Dielectronic Recombination of Complex Heavy Ions

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Motivation

- Dielectronic recombination (DR) establishes the ionization balance in non-LTE plasmas and contributes to line emission e.g. DR satellites.

- Collisional–radiative modelling is necessary for magnetic fusion plasmas — *adf09* files deliver the required initial metastable and partial final-state resolved data.

- DR project (Badnell et al. 2003) has delivered LS term and J-level resolved *adf09* files for H-like thru Al-like sequences — latest Abdel-Naby et al. A&A **537**, A40 (2012).

- For ITER and ITER-like devices we need to consider W and its brethren. The highest charge-state likely to be seen in ITER is nominally 60+ (Si-like). So much for 10 years of the DR project...

Problems

- Have you looked at the size of the latest *adf09* files?

- Atomic physics problem is ‘challenging’.

Atomic Physics

Steps along the way:

- Fe $3p^q$ — Badnell Ap.J.Lett. 651, L73 (2006)
- Sn $4d^q$ — Badnell et al. JPB44, 135201 (2011)
- W^{20+} $4d^{10}4f^8$ — Badnell et al. PRA85, 052716 (2012)

A new 'hybrid' *adf09* file format

We seek to maintain the existing initial metastable level resolution — but it is expected that the user will restrict the number severely, e.g. to levels of the ground term.

The existing *adf09* specification delivers level-resolved final state data for low-lying n — but a single complex configuration can have 10,000 levels.

Next, for high-lying states the outer quantum numbers are summed-over to give $\ldots J_{\mathrm{p}} nl$ final-state resolution — the bundled-nl (and then bundled-n) picture. But, such parent resolution can run to thousands of levels.

Solution: we simply sum further to give a bundled parent configuration.

(There are some niceties: e.g. the final resolved configuration will often straddle the ionization limit, autoionizing final states talk to a level resolved electron continuum.)

This has been implemented and Hugh is working to integrate it for use within ADAS.

There are further benefits — the AUTOSTRUCTURE DR calculation can be synchronized with the desired initial/final hybrid *adf09* resolution and carry-out summations on-the-fly.

1Tb rate files $\longrightarrow$ 10's Gb.

W^{20+} ($4d^{10}4f^{8}$)

We consider both $\Delta n = 0$:

- $4f \longrightarrow 4f$ and $4d \longrightarrow 4f$

and $\Delta n = 1$ promotions:

- $4f \longrightarrow 5l$ and $4d \longrightarrow 5l$

A larger set of promotions was considered first in the configuration average approximation (this is the *a priori* analytic average over states and is not to be confused with the *a posteriori* numerical final summation — the former omits configuration mixing.)

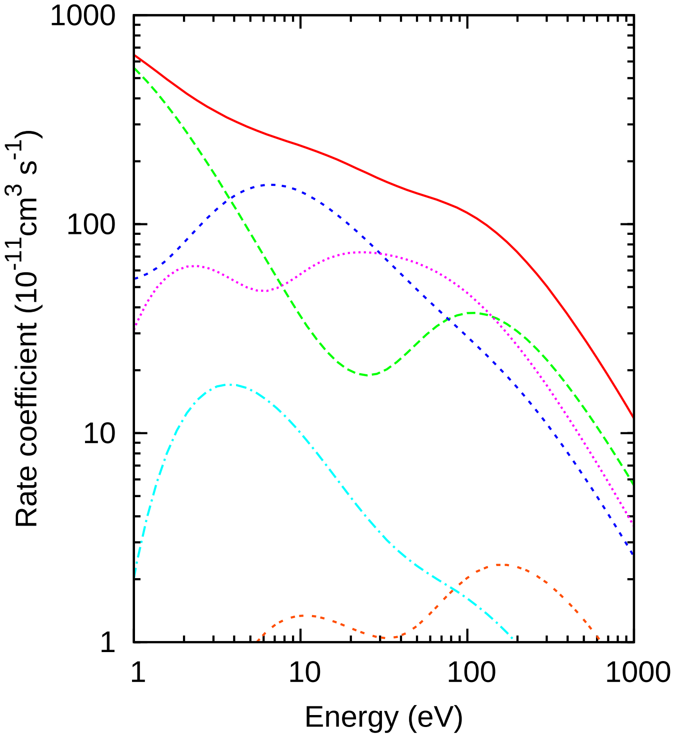

Fig 1. W^{20+} CA Maxwellian DR rate coefficient contributions for various promotions: total (solid red curve), $4d \longrightarrow 4f$ (long-dashed green curve), $4f \longrightarrow 5l$ (short-dashed blue curve), $4d \longrightarrow 5l$ (dotted magenta curve), $4p \longrightarrow 4f$ (dot-dashed cyan curve), and $4d + 4f \longrightarrow 6l$ (double-dashed orange curve).

