acx2 Documentation

Release 1.0.0

Adam Foster

CONTENTS

1	Insta	allation	•
2	Usag	ge	4
	2.1	Data Files	4
	2.2	Classes	4
	2.3	XSPEC	6
3	Vers	ion History	9
	3.1	acx2 module class reference	Ç
Pv	thon 1	Module Index	17

The AtomDB CX model is a model of charge exchange during a collision between a recombining charged ion and a donor atom or ion. The electron is transferred from the donor to the recombining ion, forming a recombined ion often in an excited state. As this recombined ion relaxes to its ground state, it releases a cascade of photons with relative intensities characteristic of CX recombination.

An original version of ACX was released in 2016, which used empirical formulae for CX emission of all ions of all the elements up to nickel. These formulae, crucially, did not include any velocity dependent effects, which are important for correctly calculating the n, l and S of the excited levels captured into. In addition, spectral information was hardwired and difficult to update, resulting in updates to AtomDB not often being reflected in the following charge exchange spectra.

We have now taken CX cross section data from the Kronos database $(^1,^2,^3)$, which covers many fully stripped and one electron recombining ions, and included it here. This has created a much improved dataset, which correctly captures the energy dependence of the process for these ions. For other ions not in the Kronos database, the model falls back on ACX1 behaviour.

Once Kronos or ACX1 have been used to calculate the correct capture cross sections for each n, l and/or S shell, the data is combined with the AtomDB database (www.atomdb.org) to calculate the cascade path to ground, and the subsequent emissivities and wavelengths. For ions with capture in to highly excited levels which AtomDB doesn't contain, AUTOSTRUCTURE calculations are preformed to get energy levels, wavelength and A-values for these transtitions. The result is a set of 3 files for each donor ion. The sigma file contains the cross section information for each ion. The line and cont[inuum] files contain the line emission and continuum emission from each shell capture in to, with a resolution appropriate for the model in question. For example, for ions with nlS resolved Kronos data, a spectrum is produced for each n, l and S capture and subsequent cascade. Thus there can be numerous spectra for each ion - there are 239 entries for Cl^{7+} reflecting each n, l and S which Kronos contains cross sections for. For ACX-level data, the spectra are calculated for each relevant n and the four l distributions, as outlined in the ACX documentation (even, statistical, Landau-Zener and separable).

For a given interaction velocity or energy, the model uses the center of mass energy to obtain the cross section for capture into each shell from Kronos. For each shell where the cross section is greater than zero, a spectrum is calculated from the *line* and *cont* files. These are then multiplied by the appropriate cross section and summed to give the spectrum for CX of a particular ion.

CONTENTS 1

¹ Mullen, P. D., et al. ApJS 224, 31 (2016)

² Mullen, P. D., et al. ApJ 844, 7 (2017)

³ Cumbee, R. S., et al. ApJ 852, 7 (2018)

2 CONTENTS

CHAPTER

ONE

INSTALLATION

Standard python installation

python setup.py install

Note: ACX2 is a python 3 only module. Depending on your system's setup, you may need to substitute python3 for all references to python.

There are several useful flags that can be provided to this call, depending on your system:

- --user flag causes installation in the user's home directory (useful if you lack root priviliges)
- develop instead of install will install links to the current directory. This is useful if you want to edit/debug/develop the files further.

USAGE

Each model in ACX2 can have an arbitrary set of donors. By default for the XSPEC model these are neutral H and He, but others may be selected. Additional input files will be required for these - please contact the project via the AtomDB or GitHub pages to make or discuss requests.

2.1 Data Files

Each model requires a set of data files to be installed with it. As these files are large they cannot be exported through GitHub, and they should instead be downloaded from the AtomDB CX webpage, www.atomdb.org/CX.

The files for each donor are:

- sigma files: the cross sections for capture into each n, l and S (depending on the ion) from the Kronos database
- line files: the line emission for capture into each n, l and S (depending on the ion) or each n and ACX1 l distribution for ions with no Kronos data
- cont files: same as line files, but including continuum emission. True continuum in CX is entirely 2-photon emission from H-, He- and Be-like ions.

Note: The emissivity data files have thousands of HDUs as currently assembled. Although these files read quickly in python, when opening in some programs (e.g. fv) the load times can be upwards of 10 minutes. Rearranging these files to not cause this issue is a priority to fix.

