Oct18-00 ADAS Bulletin

In this release there is a new code, ADAS704, a substantial extension to the cross-referencing file outputs from ADAS807 and many smaller alterations to codes, improving their robustness and capabilities. The main content of this release and the thrust of this bulletin is concerned with new data and developments in our handling of data. Firstly, Martin has completed the generalised collisional-radiative data for neon which is included in this release. Essentially the computations of the GCR project are now complete although we do intend to fill in remaining first period elements (lithium, beryllium, boron and fluorine) to the same quality and believe that we can do this quite soon. It has taken great effort by Martin, Ralph Dux and others to convert the execution of a complete GCR calculation at the highest quality level from a process with many hand interventions and steps by the producer to an integrated semi-automatic procedure within ADAS. This does not of course absolve the producer from effort, but this is now principally targetted on the assembly of best available electron impact excitation data from the general literature (accompanied by precision A-values and energy levels) or by off-line calculation (such as R-matrix).

The time and effort involved has been considerable which has had an effect on the regularity of ADAS releases. This matter, together with comments and suggestions from the Sept. ADAS workshop, has caused us to reappraise how we manage error correction and new code releases. Also, we have been concerned with the shear volume of ADAS fundamental and derived data and the perennial problem of providing enough information on how to find the 'best' data for a particular purpose. There are four parts to our plan here. Firstly, we have now placed the whole database under SCCS control. It is currently under test and we shall swap to the SCCS controlled data at the next release in March 2001. This will help to moderate dataset proliferation since we can recall older versions if necessary for code checking. Secondly, we do have particular types of fundamental data (for example: adf01, adf02, adf04, adf07) which are assessed and re-assessed over many years. We are intending to improve the sustainability of such efforts by different workers by providing the underlying spread-sheets used in maintenance of some of the data (see 'adas_excel'). Thirdly, I shall try to improve the usefulness and visibility of the 'datastatus' documents. Finally, Martin and Ricky have updated and extended our lists of ADAS users and seek to increase markedly the use of brief 'ADAS Technical Notes'which will be emailed to users. On the release pattern, I shall issue a new 'ADAS Code and Data Practice' which I hope will be helpful.

ADAS108 A duplicate subroutine name, which clashed with an IDL subroutine name, has been replaced. Note that this error only appeared at one site where the order of ADAS and IDL library scanning was reversed.

ADAS208 This main excited population code has been extended to allow ionisation rate coefficient data from any excited state to be entered from the input *adf04* file. In a prior adjustment, an alteration was made to allow such data to be present in the *adf04* file, but only for ionisation from metastables. The latest extension has been to allow such data for <u>any</u> excited level. Note that data of this type in the adf04 file is signalled by a letter 'S' in the first column of the transition line. The full specification of an adf04 file is now quite versatile (and complex) and the detailed specification is given in the '/…/adas/docs/datastatus' document. The inclusion of this capability has permitted some further testing of ADAS208 by Mathias Brix (on helium populations) which is OK.

ADAS306/308 A very long-standing error in these codes - stemming from IBM-IDL conversion days - precluded the inclusion of more than one 'experimental' charge exchange line-of-sight emissivity. In practice these codes, which have a capacity to analyse more than one charge exchange line in terms of a best estimate of the emission measure and a critique of state selective charge exchange cross-section (theory versus the experiment), have only been used in recent years to display and examine the theoretical effective emission coefficients. The situation has been corrected in response to a type of analysis being carried out at Caderache. I note that we have in development a new orientation of this type of code (focusing on the l-distribution of capture and its effect on n-n' charge exchange line profiles) which we hope to release in about a year. It will have a new ADAS code number.

