Lifting the Heavy Species Baseline: Ionisation

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Major Heavy-Species Processes

Structure calculations:		**(ADAS 8#4/8#1, now released)**
Electron impact-ionisation:		**(ADAS 8#4, now released)**
Charge-Exchange:		**(ADAS314/315, earlier release)**
Electron impact-excitation:		**(ADAS 8#2, now released)**
Recombination:	COMING SOON	**(work in progress)**

Existing methods in ADAS (case A)

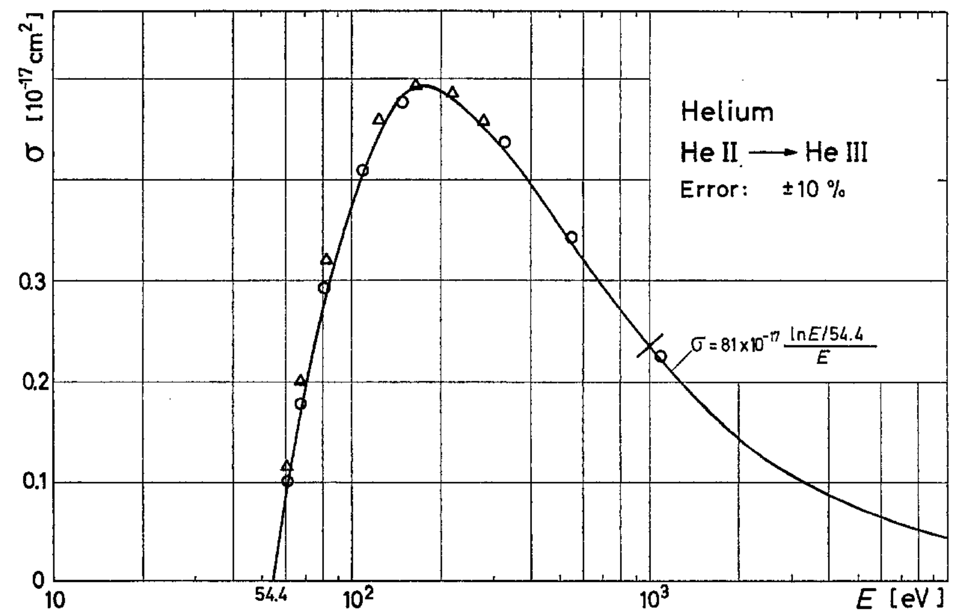
Case A: Lotz formula (1967)

No. equiv. electrons

Ionisation potential of shell i

$$\sigma(E) = \sum_{i=1}^{n} a_i \xi_i \frac{\ln(E/I_i)}{E\, I_i} \left\{1 - b_i \exp\left[-c_i\left(E/I_i - 1\right)\right]\right\} cm^2$$

Constants from fits
to experimental data



From Lotz, 1967

Existing methods in ADAS (case A)

Case A: Lotz formula (1967)

Based on comparison with available experimental data: neutral and singly ionised ions, Z ≤ 19. For +4 or more ionised, set b=0, a=const

$$\boxed{\sigma(E)=\sum_{i=1}^{n} a_i \xi_i \frac{\ln(E/I_i)}{E\, I_i}\left\{1-\cancel{b_i \exp\left[-c_i\left(E/I_i-1\right)\right]}\right\} cm^2}$$

$$\Downarrow$$

$$\boxed{\sigma(E)=4.5\times10^{-14}\sum_{i=1}^{n}\xi_i\frac{\ln(E/I_i)}{E\, I_i}cm^2}$$

Existing methods in ADAS (case B)

Case B: Burgess and Chidichimo (1983)

$$\boxed{\sigma(E) = C \sum_{i=1}^{n} \xi_i \frac{\ln(E/I_i)}{E I_i} W(E/I_i) cm^2}$$

