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*hephaestus.pod*



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## NAME

HEPHAESTUS - A souped-up periodic table for the absorption spectroscopist

## SYNOPSIS

Several simple graphical interfaces to the Xray::Absorption package and other tables of atomic data.

In his workshop he has handmaidens he has forged out of gold who can move and who help him in his work. ... With Athena, [Hephaestus is] important in the life of the city. The two [are] the patrons of handicrafts, the arts which along with agriculture are the support of civilization.

Mythology, Edith Hamilton

## DESCRIPTION

Hephaestus is a container for several utilities based on the periodic table of elements and on tables of absorption coefficients. These utilities are generally of interest to the X-ray absorption spectroscopist and are of particular value at the synchrotron.

The Hephaestus window consists of two parts. On the left is a button box containing the buttons used to access the different utilities that Hephaestus offers. On the right is the container displaying whichever utility is selected. To change utilities, simply click on one of the buttons in the button box.

The Units, Resource, and Xsec menus contains selection buttons. The Units menu sets the units used in the various utilities. The choices are energy in electron volts (eV) or wavelength in Angstroms. This sets how units are displayed in the absorption data, formula, and ion chamber utilities. The anomalous scattering and chemical data utilities do not use this setting. The unit setting is also a handy calculator for eV to wavelength and back. Simply type a number into one of the appropriate entry boxes and switch units to do the calculation.

The Resource buttons determine which tables of absorption data will be used for calculations in the absorption data, formula, and ion chamber utilities. The answers should only differ by a few percent between data resources. But it may be useful in some situations to know what these differences are.

The Xsec buttons tell Hephaestus to make computations in the Absorption and Formula pages using the total, photoelectric, coherent, or incoherent cross-sections. This is fully supported when using the Elam and McMaster resources. The Chantler resource combines the coherent and incoherent cross-sections into a single scattering cross-section, thus the scattering cross-section is used if either the coherent or incoherent buttons are selected in the Xsec menu. The other two do not include data about the coherent and incoherent cross-sections. The total cross-section is the sum of the photoelectric, coherent, and incoherent cross-sections. The Ion utility uses the full cross-section.

## Periodic Table of Absorption Data

This utility displays edge and fluorescence line energies for the elements. Simply click on an element in the periodic table and the edge and line energies will be displayed. You can also compute the absorption length of a pure element by specifying an energy value. If you specify an energy value and a thickness, the transmitted fraction at that energy will also be computed.

The absorption length calculation is made assuming the state of the element at standard temperature and pressure. To compute absorption lengths in other states, you should use the formula utility. The density of graphite is used for carbon. For diamond, again, use the formula utility.

## Absorption Lengths of Compounds

This utility computes absorption lengths of compounds using the supplied photon energy along with the chemical formula and density. There is a list of common materials, their formulas, and their densities. Clicking on that list inserts those known data into the appropriate entry boxes. Clicking the "Compute" button will display some information about the materials in the Results box, including the absorption length. If you know the formula and density of your material, you can enter those then click the "Compute" button. Hitting the return key while focus is on any of the formula, density, or energy entry boxes is the same as clicking the "Compute" button.

The formulas can be written with quite a bit of flexibility. Parends and square brackets, as commonly used in chemistry notation, will be interpreted correctly. Subscripted numbers are simply entered in line next to the element symbol or parenthesized group that they modify.

Element symbols **must** be in capitalized form. That is, "Na" is acceptable, but "na", "NA", and "nA" are not. The formula parser uses proper capitalization to determine stoichiometry.

Chemical formulas can also be written using the notation of TeX or INSPEC. This is particularly handy for cutting and pasting from other programs.  $\text{PbTiO}_3$ ,  $\text{PbTiO}_3$ , and  $\text{PbTiO}/\text{sub } 3/$  will be interpreted identically.

To compute the attenuation of the beam from the absorption length, use this formula:

$$\text{attenuation} = \exp(-1 * x / A)$$

where  $x$  is the sample thickness and  $A$  is the absorption length.

For dense materials, the mass required to make a sample that is 1 absorption length thick and 1 square centimeter wide is also reported. This mass is computed for incident photons of the specified energy. To determine the appropriate mass for your sample, multiply by the actual area of your sample and by the desired thickness in absorption lengths. This calculation is merely the product of the density and the absorption length.

### User-supplied data

You can maintain a personal database of materials, their formulas, and densities. If you wish to define a new material or update the data for one of the built-in materials, just click the Add button. This will prompt you for the name of the material then insert that material into the list on the left as well as save it in a file for future use. Any material, including one of the built-ins, can be removed by clicking the Remove button.

### Density and molarity

An alternate calculation is made by selecting "Molarity" from the density option menu. When molarity is chosen, the calculation will be made on the solute of a solution of the specified molarity. In that case, the mass of the formula unit of the sample will be computed and the specified molarity will be used to determine the density of the solute in the solution. When considering a solvated sample, don't forget that the solvent also absorbs photons.