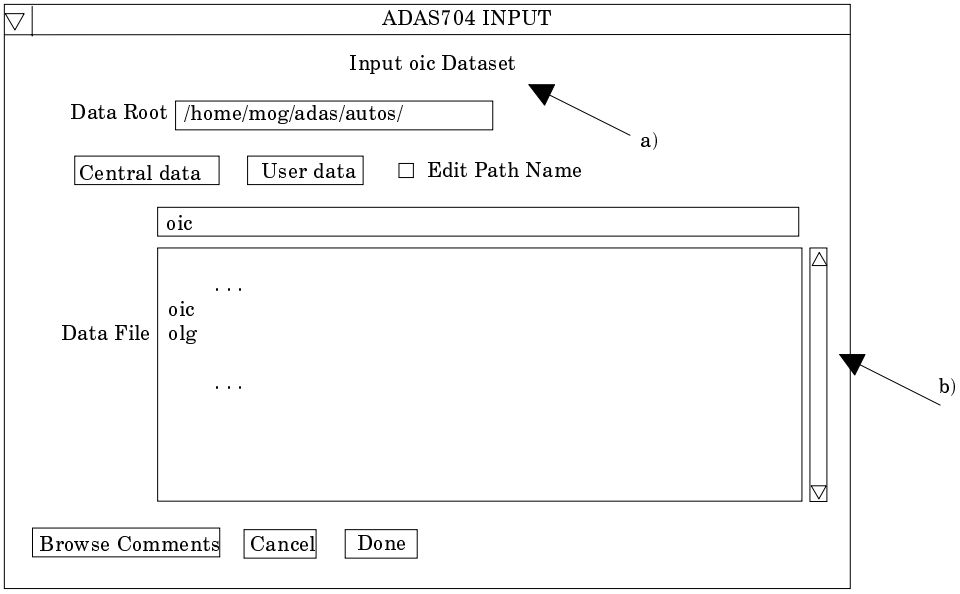
ADAS311 Internal improvements have been made to this code. This is the most complex of the population codes (although specialized to helium beams at this time) and it retains some non-ideal features from the point of view of the ADAS coding standards. A very large new population code development for heavy species at level resolution is underway with Stuart Loch. ADAS311 will receive its final 'tidy-up'in the course of this development.

ADAS603 Ricky has been spending a great deal of effort on inproving the robustness of this code. In particular, the non-linear optimisation used in the code has been compared with results of a simplex routine. A number of items came to light and this latest version is a considerable improvement. We had intended to include the improved (and much enhanced) handling of profile and instrument functions in this release of ADAS603, but we are holding this back until the next new code release. At that time ADAS604 will also be issued.

ADAS704 This is a new code which provides one of the last links in the chain of processing required in the 'GCR Project' for the generation of complete collisional-radiative data for light elements (see also ADAS807 and 'GCR Project bulletin no. 2'). The code constitutes a third post-processing option on the Auger rate coefficient data output from ADAS701 (Autostructure). It creates a part of the cross-referencing file of type /…/adas/adas/adf18/a09_p204/ which links dielectronic data into the bundle-nS population code ADAS204. The part in question is some supplementary data which allows for Auger breakup going from n-shells built on one parent metastable to a different metastable but not via a common spin system . Such Auger processes must occur via LS-coupling breakdown and, although small for light element ions, are sufficient to drop the high level populations markedly. To obtain these supplementary rates it is necessary to go back to basic ADAS701 calculations in intermediate coupling. ADAS704 then processes the intermediate coupling calculation data to give the required supplement.

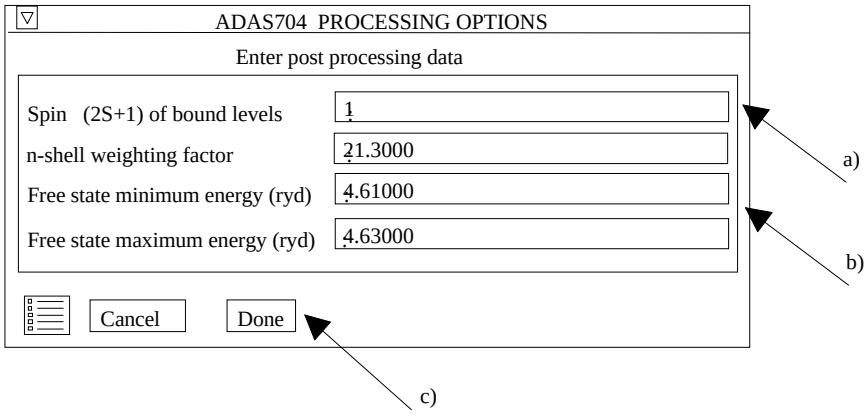
The **file selection window** has the appearance shown below

1. The input file is the intermediate coupling 'oic' file from the ADAS701 (Autostructure) run. Note that by convention a user should assign a separate '/autos/' sub-directory for such datasets from ADAS701 in his/her master '/adas/' directory rather that the usual '/pass' sub-directory. Note that the 'oic' file should be obtained for a set of n-shells in one-pass selected to match to representative levels and span n-shells up to some last n-shell from which extrapolation can safely be performed.



