

Martin O'Mullane

Photon emissivities for ArI and ArII

23 April 2008

This communication has been prepared for discussion within the ADAS and OPEN-ADAS community. It is subject to change without notice. Please contact the authors before referencing it in peer-reviewed literature. © Copyright, The ADAS Project.

Photon emissivities for ArI and ArII

Martin O'Mullane

Dept. Physics, University of Strathclyde

Abstract: *Excitation data for neutral and singly ionised argon is assessed and photon emissivities for observed transitions in PISCES are generated.*

Background

Emission from the neutral and first ionised stages of the noble gases can be used for diagnostic purposes. Photon emissivity coefficients (PEC), which are functions of plasma temperature and density, are calculated with `adas208` [1]. The quality of the calculated PECs depends, primarily, on the quality of the electron driven collision strengths, and to a lesser extent, on the energy levels and transition probabilities. Within ADAS, calculations for the light elements (hydrogen to neon) are in the full GCR picture [2] but for ArI and ArII the collisional-radiative model does not include projection of the influence of very high- n levels on the low level populations (from where the emission arises).

ArI

ArI is an ions with a special, shorthand notation for its energy levels and this Paschen notation is outlined in table 1.

Paschen label	Level	J	Energy cm^{-1}
ground	$3p^6\ ^1S_0$	0	0.0
1s ₅	$4s[3/2]_2\ ^3P_2$	2	93143.8
1s ₄	$4s[3/2]_1\ ^3P_1$	1	93750.6
1s ₃	$4s'[1/2]_0\ ^3P_0$	0	94553.7
1s ₂	$4s'[1/2]_1\ ^1P_1$	1	95399.8
2p ₁₀	$4p[1/2]_1\ ^3S_1$	1	104102.1
2p ₉	$4p[5/2]_3\ ^3D_3$	3	105462.8
2p ₈	$4p[5/2]_2\ ^3D_2$	2	105617.3
2p ₇	$4p[3/2]_1\ ^3D_1$	1	106087.3
2p ₆	$4p[3/2]_2\ ^3P_2$	2	106237.6
2p ₅	$4p[1/2]_0\ ^3P_0$	0	107054.3
2p ₄	$4p'[3/2]_1\ ^1P_1$	1	107131.7
2p ₃	$4p'[3/2]_2\ ^1D_2$	2	107289.7
2p ₂	$4p'[1/2]_1\ ^3P_1$	1	107496.4
2p ₁	$4p'[1/2]_0\ ^1S_0$	0	108722.6

Table 1: Paschen notation of energy levels of ArI. The energy levels are from NIST [3].

A baseline *adf04* dataset of these 16 levels was generated with `adas801` (Cowan code). The excitation data is calculated in the Born approximation. The energy levels were replaced by those of NIST [3]. Excitation data from the ground and the metastable levels, calculated in the distorted wave (DW) approximation [4, 5], supplemented (or replaced) the Born data where available. These data were published as cross sections and were digitised from the figures in the paper. The extracted cross sections were convolved with a Maxwellian distribution with the `h4mxw1.pro` ADAS routine to produce the effective collision strengths. Note that the A-values remain those of Cowan.

Ionisation from the ground state is that of [6] with ionisation from excited levels given by the ECIP approximation [7, 8, 9].

The PECs for the 750.4nm transition for density spanning the collisional mixing regime are shown in figure 1.

