Overview of GCR: moving to Fe and enabling transient modelling

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Introduction and motivation

Reconstructing the emission and interpreting the behaviour of elements heavier than neon is essential in both astrophysics and fusion:

- new space-borne instrumentation, in particular SPICE on-board Solar Orbiter (need of Fe^{2+}) and IRIS (need of Si^{3+}) allow observations up to the relatively dense solar upper chromosphere/lower transition region and are oriented to dynamic conditions;
- recent analysis in the lower temperature solar chromosphere and transition region (e.g. need of Si^{1+}) confirm that the use of zero-density approach and inappropriate simplification of the theoretical atomic models can lead to misinterpretation in comparing measurements and theory;
- developments in the fusion context, particularly ITER and DEMO, require advanced modelling of heavy species, such as tungsten.

The application to all densities and the distinguishing of metastable states place the issue in the environment of *Generalised Collisional-Radiative (GCR) model* (Summers et al. 2006).

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GCR approach needs to be extended to medium weight/heavy species, moving towards iron as a first step.

Towards Fe GCR: requirements

- Reformulation in terms of intermediate coupling (*ic*)

  For medium weight species and more highly ionised ions, term resolved resolution (*ls*) is not appropriate because the fine structure separation within a term becomes significant and the relative populations begin to deviate from statistical.

  Level separation increases with Z that is going to medium weight/heavy element ions.