2. Buttons and controls follow the usual pattern

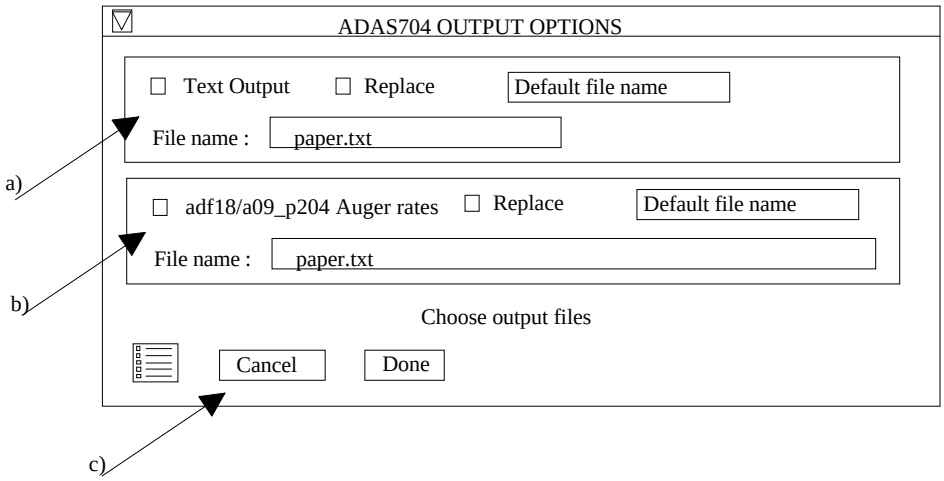
The **processing options window** has the appearance shown below.



3. There are only limited options on the processing screen. At a), the *Spin* of the recombined system targetted is specified. That is spin system of the initial metastable + nl-electron system.
4. The *n-shell weighting factor* is a little complicated. It is defined as 2*(indistinquishable composite metastable parent weight)*(spin system weight fraction of total possible spin weight for the composite parent)/(proportion of required metastable parent in the indistinquishable parent composite). For example $(2s^2 2p^3)n^{\ 1}$ for the ^{2}D parent n-shell weighting factor = 12.8 arising from: composite parent weight = 16 (^{2}D and ^{2}P are indistinquishable both contributing to the $n^{\ 1}$ system); spin weight fraction = 0.25 (from 1/[1+3] since singlet and triplet spin systems can result from these parents); proportion =0.625 (since ^{2}D is 10/[10+6] of the indistinguishablecomposite parents). Further examples are given in the archived adf18 files.
5. At b), the 'Free state maximum and minimum energies' span the range of resonances (n-shells built on metastables) and must be used to isolate the band of free-electron energies which pick up the correct final metastable.

The **output options window** appearance is shown below

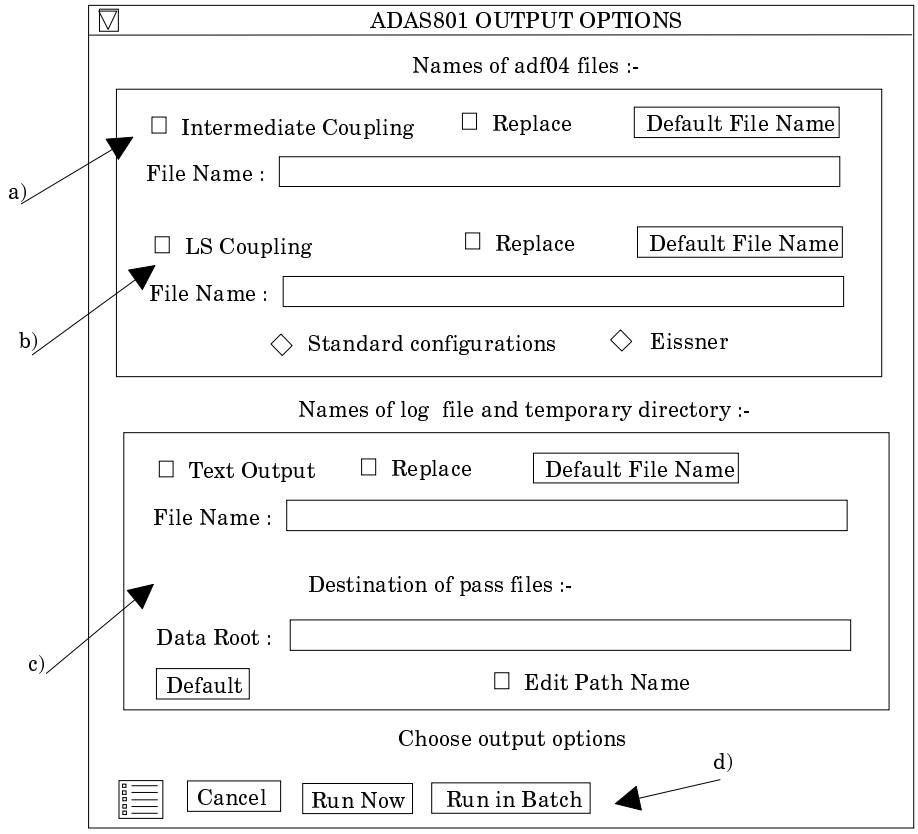
1. There is no graphical display
2. The output file sought at b) is the supplementation data . Note that the rest (first part) of the /adf18/a09_p204 cross-reference file is straightforward and existing samples can be modified quickly for other cases.



