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ADAS
Atomic Data and Analysis Structure

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Generalised Collisonal Radiative data for hydrogen

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Abstract: *New GCR data for hydrogen have been added to ADAS with the year identifier 12. The excitation data in the 96 data exhibited a kink at 10eV which is not present with the more up to data data. The PEC, SXB, PLT, SCD coefficients have changed with minor differences in the ACD and PRB. The charge exchange CCD data are unchanged.*

1 A kink in PEC and SXB 96 data

There is a kink in the hydrogen generalized collisional radiative (GCR) coefficients which is most clearly seen in the SXB and PEC data (figure 1). The electron excitation data for the *96* GCR data

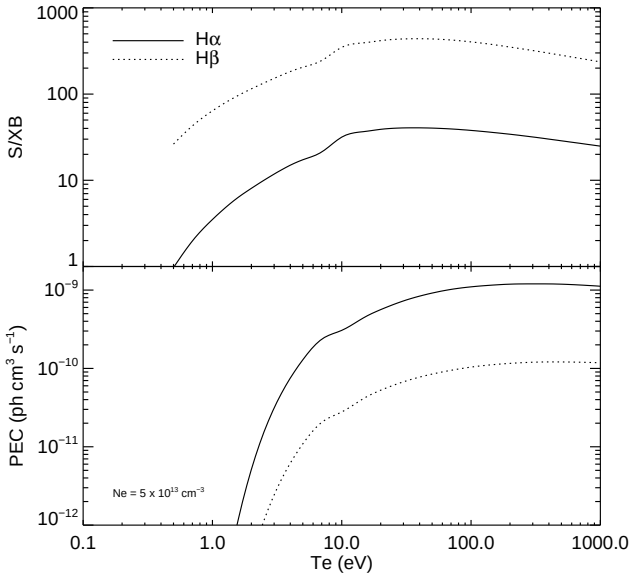

Figure 1: Ionisation per photon and photon emissivity coefficients for hydrogen Balmer-α and Balmer-β. From central ADAS files: `adas/adf13/sxb96#h/sxb96#h_pju#h0.dat` and `adas/adf15/pec96#h/pec96#h_pju#h0.dat`

is stored in two *adf04* files which hold the low temperature effective collision strengths (0.1–10eV) and the high temperature selection (10eV–70keV) separately. However there is a discontinuity at the common temperature point for high lying transitions (figure 2).

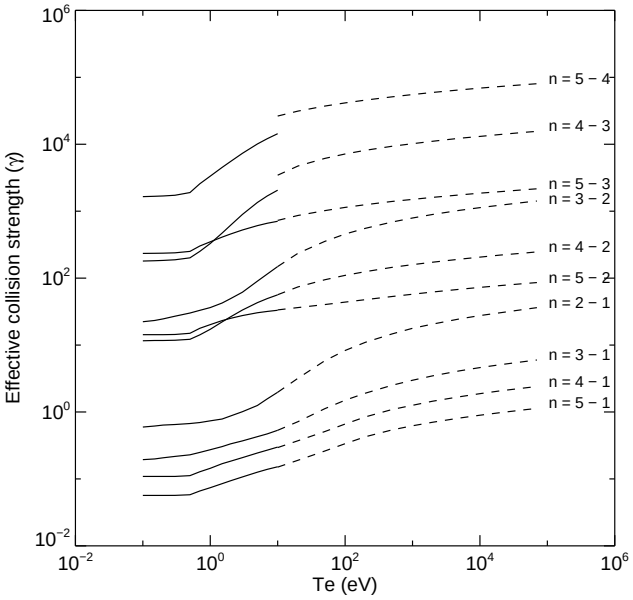

Figure 2: The discontinuity at the cross-over temperature.

The population code extracts data from each *adf04* file depending on temperature and this discrepancy propagates through to the coefficients.

The *adf04* files used in the 96 data are `adas/adf04/copha#h/copha#h_bn#l96h.dat` and `adas/adf04/copha#h/copha#h_bn#h96h.dat`. These have been assembled from LS resolved data, from calculations by Callaway [1, 2] and private data supplied by A Kingston. These precursor data are stored in the central ADAS *adf04* files, `adas/adf04/hlike/hlike_call87h.dat` and `adas/adf04/hlike/hlike_aek89h.dat`. A further supplementation with later data from Callaway [3] completed the primary data. The final assembly was made by Harvey Anderson (the *ha* in the file names) in Burgess-Tully space [4] in a spreadsheet. The resulting files were then bundled to n-resolution for the *copha#h* files.