No. equiv. elec now varied to account for E-A

Threshold parameter

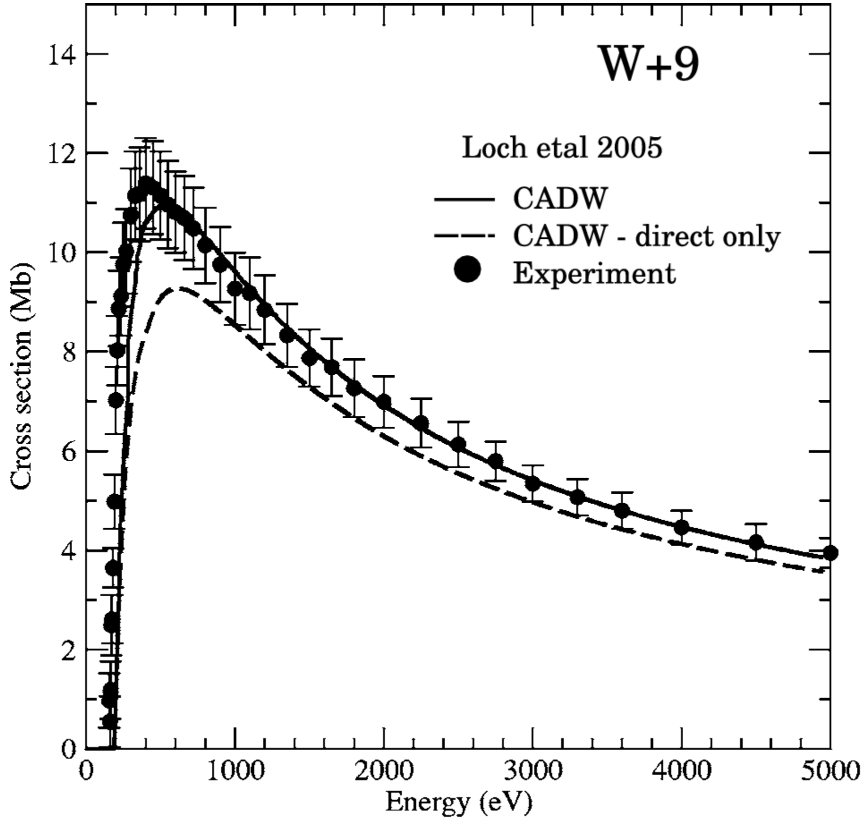
Values of constants again found from comparison with experimental data (up to Ar^{+5})

However, argon is a long way from tungsten...

CADW method for heavy species

Configuration Averaged Distorted Wave calculations have been available for some time (Pindzola, Loch).

CADW code explicitly calculates direct and excitation-autoionisation cross sections.



Comparison with experimental data for Ar, Fe, Ni, Kr, W & lots more exist in the literature.

Executive summary: works well, although some problems with neutrals.