ADAS801 A small extension has been made to the output options. This allows either the 'ADAS standard convention' or the 'Eissner convention' for the configuration descriptor string in the adf04 output file. It should be noted that, although the specification of the adf04 file allows the configuration for a level or term to be an arbitrary string at the choice of the ADAS user, some of the powerful automatic codes of ADAS series 4, series 7 and series 8 do depend on the configuration string being recognizable as either of standard or Eissner form. In actual execution of such automatic ADAS

codes, a fortran subroutine '/…/adas/idl_adas/fortran/adaslib/xxdtes.for' checks to see if the configuration string can be interpreted and if not stops with an error message. I recommend now as preferred practice to use the ADAS standard or Eissner conventions when possible.

The new **output options window** has the appearance shown below with the configuration string choice made below the File Name at b)

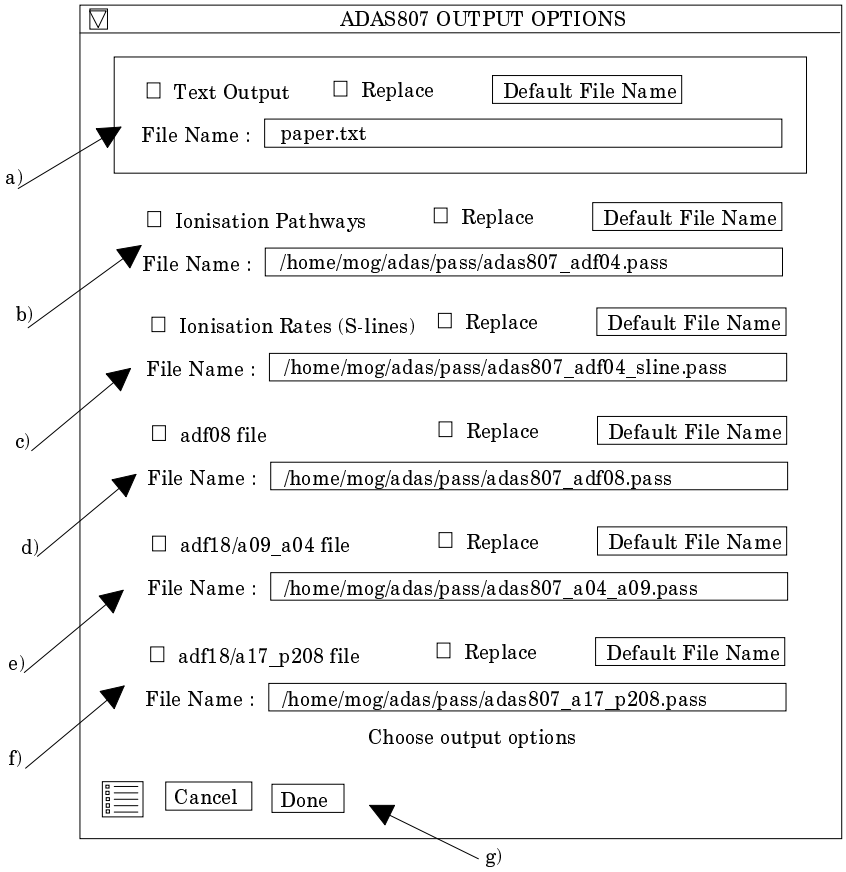


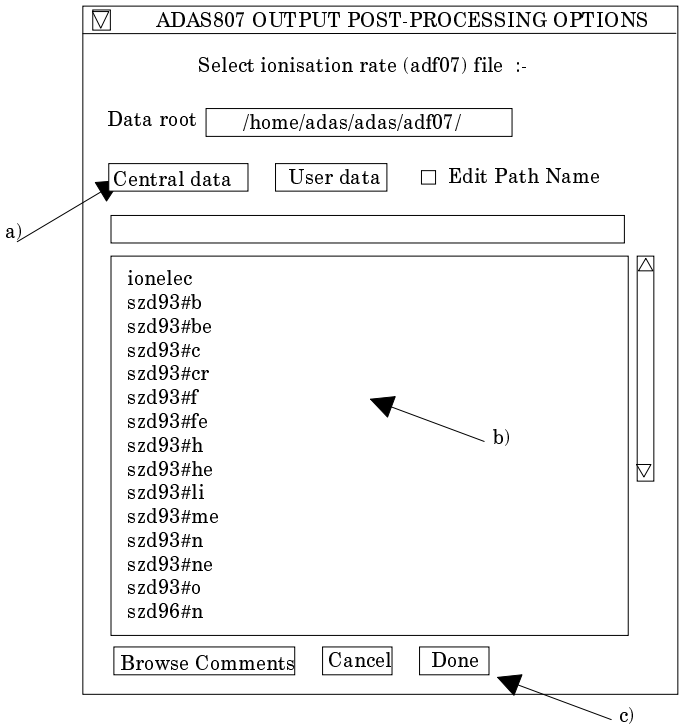
ADAS807 The code, which was first released on 18 March 2000 prepares the set of augmented, cross-reference and template files which are required for complete generalised collisional radiative modelling using the codes of ADAS series 2 and 4. Martin has added extra features so that all the intermediate and corss-referencing files and data blocks required in the 'GCR Project' can be generated automatically now by the user.

The **file selection window** and the **metastable selection** windows are before. Note however that the code now makes an automatic initial selection of the metastable levels. This may be overridden by the user