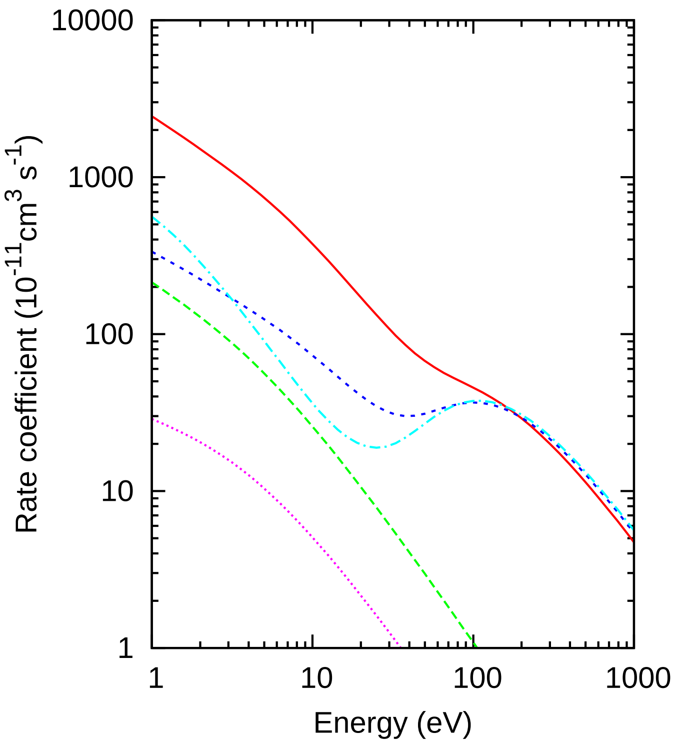

Fig 2. W^{20+} Maxwellian DR rate coefficient contributions for $\Delta n = 0$ promotions: IC $4d \rightarrow 4f$ (solid red curve), IC $4f \rightarrow 4f$ (long-dashed green curve), LS $4d \rightarrow 4f$ (short-dashed blue curve), LS $4f \rightarrow 4f$ (dotted magenta curve), and CA $4d \rightarrow 4f$ (dot-dashed cyan curve).

$\Delta n = 1$ shows a similar pattern of behaviour (not shown).

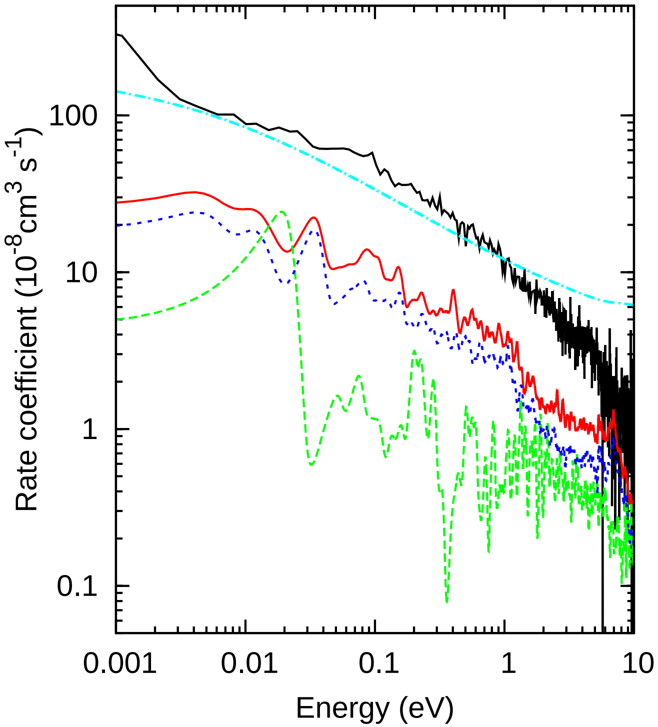

Fig 3. W^{20+} merged-beams DR rate coefficients: experiment Schippers et al. (PRA83, 012711, 2011) (solid black curve), partitioned total (dot-dashed cyan curve), IC total (solid red curve), LS total (long-dashed green curve), and IC $4d \longrightarrow 4f$ only (short-dashed blue curve).