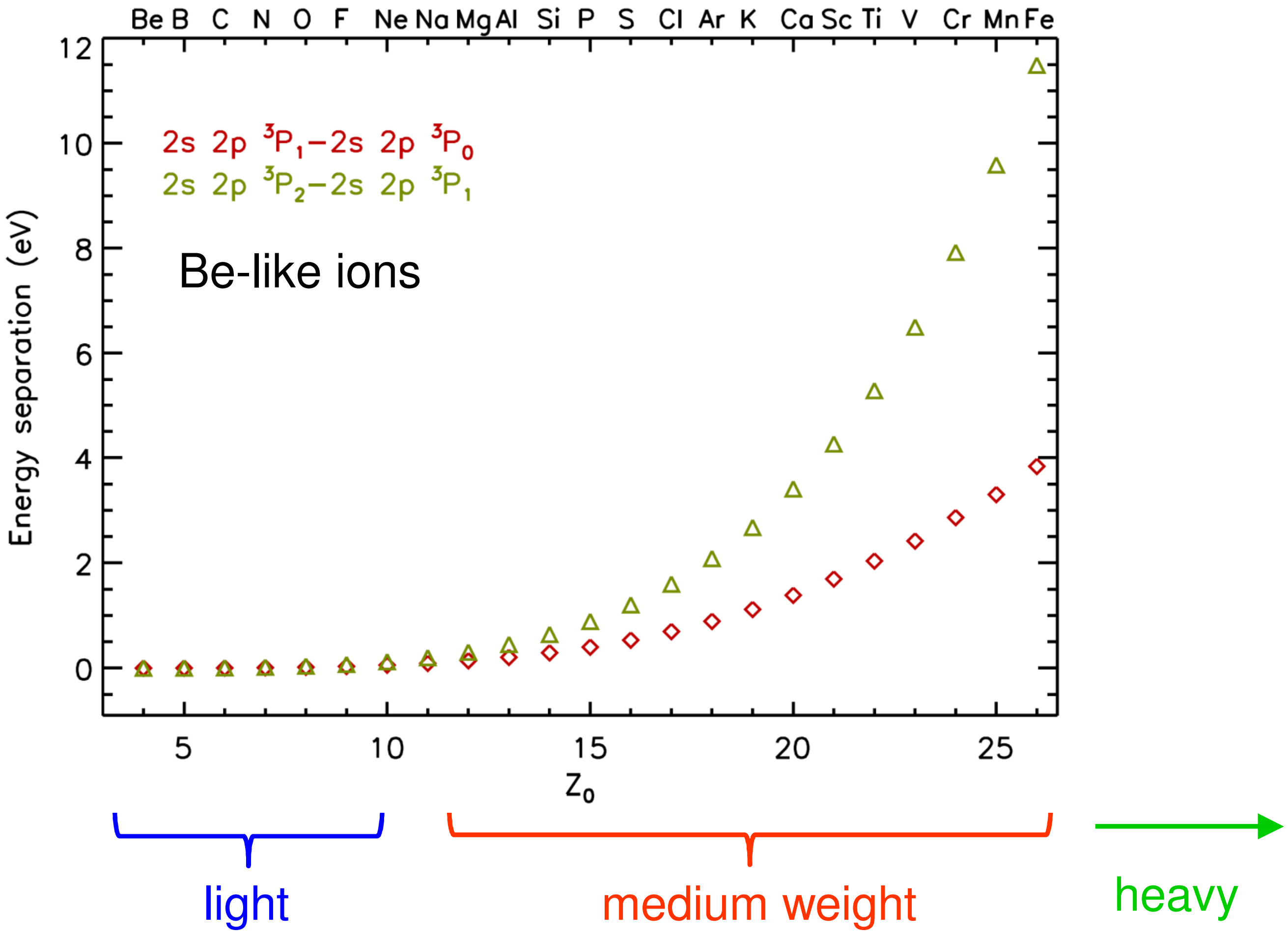
- Revision of metastability

  Moving towards Fe, level resolved metastable states need to be taken into account. This implies a large set of metastables (e.g. for Si from 32 *ls* metastables to 55 *ic* metastables), which may become huge for heavier species.

