

# ADAS204: Specific z recom/ionis - process collisional radiative coefficients and populations

The code is a mass production program for providing collisional-radiative coefficients linking two ionisation stages of an element. It is designed to handle correctly the very many n-shells required for treatment of dielectronic recombination and the influence of finite plasma density upon it. Thus it operates in the bundle-n model but resolved according to initial recombining parent metastable and recombined state spin system. It provides acceptable generalised collisional-radiative recombination, ionisation and recombination / Bremsstrahlung power coefficients. However it cannot handle low level line power and individual line emission with sufficient precision for spectroscopy. Thus we use it in ADAS to provide condensed projection matrices (adf17) which are picked up by the high precision low level population code ADAS208. This code in turn generates the final highest quality, complete generalised collisional-radiative data.

## Background theory:

For hydrogen or hydrogenic ions in a plasma, the largest collision cross-sections are those for which  $n=n'$  and  $l=l\pm 1$ . For these cases the transition energy is nearly zero and the cross-sections are so large for electron densities of relevance for fusion that it is very good approximation to assume relative statistical population for the l-states. Thus for hydrogenic systems only populations of complete n-shells need be evaluated, the *bundle-n* approximation. The equilibrium populations of the n-shells,  $N_n$ , are the solution of the statistical balance equations

$$\begin{aligned}
 & \sum_{n'>n} [A_{n'\rightarrow n} + u(\nu)B_{n'\rightarrow n} + N_e q_{n'\rightarrow n}^{(e)} + N_e q_{n'\rightarrow n}^{(p)}] N_{n'} \\
 & + \sum_{n''<n} [u(\nu)B_{n''\rightarrow n} + N_e q_{n''\rightarrow n}^{(e)} + N_e q_{n''\rightarrow n}^{(p)}] N_{n''} \\
 & + N_e N_+ \alpha_n^{(r)} + N_e^2 N_+ \alpha_n^{(3)} + N_e N_+ \int u(\nu) B_{\kappa\rightarrow n} d\kappa \\
 & = \left\{ \sum_{n'>n} [u(\nu)B_{n\rightarrow n'} + N_e q_{n\rightarrow n'}^{(e)} + N_e q_{n\rightarrow n'}^{(p)}] \right. \\
 & + \sum_{n''<n} [A_{n\rightarrow n''} + u(\nu)B_{n\rightarrow n''} + N_e q_{n\rightarrow n''}^{(e)} + N_e q_{n\rightarrow n''}^{(p)}] \\
 & \left. + \int u(\nu) B_{n\rightarrow \kappa} d\kappa + N_e q_{n\rightarrow \epsilon}^{(e)} + N_e q_{n\rightarrow \epsilon}^{(p)} \right\} N_n
 \end{aligned} \tag{3.4.1}$$

$N_n$  is the population of the state  $X_n^{+z_0-1}$  and  $N_+$  of the parent ion  $X^{+z_0}$ .  $N_e$  is the free electron density and  $N_p$  the free proton density.  $A$  and  $B$  are the usual Einstein coefficients,  $q^{(e)}$  and  $q^{(p)}$  denote collisional rates due to electrons and protons,  $\alpha_n^{(r)}$  and  $\alpha_n^{(3)}$  denote radiative and three-body recombination and  $u(\nu)$  is the energy density of the radiation field. There is one such equation for each value of n from 1 to  $\infty$ . Details of the hydrogenic rate coefficients entering these equations can be found in the background theory to the code ADAS310. For the present purposes, it is necessary to extend the above system to complex ions with multiple parents and up to two spin systems (in LS coupling) built on each parent.

## Statistical weights, energies spin systems, b-factors and scaling

Let  $X^{+z_1-1}$  denote the recombining ion and  $X^{+z_1-1}$  the recombined ion so that  $z = z_1 - 1$  is the ion charge of the latter.  $z_1$  is the effective ion charge and takes the place of the nuclear charge in the reduction of hydrogenic rate coefficients to compact forms in the statistical balance equations. Denote the parent terms, that is terms of the recombining ion by  $\gamma \equiv L_p S_p$ . The recombined system levels are distinguished by parent, n-shells and spin S under the assumption is that the populations of principal quantum shells of the same value of n but with different spins are separable. Introduce  $SSYSWT$ , the fractional spin system weight of the recombined spin system. Then

$$ssyswt = \frac{(2S+1)}{2(2S_p+1)} \quad 3.4.2$$

and the nS-shell statistical weight is given by

$$\omega_{\gamma,nS} = ssyswt.2n^2\omega_{\gamma} \quad 3.4.3$$

in terms of the parent statistical weight  $\omega_{\gamma} \equiv (2S_p+1)(2L_p+1)$ . Denote the number of accessible spin systems open to an electron added to the parent ion be  $NSYS$  and introduce  $N_{min}$  and  $N_0$  giving the lowest n-shell of the recombined ion for the calculation and the lowest n-shell accessible by recombination from the parent into the spin system respectively. A separate calculation is performed for each excited state parent/spin system formed by such a recombination pathway. Table 4.0 summarises these parameters for first period iso-electronic sequences up to nitrogen/oxygen. For hydrogenic ions it was advantageous to write the statistical equations in terms of Saha-Boltzmann deviation factors. This remains true for complex ions,  $X^{+z_1-1}$  with ion charge  $z = z_1 - 1$  but the definition must be generalised. The deviation  $b_{\gamma,nS}$  is defined by

