Updating of ionisation data for ionisation balance evaluations of atoms and ions for the elements hydrogen to germanium

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Recombination is not considered since a review has been recently published
(Brians et al. AphJS 167 (2006) 343)

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complete data sets (including both ionisation and recombination) are proposed and can be made available

1 ‘reference’ paper for the updating: Mazzotta et al A&AS 133 (1998) 403

other papers to be mentioned in this talk:

2 Arnaud and Raymond AphJ 398 (1992) 394
3 Arnaud and Rothenflug A&AS 60 (1985) 425
4 Dere A&A 466 (2007) 771
5 Mattioli et al JPhysB 39 (2006) 4457
6 Pindzola et al Phys. Scripta T37 (1991) 35

2 updating paper for Fe only, included in 1
3 ‘reference’ updating paper in the Eighties
4 same title as our paper, giving scaled ionisation rates obtained with different fits
5 ‘complete’ updating for Kr + Mo
6 Ni ionisation (not considered in 1)

Experimental cross sections, along with specific theoretical calculations when experimental data are missing, are fitted as functions of the electron energy, and from these fits ionisation rate coefficients can be evaluated.

It has been possible to take into account all elements from H to Ge but not all charge states of every element.

Since the purpose of the paper is to update the ionisation data evaluated and proposed in paper 1, it has to be discussed if modifications are needed for the ions not considered.

Fitting formulae for electron ionisation

Formula (proposed by Younger) for direct ionisation used for smooth σ (E) curves

$$\sigma(E) = \frac{1}{uI^2}\left[A(1-1/u) + B(1-1/u)^2 + C\,Ln(u) + D\,Ln(u)/u\right]$$

u=E/I ratio between the electron energy E and the ionisation potential I

Formula (proposed by Arnaud-Raymond) used in presence of ISEA edges

$$\sigma_{EA}(u) = \frac{1}{uI_{EA}}\left[A + B(1-1/u) + C(1-1/u^2) + D(1-1/u^3) + E(1-1/u^4) + F\,Ln(u)\right]$$

u=E/IEA ratio between E and the ISEA ionisation threshold IEA taken at ‘bump’ edge

