
ADAS701: Autostructure

The code is a full implementation of the program AUTOSTRUCTURE developed by N. R. Badnell. The entire capability of the original program for arbitrary structure, Auger rate and Radiative rate calculation has been retained. However input driver file selection, driver templates, output selection and output routing have been enabled within the ADAS framework to simplify the production of two types of data, namely dielectronic recombination rates and data for doubly excited state (satellite line) models.

Background theory:

AUTOSTRUCTURE [1] is a general program for the calculation of atomic and ionic energy levels, radiative and autoionization rates, and photoionization cross sections in LS or intermediate coupling using non-relativistic (IC) or semi-relativistic (ICR) wavefunctions. It is, in effect, a superset of SUPERSTRUCTURE [2] on which it was initially based.

The nuclear charge and the level of accuracy desired determines whether LS, IC or ICR coupling should be chosen. The configurations to be chosen include those for which data is wanted plus, optionally, additional configurations to improve accuracy - a configuration interaction (CI) expansion. This defines a unique angular algebra problem. The CI expansion is related closely to the choice of radial functions. The better the choice of radial functions, the smaller the CI expansion required to obtain a given level of accuracy which in turn leads to a smaller computational problem. Each (nl) radial function is calculated in a model potential - Thomas-Fermi (TF) or Slater-Type-Orbital (STO). Both contain scaling parameters. These scaling parameters can be optimized automatically by minimizing a weighted sum of term energies chosen by the user.

The LS, IC or ICR Hamiltonian is diagonalized to obtain e-energies and e-vectors with which to construct the rates. In the case of autoionization, the target N-electron and (N+1)-electron Hamiltonians are automatically diagonalized separately. The continuum orbitals are (TF or STO) distorted waves, their energy being uniquely determined by energy conservation for a given autoionizing state and continuum. (Integrals of) the continuum orbitals are efficiently and accurately interpolated from a small (~ 10) basis set which spans the range of possible energies (zero to the highest core excitation energy). Entire Rydberg series can be efficiently looped over for user supplied representative n (and l -range) for the nl Rydberg orbital. There is no limit on the size of n . The program seamlessly and accurately moves through $n=2-1000$, say. It does so by using suitably normalized zero-energy continuum orbitals in place of explicit high- nl bound orbitals, along with numerical techniques adopted from scattering theory. The two are identical in the limit: n tends to infinity. While this correspondence is the root of the (approximate) n^{-3} scaling of autoionization rates used by many codes, no such scaling is done here. The full Hamiltonians are diagonalized for each n , so tracking the variation in CI mixing along a series and the opening-up of new high-lying autoionizing channels.

The data calculated here, in part or in total, can be post-processed to generate dielectronic rate coefficient data in ADAS data format *adf09* and data for doubly excited state population and satellite line emission modelling in ADAS specific ion file data format *adf04*.

[1] N. R. Badnell, J.Phys.B19, 3827 (1986)

[2] W. Eissner, M. Jones and H. Nussbaumer, CPC8, 270 (1974)

Setting up the driver data set

Configuration Input: If the first four characters of the first line are S.S. then configurations are read in fixed-format Eissner notation (detailed below in an appendix) followed by an orbital redefinition line, exactly as in SUPERSTRUCTURE. If the first four characters of the first line are A.S. then the NAMELIST SALGEB is read first then free-format orbital definitions and configuration occupation numbers follow.

Example 1.

(Cr).

```
S.S.  
123456789 46518519 46517519 56518 46517518 4651751C 4651851B 56517  
         4651B51C  
         10 20 21 30 31 32 40 41 42 43 50 51 52 53 54
```

Notes The configurations and (optional) orbital (re-) definition are as in SUPERSTRUCTURE (because of S.S. tag). However, nothing is read from line 2 in columns 1-10, while columns 73-80 should be left blank. See the Appendix for an explanation of how to specify new, or read existing, configuration lists.

