MDANSE 2018

Virtual Experiments: Molecular Spectroscopy Practical

In this practical the aim is to use the phonon file from a CASTEP lattice dynamics calculation as a sample. The sample is used for the virtual experiment in a McStas generated TOF indirect geometry inelastic neutron instrument. The sample environments and containers are incorporated as they are used in actual experiments as McStas components. The resultant spectra is plotted in Mantid exactly we do in actual experiment.

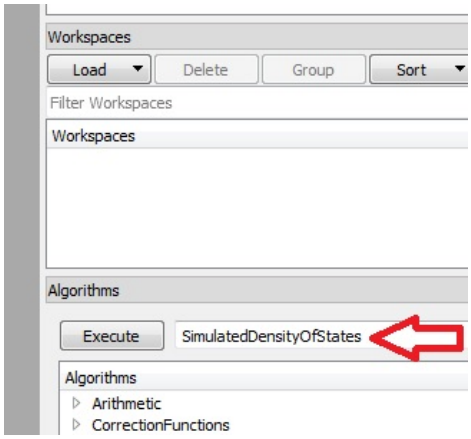
From the Practical I Molecular Spectroscopy, the .phonon and .castep files will be used as generated by the benzene Energy CASTEP calculation. Get those files as prepared previously.

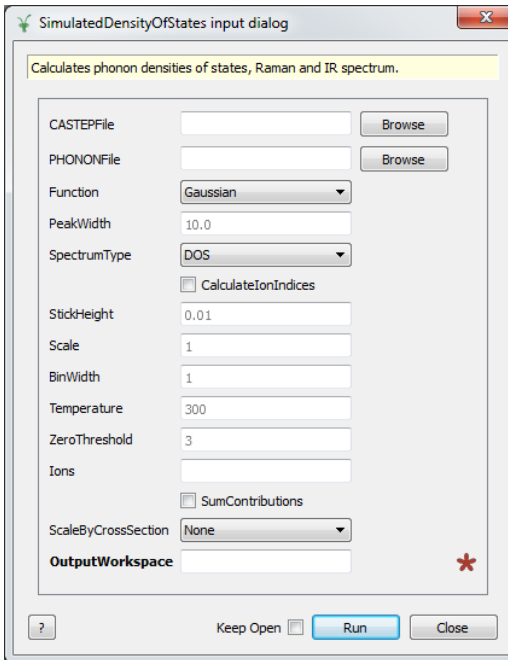
This calculation was done using an ICSD Benzene structure and the CASTEP code.

The McStas instrument is designed as similar to TOSCA in ISIS

Generating the Density of States into a NeXus file from CASTEP phonon file

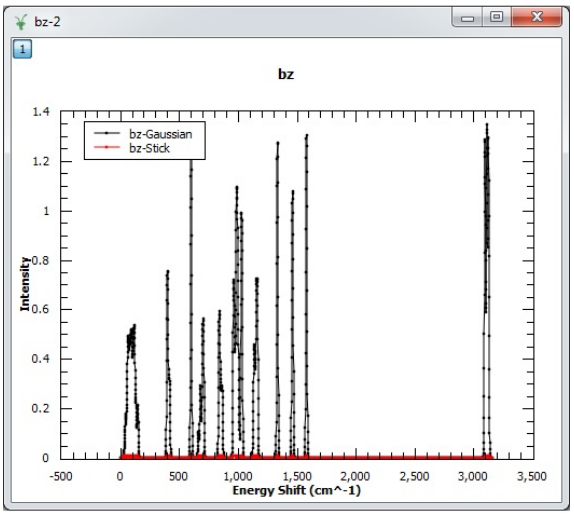
- Start MantidPlot and find the Algorithm (in the input box just above the Algorithm list) 'SimulatedDensityOfStates'. Press the Execute button.





- In the SimulatedDensityOfStates dialog box Enter the CASTEP file as: *csd_benzen11_PhonDOS.castep*
- Enter the PHONON file as: *csd_benzen11_PhonDOS.phonon*

- Keep Spectrum Type : DOS
- Set the output workspace to something (e.g. bz).
- Keep all other parameters as default
- Press the Run button.
  A new workspace appears in the main Mantid WorkSpaces window (e.g. bz).
- Right click on it to get the contextual menu, select Plot spectrum, then Plot All. The vDOS is shown.
- Right click again and select Save NeXus. Enter a file name, e.g. bz_dos.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 Temperature 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’.

