xraydb

Release 4.4

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CONTENTS

XrayDB provides atomic data, characteristic X-ray energies, and X-ray cross sections for the elements in an SQLite3 database, `xraydb.sqlite`. This file can be used directly with SQLite [sqlite] using standard SQL, or from the many programming language that suppor SQLite. A Python module providing such an interface is provided here.

Because some of the components of the database hold arrays of numbers (for example, coefficients for interpolation), the arrays are stored in the database as JSON-encoded strings, and will need to be unpacked to be used.

The project began with the data from the compilation of basic atomic properties and X-ray absorption edge energies, emission energies, and absorption cross sections from [Elam_Ravel_Sieber], who assembled data from a several sources. More data has been added from other sources. Energy widths of core holes for excited electronic levels from [Keski_Krause] and [Krause_Oliver]. Elastic X-ray scattering data, $f_0(q)$ is taken from [Waasmaier_Kirfel]. Resonant scattering cross sections $f'(E)$ and $f''(E)$ and absorption cross sections from [Chantler] as from the FFAST webpage (but on a finer energy grid, data from [Chantler2016]) are also included.

In general, the values here use units that are SI and in common usage in X-ray work. Cross sections are in cm^2/gr, and energies are in eV. Energy-dependent data for cross-sections are typically most reliable between about 250 eV to about 250,000 eV. Elements from Z=1 to 92 are supported, with some data are included for elements between Z=93 and Z=98.

The current version of the XrayDB is **7.0**, and the version of the Python module is 4.4.

See Also:

- PDF Version of this documentation
- XrayDB Github Page has data sources, code, development and issues.
- XrayDB Web App (beta!) is an interactive web page to browse some of the data in this database and make plots of X-ray attenuation, mirror reflectivity, and more.
- *X-ray Periodic Table of the Elements*.

CHAPTER

ONE

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1.1 Installation

The X-ray database is held in the SQLite3 file `xraydb.sqlite`. If you are looking for direct use with SQLite, you can download this from xraydb.sqlite.

If you want to use XrayDB from Python, install the XrayDB Python module (which includes the sqlite database), with:

```
pip install xraydb
```

If you are using Anaconda Python, you can also install with:

```
conda install -c gsecars xraydb
```

Depending on your system and Python installation, you may need administrative privileges to install any python library. For many linux and Mac OS X systems, you may need to use *sudo*.

Note: The Python module supports Python 3.5 and above.

1.1.1 Development Version

To work with the data sources or to add or modify data in the XrayDB, you will want to clone or download the full source code kit xrayDB on github.com which contains the current database, original source data, python module, and files for generating the Periodic Table posters. To get the latest development version, use:

```
git clone https://github.com/xraypy/XrayDB.git
```

1.1.2 Testing

There are a set of tests scripts for the Python interface that can be run with the pytest testing framework. These are located in the `python/tests` folder. These tests are automatically run as part of the development process. For any release or any master branch from the git repository, running `pytest` should run all of these tests to completion without errors or failures.

1.1.3 Copyright, Licensing, and Re-distribution

```
Public Domain

To the extent possible, the data, code, and documentation here are placed in
the public domain.  No claim of copyright is made by the authors and no
restrictions of any kind placed on the use of the work here.

The original sources of the data are mostly based on published works with
the clear intent of providing data to the general public.  Some of the
datasets have may not have clear statements of copyright or license, but
have been freely available for many years. The work here is a compilation
and reformatting of those datasets.

If you use these resources and wish to cite the original data source, please
see the documentation for more details.
```

1.2 X-ray Periodic Table of the Elements

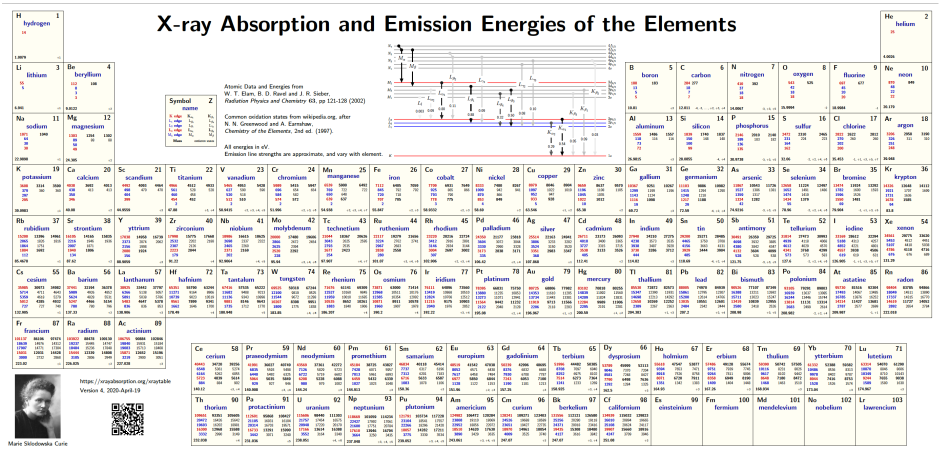
XrayDB has been used to generate X-ray Periodic Tables of the Elements.

There is a choice of two sizes, and a choice of an image of one of four prominent scientists associated with the Periodic Table and X-ray spectroscopies.

Table of X-ray Periodic Tables of the Elements The poster comes in two sizes: Large is 127.5x61 cm (about 50x24 inches) and Medium is 91x45.5 cm (about 36x17 inches).

Scientist	Large Periodic Table	Medium Periodic Table
Charles Barkla	Barkla (Large)	Barkla (Medium)
Marie Curie	Curie (Large)	Curie (Medium)
Dmitri Mendeleev	Mendeleev (Large)	Mendeleev (Medium)
Henry Moseley	Moseley (Large)	Moseley (Medium)

In general, these table look like this:



but you should definitely download the PDFs linked for high-quality results.

1.3 Example Calculations of X-ray properties of materials

Here, a few detailed examples of using the *xraydb.sqlite* to calculate the X-ray properties of materials are shown. These all use the functions in the python *xraydb* module, which is describe in more detail in the next chapter, *Using XrayDB from Python*. The examples will explore some aspects of X-ray physics, but will not give a complete tutorial on the concepts here. For reference see [AlsNielson_McMorrow2011] for example. Some of these calculations are also available at XrayDB Web App (beta!).

1.3.1 X-ray attenuation by elements

The XrayDB database tabulates values of the X-ray mass attenuation coefficient, μ/ρ, for each element. In most of the X-ray regime used in materials characterization (say, up to 150 keV), the photo-electric effect is the main process that causes X-ray attenuation. When the photo-electric process is dominant, the values for μ/ρ depends strongly on Z of the atom and on X-ray energy E. In addition to these strong dependencies, sharp increases – so-called absorption edges – with be see at energies of bound core electron levels of atoms. To illustrate these characteristics, the following script will plot μ/ρ for selected elements:

```
#!/usr/bin/env python
# XrayDB example script python/examples/mu_elements.py
#
# plot X-ray mass attenuation for selected elements
#
import numpy as np
import matplotlib.pyplot as plt
import wxmplot.interactive as wi
from xraydb import mu_elam , atomic_symbol

energy = np.arange(500, 120000, 10)  # energy in eV

for elem in ('C', 'Cu', 'Au'):
    mu = mu_elam(elem, energy)
    plt.plot(energy, mu, label=elem, linewidth=2)

plt.title('X-ray mass attenuation')
plt.xlabel('Energy (eV)')
plt.ylabel(r'$\mu/\rho \rm\, (cm^2/gr)$')
plt.legend()
plt.yscale('log')
plt.xscale('log')
plt.show()
```

As you can see in Figure from this figure, the attenuation drops very strongly with E – approximately as E^3. μ also depends strongly with Z, though the sharp absorption edges make this more complicated.

You can also observe that at relatively high energies for relatively low-Z elements (such as C above about 20 keV) that the attenuation levels off. This is because the coherent (Rayleigh) and incoherent (Compton) scattering processes dominate, so that the photo-electric absorption is no longer the dominant X-ray scattering process. This can be illustrated by plotting the different components of μ/ρ for C, as with the following script:

```
#!/usr/bin/env python
# XrayDB example script python/examples/mu_components_C.py
#
# plot components of X-ray mass attenuation for C
#
import numpy as np
```

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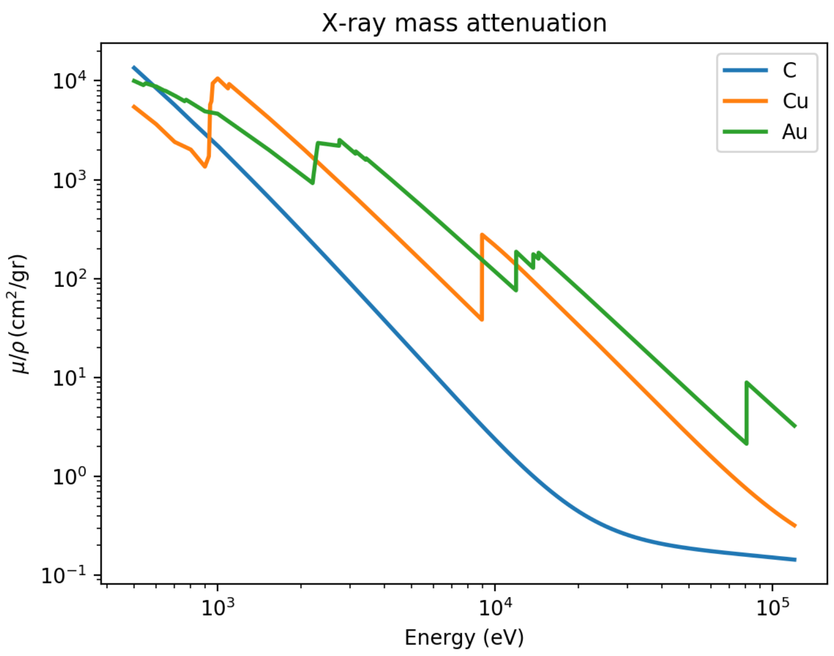

Fig. 1: X-ray mass attenuation coefficient for C, Cu, and Au.