$$N_{\gamma,nS} = N_e N_{\gamma}^+ 8 \left( \frac{\pi a_0^2 I_H}{kT_e} \right)^{3/2} \frac{\omega_{\gamma,nS}}{2\omega_{\gamma}} \exp(I_{\gamma,nS} / kT_e) b_{\gamma,nS} \quad 3.4.4$$

That is defined with respect to the parent ion  $X_{\gamma}^{+z_1}$  and the ionisation energy  $I_{\gamma,nS}$  is also referred to that parent. It is convenient to introduce  $c_{\gamma,nS} = b_{\gamma,nS} - 1$  and scaled temperatures and densities

$$t_e = \left( \frac{kT_e}{I_H} \right) \frac{1}{z_1^2}, \quad t_r = \left( \frac{kT_r}{I_H} \right) \frac{1}{z_1^2} \quad \text{and} \quad \rho_e = 2^5 \sqrt{\frac{\pi}{3}} \frac{\pi a_0^2 N_e}{\alpha^3 z_1^7} \quad 3.4.5$$

with similar forms for the proton temperature and density. In these terms the statistical balance equations become particularly suitable for calculation.

A problem of the parent/spin system model is that it does not distinguish recombined metastables within the same spin system. For example, the  $2s^2 2p^2 P$  parent in the B-like system is considered as recombining into the singlet system of the C-like ion. This system has two metastables,  $2s^2 2p^2 {}^1D$  and  $2s^2 2p^2 {}^1S$ . In this calculation, the effective ground state is taken as the lowest energy metastable (the  $2s^2 2p^2 {}^1D$  state in this example). As a prescription for completeness, statistically weighted populations may be used to obtain coefficients which tentatively resolve between recombined metastables. No such provision is made in ADAS204 since the true solution is given by the condensation matrix transfer and final solution by ADAS208 which distinguishes explicitly between the LS terms in the lowest few quantum shells from the beginning.

It is necessary to represent the energies of the lowest few quantum shells by effective quantum numbers and this is done in principle by taking statistically weighted averages of the energies of LS terms associated with each parent and spin system group. In general, the quantum defect corrections are only necessary for the ground and first excited quantum shells. Nonetheless for the collisional-radiative coefficient output (especially ionisation) of ADAS204 to be independently useful, there is an issue concerning the quantum defect for the lowest quantum shell of each system. There is often a substantial difference between the quantum defect of the lowest state itself and the mean quantum defect arising from a weighted average of the lowest n-shell terms. For example, in  $Be^{+1}$ , the  $2s {}^2S$  ground term has a quantum defect of 0.271 whereas the averaged quantum defect of  $2s {}^2S$  and  $2p {}^2P$  is 0.102. The n=3 and n=4 shells have averaged quantum defects of 0.05 and 0.03 respectively. The problem concerns which ground state energy will best represent excitation between n=2 and n=3 in general calculation. At low electron densities, the ground state has the only significant population so that the ground state energy is more appropriate. However at high electron densities, the 2p state will be significantly populated and will contribute to the excitation to n=3. In these circumstances the averaged energy will be more appropriate. The choice of this parameter is important as it influences the stepwise part of the collisional-radiative ionisation coefficient. It is one of the

limitations of a bundle-n population structure (a situation corrected by ADAS208). For practical use of ADAS204, we have normally chosen the quantum defect of the lowest n-shell to be that of the lowest state configuration for the spin system, although this is at the choice of the user.

Table 3.4a Bundle-n S calculation pathways. The parameters  $N_{sys}$ ,  $N_{min}$  and  $N_0$  are as described in the text.

