



**Update on OPEN-ADAS
and
Recent work on excitation data and
population modelling**

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OPEN-ADAS has a new look

OPEN-ADAS

Atomic Data and Analysis Structure

Tb I (5331A)

Freeform Wavelength Ion

About OPEN-ADAS

OPEN-ADAS is a system to search and disseminate key data from the Atomic Data and Analysis Structure (ADAS).

ADAS is a computer program managed by the University of Strathclyde and made up of a consortium of over twenty members.

The OPEN-ADAS system enables non-members, with an interest in fusion and astrophysics, to download and use ADAS data.

[More about OPEN-ADAS](#)

26 Feb 2013 – Major update to the website

The OPEN-ADAS website has been updated with a new visual interface and the addition of three new data classes... [Read more](#)

The OPEN-ADAS data classes

The data contained within ADAS is strictly organised and precisely formatted. There are over fifty distinct types of data file. The scope of OPEN-ADAS is targetted on and limited to the release and organisation of general user relevant data from the ADAS databases and the provision of code, subroutines and procedures to enable such users of OPEN-ADAS to read the released data. These data classes are given below.

FUNDAMENTAL CLASSES

ADF 01 **Charge exchange cross sections**
nl-resolved charge exchange cross-sections over a range of n-shells for a donor neutral atom and ionised impurity receiver

DERIVED CLASSES

ADF 11 **Iso-nuclear master files**
Effective (collisional-radiative) coefficients which are required to establish the ionisation state of a dynamic or steady-state plasma.