2.2 Classes

The acx2.py file contains a range of classes which can be used to model different aspects of the charge exchange. The basic principal is that the fits files contain the emissivity for each ion, broken down to reflect the way that Kronos handles the data.

Kronos Resolution	Typical recombining ion	ACX2 handling
n, l, S resolved	hydrogenic bare C,N,O,Ne	Capture into each n, l, S
n resolved	bare	Capture into each n, ACX for l distribution
not included	all others	Capture into 2 n shells, ACX for l distribution

To handle this, the acx2 module contains 4 levels of classes:

• ACXModel: The overall ACX model. Can include multiple donor ACXDonorModel objects.

- ACXDonorModel: The ACX model for one donor. Contains spectra from each recombining ion.
- CXIonSpectrum: The spectrum for one recombining ion. Placeholder for CXIonSpectrum_ACX1, CXIonSpectrum_N, CXIonSpectrum_NLS classes, which handle the 3 cases is the table above. Contains CXShellSpectrum as required to get the data.
- CXShellSpectrum: The actual spectrum from a single each n, l, S shell (or n, ldist shell).

2.3 XSPEC

To use the model in XSPEC, one can ignore the class details above. Unfortunately, the code only works with the XSPEC python interface, pyxspec for now. Before loading the code, you will need to edit the acx2_xspec.py file to change the data file paths.

Note: You will need to edit the acx2_xspec.py file: #. It may need to be moved into your path (depending on the data) #. The data file locations are hardcoded, you will need to update them to reflect where you have installed the line, continuum and cross section files.

To load the ACX2 model into XSPEC, acx2_xspec module contains what you need. From a python3 shell:

```
# import the xspec python module
import xspec
# import acx2 wrapper
import acx2_xspec
```

Once this is done, the data will load.

Three different models are loaded:

- acx2: Emission from CX with the 14 main elements. Abundance is tied between all elements (so there is only 1 abundance keyword). Analogous to the apec model.
- vacx2: Emission from CX with the 14 main elements. Abundance is free to vary between all the elements (though it starts frozen). Analagous to the vapec model.
- vvacx2 : Emission from 27 elements, H through Ni excluding Co. Abundance is free to vary between all the elements.

Note: Note that in the acx and vacx cases, unlike in the apec and vapec models, the effective abundance of the minor recombining elements is 0, not solar. This speeds up calculation time and does not significantly effect the resulting emission.

Once you have this, models can be used in pyxspec in the usual way, e.g.

```
m = xspec.Model('tbabs(pow+vacx2)')
```

6 Chapter 2. Usage

2.3.1 Model parameters

Parameter	Definition		
temperature	Plasma temperature (keV). Used for recombining particle ion fraction		
collnpar	Collsion parameter (kev/u,km/s). Reduced energy or velocity of collision		
collntype	rpe Sets meaning of collnpar:		
	1 - center of mass energy (kev/u)		
	2 - center of mass velocity (km/s)		
	3 - donor ion velocity (km/s)		
	4 - recombining ion velocity (km/s)		
acxmodel	ACX model to fall back on, from 1 to 8.		
recombtype	single recombination (1) or all the way to neutral (2)		
Hefrac	fefrac Number fraction of donor which is He (remainder is H).		
abund recombining elemental abundances. (given by individual element in vacx and vvac			

Note: The units for collision velocity in XSPEC are km/s, not cm/s as in the underlying ACX models. This is to keep the numbers closer to 1, which XSPEC likes.

2.3.2 Normalization of the model

This model deals with two emissivities, which can get confusing. The photon emissivity of a line $i \to j$ is defined as:

$$\epsilon_{ij} = N_i A_{ij}$$

That is, the number of emitted photons $cm^{-3}s^{-1}$ is the number density N_i of ions in state i, times the spontaneous transition probability A_{ij} .

We can ease the calculation of N_i by separating out the calculation:

$$N_i = \frac{N_i}{N_{z1}} \frac{N_{z1}}{N_Z} \frac{N_Z}{N_H^r} N_H^r$$

where N_{z1} is the ion abundance and N_Z is the element abundance. The N_{z1}/N_Z term is set by the temperature parameter, which is used to set the ion fraction. The N_Z/N_H^r is set for the recombining plasma by the abundance parameter, relative to the solar values of Anders and Grevesse 1989.