The low and high temperature files were assessed and generated *separately* — hence a check on the continuity in temperature was overlooked.

Note that the discontinuity is only present among transitions with $n = 3-5$. The source data for these is not as secure as the Callaway data, which is only for transition among the $n = 1-3$ levels. In fact, the effective collision strengths are from extrapolations of data supplied by Kingston.

2 Better *adf04* data

An R-matrix with pseudo-states calculation, for all levels between $n = 1-5$, is available [5, 6] and has the correct asymptotic behaviour at high temperatures. This is in central ADAS as `adas/adf04/hlike/hlike_ha00#h0ls.dat`. The n-resolved dataset, with NIST energy levels and S and R lines, is `adas/adf04/adas#1/ha00_n#h0.dat`.

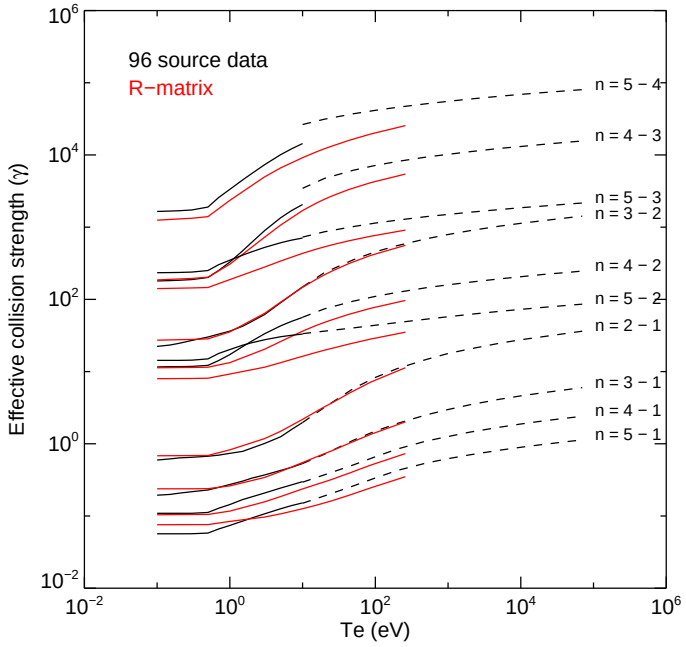

Figure 3: The 96 excitation data, with discontinuity in temperature, and the newer R-matrix effective collision strengths (red).

Transitions from ground are not greatly changed but there are significant difference among the higher levels. However the influence on the spectral emission, and other GCR coefficients, depends on both this primary difference but also on indirect effects arising from the population calculation.

3 Changes in *adf11*, *adf13* and *adf15* coefficients

A new calculation was made with the same ionisation and radiative recombination data as before and the same bundle-n population codes is used. Any differences in the derived GCR coefficients are due solely to the different excitation data.