Implementation

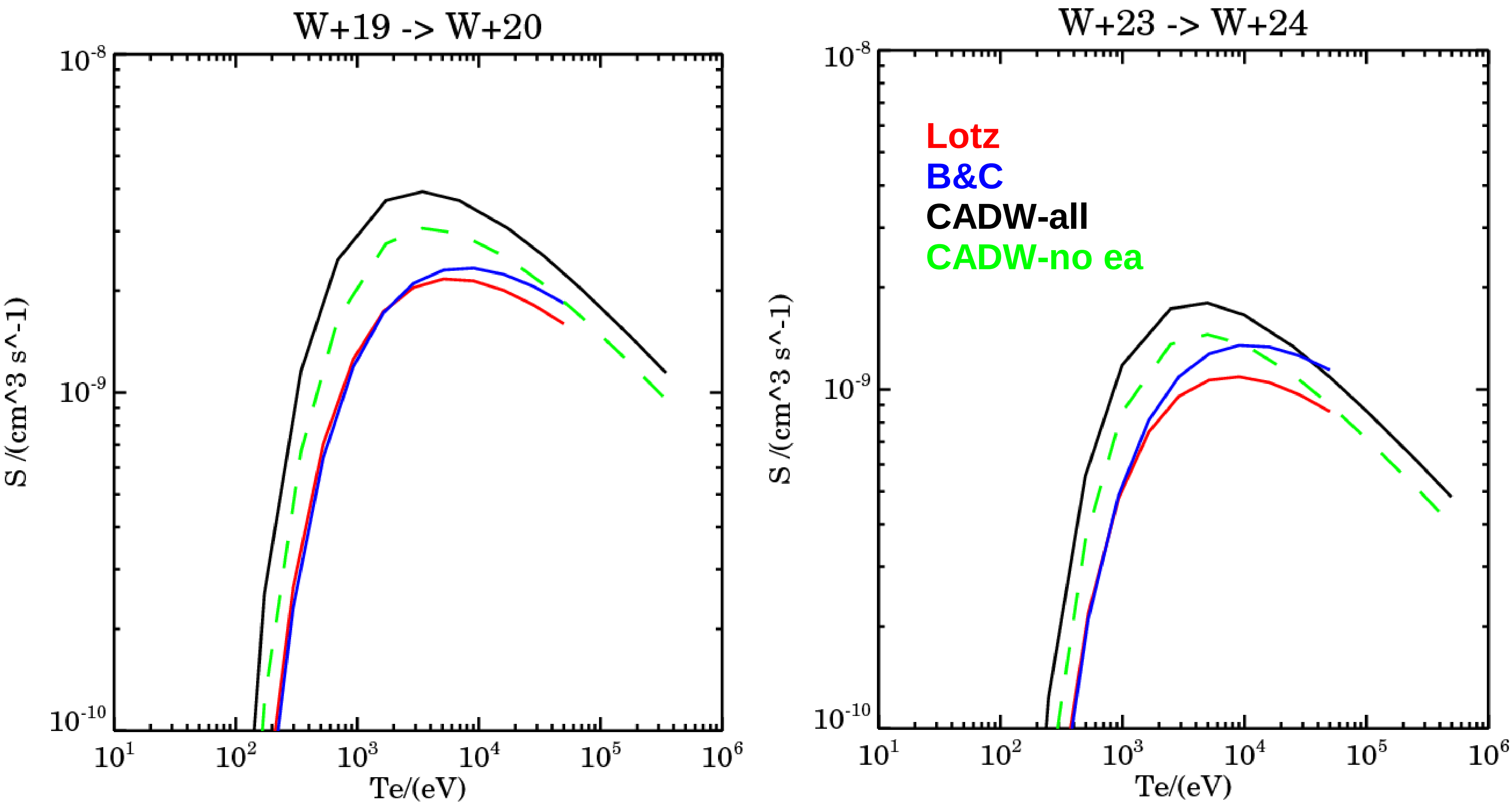
ADF56	List configurations for direct and indirect ionisation
adas8xx_ionis_ promotion_rules.pro	Interpret promotion rules to produce ADF32
ADF32	Driver for adas8#2
adas8#2.pl	Performs CADW calculation
ADF23	State selective electron-impact ionisation coeffts
process_adf23_ adf07.pro	Sum direct and indirect rates
ADF07	Total electron-impact ionisation coeffts.