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```
import matplotlib.pyplot as plt
from xraydb import mu_elam

energy = np.arange(500, 120000, 10)  # energy in eV

elem = 'C'
mu_total = mu_elam(elem, energy, kind='total')
mu_photo = mu_elam(elem, energy, kind='photo')
mu_incoh = mu_elam(elem, energy, kind='incoh')
mu_coher = mu_elam(elem, energy, kind='coh')

plt.title('X-ray mass attenuation for %s' % elem)
plt.plot(energy, mu_total, linewidth=2, label='Total')
plt.plot(energy, mu_photo, linewidth=2, label='Photo-electric')
plt.plot(energy, mu_incoh, linewidth=2, label='Incoherent')
plt.plot(energy, mu_coher, linewidth=2, label='Coherent')

plt.xlabel('Energy (eV)')
plt.ylabel(r'$\mu/\rho \rm\, (cm^2/gr)$')
plt.legend()
plt.yscale('log')
plt.show()
```

which will generate the following plot:

Note that above 20 keV, the photo-electric absorption and incoherent Compton contributions are about equal, and that the Compton scattering dominates above 50 keV. As shown above, the photo-electric scattering will be much higher for heavier elements. The Rayleigh and Compton scattering have a much weaker dependence on *Z*, so that the photo-electric process dominates to higher energies. Replacing ‘C’ with ‘Fe’ in the script above will generate the following

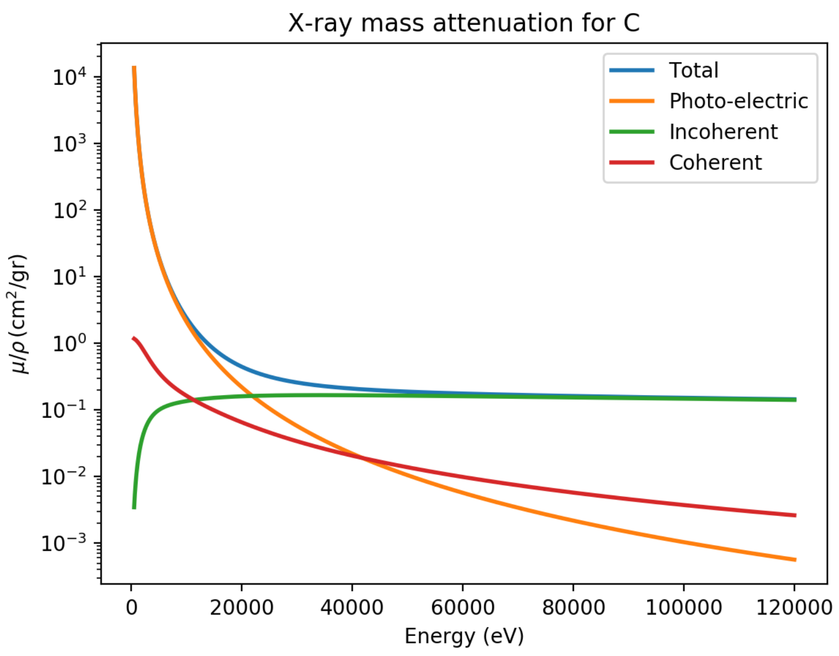

Fig. 2: X-ray scattering and attenuation factors for C.

plot:

which shows that the Compton scattering reaching about 0.1 to 0.25 $\mathrm{cm}^2/\mathrm{gr}$ for Fe, about the same value as it was for C, while the photo-electric cross-section dominates past 100 keV.

1.3.2 μ calculations for materials

While one can use the above values for μ/ρ to calculate the attenuation of X-rays by multi-element materials, the `material_mu()` function is available to do the more convenient calculation of the X-ray absorption coefficient μ in units of 1/cm for a material and energy value and density (which are known for several common materials). This gives the length for which X-ray intensity is reduced by a factor of e, and so can be used to calculate the fraction of the X-rays transmitted through a material of known thickness, as $\exp(-t\mu)$ for a material of thickness t. As a first example, we calculate the the fraction of X-ray transmitted through 1 mm of the water as a function of X-ray energy:

```
#!/usr/bin/env python
# XrayDB example script    python/examples/mu_water.py
#
# calculate the fraction of X-rays transmitted through 1 mm of water
#
import numpy as np
import matplotlib.pyplot as plt

from xraydb import material_mu

energy = np.linspace(1000, 41000, 201)

mu = material_mu('H2O', energy)

# mu is returned in 1/cm
```

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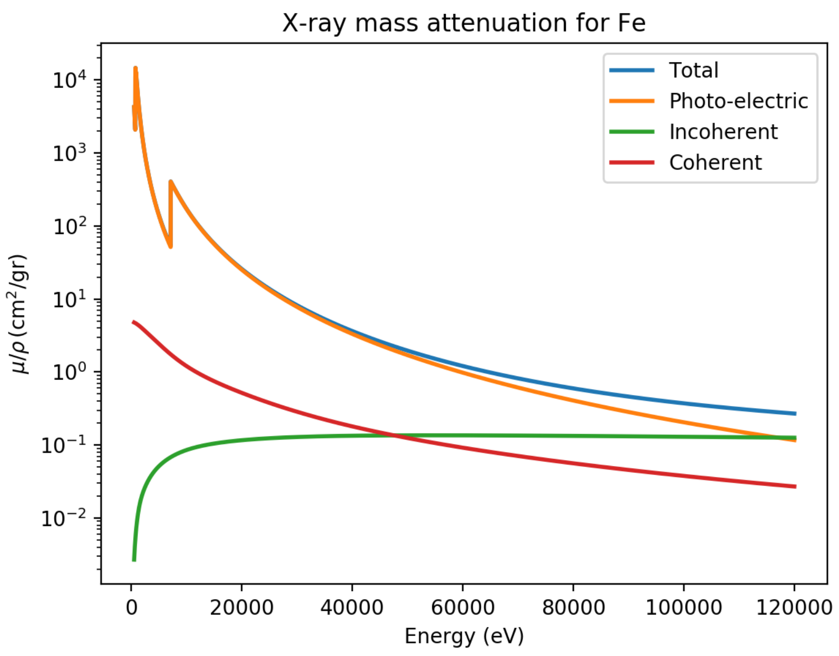

Fig. 3: X-ray scattering and attenuation factors for Fe.

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```
trans = np.exp(-0.1 * mu)

plt.plot(energy, trans, label='transmitted')
plt.plot(energy, 1-trans, label='attenuated')
plt.title('X-ray absorption by 1 mm of water')
plt.xlabel('Energy (eV)')
plt.ylabel('Transmitted / Attenuated fraction')
plt.legend()
plt.show()
```

replacing:

```
mu = material_mu('H2O', energy)
```

with:

```
mu = material_mu('CaCO3', energy, density=2.71)
```

would generate the following plot

For many X-ray experiments, selecting the size of a material size so that its thickness is approximately 1 to 2 absorption length is convenient so that X-ray scattering and emission can be observed strongly, with neither all primary and scattered X-rays being absorbed by the material itself, but also not simply passing through the material without any interaction. For example, one can simply do:

```
>>> from xraydb import material_mu
>>> mu_20kev = xraydb.material_mu('CaCO3', 20000, density=2.71)
>>> print("CaCO3 1/e depth at 20keV = {:.3f} mm".format(10/mu_20kev))
CaCO3 1/e depth at 20keV = 0.648 mm
```

