Cross section calculations

This application is used to calculate scattering, absorption and total cross sections, given the chemical formula of a material, its mass density and the wavelength of the neutrons. You can select a chemical formula from an existing database or type in a new formula. Then enter the mass density, packing fraction and wavelength. Various quantities will be displayed, including the molecular weight, the number density, and microscopic and macroscopic cross sections.

The following disclaimer describes what is calculated. The main point, which is not always fully appreciated, is that the total scattering cross section (used, for example, - together with the absorption cross section - to calculate the transmission of a sample) is generally different from the sum of coherent and incoherent bound atom scattering cross sections, which is what this application calculates. (Think of polycrystalline Be, or think of a hydrogenous material such as water.)

Disclaimer

Within this application total scattering cross sections are obtained by summing the total (coherent plus incoherent) bound atom scattering cross sections of the constituent atoms. (There is also an option to exclude the coherent scattering from the total scattering cross section.) This procedure is never completely correct. In general the scattering cross section, which is the double differential scattering cross section integrated over all directions and all final energies, is a function, inter alia, of the incident neutron energy, the temperature of the material, the morphology of the material (e.g. powder, amorphous, single crystal etc), in some cases the orientation of the material, and the chemical and magnetic structures of the material. (Magnetic scattering is not taken into consideration.) For non-hydrogenous materials the procedure is probably (possibly) justified. For hydrogenous materials it should be used with considerable caution.

Total absorption cross sections are obtained by summing the absorption cross sections of the constituent atoms. To the extent that the cross section goes as 1/v this is OK, but for nuclides that have an (n,γ) resonance at thermal neutron energies, e.g. ^{113}Cd, it is not OK.

Chemical formulae

Here are some examples of acceptable syntax for the chemical formula:

V

NaCl

Cu(ClO4)2, i.e. $Cu(ClO_4)_2$

\62Ni0.45Pt0.55, i.e. $^{62}Ni_{0.45}Pt_{0.55}$ (note the use of "\" to specify an isotope)

Na2\11B8O13, i.e. $Na_2{}^{11}B_8O_{13}$

C3H6.6(H2O)5, i.e. $C_3H_{6.6}(H_2O)_5$, more commonly written $C_3H_{6.6}.5H_2O$

CD3COOD (note that "D" and "T" are recognized)

Mn(N(CN)2)2(N2C4D4), i.e. $Mn(N(CN)_2)_2(N_2C_4D_4)$

Fe10(OCD3)20(C2D2O2Cl)10, i.e. $Fe_{10}(OCD_3)_{20}(C_2D_2O_2Cl)_{10}$

Note that a notation such as ".4H2O" will be misinterpreted; for example "Cu(NO3)2.4H2O", intended to denote $Cu(NO_3)_2.4H_2O$, is interpreted as $Cu(NO_3)_{2.4}H_2O$.

Databases

The application uses two databases.

The read-only database "xsecsdb.dat" contains atomic weight, atomic number, abundance and cross section information for elements and isotopes from ^{1}H to ^{248}Cm. The atomic weights, atomic numbers and abundances were imported from the Web page physics.nist.gov/cgi-bin/Compositions/stand_alone.pl?ele=&ascii=ascii2&isotype=some and the cross sections originated with www.ncnr.nist.gov/resources/n-lengths/list.html.

A second database, "chemical_formulae.sav", contains formulae, mass densities and packing fractions. If the "Save formulae, densities etc" button is grayed out this database cannot be modified because the file is write-protected. If the button appears like the other buttons the database can be modified.

- The database is loaded to memory when the application is launched and when the "Restore formulae, densities etc" button is pressed.
- The currently selected item may be removed from the database *in memory* by pressing the "Remove selected item from list" button.
- When a new formula is typed in it is added to the database *in memory*.
- The database in memory may be saved by pressing the "Save formulae, densities etc" button (unless this button is grayed out).
- If the "Exit" button is pressed the database in memory is not saved.

The "Options" menu

- The selections "Express Sigma (1/Sigma) in mm (mm-1)", "Show 1/Sigma values" and "Only include incoherent scattering (exclude coherent)" are self-explanatory.
- The selection "Calculate number density from lattice parameters" is discussed below.
- Selecting "Quit" has the same effect as pressing the "Exit" button; the database in memory is not saved.

The "Information" menu

- The selection "Program description" displays this file.
- The selection "Table of cross sections" displays the contents of "xsecsdb.dat", the read-only database that contains neutron scattering lengths and cross sections as well as abundances, atomic weights and atomic numbers, for ^{1}H to ^{248}Cm. The buttons and menu items should be self-explanatory.

The "pdf reader" menu

- The selection "Define pdf reader" is used to define the user's pdf reader.

Other buttons

There can be occasions when the calculation needs to be updated. This is achieved by pressing the "Calculate cross sections" button.
The "Show details of calculation" button opens a window that shows a breakdown of the calculation in two forms, "unsorted" or "sorted and simplified". Exit by pressing the "Done" button.

Calculating the number density from lattice parameters

Checking "Calculate number density from lattice parameters" in the Options menu opens a "Unit cell volume and number density calculator" window. Given the unit cell parameters a, b, c, α, β, γ, and the number of molecules (formula units) in the unit cell, the number density is calculated, sent to the parent window and used to update the calculation of macroscopic cross sections.
The "Calculate", "Send result" and "Quit" buttons are self-explanatory. If "Calculate number density from lattice parameters" in the main window's Options menu is unchecked, the density and molecular weight are used to compute the number density.