Codes

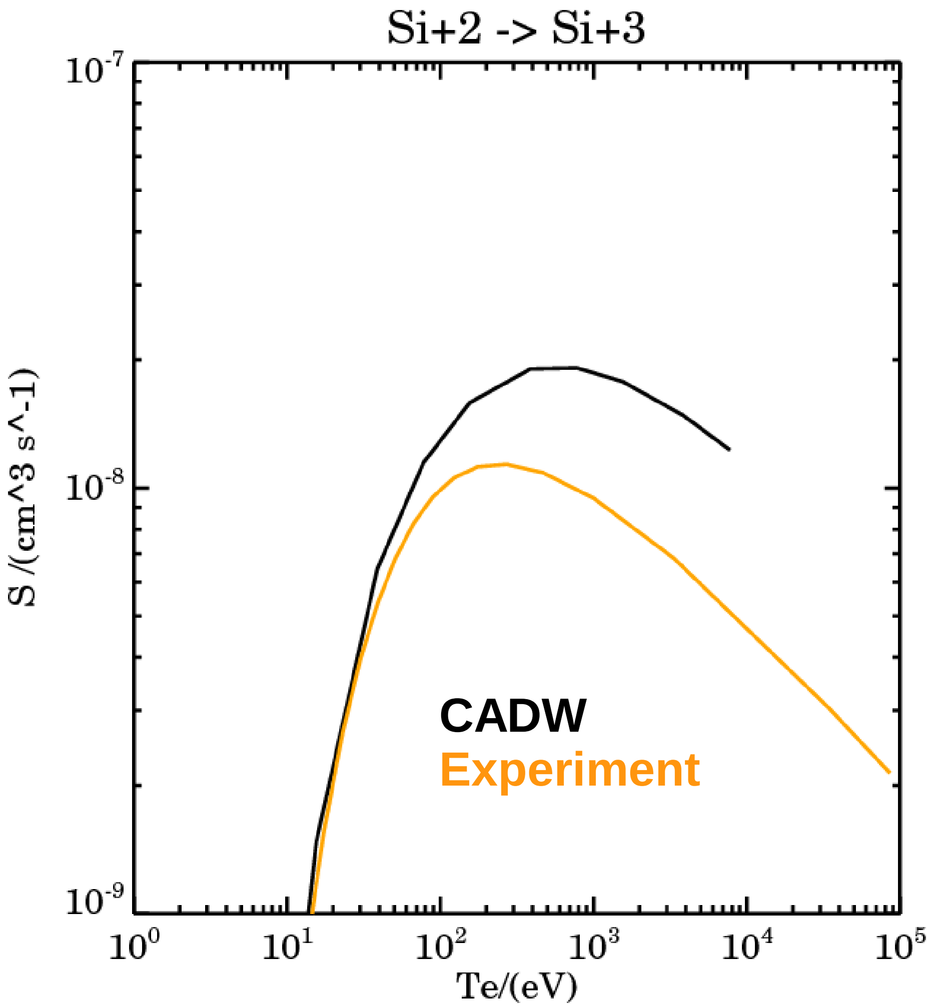
Files

Tested with C, Ne, Si, Ar, Fe, Kr, Xe, W

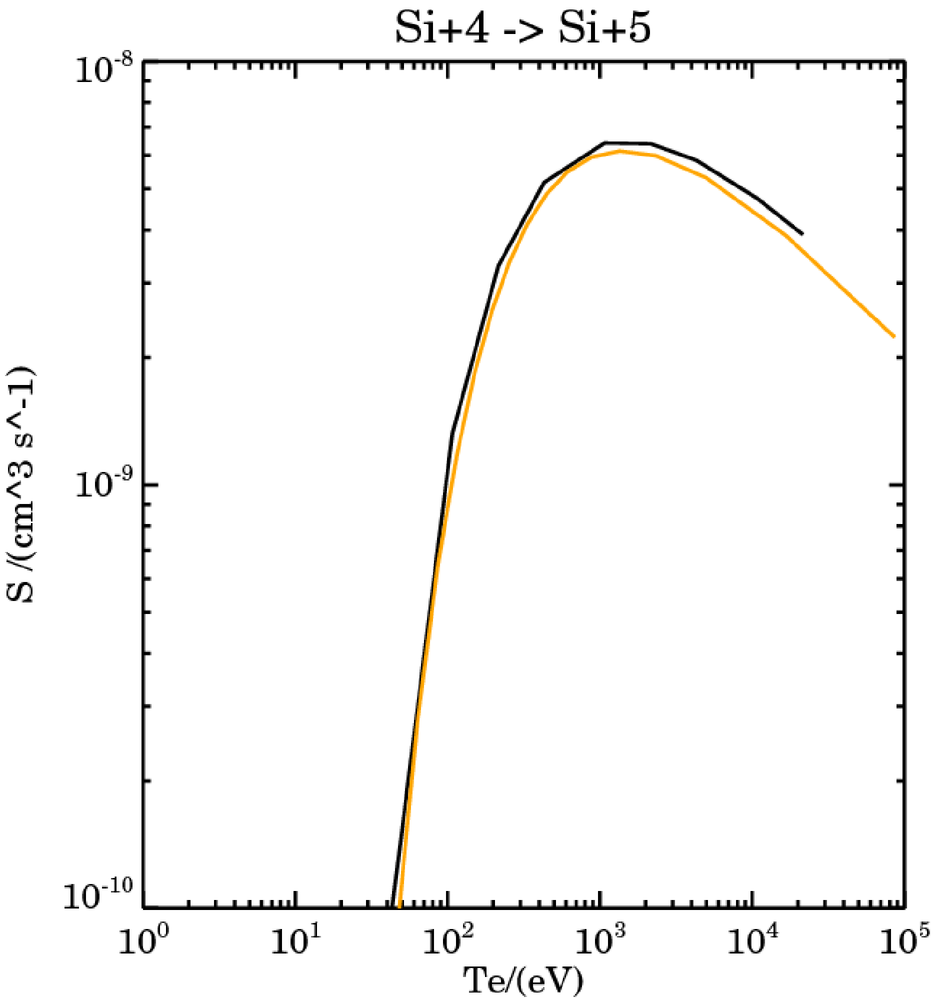
Tungsten Ionisation rates



Comparison with Experimental/FAC data



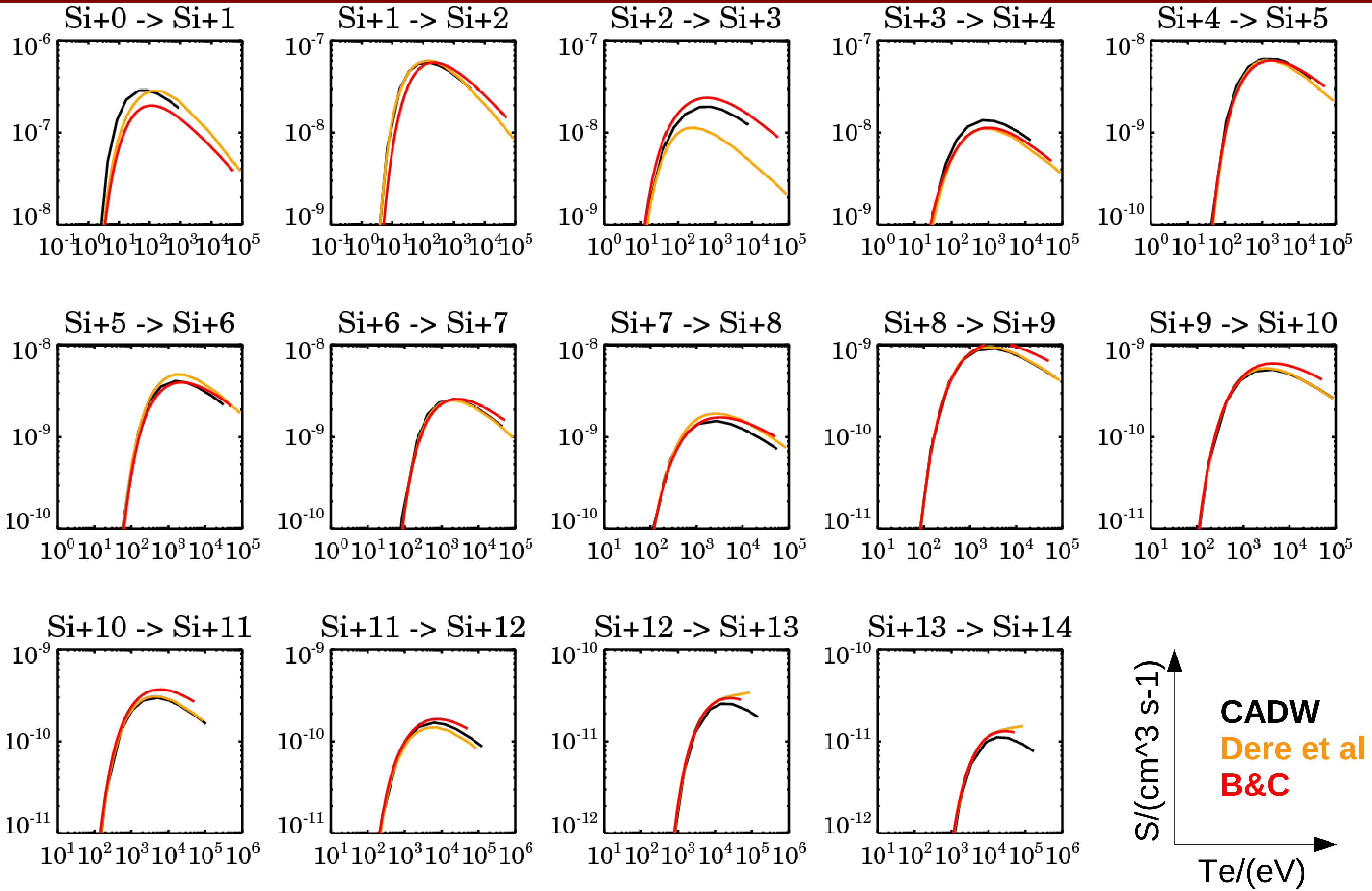
Worst fit



Best fit

Experimental data from Dere et al 2007 (prepared by A. Giunta)

Comparison with Experimental/FAC data



Summary

- CADW calculations of ionisation rates are now fully incorporated into ADAS.

- Modest but important effect on ionisation balances

- Current ADAS release contains both the CADW code and a selection of pre-generated data (ADF23, ADF07) for Ar, Mg, Si and W

- ADAS8#2 can rapidly generate more ions as required (you have the power...)

- Heavy species baseline improvement is all but complete (just add recombination)