The new **output options window** appearance is shown below

1. At c) the option to add electron impact ionisation rate coefficient data to the output adf04 file as 'S-lines' is given. As indicated in the comments for code ADAS208, S-lines can include true excited levels as well as ground and metastable levels. Within the ADAS databases, we have only explicit data for electron impact ionisation from ground and metastables. Ionisation from true excited states is included in ADAS population codes but via internal subroutines (reflecting fairly simple approximate methods such as ECIP or fits). This does correspond to reality in that that there is almost no high quality theoretical data and no experimental data for excited state ionisation.
2. Selection at c) pops up an input file selection widget as shown below. It points to the adf07 formatted section of the adas database where ionisation rate tabulations are located. It is metastable resolved initial and final state ionisation data which is relevant here.

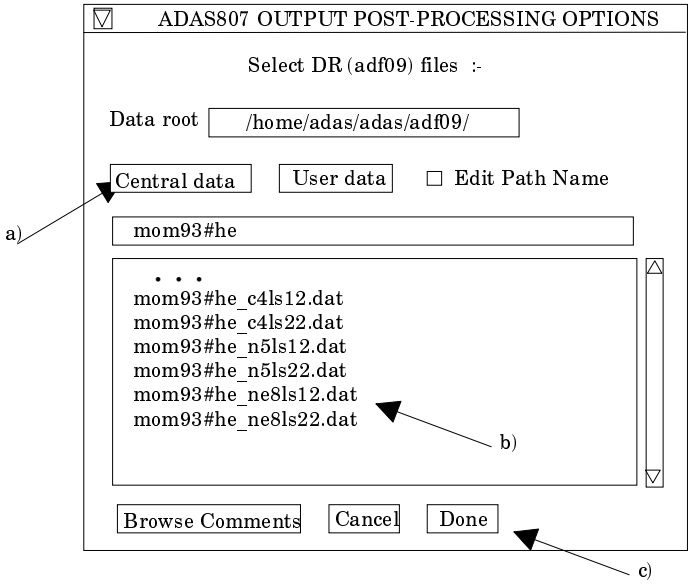




3. Select by element. It is important to *Browse Comments* and verify that the data set chosen in appropriate. The provision of initial and final state resolved ionisation data is an important issue which we have been working on extensively. Details are given the new data description part of the bulletin below, but note that we have prescriptions for creating approximate

resolved data form unresolved stage-to-stage data for 1st and 2nd period iso-electronic series.