- Inclusion of ion impact

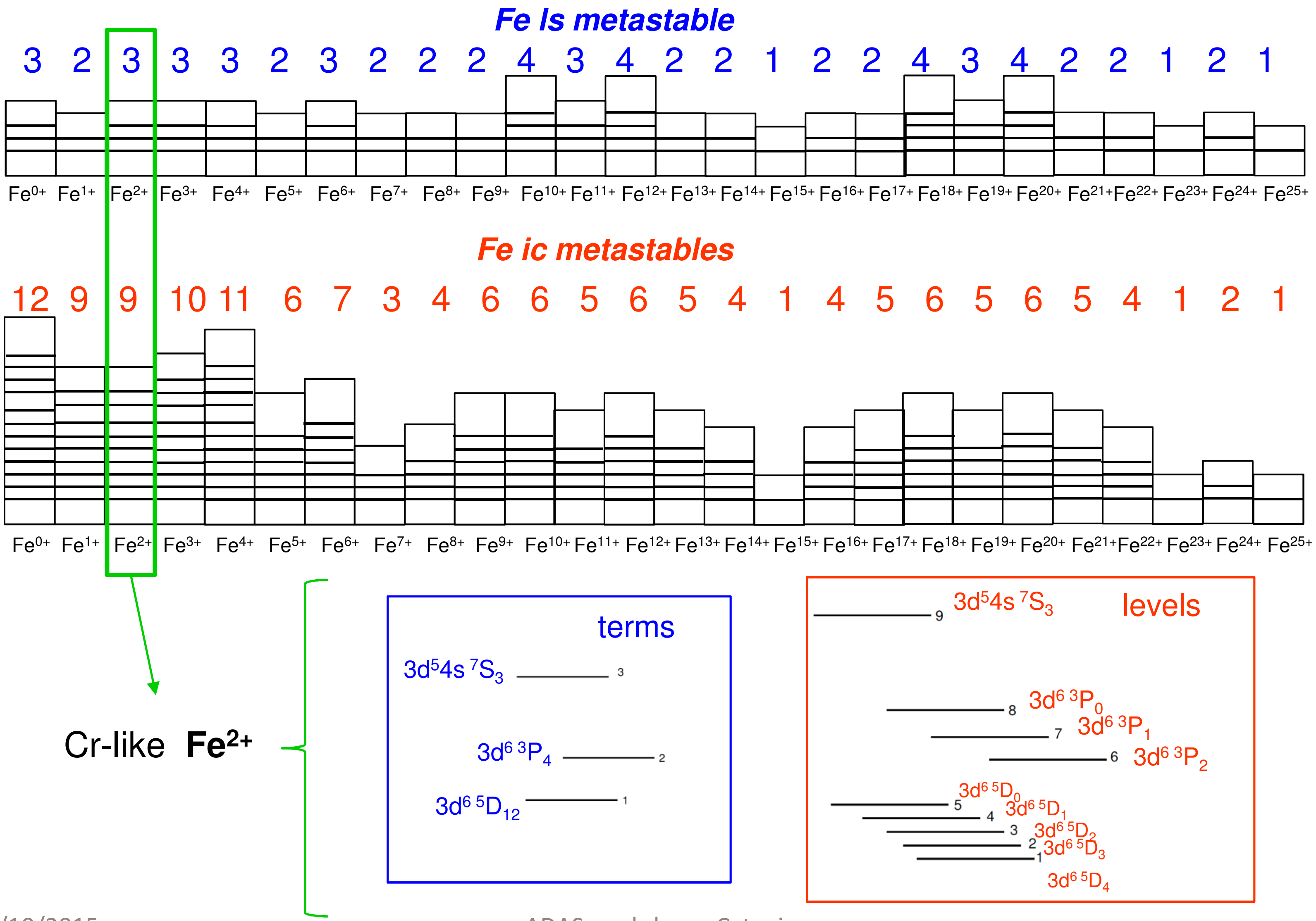
  Ion impact affects transition between close lying levels, and so the fine structure, and *ic* GCR involves interaction between levels. Therefore, ion impact cross sections need to be included in the population calculations.