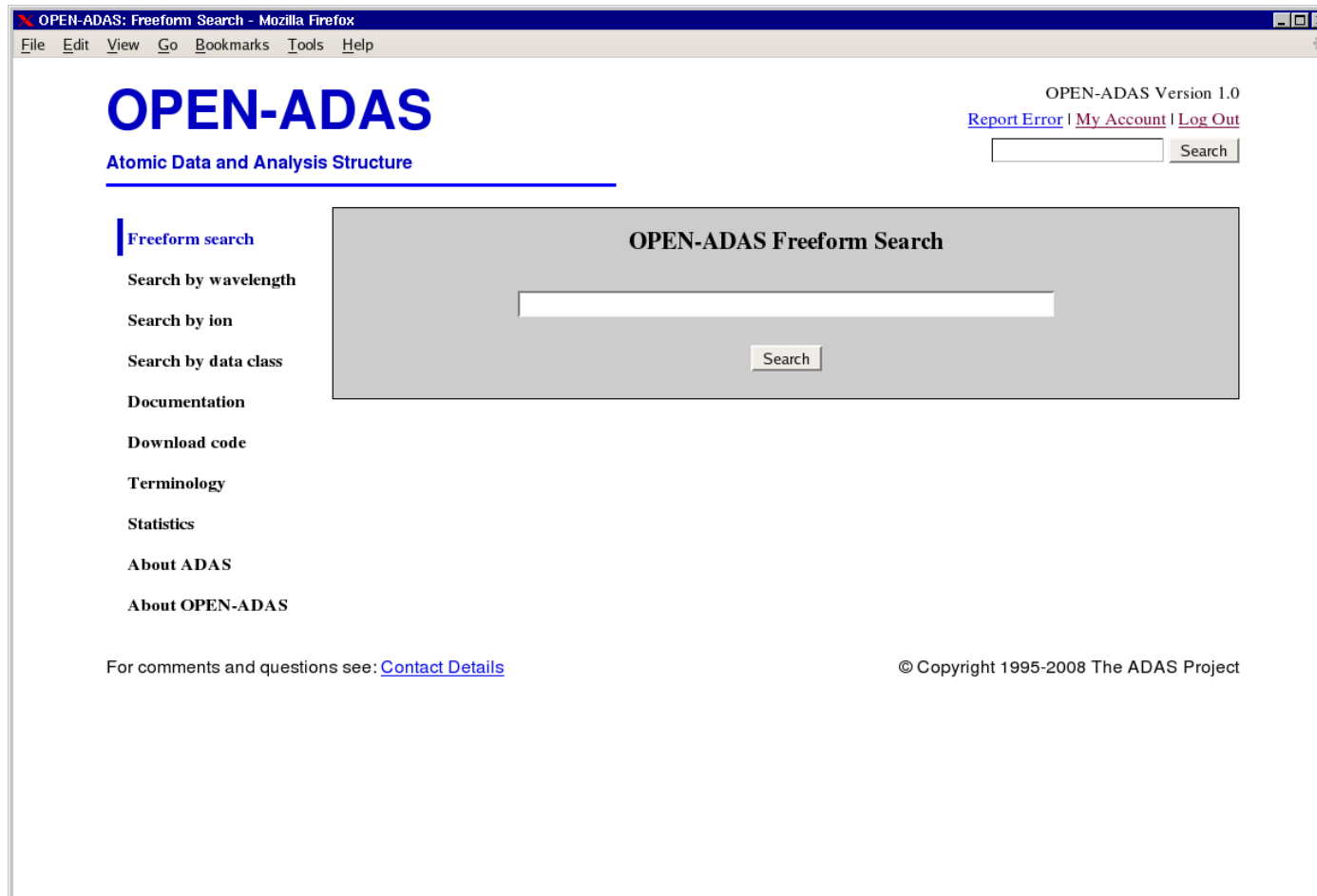
Freeform search

Search [Freeform search examples](#)

Freeform search Search by wavelength Search by ion

OPEN-ADAS has a new look

A reminder of the previous incarnation:



OPEN-ADAS: new search dialogues

A) Search by: Freeform Wavelength Ion

Select an element from the periodic table

H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															
		Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu		
			Th	Pa	U												

Or specify an element and/or charge

Element + Charge

1.1A) Search by: Freeform Wavelength Ion

Minimum wavelength / Å → Maximum wavelength / Å

Resolve results by Transition (longer list) File (shorter list)

- ▶ Functionality remains broadly similar.
- ▶ Always available — can pop-over the current screen.

OPEN-ADAS: download a dataset

- ▶ Delivery of a complete *adf* dataset remains the paradigm.
- ▶ Actual use of ADAS data is via direct use of its complete datasets — *not* via web access.

The screenshot displays the OPEN-ADAS website interface. At the top, the logo 'OPEN-ADAS' is followed by the text 'Atomic Data and Analysis Structure | Ra II (4533.1Å)'. A search bar is present with three icons: a magnifying glass labeled 'Freeform', a wavelength symbol labeled 'Wavelength', and a Z^{q+} symbol labeled 'Ion'. The main content area is titled 'DATA CLASSES' and 'lilike_lgy10#si11.dat'. Under 'FUNDAMENTAL', it lists 'Resolved Specific Ion Data Collections' for 'Si¹¹⁺' with a 'Temperature Range' of '2.482 eV → 2.482 x 10⁴ eV'. A 'Download data' button is highlighted, with a 'Download data' label and a 'ADF 04' badge. Below this, there are links for 'Documentation' and 'Software libraries'. A table with tabs 'Processes', 'States', 'Comments', and 'Origins' is visible. Under 'DERIVED', it lists 'ADF11' (Spontaneous Emission: Si¹¹(j) → Si¹¹(j) + hv) and 'ADF12' (Electron Impact Excitation: Si¹¹(i) + e → Si¹¹(j) + e). The footer includes '© Copyright 1995-2013 The ADAS Project, Version 2.0', logos for EURATOM, IAEA, and University of Strathclyde Glasgow, and a list of links: 'OPEN-ADAS news', 'Documentation', 'Download code', 'Terminology', 'Statistics', 'About ADAS', 'About OPEN-ADAS', 'Contact OPEN-ADAS', 'Terms & Conditions', and 'Privacy'.

OPEN-ADAS: reasons for upgrading

- ▶ The ADAS-EU Project placed a strong emphasis on knowledge exchange.
- ▶ OPEN-ADAS is a key (data) dissemination route.
- ▶ A new server for OPEN-ADAS was installed.
- ▶ The internet is becoming an even more hostile environment — security hardening was essential.
- ▶ A significant quantity of new data has been produced during normal ADAS activities since the first version.
- ▶ New classes of data — photo-excitation and photo-ionisation needed an authoritative distribution method.
- ▶ Internal tool chain streamlining to make OPEN-ADAS updates a simpler process.