Recomb- ining seq.	Parent index	Parent term	Recombined system	$N_{SYS}$	System index	System spin	$SSYSWT$	$N_{min}$	$N_0$	Metastables	
H-like	1	$1s^2S$	$(1s^2S)n$	2	1	1	0.250	1	1	$1s^2^1S$	
					2	3	0.750	2	2	$1s2s^3S$	
He-like	1	$1s^2^1S$	$(1s^2^1S)n$	1	1	2	1.000	2	2	$1s^22s^2S$	
					2	2	1.000	1	2	$1s^22s^2S$	
Li-like	1	$1s^22s^2S$	$(1s^22s^2S)n$	2	1	1	0.250	2	2	$1s^22s^2^1S$	
					2	3	0.750	2	2	$1s^22s2p^3P$	
Be-like	1	$1s^22s^2^1S$	$(1s^22s^2^1S)n$	1	1	2	1.000	2	2	$1s^22s^2p^2P$	
					2	1	2	0.333	2	2	$1s^22s^2p^2P$
					2	4	0.667	2	2	$1s^22s2p^2^4P$	
B-like	1	$1s^22s^2p^2P$	$(1s^22s^2p^2P)n$	2	1	3	0.750	2	2	$1s^22s^2p^2^3P$	
					2,(3)	1	0.250	2	2	$1s^22s^2p^2^1D$	
					1	3	0.375	2	2	$1s^22s^2p^2^3P$	
C-like	1	$1s^22s^2p^2^3P$	$(1s^22s^2p^2^3P)n$	2	4	5	0.625	2	2	$1s^22s2p^3^5S$	
					1	4	0.667	2	2	$1s^22s^2p^3^4S$	
					2,(3)	2	0.333	2	2	$1s^22s^2p^3^2D$	
N-like	1	$1s^22s^2p^2^1D$	$(1s^22s^2p^2^1D)n$	1	2,(3)	2	1.000	2	2	$1s^22s^2p^3^2D$	
					3	2,(3)	2	1.000	2	2	$1s^22s^2p^3^2D$
					4	1	4	1.000	2	2	$1s^22s2p^3^5S$
N-like	1	$1s^22s^2p^3^4S$	$(1s^22s^2p^3^4S)n$	2	1	3	0.375	2	2	$1s^22s^2p^3^4S$	
					4	5	0.625	2	2		
					2	1	3	0.750	2	2	
3	$1s^22s^2p$	$(1s^22s^2p^3^2P)n$	2	1	2,(3)	1	0.250	2	2		
					2,(3)	1	0.250	2	2		

### Auto-ionisation and alternate parents

Let the metastable states which represents the lowest level of recombined parent/spin system be indexed by  $\rho$ ,  $\sigma$  and parents be indexed by  $\gamma$ ,  $\delta$ .

The calculation for a given pathway involves the excited state population structure connecting the recombining parent  $\gamma$  and metastable  $\rho$ . However, alternative parents, which do not act as a recombination starting point, must also be considered. These can be populated by Auger transitions from excited states above the auto-ionisation threshold. For example, consider table 3.4a. The parent and ground states of the pathway are indexed by  $\gamma$  and  $\rho$  respectively and the alternative parent is indexed by  $\delta$ . In ADAS204, the excited state populations are calculated by first establishing the complete collisional-radiative matrix for the parent/spin system, but with the inclusion of auto-ionisation processes. The definitions of generalised collisional-radiative ionisation and recombination coefficients are still relevant and give the recombination rate from  $\gamma$  to  $\rho$  and the total loss rate from  $\rho$  (i.e. with no resolution of final parent after ionisation). The recombination coefficient is already correctly parent/metastable resolved and needs no further adjustment. The parent resolved ionisation coefficients and parent cross coupling coefficients are derived by constructing the loss vector from each level.

Because the model considers the excited state populations  $N_{\gamma,nS}$ , direct ionisation only

populates  $X_{\gamma}^{+z_1}$ . The alternative parents are populated by auto-ionisation. The parent resolved loss vectors are thus given by

$$\begin{aligned} L_{\gamma nS \rightarrow \gamma} &= N_e S_{\gamma nS \rightarrow \gamma} \\ L_{\gamma nS \rightarrow \delta} &= L_{\gamma nS \rightarrow \delta}^a \end{aligned} \quad 3.4.6$$

The  $\gamma, nS$  excited state structure is assumed built upon an metastable parent  $\gamma$ , so that the excited states can decay by either direct or auto-ionisation. Above the auto-ionisation threshold, and at low electron densities, auto-ionisation is the dominant loss mechanism. However, the auto-ionisation transition probabilities scale as  $n^{-5}$  and are independent of electron density, whereas direct ionisation loss rates scale as  $n^4$  and vary directly with electron density. For high n-shells, direct ionisation is the dominant loss process. As the electron density increases, direct ionisation becomes the dominant loss process for all n-shells and auto-ionisation is quenched. This has the consequence that not only *parent resolved ionisation coefficients* but a new type of coefficient called *the parent cross coupling coefficient* are obtained from expressions 3.4.6. The inclusion of auto-ionisation transition probabilities in the statistical balance equations leads to dramatic changes in the population structure. For example, the populations of  $C^{+1} (2s^2 \ ^1S) \ ^2n$ , which are built upon a ground state parent so no auto-ionisation pathways are accessible from the excited states. If the populations are expressed in terms of the Saha-Boltzmann  $b$  factors, then they show strong overpopulation of the high n-shells at low electron density due to dielectronic recombination. As the electron density is increased, the dielectronic recombination influence becomes less due to ionisation of the high n-shell populations with all the  $b$  factors tending to 1. This behaviour is typical for a recombined system built on a ground state parent. By contrast, the populations of  $C^{+1} (2s2p \ ^3P) \ ^2n$ , built upon an excited metastable parent shows powerful depopulation above the auto-ionisation threshold. However, as the electron density increases, the direct ionising collisions from the excited states compete more strongly and the  $b$  factors tend to 1.

