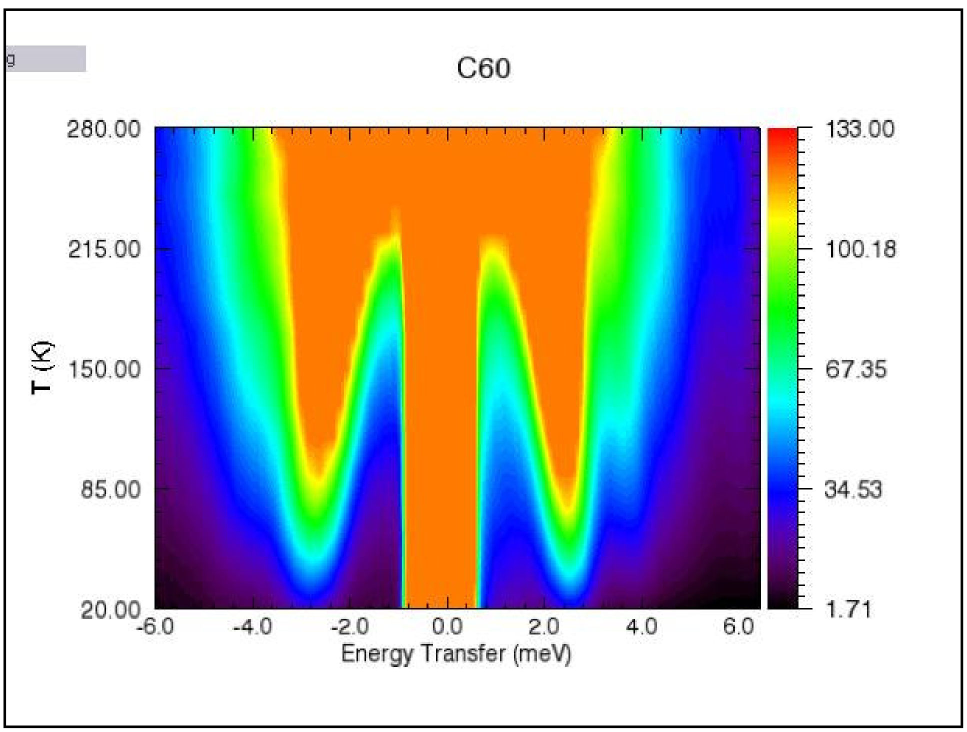
~ 0.7% change in lattice constant

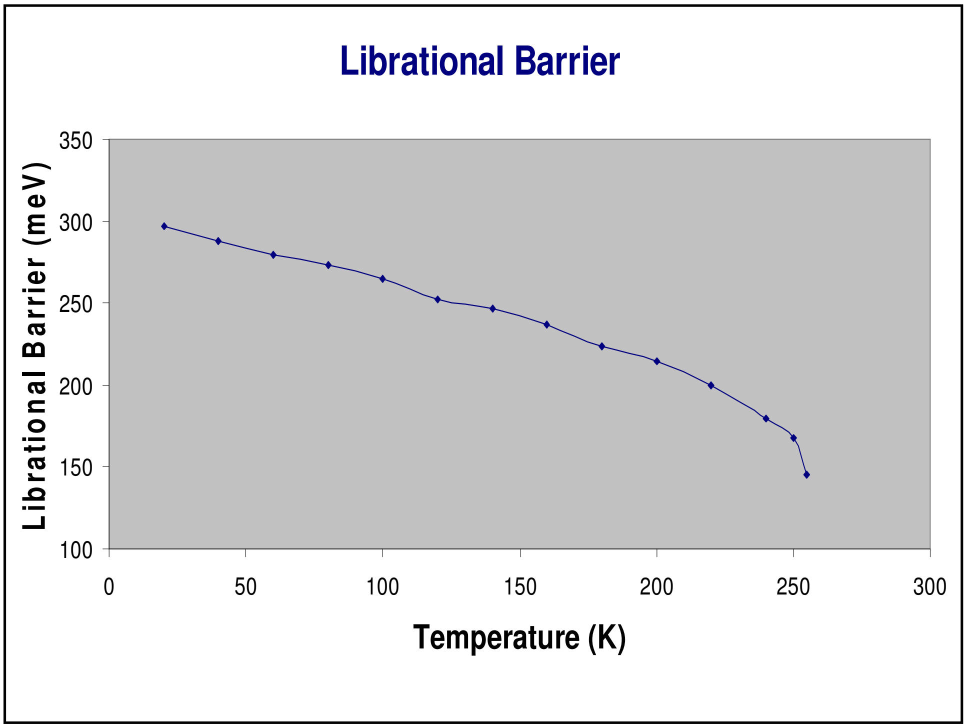


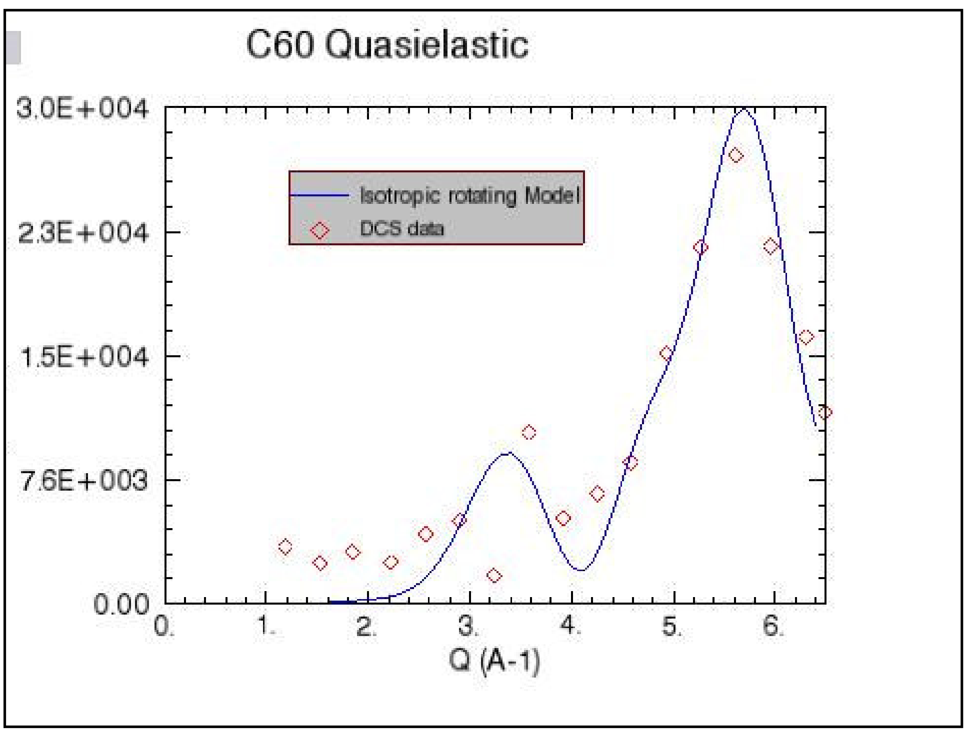

C60 gpC 15g 2.6 A/low/m=1 T=100K
E (meV)
1.0
0.5
0.0
-0.5
-1.0
-1.5
1
2
3
4
5
|Q| (Å^{-1})
1400
1200
1000
800
600
400
200
0


C60 gpC 15g 2.6 A/low/m=1 T=100K
E (meV)
4
2
0
-2
-4
2.5
3.0
3.5
4.0
4.5
5.0
|Q| (Å^{-1})
1400
1200
1000
800
600
400
200
0


C60 15g 280K 1.81A/med/m=1
E (meV)
|Q| (Å^{-1})
10
5
0
-5
-10
1
2
3
4
5
6
7
1400
1200
1000
800
600
400
200
0


C60
T (K)
280.00
215.00
150.00
85.00
20.00
-6.0
-4.0
-2.0
0.0
2.0
4.0
6.0
Energy Transfer (meV)
133.00
100.18
67.35
34.53
1.71


Librational Barrier
Librational Barrier (meV)
350
300
250
200
150
100
0
50
100
150
200
250
300
Temperature (K)


C60 Quasielastic
3.0E+004
2.3E+004
1.5E+004
7.6E+003
0.00
Isotropic rotating Model
DCS data
0.
1.
2.
3.
4.
5.
6.
Q (A-1)