OPEN-ADAS: fundamental and derived data

FUNDAMENTAL CLASSES

ADF
01

Charge exchange cross sections

nI-resolved charge exchange cross-sections over a range of n-shells for a donor neutral atom and ionised impurity receiver

ADF
04

Resolved specific ion data collections

Coefficient data for a given ion which includes spontaneous emission coefficients and electron impact collisional rates and other optional processes.

ADF
07

Electron impact ionisation coefficients

Collections of Maxwell averaged electron impact ionisation rate coefficients for both direct ionisation and excitation/autoionisation.

ADF
08

Radiative recombination coefficients

Maxwell-averaged radiative recombination coefficients i.e. spontaneous free-bound transitions of Maxwellian electrons excluding dielectronic recombination.

ADF
09

Resolved dielectronic recombination coefficients

Collections of state-selective dielectronic recombination coefficients of Maxwellian free electrons resolved by initial and final metastable and captured n-shell.

ADF
38

Photoexcitation-autoionisation rate coefficients

Fundamental data for inner shell excitation followed by autoionisation

ADF
39

Photoionisation cross-sections

Fundamental data for direct (including and especially inner shell) photoionisation.

ADF
48

Radiative recombination rate coefficients

Partial final-state resolved radiative recombination rate coefficients from both ground and metastable levels.

DERIVED CLASSES

ADF
11

Iso-nuclear master files

Effective (collisional-radiative) coefficients which are required to establish the ionisation state of a dynamic or steady-state plasma.

ADF
12

Charge exchange effective emission coefficients

Collections of effective emission coefficients for spectrum lines emitted by ions of elements following charge transfer from neutral beam donor atoms.

ADF
13

Ionisation per photon coefficients

Data collections useful in analysis of a spectrum line from an ionisation stage of an element, which is inflowing into a plasma from a surface.

ADF
15

Photon emissivity coefficients

Fully density dependent and metastable resolved effective emissivity coefficients from a collisional-radiative model.

ADF
21

Effective beam stopping/excitation coefficients

They are effective ionisation coefficients, including charge transfer losses, which leave the beam atoms ionised.