Namelists:

SALGEB:

RUN = ' ', default. Allows calculation of energies (LS or IC), radiative rates (if RAD is set) and autoionization rates (if continuum present - see optional input below).

= 'PI', will calculate (non-resonant) photo-ionization as well if continuum orbitals are present.

= 'DR','RR','RE','DI','REDA' or 'YES'. All expect one or more Rydberg orbitals to be defined (via the orbital definition list - see optional input below) and will read the optional namelist DRR to define the *nl* values of the Rydberg series to be run over. 'DR' calculates energies, radiative and autoionization rates. 'RR' calculates non-resonant radiative recombination in addition. In both these cases, if no radiation is specified, E1 will be switched on. 'RE','DI','REDA' are all equivalent and differ from 'DR' only via 'NO' radiation being a valid option.

RAD = 'E1' or 'YES' for electric dipole radiation. (Default for RUN='DR' etc.)

= 'NO' for no radiative data. (Default for RUN=' ')

= 'E2' or 'M1' for electric quadrupole and magnetic dipole radiative transitions, in addition to electric dipole.

CUP = 'LS' for LS-coupling. (Default)

= 'IC' for intermediate coupling.

= 'ICR' for IC using semi-relativistic wavefunctions.

KORB1 and KORB2 or KCOR1 and KCOR2 denote closed shells (use one or the other) e.g. KORB1=1 KORB2=3 denotes a Ne-like core (assuming standard order).

MSTART=0 (default) does nothing.

=1 writes the angular algebra to file RESTART

=4 reads the angular algebra from RESTART. This is useful for iso-electronic runs in cases when the angular algebra takes a significant time to compute.

(=2,3 restarts an incomplete calculation of RESTART.)

KUTSS controls valence-valence two-body fine-structure interactions.

=-1 None. (Default)

=-9 All.

|KUTSS| .gt. 1 includes the interactions for the first |KUTSS| configurations, KUTSS positive neglects the interaction between distinct configurations.

KUTSO controls the evaluation of the generalized spin-orbit parameter.

= 0 All.

< 0; include interactions between the first -KUTSO configurations and within a configuration for the remainder. (Default=-1)

> 0; include interactions within a configuration for the first KUTSO configurations and neglect all for the remainder.

KUTOO controls the evaluation of the two-body non-fine-structure interactions viz. contact spin-spin, two-body Darwin and orbit-orbit (only available in IC).

= 0 or -1 neglected. (Default)

else all included.

NAST= The number of distinct S_Lp terms (listed following if .gt. 0 as 2S+1 L p) generated from the configuration list, can be used with care in IC. If .eq. 0 all possible terms are generated (default).

KCUT= 0 all configurations are treated as spectroscopic (default).

> 0 configuration numbers greater than KCUT are treated as correlation, terms are only generated from them if they also exist in the spectroscopic list. Correlation terms are ignored when forming the energy functional during optimization and no transition probabilities (autoionization or radiative) are calculated for them.

If the first four characters of line 1 are A.S. then two new variables must be defined:

MXVORB is the number of distinct valence orbitals required to describe the configurations.

MXCONF is the number of configurations.

Example 2.

(Cr again).

```
A.S. The rest of the first line can be used as a header e.g. Cr 7S-7P
&SALGEB  RUN=' ' RAD='YES' CUP='LS' MXVORB=7 MXCONF=8
          KORBI=1 KORB2=5 NAST=2 KUTSS=-1 KUTSO=-1 KUTOO=-1 &END
3 2 4 0 4 1 4 2 4 3 5 0 5 1
4 0 1 1 0 0 0
4 1 0 1 0 0 0
5 0 1 0 0 0 0
4 1 1 0 0 0 0
4 1 0 0 0 0 1
4 0 1 0 0 1 0
5 1 0 0 0 0 0
4 0 0 0 0 1 1
7 0 0
7 1 1
```

- Notes
1. The alternative (new) way of inputting configurations.
 2. Using the configurations of the first example would have been time consuming without the use of NAST as they contain hundreds of terms.
 3. The NAMELIST specification must start in column 2 or greater (at least with many FORTRAN77 compilers).