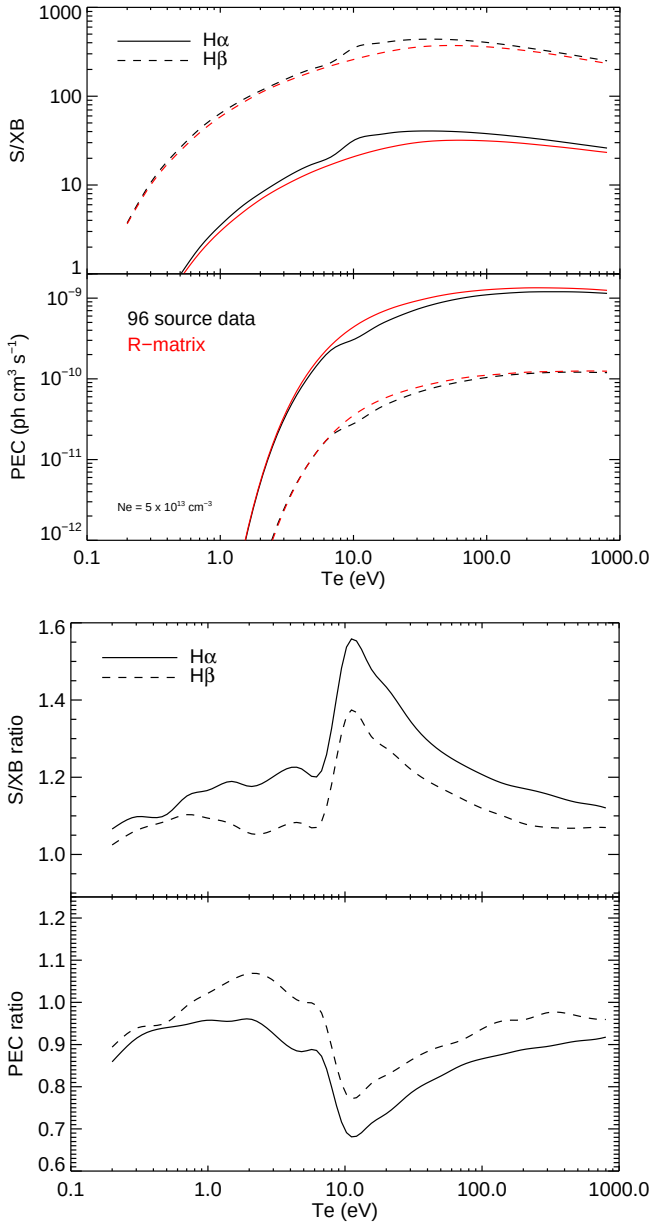

Figure 4: (top) The central (96) data and the new SXB and PEC coefficients. (bottom) The ratio of the old to the new coefficients.

The new coefficients eliminate the discontinuity but show a baseline difference of the order of 10–20%. The difference is exacerbated around the zone of influence of the discontinuity (8–30eV).

The sensitive Hγ/Hα ratio, used to distinguish divertor detachment via the switch from excitation to recombination driven emission, highlights the sensitivity of the change in data. Fig 5 reproduces figure 3 of [7] and shows an improved regularity in the shape of the ratio but the magnitude shows a baseline difference of 30–50%, but this increases to a factor of 2 in the discontinuity region.

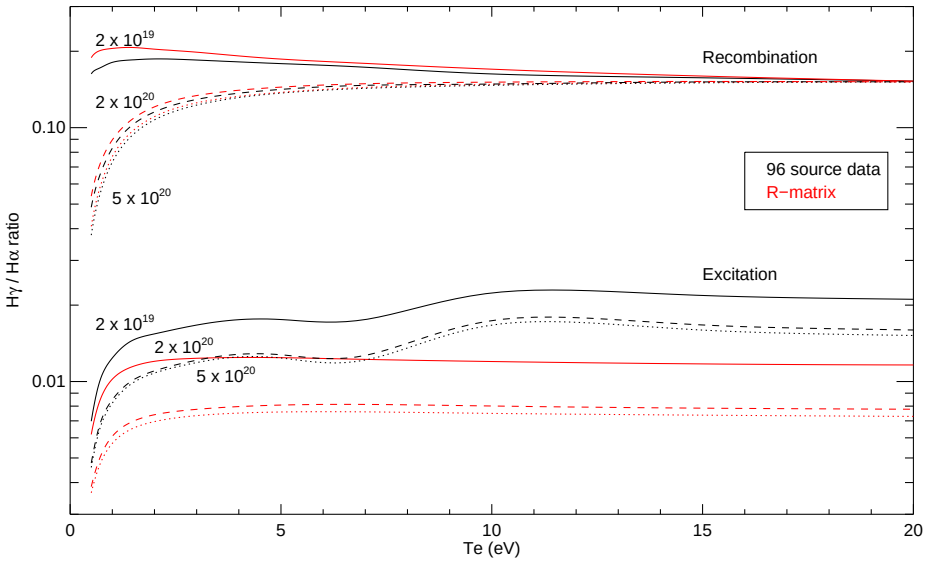

Figure 5: Following figure 3 of [7]. The three lines are for different densities ($2, 20, 50 \times 10^{19} \mathrm{m}^{-3}$).

The recombination PECs are relatively unchanged with the most noticeable difference at low temperature which reflects the modification of the 3-body contribution due to the changed excitation pathways.

The influence of new excitation data will also be evident in the effective source and power coefficients. Figure 6 illustrates the minor change in recombination and the larger modification of the effective ionisation rate. The total line power follows the trend of the ionisation coefficient whereas the continuum power coefficient is mostly unaffected. It is important to note that the change is no more than 10%.