ADF
22

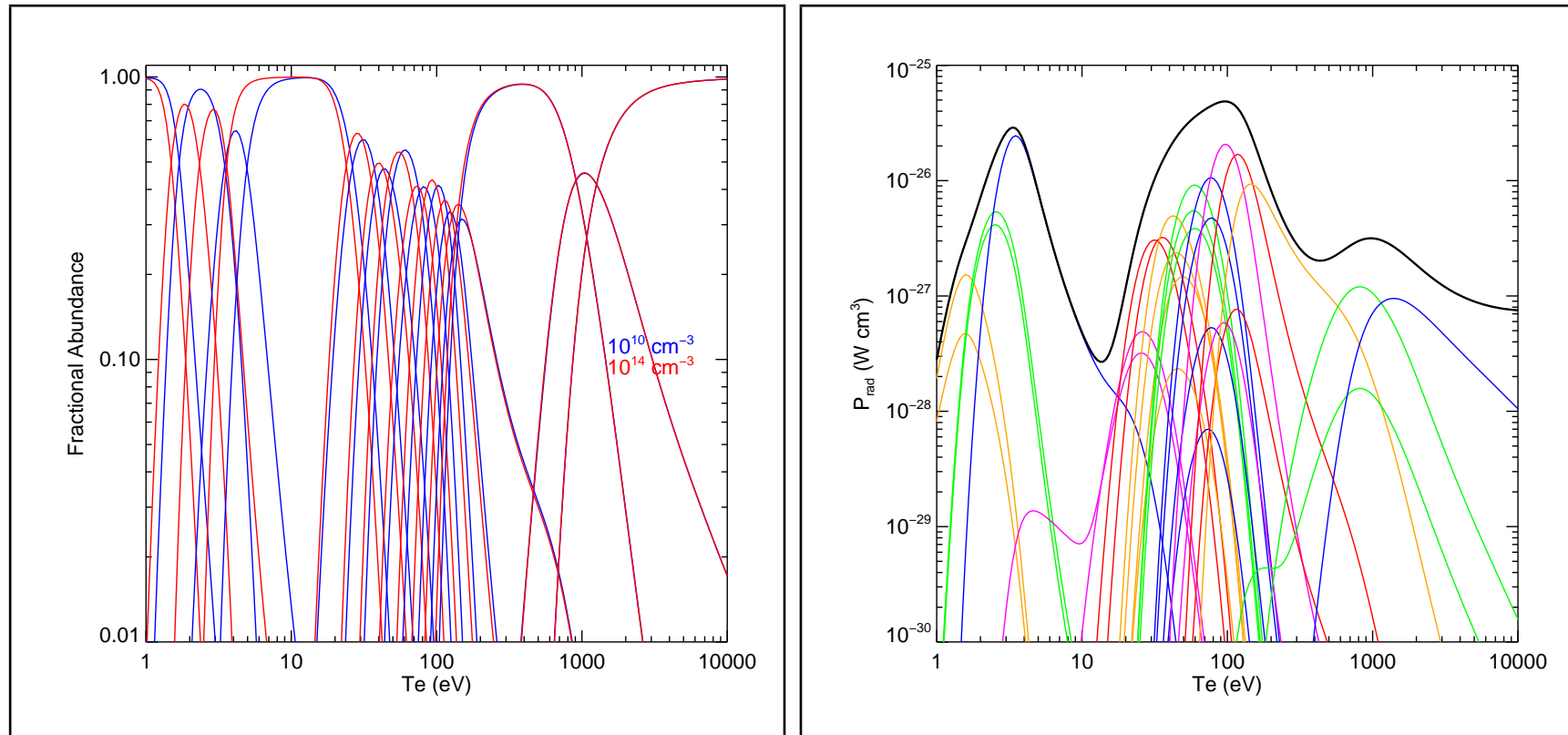
Effective beam emission/population coefficients

Coefficients for the emission from a beam when it enters an ionised plasma including impurities. Results are fully density dependent output from a collisional-radiative model.

OPEN-ADAS: new data classes

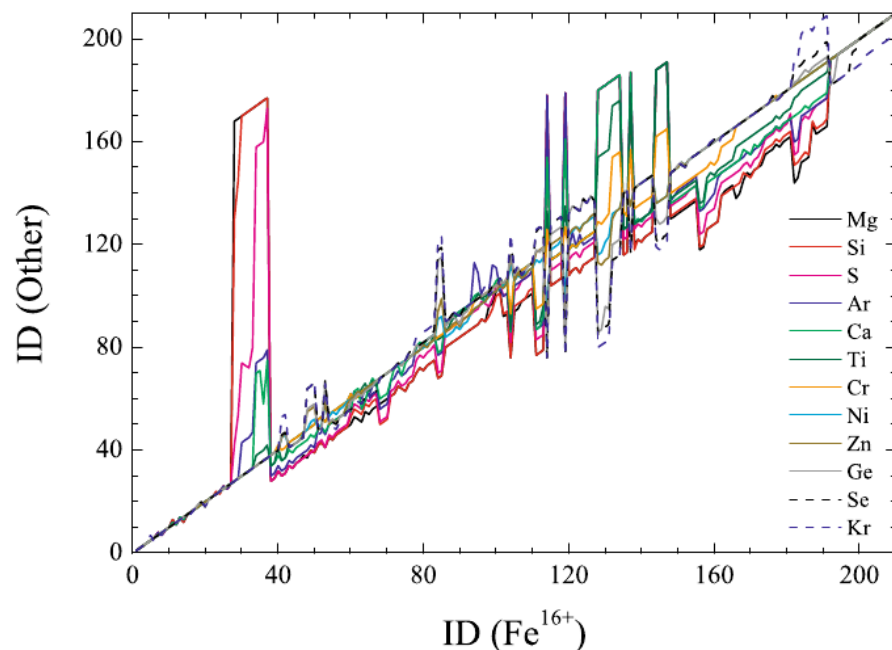
- ▶ *adf38* state resolved photo-excitation cross sections.
 - Inner- and outer-shell final-state resolved partial dipole photoionization cross sections for all states of the initial ground complex.
- ▶ *adf39* state resolved photo-ionisation rates.
 - Inner-shell final-state resolved partial photoexcitation-autoionization data for all states of the initial ground complex.
- ▶ *adf48* state resolved radiative recombination rates.
 - Final-state resolved partial RR rate coefficients for ground and metastable initial states.
- ▶ Bare ion to Mg-like sequences.
- ▶ Elements considered are: Hydrogen to Zinc (and Xenon).