Fine structure and energy separation

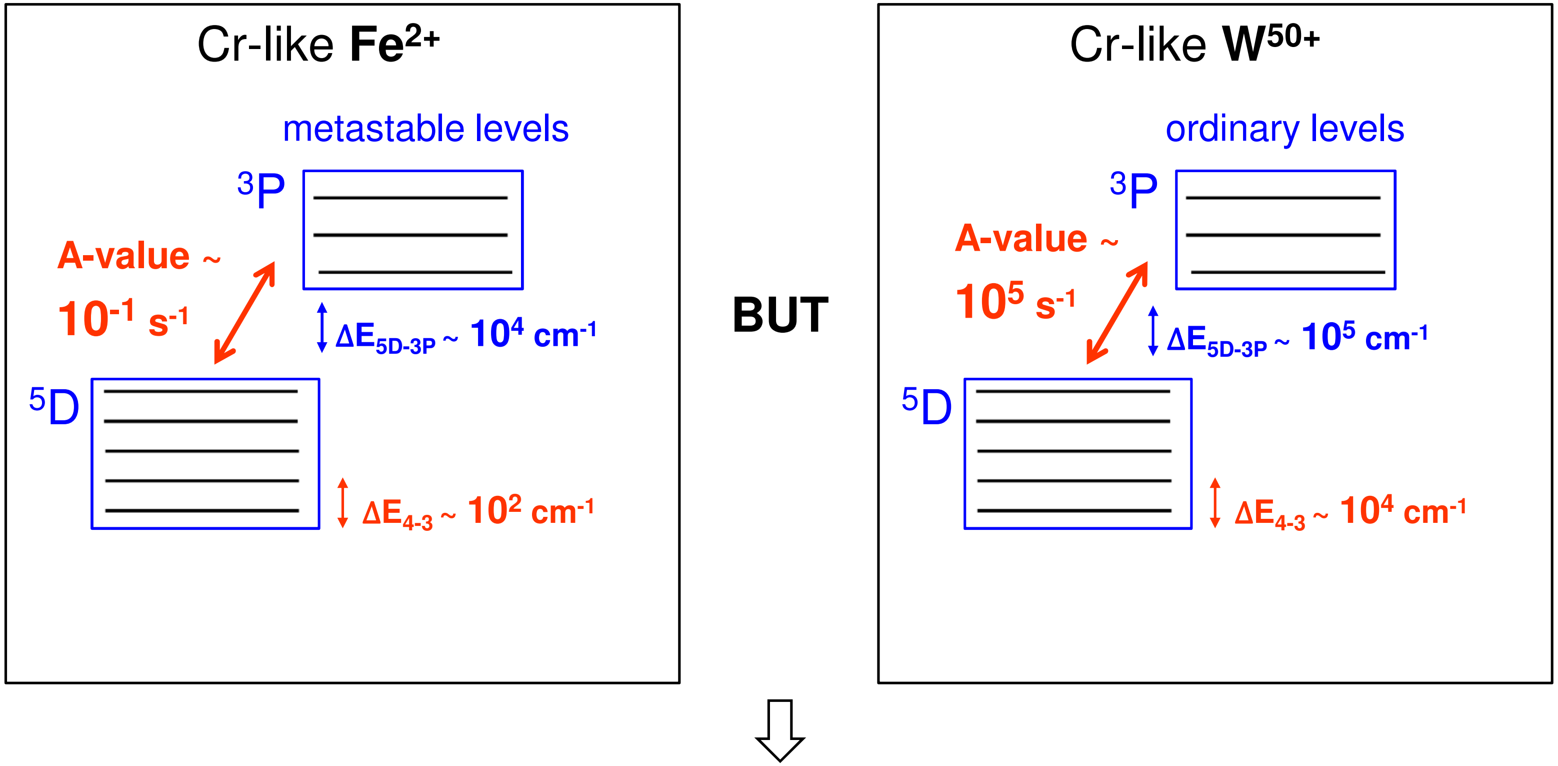


Metastability: *medium weight elements* and beyond

Number of metastable terms and levels for each Fe ionisation stage



Metastability: medium weight elements *and beyond*



Moving towards heavy elements, the metastability is lost [*A-value*(W_{5D-3P})>>*A-value*(Fe_{5D-3P})], unless the plasma is highly dynamic and in transient conditions.