4. At e), the automatic creation of the mapping file of type adf18/a09_a04, which carries state selective dielectronic data into the adf04 file as 'R-lines', is implemented. It pops up the widget shown below:



5. The mapping file is used in a subsequent execution of the mapping by ADAS212

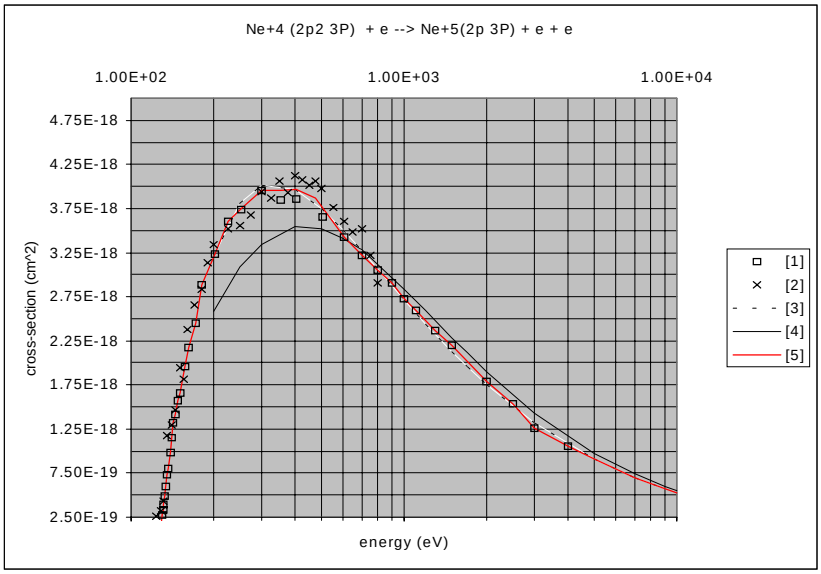
READ_ADFXX Two new routines have been added for accessing adf files from IDL, namely, *read_adf12* and *read_adf21*.

ADF02 A mistyped power in /…/adas/adas/adf02/sia#h/sia#h_tos#h.dat has been corrected.
ADF07 A kink due to mistyping in the helium-like to hydreogen-like electron impact ionisation file for nitrogen /…/adas/adas/adf07/szd93#n/szd93#n_n.dat has been corrected.
ADF11 '89' data for iron has been added. The adf03 (atompars) files existed but inadvertedly had not been run trhough to the adf11 files..
ADF13/ADF15 New CIII (C^{+2}) pecs and sxbs for visible transitions have been put in place. We missed the crucial 4650A line from the standard ones. These files suited to vsible spectroscopy are named as /…/adas/adas/adf13/pec96#c/pec96#c_vsr#c2.dat and so on in the usual manner
ADF14 A long-standing typing error in /…/adas/adas/adf14/tcx#h0/tcx#h0_h.dat has been corrected.

ADFXX for Neon There are many new files associated with the neon GCR calculations including adf04 (copmm#10/ls#ne9.dat), adf07 (metastable resolved ionisation rates), adf10, adf11, , adf17 ('cbnm96' bundle-n projection files), adf18/a09_p204 ('drm96' bundle-n dielectronic recombination mapping files), adf25 (drivers for neon and a missing neutral oxygen file), adf27 (driver files to calculate spin breakdown Auger rates for the adf18/a09_p204 mapping files).

ADAS_EXCEL At this time, I draw your attention to three sets of spread sheets which may be of interest to those of you working on extending the ADAS databas . These can be downloaded to you on request from Ricky, but do take note of our need to keep track of who is working on what (I shall issue guidelines in the 'ADAS Code and Data Practice' document with the next bulletin). They are Microsoft 1998 format EXCEL spreadsheets. Note that Martin can provide code to adjust formatting of the 'comma-delimited' EXCEL to ASCII file to the appropriate ADAS *adf* file type

/adas_excel/electron_impact_xsects/neon_ground_ionisation.xls A revision of the stage to stage ionisation cross-sections by Martin, prior to conversion to rate coefficients and then to metastable resolution. The conversion code can also be provided by Martin.