The presence of auto-ionisation transition probabilities in the population structure equations also means that the particular excited state structure, for which the population calculation is performed, is only specifying an intermediate parent or ground state. Electrons excited from  $\rho$  toward  $\gamma$  may auto-ionise so that the final state is  $\delta$ . Similarly, electrons recombining from parent  $\gamma$  towards  $\rho$  may auto-ionise to the final state  $\delta$ . In both these cases,  $\rho$  or  $\gamma$  are acting as intermediate states. The calculated generalised collisional radiative coefficients for a given pathway must therefore be indexed by initial, intermediate and final state -  $S_{\rho \rightarrow \gamma, \delta}^{eff}$ ,  $\alpha_{\delta \rightarrow \sigma, \rho}^{eff}$  and  $X_{\gamma \rightarrow \sigma, \delta}^{eff}$ .

Table 3.4b Excited state structures and ionisation coefficients calculated for the Be-B series. Ionisation coefficients are indexed by  $S_{\rho \rightarrow \gamma, \delta}^{eff}$  where  $\rho$  and  $\gamma$  index the recombined lowest metastable of the spin system and parent states of the calculation respectively and  $\delta$  indexes the final parent. 'd' denotes direct ionisation and 'e-a' denotes inner shell excitation-ionisation contributions.

Parent	Excited State Structure	Met.	Derived Ionis. Coef.	Type
1	$(2s^2 \ ^1S) \ ^2n$	1	$S_{1 \rightarrow 1, 1}^{eff}$	d
2	$(2s2p \ ^3P) \ ^2n$	1	$S_{1 \rightarrow 2, 1}^{eff}$	e-a
			$S_{1 \rightarrow 2, 2}^{eff}$	d
	$(2s2p \ ^3P) \ ^4n$	2	$S_{2 \rightarrow 2, 1}^{eff}$	e-a
			$S_{2 \rightarrow 2, 2}^{eff}$	d

*Direct Ionisation and Excitation-Auto-ionisation from Ground and Metastable Configurations*). The zero density ionisation coefficients which are used as preferred data thus contain auto-ionisation corrections. Because of this, the excitation auto-ionisation contributions explicitly derived by the bundle-nS population structure calculation are not used

as adjustments to the ionisation rate coefficient. However, these coefficients are of interest because they allow the collisional-radiative behaviour of the excitation-auto-ionisation contributions to be investigated. After the calculations for all relevant pathways for a given ion, it is necessary to obtain the final composite parent cross coupling coefficient by summing over intermediate states

$$\beta_{\sigma\gamma}^{eff} = \sum_{\rho} \beta_{\gamma \rightarrow \rho, \sigma}^{eff} \quad 3.4.7$$

For example, the parent cross coupling coefficient from  $2s2p \ ^3P \rightarrow 2s^2 \ ^1S$  includes contributions from recombination from  $2s2p \ ^3P$  towards  $2s^2 2p \ ^2P$  and  $2s2p^2 \ ^4P$ . There is no ambiguity over the final state of the ionisation and recombination coefficient. These are simply

$$S_{\gamma\rho}^{eff} = S_{\rho \rightarrow \gamma, \gamma}^{eff} \quad 3.4.8$$

$$\alpha_{\sigma\gamma}^{eff} = \alpha_{\gamma \rightarrow \rho, \rho}^{eff} \quad 3.4.9$$

If the auto-ionisation contributions derived by the bundle-nS population structure calculation coefficient were being used as adjustments to the composite ionisation coefficient, it would have been necessary to sum over intermediate states so that

$$S_{\sigma\rho}^{eff} = \sum_{\gamma} S_{\rho \rightarrow \gamma, \sigma}^{eff} \quad 3.4.10$$

The model is also used to calculate parent and spin system resolved recombination power coefficients. These were again derived for each parent and spin system excited state structure. The separate components arising from dielectronic stabilisation, cascade and recombination radiation (see Section 2.4, *Radiative Power Loss Coefficients*) were calculated as described in Appendix A4. For convenience an effective spin system resolved Bremsstrahlung coefficient was defined so that the parent/spin system resolved composite radiated power coefficient is given as

$$P_{\gamma \rightarrow \rho}^{RB} = SSYSWT_{\gamma \rightarrow \rho} \cdot P_{\gamma}^B + P_{\gamma \rightarrow \rho}^{RC} + P_{\gamma \rightarrow \rho}^{RS} + P_{\gamma \rightarrow \rho}^{RR} \quad 3.4.11$$

where SSYSWT is the spin system weight of the recombined spin system. As for the effective recombination coefficients, the radiated power coefficients do not need to be summed over intermediate states.

## Numerical Evaluation of Ionisation Coefficients

This section has to be completed.