However, for heavy species *ic* separation becomes close to *ls* separation and so the relative populations deviate from statistical.

Ion impact: the metastable cross-coupling coefficient

Considering the metastable level (or term) populations:

$$\frac{dN_{\rho}^{+z}}{dt} = -(N_e S_{CD,\sigma\to\nu} N_{\sigma}^{+z} + N_e \alpha_{CD,\nu'\to\rho} N_{\nu'}^{+z+1} + N_e \boxed{Q_{CD,\sigma\to\rho}} N_{\sigma}^{+z}) + \ldots$$

Metastable cross-coupling coefficient

Since the transitions which are readily excited by ions are those between close lying levels, ion impact can be included in the GCR modelling through the metastable cross-coupling coefficient in the form:

$$Q_{CD,\sigma\to\rho}^{total} \simeq Q_{CD,\sigma\to\rho}^{(e)} + (N_{ion} q_{\sigma\to\rho}^{ion})/N_e$$

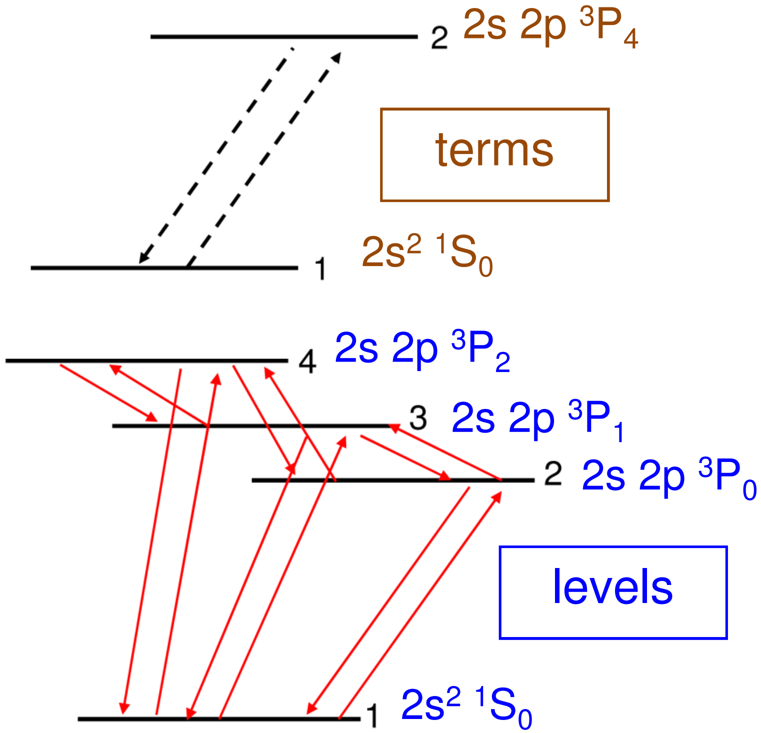
In practice, there may be several ion collider species and so:

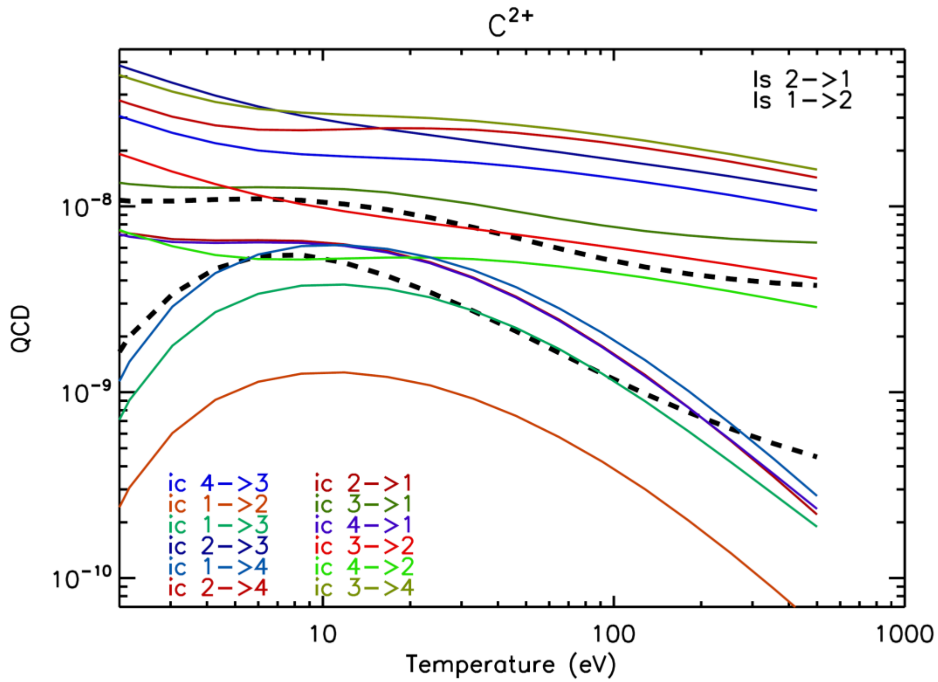
$$Q_{CD,\sigma\to\rho}^{total} \simeq Q_{CD,\sigma\to\rho}^{(e)} + \left(\sum_{ion} N_{ion} q_{\sigma\to\rho}^{ion} \right) / N_e$$