Silicon GCR data



- Metastable-resolved and density dependent ionisation balance for silicon.
- Work is progressing on Magnesium, Aluminium and Argon.
- Re-formulating to an intermediate coupling ion state description with the target plasma determining the metastables.

R-Matrix sequence data



G Liang, N R badnell, M Witthoef

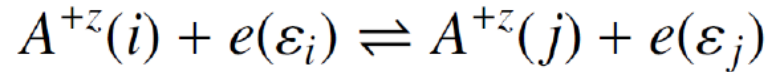
- ▶ Work programme to maximize utility of R-matrix codes.
- ▶ He, Li, F, Na, Ne sequences.
- ▶ Elements up to Zinc.
- ▶ Neutral and singly ionized are excluded.
- ▶ Be-like and B-like under way.
- ▶ H-like has somehow dropped between the cracks.
- Preparing a repository for the resonance-resolved OMEGA files is under consideration.

Improving ADAS baseline excitation data

- ▶ Completeness is important for fusion models
 - Iso-nuclear rather than iso-electronic!
- ▶ *adf04* produced with Cowan code was the ADAS baseline method
 - very good structure
 - but no inter-system rates
- ▶ Extend AUTOSTRUCTURE with distorted wave method.
- ▶ H-like to Ar-like sequences produced.
- ▶ H to Zn with selected higher Z — increases database by 10Gb.
- ▶ Collision strengths and effective collision strengths produced.

Non-Maxwellian population modelling: rate coefficients

Consider the reaction



Maxwellian: detailed balance

$$\Upsilon_{ij}(T_e) = \int_0^\infty \Omega_{ij}(\varepsilon_j) \exp\left(-\frac{\varepsilon_j}{kT_e}\right) d\left(\frac{\varepsilon_j}{kT_e}\right)$$

$$q_{i \rightarrow j}(T_e) = 2\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_e}\right)^{1/2} \frac{1}{\omega_i} \exp\left(-\frac{\Delta E_{ij}}{kT_e}\right) \Upsilon_{ij}(T_e)$$

$$q_{j \rightarrow i}(T_e) = 2\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_e}\right)^{1/2} \frac{1}{\omega_j} \Upsilon_{ij}(T_e)$$

same

Non-Maxwellian: no detailed balance

$$\Upsilon_{i \rightarrow j}(T_{eff}) = \frac{\sqrt{\pi}}{2} \exp\left(\frac{\Delta E_{ij}}{kT_{eff}}\right) \int_0^\infty \Omega_{ij}(\varepsilon_i) \left(\frac{\varepsilon_i}{kT_{eff}}\right)^{-1/2} f(\varepsilon_i) d\varepsilon_j$$

$$\mathcal{J}_{j \rightarrow i}(T_{eff}) = \frac{\sqrt{\pi}}{2} \int_0^\infty \Omega_{ij}(\varepsilon_j) \left(\frac{\varepsilon_j}{kT_{eff}}\right)^{-1/2} f(\varepsilon_j) d\varepsilon_j$$