## Calculation Methodology

This section has to be completed

Table 3.4c

Driver data set `./.../adas/adj25/bns97#b/bns97#b_c1.dat` for population calculation

&FILLINFO							
24	24	4.00D+06	0.00D+00	2.00D+00	1.00D+00	1.00D+00	1.00D+00
0	4	1	0				
1.28D+03	1.28D+04	1.28D+05	1.28D+06	1.28D+07	1.28D+08	3.84D+08	
1.28D+09	3.84D+09	1.28D+10	3.84D+10	1.28D+11	3.84D+11	1.28D+12	
3.84D+12	1.28D+13	3.84D+13	1.28D+14	3.84D+14	1.28D+15	3.84D+15	
1.28D+16	3.84D+16	1.28D+17					
2.00D+03	2.80D+03	4.00D+03	6.00D+03	8.00D+03	1.20D+04	2.00D+04	
2.80D+04	4.00D+04	6.00D+04	8.00D+04	1.20D+05	2.00D+05	2.80D+05	
4.00D+05	6.00D+05	8.00D+05	1.20D+06	2.00D+06	2.80D+06	4.00D+06	

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6.00D+06 8.00D+06 1.20D+07
0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00
0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00
0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00
0.00D+00 0.00D+00 0.00D+00
2.00D+03 2.80D+03 4.00D+03 6.00D+03 8.00D+03 1.20D+04 2.00D+04
2.80D+04 4.00D+04 6.00D+04 8.00D+04 1.20D+05 2.00D+05 2.80D+05
4.00D+05 6.00D+05 8.00D+05 1.20D+06 2.00D+06 2.80D+06 4.00D+06
6.00D+06 8.00D+06 1.20D+07
2.50D 04 0.00D 00
1 520 24
1 2 3 4 5 6 7 8 9 10 12 15 20 30
40 50 70 100 150 200 250 300 400 500
0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00
0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00
0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00 0.00D+00
0.00D+00 0.00D+00 0.00D+00
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PRT= 1 TRMPRT= (1S) SPNPRT= 1 NCTPRT=1000 SYS= 1 SPNSYS= 2
NMNIN= 2 JDEF= 5 .506 .000 .000 .000 .000
2 1.49413 .75000 .00000 1.00000
4
4 3 2.3250 1.0000 1000 .09690 .80543 .00000 0.00D+00
2 2 1.3704 .8750 1000 .26006 .26181 .00000 0.00D+00
2 2 1.3704 .8750 3 .31078 .01690 .00000 0.00D+00
7 2 1.3704 .8750 3 .34408 .02847 .00000 0.00D+00
FIT PARAMETERS FOR GP
1 0 IBSEL1= 1
JPRT= 1 PRTWHT= 1.000 IBSEL= 14
JPRT= 2 PRTWHT= .000 IBSEL= 0
3
1.000 2 6.20750 2 .76750 1 .44804
5.08D-12 4.10D-12 3.55D-12 3.72D-12 4.17D-12 4.73D-12 6.89D-12
1.41D-11 2.86D-11 4.56D-11 5.20D-11 5.08D-11 3.89D-11 2.96D-11
2.07D-11 1.30D-11 9.13D-12 5.37D-12 2.65D-12 1.65D-12 9.85D-13
5.45D-13 3.57D-13 1.96D-13
4.75D-71 2.05D-53 3.66D-40 7.93D-30 1.22D-24 2.00D-19 3.23D-15
2.17D-13 5.35D-12 6.89D-11 2.59D-10 1.05D-09 3.52D-09 6.16D-09
9.56D-09 1.36D-08 1.63D-08 1.93D-08 2.18D-08 2.26D-08 2.28D-08
2.24D-08 2.18D-08 2.06D-08
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PRT= 2 TRMPRT= (3P) SPNPRT= 3 NCTPRT= 4 SYS= 1 SPNSYS= 2
NMNIN= 2 JDEF= 5 .672 .000 .000 .000 .000
2 1.65579 .75000 .00000 1.00000
4
4 3 2.3250 1.0000 1000 .08546 .29255 .00000 0.00D+00
3 3 2.3250 .9444 1000 .18864 .05456 .00000 0.00D+00
2 3 2.3250 .9444 1000 .22059 .56857 .00000 0.00D+00
2 3 2.3250 .9444 5 .27495 .11796 .00000 0.00D+00
FIT PARAMETERS FOR GP
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JPRT= 1 PRTWHT= .000 IBSEL= 0
JPRT= 2 PRTWHT= 1.000 IBSEL= 15
3
1.000 2 6.20750 1 .76750 2 .39080
2.56D-12 2.78D-12 2.59D-12 2.07D-12 1.65D-12 1.13D-12 6.73D-13
4.90D-13 3.80D-13 3.43D-13 3.55D-13 3.72D-13 3.33D-13 2.75D-13
2.06D-13 1.37D-13 9.91D-14 6.01D-14 3.07D-14 1.94D-14 1.18D-14
6.61D-15 4.38D-15 2.44D-15
8.89D-63 2.20D-47 8.14D-36 8.67D-27 2.96D-22 1.07D-17 5.18D-14
2.07D-12 3.43D-11 3.20D-10 1.00D-09 3.26D-09 8.77D-09 1.36D-08
1.92D-08 2.50D-08 2.85D-08 3.21D-08 3.45D-08 3.48D-08 3.44D-08
3.32D-08 3.19D-08 2.98D-08
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NMNIN= 2 JDEF= 5 .540 .000 .000 .000 .000
2 1.49144 .75000 .00000 1.00000
4
4 3 2.3250 1.0000 1000 .08546 .29255 .00000 0.00D+00
3 3 2.3250 .9444 1000 .18864 .05456 .00000 0.00D+00
2 3 2.3250 .9444 1000 .22059 .56857 .00000 0.00D+00
2 3 2.3250 .9444 5 .27495 .11796 .00000 0.00D+00
FIT PARAMETERS FOR GP
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JPRT= 1 PRTWHT= .000 IBSEL= 0
JPRT= 2 PRTWHT= 1.000 IBSEL= 18
3
1.000 2 6.20750 1 .76750 2 .45794
5.19D-12 5.61D-12 5.23D-12 4.18D-12 3.34D-12 2.29D-12 1.37D-12
9.98D-13 7.74D-13 6.99D-13 7.21D-13 7.52D-13 6.73D-13 5.56D-13
4.17D-13 2.78D-13 2.00D-13 1.22D-13 6.23D-14 3.94D-14 2.40D-14
1.35D-14 8.98D-15 5.02D-15
3.97D-72 4.20D-54 1.46D-40 5.35D-30 1.07D-24 2.27D-19 4.53D-15
3.33D-13 8.74D-12 1.17D-10 4.42D-10 1.75D-09 5.52D-09 9.26D-09
1.38D-08 1.89D-08 2.20D-08 2.55D-08 2.80D-08 2.87D-08 2.86D-08
2.78D-08 2.69D-08 2.53D-08
-----
&FILINFO NUCCHG=-1, NPARNT=0, SEQ='--', XRMEMB=' ', &END

```

Table 3.4d

Cross-referencing data set `./../adas/adf18/a09_p204/nrb96#b#b/nrb96#b_c1n.dat` for access to bundle-nS dielectronic recombination data for population calculation.

