PyAtomDB Documentation

Release 0.0.3.4

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Contents

CHAPTER 1

Introduction

PyAtomDB is a selection of utilities designed to interact with the AtomDB database . These utilities started life as routines scattered around my laptop, so some produce lots of unhelpful onscreen output.

There are several different modules currently. These are:

- *atomdb* : a series of codes for interacting with the AtomDB atomic database
- *atomic* : basic atomic data routines - e.g. converting element symbols to atomic number, etc.
- *const* : a series of physical constants
- *spectrum* : routines for generating spectra from the published AtomDB line and continuum emissivity files
- *util* : sumple utility codes (sorting etc) that pyatomdb relies on.
- *apec* : ultimately, the full apec code. For now, incomplete.

Expect bugs. Report those bugs! Make feature requests! Email the code authors or raise an issue at the github page

CHAPTER 2

Contents

Contents

PyAtomDB APEC module

This modules contains the APEC code. It calls many different subroutines from throughout the PyAtomDB module. Currently largely unwritten, as APEC code needs to be tidied up for transfer. The apec module contains routines crucial for the APEC code. This also includes some interfaces to external C libraries (or will, eventually).

Version 0.1 - initial release Adam Foster September 16th 2015

`pyatomdb.apec.`**`calc_brems_gaunt`**(*E*, *T*, *z1*, *brems_type*, *datacache=False*, *settings=False*)

calculate the bremstrahulung free-free gaunt factor

Parameters **E** : float

Energy (in keV) to calculate gaunt factor

T : float

Temperature (in K) of plasma

z1 : int

Ion charge +1 of ion (e.g. 6 for C VI)

brems_type : int

Type of bremstrahlung requested: 1 = HUMMER = Non-relativistic: 1988ApJ...327..477H 2 = KELLOGG = Semi-Relativistic: 1975ApJ...199..299K 3 = RELATIVISTIC = Relativistic: 1998ApJ...507..530N 4 = BREMS_NONE = no bremstrahlung

settings : dict

See description in atomdb.get_data

datacache : dict

Used for caching the data. See description in atomdb.get_data

Returns **gaunt_ff** : float

The gaunt factor for the free-free process.

pyatomdb.apec.**calc_cascade_population**(*matrixA*, *matrixB*)

pyatomdb.apec.**calc_ee_brems**(*E*, *T*, *N*)

calculate the electron-electron bremsstrahlung.

Parameters **E** : array (float)

energy grid (keV)

T : float

Electron temperature (keV)

N : float

electron density (cm^-3)

Returns array(float)

ee_brems in photons cm^s s^-1 keV-1 at each point E. This should be multiplied by the bin width to get flux per bin.

References

Need to check this!

pyatomdb.apec.**calc_full_ionbal**(*Te*, *tau=100000000000000.0*, *init_pop=False*, *Te_init=False*, *Zlist=False*, *teunit='K'*, *extrap=True*, *cie=True*, *settings=False*)

Calculate the ionization balance for all the elements in Zlist.

One of init_pop or Te_init should be set. If neither is set, assume all elements start from neutral.

Parameters **Te** : float

electron temperature in keV or K (default K)

tau : float

N_e * t for the non-equilibrium ioniziation (default 1e14)

init_pop : dict of float arrays, indexed by Z

initial populations. E.g. init_pop[6]=[0.1,0.2,0.3,0.2,0.2,0.0,0.0]

Te_init : float

initial ionization balance temperature, same units as Te

Zlist : int array

array of nuclear charges to include in calculation (e.g. [8,26] for oxygen and iron)

teunit : {'K' , 'keV'}

units of temperatures (default K)

extrap : bool

Extrappolate rates to values outside their given range. (default False)

cie : bool

If true, collisional ionization equilbrium calculation (tau, init_pop, Te_init all ignored)

Returns **final_pop** : dict of float arrays, indexed by Z

final populations. E.g. final_pop[6]=[0.1,0.2,0.3,0.2,0.2,0.0,0.0]

pyatomdb.apec.**calc_ioniz_popn**(*levpop*, *Z*, *z1*, *z1_drv*, *T*, *Ne*, *settings=False*, *datacache=False*, *do_xi=False*)

Calculate the level population due to ionization into the ion

Parameters **levpop: array(float)**

The level population of the parent ion. Should already have abundance and ion fraction built in.

Z: int

z1: int

z1_drv: int

T: float

Ne: float

settings: dict

datacache: dict

do_xi: bool

Include collisional ionization

Returns levpop_out: array(float)

The level populations of the Z,z1 ion

pyatomdb.apec.**calc_recomb_popn**(*levpop*, *Z*, *z1*, *z1_drv*, *T*, *dens*, *drlevrates*, *rrlevrates*, *settings=False*, *datacache=False*, *dronly=False*, *rronly=False*)

Calculate the level population of a recombined ion

Parameters **levpop: array(float)**

Level populations, already taking into account elemental abundance and ion fraction of z1_drv

Z: int

z1: int

z1_drv: int

T: electron temperature (K)

dens: electron density (cm^-3)

drlevrates: array(float)

Rates into each level from DR calculations

rrlevrates: array(float)

Rates into each level from RR calculations

Returns array(float)

Level population

pyatomdb.apec.**calc_satellite**(*Z*, *z1*, *T*, *datacache=False*, *settings=False*)
Calcaulate DR satellite lines

Parameters **Z: int**

The nuclear charge of the element Z: int

z1 : int

Recombined Ion charge +1 of ion (e.g. 5 for C VI -> C V)

te: float

The electron temperature (K)

settings: dictionary

The settings read from the apec.par file by parse_par_file

Returns array(linelist)

List of DR lines

array(levlistin)

Rates into each lower level, driven by DR

pyatomdb.apec.**calc_total_coco**(*cocodata*, *settings*)
Calculate the total emission in erg cm^3 s^-1

pyatomdb.apec.**compress_continuum**(*xin*, *yin*, *tolerance*, *minval=0.0*)
Compress the continuum into linear interpolatable grids

Parameters **xin** : array(float)

The bin edges (keV)

yin : array(float)

The continuum in photons (or ergs) cm^3 s^-1 bin^-1. Should be 1 element shorter then xin

tolerance : float

The tolerance of the final result (if 0.01, the result will always be within 1% of the original value)

Returns **xout** : array (float)

The energy points of the compressed energy grid (keV)

yout : array (float)

The continuum, in photons(or ergs) cm^3 s^-1 keV^-1

pyatomdb.apec.**continuum_append**(*a*, *b*)
Join two continuum arrays together, expanding arrays as necessary

Parameters **a: numpy.array(dtype=continuum)**

The first array

b: numpy.array(dtype=continuum)

The second array

Returns

c: numpy.array(dtype=continuum)

The two arrays combined, with continuum arrays resized as required.

pyatomdb.apec.**create_chdu_cie**(*cocodata*)

pyatomdb.apec.**create_cparamhdu_cie**(*cocodata*)

pyatomdb.apec.**create_lhdu_cie**(*linedata*)

pyatomdb.apec.**create_lhdu_nei**(*linedata*)

pyatomdb.apec.**create_lparamhdu_cie**(*linedata*)

pyatomdb.apec.**do_brems**(*Z*, *z1*, *T*, *abund*, *brems_type*, *eedges*)

Calculate the bremstrahlung emission in units of photon cm^3 s^-1 bin^-1

Parameters **Z** : int

nuclear charge for which result is required

z1 : int

ion charge +1

T : float

temperture (Kelvin)

abund : float

elemental abundance (should be between 1.0 and 0.0)

brems_type : int

Type of bremstrahlung requested: 1 = HUMMER = Non-relativistic: 1988ApJ...327..477H 2 = KELLOGG = Semi-Relativistic: 1975ApJ...199..299K 3 = RELATIVISTIC = Relativistic: 1998ApJ...507..530N 4 = BREMS_NONE = no bremstrahlung

eedges : array(float)

The energy bin edges for the spectrum (keV)

Returns array(float)

bremstrahlung emission in units of photon cm^3 s^-1 bin^-1

pyatomdb.apec.**do_lines**(*Z*, *z1*, *lev_pop*, *N_e*, *datacache=False*, *settings=False*, *z1_drv_in=-1*)

Convert level populations into line lists

Parameters **Z: int**

The nuclear charge of the element

z1 : int

Ion charge +1 of ion (e.g. 6 for C VI)

lev_pop : array(float)

The level population for the ion. Should already have elemental abundance and ion fraction multiplied in.

N_e : float

Electron Density (cm^-3)

datacache : dict

Used for caching the data. See description in atomdb.get_data

settings : dict

See description in atomdb.get_data

z1_drv_in : int

the driving ion for this calculation, if not z1 (defaults to z1)

Returns linelist: numpy.dtype(linetype)

The list of lines and their emissivities. see generate_datatypes

twophot: array(float)

The two-photon continuum on the grid specified by the settings If settings['TwoPhoton'] is False, then returns a grid of zeros.

pyatomdb.apec.**extract_gauntff**(*Z*, *gamma2*, *gaunt_U*, *gaunt_Z*, *gaunt_Ng*, *gaunt_g2*, *gaunt_gf*)

Extract the appropriate Gaunt free-free factor from the relativistic data tables of Nozawa, Itoh, & Kohyama, 1998 ApJ, 507,530

Parameters **Z** : int

Z for which result is required

gamma2 : array(float)

gamma^2 in units of Z^2 Rydbergs/kT

gaunt_U : array(float)

u=E/kT

gaunt_Z : array(int)

nuclear charge

gaunt_Ng : array(int)

number of gamma^2 factors

gaunt_g2 : array(float)

gamma^2 factors

gaunt_gf : array(float)

ff factors

Returns array(float)

Gaunt factors.

References

Nozawa, Itoh, & Kohyama, 1998 ApJ, 507,530

pyatomdb.apec.**gather_rates**(*Z*, *z1*, *te*, *dens*, *datacache=False*, *settings=False*, *do_la=True*, *do_ai=True*, *do_ec=True*, *do_pc=True*, *do_ir=True*)

fetch the rates for all the levels of Z, z1

Parameters **Z: int**

The nuclear charge of the element

z1 : int

ion charge +1

te : float

temperture (Kelvin)

dens: float

electron density (cm^-3)

settings : dict

See description in atomdb.get_data

datacache : dict

Used for caching the data. See description in atomdb.get_data

Returns up: numpy.array(float)

Initial level of each transition

lo: numpy.array(float)

Final level of each transition

rate: numpy.array(float)

Rate for each transition (in s-1)

pyatomdb.apec.**generate_apec_headerblurb**(*settings*, *linehdulist*, *cocohdulist*)

Generate all the headers for an apec run, and apply them to the HDUlist.

Parameters **settings: dict**

The output of read_apec_parfile

hdulist : list or array of fits HDUs

The hdus to have headings added.

Returns None

pyatomdb.apec.**generate_cie_outputs**(*settings*, *Z*, *linelist*, *contlist*, *pseudolist*)

Convert a linelist and continuum values into an equilibrium AtomDB fits output

Parameters **settings: dictionary**

The settings read from the apec.par file by parse_par_file

Z: int

The nuclear charge of the element

linelist: numpy.array(dtype=linelisttype)

The list of lines, separated by ion

contlist: dict

Dictionary with the different continuum contributions from each ion. Each is an array of ph cm^3 s^-1 bin^-1

pseudolist: dict

Dictionary with the different pseudocontinuum contributions from each ion. Each is an array of ph cm^3 s^-1 bin^-1

Returns None

pyatomdb.apec.**generate_datatypes**(*dtype*, *npseudo=0*, *ncontinuum=0*)

returns the various data types needed by apec

Parameters **dtype** : string

One of “linetype”, “cielinetype”, “continuum”

npseudo : int (default=0)

Number of pseudocontinuum points for “continuum” type

ncontinuum : int (default=0)

Number of continuum points for “continuum” type

Returns numpy.dtype

The data dtype in question

pyatomdb.apec.**generate_nei_outputs**(*settings*, *Z*, *linelist*, *contlist*, *pseudolist*, *ionfrac_nei*)

Convert a linelist and continuum values into a non-equilibrium AtomDB fits output

Parameters **settings: dictionary**

The settings read from the apec.par file by parse_par_file

Z: int

The nuclear charge of the element

linelist: numpy.array(dtype=linelisttype)

The list of lines, separated by ion

contlist: dict

Dictionary with the different continuum contributions from each ion. Each is an array of ph cm^3 s^-1 bin^-1

pseudolist: dict

Dictionary with the different pseudocontinuum contributions from each ion. Each is an array of ph cm^3 s^-1 bin^-1

Returns None

pyatomdb.apec.**kurucz**(*uin*, *gam*)

Correction factors to Kellogg bremstrahlung calculation by Bob Kurucz

Parameters **uin** : array(float)

energy grid, units of E/kT (both in keV)

gam : array(float)

Z**2/T, in units of Rydbergs

Returns array(float)

gaunt factors at high gam (> 0.1)

pyatomdb.apec.**make_vector**(*linear*, *minval*, *step*, *nstep*)

Create a vector from the given inputs

Parameters **linear: boolean**

Whether the array should be linear or log spaced

minval: float

initial value of the array. In dex if linear==False

step: float

step between points on the array. In dex if linear==False

nstep: int

number of steps

Returns array(float)

array of values spaced out use the above parameters

pyatomdb.apec.**make_vector_nbins**(*linear*, *minval*, *maxval*, *nstep*)

Create a vector from the given inputs

Parameters **linear: boolean**

Whether the array should be linear or log spaced

minval: float

initial value of the array. In dex if linear==False

maxval: float

maximum value of the array. In dex if linear==False

nstep: int

number of steps

Returns array(float)

array of values spaced out use the above parameters

pyatomdb.apec.**parse_par_file**(*fname*)

Parse the apec.par input file for controlling APEC

Parameters **fname** : string

file name

Returns dict

The settings in "key:value" pairs.

pyatomdb.apec.**run_apec**(*fname*)

Run the entire APEC code using the data in the parameter file fname

Parameters **fname** : string

file name

Returns None

pyatomdb.apec.**run_apec_element**(*settings*, *te*, *dens*, *Z*)

Run the APEC code using the settings provided for one element

Parameters **settings: dictionary**

The settings read from the apec.par file by parse_par_file

te: float

The electron temperature (K)

dens: float

The electron density (cm^-3)

Z: int

The nuclear charge of the element

Returns None

pyatomdb.apec.**run_apec_ion**(*settings*, *te*, *dens*, *Z*, *z1*, *ionfrac*, *abund*)

Run the APEC code using the settings provided for an individual ion.