### Computing sample length for unit edge step

If any of the elements in the material has a K or L edge energy within 100 eV of the value supplied in the energy box, the sample length for unit edge step will be calculated. This is done by calculating the total absorption 50 volts above and 50 volts below the edge and subtracting the difference. This difference is converted into the sample length required to make a transmission edge step of 1.

This calculation will be suspect in the odd case where the material has two absorption edges within 50 volts.

When preparing a sample for a transmission measurement, both the absorption length and the unit edge step length should be considered.

### Periodic Table of Chemical Data

This utility is quite simple. Click on an element and several interesting factoids will be reported. That's it.

### Absorption of Ion Chambers

This utility tells you how much of the beam your ion chambers will absorb at a chosen energy and when filled with a combination of two gases. The selection buttons allow you to choose from several standard detector lengths or a length that you provide. The sliders are used to adjust the fractions of two gasses in the chamber. Only the common gasses (He, N<sub>2</sub>, Ne, Ar, Kr, and Xe) are available. As you slide the sliders back and forth to change the mixing fractions, the percentage absorption is reported in the space below the sliders.

The third slider allows you to change the pressure in the ion chamber for the calculation. The pressure slider is measured in Torr. One atmosphere is 760 Torr.

One shortcoming of this utility is that the percentage is not updated as you type the photon energy or the user supplied chamber length. After changing one of those values, hit the return key or tweak any slider to update the calculation.

The photon flux calculation will tell you the flux incident upon the detector using the formula for voltage measured at a given photon energy using a current-to-voltage amplifier (such as a Keithley 527 or 528)

$$V = \frac{e * \text{energy} * \text{flux} * \text{gain}}{\text{ionization\_energy}}$$

The ionization energy is about 32 volts for most gasses and the electron charge  $e$  is about 1.6E-19 Coulombs. The flux calculation uses the result for percent absorption, thus this result is the **net flux** upon the chamber and not the measured flux.

A rule of thumb that sometimes works for the IO chamber is to choose gases such that about 10% of the incident photons are absorbed. That is enough for a good measurement while still leaving most of the photons to interact with the sample. For the transmission chamber, a good rule of thumb is to choose gases that absorb about 2/3 to 3/4 of the photons. This spreads the measurement out more or less evenly over the length of the capacitor plate and still allows some photons to reach the reference chamber. The 2/3 to 3/4 rule works well for the gases in the fluorescence chamber as well.

## Emission Line Transitions

This displays a chart of the electronic transitions corresponding to the various fluorescence emission lines. There is no interactive component to this page. The chart follows Figure 1.1 in the Center for X-Ray Optics *X-Ray Data Booklet*.

## Edge and Line Finders

These utility displays a list of absorption edges or fluorescence lines in order of increasing energy. Clicking the button centers the view of the list box around the edge just below the specified energy. This tool is useful in any situation where you need to know what edge or line is in the vicinity of the specified energy.

It may be useful to know what edge energy is at an integer multiple of the specified energy. For instance, you may be suspicious that a harmonic of the monochromator is exciting an edge in your sample. Suppose you are seeing a feature at about 6000 eV in your spectrum while using a Si(111) monochromator. You might then suspect that the third harmonic at 18000 eV (the Zr K edge is at 17998 eV) is the culprit. To check, enter 6000 in the entry box and click the third harmonic button on the edge finder page.

The information in the edge finder list is the element symbol, the edge symbol, and edge energy. The information in the line finder list is the element symbol, the full Siegbahn line symbol, the IUPAC line designation, a measure of the line intensity, and the line energy. The intensity values are such that all lines of a type (e.g. all K $\alpha$  lines) have intensities which sum to 1. Thus these numbers are — for several reasons — a **very** crude measure of how different lines which are nearby in energy might relate in a real measurement.

Hitting the return key while the focus is on the energy entry box in either page is the same as clicking the "Find it" button.

## Complex Scattering Factors for the Elements

This utility plots the complex corrections to the scattering factors for the elements, i.e. the energy dependent  $f'(E)$  and  $f''(E)$  terms. These functions are tabulated from the Cromer-Lieberman calculations for the isolated, neutral atom. Solid state effects are ignored.

To make plot, click and element. There are selection buttons for plotting one or both parts of the complex scattering function. There are also selection buttons for setting whether the next plot will be a new plot or if it will add to the previous plot.

You can set the energy range of the plot along with the spacing of the grid in energy that is used to interpolate from the tabulated values. Finally, you have the option of convoluting the scattering functions by a Lorentzian of a specified width or, by clicking the checkbox, using the natural line width of the element. Any negative value for the line width will be set to the natural line width.

The most recently displayed complex scattering function can be saved to a file by clicking the button at the bottom of the screen. Only the most recent element and only those parts that were displayed in the most recent plot is saved. The energy range and grid size of the most recent display is used in the output file. To change the element, energy axis, or the parts of the function for a saved file, it is necessary to redisplay the function using the desired parameters.