Edit the McStas File

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 (or by any editor).

In the file header anywhere, 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 geometry 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 appears. 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.

Q1. Estimate the proportion of multiple scattering. Is it large ? How can you explain that ? How can this be reduced ?

Q2. Perform an other simulation with half radius, and compare. Does it help ?

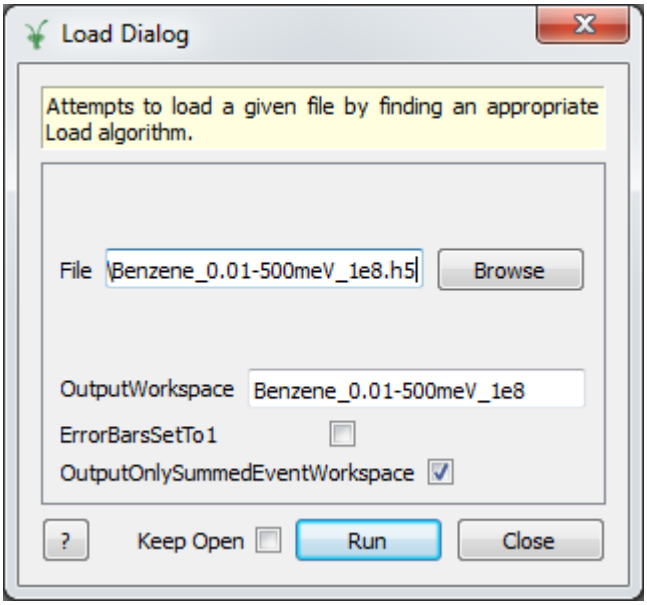
Scattering of benzene in TOSCA using McStas

- Open the ToscaPreUpgrade_focused_modified.instr McStas instrument file and Run it. It has a Rubidium sample by default. Change it to benzene and Run with 1e8 events.

Since the calculation takes some time, a hdf file is supplied, which can be loaded in Mantid for further processing.

Reducing the data from virtual experiment using Mantid

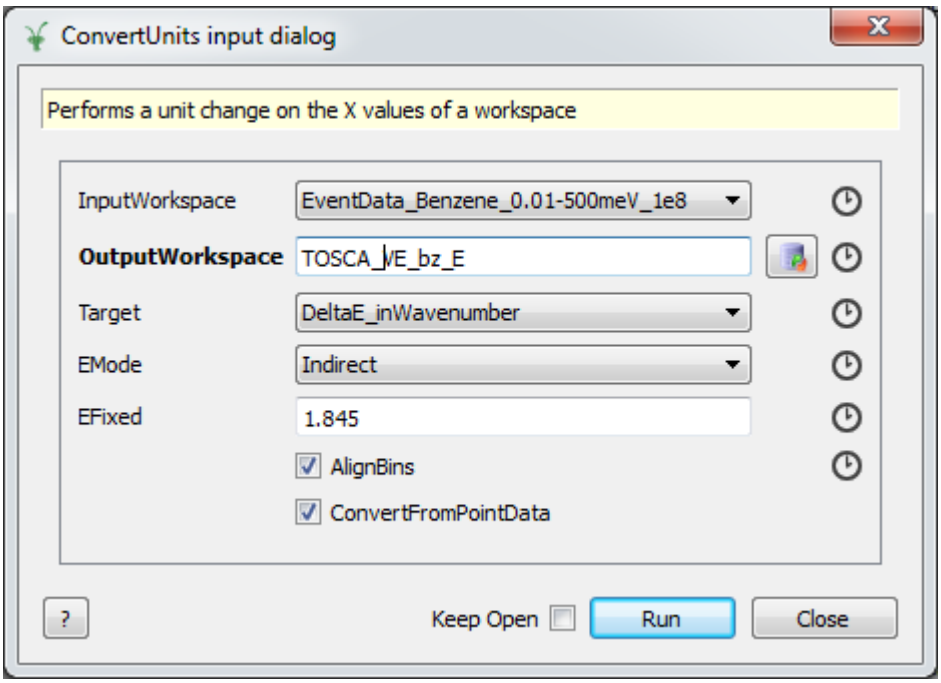
- Open Mantid and Load the hdf file as a File