The ACX2 model solves the N_i/N_{z1} problem by setting up a radiative matrix, with levels populated by CX and then radiative decay to the ground state forming the rest of the matrix. The CX rate coefficient into level i is given by

$$\alpha_i^{CX}(cm^{-3}s^{-1}) = \langle v_{com}\sigma_i(E) \rangle$$

and the rate is

$$\alpha_i^{CX}(cm^{-3}s^{-1}) = \langle v_{com}\sigma_i(E)\rangle \ N_H^d$$

We solve the radiative matrix to obtain N_i/N_{z1} , without the donor densities included (as they are multipliers on all the diagonal matrix elements we are effectively just moving them outside the matrix). This leaves us with:

$$\epsilon_{ij} = \frac{N_i}{N_{z1}} \frac{N_{z1}}{N_Z} \frac{N_Z}{N_H} N_H^r A_{ij} N_H^d$$

2.3. XSPEC 7

ACX2 calculates the photon emissivity coefficient, $\varepsilon_{ij} = \frac{N_i}{N_{z1}} A_{ij}$, and multiplies in the elemental and ion abundances based on the abundance and temperatures specified. This leaves:

$$\epsilon_{ij} = \varepsilon_{ij} \frac{N_{z1}}{N_Z} \frac{N_Z}{N_H} N_H^r N_H^d$$

$$\epsilon_{ij} = (\text{ACX2output}) N_H^r N_H^d$$

To convert this to a flux from a source to our instrument we integrate over the emitting volume and account for radiation over 4π . We also, at this point, repeat the process for the He donor and add the results, accounting for the different donor ion fractions.

$$\Gamma_{ij}(cm^{-2}s^{-1}) = \frac{\int (\text{ACX2output}) N_H^r N_{(H+He)}^d dV}{4\pi D^2}$$

out of the line is defined as is calculated in photons cm³ s⁻¹, as:

$$\varepsilon_{ij}(cm^3s^{-1}) = v_{com}\sigma_i(E)A_{ij}$$

2.3.3 XSPEC Normalization of the model

The geometric norm represents the geometric parts of the flux calculation with a single number:

$$\mathrm{norm}_{\mathrm{geom}}(cm^{-5}) = \frac{\int N_H^r N_{(H+He)}^d dV}{4\pi D^2}$$

The XSPEC normalization is adjusted from the above in a few ways to make fitting more reliable. First, there is a factor of 10^{10} applied to bring the value closer to 1, which makes XSPEC fitting more reliable.

Secondly, for versions $\geq 1.1.0$, the normalization is divided by the center of mass velocity. This has been implemented to compensate for the increase in flux with an increase in velocity (since $\varepsilon_{ij} \propto \langle v_{com} \sigma_i(E) \rangle$), which resulted in the norm being anticorrelated with the collnpar. As this value would be different for every ion, the correction factor is based on a carbon-12 recombining ion and a hydrogen donor.

To recover the true emissivity of the plasma given an XSPEC fit result:

- 1. If using version \geq 1.1.0, calculate the correction factor, cf:
 - 1. If collntype == 1: cf = numpy.sqrt(4786031.3*collnpar/25.)
 - 2. If collntype == 2: cf = 1.0
 - 3. If collntype == 3: cf = 1.0 * collnpar/(1.0+12.0) = collnpar/13
 - 4. If collntype == 4: cf = 12.0 * collnpar/(1.0+12.0) = collnpar*12/13
- 2. Else, cf = 1
- 3. $\operatorname{norm}_{\text{geom}} = \operatorname{norm}_{\text{XSPEC}} * \operatorname{cf} * 10^{-10}$

8 Chapter 2. Usage

CHAPTER

THREE

VERSION HISTORY

1.0.0 March 15th 2019 Initial release

- 1.0.1 October 25th 2019 Fixed error in vacx2 XSPEC interface, which specified but did not implement fluorine leading to an off-by-one error for all higher-Z elements
- 1.0.2 February 27th 2020 Error in velocity unit conversion corrected, thanks to Gabrielle Betancourt-Martinez for reporting the bug. This will not have affected fits performed through XSPEC
- 1.0.3 July 9th 2020 Updated code for compatibility with changes in the PyAtomDB interface
- 1.1.0 November 16th 2022 Major changes to the normalization. It now has the center of mass velocity of carbon-12 divided out of it. This removed the velocity-normalization correlation which was otherwise present.