## Initialization file

The initialization file is `~/horae/hephaestus.ini` on unix or Mac and `C:\Program Files\Ifeffit\horae\hephaestus\hephaestus.ini`.

You can edit this file to change the startup values of several of the parameters used in Hephaestus, including the utility shown at startup and the initial values of the data resource, units, and cross section.

The most important use of the initialization file is to enable or disable the use of Ifeffit in Hephaestus. Set the general-ifeffit parameter to 1 or 0 enable or disable the use of Ifeffit. Disabling Ifeffit removes the  $f'/f''$  utility from the button bar and disables the Cromer-Lieberman entry in the Resources menu.

So why would you want to do that? Well, importing Ifeffit into Hephaestus increases its memory use dramatically. This may be undesirable on a beamline's data collection computer. The Ifeffit-less Hephaestus is quite a bit more slender.

## Keyboard shortcuts

Shortcut	effect
Control-1	display the absorption data utility
Control-2	display the formulas utility
Control-3	display the chemical data utility
Control-4	display the ion chamber utility
Control-5	display the emission line transitions chart
Control-6	display the edge finder utility
Control-7	display the line finder utility
Control-8	display the anomolous scattering utility
Control-0	display the document
Control-q	quit
Alt-F	post the File menu
Alt-U	post the Units menu
Alt-R	post the Resources menu
Alt-X	post the Cross Sections menu
Alt-H	post the Help menu

## BUGS AND MISSING FEATURES

Every calculation at high temperature is inaccurate in Hephaestus. Xray::Absorption does not correctly handle the mass-energy absorption coefficients at high energy, although the ion chamber utility does attempt a crude correction.

More types of information can be added to the chemical data utility. If there is something you would like to see, you should send the data in an easily readable format (i.e. plain text — spreadsheet or word processor files should not be considered "easily readable"). Merely suggesting new data types is unlikely to have any effect. Supplying the data is highly likely to have an effect.

Wish list includes a utility for mirrors and including auger/fluoro branching ratios in one of the periodic table utilities.

## ACKNOWLEDGMENTS

The layout of Hephaestus — with its button bar on the left side which changes the mode of the main part of the program — was inspired by programs I use on my KDE systems. Kontakt and the KDE Control Center use that motif. I found it effective so I swiped it for this program.

The pictures used on the buttons were cropped from images I found using <http://images.google.com/>. The picture of the ion chamber is from Advanced Designed Consulting's web site (<http://www.adc9001.com/index.html>). Their ion chambers are quite nice. The edge finder icon was swiped from the find.png icon in the kid's icon theme for KDE. The line finder icon is from a web page by the Alberta Synchrotron Institute and depicts a fluorescence map of some rock.

The absorption data resources all have literature references.

The Elam tables are from W.T. Elam, B.Ravel, and J.R. Sieber, Radiat. Phys. Chem. v.63 (2002) pp 121-128. This is the source of data for the edge and line finders.

The McMaster tables were published as W.H. McMaster et al. Compilation of X-ray Cross Sections. Lawrence Radiation Laboratory Report UCRL-50174, National Bureau of Standards, pub. (1969). These data were originally compiled in machine readable form by Pathikrit Bandyopadhyay.

The Henke tables are derived from B. L. Henke, E. M. Gullikson, and J. C. Davis, Atomic Data and Nuclear Data Tables Vol. 54 No. 2 (1993). Data is available on the web at [http://www-cxro.lbl.gov/optical\\_constants/](http://www-cxro.lbl.gov/optical_constants/)

The Chantler tables are derived from C. T. Chantler, J. Phys. Chem. Ref. Data 24, 71 (1995) and the data files can be found on the web at <http://physics.nist.gov/PhysRefData/FFast/html/form.html>

The Cromer-Lieberman tables are derived from S. Brennan and P.L. Cowen, Rev. Sci. Instrum, vol 63, p.850 (1992).

The formulas utility owes much to Gerry Roe, who pointed out a bug, and Erik Gullikson, whose similar utility on the web set me straight.

The information used in the chemical data utility is from the kalziumrc file, which was swiped from the Kalzium package. See <http://edu.kde.org/kalzium/> for more details.

Plotting and function generation in the anomalous scattering utility is provided by Matt Newville's Iffeffit.

The ion chamber and edge finder utilities were inspired by the similar utilities in the data acquisition program by Lars Fuerenlid and Johnny Kirkland and in wide use at NSLS. Lars and Johnny seem to have a deeper love of pastel than do I.

The electronic transitions chart was created from scratch but slavishly following Figure 1.1 in the Center for X-Ray Optics *X-Ray Data Booklet*.

Hephaestus makes use of the *Xray::Absorption*, *Chemistry::Formula*, *Iffffit*, and *Iffffit::Tools* modules as well as *Tk* and several things from <http://www.cpan.org>.

And, of course, the users of my various software efforts deserve all the credit for kind praise and useful feedback over these many years.

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