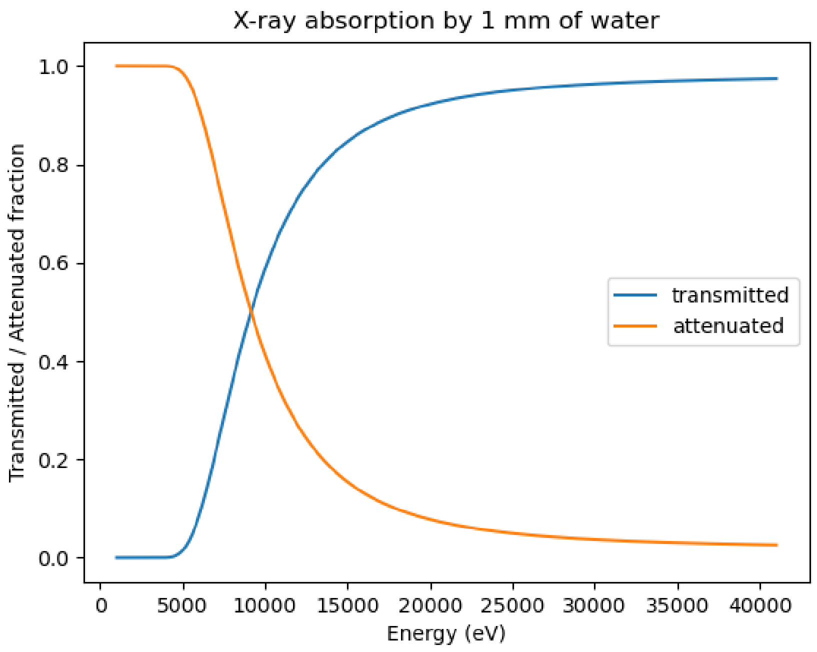

Fig. 4: Fraction of X-rays absorbed and transmitted by water

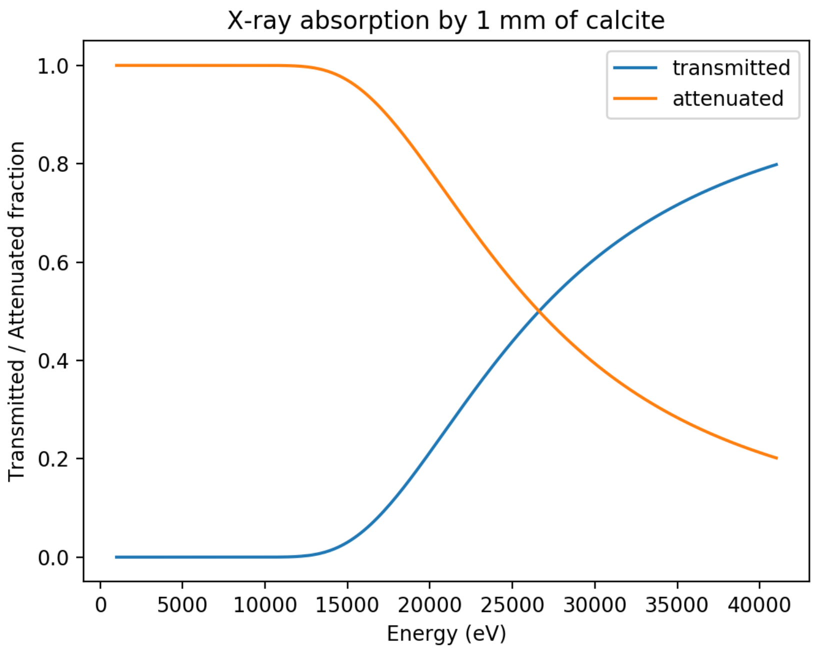

Fig. 5: Fraction of X-rays absorbed and transmitted by calcite

1.3.3 Ionization chamber calculation of X-ray flux

A gas-filled ionization chamber is a widely used form an X-ray detector, used because it is simple, cheap, and can absorb a fraction of an incident X-ray beam and be linear in estimating the photon flux over many orders of magnitude. X-rays entering a chamber filled with an inert gas (often a He, N2, or one of the noble gases, or a mixture of two of these) will be partially absorbed by the gas, with the strong energy dependence shown above. The absorption will *ionize* the gas, generating free electrons and energetic ions. In fact, the first ionization will generate an electron-ion pair with the energy of the X-ray minus the binding energy of the core electron, but the high-energy electron and ion will further ionize other gas molecules. With an electric potential (typically on the order of 1 kV /cm) across the chamber, a current can be measured that is proportional to the X-ray energy and fluence of the X-rays.

The process of converting the photo-current into X-ray fluence involves several steps. First, the energy from a single X-ray generates a number of electron-ion pairs given by the *effective ionization potential* of the gas. These are reasonably well-known values (see [Knoll2010]) that are all between 20 and 40 eV, given in the *Table of Effective Ionization Potentials*.

Table of Effective Ionization Potentials. Many of these are taken from [Knoll2010], while others appear to come from International Commission on Radiation Units & Measurement, Report 31, 1979. The names given are those supported by the functions `ionization_potential()` and `ionchamber_fluxes()`.

gas name(s)	potential (eV)
hydrogen, H	36.5
helium, He	41.3
nitrogen, N, N2	34.8
oxygen, O, O2	30.8
neon, Ne	35.4
argon, Ar	26.4
krypton, Kr	24.4
xenon, Xe	22.1
air	33.8
methane, CH4	27.3
carbondioxide, CO2	33.0

From this, we can see that the absorption of 1 X-ray of energy 10 keV will generate about 300 electron-ion pairs. That is not much current, but if 10^8 Hz are absorbed per second, then the current generated will be around 5 nA. Of course, the thickness of the gas or more importantly the length of gas under ionizing potential will have an impact on how much current is generated. The photo-current will then be amplified and converted to a voltage using a current amplifier, and that voltage will then recorded by a number of possible means. Note that while the ion chamber itself will be linear over many orders of magnitude of flux (provided the potential between the plates is high enough), a current amplifier at a particular setting of sensitivity will be linear only over a couple orders of magnitude (typically between output voltage of 0.05 to 5 V). Because of this, the sensitivity of the ion chamber current amplifier needs careful attention.

The function `ionchamber_fluxes()` will help generate X-ray fluxes associated with an ion chamber and help handle all of these subtle issues, using the following inputs:

- *gas*: the gas, or mixture of gases, used.
- *length*: the length of the ion chamber, in mm.
- *energy*: the X-ray energy, in eV.
- *volts*: the output voltage of the current amplifier
- *sensitivity* and *sensitivity_units*: the sensitivity or gain of the amplifier used to convert the photo-current to the recorded voltage.

The default *sensitivity_units* is 'A/V' but can be set to any of the common SI prefixes such as 'p', 'pico', 'n', 'nano', μ, (unicode '03bc'), 'u', 'micro', 'm', or 'milli', so that:

```
>>> fluxes = ionchamber_fluxes('N2', volts=1, energy=10000, length=100,
                               sensitivity=1.e-9)
>>> fluxes = ionchamber_fluxes('N2', volts=1, energy=10000, length=100,
                               sensitivity=1, sensitivity_units='nA/V')
```

will give the same results.

The output from `ionchamber_fluxes()` is a named tuple with 3 fiels:

- *photo* - the flux absorbed by the photo-electric effect, in Hz.
- *incident* - the flux incident on the ion chamber, in Hz.
- *transmitted* - the flux beam leaving the ion chamber, in Hz.

Note that the ion chamber current is generated only by the photo-electric effect, which dominates for heavy elements and relatively low X-ray energies, but does not necessarily dominate at high X-ray energies for gases such as helium, nitrogen which are often used in ion chambers. The coherent and incoherent scattering processes are included in the calculations done in `ionchamber_fluxes()` so that estimated incident flux from the measured current can be somewhat larger than if only the photo-electric effect was considered.

As an example calculation of ion chamber currents:

```
>>> fluxes = ionchamber_fluxes(gas='nitrogen', volts=1.25, energy=18000,
                               length=100.0, sensitivity=1.e-6)
>>> print("Incident flux= %g Hz" % fluxes.incident)
Incident flux= 1.1632e+11 Hz
>>> print("Downstream flux= %g Hz" % fluxes.transmitted)
Incident flux= 1.1632e+11 Hz
>>> print("Downstream flux= %g Hz" % fluxes.transmitted)
Downstream flux= 1.05463e+11 Hz

>>> print("Absorbed Photo flux= %g Hz" % fluxes.photo)
Absorbed Photo flux= 7.54182e+09 Hz
>>> print("Scattered flux= %g Hz" % (fluxes.incident - fluxes.transmitted - fluxes.
↪photo))
Scattered flux= 3.31569e+09 Hz
```

As for the example for carbon above, the non-photo-electric effects are not negligible for nitrogen at 18 keV.

It is not uncommon for an ion chamber to be filled with a mixture of 2 or more gases so as to better control the fraction of X-rays absorbed in a chamber of fixed length. This can be specified by passing in a dictionary of gas name and fractional density, as with:

```
>>> fluxes = ionchamber_fluxes(gas={'N2':0.75, 'Ar': 0.25}, volts=1.25,
                               energy=18000, length=100,
                               sensitivity=0.2, sensitivity_units='microA/V')
>>> "%g" % fluxes.incident
'1.77786e+10'
```

Finally, the pressure of the gas is sometimes adjusted to alter the fraction of the beam absorbed. The calculations here all use the densities at STP, but changes in gas density will be exactly linear to changing the length of the ion chamber.

1.3.4 X-ray mirror reflectivities

At very shallow angles of incidence X-rays can be reflected by total external reflection from a material. The reflectivity can be very high at relatively low energies and shallow angles, but drops off dramatically with increasing energy, increasing angle, and decreasing electron density. Still, this reflectivity is one of the few ways to steer X-ray beams and so is widely used in synchrotron radiation sources.

The reflectivity can be calculated with the `mirror_reflectivity()` function which takes X-ray energy, incident angle, and mirror material as arguments.