Reaction: Ne^{+4} ($2p^2\ ^3P$) + e --> Ne^{+5}($2p\ ^3P$) + e + e
Last reviewed: 15-Nov-00
Reviewer: M. G. O'Mullane

Sources:
[1] Duponchelle et al, J> Phys. B 30, p729, 1997
[2] Bannister, Phys. Rev. A 54, p1435, 1996
[3] Godunov & Ivanov, Physica Scripta, 59, p 277, 1999 - recommended
[4] Lennon et al, J. Phys. Chem. Ref. Data, 17, p1285, 1988 - recommended
[5] ADAS 2000 preferred:

[1]		[2]		[3]		[4]		[5]
energy (eV)	x-sect. (cm^2)	energy (eV)	x-sect. (cm^2)	energy (eV)	x-sect. (cm^2)	energy (eV)	x-sect. (cm^2)	energy (eV)
1.22E+02	-1.90E-21	1.16E+02	-7.00E-20	2.00E+02	3.21E-18	2.00E+02	2.59E-18	1.22E+02
1.25E+02	5.00E-22	1.21E+02	-7.00E-20	2.50E+02	3.81E-18	2.50E+02	3.08E-18	1.25E+02
1.27E+02	7.00E-20	1.23E+02	2.60E-19	3.00E+02	4.01E-18	3.00E+02	3.34E-18	1.27E+02
1.29E+02	1.70E-19	1.26E+02	2.40E-19	4.00E+02	3.97E-18	4.00E+02	3.54E-18	1.29E+02
1.30E+02	2.70E-19	1.28E+02	3.20E-19	5.00E+02	3.75E-18	5.00E+02	3.52E-18	1.30E+02
1.31E+02	3.30E-19	1.31E+02	4.30E-19	6.00E+02	3.50E-18	6.00E+02	3.42E-18	1.31E+02
1.32E+02	3.90E-19	1.36E+02	1.17E-18	7.00E+02	3.27E-18	7.00E+02	3.28E-18	1.32E+02
1.33E+02	4.90E-19	1.41E+02	1.30E-18	1.00E+03	2.72E-18	1.00E+03	2.84E-18	1.33E+02
1.34E+02	6.00E-19	1.46E+02	1.46E-18	1.20E+03	2.44E-18	1.20E+03	2.59E-18	1.34E+02
1.36E+02	7.30E-19	1.51E+02	1.95E-18	1.50E+03	2.13E-18	1.50E+03	2.28E-18	1.36E+02
1.37E+02	8.00E-19	1.56E+02	1.81E-18	1.70E+03	1.96E-18	1.70E+03	2.11E-18	1.37E+02
1.39E+02	9.80E-19	1.61E+02	2.38E-18	2.00E+03	1.76E-18	2.00E+03	1.90E-18	1.39E+02
1.41E+02	1.15E-18	1.71E+02	2.66E-18	3.00E+03	1.32E-18	3.00E+03	1.43E-18	1.41E+02
1.42E+02	1.32E-18	1.81E+02	2.84E-18	5.00E+03	9.06E-19	5.00E+03	9.66E-19	1.42E+02
1.46E+02	1.42E-18	1.91E+02	3.14E-18	7.00E+03	6.99E-19	7.00E+03	7.39E-19	1.46E+02
1.49E+02	1.57E-18	2.01E+02	3.34E-18	9.00E+03	5.74E-19	9.00E+03	6.02E-19	1.49E+02
1.52E+02	1.66E-18	2.26E+02	3.52E-18	1.00E+04	5.28E-19	1.00E+04	5.51E-19	1.52E+02
1.57E+02	1.96E-18	2.51E+02	3.56E-18					1.57E+02
1.62E+02	2.17E-18	2.76E+02	3.68E-18					1.62E+02
1.72E+02	2.45E-18	3.01E+02	3.94E-18					1.72E+02
1.82E+02	2.88E-18	3.26E+02	3.87E-18	ip=	1.26E+02	ip=	1.26E+02	1.82E+02
2.02E+02	3.23E-18	3.51E+02	4.06E-18	a=	1.35E+03	a=	1.07E+03	2.02E+02
2.27E+02	3.61E-18	3.76E+02	3.93E-18	b1=	3.54E+02	b1=	4.42E+02	2.27E+02
2.52E+02	3.74E-18	4.01E+02	4.12E-18	b2=	4.41E+02	b2=	4.75E+02	2.52E+02
3.02E+02	3.95E-18	4.26E+02	4.07E-18			b3=	-2.96E+03	3.02E+02
3.52E+02	3.85E-18	4.51E+02	4.01E-18			b4=	4.47E+03	3.52E+02
4.02E+02	3.86E-18	4.76E+02	4.06E-18					4.02E+02
5.02E+02	3.65E-18	5.01E+02	3.98E-18					4.75E+02
6.02E+02	3.42E-18	5.51E+02	3.76E-18					6.02E+02
7.02E+02	3.22E-18	6.01E+02	3.61E-18					7.02E+02
8.02E+02	3.05E-18	6.51E+02	3.48E-18					8.02E+02
9.02E+02	2.91E-18	7.01E+02	3.52E-18					9.02E+02
1.00E+03	2.73E-18	7.51E+02	3.22E-18					1.00E+03
1.10E+03	2.60E-18	8.00E+02	2.91E-18					1.10E+03
1.30E+03	2.37E-18							1.30E+03
1.50E+03	2.20E-18							1.50E+03
2.00E+03	1.79E-18							2.00E+03
2.50E+03	1.54E-18							2.50E+03
3.00E+03	1.26E-18							3.00E+03
4.00E+03	1.06E-18							4.00E+03
								5.00E+03
								7.00E+03
								9.00E+03
								1.00E+04

