

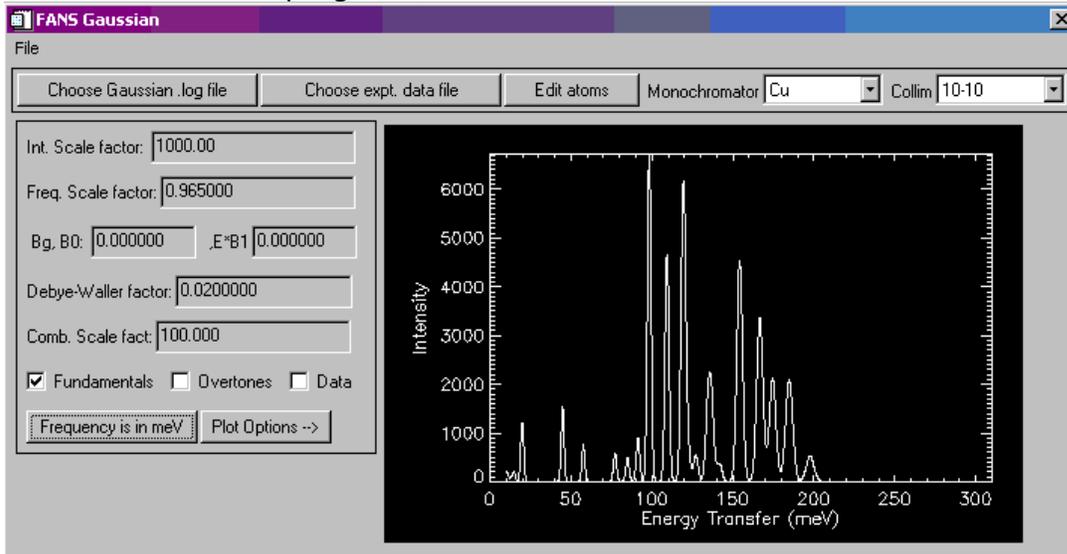
Gaussian98 Analysis within DAVE

Users of FANS can crudely compare vibrational calculations from molecular fragments using the Gaussian98 code within DAVE (Data Analysis and Visualization Environment). This package is freely available from the NIST Center for Neutron Research and can be downloaded from <http://www.ncnr.nist.gov/dave>.

In this document we will describe how and what you need to do.

Getting started

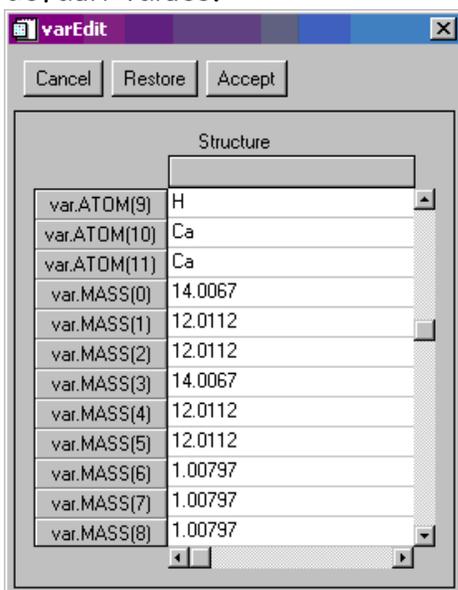
After launching DAVE and selecting the module from Tools-> FANS Tools-> Gaussian98 calculation, you need to load a Gaussian98 LOG file (i.e. the text output from Gaussian98). Since I use Gaussian in one particular style, there may be cases when the program has problems reading how you performed your vibrational analysis. The program can definitely read data from a geometry minimization followed by a frequency calculation. Any other permutations of Gaussian jobs are not guaranteed to work. Data can be loaded from the "Choose expt. data file" button. From the file extension the program will understand to load a .bt4 file, a traditional ICP type .bta file (i.e. all individual detector information from the .bt4 file is removed) or even a .dave file. Any dave file can be read, but this program will only plot the first dimension of an array of data (ideal for FANS, and `_ge.dave` files from the FCS reduction program.)



Upon reading in the atoms, the program assigns a mass and incoherent scattering cross-section to them and, after normalizing the eigenvectors, weighs the vibrational modes accordingly. The default plot is to show the fundamental frequencies of the calculation convoluted with the instrument resolution, but by checking/un-checking the fundamental/overtone/data boxes you can plot (if available) combinations of the three types.

The calculated spectrum can be adjusted for instrument resolution depending on the monochromator used to collect data and the collimations before and after the monochromator. You just select from the drop down list box (bear in mind that even though you can plot calculated spectra for graphite to high energies, this is unfeasible in practice.)

To inspect the atoms use the 'Edit atoms' button from which you can also change mass and scattering cross-section for the calculation. (NOTE: changing the mass of the atom does not alter the normal mode frequencies, only modulating the intensity. Do not expect to get the correct frequencies if you perform a H to D substitution.) The Restore button will reset the default values.



Options

Intensity Scale Factor:

A multiplying factor to get the calculation on the same vertical scale as the experimental data.

Frequency Scale Factor:

It is well known the DFT overestimates the frequencies, so here is an option to set that empirical offset.

Bg:

A linear background added to the calculation defined by $B_0 + B_1 * E$.

Debye-Waller Factor:

A factor that reduces the calculated intensity at higher energy transfers as determined from Debye-Waller.

Combination Scale Factor:

The scaling factor for the combination and overtone spectra that is added to the fundamental spectrum. Typically this is very weak and may just be adding to the background of your data.

The spectra and data can be displayed in either meV or wavenumbers as displayed on the button next to "plot options". The "plot options" button controls text input for the graph axes limits.

To save the calculated spectra, just select File-> "Save spectra as ascii". The output will be your chosen calculation plot array and the infrared intensities if available from the gaussian calculation.