

ADAS

Atomic Data and Analysis Structure

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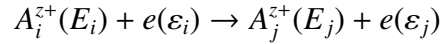
Cross sections, collision strengths and effective collision strengths as used in *adf04* and *adf06* files

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1 Electron impact excitation

For the reaction



where $\varepsilon_i + E_i = \varepsilon_j + E_j$ and $\Delta E_{ij} = E_j - E_i$ where E_i is the excitation energy of state i and ε_i is the energy of the incident (i) or scattered (j) electron.

The reaction is described by the cross section, $\sigma_{i \rightarrow j}(\varepsilon_i)$, which is only energetically possible if $\varepsilon_i \geq \Delta E_{ij}$.

Define $X = \varepsilon_i / \Delta E_{ij}$ where $X \in [1, \infty]$

The collision strength is dimensionless and symmetrical between initial and final states,

$$\Omega_{ij} = g_i(E_i/I_H)(\sigma_{i \rightarrow j}(\varepsilon_i)/\pi a_0^2) = g_j(E_j/I_H)(\sigma_{j \rightarrow i}(\varepsilon_j)/\pi a_0^2)$$

with g_i and g_j the statistical weights and I_H the Rydberg energy.

To convert (measured/calculated) cross sections (σ) to collision strengths ($\Omega_{ij} \equiv \Omega_{ij}$) which are tabulated against incident energy,

$$\Omega_{ij} = g_i * (\Delta E_{ij} * X / 109737.26) * (\sigma / 8.7972e-17)$$

where X is defined by the user and σ (as a function of energy in cm^2) is interpolated for $X * \Delta E_{ij}$.

A *type 1*, *adf04* file tabulates Ω_{ij} as a function of X .

A *type 5*, *adf04* file tabulates Ω_{ij} as a function of $\varepsilon_i - \Delta E_{ij}$.

The default *adf04* output for AUTOSTRUCTURE (*adas7#1*) is *type 5* whereas Cowan (*adas8#1*) produces *type 1* *adf04* files.

The Maxwellian distribution function for free particles is:

$$f(v) = 4\pi \left(\frac{m}{2\pi kT} \right)^{3/2} v^2 \exp\left(-\frac{mv^2}{2kT}\right)$$

$$f(E) = 2\pi \left(\frac{1}{\pi kT} \right)^{3/2} E^{1/2} \exp(-E/kT)$$

where m is the particle mass and T the temperature and $\int_0^\infty f(v) dv = 1$. Note that $v^2 = 2E/m$ and $dv = 1/(2mE)^{1/2} dE$.

The excitation rate is then

$$q_{i \rightarrow j}(T) = \langle v_i \sigma_{i \rightarrow j}(v_i) \rangle$$

$$= \int_{\Delta E_{ij}}^{\infty} f(v_i) v_i \sigma_{i \rightarrow j}(v_i) dv_i$$

$$\begin{aligned}
&= 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} \int_{\Delta E_{ij}}^{\infty} v_i^2 v_i \exp(-\varepsilon_i/kT) \sigma_{i \rightarrow j}(\varepsilon_i) dv_i \\
&= 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} \left(\frac{2}{m}\right)^{3/2} \left(\frac{1}{2m}\right)^{1/2} \int_{\Delta E_{ij}}^{\infty} \varepsilon_i \exp(-\varepsilon_i/kT) \sigma_{i \rightarrow j}(\varepsilon_i) dE_i \\
&= \frac{2\sqrt{2}}{\sqrt{\pi}} \left(\frac{1}{kt}\right)^{3/2} \left(\frac{1}{m}\right)^{1/2} \frac{\pi a_0^2 I_H}{g_i} \int_{\Delta E_{ij}}^{\infty} \Omega_{ij} \exp(-\varepsilon_i/kT) (\varepsilon_i) dE_i
\end{aligned}$$

where the cross section is replaced by the collision strength.

When the integral is further transformed from v_i to E_j ($\varepsilon_i = \varepsilon_j + \Delta E_{ij}$), and noting that $\alpha c = (2I_H/m_e)^{1/2}$, the excitation rate coefficient for electron impact excitation becomes

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

where Υ_{ij} is the effective collision strength,

$$\Upsilon_{ij} = \int_0^{\infty} \Omega_{ij}(\varepsilon_j) \exp(-\varepsilon_j/kT_e) d(\varepsilon_j/kT_e).$$

The limits reflect that this integral is defined over electron energies, ε_j , with respect to the final, excited, state. However Υ_{ij} is symmetrical between excitation and de-excitation concordant with the collision strength.