Parameters **settings: dictionary**

The settings read from the apec.par file by parse_par_file

te: float

The electron temperature (K)

dens: float

The electron density (cm^-3)

Z: int

The nuclear charge of the element

z1: int

The ion charge +1 of the ion

ionfrac: float

The fractional abundance of this ion (between 0 and 1)

abund: float

The elemental abundance of the element (normalized to H)

Returns **linelist** : numpy array

List of line details and emissivities

continuum : array

Continuum emission in photons bin-1 s-1. This is a 3-item dict, with "rrc", "twophot", "brems" entries for each continuum source

pseudocont : array

Pseudo Continuum emission in photons bin-1 s-1

pyatomdb.apec.**run_wrap_run_apec**(*fname*, *Z*, *iTe*, *iDens*)

After running the APEC code ion by ion, use this to combine into FITS files.

Parameters **fname** : string

file name of par file

Z: int

The atomic numbers

iTe: int

The temperature index

iDens: int

The density index

Returns None

pyatomdb.apec.**solve_ionbal**(*ionrate*, *recrate*, *init_pop=False*, *tau=False*)

solve_ionbal: given a set of ionization and recombination rates, find the equilibrium ionization balance. If init_pop and tau are set, do an non-equilibrium calculation starting from init_pop and evolving for n_e * t = tau (cm^-3 s)

Parameters **ionrate** : float array

the ionization rates, starting with neutral ionizing to +1

recrate : float array

the recombination rates, starting with singly ionized recombining to neutral

init_pop : float array

initial population of ions for non-equlibrium calculations. Will be renormalised to 1.

tau : float

N_e * t for the non-equilibrium ioniziation

Returns **final_pop** : float array

final populations.

Notes

Note that init_pop & final_pop will have 1 more element than ionrate and recrate.

pyatomdb.apec.**solve_ionbal_eigen**(*Z*, *Te*, *init_pop=False*, *tau=False*, *Te_init=False*, *teunit='K'*, *filename=False*, *datacache=False*)

Solve the ionization balance for a range of ions using the eigenvector approach and files as distributed in XSPEC.

Parameters **Z** : int

atomic number of element

Te : float

electron temperature, default in K

init_pop : float array

initial population of ions for non-equlibrium calculations. Will be renormalised to 1.

tau : float

N_e * t for the non-equilibrium ioniziation

Te_init : float

initial ionization balance temperature, same units as Te

teunit : {'K' , 'keV'}

units of temperatures (default K)

filename : string

Can optionally point directly to the file in question, i.e. to look at older data look at $HEADAS/../spectral/modelData/eigenELSYMB_v3.0.fits. If not set, download from AtomDB FTP site.

Returns **final_pop** : float array

final populations.

pyatomdb.apec.**solve_level_pop**(*init*, *final*, *rates*, *settings*)
Solve the level population

Parameters **init** : array(int)

The initial level for each transition

final : array(int)

The initial level for each transition

rates : array(float)

The rate for each transition

settings: dictionary

The settings read from the apec.par file by parse_par_file

Returns array(float)

The level population

pyatomdb.apec.**wrap_ion_directly**(*fname*, *ind*, *Z*, *z1*)

pyatomdb.apec.**wrap_run_apec**(*fname*, *readpickle=False*)
After running the APEC code ion by ion, use this to combine into FITS files.

Parameters **fname** : string

file name

readpickle : bool

Load apec results by element from pickle files, instead of regenerating

Returns None

pyatomdb.apec.**wrap_run_apec_element**(*settings*, *te*, *dens*, *Z*, *ite*, *idens*, *writepickle=False*, *readpickle=False*)
Combine wrap_run_apec_ion results for an element

Parameters **settings: dictionary**

The settings read from the apec.par file by parse_par_file

te: float

The electron temperature (K)

dens: float

The electron density (cm^-3)

Z: int

The nuclear charge of the element

ite: int

The temperature index

idens: int

The density index

writepickle: bool

Dump data into a pickle file. Useful for rapidly combining data after runs.

readpickle: bool

Read data from a pickle file. Useful for rapidly combining data after runs. Usually the result of a previous call using writepickle=True

Returns None

PyAtomDB Atomic module

This modules contains basic atomic parameters (i.e. atomic numbers, element symbols) atomic.py contains routines related to basic atomic data, e.g. converting integer nuclear charge to element symbols, etc.

Version -.1 - initial release Adam Foster July 17th 2015

pyatomdb.atomic.**Z_to_mass**(*Z*)

Converts element symbol to atomic mass, e.g. "C" -> 12.0107

Isotope fractions based on those found in earth's crust samples, your astrophysical object may vary.

Parameters **Z** : int

nuclear charge, e.g 6 for C

Returns float

mass in a.m.u. for the element. (e.g. 12.0107 for C)

References

Atomic masses are taken from: Pure Appl. Chem. 81 NO 11, 2131-2156 (2009) Masses for Technetium, Promethium, Polonium, Astatine, Radon, Francium, Radium & Actinum are estimates. If you need these you probably aren't doing astronomy...

pyatomdb.atomic.**Ztoelname**(*Z*)

Returns element name of element with nuclear charge Z.

Parameters **Z** : int

nuclear charge of element (e.g. 6 for carbon)

Returns str

element name (e.g. "Carbon" for carbon)

pyatomdb.atomic.**Ztoelsymb**(*Z*)

Returns element symbol of element with nuclear charge Z.

INPUTS Z - nuclear charge of element (e.g. 6 for carbon)

RETURNS element symbol (e.g. "C" for carbon)

Version 0.1 28 July 2009 Adam Foster

pyatomdb.atomic.**config_to_occup**(*cfgstr, nel=-1, shlmax=-1, noccup=[-1]*)

pyatomdb.atomic.**elsymb_to_Z**(*elsymb*)

Converts element symbol to nuclear charge, e.g. "C" -> 6

Parameters **elsymb** : str

Element symbol, e.g. "C". Case insensitive.

Returns int

Z for the ion. (e.g. 6 for C)

pyatomdb.atomic.**elsymb_to_z0**(*elsymb*)
Converts element symbol to nuclear charge, e.g. "C" -> 6 (wrapper to elsymb_to_Z, retained for consistency)

Parameters **elsymb** : str

Element symbol, e.g. "C". Case insensitive.

Returns int

Z for the ion. (e.g. 6 for C)

pyatomdb.atomic.**get_maxn**(*cfgstr*)

pyatomdb.atomic.**get_parity**(*cfgstr*)

pyatomdb.atomic.**int2roman**(*number*)

pyatomdb.atomic.**int_to_roman**(*input*)
Convert an integer to Roman numerals.

pyatomdb.atomic.**occup_to_cfg**(*occlist*)

pyatomdb.atomic.**occup_to_config**(*occup*)

pyatomdb.atomic.**parse_config**(*cfgstr*)

pyatomdb.atomic.**parse_eissner**(*cfgstr*, *nel=0*)

pyatomdb.atomic.**roman_to_int**(*input*)
Convert a roman numeral to an integer.

pyatomdb.atomic.**spectroscopic_name**(*Z*, *z1*)
Converts Z,z1 to spectroscopic name, e.g. 6,5 to "C V"

Parameters **Z** : int

nuclear charge (e.g. 6 for C)

z1 : int

ion charge +1 (e.g. 5 for C4+)

Returns str

spectroscopic symbol for ion (e.g. "C V" for C+4)

pyatomdb.atomic.**spectroscopictoz0**(*name*)
Converts spectroscopic name to Z, z1, e.g. "C V" to 6,5

Parameters **name** : str

Ion name, e.g. "C V"

Returns int, int

Z, z1 for the ion. (e.g. 6,5 for C V)

pyatomdb.atomic.**z0_to_mass**(*z0*)
Converts element symbol to atomic mass, e.g. "C" -> 12.0107

(wrapper to Z_to_mass, retained for consistency)

Isotope fractions based on those found in earth's crust samples, your astrophysical object may vary.

Parameters **z0** : int

nuclear charge, e.g 6 for C

Returns float

mass in a.m.u. for the element. (e.g. 12.0107 for C)

References

Atomic masses are taken from: Pure Appl. Chem. 81 NO 11, 2131-2156 (2009) Masses for Technetium, Promethium, Polonium, Astatine, Radon, Francium, Radium & Actinum are estimates. If you need these you probably aren't doing astronomy...

pyatomdb.atomic.**z0toelname**(*z0*)

Returns element name of element with nuclear charge z0. (wrapper to Ztoelname for compatibility purposes)

Parameters **z0** : int

nuclear charge of element (e.g. 6 for carbon)

Returns str

element name (e.g. "Carbon" for carbon)

pyatomdb.atomic.**z0toelsymb**(*z0*)

Returns element symbol of element with nuclear charge z0. (wrapper to Ztoelsymb for compatibility purposes)

Parameters **z0** : int

nuclear charge of element (e.g. 6 for carbon)

Returns str

element symbol (e.g. "C" for carbon)

PyAtomDB AtomDB module

This modules is designed to interact with the main atomic database, extracting real values of coefficients and so on. The atomdb module contains several routines for interfacing with the AtomDB database to extract useful physical quantities, line lists, write new fits files and more. It is currently a dump of everything I've done with AtomDB. This should all be considered unstable and possibly susceptible to being wrong. It will be fixed, including moving many routines out of this library, as time goes on.

Version 0.1 - initial release Adam Foster July 17th 2015

Version 0.2 - added PI reading routines and get_data online enhancements. Adam Foster August 17th 2015

Version 0.3 - added RRC generation routines Adam Foster August 28th 2015

pyatomdb.atomdb.**A_twoph**(*A*, *E0*, *E*)

Convert the A value into energy distribution for 2-photon transitions

Parameters **A** : float

Einstein A for transition

E0 : float

Energy in keV of transition

E : array(float)

Energies of each bin to output continuum at (keV)

Returns

——-

array(float)

Distribution of transtion rate amongst bins E (s^-1)

References

From Nussbaumer & Schmutz, 1984, A+A, 138,495 Z is the element, and E is the energy of the bin, in keV y is unitless, and is equal to nu/nu0 = lambda0/lambda, where lambda0 = 1215.7 A for hydrogen–the base wavelength of the 2s->1s transition. This fit is accurate to better than 0.6% for 0.01 < y < 0.99

The A_norm is the A value for neutral hydrogen for this transition. For other transitions, we renormalize to the appropriate A value.

This routine is used for BOTH hydrogenic and He-like two-photon distributions. This is justified using the result of Derevianko & Johnson, 1997, Phys Rev A, 56, 1288 who show in Figures 5 and 2 of that paper that the difference is everywhere less than 10% between these two for Z=6-28 – it is about 5% or so.

pyatomdb.atomdb.**B_hyd**(*s*, *l*, *m*, *eta*)

pyatomdb.atomdb.**G_hyd**(*l*, *m*, *eta*, *rho*)

pyatomdb.atomdb.**addline**(*xbins*, *yvals*, *wv*, *amp*, *dx*)

pyatomdb.atomdb.**addline2**(*xbins*, *wv*, *amp*, *dx*)

pyatomdb.atomdb.**calc_ci_dere**(*Te*, *ionpot*, *Tscal*, *Upsscal*)

Calculate the collisional ionization rates using the Dere 2007 method

Parameters **Te** : float or array(float)

Electron temperature (K)

ionpot : float

Ionization potential (eV)

Tscal : array(float)

scaled temperatures

Upsscal : array(float)

scaled upsilons

Returns float or array(float)

Ionization rate in cm^3 s^-1

References

2007A&A...466..771D

pyatomdb.atomdb.**calc_ionrec_ci**(*cidat*, *Te*, *extrap=False*, *ionpot=False*)

pyatomdb.atomdb.**calc_ionrec_dr**(*cidat*, *Te*, *extrap=False*)

pyatomdb.atomdb.**calc_ionrec_ea**(*cidat*, *Te*, *extrap=False*)

pyatomdb.atomdb.**calc_ionrec_rr**(*cidat*, *Te*, *extrap=False*)

pyatomdb.atomdb.**calc_kato**(*coll_type*, *par*, *Z*, *Te*)

pyatomdb.atomdb.**calc_maxwell_rates**(*coll_type*, *min_T*, *max_T*, *Tarr*, *om*, *dE*, *T*, *Z*, *degl*, *degu*, *quiet=False*, *levdat=False*, *ladat=False*, *lolev=False*, *uplev=False*, *force_extrap=False*, *did_extrap=False*, *datacache=False*)

pyatomdb.atomdb.**calc_rad_rec_cont**(*Z*, *z1*, *z1_drv*, *T*, *ebins*, *abund=1.0*, *ion_pop=1.0*, *settings=False*, *datacache=False*)

Calculate the radiative recombination continuum for an ion at temperature T

Parameters **Z** : int

nuclear charge

z1 : int

recombined ion charge+1

z1_drv : int

recombining ion charge+1

T : float

temperautre (K)

ebins : array(float)

energy bins (in keV) on which to caclulate the spectrum

abund : float

elemental abundance, relative to hydrogen

ion_pop : float

the ion's population fraction of that element (i.e. sum of all ion_pop for an element = 1)

Returns array(float)

RRC in photons cm^3 s^-1 bin^-1, in an array of length(ebins)-1

array(float)

Recombination rates into the excited levels, in s-1

pyatomdb.atomdb.**calc_rrc**(*Z*, *z1*, *eedges*, *Te*, *lev*, *xstardat=False*, *xstarlevfinal=1*, *settings=False*, *datacache=False*, *returntotal=False*)

Calculate the radiative recombination continuum for a given ion

Parameters **Z** : int

Atomic number

z1 : int

recombined ion charge

eedges : array(float)

the bin edges for the spectrum to be calculated on (keV)

Te : float

The electron temperature (K)

lev : int

The level of the ion for the recombination to be calculated into

xstardat : dict or HDUList

The xstar PI data. This can be an already sorted dictionary, as returned by sort_xstar_data, or the raw results of opening the PI file

xstarlevfinal : int

If you need to identify the recombining level, you can do so here. Should normally be 1.

settings : dict

See description in read_data

datacache : dict

See description in read_data

returntotal : bool

If true, return the total recombination rate as well

Returns array(float)