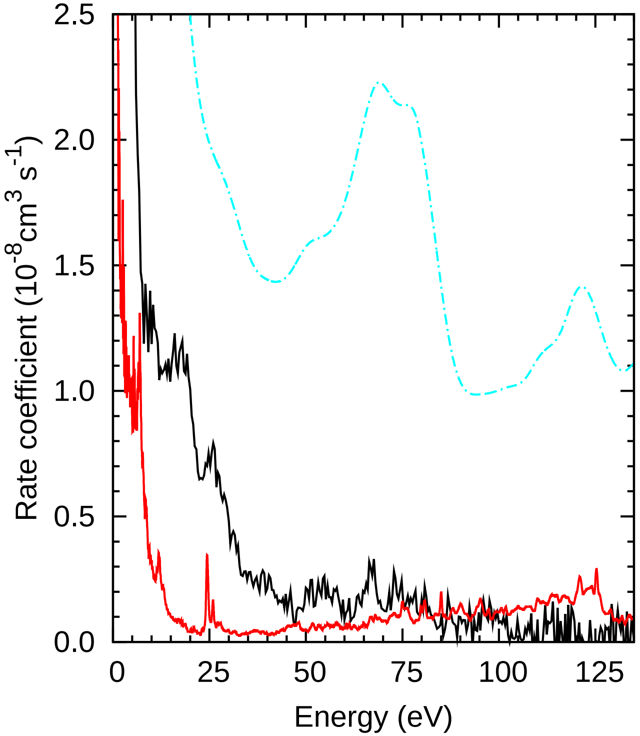

Fig 4. W^{20+} merged-beams DR rate coefficients: experiment Schippers et al. (2011) (solid black curve), partitioned total (dot-dashed cyan curve), IC total (solid red curve).

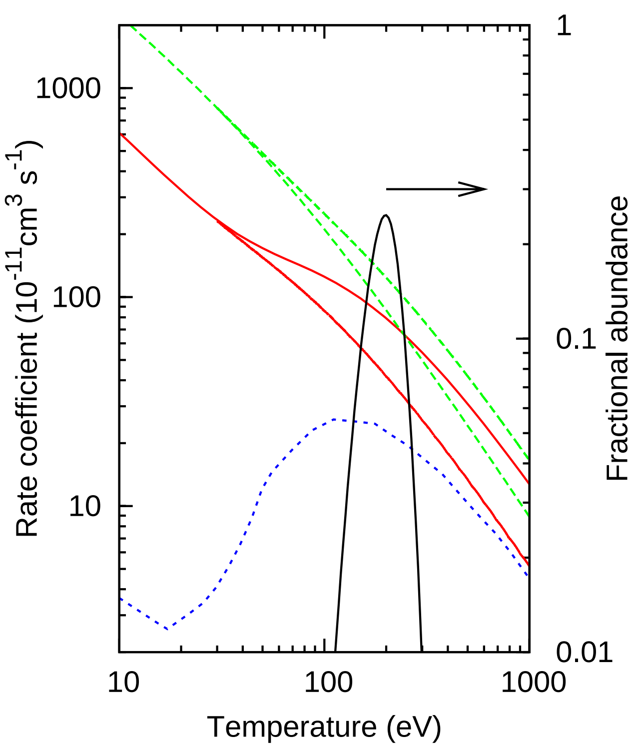

Fig 5. W^{20+} total Maxwellian DR rate coefficients: IC all resonances and to 140 eV only (solid red curves), experiment Schippers et al. (2011) to 140 eV and with theory top-up for resonances above 140eV (long-dashed green curves), and ADAS (Foster, Ph.D. Thesis 2008) (short-dashed blue curve). The fractional abundance of W^{20+} in a magnetic fusion plasma is shown also (solid black curve).

Follow-up

- CR modelling to assess density effects and revise ionization balance for W with open f-shell; DR of adjacent ions expected to be similar.
- Experiments on adjacent ions being analyzed (Schippers, private communication).
- Can the validity of the model calculation be extended to higher energy?

Hot off the press!

Hybrid *adf09* data for K-like thru Ni-like sequences: $3\mathrm{d}^q(q = 1 - 10)$

Coverage: all elements to Zn plus Kr, Mo, Xe and W, ~ 100 ions.

(Entire disk usage — still holding all necessary rates from AS to adasdr — is < 300Gb.)

This is part of "The DR of Everything Else (for Astrophysics) Project".

Thanks

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