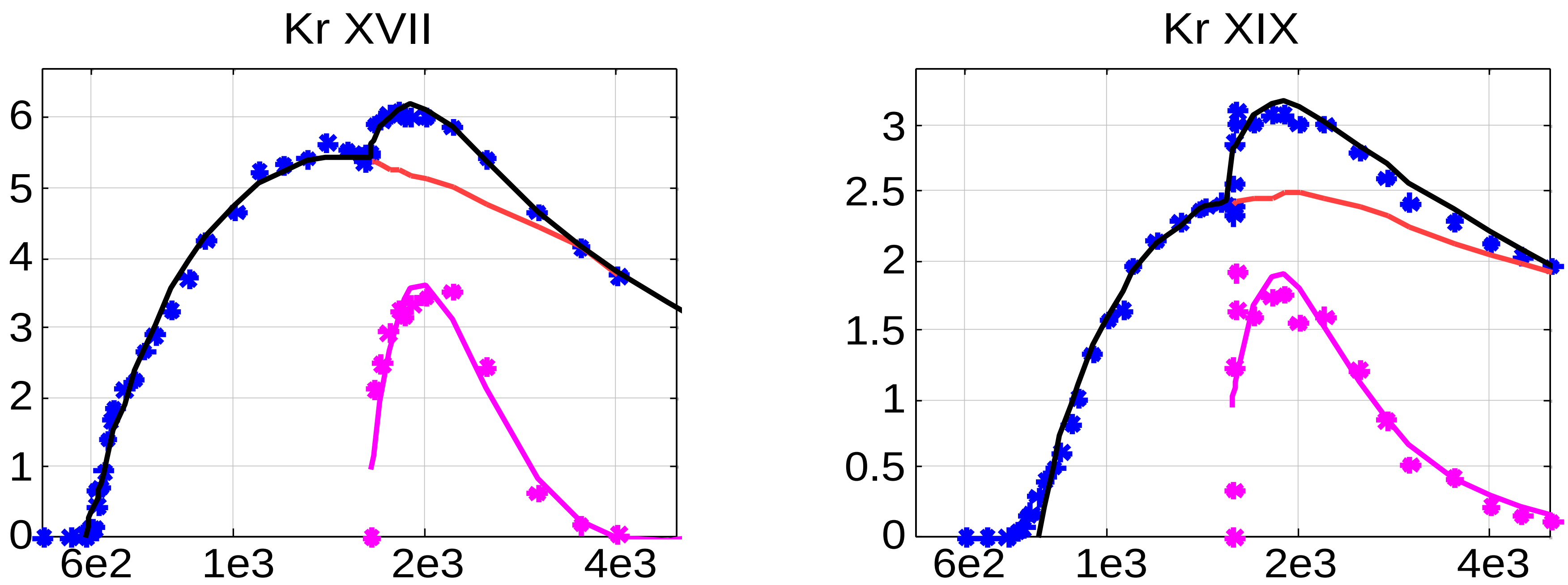
I and IEA are not fitting parameters

Both curves can integrated analytically over a Maxwellian electron distribution

Experimental ionisation data are considered, even when the presence of populated metastable levels (related to the electron density inside the source) is reported in the ion beams involved in the cross-section data measurements
(this is contrary to paper 4, where theoretical calculations, based on the Gu's flexible atomic code (FAC), were preferred)
We deem such a procedure acceptable when the proposed rates have to be included in codes that simulate the impurity behavior