SMINIM:

NZION = Nuclear charge. This must be set.

.gt. 0 radial functions are calculated in TFDA potential.

.lt. 0 radial functions are calculated in Hartree potential evaluated with Slater-Type-Orbitals. (Preferred)

By default, nl-dependent operation is assumed and the orbitals are Schmidt orthogonalised. Even if the orbitals happen to be orthogonal there is little overhead to the nl-dependent operation and it is not worth the hassle switching it off.

.eq. 0 stops the code after computation of the angular algebra. Useful for restart.

INCLUDE .eq. 0 no variational procedure. (Default)

.gt. 0 include the lowest INCLUDE terms in the energy-sum to be minimised.

.lt. 0 include -INCLUDE terms in energy sum, the T-index labels and weighting factors follow next (before the lambdas, see below).

Note: the T-index is required, not the I-index. This is output on the term energy list from a trial run.

NLAM is the number of (lambda) scaling parameters. Both TFDA and STO Hartree potentials contain a radial scaling parameter.

= 0 all lambda's equal unity. (Default)

If NLAM is less than the number of orbitals then the last scaling parameter read will be used for the remaining orbitals.

NVAR is the number of variational parameters. This decoupling of NVAR and NLAM greatly simplifies the variational operation. NVAR orbital numbers will be read and their scaling parameters varied. (The variation only takes place when INCLUDE is set non-zero.) Default=0.

Note: The scaling/variational parameters are normally positive numbers around 1. This gives a "physical" orbital. Pseudo-orbitals are generated with negative lambdas. The default is a screened hydrogenic potential of charge $|\lambda * NZION|$. However, if

ORTHOG='LPS' then Laguerre pseudo-states are generated for that nl. The lambda is then the scaling parameter associated with the Laguerre orbital, with the Z dependence factored out so that |1.0| is usual. Only specify if needed.

MCFMX: Case of STO Hartree/X potentials. MCFMX configuration numbers are read, one for each orbital. The Hartree potential, for each orbital, uses the occupation numbers from the specified configuration. If the number of orbitals is .gt. MCFMX the last configuration is used for the remaining orbitals. Default=0, and an average of all configurations is used.

MEXPOT = 0 (default) the STO potential is Hartree.

= 1 a local exchange term is added to the Hartree potential.

PRINT='FORM' (default) gives detailed formatted output (to file olg) for a structure run. Energy/Rate files for DR/RE run are formatted (ols, oic, opls, opic).

= 'UNFORM', limited writes to file olg and the Energy/Rate files for DR/RE are unformatted (olsu, oicu) but opls & opic are still formatted.

RADOUT='YES' produces a radial file (radout) suitable for R-matrix STG1 S.S. style.

= 'NO' doesn't. (Default)

RAD='BF' only produces radiative rates between autoionizing and true bound states (useful for DR).

= ' ' Default, all.

Example 3.

(Cr still).

```
&SMINIM NZION=24 INCLUDE=-1 NLAM=12 NVAR=2 PRINT='FORM' RADOUT='NO' &END
6 1.0
1.4361 1.1326 1.0754 1.0816 1.0636 1.0878 0.9223 0.9446 -0.4324 0.0000
1.0000 1.0000
11 12
```

Note: The 5s and 5p orbitals (11 and 12) are being optimised on term number 6 of the term table, which wasn't the lowest in energy hence INCLUDE=-1. Note also that the 4d is a scaled hydrogenic orbital and the 4f orbital is not being used, its lambda value is irrelevant.

Example 4.