```

ADAS204 driver dataset.
-----
"ADASCENT"/adf25/bns96#b/bns96#b_c1.dat

```

```

Dielectronic recombination files.
-----
"ADASCENT"/adf09/nrb93#be/nrb93#be_c2ls22.dat      : 1st. file of diel. data
"ADASCENT"/adf09/nrb93#be/nrb93#be_c2ls23.dat      : 2nd. file of diel. data

Output file.
-----
"ADASUSER"/pass/adas204.pass      : passing file (not used at present)

Parent cross-reference lists for maincl and Badnell files
-----

   mn.      bd1.      bd2.      bd3.      bd4.      bd5.      bd6.
   ---      ---      ---      ---      ---      ---      ---
     1         1         1         1         1         1         1
     2         2         2         2         2         2         2

Supplementary LS-breakdown autoionisation data between parent spin pairs
-----

(pmni,isysi ; pmnf)      ncut1      A Auger      slope
-----
   2      2      1         4      1.509d+09
   5      2      1         5      1.401d+09
   6      2      1         6      1.454d+09
   7      2      1         7      1.454d+09
   8      2      1         8      1.278d+09
   9      2      1         9      1.048d+09
  10      2      1        10      8.889d+08
  11      2      1        11      7.198d+08
  12      2      1        12      6.187d+08
  13      2      1        13      4.824d+08
  14      2      1        14      4.139d+08
  15      2      1        15      3.592d+08
  16      2      1        16      3.993d+08
  18      2      1        18      2.227d+08
  20      2      1        20      1.581d+08
  22      2      1        22      1.083d+08
  25      2      1        25      6.297d+07      -5.00

```

**Concluding Remarks**

This section has to be completed

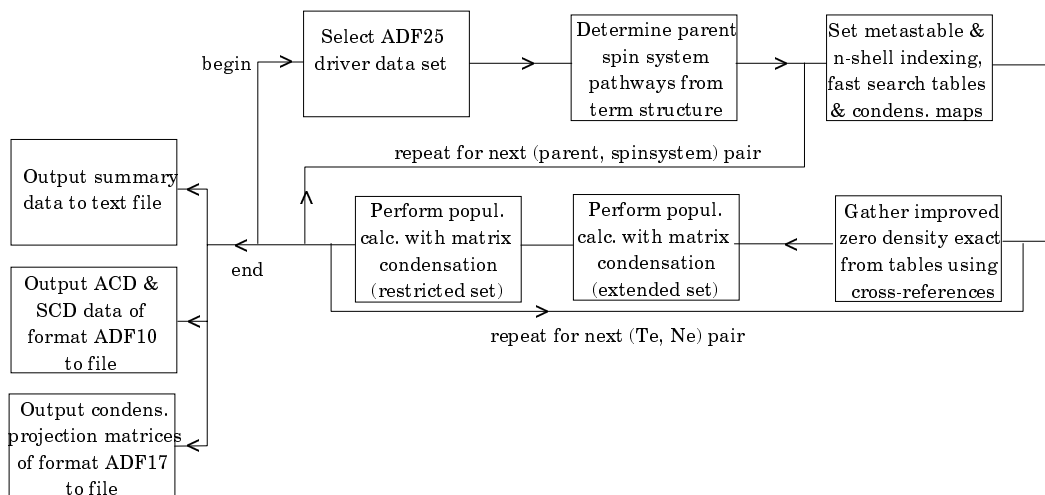
**Auto-ionisation From Excited States**

This section has to be completed

**Program steps:**

These are summarised in figure 3.4.

Figure 3.4



## Interactive parameter comments:

Move to the directory in which you wish any ADAS created files to appear. These include the output text file produced after executing any ADAS program (*paper.txt* is the default). There is no graphical output from ADAS204. Initiate ADAS204 from the program selection menus in the usual manner.

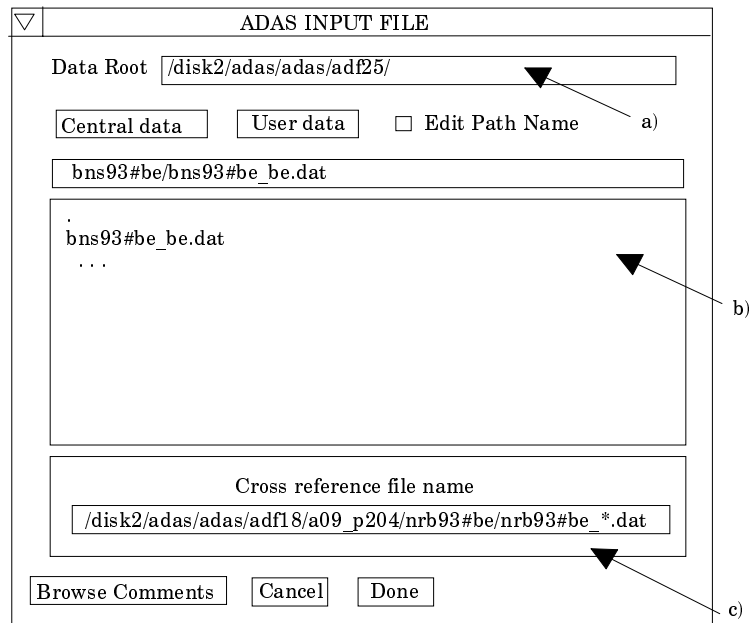
The **file selection window** appears first as illustrated below.

1. Driver data sets for ADAS204 are defined by ADAS data format *adf25*. The program automatically sets the Data Root at a) to this class.