in magnetic-confinement fusion devices, i.e., when radial transport is added to ionisation and recombination to predict spatially resolved charge-state distributions.

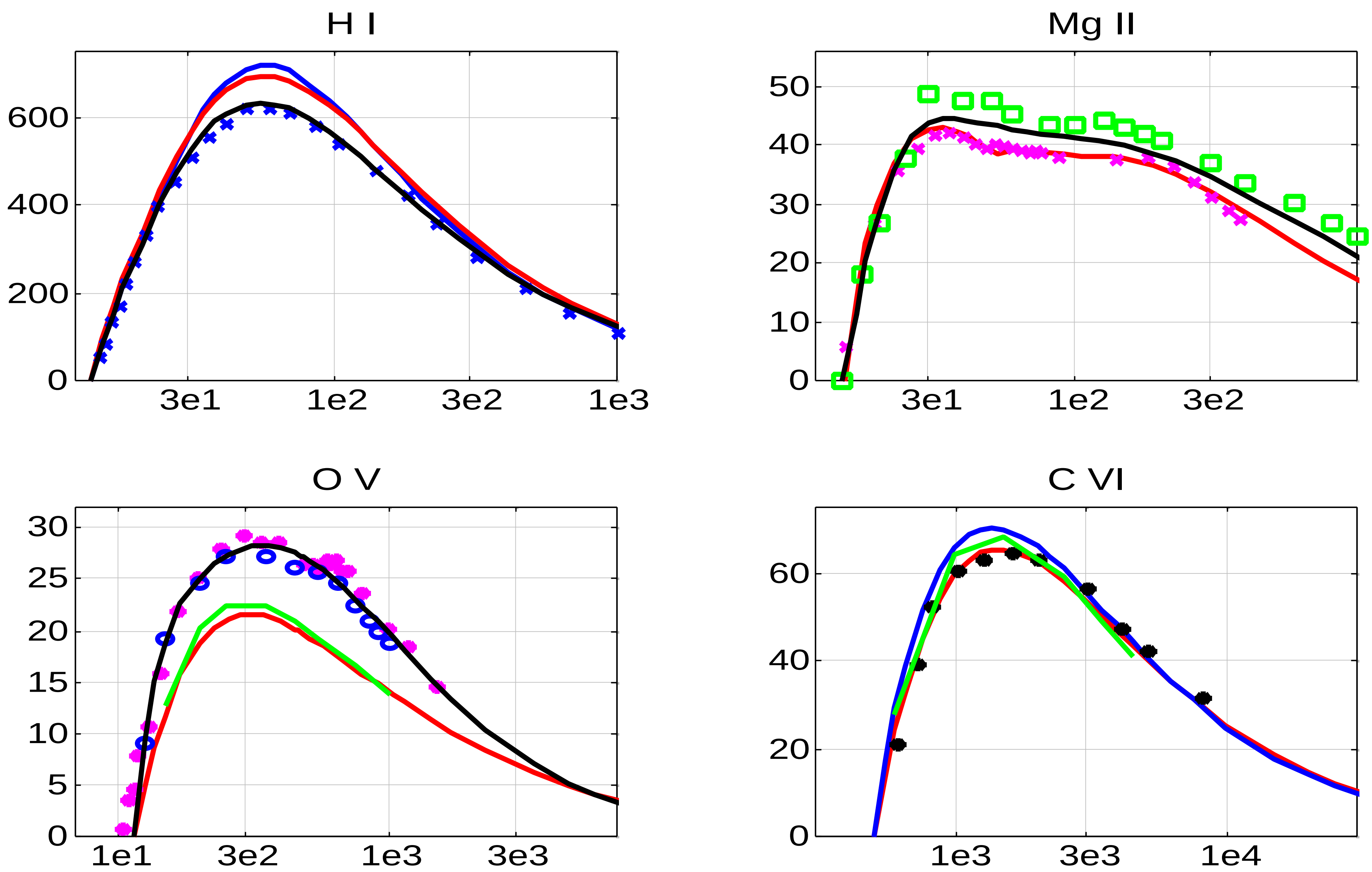
On the other hand, for astrophysical plasmas the contributions of metastable levels to the experimental data may represent a serious problem since, generally, the values of the electron densities that are involved are much lower than those in the ion sources.
From critical investigation it has been found that the presence of metastables does not significantly modify the rates of most of the ions apart from a dozen.