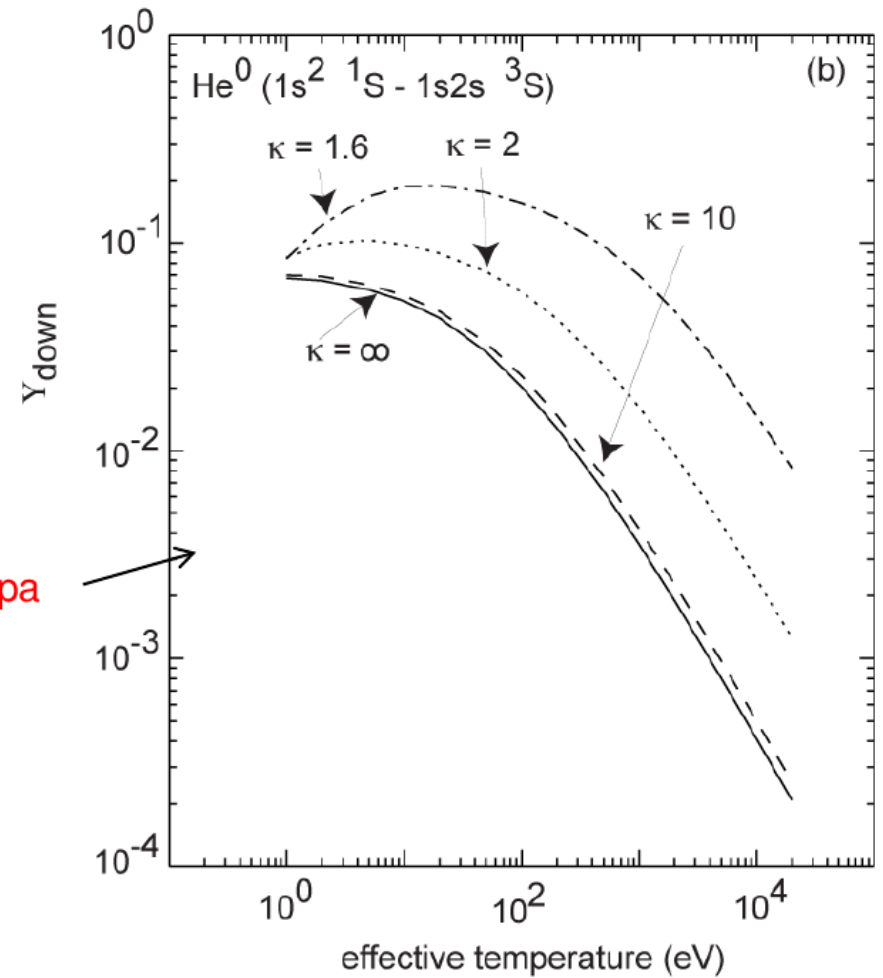
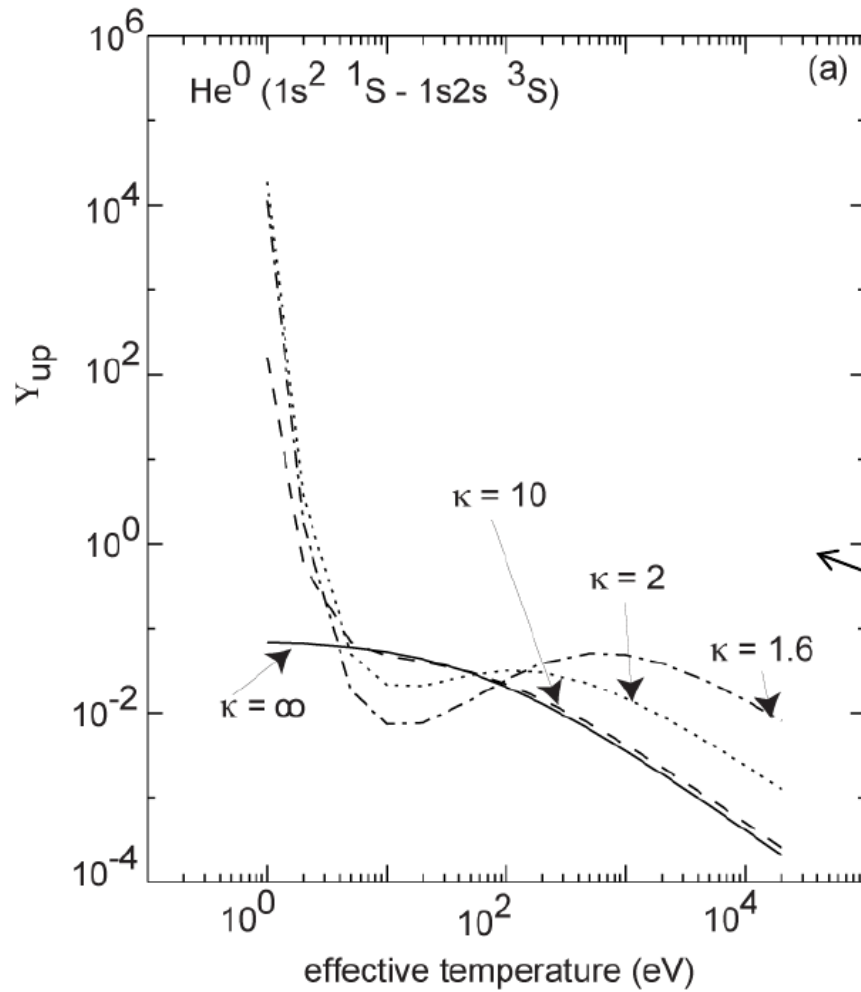
$$q_{i \rightarrow j}(T_{eff}) = 2\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_{eff}}\right)^{1/2} \frac{1}{\omega_i} \exp\left(-\frac{\Delta E_{ij}}{kT_{eff}}\right) \Upsilon_{i \rightarrow j}(T_{eff})$$