An example script, comparing the energy-dependence of the reflectivity for a few common mirror materials is given as

```
import numpy as np
from xraydb import mirror_reflectivity
import matplotlib.pyplot as plt

energy = np.linspace(1000, 51000, 501)

r_si = mirror_reflectivity('Si', 0.002, energy)
r_ni = mirror_reflectivity('Ni', 0.002, energy)
r_rh = mirror_reflectivity('Rh', 0.002, energy)
r_pt = mirror_reflectivity('Pt', 0.002, energy)

plt.plot(energy, r_si, label='Si')
plt.plot(energy, r_ni, label='Ni')
plt.plot(energy, r_rh, label='Rh')
plt.plot(energy, r_pt, label='Pt')

plt.title('X-ray reflectivity at $\\theta=2 \mathrm{mrad}$')
plt.xlabel('Energy (eV)')
plt.ylabel('Reflectivity')
plt.legend()
plt.show()
```

1.3.5 Darwin widths of monochromator crystals

Bragg's law describes X-ray diffraction from crystals as

$$m\lambda = 2d\sin(\theta)$$

where λ is the X-ray wavelength, d the d-spacing of the crystal lattice plane, θ the incident angle, and m the order of the reflection. For imperfect crystals, in which the lattice planes are not stacked perfectly over extended distances, the angular width of any particular reflection is dominated by the spread in d-spacing and the mosaicity inherent in the crystal. For perfect crystals, however, the angular width of a reflection is dominated by the fact that effectively all of the X-rays will scatter from the lattice well before any attenuation of the X-ray beam occurs. This *dynamical* diffraction gives a finite angular width to reflection usually called the Darwin width (named for Charles G. Darwin, grandson of the more famous Charles R. Darwin). In addition, the refraction and absorption effects that give anomalous scattering (as calculated with `xray_delta_beta()`) give non-symmetric attenuation of this reflectivity.

All of these effects are included in the `darwin_width()` function, which follows very closely the description from chapter 6.4 in [AlsNielson_McMorrow2011]. The function takes inputs of

- *energy*: the X-ray energy, in eV.
- *crystal*: the atomic symbol for the crystal: 'Si', 'Ge', or 'C'. ['Si']
- *hkl*: a tuple with (h, k, l) of the reflection used. [(1, 1, 1)]

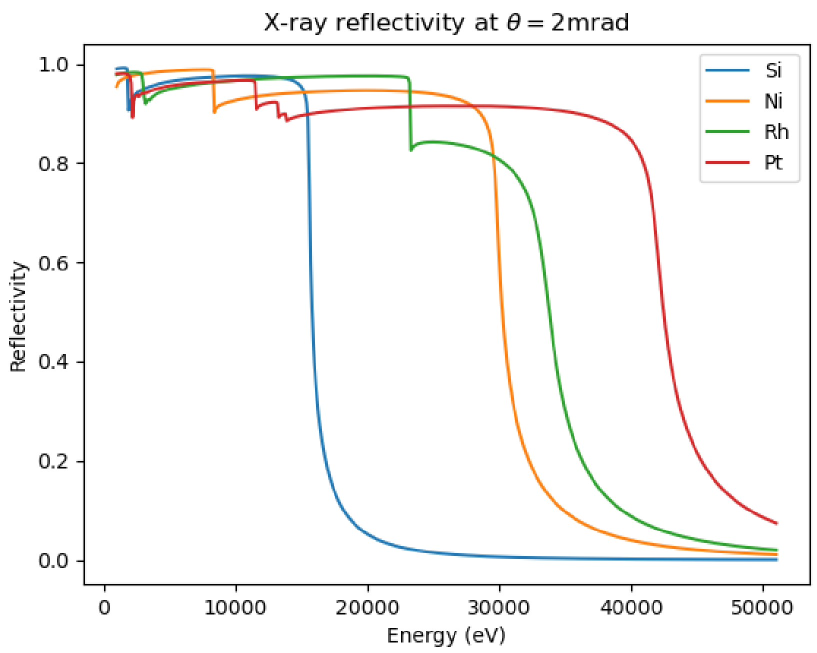

Fig. 6: X-ray mirror reflectivity at $\theta = 2\mathrm{mrad}$ for selected mirror surfaces and coatings used for mirrors.

- *m*: the order of the reflection. [1]

As with `ionchamber_fluxes()`, the output here is complicated enough that it is put into a named *DarwinWidth* tuple that will contain the following fields:

- *theta* - the nominal Bragg angle, in rad
- *theta_fwhm* - estimated angular Darwin width, in rad
- *energy_fwhm* - estimated energy Darwin width, in eV
- *zeta* - nd-array of $\zeta = \Delta\lambda/\lambda$.
- *dtheta* - nd-array of angles around from Bragg angle, in rad
- *denergy* - nd-array of energies around from Bragg energy, in eV
- *intensity* - nd-array of reflected intensity at *zeta* values.

Here, *dtheta* will be given by $\Delta\theta = \zeta\tan(\theta)$, and *denergy* will be given by $\Delta E = \zeta E$. All of the nd-arrays will be the same size, so that plots of reflectivity can be readily made. An example usage, printing the predicted energy and angular widths and plotting the intensity profile or "rocking curve" is

```
import numpy as np
from xraydb import darwin_width
import matplotlib.pyplot as plt

dw_si111 = darwin_width(10000, 'Si', (1, 1, 1))
dw_si333 = darwin_width(10000, 'Si', (1, 1, 1), m=3)

fmt_string = "Darwin Width for {:s} at {:.0f} keV: {:.2f} microrad, {:.2f} eV"
print(fmt_string.format('Si(111)', 10, dw_si111.theta_fwhm*1e6,
                        dw_si111.energy_fwhm))
```

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```
print(fmt_string.format('Si(333)', 10, dw_si333.theta_fwhm*1e6,
                        dw_si333.energy_fwhm))


dtheta  = dw_si111.dtheta*1e6
denergy = dw_si111.denergy[::-1]

#  slightly advanced matplotlib hackery:
fig, ax = plt.subplots(constrained_layout=True)


ax.plot(dtheta, dw_si111.intensity, label='Si(111)', linewidth=2)
ax.plot(dw_si333.dtheta*1e6, dw_si333.intensity, label='Si(333)', linewidth=2)

ax.set_title('X-ray diffraction intensity at 10keV')
ax.set_xlabel('Angle ($ \mu \mathrm{rad}$)')
ax.set_ylabel('Reflectivity')
ax.legend()

def foreward(x): return np.interp(x, dtheta, denergy)
def backward(x): return np.interp(x, denergy, dtheta)

axtop = ax.secondary_xaxis('top', functions=(foreward, backward))
axtop.set_xlabel('Energy (eV)')

plt.show()
```

which will print out values of:

```
Darwin Width for Si(111) at 10 keV: 20.84 microrad, 1.03 eV
Darwin Width for Si(333) at 10 keV: 2.32 microrad, 0.11 eV
```

and generates a plot of

Note here that the width of the 3rd harmonic peak is specified not as the Si (3, 3, 3) peak, but as the (1, 1, 1) peak with m=3, as we want to ensure that the Bragg angle used is for the (1, 1, 1) reflection.

1.4 Using XrayDB from Python

The *python* directory contains the source code for a Python module for XrayDB. This module gives a user-friendly wrapping of the XrayDB, and automates the the conversion of data from sqlite database into Python and numpy arrays. The module requires the *numpy*, *scipy* and *sqlalchemy* modules, all of which are readily available and can be installed with:

```
pip install xraydb
```

The current version of the Python module is 4.4, corresponding to version 6 of *xraydb.sqlite*.

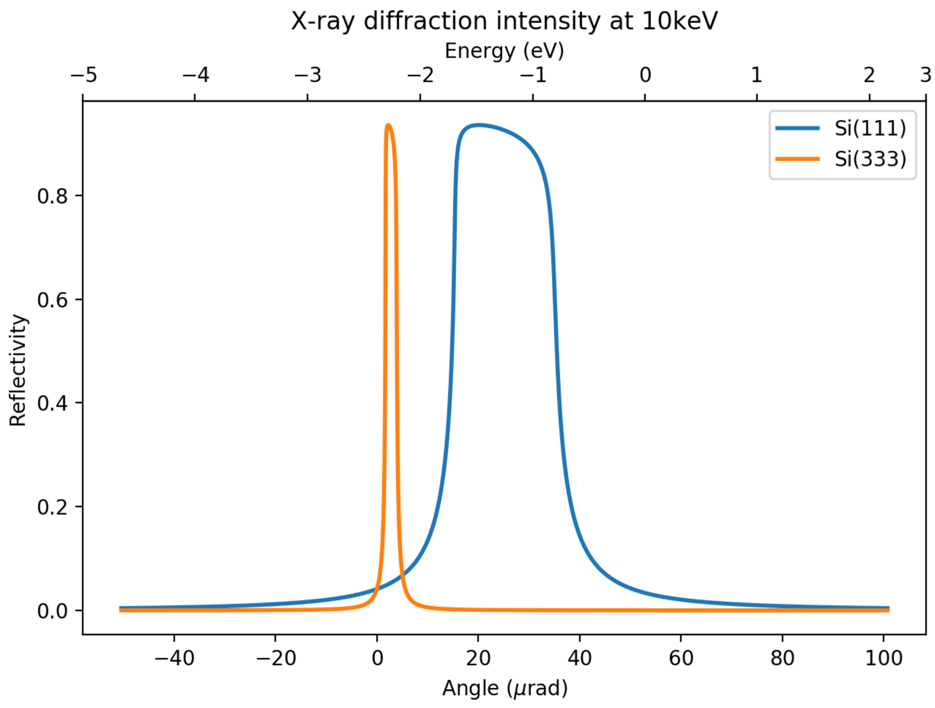

Fig. 7: X-ray monochromator diffracted intensities around the Si(111) reflection.

1.4.1 The Python xraydb module

To use the XrayDB from Python, you can import the *xraydb* module and start using it:

```
>>> import xraydb
>>> xraydb.atomic_number('Ag')
47
#
# X-ray elastic (Thomson) scattering factors:
>>> import numpy as np
>>> q =np.linspace(0, 5, 11)
>>> xraydb.f0('Fe', q)
array([25.994603  , 11.50848469,  6.55945765,  4.71039413,  3.21048827,
        2.20939146,  1.65112769,  1.36705887,  1.21133507,  1.10155689,
        1.0035555 ])
#
# X-ray emission lines:
>>> for name, line in xraydb.xray_lines('Zn', 'K').items():
...     print(name, ' = ', line)
...
Ka3  =  XrayLine(energy=8462.8, intensity=0.000316256, initial_level='K', final_level=
↪'L1')
Ka2  =  XrayLine(energy=8614.1, intensity=0.294353, initial_level='K', final_level='L2
↪')
Ka1  =  XrayLine(energy=8637.2, intensity=0.576058, initial_level='K', final_level='L3
↪')
Kb3  =  XrayLine(energy=9567.6, intensity=0.0438347, initial_level='K', final_level=
↪'M2')
Kb1  =  XrayLine(energy=9570.4, intensity=0.0846229, initial_level='K', final_level=
↪'M3')
```

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```
Kb5  =  XrayLine(energy=9648.8, intensity=0.000815698, initial_level='K', final_level=
↪'M4,5')
#
# X-ray absorption edges:
>>> xraydb.xray_edge('As', 'K')
XrayEdge(energy=11867.0, fyield=0.548989, jump_ratio=7.314)
#
# X-ray attenuation factors:
>>> as_kedge = xraydb.xray_edge('As', 'K').energy
>>> energies = np.linspace(-50, 50, 5) + as_kedge
>>> muvals = xraydb.mu_elam('As', energies)
>>> for en, mu in zip(energies, muvals):
...     print("{:.0f}   {:8.2f}".format(en, mu))
...
11817      26.07
11842      25.92
11867      25.77
11892     178.32
11917     177.38
```

Table of XrayDB function for Atomic and X-ray data for the elements

Most of these function return some element-specific property from the element symbol or atomic number. Some of the data extends to Z=98 (Cf), but some data may not be available for Z > 92 (U). Except where noted, the data comes from [Elam_Ravel_Sieber].

xraydb functions	description
atomic_number()	atomic number from symbol
atomic_symbol()	atomic symbol from number
atomic_mass()	atomic mass
atomic_density()	density of pure element
f0()	elastic scattering factor ([Waasmaier_Kirfel])
f0_ions()	list of valid "ions" for *f0()* ([Waasmaier_Kirfel])
xray_edge()	xray edge data for a particular element and edge
xray_edges()	dictionary of all X-ray edges data for an element
xray_lines()	dictionary of all X-ray emission line data for an element
fluor_yield()	fluorescent yield for an X-ray emission line
ck_probability()	Coster-Kronig transition probability between two atomic levels
mu_elam()	absorption cross-section, photo-electric or total for an element
coherent_cross_section_elam()	coherent scattering cross-section for an element
incoherent_cross_section_elam()	incoherent scattering cross-section for an element
chantler_energies()	energies of tabulation for Chantler data ([Chantler])
f1_chantler()	$f'(E)$ anomalous scattering factor ([Chantler])
f2_chantler()	$f''(E)$ anomalous scattering factor ([Chantler])
mu_chantler()	absorption cross-section ([Chantler])
guess_edge()	guess element and edge from energy of absorption edge
chemparse()	parse a chemical formula to atomic abundances
validate_formula()	test whether a chemical formula can be parsed.
get_materials()	get a dictionary of known materials {name:(formula, density)}
get_material()	get a (formula, density) tuple for a material in the materials database
find_material()	get a material instance for a material in the materials database
add_material()	add a material to local materials database
material_mu()	absorption cross-section for a material at X-ray energies

continues on next page

Table 1 – continued from previous page

xraydb functions	description
`material_mu_components()`	dictionary of elemental components of *mu* for material
`xray_delta_beta()`	anomalous index of refraction for material and energy
`darwin_width()`	Darwin widths for monochromator crystals
`mirror_reflectivity()`	X-ray reflectivities for mirror materials (thick slab limit)
`ionization_potential()`	effective ionization potential for a gas, as for ion chambers
`ionchamber_fluxes()`	calculate fluxes from ion chamber voltages, gases, and sensitivities

get_xraydb()
return instance of the XrayDB

Returns XrayDB

Example

```
>>> import xraydb
>>> xdb = xraydb.get_xraydb()
```

1.4.2 Atomic Properties

atomic_number(*element*)
z for element name

Parameters **element** (*str*) – atomic symbol

Returns atomic number

atomic_symbol(*z*)
atomic symbol for atomic number

Parameters **z** (*int*) – atomic number

Returns atomic symbol

atomic_mass(*element*)
molar mass for an element

Parameters **element** (*int, str*) – atomic number, atomic symbol for element

Returns atomic mass, in AMU

atomic_density(*element*)
density (gr/cm^3) for common for of an element

Parameters **element** (*int, str*) – atomic number, atomic symbol for element

Returns density in gm/cm^3

1.4.3 Elastic Scattering Factors

f0 (*ion*, *q*)

elastic X-ray scattering factor, f0(q), for an ion.

Parameters

- **ion** (*int or str*) – atomic number, atomic symbol or ionic symbol of scatterer
- **q** (*float, ndarray*) – Q value(s) for scattering

Returns scattering factor for each Q value

Notes

1. from D. Waasmaier and A. Kirfel, Acta Cryst. A51 p416 (1995) and International Tables for Crystallography, Vol. C.
2. *ion* can be of the form: 26, *Fe*, *Fe2+*. For a full list of ions use *f0_ions()*
3. elements supported are from Z = 1 to 98 ('H' to 'Cf')
4. q = sin(theta) / lambda, where theta=incident angle, lambda=X-ray wavelength

f0_ions (*element=None*)

list ion names supported in the f0() calculation from Waasmaier and Kirfel.

Parameters element (*None, int, str*) – scatterer

Returns list of strings for matching ion names

Notes

if element is None, all 211 ions are returned.

1.4.4 X-ray Edges

xray_edge (*element*, *edge*, *energy_only=False*)

get x-ray absorption edge data for an element: (energy(in eV), fluorescence yield, jump ratio)

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **edge** (*str*) – iupac symbol of X-ray edge
- **energy_only** (*bool*) – whether to return only the energy [False]

Returns XrayEdge namedtuple containing (energy, fluorescence_yield, edge_jump) or float of energy

xray_edges (*element*)

get dictionary of x-ray absorption edges: energy(in eV), fluorescence yield, and jump ratio for an element.

Parameters element (*int, str*) – atomic number, atomic symbol for element

Returns dictionary of XrayEdge named tuples.

Notes

1. The dictionary will have keys of edge (iupac symbol) and values containing an XrayEdge namedtuple containing (energy, fluorescence_yield, edge_jump)

`core_width`(*element*, *edge=None*)
returns core hole width for an element and edge

Parameters

- **`element`** (*`int or str`*) – element
- **`edge`** (*`None or str`*) – edge to consider

Returns core width or list of core widths

Notes

1. if edge is None, values are return for all edges
2. Data from Krause and Oliver (1979) and Keski-Rahkonen and Krause (1974)

`guess_edge`(*energy*, *edges=['K', 'L3', 'L2', 'L1', 'M5']*)
guess an element and edge based on energy (in eV)

Parameters

- **`energy`** (*`float`*) – approximate edge energy (in eV)
- **`edges`** (*`None or list of strings`*) – edges to consider

Returns a tuple of (atomic symbol, edge) for best guess

Notes

by default, the list of edges is ['K', 'L3', 'L2', 'L1', 'M5']

1.4.5 X-ray Emission Lines

`xray_lines`(*element*, *initial_level=None*, *excitation_energy=None*)
get dictionary of X-ray emission lines of an element

Parameters

- **`element`** (*`int, str`*) – atomic number, atomic symbol for element
- **`initial_level`** (*`None or str`*) – iupac symbol of initial level
- **`excitation_energy`** (*`None or float`*) – exciation energy

Returns dict of X-ray lines with keys of siegbahn notation and values of XrayLine tuples of (energy, intensity, initial level, final level)

Notes

1. excitation energy will supercede initial_level, as it means ‘all intial levels with below this energy

Exaample:

```
>>> for name, line in xraydb.xray_lines('Mn', 'K').items():
...     print(name, line)
...
Ka3 XrayLine(energy=5769.9, intensity=0.000265963, initial_level='K', final_
↪level='L1')
Ka2 XrayLine(energy=5889.1, intensity=0.293941, initial_level='K', final_
↪level='L2')
Ka1 XrayLine(energy=5900.3, intensity=0.58134, initial_level='K', final_level=
↪'L3')
Kb3 XrayLine(energy=6491.8, intensity=0.042234, initial_level='K', final_
↪level='M2')
Kb1 XrayLine(energy=6491.8, intensity=0.0815329, initial_level='K', final_
↪level='M3')
Kb5 XrayLine(energy=6537.0, intensity=0.000685981, initial_level='K', final_
↪level='M4,5')
```

fluor_yield(*element*, *edge*, *line*, *energy*)

fluorescence yield for an X-ray emission line or family of lines.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **edge** (*str*) – iupac symbol of X-ray edge
- **line** (*str*) – siegbahn notation for emission line
- **energy** (*float*) – incident X-ray energy

Returns fluorescence yield, weighted average fluorescence energy, net_probability

Examples

```
>>> xraydb.fluor_yield('Fe', 'K', 'Ka', 8000)
0.350985, 6400.752419799043, 0.874576096
```

```
>>> xraydb.fluor_yield('Fe', 'K', 'Ka', 6800)
0.0, 6400.752419799043, 0.874576096
```

```
>>> xraydb.fluor_yield('Ag', 'L3', 'La', 6000)
0.052, 2982.129655446868, 0.861899000000000
```

See also:

xray_lines which gives the full set of emission lines (‘Ka1’, ‘Kb3’, etc) and probabilities for each of these.

ck_probability(*element*, *initial*, *final*, *total=True*)

transition probability for an element, initial, and final levels.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element

- **initial** (*str*) – iupac symbol for initial level
- **final** (*str*) – iupac symbol for final level
- **total** (*bool*) – whether to include transitions via possible intermediate levels [True]

Returns transition probability, or 0 if transition is not allowed.

