From the Practical I Molecular Spectroscopy, get the benzene Energy CASTEP calculation, which has been prepared, namely the .phonon and .castep files.

This calculation was done using an ICSD Benzene structure and the CASTEP code.

**Generating the Density of States into a NeXus file**

Start MantidPlot and fill in the Algorithm input text entry (just above the Algorithm list) as ‘SimulatedDensityOfStates’. Press the Execute button.

[image of MantidPlot]

[image of SimulatedDebsityOfStates algorithm dialogue box]

Enter the CASTEP file as: csd\_benzen11\_PhonDOS.castep

Enter the PHONON file as: csd\_benzen11\_PhonDOS.phonon

Set the output workspace to something (e.g. blah).

Press the Run button. A new workspace appears in the main Mantid window (e.g. blah).

Right click on it to get the contextual menu, select Plot spectrum, then Plot All. The vDOS is shown.

Right click again and select Export NeXus. Enter a file name, e.g. blah.nxs, press Run.

Now you can close Mantid.

**Converting the vDOS into an S(q,w)**

This step is using Matlab/iFit.

Start Matlab. Ifit is already configured here.

Import the vDOS NeXus file with command (change the file name according to the one you have exported):

* g = iData('/home/mdanse2018/bz\_dos.nxs')

which reads the file and creates a Data Set object called g. Now, the NeXus data is stored as a 2-column array (Intensity), while the energy axis is a vector in cm-1.

We first get the definition of the ‘signal’ which has been guessed from the data file.

* getalias(g, ‘Signal’)

and it says:

Data.mantid\_workspace\_1.workspace.values

which is [3135 x 2]. We only want the 1st column, so we say:

* setalias(g, ‘Signal’, ‘Data.mantid\_workspace\_1.workspace.values(:,1)’ )

We can plot the vDOS:

* plot(g)

Now we convert cm-1 into meV because the method below works with meV. The syntax ‘g{n}’ gets or sets the axis values for dimension ‘n’, here 1 (vector, rows).

* g{1} = g{1}/8.065;

Now ‘g’ is the vDOS in meV. We can apply the incoherent approximation and compute the S(q,w). We have to set the mass of the material in [g/mol] for C6H6, and the Tenmperature as 300 K.

* inc = incoherent(g, ‘m’, 12\*6+6, ‘T’, 300)

Now ‘inc’ is an array of multi-phonon contributions (default is up to 6), which we have to sum up to get the total incoherent S scattering law. We create a new variable ‘sinc’ as the sum of all.

* sinc = plus(inc);

The sinc contains the Bose factor (detailed balance) for T=300. The McStas file can wotk with it, or use symmetric S(q,w) [classical]. Let’s go classical by removing the Bose population.

* sinc = deBosify(sinc);

Now we can plot the incoherent S(q,w) in log10 scale

* plot( log10( sinc ) )

Nice colors, you can rotate the view with the ‘rotate’ toolbar icon (a small circle arrow).

**Export S(q,w) for McStas**

The object must be saved in the Sqw McStas format.

* saveas( sinc, ‘bz\_inc\_castep.sqw’, ‘mcstas’)

The file is written. Now you can close Matlab/iFit. Type ‘exit’.

The density of the material and its cross setion are missing, we must add them in the header of this file. Edit the file with ‘Nedit’ (faster than gedit) or Geany

In the file header 9anywhere, but be logical, go in the Physical parameters section, add:

# weight 78 [g/mol] Material molar weight

# sigma\_inc 80 [barns]

# sigma\_coh 0

# density 0.9

# Temperature 300 [K]

There is already a TEMP keywords which collides with the temperature setting. Remove the TEMP line.

Then save the file. This also sets the coherent scattering to 0, and only remains the incoherent for this simulation.

**Scattering of benzene in a direct ToF spectrometer**

Start McStas.

Open the ‘Neutron Site’ templates/templateTOF instrument (Perl version) or ‘Open from template’ and select that same instrument.\

Click the Edit window and have a look at the instrument. It mostly contains a Source, a Sample (made of 3 shells) and a set of detectors, sensitive to various type of events.

Click Run. The instrument is compiled, and the Run dialogue apperas. Specify an incoming neutron energy of 150 meV, a broadening (energy resolution) of 1.5 meV (1%), and the material should be using the Sqw file we have generated, but no coherent contribution.

coh = NULL

inc = bz\_inc\_castep.sqw

Use 1e7 neutron events. Then press Run. You may as well use MPI to run faster. This takes a few minutes. Press the Plot button and look at the results. Identify the total scattering (Nb container + Al cryostat tail + sample), then the incoherent scattering, and the multiple scattering. The vertical axis is the radial angle, and the horizontal is the absolute neutron energy.

Estimate the proportion of multiple scattering. Is it large ? How can you explain that ? How can this be reduced ?

Perform an other simulation with half radius, and compare. Does it help ?

**Scattering of benzene in TOSCA**

Open the ToscaPreUpgrade\_focused2.out McStas instrument file and Run it. It has a Rubidium sample by default. Change it to benzene and Run with 1e6 events (not more).