To show an ISEA fitting a slide from paper 5 is reproduced.
Then two slides show how it has been proceeded in the fittings
(shown by the black curves, whereas the red ones are from paper 1)

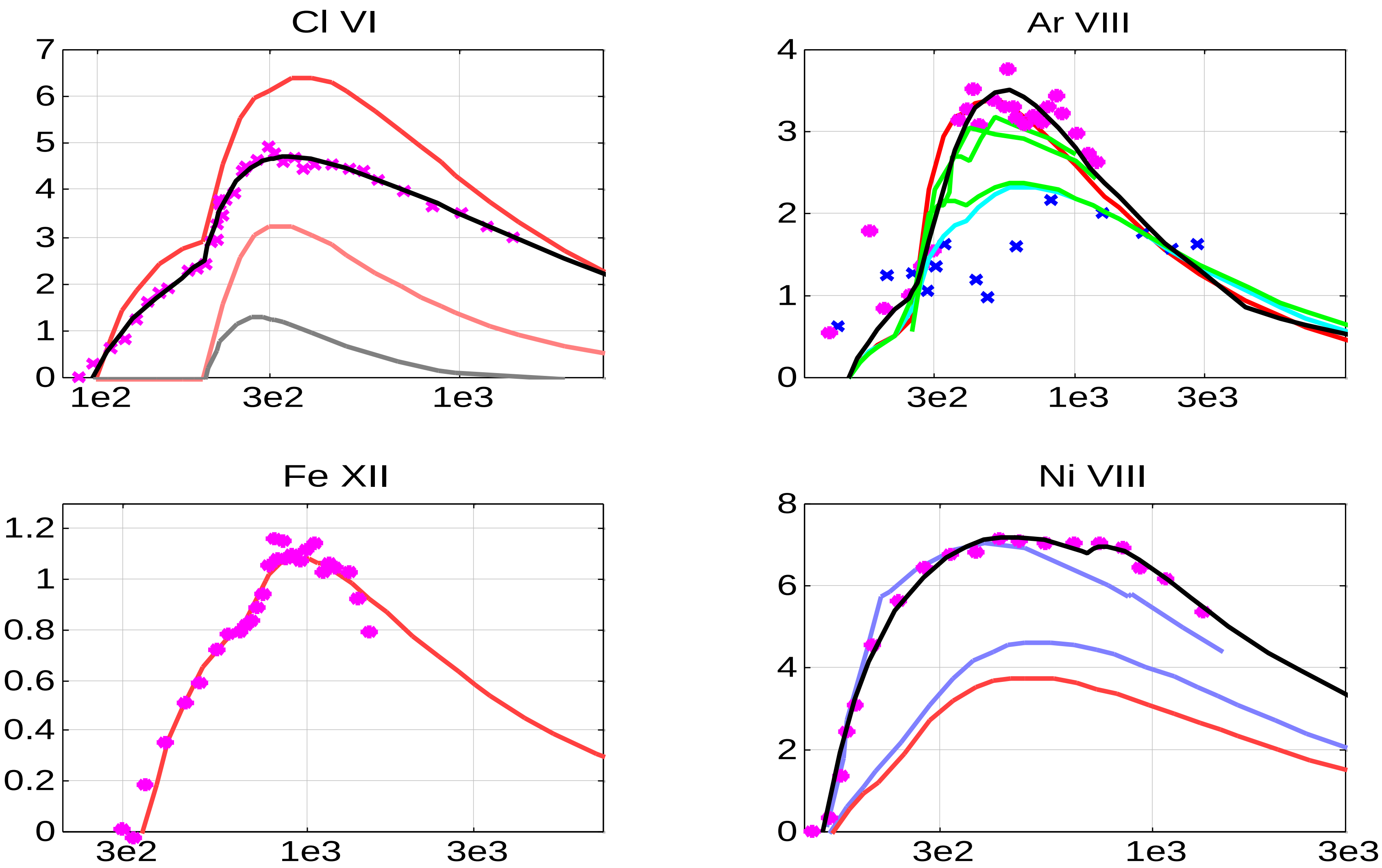


Kr XVII + XIX σ **(E),** σ_{DI}**(E) extr,** σ_{EA}**(E)**

(units 1e-19 cm^2, eV)
blue stars Louvain experimental points; red dashed DI extrapolated
magenta curves ISEA expanded Kr XVII *4 + XIX *3



σ_{ion} **f (E)** k proposed fits, r Mazzotta
other curves theory, various symbols experiment