The rrc in photons cm^3 s^-1 keV^-1

optional float

If returntotal is set, also return total RRC calculated by separate integral from the ionization edge to infinity.

pyatomdb.atomdb.**calc_sampson_h**(*om*, *Z*, *Te*)

pyatomdb.atomdb.**calc_sampson_p**(*om*, *Z*, *Te*)

pyatomdb.atomdb.**calc_sampson_s**(*om*, *Z*, *Te*)

pyatomdb.atomdb.**calc_spline_atomdb**(*xa*, *ya*, *y2a*, *n*, *x*)

pyatomdb.atomdb.**calc_two_phot**(*wavelength*, *einstein_a*, *lev_pop*, *ebins*)

Calculate two photon spectrum

Parameters **wavelength** : float

Wavelength of the transition (Angstroms)

einstein_a : float

The Einstein_A paramater for the transition

lev_pop : float

The level population for the upper level

ebins : array(float)

The bin edges for the spectrum (in keV)

Returns array(float)

The flux in photons cm-3 s-1 bin-1 array is one element shorter than ebins.

pyatomdb.atomdb.**ci_younger**(*Te*, *c*)

Calculates Collisional Ionization Rates from Younger formula

Parameters **Te** : array(float)

Temperatures in Kelvin

c : the ionrec_par from the transition in the AtomDB IR file

Returns array(float)

returns ionization rate in cm^3 s^-1

pyatomdb.atomdb.**dr_badnell**(*Te*, *c*)
Convert data from Badnell constants into a DR Rate

Parameters **Te** : float or array(float)

Electron temperature[s] in K

c : array

Constants from DR rates. Stored as alternating pairs in AtomDB, so c1,e1,c2,e2,c3,e3 etc in the IONREC_PAR column

Returns float

DR rate in cm^3 s-1

References

See http://amdpp.phys.strath.ac.uk/tamoc/DATA/DR/

pyatomdb.atomdb.**dr_mazzotta**(*Te*, *c*)

pyatomdb.atomdb.**ea_mazzotta**(*Te*, *c*, *par_type*)
Te is an array in Kelvin c is the ionrec_par par_type is the number denoting the type of the parameter returns excitation-autoionization rate in cm^3 s^-1

pyatomdb.atomdb.**ea_mazzotta_iron**(*T_eV*, *c*)

pyatomdb.atomdb.**extract_n**(*conf_str*)

pyatomdb.atomdb.**f1_fcn**(*x*)

pyatomdb.atomdb.**f2_fcn**(*x*)

pyatomdb.atomdb.**get_abundance**(*abundfile=False, abundset='AG89', element=[-1], datacache=False, settings=False*)
Get the elemental abundances, relative to H (H=1.0)

Parameters **abundfile** : string

special abundance file, if not using the default from filemap

abundset : string

Abundance set. Available:

- Allen: Allen, C. W. Astrophysical Quantities, 3rd Ed., 1973 (London: Athlone Press)
- AG89: Anders, E. and Grevesse, N. 1989, Geochimica et Cosmochimica Acta, 53, 197
- GA88: Grevesse, N, and Anders, E.1988, Cosmic abundances of matter, ed. C. J. Waddington, AIP Conference, Minneapolis, MN
- Feldman: Feldman, U., Mandelbaum, P., Seely, J.L., Doschek, G.A.,Gursky H., 1992, ApJSS, 81,387

Default is AG89

element : list of int

Elements to find abundance for. If not specified, return all.

datacache : dict

See get_data

datacache : settings

See get_data

Returns dict

abundances in dictionary, i.e :

{1: 1.0,

2: 0.097723722095581111,

3: 1.4454397707459272e-11,

4: 1.4125375446227541e-11,

5: 3.9810717055349735e-10,

6: 0.00036307805477010178,...

pyatomdb.atomdb.**get_bt_approx**(*om*, *Tin*, *Tout*, *uplev*, *lolev*, *levdat*, *ladat*)

pyatomdb.atomdb.**get_burgess_tully_extrap**(*bttype*, *lolev*, *uplev*, *Aval*, *Tarr*, *om*, *TTarg*)

pyatomdb.atomdb.**get_burgess_tully_transition_type**(*lolev*, *uplev*, *Aval*)

pyatomdb.atomdb.**get_data**(*Z*, *z1*, *ftype*, *datacache=False*, *settings=False*, *indexzero=False*, *offline=False*)

Read AtomDB data of type ftype for ion rmJ of element Z.

If settings are set, the filemap can be overwritten (see below), otherwise $ATOMDB/filemap will be used to locate the file. If indexzero is set, all levels will have 1 subtracted from them (AtomDB indexes lines from 1, but python and C index arrays from 0, so this can be useful)

Parameters **Z** : int

Element nuclear charge

rmJ : int

Ion charge +1 (e.g. 5 for C^{4+}, a.k.a. C V)

ftype : string

type of data to read. Currently available

- 'IR' - ionization and recombination
- 'LV' - energy levels
- 'LA' - radiative transition data (lambda and A-values)
- 'EC' - electron collision data
- 'PC' - proton collision data
- 'DR' - dielectronic recombination satellite line data
- 'PI' - XSTAR photoionization data
- 'AI' - autoionization data

Or, for non-ion-specific data (abundances and bremstrahlung coeffts) * 'ABUND' - abundance tables * 'HBREMS' - Hummer bremstrahlung coefficients * 'RBREMS' - relativistic bremstrahlung coefficitients * 'IONBAL' - ionization balance tables * 'EIGEN' - eigenvalue files

filemap : string

The filemap to use, if you do not want to use the default one.

settings : dict

This will let you override some standard inputs for get_data:

- settings['filemap']: the filemap to use if you do not want to use the default $ATOMDB/filemap
- settings['atomdbroot']: If you have files in non-standard locations you can replace $ATOMDB with this value

datacache : dict

This variable will hold the results of the read in a dictionary. It will also be checked to see if the requested data has already been cached here before re-reading from the disk. If you have not yet read in any data but want to start caching, provide it as an empty dictionary i.e. mydatacache={}

2 parts of the data ares stored here:

- Settings['data'] will store a copy of the data you read in. This means that if your code ends up calling for the same file multiple times, rather than re-reading from the disk, it will just point to this data already in memory. To clear the read files, just reset the data dictionary (e.g. settings['data'] ={})
- settings['datasums'] stores the datasum when read in. Can be used later to check files are the same.

Both data and datasums store the data in identical trees, e.g.: settings['data'][Z][z1][ftype] will have the data.

indexzero: bool

If True, subtract 1 from all level indexes as python indexes from 0, while AtomDB indexes from 1.

offline: bool

If True, do not search online to download data files - just return as if data does not exist

Returns HDUlist

the opened pyfits hdulist if succesful. False if file doesn't exist

`pyatomdb.atomdb.`**`get_emissivity`**(*linefile, elem, ion, upper, lower, kT=[-1], hdu=[-1], kTunits='keV'*)

`pyatomdb.atomdb.`**`get_filemap_file`**(*ftype*, *Z*, *z1*, *fmapfile='$ATOMDB/filemap'*, *atomdbroot='$ATOMDB'*, *quiet=False*, *misc=False*)

Find the correct file from the database for atomic data of type ftype for ion with nuclear charge Z and ioncharge+1 = z1

Parameters **ftype** : str

- 'ir' = ionization & recombination data
- 'lv' = energy levels
- 'la' = wavelength and transition probabilities (lambda & a-values)
- 'ec' = electron collision rates
- 'pc' = proton collision rates
- 'dr' = dielectronic recombination satellite line information

- 'ai' = autoionization rate data
- 'pi' = XSTAR photoionization data
- 'em' = emission feature data (currently unused)

Z : int

Element atomic number (=6 for C+4)

z1 : int

Ion charge +1 (=5 for C+4)

fmapfile : str

Specific filemap to use. Otherwise defaults to atomdbroot+'/filemap'

atomdbroot : str

Location of ATOMDB database. Defaults to ATOMDB environment variable. all $ATOMDB in the filemap will be expanded to this value

quiet : bool

If true, suppress warnings about files not being present for certain ions

misc : bool

If requesting "misc" data, i.e. the Bremsstrahlung inputs, use this. This is for non ion-specific data, therefore Z,z1 are ignored. types are: 10 or 'abund': elemental abundances 11 or 'hbrems': Hummer bremstrahlung gaunt factor coefficients 13 or 'rbrems': Relativistic bremstrahlung gaunt factor coefficients

Returns str

The filename for the relevant file, with all $ATOMDB expanded. If no file exists, returns zero length string.

pyatomdb.atomdb.**get_ion_lines**(*linefile*, *Z*, *z1*, *fullinfo=False*)

pyatomdb.atomdb.**get_ionbal**(*ionbalfile*, *element*, *ion=-1*)

pyatomdb.atomdb.**get_ionfrac**(*ionbalfile*, *Z*, *te*, *z1=-1*)

Reads the ionization fraction of a given ion at a given Te from an ionbalfile Assumes ionization equilibrium

Parameters **ionbalfile** : str

location of ionization balance file

Z : int

atomic number of element (e.g. 6 for carbon)

te : float

electron temperature (in K)

z1 : int

if provided, z+1 of ion (e.g. 5 for O V). If omitted, returns ionization fraction for all ions of element

Returns ionization fraction of ion or, if not specified, of all ions at Te

pyatomdb.atomdb.**get_ionpot**(*Z*, *z1*, *settings=False*, *datacache=False*)

Get the ionization potential of an ion in eV

Parameters **Z** : int

The atomic number of the element

z1 : int

The ion charge + 1 of the ion

settings : dict

See description in get_data

datacache : dict

Used for caching the data. See description in get_data

Returns float

The ionization potential of the ion in eV.

pyatomdb.atomdb.**get_ionrec_rate**(*Te_in*, *irdat_in*, *lvdat_in=False*, *Te_unit='K'*, *lvdatp1_in=False*, *ionpot=False*, *separate=False*, *Z=-1*, *z1=-1*, *settings=False*, *datacache=False*, *extrap=True*)

Get the ionization and recombination rates at temperture(s) Te from ionization and recombination rate data file irdat.

Parameters **Te_in** : float or arr(float)

electron temperature in K (default), eV, or keV

irdat_in : HDUList

ionization and recombination rate data

lvdat_in : HDUList

level data for ion with lower charge (i.e. ionizing ion or recombined ion)

Te_unit : {'K' , 'keV' , 'eV'}

temperature unit

lvdatp1_in : HDUList

level data for the ion with higher charge (i.e ionized or recombining ion)

ionpot : float

ionization potential of ion (eV).

separate : bool

if set, return DR, RR, EA and CI rates seperately. (DR = dielectronic recombination, RR = radiative recombination, EA = excitaiton autoionization, CI = collisional ionization) Note that EA & CI are not stored separately in all cases, so may return zeros for EA as the data is incorporated into CI rates.

Z : int

Element charge to get rates for (ignores "irdat_in")

z1 : int

Ion charge +1 to get rates for (ignores "irdat_in") e.g. Z=6,z1=4 for C IV (C 3+)

settings : dict

See description in read_data

datacache : dict

See description in read_data

extrap : bool

Extrappolate rates to Te ranges which are off the provided scale

Returns float, float:

(ionization rate coeff., recombination rate coeff.) in cm^3 s^-1 *unless* separate is set, in which case:

float, float, float, float:

(CI, EA, RR, DR rate coeffs) in cm^3 s^-1 Note that these assume low density & to get the real rates you need to multiply by N_e N_ion.

pyatomdb.atomdb.**get_level_details**(*level*, *Z=-1*, *z1=-1*, *filename=''*, *filemap=''*, *atomdb-root=''*)

Function returns the details in the level file for the specified level. LV file can be specified by filename, or by filemap, Z, z1

pyatomdb.atomdb.**get_line_emissivity**(*Z*, *z1*, *upind*, *loind*, *linefile='$ATOMDB/apec_line.fits'*, *ion_drv=False*, *elem_drv=False*, *use_nei=False*)

Get the emissivity of a line as fn of temperature from APEC line file

Parameters **Z** : int

Atomic number of element of line

z1 : int

Ion charge +1 of ion

upind : int

Upper level of transition

loind : int

Lower level of transition

linefile : str

line emissivity file. defaults to $ATOMDB/apec_line.fits

ion_drv : int

if set, return only the contribution from driving ion ion_drv. This is useful for non-equilibrium plasma calculations, and requires an nei_line file to be specified in linefile

elem_drv : int

same as ion_drv, but specified driving element. Currently this setting is pointless, as all transitions have the same driving element as element.

use_nei : bool

This can be useful when trying to get line emissivities which fall below the 1e-20 cut off. Applying this flag, the NEI file will be used by default and an ionization balance applied. This should give the same results as normal for strong emissivities, but go to a lower emissivity before being set to zero. Use with caution...

Returns dict

dictionary with the following data in it:

['kT'] : array(float)

the electron temperatures, in keV

['dens'] : array(float)

the electron densities, in cm^-3

['time'] : array(float)

the time (for old-style NEI files only, typically all zeros in current files)

['epsilon'] : array(float)

the emissivity in ph cm^3 s^-1

pyatomdb.atomdb.**get_lorentz_levpop**(*Z*, *z1*, *up*, *lo*, *Te*, *Ne*, *version*, *linelabel*)

calculate the level population for a particular ion

pyatomdb.atomdb.**get_maxwell_rate**(*Te*, *colldata=False*, *index=-1*, *lvdata=False*, *Te_unit='K'*, *lvdatap1=False*, *ionpot=False*, *force_extrap=False*, *silent=True*, *finallev=False*, *initlev=False*, *Z=-1*, *z1=-1*, *dtype=False*, *exconly=False*, *datacache=False*, *settings=False*)

Get the maxwellian rate for a transition from a file, typically for ionization, recombination or excitation.