/adas_excel/ionisation_fractions/neon_ionisation_fraction.xls The sheets have energy levels, transition and fractionation tables which sspecify how to breakdown state-to-stage ionisation rates to metastable resolved rates. The sheets are self-calculating and so can be adjusted easily for the hydrogen-like to neon-like ionsation states of other elements by altering energy level and orbital energy information

Transition	Metastable	Index	Purpose	Formula	Shell 1		Shell 2		Shell 3		Shell 4	
					I(1s) (Ryd)	ζ(1s)	I(2s) (Ryd)	ζ(2s)	I(2p) (Ryd)	ζ(2p)	I(3s) (Ryd)	ζ(3s)
Ne+3 ->Ne+4		f1			62.02000	2.000	7.14483	2.000	7.14483	3.000		
			Bell comparison	ratio=Bell/f1								
	2s2 2p3 (4	f2	2p via 3P direct						7.14483	3.000		
		f3	2s via 3S + auto				7.14483	2.000				
		f4	2s via 5S + auto				7.14483	2.000				
		f5	2s via 5S direct				7.94315	2.000				
		f6	1s + auto		62.02000	2.000						
		f7	1s direct		71.13000	2.000						
			2s2 2p3 (4S) total	(f2+f3+f4+f6)*ratio								
	#		2s2 2p3 (4S) -> 2s2 2p2 (3P)	(f2+f3+f4+0.375*f6-f5)*ratio								
	#		2s2 2p3 (4P) -> 2s1 2p3 (5S)	(f5+0.625*f6)*ratio								
	2s2 2p3 (2	f8	2p via 3P direct						6.76891	3.000		
		f9	2p via 1D + auto						6.76891	3.000		
		f10	2p via 1D direct						7.03807	3.000		
		f11	2s via 1D + auto				6.76891	2.000				
		f12	2s via 3D + auto				6.76891	2.000				
		f13	2s via 3D direct				8.36474	2.000				
		f14	1s + auto		62.02000	2.000						
		f15	1s direct		71.13000	2.000						
			2s2 2p3 (2D) total	(f8+f9+f11+f12+f14)*ratio								
	#		2s2 2p3 (2D) -> 2s2 2p2 (3P)	(f8+f9-f10+f12+0.750*f14)*ratio								
	#		2s2 2p3 (2D) -> 2s2 2p2 (1D)	(f10+f11+0.250*f14)*ratio								
	2s2 2p3 (2	f16	2p via 3P direct						6.57584	3.000		
		f17	2p via 1D + auto						6.57584	3.000		
		f18	2p via 1D direct						6.84501	3.000		
		f19	2p via 1S + auto						6.57584	3.000		
		f20	2p via 1S direct						7.15140	3.000		
		f21	2s via 1P + auto				6.57584	2.000				
		f22	2s via 3P + auto				6.57584	2.000				
		f23	2s via 3P direct				8.46588	2.000				
		f24	1s + auto		62.02000	2.000						
		f25	1s direct		9.11000	2.000						
			2s2 2p3 (2P) total	(f16+f17+f19+f21+f22+f24)*ratio								
	#		2s2 2p3 (2P) -> 2s2 2p2 (3P)	(f16+f17-18+f19-f20+f22+0.750*f24)*ratio								
	#		2s2 2p3 (2P) -> 2s2 2p2 (1D)	(f18+0.8*f21+0.250*0.8*f24)*ratio								
	#		2s2 2p3 (2P) -> 2s2 2p2 (1S)	(f20+0.2*f21+0.250*0.2*f24)*ratio								

/adas_excel/he0_ion_impact xsects.xls We have extensive sheets on the various types of fully stripped impurity ion impact cross-sections. At this time Mathias Brix and I are working extensively on upgrading these in preparation for the EFDA-JET helium experiments and so we shall not open them to others at this time.

H. P. Summers
18 Oct 2000