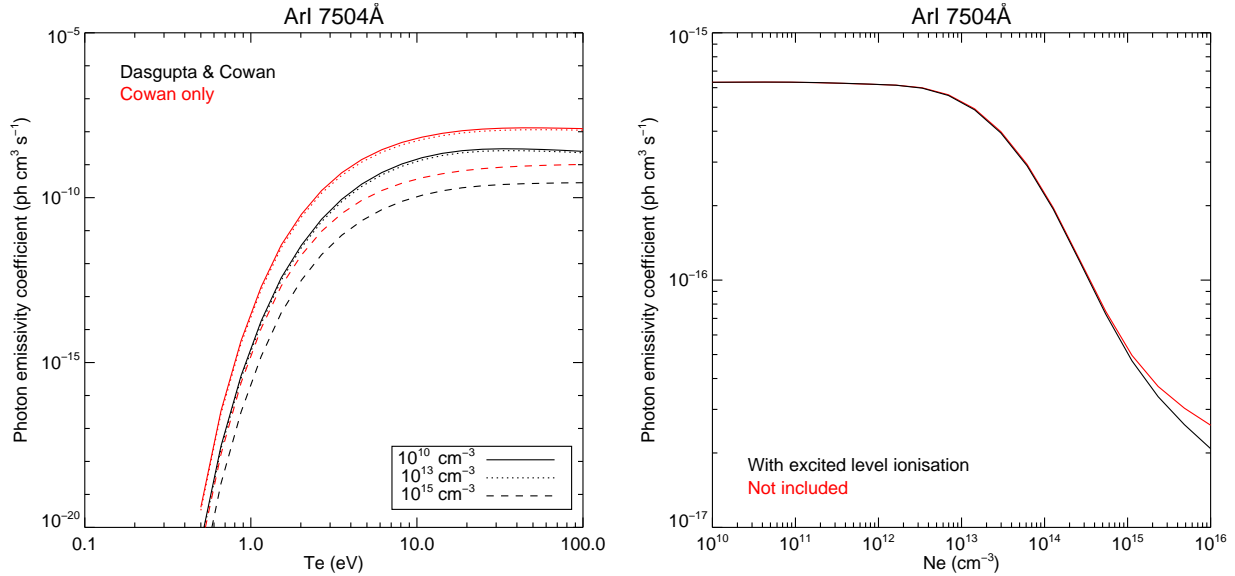


Figure 1: (lef) Photon emissivity coefficients for the 705.4nm transition of ArI generated from the Cowan excitation data and from the same data supplemented with transitions from Dasgupta [4, 5]. (right) The dependence on density and the influence of ionisation from excited levels (at a temperature of 0.9eV).

The supplementary Dasgupta DW data does make a difference. This is expected because the Born approximation does not produce good spin-changing cross sections.

A better method would be to perform an *R*-matrix calculation for the excitation data. An exploration of the *R*-matrix method has been reported [10] with the conclusion that the effects of continuum coupling are large even for transitions from the ground term to the lowest excited terms. The implication is that a full intermediate-coupling *R*-matrix with pseudo stages (RMPS) calculation between individual levels in argon is required — ‘a formidable computational challenge’ is their conclusion.

ArI

The original *adf04* dataset with *R*-matrix excitation data for singly ionised argon was based on a 40-state close-coupling calculation [11]. This data has recently been revisited [12]; the realisation that the RMPS model is a better description for neutral and near-neutral ions and improved computational facilities, permitting a 452-state description, prompted the new work.

Figure 2 compares the photon emissivities for the old and new datasets. The differences could be interpreted as an error on the calculated coefficients.