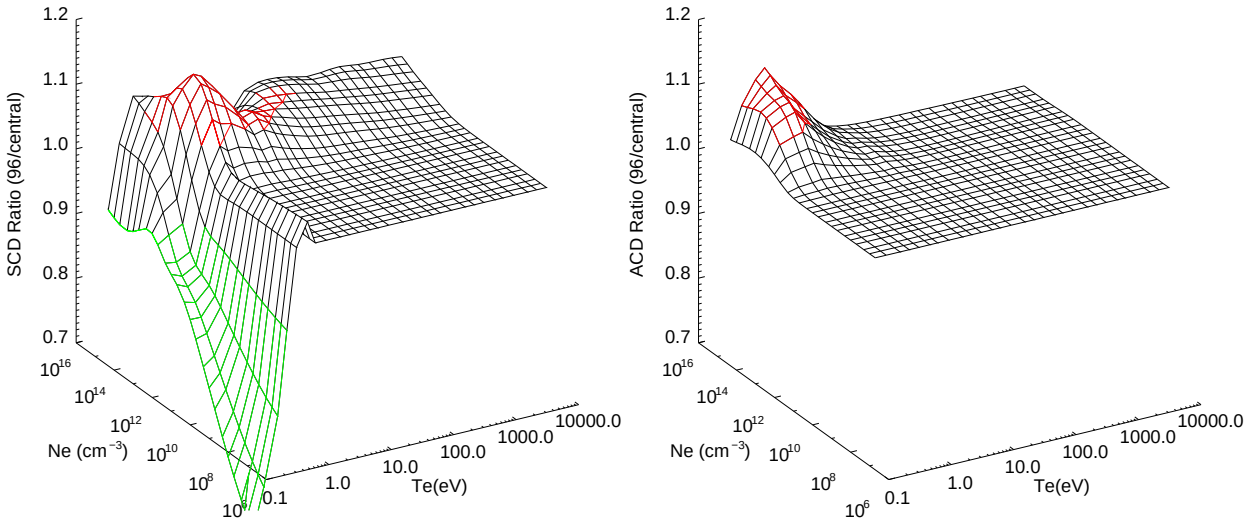

Figure 6: Surface plot of the *ratio* of the old (96) GCR rates to the new data — (left) ionisation and (right) recombination coefficients. Green indicates ratios below 95% and red ratios above 105%.

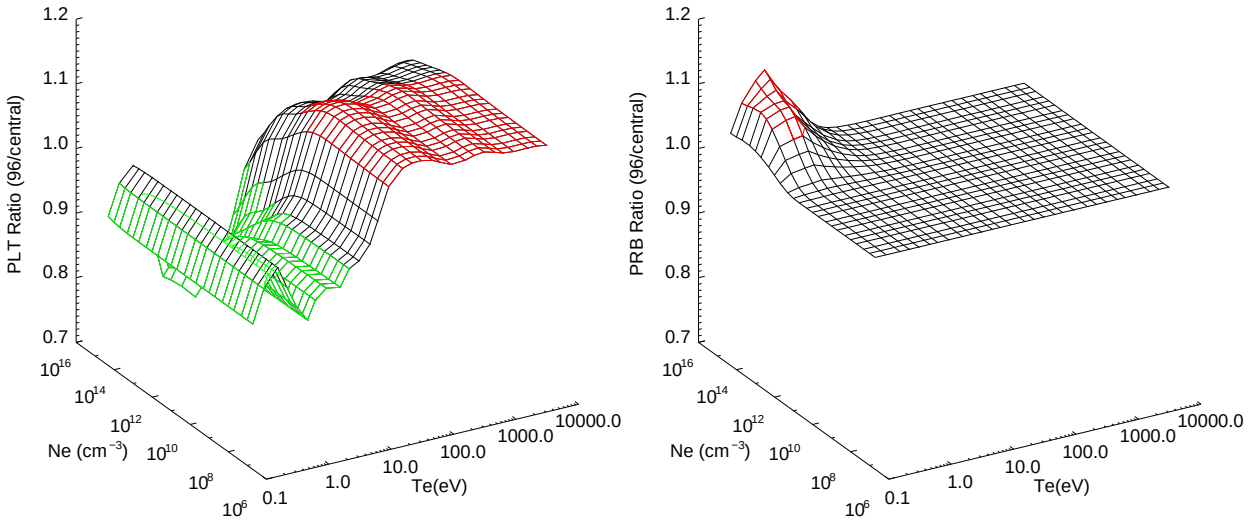

Figure 7: Surface plot of the *ratio* of the old (96) GCR rates to the new data — (left) total line power rates and (right) the continuum power (radiative recombination + bremsstrahlung). Green indicates ratios below 95% and red ratios above 105%.

The effect on ionisation balance is smaller than the change in the coefficients. Figure 8 shows the equilibrium ionisation balance and the ratio due to the changed ionisation and recombination rates. The largest difference is seen on the falling edge of the H^0 abundance curve. Over the region of maximum abundance the difference is of order 5%.