$$q_{j \rightarrow i}(T_{eff}) = 2\sqrt{\pi}\alpha c a_0^2 \left(\frac{I_H}{kT_{eff}}\right)^{1/2} \frac{1}{\omega_j} \mathcal{J}_{j \rightarrow i}(T_{eff})$$

different

Effective mean energy parameter

Non-Maxwellian upsilons and downsilons



Kappa

Non-Maxwellian population modelling: other rates

Dielectronic recombination and radiative recombination coefficients are straightforward. Electron impact ionisation and three-body recombination are more complicated.

Fowler relation is the starting point

$$\omega_i E Q_{i \rightarrow +}(E; E', E'') = \frac{16\pi m}{h^3} \omega_+ E' E'' Q_{+ \rightarrow i}(E', E''; E)$$

Collisional ionisation

$$q_{i \rightarrow +} = \int_{I_i}^{\infty} \sqrt{\frac{2E}{m}} Q_{i \rightarrow +}(E; E', E'') f(E) dE \int dE' \int dE''$$

E is the incident energy, E' and E'' the scattered and ejected energies

Three-body recombination

$$\begin{aligned} \alpha_{+ \rightarrow i}^{(3)} &= 8 \left(\frac{\pi a_0^2 I_H}{kT_{eff}} \right)^{3/2} \frac{\omega_i}{2\omega_+} e^{I_i/kT_{eff}} \\ &\times \int_{I_i}^{\infty} \sqrt{\frac{2E}{m}} Q_{i \rightarrow +}(E; E', E'') f(E) dE \\ &\times \int \int \left[\frac{\sqrt{\pi}}{2} (kT_{eff})^{3/2} e^{-I_i/kT_{eff}} \right. \\ &\times \left. \sqrt{\frac{E}{E' E''} \frac{f(E') f(E'')}{f(E)}} \right] dE' dE'' \end{aligned}$$

Thompson cross-section allows evaluation

$$Q_{i \rightarrow +}(E; E', E'') = 4\pi a_0^2 \zeta I_H^2 \frac{1}{EE'^2} \delta(E - E' - E'' - I_i)$$

Non-Maxwellian population modelling: diagnostic potential

Non-Maxwellian populations evaluated using code [ADAS218](#).

Differential variation of populations according to enhancement or depletion of regions of the appropriate distribution functions.

The numerical non-Maxwellian is from a JET simulation near the divertor plate by Tskhakaya.

The non-Maxwellian adf04 datasets were prepared for the appropriate distribution functions using [offline_adas/adas7#3/adf04_om2ups](#)