A *type 3*, *adf04* file tabulates Υ_{ij} as a function of T_e .

De-excitation and excitation rates follow:

$$\begin{aligned}
q_{j \rightarrow i}(T_e) &= 2\sqrt{\pi} a_0^2 \alpha c \frac{1}{g_j} \left(\frac{I_H}{kT_e}\right)^{1/2} \Upsilon_{ij} \\
&= \frac{g_i}{g_j} \exp(\Delta E_{ij}/kT_e) q_{i \rightarrow j}(T_e)
\end{aligned}$$

and $2\sqrt{\pi} a_0^2 \alpha c = 2.1716 \times 10^{-8} \text{ cm}^3 \text{ s}^{-1}$.

The offline code `adas7#3/adf04_om2ups.x` can convert a *type 1* or *type 5 adf04* to a *type 3* file. The reverse process is not possible. The python library function, `adf04_om2ups.py`, calls the offline code to enable a python workflow.

2 Ion impact excitation

The collision strength is the ratio of the cross section to the de Broglie wavelength squared and the generalized form (for ion impact is),

$$\Omega_{ij}^{ion} = M g_i (E_i/I_H) (\sigma_{i \rightarrow j}(\varepsilon_i)/\pi a_0^2) = M g_j (E_j/I_H) (\sigma_{j \rightarrow i}(\varepsilon_j)/\pi a_0^2)$$

where M is the reduced mass of the target-projectile system,

$$M = \frac{m_t m_p}{m_t + m_p}$$

in atomic units ($m_e = 1$). The energies ($\varepsilon_i, \varepsilon_j$) are those of the incident and scattered projectile. $M \rightarrow 1$ for electron impact (*ie* $m_p = m_e$), where the target is considered massive compared to the electron projectile. This is not the case where the projectile ion is a proton or a heavier particle.

The threshold parameter $X = \varepsilon_i/\Delta E_{ij}$ is defined the same way as for the electron impact case.

A *type 1, adf06* file tabulates Ω_{ij}^{ion} against X . Note that this includes the reduced mass value.

The effective collision strength for ion impact is defined identically as the electron impact version, assuming a Maxwellian ion temperature,

$$\Upsilon_{ij} = \int_0^{\infty} \Omega_{ij}^{ion}(\varepsilon_j) \exp(-\varepsilon_j/kT_e) d(\varepsilon_j/kT_e).$$

A *type 3, adf06* file tabulates Υ_{ij}^{ion} against T_{ion} .

The excitation rate contains an explicit mass factor,

$$q_{i \rightarrow j}^{ion}(T_{ion}) = 2 \sqrt{\pi} a_0^2 \alpha c \frac{1}{g_i} \left(\frac{I_H}{kT} \right)^{1/2} \exp(-\Delta E_{ij}/kT) \left(\frac{1}{M} \right)^{3/2} \Upsilon_{ij}$$

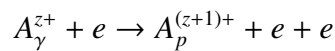
The mass used in forming the rate coefficient is the actual mass, Mm_e , but since the collision strength is defined in atomic units the reduced mass M term appears. *eg* for $p + \text{Na}$, $M = 0.958$. The electron mass is included in the above equation in αc , as in the electron impact case.

There is no ADAS code to convert between a *type 1* and *type 3 adf06* file.

The *adf06* file includes information on the masses of the target and projectile so forming the rate coefficient using the above equation is unambiguous. For ion-impact data stored as P-lines in *adf04* files this information is not stored. The population codes, *eg* `adas205`, `adas208`, `run_adas208.pro`, `run_adas208.py` etc., form rate coefficients using just the P-line data. The rate used in these codes may be scaled by a user supplied Z_{eff} parameter to the code it is preferable that this step should not be required. Therefore the ADAS *adf04* data files archive $\Upsilon_{ij}/M^{3/2}$ in the P-lines.

3 Electron impact ionization

The reaction



where the ion in its initial state, γ , is ionised to a residual state p . The final state may be metastable but often is not specified, being the sum over all possible final states. This direct ionisation may be augmented by indirect auto-ionisation channels which are manifest as steps in the cross section.