σ_{ion} **f (E)** k proposed fits, r Mazzotta

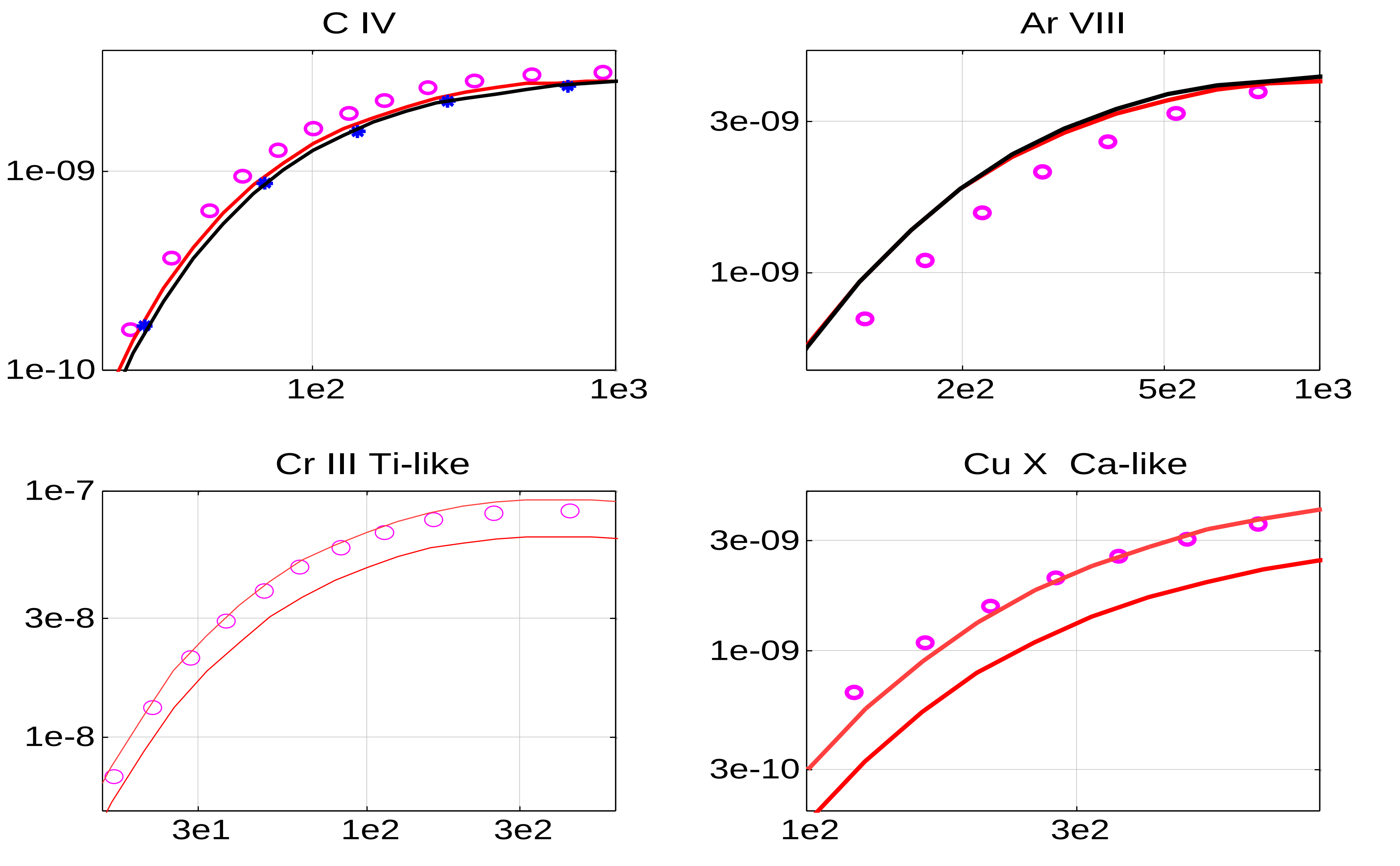
stars + crosses experiment, other curves theory

As already said, the purpose being to update the ionisation data evaluated and proposed in paper 1, it has to be discussed if modifications are needed for the ions not fitted.

For highly ionized ions starting from the Ne-like iso-electronic sequence corrections don't appear necessary. On the other hand, except for Fe, for slightly ionized ions, specifically below the S-like iso-electronic sequence, the data proposed in paper 1 often underestimate the total ionisation cross section, since only direct ionisation channels have been considered and indirect processes have been neglected.

ISEA was considered in paper 1 starting from the S-like iso-electronic sequence following the formulae proposed in paper 3

Multiplicative correction coefficients of the rates of paper 1 are given to agree with the tabulated rates of paper 4. In the next slide the latter are given by the magenta circles.



Ionisation rates Sion (Te)
k proposed fits, mo Dere, r Mazzotta
r dashed proposed correction, b* ORNL database