1.4.6 Absorption and Scattering Cross-sections

mu_elam(*element*, *energy*, *kind='total'*)

X-ray mass attenuation coefficient, mu/rho, for an element and energy or array of energies. Data is from the Elam tables.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **energy** (*float or ndarray*) – energy or array of energies
- **kind** (*str*) – type of cross-section to use, one of ('total', 'photo', 'coh', 'incoh') ['total']

Returns float value or ndarray

Notes

1. Values returned are in units of cm^2/gr
2. The default is to return total attenuation coefficient.

coherent_cross_section_elam(*element*, *energy*)

coherent scaattering cross-section for an element and energy or array of energies. Data is from the Elam tables.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **energy** (*float or ndarray*) – energy or array of energies

Returns float value or ndarray

Notes

1. Values returned are in units of cm^2/gr

incoherent_cross_section_elam(*element*, *energy*)

incoherent scaattering cross-section for an element and energy or array of energies. Data is from the Elam tables.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **energy** (*float or ndarray*) – energy or array of energies

Returns float value or ndarray

Notes

1. Values returned are in units of cm^2/gr

chantler_energies(*element*, *emin=0*, *emax=1000000000.0*)
energies at which Chantler data is tabulated for a particular element.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **emin** (*float*) – lower bound of energies (default=0)
- **emax** (*float*) – upper bound of energies (default=1.e9)

Returns ndarray of energies

Notes

energies are in eV

f1_chantler(*element*, *energy*, ***kws*)
real part of anomalous x-ray scattering factor for an element and energy or array of energies. Data is from the Chantler tables.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **energy** (*float or ndarray*) – energy or array of energies

Returns float value or ndarray

Notes

1. Values returned are in units of electrons

f2_chantler(*element*, *energy*)
imaginary part of anomalous x-ray scattering factor for an element and energy or array of energies. Data is from the Chantler tables.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **energy** (*float or ndarray*) – energy or array of energies

Returns float value or ndarray

Notes

1. Values returned are in units of electrons

mu_chantler (*element*, *energy*, *incoh=False*, *photo=False*)
X-ray mass attenuation coeficient, mu/rho, for an element and energy or array of energies. Data is from the Chantler tables.

Parameters

- **element** (*int, str*) – atomic number, atomic symbol for element
- **energy** (*float or ndarray*) – energy or array of energies
- **incoh** (*bool*) – whether to return only the incoherent contribution [False]
- **photo** (*bool*) – whether to return only the photo-electric contribution [False]

Returns float value or ndarray

Notes

1. Values returned are in units of cm^2/gr
2. The default is to return total attenuation coefficient.

1.4.7 Chemical and Materials database

chemparse (*formula*)
parse a chemical formula to a dictionary of elemental abundances

Parameters **formula** (*str*) – chemical formula

Returns dict of element symbol and abundance.

Examples

```
>>> from xraydb import chemparse
>>> chemparse('Mn(SO4)2(H2O)7)')
{'H': 14.0, 'S': 2.0, 'Mn': 1, 'O': 15.0}
```

```
>>> chemparse('Zn1.e-5Fe3O4')
{'Zn': 1e-05, 'Fe': 3.0, 'O': 4.0}
```

```
>>> chemparse('CO')
{'C': 1, 'O': 1}
>>> chemparse('Co')
{'Co': 1}
```

```
>>> chemparse('co')
ValueError: unrecognized element or number:
co
```

validate_formula (*formula*)
return whether a chemical formula is valid and can be parsed to a dictionary with chemparse()

Parameters **`formula`** (*str*) – chemical formula

Returns bool (True or False) for whether chemparse() will succeed

Examples

```
>>> from xraydb import validate_formula
>>> validate_formula('Mn(SO4)2(H2O)7)')
True
```

```
>>> validate_formula('Mn(SO4)2(H2O7')
False
```

```
>>> validate_formula('Z')
False
```

`get_materials` (*force_read=False*, *categories=None*)
get dictionary of all available materials

Parameters

- **`force_read`** (*bool*) – whether to force a re-reading of the materials database [False]
- **`categories`** (*list of strings or None*) – restrict results to those that match category names

Returns dict with keys of material name and values of Materials instances

Examples

```
>>> for name, m in xraydb.get_materials().items():
...     print(name, m)
...
water H2O 1.0
lead Pb 11.34
aluminum Al 2.7
kapton C22H10N2O5 1.42
polyimide C22H10N2O5 1.42
nitrogen N 0.00125
argon Ar 0.001784
...
```

`find_material` (*name*)
look up material name, return material instance

Parameters **`name`** (*str*) – name of material or chemical formula

Returns material instance

Examples

```
>>> xraydb.find_material('kapton')
Material(formula='C22H10N2O5', density=1.42, name='kapton', categories=['polymer
↪'])
```

See also:

get_material()

get_material(*name*)
look up material name, return formula and density

Parameters **name** (*str*) – name of material or chemical formula

Returns chemical formula, density of material

Examples

```
>>> xraydb.get_material('kapton')
('C22H10N2O5', 1.43)
```

See also:

find_material()

add_material(*name*, *formula*, *density*, *categories=None*)
add a material to the users local material database

Parameters

- **name** (*str*) – name of material
- **formula** (*str*) – chemical formula
- **density** (*float*) – density
- **categories** (*list of strings or None*) – list of category names

Returns None

Notes

the data will be saved to $HOME/.config/xraydb/materials.dat in the users home directory, and will be useful in subsequent sessions.

Examples

```
>>> xraydb.add_material('becopper', 'Cu0.98e0.02', 8.3, categories=['metal'])
```

1.4.8 X-ray properties of materials

For some further examples, see *Example Calculations of X-ray properties of materials*.

material_mu (*name*, *energy*, *density=None*, *kind='total'*)
X-ray attenuation length (in 1/cm) for a material by name or formula

Parameters

- **name** (*str*) – chemical formul or name of material from materials list.
- **energy** (*float or ndarray*) – energy or array of energies in eV
- **density** (*None or float*) – material density (gr/cm^3).
- **kind** (*str*) – 'photo' or 'total' for whether to return the photo-absorption or total cross-section ['total']

Returns absorption length in 1/cm

Notes

1. material names are not case sensitive, chemical compounds are case sensitive.
2. mu_elam() is used for mu calculation.
3. if density is None and material is known, that density will be used.

Examples

```
>>> material_mu('H2O', 10000.0)
5.32986401658495
```

material_mu_components (*name*, *energy*, *density=None*, *kind='total'*)
material_mu_components: absorption coefficient (in 1/cm) for a compound

Parameters

- **name** (*str*) – chemical formul or name of material from materials list.
- **energy** (*float or ndarray*) – energy or array of energies in eV
- **density** (*None or float*) – material density (gr/cm^3).
- **kind** (*str*) – 'photo' or 'total'for whether to return photo-absorption or total cross-section ['total']

Returns

dict for constructing mu per element, with elements 'mass' (total mass), 'density', and

'elements' (list of atomic symbols for elements in material). For each element, there will be an item (atomic symbol as key) with tuple of (stoichiometric fraction, atomic mass, mu)

Examples

```
>>> xraydb.material_mu('quartz', 10000)
50.36774553547068
>>> xraydb.material_mu_components('quartz', 10000)
{'mass': 60.0843, 'density': 2.65, 'elements': ['Si', 'O'],
'Si': (1, 28.0855, 33.87943243018506), 'O': (2.0, 15.9994, 5.952824815297084)}
```

`xray_delta_beta` (*material*, *density*, *energy*)
anomalous components of the index of refraction for a material, using the tabulated scattering components from Chantler.

Parameters

- **`material`** – chemical formula ('Fe2O3', 'CaMg(CO3)2', 'La1.9Sr0.1CuO4')
- **`density`** – material density in g/cm^3
- **`energy`** – x-ray energy in eV

Returns (delta, beta, atlen)

where delta : real part of index of refraction beta : imag part of index of refraction atlen : attenuation length in cm

These are the anomalous scattering components of the index of refraction:

n = 1 - delta - i*beta = 1 - lambda**2 * r0/(2*pi) Sum_j (n_j * fj)

Adapted from code by Yong Choi

`darwin_width` (*energy*, *crystal='Si'*, *hkl=1, 1, 1*, *m=1*)
darwin width for a crystal reflection and energy

Parameters

- **`energy`** (*`float`*) – X-ray energy in eV
- **`crystal`** (*`string`*) – name of crystal (one of 'Si', 'Ge', or 'C') ['Si']
- **`hkl`** (*`tuple`*) – h, k, l for reflection [(1, 1, 1)]
- **`m`** (*`int`*) – order of reflection [1]

Returns

A named tuple 'DarwinWidth' with the following fields

theta float, nominal Bragg angle, in rad,

theta_fwhm float, estimated angular Darwin width, in rad,

energy_fwhm float, estimated energy Darwin width, in eV,

zeta nd-array of Zeta parameter (delta_Lambda / Lambda),

dtheta nd-array of angles away from Bragg angle, theta in rad,

denergy nd-array of energies away from Bragg energy, in eV,

intensity nd-array of reflected intensity

Notes

1. This follows the calculation from section 6.4 of Elements of Modern X-ray Physics, 2nd Edition J Als-Nielsen, and D. McMorrow.
2. Only diamond structures (Si, Ge, diamond) and sigma polarization are currently supported.