Ion impact rates $q_{\sigma\to\rho}^{ion}$ for different colliders are archived in the ***adf06*** data files.

Ion impact: term and level resolved Q_{CD} coefficients

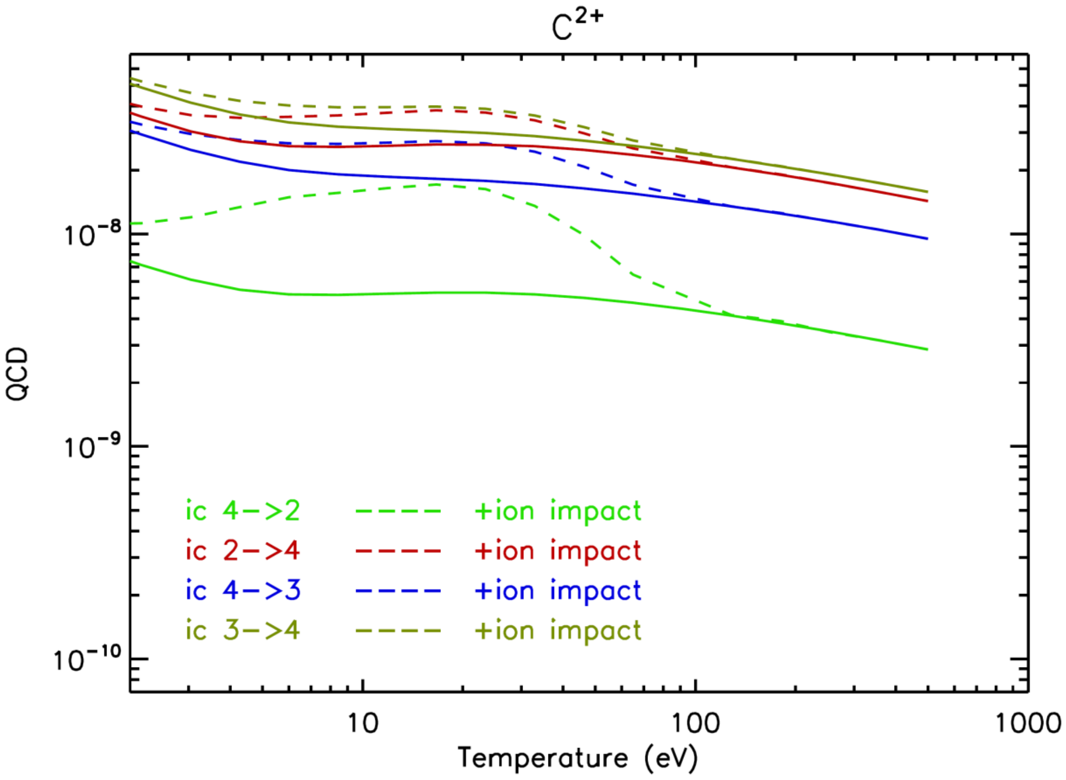
Be-like Carbon example

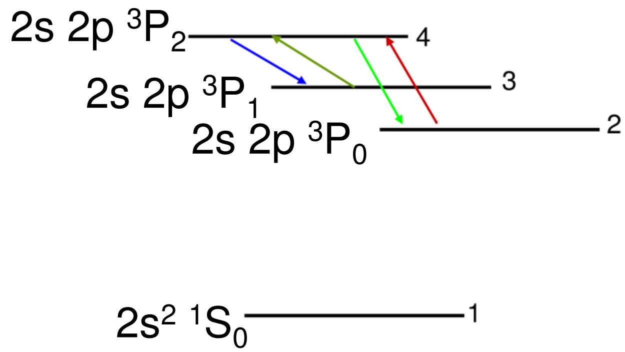




Ion impact: contribution on Q_{CD}

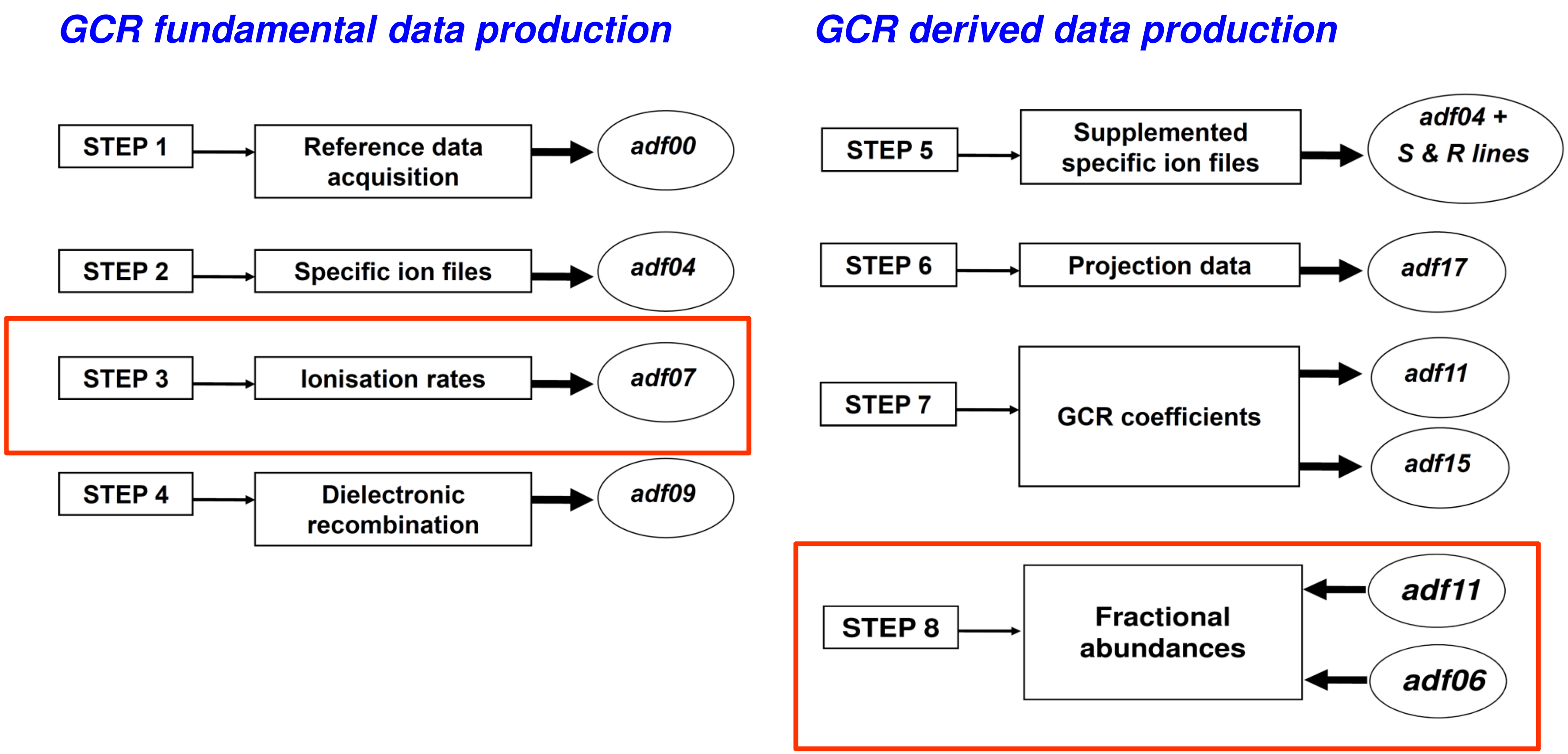
Only levels within the fine structure are affected significantly by ion impact.