Parameters **Te** : float

electron temperature(s), in K by default

colldata : HDUList

If provided, the HDUList for the collisional data

index : int

The line in the HDUList to do the calculation for. Indexed from 0.

lvdata : HDUList

the hdulist for the energy level file (as returned by pyfits.open('file'))

Te_unit : {'K' , 'eV' , 'keV'}

Units of temperature grid.

lvdatap1 : HDUList

The level data for the recombining or ionized data.

ionpot : float

The ionization potential in eV (required for some calculations, if not provided, it will be looked up)

force_extrap : bool

Force extrappolation to occur for rates outside the nominal range of the input data

silent : bool

Turn off notifications

finallev : int

Instead of specifying the index, can use upperlev, lowerlev instead.

initlev : int

Instead of specifying the index, can use upperlev, lowerlev instead

Z : int

Instead of providing colldata, can provide Z & z1. Z is the atomic number of the element.

z1 : int

Instead of providing colldata, can provide Z & z1. z1 is the ion charge +1 for the initial ion

dtype : str

data type. One of:

'EC' : electron impact excitation

'PC' : proton impact excitation

'CI' : collisional ionization

'EA' : excitation-autoionization

'XI' : excluded ionization

'XR' : excluded recombination

'RR' : radiative recombination

'DR' : dielectronic recombination

exconly : bool

For collisional excitation, return only the excitation rate, not the de-excitation rate.

settings : dict

See description in read_data

datacache : dict

See description in read_data

Returns float or array(float)

Maxwellian rate coefficient, in units of cm^3 s^-1 For collisional excitation (proton or electron) returns excitation, dexcitation rates

Examples

Te = numpy.logspace(4,9,20)

(1) Get excitation rates for row 12 of an Fe XVII file colldata = pyatomdb.atomdb.get_data(26,17,'EC') exc, dex = get_maxwell_rate(Te, colldata=colldata, index=12)

(2) Get excitation rates for row 12 of an Fe XVII file exc, dex = get_maxwell_rate(Te, Z=26,z1=17, index=12)

(3) Get excitation rates for transitions from level 1 to 15 of FE XVII exc, dex = get_maxwell_rate(Te, Z=26, z1=17, dtype='EC', finallev=15, initlev=1)

`pyatomdb.atomdb.`**`get_oscillator_strength`**(*Z*, *z1*, *upperlev*, *lowerlev*, *datacache=False*)

Get the oscillator strength f_{ij} of a transition

Parameters **Z** : int

The atomic number of the element

z1 : int

The ion charge + 1 of the ion

upperlev : int

The upper level, indexed from 1

lowerlev : int

The lower level, indexed from 1

datacache : dict

Used for caching the data. See description in get_data

Returns float

The oscillator strength. Returns 0 if transition not found. If transition is not found but the inverse transition is present the oscillator strength is calculated for this instead.

pyatomdb.atomdb.**interp_rate**(*Te*, *npar*, *Te_grid*, *ionrec_par*)

pyatomdb.atomdb.**interpol_huntd**(*x*, *y*, *z*)

pyatomdb.atomdb.**interpolate_ionrec_rate**(*cidat*, *Te*, *force_extrap=False*)

pyatomdb.atomdb.**lorentz_cie**(*version*)

Calculate the CSD of equilibrium plasmas at 1e6, 6e6K and 4keV.

Parameters **version** : string

The version string

Returns None

pyatomdb.atomdb.**lorentz_levpop**(*version*)

Calculate the level populating processes for each line in the stronglines Files. This will require a significant rerun of APEC. Hmmmmm

Processes to be tracked: electron excitation, electron de-excitation, proton excitation and dexcitation, cascade into the level, radiative out, recombination (incl. cascade) in, DR (incl cascade) in, and inner-shell ionization in (why only inner shell?)

pyatomdb.atomdb.**lorentz_neicont**(*version*)

Full spectrum of a gas ionizing from 1e4K to 2.321e7K (=2keV) at a fluence (n_e * t, or $ au$) of 10^{10} cm$^-3$ s

Parameters **version** : string

The version string

Returns None

pyatomdb.atomdb.**lorentz_neicsd**(*version*)

Charge state distribution of a gas ionizing from 1e4K to 2.321e7K (=2keV) at a fluence (n_e * t, or $ au$) of 10^{10} cm$^-3$ s

Parameters **version** : string

The version string

Returns None

pyatomdb.atomdb.**lorentz_neilines**(*version*)

100 strongest lines with wavelength < 1000A for a 1cm^3 plasma (1) starting at 1e4K, going to 2.321e7K at a fluence (n_e * t, or $ au$) of 10^{10} cm$^-3$ s (2) starting at 3.5keV, going to 1.5keV at a fluence (n_e * t, or $ au$) of 10^{10} cm$^-3$ s

Parameters **version** : string

The version string

Returns None

pyatomdb.atomdb.**lorentz_power**(*version*)
Calculate the power emitted from 13.6eV to 13.6keV in a 1m^3 slab of plasma with n_e=1e6m^-3.

Parameters **version** : string

The version string

Returns None

pyatomdb.atomdb.**lorentz_stronglines**(*version*)
Calculate the 100 strongest lines below 1000A from a 1m3 slab of plasma with n_e = 1e6m-3, at 3 different temperatures: 10^6K, 6e6K, 4.642e7K

Parameters **version** : string

The version string

Returns None

pyatomdb.atomdb.**make_level_descriptor**(*lv*)

pyatomdb.atomdb.**make_lorentz**(*version=False*, *do_all=True*, *cie=False*, *power=False*, *strong-lines=False*, *neicsd=False*, *neilines=False*, *neicont=False*, *lev-pop=False*)
This makes all the Lorentz data comparison files from the Astrophysical Collisional Plasma Test Suite, version 0.4.0

Parameters **version** : string (optional)

e.g. "3.0.7" to run the suite for v3.0.7. Otherwise uses latest version.

Returns none

pyatomdb.atomdb.**prep_spline_atomdb**(*x*, *y*, *n*)

pyatomdb.atomdb.**read_filemap**(*filemap='$ATOMDB/filemap'*, *atomdbroot='$ATOMDB'*)
Reads the AtomDB filemap file in to memory. By default, tries to read $ATOMDB/filemap, replacing all instances of $ATOMDB in the filemap file with the value of the environment variable $ATOMDB

Parameters **filemap: str**

the filemap file to read

atomdbroot: str

location of files, if not $ATOMDB.

pyatomdb.atomdb.**rr_badnell**(*Te*, *c*)
Convert data from Badnell constants into a RR Rate

Parameters **Te** : float or array(float)

Electron temperature[s] in K

c : array

Constants from DR rates. Stored as alternating pairs in AtomDB, so c1,e1,c2,e2,c3,e3 etc in the IONREC_PAR column

Returns float

RR rate in cm^3 s-1

References

See http://amdpp.phys.strath.ac.uk/tamoc/DATA/RR/

pyatomdb.atomdb.**rr_shull**(*Te*, *c*)

pyatomdb.atomdb.**rr_verner**(*Te*, *c*)

pyatomdb.atomdb.**rrc_ph_value**(*E*, *Z*, *z1*, *rrc_ph_factor*, *IonE*, *kT*, *levdat*, *xstardata=False*, *xstarfinallev=False*)

Returns RRC in photons cm3 s-1 keV-1

Parameters **E:**

Z: int

Atomic number of element (i.e. 8 for Oxygen)

z1: int

Ion charge +1 e.g. 5 for C+4, a.k.a. C V

rrc_ph_factor: float

Conversion factor for RRC.

IonE: float

Ionization potential of ion

kT: float

Temperature (keV)

levdat: lvdat line

Line from the lvdat file

xstardata : dict, str or HDUList

if the data is XSTAR data (pi_type=3), supply the xstardata. This can be a dictionary with 2 arrays, one "Energy", one "sigma", the file name, or the entire PI file (already loaded):

```
# load level data
lvdata = atomdb.get_data(26, 24, 'LV', settings)

# load XSTAR PI data if it exists
pidata = atomdb.get_data(26, 24, 'PI', settings)

# get pi xsection at energy E for the ground state to ground state
sigma_photoion(E,
               lvdata[1].data['pi_type'][0],
               lvdata[1].data['pi_param'][0],
               xstardata=pidata,
               xstarfinallev=1)
```

xstarfinallev: the level to ionize in to. Defaults to 1.

Returns float

The RRC in photons cm3 s-1 keV-1 at energy(ies) E.

pyatomdb.atomdb.**sigma_hydrogenic**(*Z*, *N*, *L*, *Ein*)

Calculate the PI cross sections of type hydrogenic.

Parameters **N** : int

n shell

L : int

l quantum number

Z : int

nuclear charge

Ein : array(float)

energy grid for PI cross sections (in keV)

Returns array(float)

Photoionization cross section (in cm^2)

pyatomdb.atomdb.**sigma_photoion**(*E*, *Z*, *z1*, *pi_type*, *pi_coeffts*, *xstardata=False*, *xstarfinallev=1*)

Returns the photoionization cross section at E, given an input of sig_coeffts.

Parameters **E: float or array of floats**

Energy/ies to find PI cross section at (keV)

Z: int

Atomic number of element (i.e. 8 for Oxygen)

pi_type : int

the "PI_TYPE" from the energy level file for this level, can be:

-1. No PI data 0. Hydrogenic 1. Clark 2. Verner 3. XSTAR

pi_coeffts : array(float)

the "PI_PARAM" array for this level from the LV file

xstardata : dict, str or HDUList

if the data is XSTAR data (pi_type=3), supply the xstardata. This can be a dictionary with 2 arrays, one "Energy", one "sigma", the file name, or the entire PI file (already loaded):

```
# load level data
lvdata = atomdb.get_data(26, 24, 'LV', settings)

# load XSTAR PI data if it exists
pidata = atomdb.get_data(26, 24, 'PI', settings)

# get pi xsection at energy E for the ground state to ground state
sigma_photoion(E,
               lvdata[1].data['pi_type'][0],
               lvdata[1].data['pi_param'][0],
               xstardata=pidata,
               xstarfinallev=1)
```

xstarfinallev: the level to ionize in to. Defaults to 1.

Returns array(float)

pi cross section in cm^2 at energy E.

pyatomdb.atomdb.**sort_pi_data**(*pidat*, *lev_init*, *lev_final*)

Given the pidat (returned by opening the PI data file, i.e. pyfits.open('XX_YY_PI.fits'), and the initial and final levels, return the PI cross section data.

Parameters **pidat** : hdulist

The photoionization data for the ion

lev_init : int

The initial level

lev_final : int

The final level

Returns dict:

which contains the following information: pi['ion_init'] - the initial ion charge +1 pi['lev_init'] - the initial level pi['ion_final'] - the final ion charge+1 (should be ion_init+1) pi['lev_final'] - the final level pi['pi_type'] - the type. (best to ignore) pi['g_ratio'] - the ratio of the statistical weight of the intitial and final levels pi['energy'] - the array of energies (keV) pi['pi_param'] - the array of pi cross sections in Mbarn.

pyatomdb.atomdb.**write_filemap**(*d*, *filemap*, *atomdbroot=''*)

Write filemap to file

Parameters **d** : dict

Dictionary with filemap data in it. Structure defined as return value from read_filemap.

filemap : str

Name of filemap file to read. If zero length, use "$ATOMDB/filemap"

atomdbroot : str

Replace any $ATOMDB in the file names with this. If not provided, use "ATOMDB" environment variable instead

Returns none

PyAtomDB Const module

A series of physical constants and constants relevant to running the APEC code. This contains a list of constants, both physical and apec code related.

Version 0.1 - initial release Adam Foster July 17th 2015

PyAtomDB Spectrum module

This module contains codes for creating spectra from the AtomDB emissivity files This module contains methods for creating spectra from the AtomDB files. Some are more primitive than others...

class pyatomdb.spectrum.**CXSession**(*linefile='$ATOMDB/apec_line.fits'*, *cocofile='$ATOMDB/apec_coco.fits'*, *elements=False*, *abundset='AG89'*, *collisionunits='kev/amu'*)

Bases: pyatomdb.spectrum.Session

A Charge Exchange session using the same line and coco files, and/or responses

Attributes

linefile	(string) The line emissivity data file
cocofile	(string) The continuum emissivity data file
linedata: **HDUList**	The line emissivity data
cocodata: **HDUList**	The line emissivity data
elements	(array_like, int) The atomic number of the elements to include. Defaults to all.
abundset	(string) The elemental abundances to be used. Defaults to Anders and Grevesse 1989.
collisionunits	(string) Whether the units are given in energy (kev/amu) or velocity (cm/s)
veltype	(int) Whether the velocity is in terms of (1) center of mass, (2) donor ion or (3) receiver ion
ready	(bool) Set when line, continuum and spectral bin data has been read in, and a spectrum can be calculated.
default_abundset	(string) The abundance set used in line and continuum files
abundset	(string) The abundance set to be used in calculating the spectra.
response_set	(bool) If a response (rmf & arf) have been loaded, set to true
spectra	(dict of array_like) Holds the spectra at each temperature.
rmffile	(string) Filename of RMF file
arffile	(string) Filename of ARF file
rmf	(HDUList) RMF data
arf	(HDUList) ARF data
ionbal	(dict of array like) ionization balance of each ion, normalized to 1 e.g. ionbal[6]=numpy.array([0.5,0.4,0.1,0,0,0,0]) for Carbon

class `IonSpec`(*session*, *index*, *Z*, *z1*)

An individual ion spectrum within a session, from a specifically tabulated energy in a line/coco file.

Attributes

energy	(float) The energy of this spectrum, in keV/amu
index	(int) The index in the line file for this spectrum
Z	(int) The element
z1	(int) The the recombining ion charge+1 (so 5 for C4+ + H -> C3+ + H+)

`calc_spectrum`(*session*, *dolines=True*, *docont=True*, *dopseudo=True*)

Calculates the spectrum for each ion on a single energy

Parameters **session** : Session
The parent Session
dolines : bool
Include lines in the spectrum
docont : bool
Include continuum in the spectrum
dopseudo : bool
Include pseudocontinuum in the spectrum
Outputs

———-

none

Notes

Modifies:

dict : self.spectrum the spectrum of the ion

dict : self.spectrum_withresp the spectrum of the ion, folded through response

Then calls *recalc()* to update the spectra

recalc(*session*)

Recalculate the spectrum - just for changing abundances etc. Does not recalculate spectrum fully, just changes the multipliers. Does nothing if self.ready is False, should be run after calc_spectrum.

Parameters **session** : Session
The parent session

Returns none

Notes

Modifies:

self.spectrum : array_like (float)

self.spectrum_withresp : array_like (float)

set_index(*E*, *Eunit='kev/amu'*, *logscale=False*)

Finds HDU with kT closest to desired kT in given line or coco file.