Examples

```
>>> dw = darwin_width(10000, crystal='Si', hkl=(1, 1, 1)
>>> dw.theta_fwhm, dw.energy_fwhm
(2.0841049436681097e-05, 1.0333427816952565)
```

`mirror_reflectivity`(*formula*, *theta*, *energy*, *density=None*, *roughness=0.0*, *polarization='s'*)
mirror reflectivity for a thick, singl-layer mirror.

Parameters

- **`formula`** (*`string`*) – material name or formula ('Si', 'Rh', 'silicon')
- **`theta`** (*`float or nd-array`*) – mirror angle in radians
- **`energy`** (*`float or nd-array`*) – X-ray energy in eV
- **`density`** (*`float or None`*) – material density in g/cm^3
- **`roughness`** (*`float`*) – mirror roughness in Angstroms
- **`polarization`** (*`'s' or 'p'`*) – mirror orientation relative to X-ray polarization

Returns mirror reflectivity values

Notes

1. only one of theta or energy can be an nd-array
2. density can be *None* for known materials
3. polarization of 's' puts the X-ray polarization along the mirror surface, 'p' puts it normal to the mirror surface. For horizontally polarized X-ray beams from storage rings, 's' will usually mean 'vertically deflecting' and 'p' will usually mean 'horizontally deflecting'.

`ionization_potential`(*gas*)
return effective ionization potential for a gas, as appropriate for ionization chambers in the linear regime (not 'proportional counter' regime)

Parameters **`gas`** (*`string`*) – name of gas

Returns ionization potential in eV

Notes

Data from G. F. Knoll, Radiation Detection and Measurement, Table 5-1, and from ICRU Report 31, 1979. Supported gas names and effective potentials:

gas names	potential (eV)
hydrogen, H	36.5
helium, He	41.3
nitrogen, N, N2	34.8
oxygen, O, O2	30.8
neon, Ne	35.4
argon, Ar	26.4
krypton, Kr	24.4
xenon, Xe	22.1
air	33.8
methane, CH4	27.3
carbondioxide, CO2	33.0

If the gas is not recognized the default value of 32.0 eV will be returned.

`ionchamber_fluxes` (*gas='nitrogen'*, *volts=1.0*, *length=100.0*, *energy=10000.0*, *sensitivity=1e-06*, *sensitivity_units='A/V'*)

return ion chamber fluxes for a gas or mixture of gases, ion chamber length, X-ray energy, recorded voltage and current amplifier sensitivity.

Parameters

- **`gas`** (*`string or dict`*) – name or formula of fill gas (see note 1) ['nitrogen']
- **`volts`** (*`float`*) – measured voltage output of current amplifier [1.0]
- **`length`** (*`float`*) – active length of ion chamber in mm [100]
- **`energy`** (*`float`*) – X-ray energy in eV [10000]
- **`sensitivity`** (*`float`*) – current amplifier sensitivity [1.e-6]
- **`sensitivity_units`** (*`string`*) – units of current amplifier sensitivity (see note 2 for options) ['A/V']

Returns

named tuple IonchamberFluxes with fields

photo flux absorbed by photo-electric effect in Hz,

incident flux of beam incident on ion chamber in Hz,

transmitted flux of beam output of ion chamber in Hz

Notes

1. The gas argument can either be a string for the name of chemical formula for the gas, or dictionary with keys that are gas names or formulas and values that are the relative fraction for mixes gases.

   The gas formula is used in two ways:

   a) to get the photo- and total- absorption coefficient, and

   b) to get the effective ionization potential for the gas.

   The effective ionization potentials are known for a handful of gases (see *ionization_potential* function), all ranging between 20 and 45 eV. For unknown gases the value of 32.0 eV will be used.

2. The *sensitivity* and *sensitivity_units* arguments have some overlap to specify the sensitivity or gain of the current amplifier. Generally, the units in *A/V*, but you can add a common SI prefix of

   'p', 'pico', 'n', 'nano', (unicode 'u03bc'), 'u', 'micro', 'm', 'milli'

   so that, for example ionchamber_fluxes(..., sensitivity=1.e-6)

   and ionchamber_fluxes(..., sensitivity=1, sensitivity_units='uA/V')

   will both give a sensitivity of 1 microAmp / Volt .

Examples

```
>>> ionchamber_fluxes(gas='helium', volts=1.25, length=200.0,
                      energy=10000.0, sensitivity=1.e-9)
IonChamberFluxes(photo=16110895.3, incident=15452608024.6,␣
↪transmitted=15316549138.8)
>>> ionchamber_fluxes(gas='nitrogen', volts=1.25, length=200.0,
                      energy=10000.0, sensitivity=1.e-9)
IonChamberFluxes(photo=13575282.2, incident=23102328.0, transmitted=8759458.7)
>>> ionchamber_fluxes(gas={'nitrogen':0.5, 'helium': 0.5}, volts=1.25,
                      length=200.0, energy=10000.0, sensitivity=1.e-9)
IonChamberFluxes(photo=14843088.8, incident=7737855176.4, transmitted=7662654298.
↪8)
```

1.5 Overview of Atomic and X-ray Data

The data provided in XrayDB includes Atomic data and characteristic energies and cross sections for the interaction of X-rays with elements. A few definitions and conventions necessary for using this data are discussed here.

1.5.1 Elements

Most of the data resources are accessed by an elements *Atomic Symbol*. For the Python module, most methods will take *element* as the first argument, and this can either be the integer atomic number or the string for the atomic symbol.

1.5.2 Physical Units

Elemental densities are given in gr/cm^3, and molar masses are given in AMU. Unless otherwise stated, all energies are in units of eV.

1.5.3 X-ray Edges

Several resources (database tables, python methods) take either an `edge` or a `level` argument to signify a core electronic level. These are strings and must be one of the levels listed in the *Table of X-ray edge names*.

Table of X-ray Edges and Core electronic levels. The Names are the IUPAC symbols for the core electronic levels.

Name	electronic level	Name	electronic level
K	$1s$	N5	$4d_{5/2}$
L3	$2p_{3/2}$	N4	$4d_{3/2}$
L2	$2p_{1/2}$	N3	$4p_{3/2}$
L1	$2s$	N2	$4p_{1/2}$
M5	$3d_{5/2}$	N1	$4s$
M4	$3d_{3/2}$	O3	$5p_{3/2}$
M3	$3p_{3/2}$	O2	$5p_{1/2}$
M2	$3p_{1/2}$	O1	$5s$
M1	$3s$	P3	$6p_{3/2}$
N7	$4f_{7/2}$	P2	$6p_{1/2}$
N6	$4f_{5/2}$	P1	$6s$

1.5.4 X-ray Lines

Many resources (database tables or methods) take emission line arguments. These are all strings and follow the latinized version of the Siegbahn notation as indicated in the *Table of X-ray emission line names*.

Table of X-ray emission line names and the corresponding Siegbahn and IUPAC notations

Name	IUPAC	Siegbahn	Name	IUPAC	Siegbahn
Ka1	K-L3	$K\alpha_1$	Lb4	L1-M2	$L\beta_4$
Ka2	K-L2	$K\alpha_2$	Lb5	L3-O4,5	$L\beta_5$
Ka3	K-L1	$K\alpha_3$	Lb6	L3-N1	$L\beta_6$
Kb1	K-M3	$K\beta_1$	Lg1	L2-N4	$L\gamma_1$
Kb2	K-N2,3	$K\beta_2$	Lg2	L1-N2	$L\gamma_2$
Kb3	K-M2	$K\beta_3$	Lg3	L1-N3	$L\gamma_3$
Kb4	K-N4,5	$K\beta_2$	Lg6	L2-O4	$L\gamma_6$
Kb5	K-M4,5	$K\beta_3$	Ll	L3-M1	Ll
La1	L3-M5	$L\alpha_1$	Ln	L2-M1	$L\nu$
La2	L3-M4	$L\alpha_1$	Ma	M5-N6,7	$M\alpha$
Lb1	L2-M4	$L\beta_1$	Mb	M4-N6	$M\beta$
Lb2,15	L3-N4,5	$L\beta_2, L\beta_{15}$	Mg	M3-N5	$M\gamma$
Lb3	L1-M3	$L\beta_3$	Mz	M4,5-N6,7	$M\zeta$

1.5.5 Cross Sections

The photo-absorption and scattering cross sections from [Elam_Ravel_Sieber] and [Chantler] are in cm^2/gr.

The data from [Elam_Ravel_Sieber] is held as logarithms of energy, cross section, and logarithm of the 2nd derivative of cross section that allows for cubic spline interpolation in log-log space.