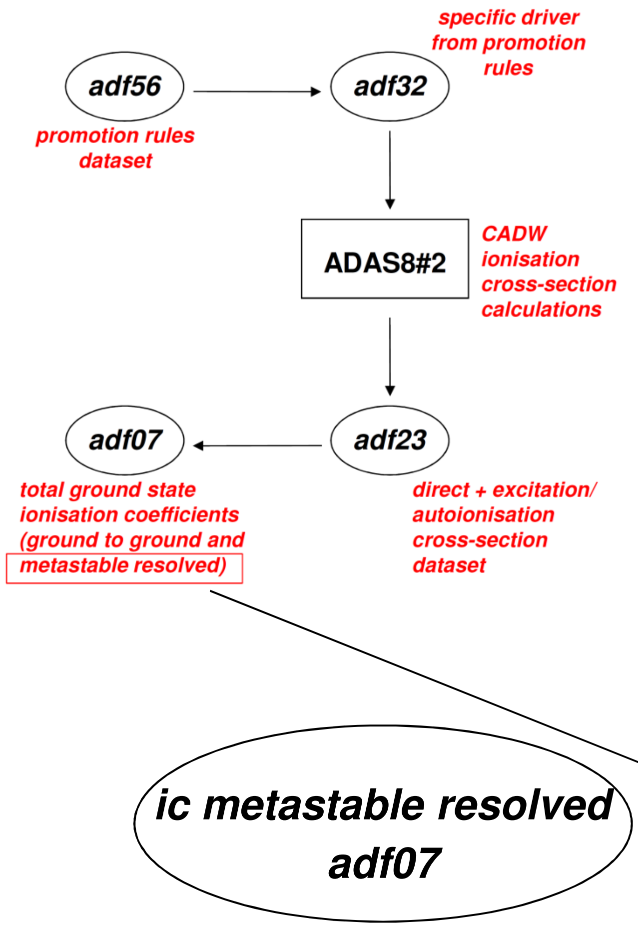
The GCR picture

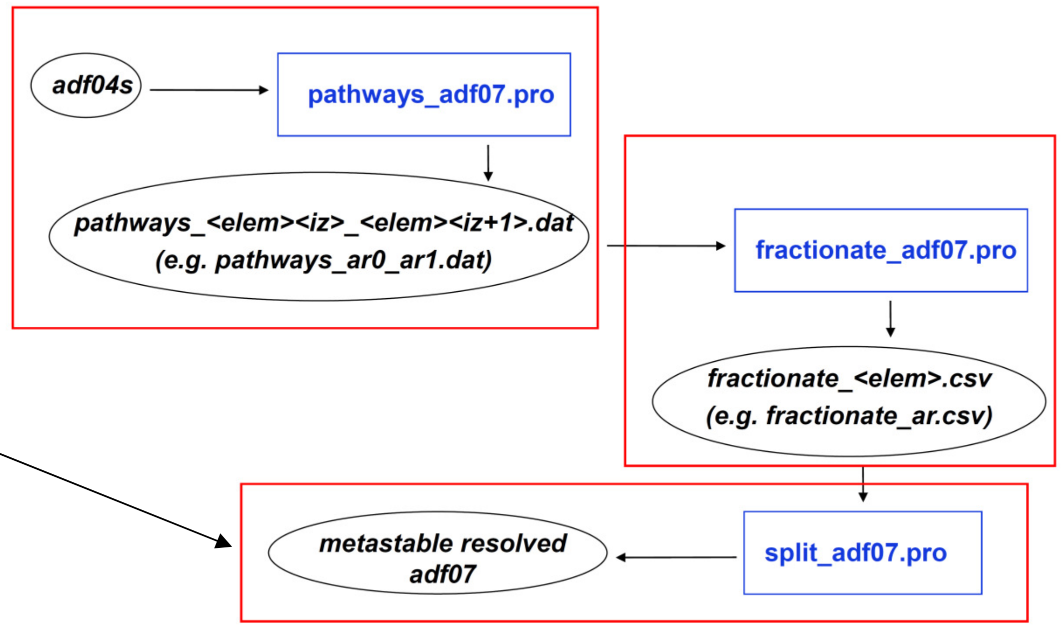
The GCR approach needs to be reformulated in terms of *ic* resolution.



Step 3 – Ionisation rates and *ic* fractionation

The need of ionisation resolved into ground and metastable terms has been addressed using the semi-empirical formula of Burgess & Chidichimo (1983) and adjusted to the CADW calculations. For *ic* GCR, the fractionation needs to be extended to ground and metastable levels.