Opens the line or coco file, and looks for the header unit with temperature closest to te. Use result as index input to make_spectrum

Parameters **E** : float
Energy in keV/amu

Eunit : {'keV' , 'K', 'eV'}
Units of E (kev/amu default)

logscale : bool
Search on a log scale for nearest temperature if set.

Returns none

Notes

modifies self.index : int Index in HDU file with nearest temperature to te.

class CXSession.**Spec**(*session*, *index*)

An individual spectrum within a session, from a specifically tabulated temperature in a line/coco file.

Attributes

temperature	(float) The temperature of this spectrum, in keV
index	(int) The index in the line file for this spectrum

calc_spectrum(*session*)

Calculates the spectrum for each element on a single temperature

Parameters **session** : Session
The parent Session

dolines : bool
Include lines in the spectrum

docont : bool
Include continuum in the spectrum
dopseudo : bool
Include pseudocontinuum in the spectrum
Outputs

———-

none

Notes

Modifies:

dict : self.spectrum_by_Z the spectrum of each element

dict : self.spectrum_by_Z_withresp the spectrum of each element, folded through response

Then calls *recalc()* to update the spectra

recalc(*session*)
Recalculate the spectrum - just for changing abundances etc. Does not recalculate spectrum fully, just changes the multipliers. Does nothing if self.ready is False, should be run after calc_spectrum.
Parameters **session** : Session
The parent session
Returns none

Notes

Modifies:

self.spectrum : array_like (float)

self.spectrum_withresp : array_like (float)

set_index(*T*, *teunit='K'*, *logscale=False*)
Finds HDU with kT closest to desired kT in given line or coco file.

Opens the line or coco file, and looks for the header unit with temperature closest to te. Use result as index input to make_spectrum
Parameters **te** : float
Temperature in keV or K
teunits : {'keV' , 'K', 'eV'}
Units of te (kev or K, default keV)
logscale : bool
Search on a log scale for nearest temperature if set.
Returns none

Notes

modifies self.index : int Index in HDU file with nearest temperature to te.

CXSession.**recalc**()
Recalculate the spectrum - just for changing abundances etc. Does not recalculate spectrum fully, just changes the multipliers. Does nothing if self.ready is False, should be run after calc_spectrum.

Parameters **none**

Returns none

Notes

modifies self.spectrum

CXSession.**return_spectra**(*collision*, *veltype=False*, *raw=False*, *nearest=False*)
Get the spectrum at an exact temperature. Interpolates between 2 neighbouring spectra

Finds HDU with kT closest ro desired kT in given line or coco file.

Opens the line or coco file, and looks for the header unit with temperature closest to te. Use result as index input to make_spectrum

Parameters **collision** : float

The energy (kev/amu) or velocity (cm/s) of the collision

raw : bool

If set, return the spectrum without response applied. Default False.

Returns **spectrum** : array(float)

The spectrum in photons cm^5 s^-1 bin^-1, with the response, or photons cm^3 s^-1 bin^-1 if raw is set.

CXSession.**set_abund**(*elements*, *abund*)
Set the elemental abundance, relative to the abundset. Defaults to 1.0 for everything

Parameters **elements** : int or array_like(int)

The elements to change the abundance of

abund : float or array_like(float)

The new abundances. If only 1 value, set all *elements* to this abundance Otherwise, should be of same length as elements.

Returns None

Examples

Set the abundance of iron to 0.5

```
>>> myspec.set_abund(26, 0.5)
```

Set the abundance of iron and nickel to 0.1 and 0.2 respectively

```
>>> myspec.set_abund([26, 28], [0.1,0.2])
```

Set the abundance of oxygen, neon, magnesium and iron to 0.1

```
>>> myspec.set_abund([8,10,12,26],0.1)
```

CXSession.**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 none

updates self.abundset and self.abundsetvector.

CXSession.**set_apec_files**(*linefile='$ATOMDB/apec_line.fits'*, *cocofile='$ATOMDB/apec_coco.fits'*)

Set the apec line and coco files

Parameters **linefile** : str or HDUList

The filename of the line emissivity data, or the opened file.

cocofile : str or HDUList

The filename of the continuum emissivity data, or the opened file.

elements : array_like(int)

The atomic numbers of the elements to include. Defaults to all (1-30)

abundset : string

The abundance set to use. Defaults to AG89. See atomdb.set_abundance

Returns None

Notes

Updates self.linefile, self.linedata, self.cocofile and self.cocodata

CXSession.**set_ionbal_temperature**(*te*, *teunit='keV'*)

Set the ionization balance to that of a given electron temperature

Parameters **te** : float

Electron Temperature

teunit : string

Units for the temperature. keV or A.

Notes

Modifies self.ionbal

CXSession.**set_response**(*rmf*, *arf=False*)

Set the response. rmf, arf can either be the filenames or the opened files (latter is faster if called repeatedly)

Amends the following items:

self.rmffile [string] The rmf file name

self.rmf [string] The response matrix

self.arffile [string] The arf file name

self.arf [string] The arf data

Parameters **rmf: string or HDUlist**

The response matrix file

arf: string or HDUlist

The ancillary response file

Returns none

CXSession.**set_specbins**(*specbins*, *specunits='A'*)

Set the energy or wavelength bin for the raw spectrum

Note that this is overridden if a response is loaded

Parameters **ebins** : array(float)

The edges of the spectral bins (for n bins, have n+1 edges)

specunits : {'a','kev'}

The spectral bin units to use. Default is angstroms

Returns None

Notes

updates self.specbins, self.binunits, self.specbins_set

class pyatomdb.spectrum.**Session**(*linefile='$ATOMDB/apec_line.fits'*, *cocofile='$ATOMDB/apec_coco.fits'*, *elements=False*, *abundset='AG89'*)

A session using the same line and coco files, and/or responses

Attributes

linefile	(string) The line emissivity data file
cocofile	(string) The continuum emissivity data file
linedata: HDUList	The line emissivity data
cocodata: HDUList	The line emissivity data
elements	(array_like, int) The atomic number of the elements to include. Defaults to all.
abundset	(string) The elemental abundances to be used. Defaults to Anders and Grevesse 1989.
ready	(bool) Set when line, continuum and spectral bin data has been read in, and a spectrum can be calculated.
default_abundset	(string) The abundance set used in line and continuum files
abundset	(string) The abundance set to be used in calculating the spectra.
response_set	(bool) If a response (rmf & arf) have been loaded, set to true
spectra	(dict of array_like) Holds the spectra at each temperature.
rmffile	(string) Filename of RMF file
arffile	(string) Filename of ARF file
rmf	(HDUList) RMF data
arf	(HDUList) ARF data

class **Spec**(*session*, *index*)

An individual spectrum within a session, from a specifically tabulated temperature in a line/coco file.

Attributes

temperature	(float) The temperature of this spectrum, in keV
index	(int) The index in the line file for this spectrum

calc_spectrum(*session*)

Calculates the spectrum for each element on a single temperature

Parameters **session** : Session
The parent Session
dolines : bool
Include lines in the spectrum
docont : bool
Include continuum in the spectrum
dopseudo : bool
Include pseudocontinuum in the spectrum
Outputs

———-

none

Notes

Modifies:

dict : self.spectrum_by_Z the spectrum of each element

dict : self.spectrum_by_Z_withresp the spectrum of each element, folded through response

Then calls *recalc()* to update the spectra

recalc(*session*)

Recalculate the spectrum - just for changing abundances etc. Does not recalculate spectrum fully, just changes the multipliers. Does nothing if self.ready is False, should be run after calc_spectrum.

Parameters **session** : Session
The parent session
Returns none

Notes

Modifies:

self.spectrum : array_like (float)

self.spectrum_withresp : array_like (float)

set_index(*T*, *teunit='K'*, *logscale=False*)

Finds HDU with kT closest to desired kT in given line or coco file.

Opens the line or coco file, and looks for the header unit with temperature closest to te. Use result as index input to make_spectrum

Parameters **te** : float
Temperature in keV or K
teunits : {'keV' , 'K', 'eV'}
Units of te (kev or K, default keV)
logscale : bool
Search on a log scale for nearest temperature if set.
Returns none

Notes

modifies self.index : int Index in HDU file with nearest temperature to te.

Session.**recalc**()

Recalculate the spectrum - just for changing abundances etc. Does not recalculate spectrum fully, just changes the multipliers. Does nothing if self.ready is False, should be run after calc_spectrum.

Parameters **none**

Returns none

Notes

modifies self.spectrum

Session.**return_spectra**(*te*, *teunit='keV'*, *raw=False*, *nearest=False*, *get_nearest_t=False*)

Get the spectrum at an exact temperature. Interpolates between 2 neighbouring spectra

Finds HDU with kT closest ro desired kT in given line or coco file.

Opens the line or coco file, and looks for the header unit with temperature closest to te. Use result as index input to make_spectrum

Parameters **te** : float

Temperature in keV or K

teunit : {'keV' , 'K'}

Units of te (kev or K, default keV)

raw : bool

If set, return the spectrum without response applied. Default False.

nearest : bool

If set, return the spectrum from the nearest tabulated temperature in the file, without interpolation

get_nearest_t : bool

If set, and *nearest* set, return the nearest tabulated temperature as well as the spectrum.

Returns **spectrum** : array(float)

The spectrum in photons cm^5 s^-1 bin^-1, with the response, or photons cm^3 s^-1 bin^-1 if raw is set.

nearest_T : float, optional

If *nearest* is set, return the actual temperature this corresponds to. Units are same as *teunit*

Session.**set_abund**(*elements*, *abund*)

Set the elemental abundance, relative to the abundset. Defaults to 1.0 for everything

Parameters **elements** : int or array_like(int)

The elements to change the abundance of

abund : float or array_like(float)

The new abundances. If only 1 value, set all *elements* to this abundance Otherwise, should be of same length as elements.

Returns None

Examples

Set the abundance of iron to 0.5

```
>>> myspec.set_abund(26, 0.5)
```

Set the abundance of iron and nickel to 0.1 and 0.2 respectively

```
>>> myspec.set_abund([26, 28], [0.1,0.2])
```

Set the abundance of oxygen, neon, magnesium and iron to 0.1

```
>>> myspec.set_abund([8,10,12,26],0.1)
```

Session.**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 none

updates self.abundset and self.abundsetvector.

Session.**set_apec_files**(*linefile='$ATOMDB/apec_line.fits'*, *cocofile='$ATOMDB/apec_coco.fits'*)

Set the apec line and coco files

Parameters **linefile** : str or HDUList

The filename of the line emissivity data, or the opened file.

cocofile : str or HDUList

The filename of the continuum emissivity data, or the opened file.

elements : array_like(int)

The atomic numbers of the elements to include. Defaults to all (1-30)

abundset : string

The abundance set to use. Defaults to AG89. See atomdb.set_abundance

Returns None

Notes

Updates self.linefile, self.linedata, self.cocofile and self.cocodata

Session.**set_response**(*rmf*, *arf=False*)

Set the response. rmf, arf can either be the filenames or the opened files (latter is faster if called repeatedly)

Amends the following items:

self.rmffile [string] The rmf file name

self.rmf [string] The response matrix

self.arffile [string] The arf file name

self.arf [string] The arf data

Parameters **rmf: string or HDUlist**

The response matrix file

arf: string or HDUlist

The ancillary response file

Returns none

`Session.`**`set_specbins`**(*specbins*, *specunits='A'*)

Set the energy or wavelength bin for the raw spectrum

Note that this is overridden if a response is loaded

Parameters **ebins** : array(float)

The edges of the spectral bins (for n bins, have n+1 edges)

specunits : {'a','kev'}

The spectral bin units to use. Default is angstroms

Returns None

Notes

updates self.specbins, self.binunits, self.specbins_set

`pyatomdb.spectrum.`**`add_lines`**(*Z*, *abund*, *lldat*, *ebins*, *z1=False*, *z1_drv=False*, *broadening=False*, *broadenunits='A'*)

Add lines to spectrum, applying gaussian broadening.

Add the lines in list lldat, with atomic number Z, to a spectrum delineated by ebins (these are the edges, in keV). Apply broadening to the spectrum if broadening != False, with units of broadenunits (so can do constant wavelength or energy broadening)

Parameters **Z** : int

Element of interest (e.g. 6 for carbon)

abund : float

Abundance of element, relative to AG89 data.

lldat : dtype linelist

The linelist to add. Usually the hdu from the apec_line.fits file, often with some filters pre-applied.

ebins : array of floats

Energy bins. Will return spectrum with nbins-1 data points.

z1 : int

Ion charge +1 of ion to return

z1_drv : int

Driving Ion charge +1 of ion to return

broadening : float

Apply spectral broadening if > 0. Units of A of keV

broadenunits : {'A' , 'keV'}

The units of broadening, Angstroms or keV

Returns array of float

broadened emissivity spectrum, in photons cm^3 s^-1 bin^-1. Array has len(ebins)-1 values.

pyatomdb.spectrum.**apply_response**(*spectrum*, *rmf*, *arf=False*)

Apply a response to a spectrum

Parameters **spectrum** : array(float)

The spectrum, in counts/bin/second, to have the response applied to. Must be binned on the same grid as the rmf.

rmf : string or pyfits.hdu.hdulist.HDUList

The filename of the rmf or the opened rmf file

arf : string or pyfits.hdu.hdulist.HDUList

The filename of the arf or the opened arf file

Returns

——-

array(float)

energy grid (keV) for returned spectrum

array(float)

spectrum folded through the response

pyatomdb.spectrum.**broaden_continuum**(*bins*, *spectrum*, *binunits='keV'*, *broadening=False*, *broadenunits='keV'*)

Apply a broadening to the continuum

Parameters **bins** : array(float)

The bin edges for the spectrum to be calculated on, in units of keV or Angstroms. Must be monotonically increasing. Spectrum will return len(bins)-1 values.

spectrum : array(float)

The emissivities in each bin in the unbroadened spectrum

binunits : {'keV' , 'A'}

The energy units for bins. "keV" or "A". Default keV.

broadening : float

Broaden the continuum by gaussians of this width (if False, no broadening is applied)

broadenunits : {'keV' , 'A'}

Units for broadening (kev or A)

Returns array(float)

spectrum broadened by gaussians of width broadening

pyatomdb.spectrum.**expand_E_grid**(*eedges*, *n*, *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

n : int

The number of good data points in the continuum array

Econt_in_full: float(array)

The compressed continuum energies

cont_in_full: float(array)

The compressed continuum emissivities

Returns float(array)

len(bins)-1 array of continuum emission, in units of photons cm^3 s^-1 bin^-1

pyatomdb.spectrum.**get_effective_area**(*rmf*, *arf=False*)

Get the effective area of a response file

Parameters **rmf** : string or pyfits.hdu.hdulist.HDUList

The filename of the rmf or the opened rmf file

arf : string or pyfits.hdu.hdulist.HDUList

The filename of the arf or the opened arf file

Returns

———-

array(float)

energy grid (keV) for returned response

array(float)

effective area for the returned response

pyatomdb.spectrum.**get_index**(*te*, *filename='$ATOMDB/apec_line.fits'*, *teunits='keV'*, *logscale=False*)

Finds HDU with kT closest ro desired kT in given line or coco file.

