ADAS-C(24)01

# 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

$$A_i^{z+}(E_i) + e(\varepsilon_i) \rightarrow A_j^{z+}(E_j) + e(\varepsilon_j)$$

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 $\varepsilon_i$ 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 (`sigma`) to collision strengths (`omega` $\equiv \Omega ij$) which are tabulated against incident energy,

```
omega = gi * (delta_e * X / 109737.26) * (sigma / 8.7972e-17)
```

where `X` is defined by the user and `sigma` (as a function of energy in $\text{cm}^2$) is interpolated for `X * delta_e`.

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

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

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:

$$\begin{aligned} f(v) &= 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} v^2 \exp(-\frac{mv^2}{2kT}) \\ f(E) &= 2\pi \left(\frac{1}{\pi kT}\right)^{3/2} E^{1/2} \exp(-E/kT) \end{aligned}$$

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

$$\begin{aligned} q_{i\rightarrow j}(T) &= \langle v_i\, \sigma_{i\rightarrow j}(v_i)\rangle \\ &= \int_{\Delta E_{ij}}^{\infty} f(v_i)\, v_i\, \sigma_{i\rightarrow j}(v_i)\, dv_i \end{aligned}$$

$$= 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2}\int_{\Delta E_{ij}}^{\infty} v_i^2 v_i \exp(-\varepsilon_i/kT)\sigma_{i\to j}(\varepsilon_i)\,dv_i$$

$$= 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2}\left(\frac{2}{m}\right)^{3/2}\left(\frac{1}{2m}\right)^{1/2}\int_{\Delta E_{ij}}^{\infty} \varepsilon_i \exp(-\varepsilon_i/kT)\sigma_{i\to j}(\varepsilon_i)\,dE_i$$

$$= \frac{2\sqrt{2}}{\sqrt{\pi}}\left(\frac{1}{kt}\right)^{3/2}\left(\frac{1}{m}\right)^{1/2}\frac{\pi a_0^2 I_H}{g_i}\int_{\Delta E_{ij}}^{\infty} \Omega_{ij}\exp(-\varepsilon_i/kT)(\varepsilon_i)\,dE_i$$

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

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

where $\Upsilon_{ij}$ 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, $\varepsilon_j$, with respect to the final, excited, state. However $\Upsilon_{ij}$ is symmetrical between excitation and de-excitation concordant with the collision strength.

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

De-excitation and excitation rates follow:

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

and $2\sqrt{\pi}a_0^2\alpha c = 2.1716\times10^{-8}\ \mathrm{cm^3\ s^{-1}}$.

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),

$$\Omega_{ij}^{ion} = Mg_i(E_i/I_H)(\sigma_{i\to j}(\varepsilon_i)/\pi a_0^2) = Mg_j(E_j/I_H)(\sigma_{j\to i}(\varepsilon_j)/\pi a_0^2)$$

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. $M \to 1$ 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 $\Omega^{ion}_{ij}$ 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,

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

A *type 3, adf06* file tabulates $\Upsilon^{ion}_{ij}$ against $T_{ion}$.

The excitation rate contains an explicit mass factor,

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

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 $p$ + Na, $M = 0.958$. The electron mass is included in the above equation in $\alpha c$, 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 $Z_{\text{eff}}$ 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

$$A^{z+}_\gamma + e \to A^{(z+1)+}_p + e + e$$

where the ion in its initial state, $\gamma$, 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:

$$\Omega^{ionis}_{\gamma p} = g_\gamma \frac{E}{I_H} \frac{\sigma^{ionis}_{\gamma\to p}}{\pi a_0^2}$$

where $E$ is the energy of the impacting electron and $g_\gamma$ the statistical weight of the ionising level.

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

```
omega_s = gi * (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 `sigma` (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 $\Omega^{ionis}_{ij}$ as a function of $X = E/I_{ionis}$.

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

$$S^{ionis}_{\gamma\to p} = 2\sqrt{\pi}\alpha a_0^2 \frac{1}{g_\gamma} \exp(-I_{ionis}/kT)\, \Upsilon^{ionis}_{\gamma\to p}$$

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 ($\Upsilon_{\gamma\to p}$) 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:

$$S^{scaled}_{\gamma\to p} = \exp(I_{ionis}/kT)\, S_{\gamma\to p}$$

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

# 4 Ion impact ionization

The reaction,

$$A^{z+}_\gamma + p \to A^{(z+1)+}_p + p + e$$

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

The ion impact collision strength for ionisation is defined as:

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

where $M = m_t m_p/(m_t + m_p)$ 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:

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

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

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

# 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.