Added redshift to parameters.

Converted XSPEC interface collntype, acxmodel and recombtype into integer switches

3.1 acx2 module class reference

class acx2.**ACXDonorModel** (donor, donor_linefile, donor_contfile, donor_crosssectionfile, abund-set='AG89', elements=[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30], acxmodel=8, recombtype=1, collisiontype=1)

A model of the ACX Donor

Parameters

- **donor** (*string*) The donor symbol (e.g. "H")
- **donor_linefile** (*string*) The file with the donor line emision
- donor_contfile (string) The file with the donor continuum emision
- donor_crosssectionfile (string) The cross section file for donor
- abundset (optional, { "AG89"}) The abundance set. Only AG89 works currently
- **elements** (optional, array-like int) The recombining element atomic numbers. Default is all.
- acxmodel (optional, int, default=8) The acx model l, n distribution to fall back on.

linedata

The data in the donor_linefile

Type HDUList

contdata

The data in the donor_contfile

Type HDUList

crosssectiondata

The data in the donor_crosssectionfile

Type HDUList

donorAbundance

The donor abundance. Defaults to 1.0. Intended for correctly mixing donors, e.g. in 10%He, 90%H donor plasma, set to 0.1 and 0.9 respectively, though no normalization is checked for.

Type float

donormass

mass of the donor in a.m.u.

Type float

abund

abundance of each element, relative to abundset. e.g. abund[6] = 2.0 means 2x solar C

Type dict of float

ionfrac_from_temperature

was the ionfracance calculated from the temperature

Type bool

temperature

the temperature in keV

Type float

ionfrac

the ionization fraction, normalized to 1 for each element, e.g. ionfrac[2] = ndarray([0.01,0.1,0.89])

Type dict of arrays of float

calc_ionfrac_equilibrium()

Recalculate the ionization balance based on equilibrium electron temperature

Parameters None -

Returns

Return type None

Notes

Uses self.temperature (in keV) to set self.ionfrac

calc_spectrum(collparam)

Calculate the spectrum we want

Parameters collparam (*float*) – Collision energy, or velocity, as determined by set_collisiontype, in kev/u, cm/s or km/s

Returns self.emiss – The emissivity in photons cm³ bin-1 s-1

Return type array(float)

find_crosssection_type (Z, z1)

Find the cross section type, to assign correct CXIonSpectrum type

Parameters

- **Z** (int) element charge
- **z1** (*int*) recombining ion charge +1.

Returns

- resolution (string) The coupling, currently N, NLS or ACX1 (returned in upper case)
- ihdu (int) The HDU with the cross section data for the ion. Set to -1 for none.

```
hashlib = <module 'hashlib' from '/usr/lib/python3.8/hashlib.py'>
```

```
numpy = <module 'numpy' from '/home/afoster/.local/lib/python3.8/site-packages/numpy-1
os = <module 'os' from '/usr/lib/python3.8/os.py'>
```

```
set_abund (abund, elements=None)
```

Set the elemental abundance, also in each donor model

Parameters abund (array (float)) – Abundances, relative to defulat

Returns

Return type None

set_abundset (abundstring)

Set the abundance set.

Parameters abundstring (*string*) – The abundance string (e.g. "AG89", "uniform"). Case insensitive. See atomdb.get_abundance for list of possible abundances

Returns updates self.abundset and self.abundsetvector.

Return type none

set_acxmodel (acxmodel)

Set the ACX spectrum type

Parameters acxmodel (int) – The acxmodel (between 1 and 8)

set_collisionparam(collisionparam)

Set the collision velocity or energy

Parameters collisionparam (*float*) – The collision velocity or energy. Units and parameter type are set in ACXModel.set_collisiontype

Returns

Return type None

```
set_collisiontype (colltype, collunits='default')
```

Set the collision type and units

Parameters

- **colltype** (*int*) Parameter for provided collision type Collision type 1=energy/mass of center of mass Collision type 2=velocity of center of mass Collision type 3=velocity of donor Collision type 4=velocity of receiver
- **collunits** (*string*, *optional*) Units of collision paramter. Defaults to "kev/u" for colltype=1, "cm/s" for others

Returns

Return type None

set_donorabund(abund)

Set the donor abundance

Parameters abund (float) – The abundance of the donor.

```
set_ebins (ebins, ebins_checksum=False)
```

Set the energy bins for the spectrum being returned.