- The opened dialog will look like above. Keep everything as default and click on Run

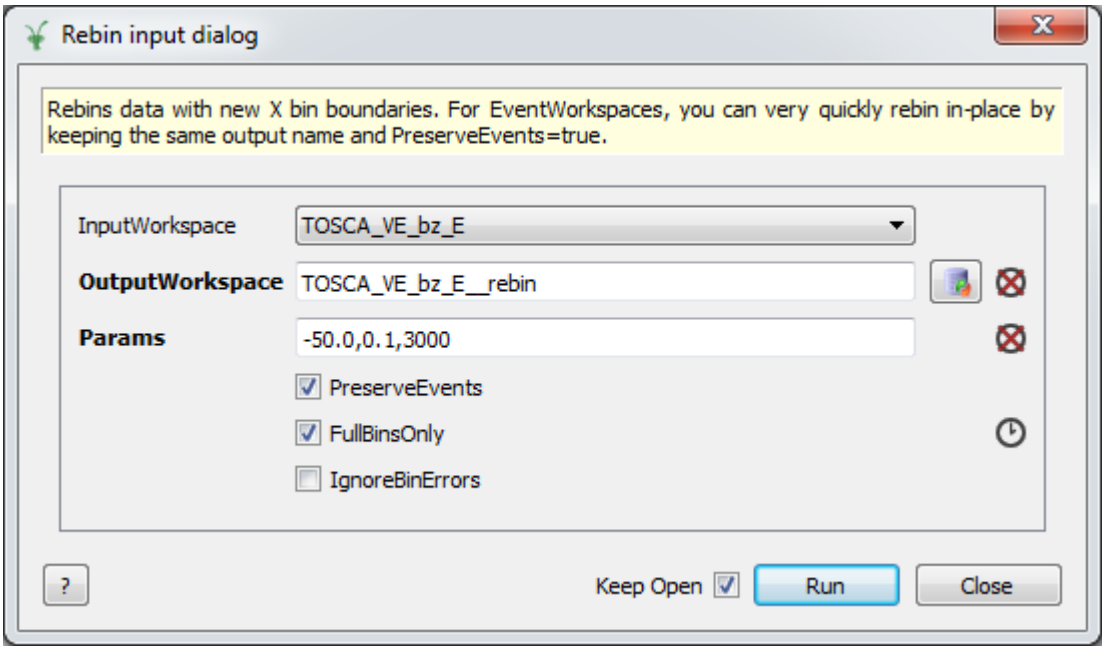
- A new Workspace called Benzene_0.01-500meV_1e8 will be available in the Mantid Workspace region.

- Execute **ConvertUnits** algorithm from the Algothim-> Execute field. The dialog as below will appear. Load the *Benzene_0.01-500meV_1e8* workspace as Input and give any name (such as TOSCA_VE_bz_E) as output. Keep Target as DeltaE_inWavenumberClick on Run.