1.6 Using the XrayDB xraydb.sqlite

All the data for the X-ray database is held in the SQLite3 file `xraydb.sqlite`. To use with SQLite, this file is all you need. While many programs and languages can access SQLite files, basic usage with the `sqlite3` program (available from Windows, Mac OS X, and Linux) can be as simple as:

```
system~> sqlite3 xraydb.sqlite
sqlite> .headers on
sqlite> select * from elements where atomic_number=47;
atomic_number|element|molar_mass|density
47|Ag|107.868|10.48
```

That is, you can retrieve the data using standard SQL queries built-in to SQLite. Of course, the expectation is that you'd want to use this database within a programming environment. Currently, wrappers exist only for Python.

1.6.1 Overall Database Schema

The schema for the SQLite3 database describes where data is held in the database, and how to access it. The schema for the current version (4) looks like this:

```
Table Version (id integer primary key,
               tag text,
               date text,
               notes text);
Table elements (atomic_number integer primary key,
                element text,
                molar_mass real,
                density real);
Table xray_levels (id integer primary key,
                   element text,
                   iupac_symbol text,
                   absorption_edge real,
                   fluorescence_yield real,
                   jump_ratio real);
Table xray_transitions (id integer primary key,
                        element text,
                        iupac_symbol text,
                        siegbahn_symbol text,
                        initial_level text,
                        final_level text,
                        emission_energy real,
                        intensity real);
Table Coster_Kronig (id integer primary key,
                     element text,
                     initial_level text,
                     final_level text,
                     transition_probability real,
```

(continues on next page)

(continued from previous page)

```
                     total_transition_probability real);
Table photoabsorption (id integer primary key,
                       element text,
                       log_energy text,
                       log_photoabsorption text,
                       log_photoabsorption_spline text);
Table scattering (id integer primary key,
                  element text,
                  log_energy text,
                  log_coherent_scatter text,
                  log_coherent_scatter_spline text,
                  log_incoherent_scatter text,
                  log_incoherent_scatter_spline text);
Table Waasmaier (id integer primary key,
                 atomic_number integer,
                 element text,
                 ion text,
                 offset real,
                 scale text,
                 exponents text);
Table KeskiRahkonen_Krause (id integer primary key,
                            atomic_number integer,
                            element text,
                            edge text,
                            width float);
Table Krause_Oliver (id integer primary key,
                     atomic_number integer,
                     element text,
                     edge text,
                     width float);
Table corelevel_widths (id integer primary key,
                        atomic_number integer,
                        element text,
                        edge text,
                        width float);
Table Chantler (id integer primary key,
                element text,
                sigma_mu real,
                mue_f2 real,
                density real,
                corr_henke float,
                corr_cl35 float,
                corr_nucl float,
                energy text,
                f1 text,
                f2 text,
                mu_photo text,
                mu_incoh text,
                mu_total text);
```

More details for each table are given below.

Note: in the tables below the type of *json array* means that arrays of numerical data are stored in the database as text of JSON-encoded arrays.

1.6.2 Version Table

The *Version* table holds data about the revisions to the database file itself. Each row represents a single revision.

DB Table of Database Versions

Column	Type	Description
id	integer	counter (primary tag)
tag	text	version name
date	text	date string
notes	text	notes on changes for version

1.6.3 Elements Table

The *elements* table holds basic data about each element. Each row represents an element.

DB Table of Basic Properties of the Elements

Column	Type	Description
atomic_number	integer	Atomic Number, Z
element	text	Atomic symbol
molar_mass	float	Atomic mass in AMU
density	float	Density of pure element (gr/cm^3)

1.6.4 Xray_Levels Table

The *xray_levels* table holds data for electronic levels of atoms. Each row represents a core electronic level.

DB Table of X-ray and core electronic levels. *fluorescence yield* gives the probability of an empty level refilling by X-ray fluorescence. The *jump ratio* is the ratio of values for photo-electric cross section (that is, from *Photoabsorption Table*) 1 eV above the absorption edge to that 1 eV below the absorption edge. See *Table of X-ray Edges*

Column	Type	Description
id	integer	Index (primary key)
element	text	Atomic symbol for element
iupac_symbol	text	IUPAC symbol for level (‘K’,’L3’,. . .)
absorption_edge	float	binding energy for level (eV)
fluorescence_yield	float	fluorescence yield (fraction)
jump_ratio	float	ratio of mu_photo across edge

1.6.5 Xray_Transitions Table

The *xray_transitions* table holds data for transitions between electronic levels of atoms. Each row represents a transition between two levels.

DB Table of X-ray Transitions. Both IUPAC and Siegbahn symbols are given (see *Table of X-ray emission lines*), as well as the initial and final levels. The *intensity* is the relative intensity of the transition for a given *initial level*.

Column	Type	Description
id	integer	Index (primary key)
element	text	Atomic symbol for element
iupac_symbol	text	IUPAC symbol for transition
siegbahn_symbol	text	Siegbahn symbol for transition
initial_level	text	IUPAC symbol for initial level
final_level	text	IUPAC symbol for final level
emission_energy	float	fluorescence energy (eV)
intensity	float	relative intensity for transition

1.6.6 Photoabsorption Table

The *photoabsorption* table holds data for the photo-electric absorption cross sections in cm^2/gr. Each row represents an element.

DB Table of Photoabsorption Cross Sections. JSON-encoded arrays are held for logs of energy, cross section, and cross section spline (second derivative useful for spline interpolation).

Column	Type	Description
id	integer	Index (primary key)
element	text	Atomic symbol for element
log_energy	json array	log of Energy values (eV)
log_photoabsorption	json array	log of cross section (cm^2/gr)
log_photoabsorption_spline	json array	log of cross section spline

1.6.7 Scattering Table

The *scattering* table holds data for the coherent and incoherent X-ray scattering cross sections, in cm^2/gr. Each row represents an element.

DB Table of Coherent and Incoherent Scattering Cross Sections. JSON-encoded arrays are held for logs of energy, cross section, and cross section spline (second derivative useful for spline interpolation).

Column	Type	Description
id	integer	Index (primary key)
element	text	Atomic symbol for element
log_energy	json array	log of Energy values (eV)
log_coherent_scatter	json array	log of cross section (cm^2/gr)
log_coherent_scatter_spline	json array	log of cross section spline
log_incoherent_scatter	json array	log of cross section (cm^2/gr)
log_incoherent_scatter_spline	json array	log of cross section spline

1.6.8 Coster_Kronig Table

The *Coster_Kronig* table holds data for energy levels, partial and total transition probabilities for the Coster-Kronig transitions (Auger processes in which the empty core level is filled from an electron in a higher level with the same principle quantum number). The partial probability describes direct transitions, while the total probability includes cascade effects. Each row represents a transition.

DB Table of Coster-Kronig Transitions.

Column	Type	Description
id	integer	Index (primary key)
element	text	Atomic symbol for element
initial_level	text	IUPAC symbol for initial level
final_level	text	IUPAC symbol for final level
transition_probability	float	direct transition probability
total_transition_probability	float	total transition probability

1.6.9 Waasmaier Table

The *Waasmaier* table holds data for calculating elastic X-ray scattering factors $f_0(k)$, from [Waasmaier_Kirfel]. The scattering factor is unitless, and $k = \sin(\theta)/\lambda$ where θ is the scattering angle and λ is the X-ray wavelength. available for many common ionic states for each element. Each row represents an ion.

DB Table of Elastic Scattering Cross Section Coefficients

Column	Type	Description
id	integer	Index (primary key)
atomic_number	integer	Atomic Number, Z
element	text	Atomic symbol for element
ion	text	symbol for element and ionization
offset	float	offset value
scale	json array	coefficients for calculation
exponents	json array	coefficients for calculation

1.6.10 KeskiRahkonen_Krause Table

The *KeskiRahkonen_Krause* table holds data for energy widths of the core electronic levels from [Keski_Krause]. Values are in eV, and each row represents an energy level for an element.

DB Table of Core Hole Widths from Keski-Rahkonen and Krause

Column	Type	Description
id	integer	Index (primary key)
atomic_number	integer	Atomic Number, Z
element	text	Atomic symbol for element
edge	text	IUPAC symbol for energy level (‘K’)
width	float	width of level (eV)

1.6.11 Krause_Oliver Table

The *Krause_Oliver* table holds data for energy widths of the core electronic levels from [Krause_Oliver]. Values are in eV, and each row represents an energy level for an element.

DB Table of Core Hole Widths from Krause and Oliver

Column	Type	Description
id	integer	Index (primary key)
atomic_number	integer	Atomic Number, Z
element	text	Atomic symbol for element
edge	text	IUPAC symbol for energy level ('K')
width	float	width of level (eV)

1.6.12 Chantler Table

The *Chantler* table holds data for resonant X-ray scattering factors $f'(E)$ and $f''(E)$ as well as photo-electric absorption, coherent, and incoherent scattering factors from [Chantler]. As with other tables, scattering factors are unitless, and cross sections are in cm^2/gr. Each row represents an element.

DB Table of resonant scattering and mass attenuation coefficients from Chantler.

Column	Type	Description
id	integer	Index (primary key)
element	text	Atomic symbol for element
mue_f2	float	factor to convert mu(E) to f"(E)
density	float	atomic density (gr/cm^3)
corr_henke	float	Henke correction to f`(E)
corr_cl35	float	Cromer-Liberman correction to f`(E)
corr_nucl	float	nuclear correction to f`(E)
energy	json array	energies for interpolation
f1	json array	f'(E) (e)
f2	json array	f"(E) (e)
mu_photo	json array	photoabsorption mu(E) (cm^2/gr)
mu_incoh	json array	incoherent scattering (cm^2/gr)
mu_total	json array	total attenuation (cm^2/gr)

1.7 References

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