Opens the line or coco file, and looks for the header unit with temperature closest to te. Use result as index input to make_spectrum

Parameters **te** : float

Temperature in keV or K

teunits : {'keV' , 'K'}

Units of te (kev or K, default keV)

logscale : bool

Search on a log scale for nearest temperature if set.

filename : str or hdulist

line or continuum file, already opened or filename.

Returns int

Index in HDU file with nearest temperature to te.

pyatomdb.spectrum.**get_response_ebins**(*rmf*)

Get the energy bins from the rmf file

Parameters **rmf** : string or pyfits.hdu.hdulist.HDUList

The filename of the rmf or the opened rmf file

Returns array(float)

input energy bins used. nbins+1 length, with the last item being the final bin This is the array on which the input spectrum should be calculated

pyatomdb.spectrum.**list_lines**(*specrange*, *lldat=False*, *index=False*, *linefile=False*, *units='angstroms'*, *Te=False*, *teunit='K'*, *minepsilon=1e-20*)

Gets list of the lines in a given spectral range

Note that the output from this can be passed directly to print_lines

Parameters **specrange** : [float,float]

spectral range [min,max] to return lines on

lldat : see notes

line data

index : int

index in lldat, see notes

linefile : see notes

line data file, see notes

units : {'A' , 'keV'}

units of specrange (default A)

Te : float

electron temperature (used if index not set to select appropriate data HDU from line file)

teunit : {'K','keV','eV'}

units of Te

minepsilon : float

minimum epsilon for lines to be returned, in ph cm^3 s^-1

Returns **linelist** : dtype=([('Lambda', '>f4'), ('Lambda_Err', '>f4'), ('Epsilon', '>f4'), ('Epsilon_Err', '>f4'), ('Element', '>i4'), ('Ion', '>i4'), ('UpperLev', '>i4'), ('LowerLev', '>i4')])

A line list filtered by the various elements.

Notes

The actual line list can be defined in one of several ways:

specrange = [10,100]

1.lldat as an actual list of lines:

```
a = pyfits.open('apec_line.fits')
llist = a[30].data
l = list_lines(specrange, lldat=llist)
```

2.lldat as a numpy array of lines:

```
a = pyfits.open('apec_line.fits')
llist = numpy.array(a[30].data)
l = list_lines(specrange, lldat=llist)
```

3.lldat is a BinTableHDU from pyfits:

```
a = pyfits.open('apec_line.fits')
llist = numpy.array(a[30])
l = list_lines(specrange, lldat=llist)
```

4.lldat is a HDUList from pyfits. In this case index must also be set:

```
a = pyfits.open('apec_line.fits')
index = 30
l = list_lines(specrange, lldat=a, index=index)
```

5.lldat NOT set, linefile contains apec_line.fits file location, index identifies the HDU:

```
linefile = 'mydir/apec_v2.0.2_line.fits'
index = 30
l = list_lines(specrange, linefile=linefile, index=index)
```

6.lldat NOT set & linefile NOT set, linefile is set to $ATOMDB/apec_line.fits. index identifies the HDU:

```
index = 30
l = list_lines(specrange, index=index)
```

pyatomdb.spectrum.**list_nei_lines**(*specrange*, *Te*, *tau*, *Te_init=False*, *lldat=False*, *linefile=False*, *units='angstroms'*, *teunit='K'*, *minepsilon=1e-20*, *datacache=False*)

Gets list of the lines in a given spectral range for a given NEI plasma

For speed purposes, this takes the nearest temperature tabulated in the linefile, and applies the exact ionization balance as calculated to this. This is not perfect, but should be good enough.

Note that the output from this can be passed directly to print_lines

Parameters **specrange** : [float,float]

spectral range [min,max] to return lines on

Te : float

electron temperature

tau : float

electron density * time (cm^-3 s)

Te_init : float

initial ionization balance temperature

lldat : see notes

line data

linefile : see notes

line data file, see notes

units : {'A' , 'keV'}

units of specrange (default A)

teunit : {'K' , 'keV'}

units of temperatures (default K)

minepsilon : float

minimum emissivity (ph cm^3 s^{-1}) for inclusion in linelist

Returns linelist : dtype=([('Lambda', '>f4'), ('Lambda_Err', '>f4'), ('Epsilon', '>f4'), ('Epsilon_Err', '>f4'), ('Element', '>i4'), ('Elem_drv', '>i4'), ('Ion', '>i4'), ('Ion_drv', '>i4'), ('UpperLev', '>i4'), ('LowerLev', '>i4')])

A line list filtered by the various elements.

Notes

The actual line list can be defined in one of several ways:

specrange = [10,100]

1.lldat as an actual list of lines:

```
a = pyfits.open('apec_nei_line.fits')
llist = a[30].data
l = list_nei_lines(specrange, lldat=llist)
```

2.lldat as a numpy array of lines:

```
a = pyfits.open('apec_nei_line.fits')
llist = numpy.array(a[30].data)
l = list_nei_lines(specrange, lldat=llist)
```

3.lldat is a BinTableHDU from pyfits:

```
a = pyfits.open('apec_nei_line.fits')
llist = numpy.array(a[30])
l = list_nei_lines(specrange, lldat=llist)
```

4.lldat is a HDUList from pyfits. In this case index must also be set:

```
a = pyfits.open('apec_nei_line.fits')
index = 30
l = list_nei_lines(specrange, lldat=a, index=index)
```

5.lldat NOT set, linefile contains apec_line.fits file location, index identifies the HDU:

```
linefile = 'mydir/apec_v3.0.2_nei_line.fits'
index = 30
l = list_nei_lines(specrange, linefile=linefile, index=index)
```

6.lldat NOT set & linefile NOT set, linefile is set to $ATOMDB/apec_line.fits. index identifies the HDU:

```
index = 30
l = list_nei_lines(specrange, Te, tau)
```

pyatomdb.spectrum.**make_ion_index_continuum**(*bins*, *element*, *index=False*, *cocofile='$ATOMDB/apec_coco.fits'*, *binunits='keV'*, *fluxunits='ph'*, *no_coco=False*, *no_pseudo=False*, *ion=0*, *broadening=False*, *broadenunits='keV'*)

Creates the continuum for a given ion.

Parameters **bins** : array(float)

The bin edges for the spectrum to be calculated on, in units of keV or Angstroms. Must be monotonically increasing. Spectrum will return len(bins)-1 values.

element : int

Atomic number of element to make spectrum of (e.g. 6 for carbon)

binunits : {'keV' , 'A'}

The energy units for bins. "keV" or "A". Default keV.

fluxunits : {'ph' , 'erg'}

Whether to return the emissivity in photons ('ph') or ergs ('erg'). Defaults to photons

no_coco : bool

If true, do not include the compressed continuum

no_pseudo : bool

If true, do not include the pseudo continuum (weak lines)

ion : int

Ion to calculate, e.g. 4 for C IV. By default, 0 (whole element).

index : int

The index to generate the spectrum from. Note that the AtomDB files the emission starts in hdu number 2. So for the first block, you set index=2. Only required if cocofile is a filename or an HDULIST

cocofile : HDUList, HDU or str

The continuum file, either already open (HDULIST) or filename. alternatively, provide the HDU itself, and then do not need to define the index

broadening: float

Broaden the continuum by gaussians of this width (if False, no broadening is applied)

broadenunits: {'keV' , 'A'}

Units for broadening (kev or A)

Returns array(float)

len(bins)-1 array of continuum emission, in units of photons cm^3 s^-1 bin^-1 (fluxunits = 'ph') or ergs cm^3 s^-1 bin^-1 (fluxunits = 'erg')

pyatomdb.spectrum.**make_ion_spectrum**(*bins*, *index*, *Z*, *z1*, *linefile='$ATOMDB/apec_nei_line.fits'*, *cocofile='$ATOMDB/apec_nei_comp.fits'*, *binunits='keV'*, *broadening=False*, *broadenunits='keV'*, *abund=False*, *dummyfirst=False*, *nei=True*, *dolines=True*, *docont=True*, *dopseudo=True*)

make_spectrum is the most generic "make me a spectrum" routine.

It returns the emissivity in counts cm^3 s^-1 bin^-1.

Parameters **bins** : array(float)

The bin edges for the spectrum to be calculated on, in units of keV or Angstroms. Must be monotonically increasing. Spectrum will return len(bins)-1 values.

index : int

The index to plot the spectrum from. note that the AtomDB files the emission starts in hdu number 2. So for the first block, you set index=2

Z : int

Element of spectrum (e.g. 6 for carbon)

z1 : int

Ion charge +1 for the spectrum (e.g. 3 for C III)

linefile : str or HDUList

The file containing all the line emission. Defaults to "$ATOMDB/apec_line.fits". Can also pass in the opened file, i.e. "linefile = pyatomdb.pyfits.open('apec_nei_line.fits')"

cocofile : str or HDUList

The file containing all the continuum emission. Defaults to "$ATOMDB/apec_coco.fits". Can also pass in the opened file, i.e. "cocofile = pyatomdb.pyfits.open('apec_nei_comp.fits')"

binunits : {'keV','A'}

The energy units for bins. "keV" or "A". Default keV.

broadening : float

Line broadening to be applied

broadenunits : {'keV','A'}

Units of line broadening "keV" or "A". Default keV.

elements : iterable of int

Elements to include, listed by atomic number. if not set, include all.

abund : iterable of float, length same as elements.

If set, and array of length (elements) with the abundances of each element relative to the Andres and Grevesse values. Otherwise, assumed to be 1.0 for all elements

dummyfirst : bool

If true, add a "0" to the beginning of the return array so it is of the same length as bins (can be useful for plotting results)

nei : bool

If set, return the spectrum from the driving ion being Z, rmJ. If not set, return the spectrum for the collisional ionization equilibrium *BUT* note that the continuum will be wrong, as it is provided for each element as a whole.

dolines : bool

Include lines in the spectrum

docont : bool

Include the continuum in the spectrum

dopseudo : bool

Include the pseudocontinuum in the spectrum.

Returns array of floats

Emissivity in counts cm^3 s^-1 bin^-1.

pyatomdb.spectrum.**make_spectrum**(*bins*, *index*, *linefile='$ATOMDB/apec_line.fits'*, *cocofile='$ATOMDB/apec_coco.fits'*, *binunits='keV'*, *broadening=False*, *broadenunits='keV'*, *elements=False*, *abund=False*, *dummyfirst=False*, *dolines=True*, *docont=True*, *dopseudo=True*)

make_spectrum is the most generic "make me a spectrum" routine.

It returns the emissivity in counts cm^3 s^-1 bin^-1.

Parameters **bins** : array(float)

The bin edges for the spectrum to be calculated on, in units of keV or Angstroms. Must be monotonicallyincreasing. Spectrum will return len(bins)-1 values.

index : int

The index to plot the spectrum from. note that the AtomDB filesthe emission starts in hdu number 2. So for the first block, youset index=2

linefile : str

The file containing all the line emission. Defaults to "$ATOMDB/apec_line.fits"

cocofile : str

The file containing all the continuum emission. Defaults to "$ATOMDB/apec_coco.fits"

binunits : {'keV','A'}

The energy units for bins. "keV" or "A". Default keV.

broadening : float

Line broadening to be applied

broadenunits : {'keV','A'}

Units of line broadening "keV" or "A". Default keV.

elements : iterable of int

Elements to include, listed by atomic number. if not set, include all.

abund : iterable of float, length same as elements.

If set, and array of length (elements) with the abundances of eachelement relative to the Andres and Grevesse values. Otherwise, assumed tobe 1.0 for all elements

dummyfirst : bool

If true, add a "0" to the beginning of the return array so it is of the same length as bins (can be useful for plotting results)

dolines : bool

Include lines in the spectrum

docont : bool

Include the continuum in the spectrum

dopseudo : bool

Include the pseudocontinuum in the spectrum.

Returns array of floats

Emissivity in counts cm^3 s^-1 bin^-1.

pyatomdb.spectrum.**print_lines**(*llist*, *specunits='A'*)

Prints lines in a linelist to screen

This routine is very primitive as things stand. Plenty of room for refinement.

Parameters **llist: dtype(linelist)**

list of lines to print. Typically returned by list_lines.

specunits: {'A' , 'keV'}

units to list the line positions by (A or keV, default A)

Returns Nothing, though prints data to standard out.

PyAtomDB Util module

This modules contains simple utility codes (sorting etc) that pyatomdb relies on. util.py contains a range of miscellaneous helper codes that assist in running other AtomDB codes but are not in any way part of a physical calculation.

Version -.1 - initial release Adam Foster July 17th 2015

pyatomdb.util.**check_version**()

Checks if there is a more recent version of the database to install.

Parameters **None.**

Returns None

pyatomdb.util.**download_atomdb_emissivity_files**(*adbroot*, *userid*, *version*)

Download the AtomDB equilibrium emissivity files for AtomDB"

This code will go to the AtomDB FTP site and download the necessary files. It will then unpack them into a directory adbroot. It will not overwrite existing files with the same md5sum (to avoid pointless updates) but it will not know this until it has downloaded and unzipped the main file.

Parameters **adbroot** : string

The location to install the data. Typically should match $ATOMDB

userid : string

An 8 digit ID number. Usually passed as a string, but integer is also fine (provided it is all numbers)

version : string

The version string for the release, e.g. "3.0.2"

Returns None

pyatomdb.util.**download_atomdb_nei_emissivity_files**(*adbroot*, *userid*, *version*)

Download the AtomDB non-equilibrium emissivity files for AtomDB"

This code will go to the AtomDB FTP site and download the necessary files. It will then unpack them into a directory adbroot. It will not overwrite existing files with the same md5sum (to avoid pointless updates) but it will not know this until it has downloaded and unzipped the main file.