Parameters

- **ebins** (array (float)) Energy bin edges (keV)
- **ebins_checksum**(*string*, *optional*) The hex digest of the md5 sum of ebins. Used to check for changes.

set ionfrac(ionfrac)

Recalculate the ionization balance based on equilibrium electron temperature

```
Parameters ionfrac (dict of arrays) – ionization fraction, e.g. ion-frac[8]=numpy.array([0.0, 0.0, 0.0, 0.0, 0.1, 0.3, 0.4, 0.2, 0.0])
```

Returns

Return type None

set_recombtype (recombtype)

Set the recombination type

Parameters recombtype (int) – The type of recombination (1=single, 2=all the way to neutral)

set_temperature (temperature)

Recalculate the ionization balance based on equilibrium electron temperature

Parameters temperature (float) – electron temperature in keV

Returns

Return type None

class acx2. CXIonSpectrum (Z, z1, ebins, crosssectiondata, linedata, contdata, cxdata)

Class to store and prepare each ion's spectrum. Will have a subset of CXShellSpectrum for each shell. Can provide it a set of energy bins and get a spectrum back. This will store all the emissivity data.

```
hashlib = <module 'hashlib' from '/usr/lib/python3.8/hashlib.py'>
```

```
numpy = <module 'numpy' from '/home/afoster/.local/lib/python3.8/site-packages/numpy-1</pre>
```

```
os = <module 'os' from '/usr/lib/python3.8/os.py'>
```

return_spectrum (ebins, collision_energy, linedata, contdata, ebins_checksum=False)
Return the spectrum on the energy bins

set_acxmodel (acxmodel)

Set the ACX spectrum type

Parameters acxmodel (int) – The acxmodel (between 1 and 8)

set_ebins (ebins, ebins_checksum=False)

Set the energy bins for the spectrum being returned.

Parameters

• **ebins** (array (float)) – Energy bin edges (keV)

• **ebins_checksum** (*string*, *optional*) – The hex digest of the md5 sum of ebins. Used to check for changes.

class acx2. CXIonSpectrum_ACX1 (Z, z1, crosssectionhdu, linedata, contdata, acxmodel=8, donor=False, receivermass=False, donormass=False)

This is a class for ACX1 model data

ebins

The energy bin in keV

Type array(float)

ebins m5sum

hex digest of ebins

Type md5hash

calc_spectrum(collenergy, collvelocity)

Calculate the spectrum of the data

Parameters

- **ebins** (array (float)) The energy bins (in keV) to calcualte the spectrum on
- collenergy (flaot) The collision energy (keV/amu)
- collvelocity (float) The velocity of the center of mass (cm/s)
- linedata (hdulist) The line emissivity data
- contdata (hdulist) The continuum emissivity data
- acxmodel (int) n, 1 shell distribution, between 1 and 8:

Returns emissivity – Emissivity * velocity in photons cm4 s-2

Return type array(float)

```
hashlib = <module 'hashlib' from '/usr/lib/python3.8/hashlib.py'>
numpy = <module 'numpy' from '/home/afoster/.local/lib/python3.8/site-packages/numpy-1</pre>
```

os = <module 'os' from '/usr/lib/python3.8/os.py'>
set_ebins(ebins, ebins_checksum=False)

Set the energy bins, also in each donor model

Parameters ebins (array (float)) – The energy bins in keV for the spectrum

Returns

Return type None

class acx2. CXIonSpectrum_N (Z, z1, crosssectiondata, linedata, contdata, acxmodel=8, donor=False, receivermass=False, donormass=False)

This is a class for n resolved Kronos data

calc_spectrum(collenergy, collvelocity)