- A new workspace TOSCA_VE_bz_E will appear in the workspace section

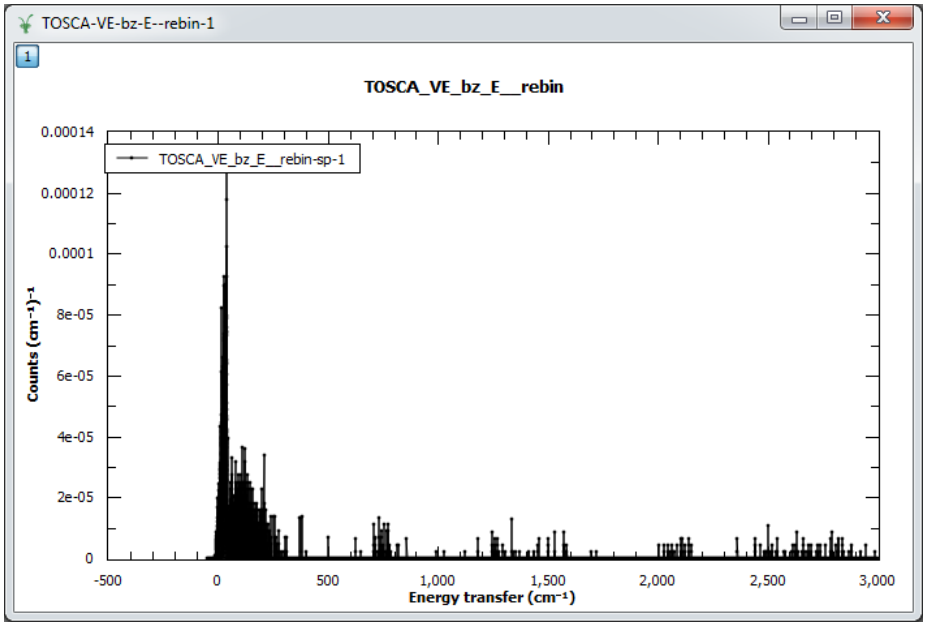
- Execute **Rebin** algorithm from the Mantid Algothim-> Execute field. The dialog will be as below.



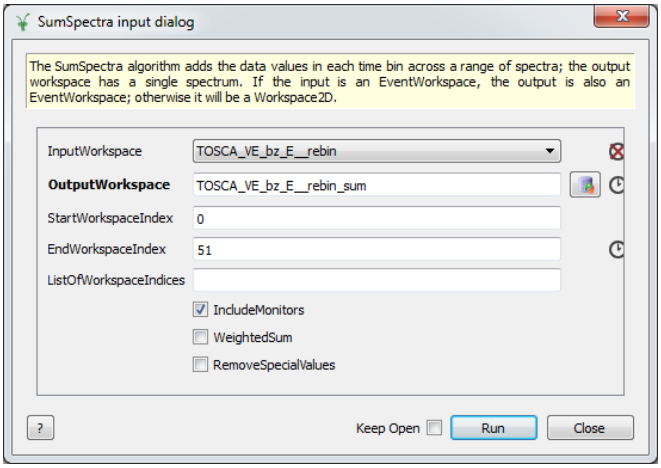
- Load the *TOSCA_VE_bz_E* as Input. Give any name as output or as given in the example *TOSCA_VE_bz_E_rebin* as Output. The rebinning option will be given in the Param field. The entry -50.0,0.1,3000 is for the X-axis range -50.0 to 3000 with bin 0.1. Click on Run.

- A New workspace *TOSCA_VE_bz_E_rebin* will appear as Mantid Workspace.

- Right click on the workspace and select Plot Spectrum. Enter Spectrum number 1 and click OK. The spectrum like below will appear.