Parameters **adbroot** : string

The location to install the data. Typically should match $ATOMDB

userid : string

An 8 digit ID number. Usually passed as a string, but integer is also fine (provided it is all numbers)

version : string

The version string for the release, e.g. "3.0.2"

Returns None

pyatomdb.util.**figcoords**(*lowxpix*, *lowypix*, *highxpix*, *highypix*, *lowxval*, *lowyval*, *highxval*, *highyval*, *xpix*, *ypix*, *logx=False*, *logy=False*)

pyatomdb.util.**generate_equilibrium_ionbal_files**(*filename*, *settings=False*)

Generate the eigen files that XSPEC uses to calculate the ionizatoin balances

Parameters **filename** : string

file to write

settings : dict

This will let you override some standard inputs for get_data:

- settings['filemap']: the filemap to use if you do not want to use the default $ATOMDB/filemap
- settings['atomdbroot']: If you have files in non-standard locations you can replace $ATOMDB with this value

Returns none

pyatomdb.util.**generate_isis_files**(*version=''*, *outfile='atomdb_VERSION_isis.tar.bz2'*)

Generate the ISIS tarball

Parameters **version** : string

version number to generate ISIS tarball for. Defaults to version in $ATOMDB/VERSION

outfile : string

the file to be generated. Defaults to atomdb_VERSION_isis.tar.bz2

Returns

——-

none

pyatomdb.util.**generate_web_fitsfiles**(*version=''*, *outdir=''*)

Split the linelist files into many small files and make an index for them

Parameters **version** : string

version number to generate this for. Defaults to version in $ATOMDB/VERSION

outdir : string

Output files will be placed in this directory. Defaults to 'webonly"

Returns

——-

none

pyatomdb.util.**generate_xspec_ionbal_files**(*Z*, *filesuffix*, *settings=False*)

Generate the eigen files that XSPEC uses to calculate the ionizatoin balances

Parameters **Z** : int

atomic number of element

filesuffix : string

the filename will be eigenELSYMB_filesuffix.fits

settings : dict

This will let you override some standard inputs for get_data:

- settings['filemap']: the filemap to use if you do not want to use the default $ATOMDB/filemap
- settings['atomdbroot']: If you have files in non-standard locations you can replace $ATOMDB with this value

Returns none

pyatomdb.util.**initialize**()

Initialize your AtomDB Setup

This code will let you select where to install AtomDB, get the latest version of the filemap, and download the emissivity files needed for various functions to work.

Parameters **None.**

Returns None

pyatomdb.util.**keyword_check**(*keyword*)

Returns False is the keyword is in fact false, otherwise returns True

Parameters **keyword: any**

The keyword value

Returns bool

True if the keyword is set to not False, otherwise False

pyatomdb.util.**load_user_prefs**(*adbroot='$ATOMDB'*)

Loads user preference data from $ATOMDB/userdata

Parameters **adbroot** : string

The AtomDB root directory. Defaults to environment variable $ATOMDB.

Returns dictionary

keyword/setting pairs e.g. settings['USERID'] = "12345678"

pyatomdb.util.**make_linelist**(*linefile*, *outfile*)

Create atomdb linelist file from line.fits file

Parameters **linefile** : string

The filename of the line file

outfile : string

The output filename of the string

Returns none

pyatomdb.util.**make_release_filetree**(*filemapfile_in*, *filemapfile_out*, *replace_source*, *destination*, *versionname*)

Take an existing filemap, copy the files to the atomdbftp folder as required.

Parameters **filemapfile_in** : string

The existing filemap file for the new release

filemapfile_out : string

The filename for the produced filemap

replace_source : string

All new files are in this directory.

destination : string

The folder to store the files in

versionname : string

The version string for the new files (e.g. 3_0_4)

Returns None

Notes

This code searches for any files which don't have $ATOMDB in the filename and assumes they are new.

It updates the file name to be $ATOMDB/elname/elname_ion/elname_ion_FTYPE_versionname.fits

Versionname will have its last number stsripped and replaced with "a". So 3_0_4_2 becomes 3_0_4_a. This reflects that 4-number versions are for revisions of a file under development, while 3 number + letter are for released data.

And then copies it to the destination folder, compressing it with gzip.

pyatomdb.util.**make_release_tarballs**(*ciefileroot*, *neifileroot*, *filemap*, *versionname*, *releasenotes*, *parfile*, *neiparfile*, *makelinelist=False*)

Create tarball for exmissivity files for a new release.

Parameters **ciefileroot** : string

The path to the CIE line and coco files, with the _line.fits and _coco.fits ommitted.

neifileroot : string

The path to the NEI line and coco files, with the _line.fits and _comp.fits ommitted.

filemap : string

The filemap file

versionname : string

The version string for the new files (e.g. 3.0.4).

releasenotes : string

The file name for the release notes.

parfile : string

The parameter file used to create the data

neiparfile : string

The parameter file used to create the NEI data

makelinelist : bool

Remake the line list from the line file. If not specified, assumes linelist file already exists.

Returns None

pyatomdb.util.**make_vec**(*d*)

Create vector version of d, return True or false depending on whether input was vector or not

Parameters **d: any scalar or vector**

The input

Returns **vecd** : array of floats

d as a vector (same as input if already an iterable type)

isvec : bool

True if d was a vector, otherwise False.

pyatomdb.util.**md5Checksum**(*filePath*)

Calculate the md5 checksum of a file

Parameters **filepath** : str

the file to calculate the md5sum of

Returns string

the hexadecimal string md5 hash of the file

References

Taken from http://joelverhagen.com/blog/2011/02/md5-hash-of-file-in-python/

pyatomdb.util.**mkdir_p**(*path*)

Create a directory. If it already exists, do nothing.

Parameters **path** : string

The directory to make

Returns none

pyatomdb.util.**question**(*question*, *default*, *multichoice=[]*)

Ask question with default answer provided. Return answer

Parameters **question** : str

Question to ask

default : str

Default answer to question

multichoice : str

if set, answer must be one of these choices

Returns str

The answer.

pyatomdb.util.**record_upload**(*fname*)
Transmits record of a file transfer to AtomDB

This simply transmits the USERID, filename, and time to AtomDB. If USERID=0, then the user has chosen not to share this information and this is skipped

Parameters **fname** : string

The file name being downloaded.

Returns None

pyatomdb.util.**switch_version**(*version*)
Changes the AtomDB version. Note this will overwrite several links on your hard disk, and will *NOT* be repaired upon quitting python.

The files affect are the VERSION file and the soft links $ATOMDB/apec_line.fits, $ATOMDB/apec_coco.fits, $ATOMDB/filemap and $ATOMDB/apec_linelist.fits

Parameters **version: string**

The version of AtomDB to switch to. Should be of the form "2.0.2"

Returns None

pyatomdb.util.**unique**(*s*)
Return a list of the elements in s, but without duplicates.

For example, unique([1,2,3,1,2,3]) is some permutation of [1,2,3], unique("abcabc") some permutation of ["a", "b", "c"], and unique(([1, 2], [2, 3], [1, 2])) some permutation of [[2, 3], [1, 2]].

For best speed, all sequence elements should be hashable. Then unique() will usually work in linear time.

If not possible, the sequence elements should enjoy a total ordering, and if list(s).sort() doesn't raise TypeError it's assumed that they do enjoy a total ordering. Then unique() will usually work in O(N*log2(N)) time.

If that's not possible either, the sequence elements must support equality-testing. Then unique() will usually work in quadratic time.

Parameters **s** : list type object

List to remove the duplicates from

Returns list type object

...with all the duplicates removed

References

Taken from Python Cookbook, written by Tim Peters. http://code.activestate.com/recipes/52560/

pyatomdb.util.**write_ai_file**(*fname*, *dat*, *clobber=False*)
Write the data in list dat to fname

Parameters **fname** : string

The file to write

dat : list

The data to write. Should be a list with the following keywords:

- Z : int: nuclear charge
- z1 : int: ion charge + 1
- comments : iterable of strings: comments to append to the file
- data : numpy.array : stores all the individual level data, with the following types:
  - ion_init : int : Inital ion state of transition
  - ion_final : int : Final ion state of transition
  - level_init : int : Initial level of transition
  - level_final : int : Final level of transition
  - auto_rate : float : Autoionization rate (s-1)
  - auto_err : float : Error in autoionization rate (s-1)
  - auto_ref : string(20) : Autoionization rate reference (bibcode)

clobber : bool

Overwrite existing file if it exists.

Returns none

pyatomdb.util.**write_develop_data**(*data*, *filemapfile*, *Z*, *z1*, *ftype*, *folder*, *froot*)

pyatomdb.util.**write_ec_file**(*fname*, *dat*, *clobber=False*)

Write the data in list dat to fname

Parameters **fname** : string

The file to write

dat : list

The data to write. Should be a list with the following keywords:

- Z : int : nuclear charge
- z1 : int : ion charge + 1
- comments : iterable of strings: comments to append to the file
- data : numpy.array : stores all the individual level data, with the following types:
  - lower_lev : int : Lower level of transition
  - upper_lev : int : Upper level of transition
  - coeff_type : int : Coefficient type
  - min_temp : float : Minimum temperature in range (K)
  - max_temp : float : Maximum temperature in range (K)
  - temperature : float(20) : List of temperatures (K)
  - effcollstrpar : float(20) : Effective collision strength parameters
  - inf_limit : float (OPTIONAL - if type 1.2.0) : High temperature limit point, if provided.
  - reference : string(20) : Collisional excitation reference (bibcode)

clobber : bool

Overwrite existing file if it exists.

Returns none

pyatomdb.util.**write_ionbal_file**(*Te*, *dens*, *ionpop*, *filename*, *Te_linear=False*, *dens_linear=False*)

Create ionization balance file

Parameters **Te** : array(float)

temperatures (in K)

dens : array(float)

electron densities (in cm^-3)

ionpop : dict of arrays

one entry for each element: ionpop[2] = numpy.array(nion,nte, ndens)

filename : str

filename to write to

Te_linear : bool

if true, temperature grid is linear

dens_linear : bool

if true, density grid is linear

pyatomdb.util.**write_ir_file**(*fname*, *dat*, *clobber=False*)

Write the data in list dat to fname

Parameters **fname** : string

The file to write

dat : list

The data to write. Should be a list with the following keywords:

- Z : int : nuclear charge
- z1 : int : ion charge + 1
- comments : iterable of strings : comments to append to the file
- ionpot : float : ionization potential (eV)
- ip_dere : float : ionization potential (eV) (from dere, optional)
- data : numpy.array : stores all the individual level data, with the following types:
  - element : int : Nuclear Charge
  - ion_init : int : Initial ion stage
  - ion_final : int : Final ion stage
  - level_init : int : Initial level
  - level_final : int : Final level
  - tr_type : string(2) : Transition type:

```
CI = collisional excitaion
EA = excitation autoionization
RR = radiative recombination
DR = dieclectronic recombination
```

```
XI = ionization, excluded from total rate calculation
XR = recombination, excluded from total rate calculation
(XR and XI are used to populate level directly)
```

- tr_index : int : index within the file
- par_type : int : parameter type, i.e. how the data is stored
- min_temp : float : Minimum temperature in range (K)
- max_temp : float : Maximum temperature in range (K)
- temperature : float(20) : List of temperatures (K)
- ionrec_par : float(20) : Ionization and recombination rate parameters
- wavelen : float : Wavelength of emitted lines (A) [not used]
- wave_obs : float : Observed wavelength of emitted lines (A) [not used]
- wave_err : float : Error in these wavelengths (A) [not used]
- br_ratio : float : Branching ratio of this line [not used]
- br_rat_err : float : Error in branching ratio [not used]
- label : string(20) : Label for the transition
- rate_ref : string(20) : Rate reference (bibcode)
- wave_ref : string(20) : Wavelength reference (bibcode)
- wv_obs_ref : string(20) : Observed wavelength reference (bibcode)
- br_rat_ref : string(20) : Branching ratio reference (bibcode)

clobber : bool

Overwrite existing file if it exists.

Returns none

`pyatomdb.util.`**`write_la_file`**(*fname*, *dat*, *clobber=False*)

Write the data in list dat to fname

Parameters **fname** : string

The file to write

dat : list

The data to write. Should be a list with the following keywords:

- Z : int : nuclear charge
- z1 : int : ion charge + 1
- comments : iterable of strings : comments to append to the file
- data : numpy.array: stores all the individual level data, with the following types:
  - upper_lev : int : Upper level of transition
  - lower_lev : int : Lower level of transition
  - wavelen : float : Wavelength of transition (A)
  - wave_err : float : Error in wavelength (A)
  - einstein_a : float : Einstein A coefficient (s-1)

- ein_a_err : float : Error in A coefficient (s-1)
- wave_ref : string(20) : wavelength reference (bibcode)
- ein_a_ref : string(20) : A-value reference (bibcode)

clobber : bool

Overwrite existing file if it exists.

Returns none

pyatomdb.util.**write_lv_file**(*fname*, *dat*, *clobber=False*)

Write the data in list dat to fname

Parameters **fname** : string

dat : list

- Z : int : nuclear charge
- z1 : int: ion charge + 1
- comments : iterable of strings: comments to append to the file
- data : numpy.array: stores all the individual level data, with the following types
  - elec_config : string (40 char max) : Electron configuration strings
  - energy : float: Level energy (eV)
  - e_error : float : Energy level error (eV)
  - n_quan : int : N quantum number
  - l_quan : int : L quantum number
  - s_quan : float : S quantum number
  - lev_deg : int : level degeneracy
  - phot_type : int : photoionization data type:

```
-1. none

 0. hydrogenic

 1. Clark

 2. Verner

 3. XSTAR data
```

  - phot_par : float(20) : photoionization paramters (see specific PI type for definition)
  - Aaut_tot : float (optional) : the total autoionization rate out of the level (s^-1)
  - Arad_tot : float (optional) : the total radiative rate out of the level (s^-1)
  - energy_ref : string(20) : energy reference (usually bibcode)
  - phot_ref : string(20) : photoionization reference (bibcode)
  - Aaut_ref : string(20) : total autoionization rate reference (bibcode)
  - Arad_ref : string(20) : total radiative decay rate reference (bibcode)

clobber : bool

Overwrite existing file if it exists.