An electron impact ionisation collision strength is defined in the same way as for excitation:

$$\Omega_{\gamma p}^{ionis} = g_{\gamma} \frac{E}{I_H} \frac{\sigma_{\gamma \rightarrow p}^{ionis}}{\pi a_0^2}$$

where E is the energy of the impacting electron and g_{γ} the statistical weight of the ionising level.

To convert (measured/calculated) cross sections (σ) to collision strengths ($\omega_s \equiv \Omega^{ionis}$) which are tabulated against incident energy,

$$\omega_s = g_i * (ip * X / 13.6) * (\sigma / 8.7972e-17)$$

where X is defined by the user, ip is the energy of the level–parent gap (in eV, equivalent to ionisation potential for ground state ionisation) and σ (cm^2) is interpolated for $X * ip$. Any steps, due to auto-ionisation, in the cross section are not scaled separately so the collision strength will retain the energy resolved structure of the cross section.

A *type 1, adf04* file tabulates Ω_{ij}^{ionis} as a function of $X = E/I_{ionis}$.

The ionisation rate coefficient, for a Maxwellian distribution, is:

$$S_{\gamma \rightarrow p}^{ionis} = 2 \sqrt{\pi} \alpha a_0^2 \frac{1}{g_{\gamma}} \exp(-I_{ionis}/kT) \Upsilon_{\gamma \rightarrow p}^{ionis}$$

where $I_{ionis} = I_p(m) - E_i$ with $I_p(m)$ being the ionisation potential of the parent metastable and E_i is the energy relative to ground of the level being ionised. The effective collision strength ($\Upsilon_{\gamma \rightarrow p}$) is defined the same way as the excitation case.

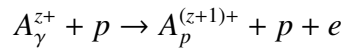
The *type 3 adf04* file stores a scaled version of the ionisation rate as a function of temperature. The S-line in the file is defined:

$$S_{\gamma \rightarrow p}^{scaled} = \exp(I_{ionis}/kT) S_{\gamma \rightarrow p}$$

where S is the ionisation rate coefficient ($\text{cm}^3 \text{s}^{-1}$) and *not* the ‘ionisation effective collision strength’.

4 Ion impact ionization

The reaction,



where the ionising particle projectile, p , can be a proton or a heavier ion.

The ion impact collision strength for ionisation is defined as:

$$\Omega_{\gamma p}^{ion;ionis} = M g_{\gamma} (E/I_H) (\sigma_{\gamma p}(E) / \pi a_0^2)$$

where $M = m_i m_p / (m_i + m_p)$ is the reduced mass of the target-projectile system, in atomic units.

The threshold parameter, $X = E/I_{ionis}$ with $I_{ionis} = I_p(m) - E_i$ with $I_p(m)$ being the ionisation potential of the parent metastable and E_i is the energy relative to ground of the level being ionised.

The *type 1 adf06* file tabulates $\Omega_{\gamma p}^{ion;ionis}$ as a function of the threshold parameter, X .

The ionisation rate is formed in a similar way as the electron impact rate with a mass scaling factor:

$$S_{\gamma \rightarrow p}^{ion;ionis}(T_{ion}) = 2 \sqrt{\pi} a_0^2 \alpha c \frac{1}{g_\gamma} \left(\frac{I_H}{kT} \right)^{1/2} \exp(-I_{ionis}/kT) \left(\frac{1}{M} \right)^{3/2} \Upsilon_{\gamma p}^{ion;ionis}$$

The *type 3 adf06* file tabulates a scaled, mass-free, rate coefficient with ion temperature,

$$S_{\gamma \rightarrow p}^{ion;ionis,scaled} = M^{3/2} \exp(I_{ionis}/kT) S_{\gamma \rightarrow p}^{ion;ionis}.$$

5 Comments

To calculate ion impact excitation and ionisation rates from the data in the *type 3 adf06* file requires that a mass factor is applied (simple multiplication) when forming the rate from the effective collision strengths. For ionisation this is inconsistent with the definition of the electron impact ionisation S-line in the *adf04* file. However the expectation should be that the way of forming the excitation and ionisation rates from one file, whether *adf04* or *adf06*, should be consistent. Formally the two formats are consistent since the electron S-line has an implicit mass factor of 1.