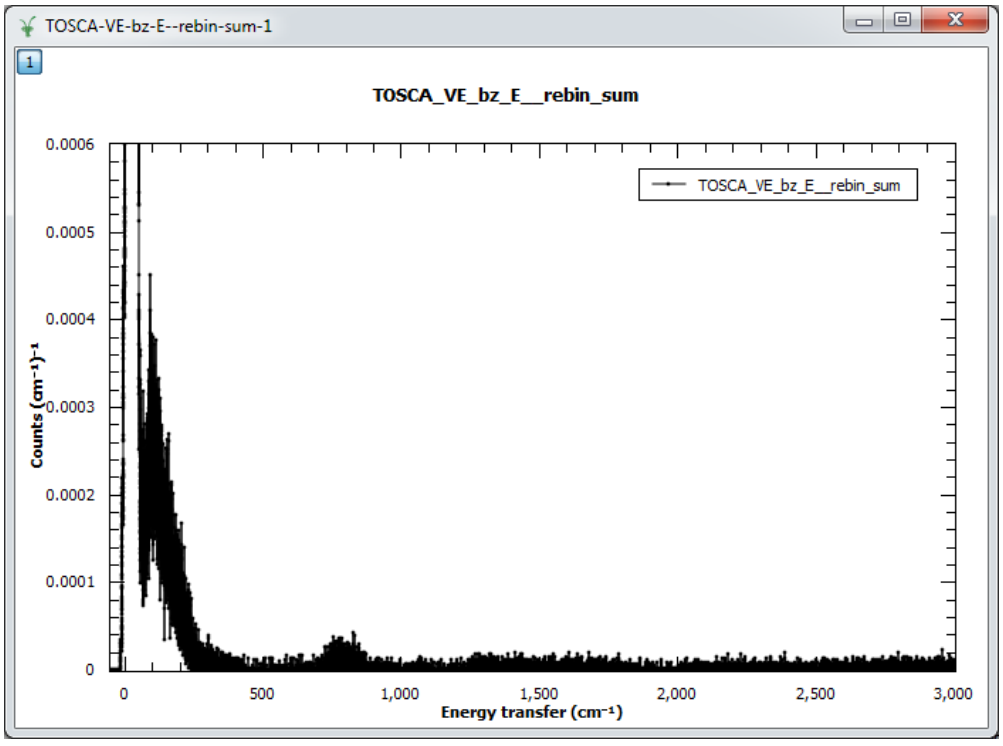


- To reduce the noise in the spectrum we have to sum over all detectors available in the simulations, 0-51. To do that execute SumSpectra algorithm with Input workspace as *TOSCA_VE_bz_E_rebin* and Output workspace as *TOSCA_VE_bz_E_rebin_sum* and click *Run.*

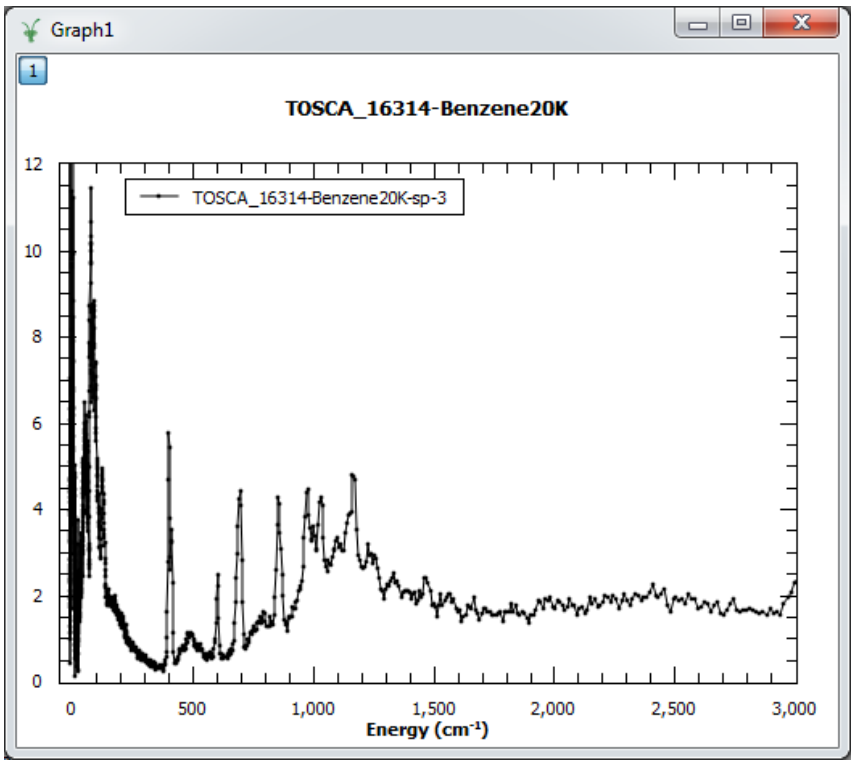


- Right click on the workspace *TOSCA_VE_bz_E_rebin_sum* and select *PlotSpectrum*.

The plot will be found as below:



The plot of the experimental data of benzene as measured on TOSCA is given below. To improve the experiment from virtual experiment one will have to use more realistic description of TOSCA instrument, realistic description of sample environment, more number of neutron events and number of detectors, etc.



More information about the TOSCA instrument can be found here:
https://www.isis.stfc.ac.uk/Pages/tosca.aspx

Database of experimental data measured on TOSCA on
http://wwwisis2.isis.rl.ac.uk/INSdatabase/Theindex.asp

In the same way you can calculate quasielastic spectrum by virtual experiments.