Calculate the spectrum of the data

Parameters

- **ebins** (array (float)) The energy bins (in keV) to calcualte the spectrum on
- **collenergy** (*flaot*) The collision energy (keV/amu)
- **collvelocity** (*float*) The velocity of the center of mass (cm/s)
- linedata (hdulist) The line emissivity data

```
• contdata (hdulist) - The continuum emissivity data
                  • acxmodel (int) - n, l shell distribution, between 1 and 8
              Returns emissivity – Emissivity * velocity in photons cm4 s-2
              Return type array(float)
     hashlib = <module 'hashlib' from '/usr/lib/python3.8/hashlib.py'>
     numpy = <module 'numpy' from '/home/afoster/.local/lib/python3.8/site-packages/numpy-1</pre>
     os = <module 'os' from '/usr/lib/python3.8/os.py'>
     set_ebins (ebins, ebins_checksum=False)
          Set the energy bins, also in each donor model
              Parameters ebins (array (float)) – The energy bins in keV for the spectrum
              Returns
              Return type None
class acx2.CXIonSpectrum_NLS(Z, z1, crosssectiondata, linedata, contdata, donor=False, receiver-
                                     mass=False, donormass=False)
     This is a class for nls resolved Kronos data
     calc_spectrum(collenergy, collvelocity)
          Calculate the spectrum of the data
              Parameters
                  • ebins (array (float)) – The energy bins (in keV) to calcualte the spectrum on
                  • collenergy (flaot) – The collision energy (keV/amu)
                  • collvelocity (float) – The velocity of the center of mass (cm/s)
                  • linedata (hdulist) - The line emissivity data
                  • contdata (hdulist) - The continuum emissivity data
                  • acxmodel (int) - n, l shell distribution, between 1 and 8
              Returns emissivity – Emissivity * velocity in photons cm4 s-2
              Return type array(float)
     hashlib = <module 'hashlib' from '/usr/lib/python3.8/hashlib.py'>
     numpy = <module 'numpy' from '/home/afoster/.local/lib/python3.8/site-packages/numpy-1</pre>
     os = <module 'os' from '/usr/lib/python3.8/os.py'>
     set_ebins (ebins, ebins_checksum=False)
          Set the energy bins, also in each donor model
              Parameters ebins (array (float)) – The energy bins in keV for the spectrum
              Returns
              Return type None
class acx2. CXShellSpectrum (Z, z1, n, l, linedata, contdata, s=False)
     Holds a single n, l, shell spectrum
     expand_E_grid (eedges, Econt_in_full, cont_in_full)
          Code to expand the compressed continuum onto a series of bins.
              Parameters
```

- **eedges** (*float* (*array*)) The bin edges for the spectrum to be calculated on, in units of keV
- Econt_in_full (float (array)) The compressed continuum energies (keV)
- cont_in_full (float (array)) The compressed continuum emissivities (ph cm3 s-1 keV-1)

Returns len(bins)-1 array of continuum emission, in units of photons cm³ s⁻¹ bin⁻¹

Return type float(array)

```
hashlib = <module 'hashlib' from '/usr/lib/python3.8/hashlib.py'>
numpy = <module 'numpy' from '/home/afoster/.local/lib/python3.8/site-packages/numpy-1
os = <module 'os' from '/usr/lib/python3.8/os.py'>
scipy = <module 'scipy' from '/home/afoster/.local/lib/python3.8/site-packages/scipy/_
set_ebins(ebins, ebins_checksum)
```

Set the energy bins, also in each donor model

Parameters ebins (array (float)) – The energy bins in keV for the spectrum

Returns

Return type None

class acx2. DummyCXShellSpectrum (Z, z1, n, l, s=False)

Placeholder for a blank spectrum

calc_spectrum(ebins, ebins_checksum)

Return zeros

Parameters

- ebinshash (string) md5 sum of ebins
- ebins (array (float)) array of floats

Returns 0.0

Return type there is no data here, so return zero.

set_ebins (ebins, ebins_checksum=False)

Dummy

Parameters

- ebinshash (string) md5 sum of ebins
- ebins (array (float)) array of floats

Returns

Return type None

```
acx2.loginterp (newx, x, y, offset=1e-40)
```

Interpolation helper function. Interpolates linearly on a log-log grid If newx < x[0], return x[0]. If newx > x[-1], extrapolate slope of last 2 points, unless y[-1] ==0 in which case return 0.

Parameters

- **newx** (float) The new X parameters (energy, kev/amu)
- **x** (array (float)) The x parameters (energy, kev/amu)
- **y** (array (float)) The y parameters (cross section, cm2)

• offset (float (optional)) - An offset to apply before interpolation. Prevents log(0) issues.

Returns newy – The interpolated cross section. Minimum of 0 in case of numerical issues.

Return type float

- genindex
- modindex
- search

PYTHON MODULE INDEX

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acx2 (posix, macos), 9