2. Data root a) shows the full pathway to the appropriate data subdirectories of type *adf25*. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. Click the *User Data* button to insert the pathway to your own data. Note that your data must be held in a similar file structure to central ADAS, but with your identifier replacing the first *adas*, to use this facility.
3. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.
4. Available sub-directories are shown in the large file display window b). Scroll bars appear if the number of entries exceed the file display window size.
5. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then its sub-directories in turn are displayed in the file display window. Ultimately the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
6. Once a data file is selected, the set of buttons at the bottom of the main window become active.
7. The driver data sets are not very informative with an unhelpful condensed layout. However they can be created automatically by execution of the code ADAS407. This latter code has several purposes. When we originally used ADAS407 to produce drivers for ADAS204, they were really just templates and required quite a bit of hand adjustment. The present version of ADAS407 produces an almost ready to use driver. It just requires setting of reference indices if you wish to access ground state ionisation data of better quality than ADAS204's default. This is a worthwhile step if you wish the '*scd*' output from ADAS204 to be accurate and are not simply concerned with relaying condensed projection data to ADAS208.
8. A second Cross-reference file must be selected at d). This file specifies what high quality n-shell resolved dielectronic data of ADAS data format *adf09* is to be used and how it should be mapped onto the n-shells of the ADAS204 calculation. The file name sub-directory is includes *adf18/a09\_p204* which reflects its purpose. *adf18* contains all the ADAS cross-referencing files in



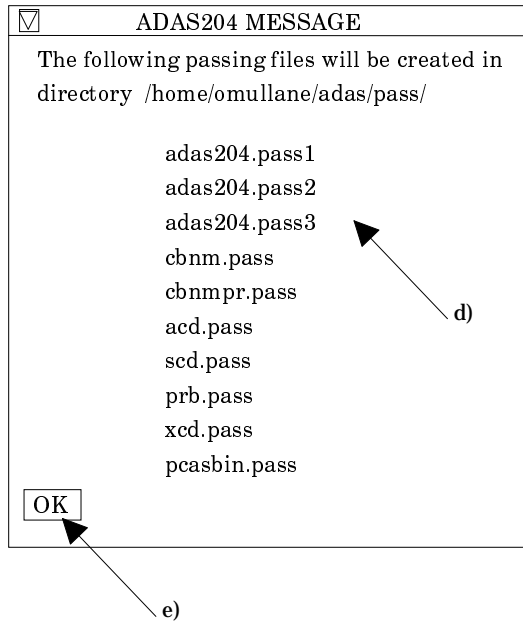
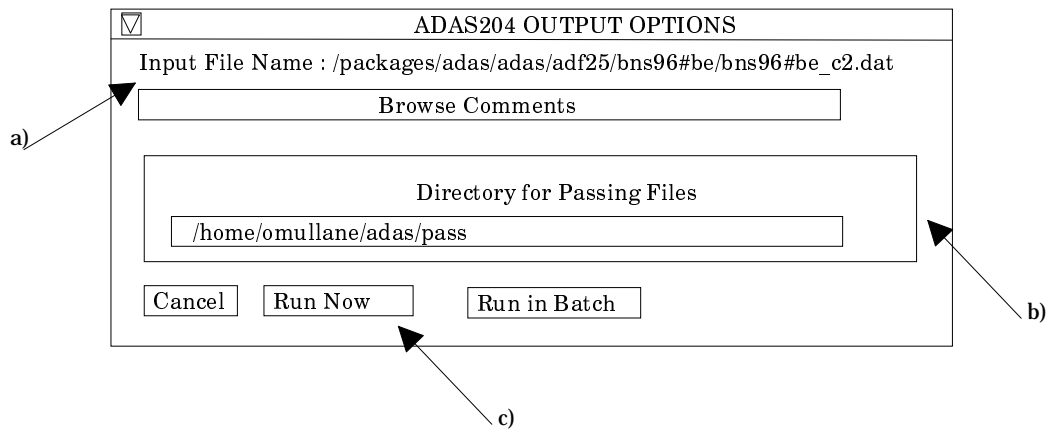
various sub-directories. ADAS204 constructs a cross-reference file name automatically according to the choice of driver data set made at c). However the file name is editable. The current default sets the *nrb93* subdirectory. Our newer dielectronic data is in *nrb96*. Note the ‘\_’ at the end of the name. This is sufficient and a fully resolved name is not required.