Step 8 – Fractional abundances and ion impact

Issue

Different colliders can contribute to the total metastable cross-coupling coefficient in different plasmas so

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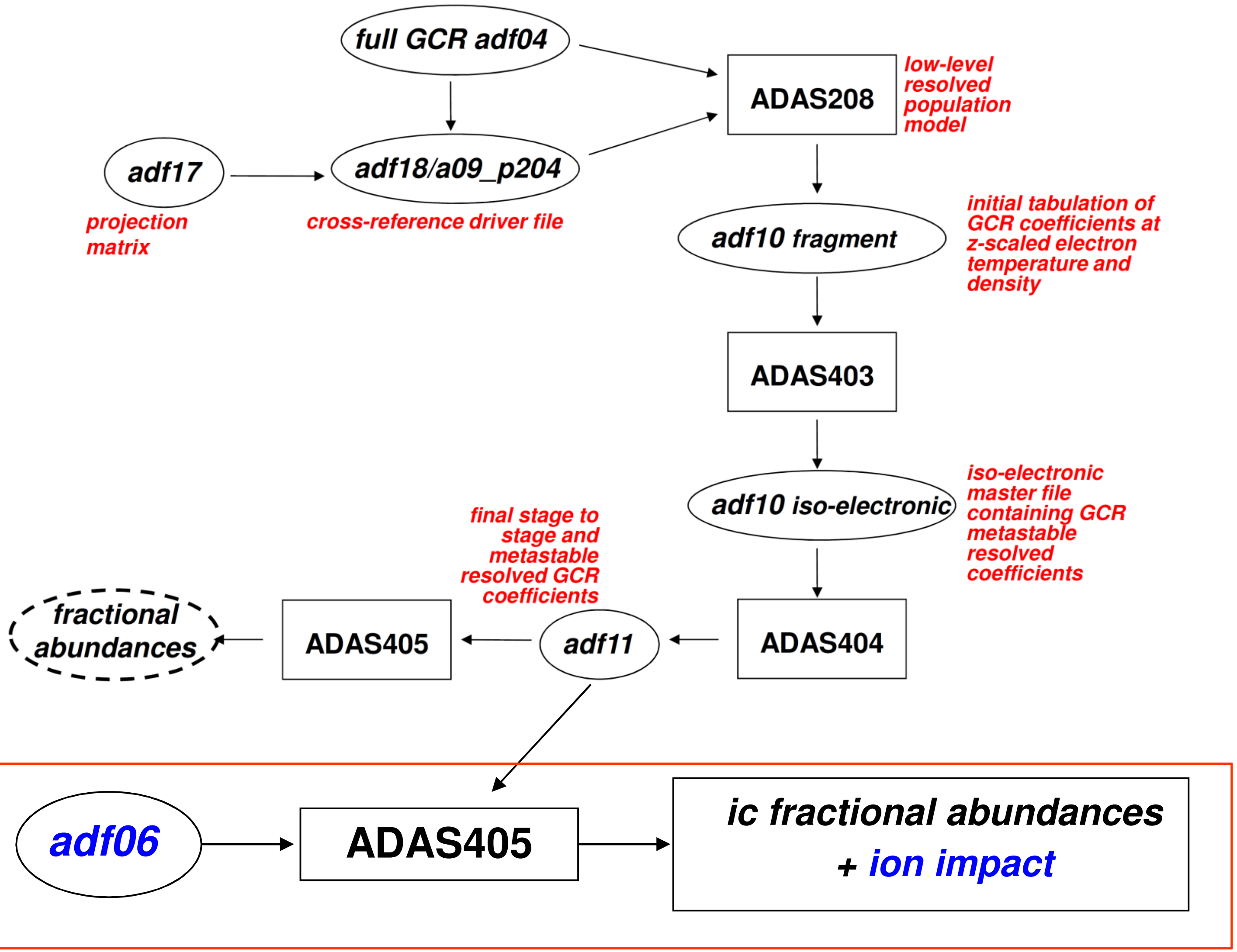
Q_{CD} with ion impact is not suitable for archiving in central ADAS

Method

Since the alteration due to ion impact is incorporated as an additive term in the Q_{CD} coefficient only, it is convenient and efficient to include its effect in the coefficient *on the fly* when establishing the ionisation state.

Step 8 – Ion impact and inclusion in *ic* GCR



Conclusions and future developments

- Finalising *ic* GCR

  - State selective ionisation (fractionation and *adf07* level resolved)

  - State selective recombination (*adf48*, *adf09*)

  - Projection

- Use a mixed resolution *adf11*

  - Bundle *ic* → *ls* → stage

  - Superstages approach (ADAS416): focus on the key spectroscopic stages

- Enabling a transient ionisation modelling

  - ADAS406 with *ic* GCR coefficients + ion impact