RR + DR recombination have been included in the complete data set

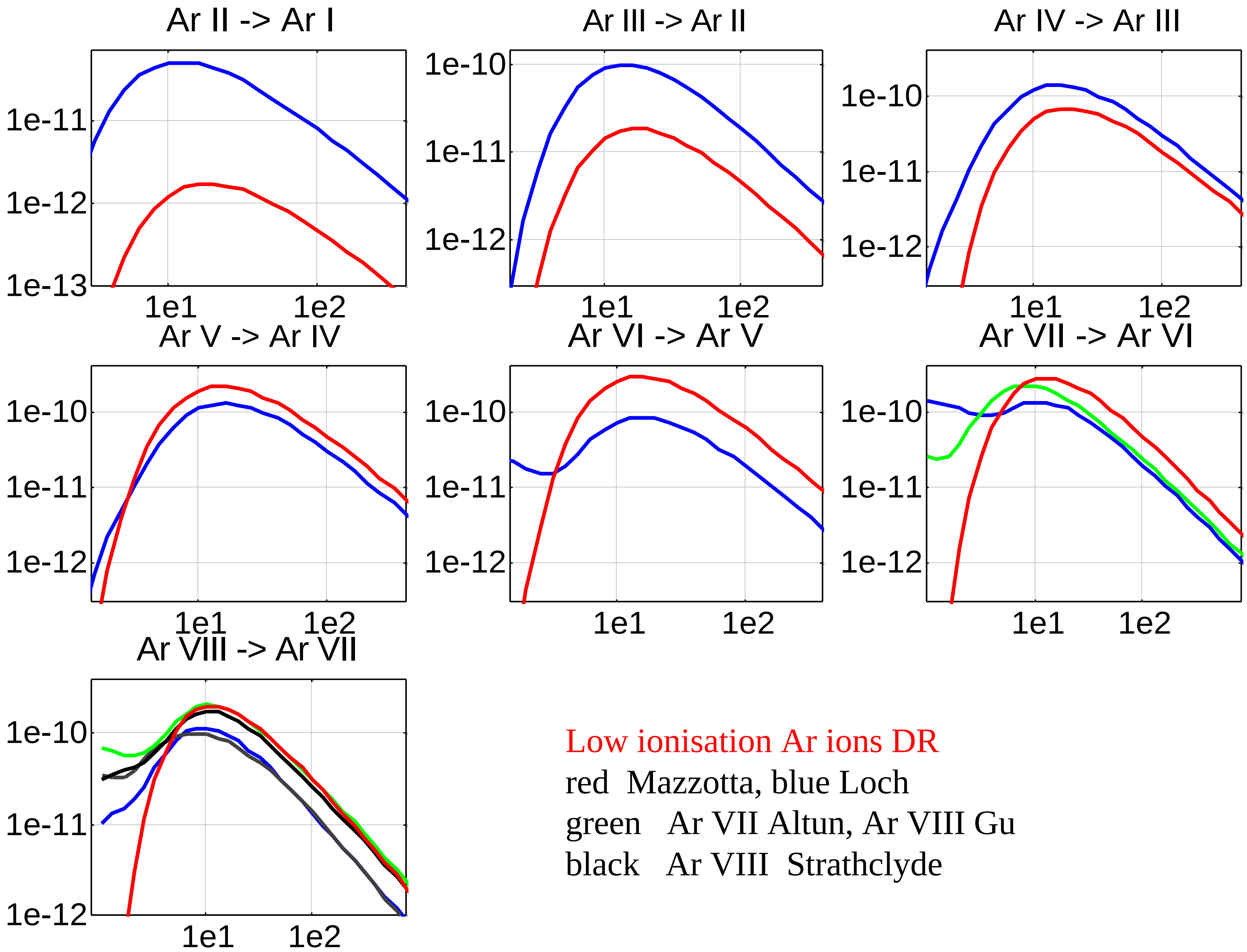
In their review of recombination data Bryans et al. propose to modify the data previously assessed in paper 1 only down to recombining Na-like ions and to follow the Strathclyde coordinated programme.
There not only the T_e range of collisionally ionised plasmas is considered (i.e., that of MCF devices), but calculations also extend down to the low-T_e astrophysical photoionised plasmas.
The tabulated coefficients for the ground levels of the up-dated fits C-20051227 and C-20060311 are considered, respectively, for RR and DR.

For less ionised isoelectronic sequences Bryans et al claim that there are no new ‘reliable’ recombination data and that those assessed in paper 1 should be kept (in spite of the general use of the Burgess-Merts BM formula, which is known to underestimate the DR rates at low T_e).
After the publication of the Brians paper a few DR and/or RR calculations have been published (Badnell down to recombining Ar-like Fe ions, Altun for recombining Mg-like ions and Loch for low ionisation Ar ions).

From our review of recombination data we reached the same conclusions as Brians, but we found a few other ions for which recombination data different from paper 1 have been proposed.

We propose these data, even if, according to the Brians' criteria, they are not 'reliable' since based on 'old fashioned' calculations.

But, given the way the values of f and Eex (to be included in the BM formula) have been chosen for low ionisation degree ions, we believe that specific calculations are in any case better (as justified for Ar ions in the next slide)



Low ionisation Ar ions DR

red Mazzotta, blue Loch

green Ar VII Altun, Ar VIII Gu

black Ar VIII Strathclyde