9. Clicking on the *Browse Comments* button displays any information stored with the selected driver dataset.
10. There is no Processing Options window with ADAS204.

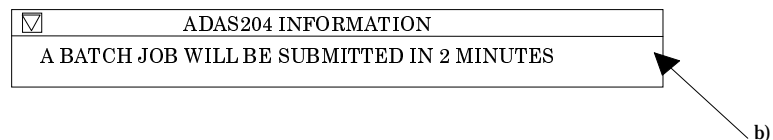
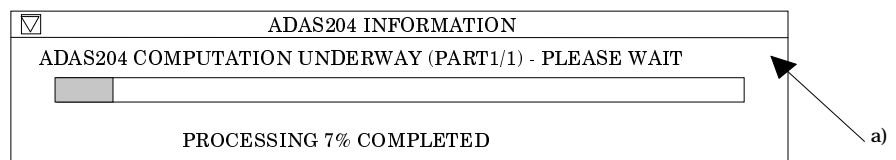


The **output options window** is shown below.

11. The driver data set name is given at a) for information and comments attached to it can be browsed as usual.
12. There is no graphical output from ADAS204.
13. The main output data set production is routed to the directory identified at b). This is your ‘pass’ directory by default, but the directory name is editable if you wish to change this. Note that several datasets are created by ADAS204 and these can be of quite substantial size if you use the current temperature and density grids set by default in the driver dataset.
14. The code can be run in foreground or in batch. Make the appropriate selection at c). The message shown below pops up to advise you of the output datasets which will be created. This message may be out of date. We are currently suppressing the *pass1*, *pass2* and *pass3* files internally. There are quite large text files and are of rather specialist interest for the progress of parts of the calculation. The *cbnm.pass* file contains the condensed projection matrices for use by ADAS208. The file is ASCII but with long lines and is not very readable. A shortened version of it is given in *cbnmpr.pass* which can be sent to a line printer. *pcasbin.pass* is a special output created by Billy Dickson and Martin O’Mullane which they may reveal the purpose of in the future! Other output datasets are the conventionally named collisional-radiative datasets.



15. On foreground launch of ADAS204, the progress meter shown at a) below appears. Note that the calculations may be quite long with 20-30 minutes on a medium power workstation typical, so batch processing is probably to be preferred.
16. On batch submission, the information pop-up at b) below appears and the job initiates in 2 minutes. If your system requires special queuing for long jobs, please let us know and we can include this in the batch submission.



**Illustration:**

This section has to be completed

**Notes:**