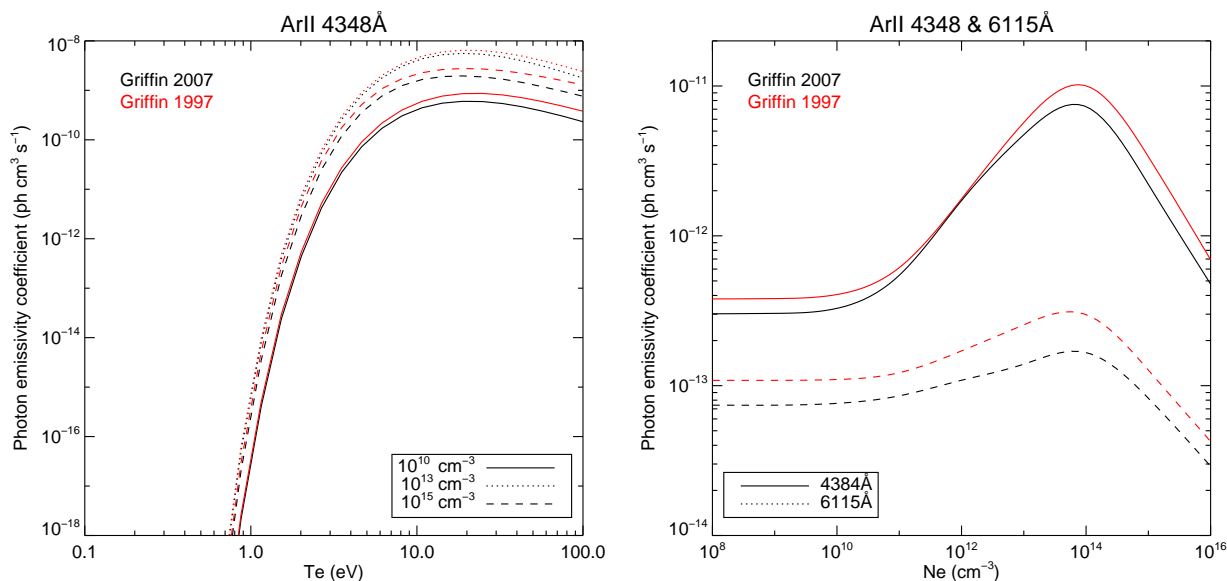


Figure 2: (left) Photon emissivity coefficients for the 434.8nm transition of ArII generated from *R*-matrix data with and without pseudo-states [11, 12]. (right) The dependence on density for two prominent ArII transitions (at a temperature of 1.95eV).

Central ADAS data for ArI and ArII

The data described in this note is available in central ADAS. The *adf04* files are:

- `adf04/arlike/arlike_mom08#ar0.dat`
- `adf04/cllike/cllike_dcg07#ar1.dat`

The *adf15* photon emissivity coefficients are:

- `adf15/transport/transport_llu#ar0.dat`
- `adf15/transport/transport_llu#ar1.dat`

References

- [1] H. P. Summers (2007). Atomic Data and Analysis Structure User Manual. Available from: <http://adas.phys.strath.ac.uk>
- [2] H. P. Summers, W. J. Dickson, M. G. O'Mullane, N. R. Badnell, A. D. Whiteford, D. H. Brooks, J. Lang, S. D. Loch and D. C. Griffin. 'Ionization state, excited populations and emission of impurities in dynamic finite density plasmas: I. The generalized collisional-radiative model for light elements'. *Plasma Phys. Control. Fusion*, **48**(2) (2006) 263–293. doi:10.1088/0741-3335/48/2/007
- [3] NIST : Atomic Spectra Database, Ar I energy levels. Available from: <http://physics.nist.gov/PhysRefData/Handbook/Tables/argontable5.htm>
- [4] A. Dasgupta, M. Blaha and J. L. Giuliani. 'Electron-impact excitation from the ground and the metastable levels of Ar I'. *Phys. Rev. A*, **61**(1) (1999) 012703. doi:10.1103/PhysRevA.61.012703
- [5] A. Dasgupta, M. Blaha and J. L. Giuliani. 'Erratum: Electron-impact excitation from the ground and the metastable levels of Ar I'. *Phys. Rev. A*, **65**(3) (2002) 039905. doi:10.1103/PhysRevA.65.039905
- [6] K. Bartschat and P. G. Burke. 'Electron impact ionisation of argon'. *J. Phys. B*, **21**(17) (1988) 2969–2975. doi:10.1088/0953-4075/21/17/010
- [7] A. Burgess. 'Semi-classical theory of electron-atom collisions'. In 'Proceedings of the symposium on atomic collision processes in plasmas', AERE-R 4818 (1964). Culham Laboratory, UK. 14–16 September.
- [8] H. P. Summers. 'Tables and graphs of collisional dielectronic recombination and ionisation equilibria of H-like to A-like ions of elements'. 367, Appleton Laboratory (1974)
- [9] A. Burgess and H. P. Summers. 'The recombination and level populations of ions. I - Hydrogen and hydrogenic ions'. *Mon. Not. R. Astr. Soc.*, **174** (1976) 345–391
- [10] C. P. Ballance and D. C. Griffin. 'An R-matrix with pseudo states calculation of electron-impact excitation in Ar'. *J. Phys. B*, **41**(6) (2008) 065201 (7pp). doi:10.1088/0953-4075/41/6/065201
- [11] D. C. Griffin, M. S. Pindzola, J. A. Shaw, N. R. Badnell, M. O'Mullane and H. P. Summers. 'Electron-impact excitation and ionization of Ar⁺ for the determination of impurity influx in tokamaks'. *J. Phys. B*, **30**(15) (1997) 3543–3565. doi:10.1088/0953-4075/30/15/023
- [12] D. C. Griffin, C. P. Ballance, S. D. Loch and M. S. Pindzola. 'Electron-impact excitation of Ar⁺ : an improved determination of Ar impurity influx in tokamaks'. *J. Phys. B*, **48**(23) (2007) 4537–4550. doi:10.1088/0953-4075/40/23/013