Returns none

pyatomdb.util.**write_user_prefs**(*prefs*, *adbroot='$ATOMDB'*)

Write user preference data to $ATOMDB/userdata. This will overwrite the entire file.

Therefore you should use "load_user_prefs", then add in additional keywords, the call write_user_prefs.

Parameters **prefs: dictionary**

keyword/setting pairs e.g. settings['USERID'] = "12345678"

adbroot : string

The AtomDB root directory. Defaults to environment variable $ATOMDB.

Returns None

PyAtomDB Example Scripts

These are examples of using the pyatomdb module in your projects. They can all be found in the examples subdirectory of the pyatomdb tarball.

Table of Contents

Initial installation

first_installation.py

```
import pyatomdb

"""
This script shows the commands you should run when you first download pyatomdb.

It is recommended that you choose the location you want to install the
AtomDB data files (not the same as the python module) and set your
ATOMDB environment variable to point to it.


Parameters
------
none

Returns
-------
none
```

```
"""

# call the setup routine
pyatomdb.util.initialize()

# this routine downloads a bunch of files and sets things up for you. It will
# take a few minutes, depending on your internet connection.

print "Install complete!"

#and that's it!

# If you want to switch versions of atomdb (in this case to 3.0.2) later, call:
# pyatomdb.util.switch_version('3.0.2')
```

Make Line List

List the strongest lines in a given temperature and wavelength region: `make_line_list.py`

```
import pyatomdb

"""
This code will produce a list of lines in a given wavelength range at a
given temperature. It also shows the use of an NEI version, where you
have to additionally specify the initial ionization temperature (or the
ionization fraction directly) and the elapsed Ne*t.

The results of the list_lines codes are numpy arrays which can be sorted any
way you wish. You can, of course, extract the lines easily at this point. There
is also a print_lines routine for a fixed format output.

Parameters
----------
none

Returns
-------
none

"""

# Adam Foster 2015-12-02
# version 0.1

#specify wavelength range, in Angstroms
wl = [8.0,9.0]

# electron temperature in K
Te = 1e7

# get equilibrium line list

res = pyatomdb.spectrum.list_lines(wl,Te=Te, teunit='K', minepsilon=1e-18)

# reprocess lines for printing
print "Unsorted line list:"
```

```
pyatomdb.spectrum.print_lines(res)

# re-sort lines, for a giggle
# for more information, look up numpy.sort: res is a numpy array.
# http://docs.scipy.org/doc/numpy/reference/generated/numpy.sort.html

res.sort(order=['Epsilon'])
print "sorted by Emissivity:"
pyatomdb.spectrum.print_lines(res)

# re-sort by element, ion then emissivity
res.sort(order=['Element','Ion','Epsilon'])
print "sorted by Element, Ion, Emissivity:"
pyatomdb.spectrum.print_lines(res)


# now do an NEI version. This is slow at the moment, but functional.
Te_init = 1e4
tau = 1e11
res_nei = pyatomdb.spectrum.list_nei_lines(wl,Te=Te, teunit='K', \
                                           minepsilon=1e-18,\
                                           Te_init=Te_init,\
                                           tau = tau)
print "NEI linelist (this takes a while):"
pyatomdb.spectrum.print_lines(res_nei)
```

Get PI Cross Sections

Extract the PI cross section data: `photoionization_data.py`

```
import pyatomdb, numpy,os, pylab
try:
  import astropy.io.fits as pyfits
except:
  import pyfits

# This is a sample routine that reads in the photoionization data
# It also demonstrates using get_data, which should download the data you
# need automagically from the AtomDB site.
#
# It also shows how to get the raw XSTAR PI cross sections.

# going to get PI cross section from iron 16+ to 17+ (Fe XVII-XVIII)
Z = 26
z1 = 17

# get the AtomDB level data
lvdata = pyatomdb.atomdb.get_data(Z, z1, 'LV')

# get the XSTAR PI data from AtomDB
pidata = pyatomdb.atomdb.get_data(Z, z1, 'PI')

# set up the figure
fig = pylab.figure()
fig.show()
ax = fig.add_subplot(111)
```

```
# to calculate the cross section (in cm^2) at a given single energy E (in keV)
# does not currently work with vector input, so have to call in a loop if you
# want multiple energies [I will fix this]

E = 10.

# get the ground level (the 0th entry in LV file) data
lvd = lvdata[1].data[0]

# This is the syntax for calculating the PI cross section of a given line
# This will work for non XSTAR data too.
sigma = pyatomdb.atomdb.sigma_photoion(E, Z, z1,lvd['phot_type'], lvd['phot_par'], \
               xstardata=pidata, xstarfinallev=1)


# To get the raw XSTAR cross sections (units: energy = keV, cross sections = Mb)
# for level 1 -> 1 (ground to ground)
pixsec = pyatomdb.atomdb.sort_pi_data(pidata, 1,1)
ax.loglog(pixsec['energy'], pixsec['pi_param']*1e-18, label='raw xstar data')

# label the plot
ax.set_title('Plotting raw XSTAR PI cross sections. Fe XVII gnd to Fe XVIII gnd')
ax.set_xlabel("Energy (keV)")
ax.set_ylabel("PI cross section (cm$^{2}$)")

pylab.draw()
zzz=raw_input('press enter to continue')
```

Make a Spectrum

Make a broadened and unbroadened spectrum: `make_spectrum.py`

```
import pyatomdb, numpy, pylab

# set up a grid of energy bins to model the spectrum on:
ebins=numpy.linspace(0.3,10,1000)

# define a broadening, in keV, for the lines
de = 0.01

# define the temperature at which to plot (keV)
te = 3.0

# find the index which is closest to this temperature
ite = pyatomdb.spectrum.get_index( te, teunits='keV', logscale=False)

# create both a broadened and an unbroadened spectrum
a = pyatomdb.spectrum.make_spectrum(ebins, ite,dummyfirst=True)
b = pyatomdb.spectrum.make_spectrum(ebins, ite, broadening=de, \
                                    broadenunits='kev',dummyfirst=True)
# The dummyfirst argument adds an extra 0 at teh beginning of the
# returned array so it is the same length as ebins. It allows
# accurate plotting using the "drawstyle='steps'" flag to plot.
```

```
# plot the results
fig = pylab.figure()
fig.show()
ax = fig.add_subplot(111)

ax.loglog(ebins, a, drawstyle='steps', label='Unbroadened')
ax.loglog(ebins, b, drawstyle='steps', label='sigma = %.2f'%(de))
ax.set_xlabel('Energy (keV)')
ax.set_ylabel('Emissivity (ph cm$^{3}$ s$^{-1}$ bin$^{-1}$)')
ax.legend(loc=0)
pylab.draw()
zzz = raw_input("Press enter to continue")

print "Listing lines between 1 and 2 A"
# now list the lines in a wavelength region
llist = pyatomdb.spectrum.list_lines([1,2.0], index=ite)
# print these to screen
pyatomdb.spectrum.print_lines(llist)
# print to screen, listing the energy, not the wavelength
print "Listing lines between 1 and 2 A, using keV."

pyatomdb.spectrum.print_lines(llist, specunits = 'keV')
```

Make a Spectrum version 2.0

Make a spectrum using the new Session class: `new_make_spectrum.py`. This is significantly faster if you need to make lots of spectra (fitting, interpolating between 2 temperatures etc). Note the example requires an RMF and ARF file - adjust to fit your available response.

```
import pyatomdb, pylab, numpy, time


rmf = '/export1/projects/atomdb_308/hitomi/resp_100041010sxs.rmf'
arf = '/export1/projects/atomdb_308/hitomi/arf_100041010sxs.arf'


# create a session object. This contains the apec files, response files,
# and any previously calculated spectrs so that simple multiplication
# can be used to get the results without recalculating everything from scratch

data = pyatomdb.spectrum.Session()

# If you want to specify custom energy bins:
ebins = numpy.linspace(1,2,1001)
data.set_specbins(ebins, specunits='A')

# alternative method: just load the response and use its binning. Note
# that this will always be in keV currently, because reasons.

data.set_response(rmf, arf=arf)
ebins = data.ebins_response

# now get the spectrum at 4keV. This calculates (and stores) the
# spectrum at each temperature nearby (~3.7, 4.3 keV)
# then linearly interpolates between the result
#
```

```
# vector is stored for each element at each temperature
# so if you change temperature/abundance, it's a simple multiplication and
# interpolation instead of a total recalculation

t0 = time.time()
s=data.return_spectra(4.0, teunit='keV')
t1 = time.time()
# let's change the abundance
data.set_abund([1,2,3,4,26],0.5)

# and see how fast this goes this time, changing temperature and abund
s2=data.return_spectra(4.1, teunit='keV')
t2 = time.time()

print "first spectrum took %g seconds" %(t1-t0)
print "second spectrum took %g seconds" %(t2-t1)
print "note how much faster the second one was as I didn't recalculate everything from scratch!"


#linedata = pyatomdb.pyfits.open('/export1/atomdb_latest/apec_v3.0.8_line.fits')


#spec = speclo*rlo + specup*rup

# some plotting of things

fig = pylab.figure()
fig.show()
ax = fig.add_subplot(111)
#ax2 = fig.add_subplot(212, sharex=ax)
s = numpy.append(0,s)
s += 1e-40

s2 = numpy.append(0,s2)
s2 += 1e-40
#spec = numpy.append(0,spec)
#spec += 1e-40

ax.plot(ebins, s, drawstyle='steps')
ax.plot(ebins, s2, drawstyle='steps')
#ax.plot(elo, spec, drawstyle='steps')


#ax2.plot(elo, s/spec, drawstyle='steps')


zzz=raw_input('Press enter to exit')
```

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Usage

Examples

Note: there are example routines demonstrating use of these features in the examples directory of the package.

Installation

PyAtomDB can be installed from pypi, using the simple `pip install pyatomdb` command.

For PyAtomDB to be useful, it requires access to a range of AtomDB database files (these are all FITS files). The database has two broad types of files, emissivity files (APEC) and fundamental atomic data files (APED, the Astrophysical Plasma Emission Database).

The emissivity files are needed for things such as producing spectra. The APED files are underlying atomic data and are not strictly needed for creating a spectrum, but can be useful for getting later information out.

In order for PyAtomDB to work efficiently, you should choose a location to store all of these files (e.g. /home/username/atomdb). It is strongly recommended that you set the environment variable ATOMDB to point to this, i.e. for bash add the following line to your .bashrc file:

```
export ATOMDB=/home/username/atomdb
```

or for csh, add this to your .cshrc or .cshrc.login:

```
setenv ATOMDB /home/username/atomdb
```

If you run the following code within a python shell, PyAtomDB will download the files you need to get started:

```
import pyatomdb
pyatomdb.util.initialize()
```

This will prompt you for an install location (defaulting to *$ATOMDB*) and whether to download the emissivity files. It is suggested that you say yes. It will also ask if you mind sharing anonymous download information with us. We would appreciate it if you say yes, but it is not necessary for the functioning of the software.

Example: Making a Spectrum

These functions are in the `spectrum` module:

```
import pyatomdb, numpy, pylab

# set up a grid of energy bins to model the spectrum on:
ebins=numpy.linspace(0.3,10,1000)

# define a broadening, in keV, for the lines
de = 0.01

# define the temperature at which to plot (keV)
te = 3.0

# find the index which is closest to this temperature
ite = pyatomdb.spectrum.get_index( te, teunits='keV', logscale=False)

# create both a broadened and an unbroadened spectrum
a = pyatomdb.spectrum.make_spectrum(ebins, ite,dummyfirst=True)
b = pyatomdb.spectrum.make_spectrum(ebins, ite, broadening=de, \
                                    broadenunits='kev',dummyfirst=True)
# The dummyfirst argument adds an extra 0 at teh beginning of the
# returned array so it is the same length as ebins. It allows
# accurate plotting using the "drawstyle='steps'" flag to plot.

# plot the results
fig = pylab.figure()
fig.show()
ax = fig.add_subplot(111)

ax.loglog(ebins, a, drawstyle='steps', label='Unbroadened')
ax.loglog(ebins, b, drawstyle='steps', label='sigma = %.2f'%(de))
ax.set_xlabel('Energy (keV)')
ax.set_ylabel('Emissivity (ph cm$^{3}$ s$^{-1}$ bin$^{-1}$)')
ax.legend(loc=0)
pylab.draw()
zzz = raw_input("Press enter to continue")

print "Listing lines between 1 and 2 A"
# now list the lines in a wavelength region
llist = pyatomdb.spectrum.list_lines([1,2.0], index=ite)
# print these to screen
pyatomdb.spectrum.print_lines(llist)
# print to screen, listing the energy, not the wavelength
print "Listing lines between 1 and 2 A, using keV."

pyatomdb.spectrum.print_lines(llist, specunits = 'keV')
```

Interrogating the atomic database

The atomic database APED contains a range of data for a host of different ions. It contains a host of different files covering a range of different processes. The full database, when uncompressed is more than 10GB of data, so we are avoiding distributing it to all users. You can, however, get the individual data you need using the `get_data` routine:

```
mydata = pyatomdb.atomdb.get_data(Z, z1, ftype)
```

This will try to open the file locally if it exists, and if it does not it will then go to the AtomDB FTP server and download the data for element Z, ion z1, with ftype a 2-character string denoting the type of data to get:

- `IR`: ionization and recombination
- `LV`: energy levels
- `LA`: radiative transition data (lambda and A-values)
- `EC`: electron collision data
- `PC`: proton collision data
- `DR`: dielectronic recombination satellite line data
- `PI`: XSTAR photoionization data
- `AI`: autoionization data

So to open the energy levels for oxygen with 2 electrons (O 6+, or O VII):

```
lvdata = pyatomdb.atomdb.get_data(8,7,'LV')
```

Downloaded data files are stored in `$ATOMDB/APED/<elsymb>/<elsymb>_<ionnum>/`. You can delete them if you need to free up space, whenever a code needs the data it will reload them. There are many routines in the atomdb module which relate to extracting the data from the files, i.e. getting collisional excitation rates or line wavelengths. If you have trouble finding a routine to do what you want, please contact us and we'll be happy to write one if we can (this is how this module will grow - through user demand!)

CHAPTER 3

Indices and tables

- *genindex*
- *modindex*
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