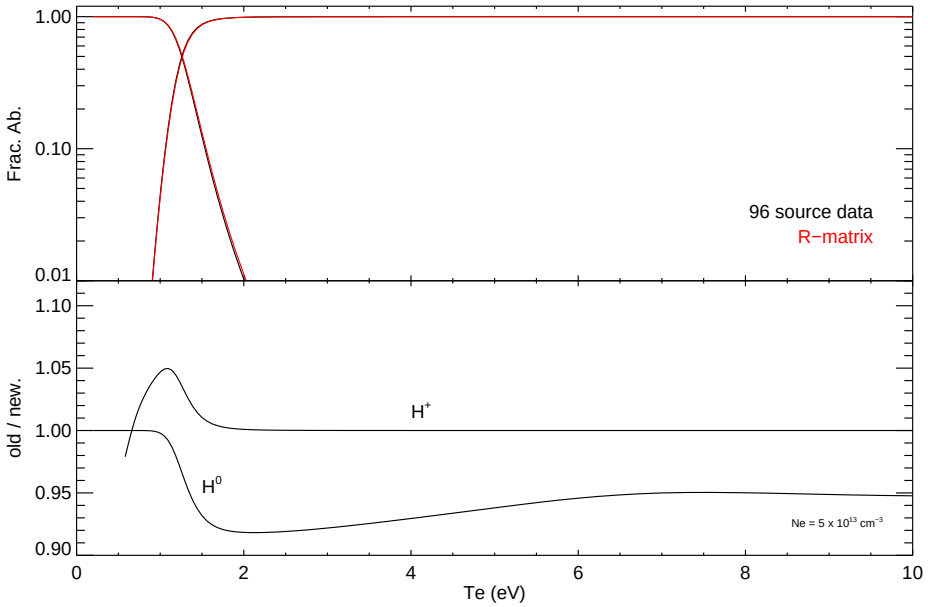

Figure 8: (top) Equilibrium ionisation balance with (bottom) ratio of change for each stage..

4 New GCR data for hydrogen — year 12 datasets

The uneven behaviour of the hydrogen CGR coefficients (*96* data) is the result of incorrect utilization of the excitation data, as a consequence of this being archived in separate low and high temperature *adf04* files. It is possible to reconcile these datasets and make them consistent in their temperature behaviour. This would result in producing new preferred curves with an additional low temperature constraint from the low-Te file.

However it is notable that the discrepancy arises from transitions which were empirical extrapolations due to the unavailability of calculated *ab initio* collision strengths when these files were assembled.

Now there is an up to date, R-matrix with pseudo-states, excitation calculation available for all transitions up to $n = 5$. This eliminates the error. However a ramification is that the new data also changes the other derived coefficients.

There are conflicting concerns for the ADAS database. The existing *96* data is erroneous and should be corrected. However the proper correction, ie using the latest excitation data, rectifies both a mistake and introduces improved fundamental data. The other consideration is that these hydrogen GCR data have been in use for an extended period.

The adopted solution is to supply new *adf11, adf13* and *adf15* coefficients with a new year

number — 12. The existing *96* data will remain unchanged (and incorrect).

The new files are:

- `adas/adf13/sxb12#h/sxb12#h_pju#h0.dat`
- `adas/adf15/pec12#h/pec12#h_pju#h0.dat`
- `adas/adf11/acd12/acd12_h.dat`
- `adas/adf11/scd12/scd12_h.dat`
- `adas/adf11/plt12/plt12_h.dat`
- `adas/adf11/prb12/prb12_h.dat`

A few observations:

1. The SXB and PEC *96* data has *pjr* variants. Since hydrogen has one metastables these are redundant and contain the same data as the metastable-unresolved *pju* file. Therefore no *pjr* version with year *12* has been generated.
2. Furthermore there was no resolved hydrogen (*adf11/xxx96r*) data.
3. There are charge exchange *adf11/ccd96* data for hydrogen, deuterium and tritium. Unlike the impurities these data are *not* produced as part of the GCR workflow. The *96* files remain valid and should be used in conjunction with the new *12* files for ionisation and recombination.

References

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[5] H. Anderson, C. P. Ballance, N. R. Badnell and H. P. Summers. 'An R-matrix with pseudostates approach to the electron-impact excitation of H I for diagnostic applications in fusion plasmas'. J. Phys. B, **33**(6) (2000) 1255–1262. doi:10.1088/0953-4075/33/6/311

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