(Si¹¹⁺).

```
S.S.
123456789 11522 11512513 11523
21512 21513
21514 21515 21516
10 20 21 30 31 32
&SALGEB RAD='E1' CUP='IC' KUTSS=-1 KUTSO=-1 KUTOO=-1 &END
&SMINIM NZION=-14 PRINT='FORM' MCFMX=6 &END
6 2 2 6 7 8
```

Note The orbital must appear in the configuration specified for its generation. Thus, if any other configuration besides 6 had been specified for orbital 4 (the 3s) an error would have resulted. No scaling parameters were specified so they would be taken to be unity, which is a much better approximation than for TFDA.

Supplementary input (required for subsequent processing by ADAS702 and ADAS703): The orbital (re-) definition list is used to "tag" orbitals for special attention if their principal quantum numbers are as follows:

n=90-99: A continuum orbital. If continuum orbitals are present then SR.RADCON is entered for their generation and a namelist SRADCON is read to control it.

SRADCON:

MENG is the number of interpolation energies. MENG energies (in Rydbergs) follow and the continuum orbitals are calculated at those energies.

.lt. 0, only the range need be specified and the -MENG interpolation energies will be chosen internally.

NREL, there is no interpolation of the bound-continuum relativistic integrals. They are calculated at a single energy. The NREL'th interpolation energy is used. Defaults to (MENG+1)/2 if not specified.

Example 5.

(LMM transitions in Si¹¹⁺).

```
S.S. A short TITLE (8 chars.) may be set in SALGEB, or a longer one here.
123456789 24 14515 14516 25 15516 26
      12518 12519 1251A 1251B 1251C
      13518 13519 1351A 1351B 1351C
      12514 12515 12516
      13514 13515 13516
          10 20 21 30 31 32   900901902903904
&SALGEB RUN=' ' RAD='E1' CUP='IC' KCOR1=1 KCOR2=1 TITLE='2-3,3' &END
&SMINIM NZION=-14 PRINT='UNFORM' MCFMX=8 &END
17 17 20 1 2 3 0 7
&SRADCON MENG=-10 &END
      2.0000 15.0000
```

Note: Ten interpolation energies are used, between 2.0 and 15.0 Rydbergs. All of the continuum orbitals will be generated using the Hartree potential with occupation numbers given by configuration 7. The requirement that the orbital belong to the configuration is relaxed for continuum orbitals, the configuration merely has to contain a continuum orbital.

For RUN=' ', as here, the continuum orbital angular momenta are those specified on the orbital definition line. Thus we have ks, kp, kd, kf and kg continua.

For RUN.ne.' ' the continuum angular momenta are "matched" to that of the valence orbital (defined by *n=80-89*, see next section) but those with *n=99* are NEVER redefined. This is important for inner-shell transitions which may have an autoionization pathway that is independent of the Rydberg orbital. Note: it makes no sense (and could cause problems here) to define two continuum orbitals *n=90-98* with the same angular momentum.

n=80-89: A valence/Rydberg orbital that will be redefined in DR/RE operation. If RUN.ne.' ' the namelist DRR is read to define the *nl*-values that AUTOSTRUCTURE will loop-over for these orbitals.

DRR:

NMIN, NMAX: Loop the valence orbital over *n=NMIN* to *NMAX* incrementing *n* by 1.

JND = 0, default.

.gt. 0, then JND additional *n*-values are read following the namelist. AS inserts an additional *n*-value between each input value to aid interpolation and numerical integration over *n* in the post-processing routines.

NRAD =50, default. In DR runs the radiation from high-*n* is negligible and the effect of the Rydberg orbital on the core is small. So, for *n.gt.NRAD* no new radiative rates are calculated. The default value is sufficient for most cases.

LMIN, LMAX: Loop the valence orbital over *l=LMIN* to *LMAX* incrementing *l* by 1. If no valid LMIN & LMAX are set then the loop over *n* is done using the

angular momenta specified in the orbital definition. This enables *l*-mixing along a Rydberg series to be investigated.

LCON is the number of continuum orbitals used with $n=90-98$. This is not used if there is no loop over valence *l*. As noted above, the continuum orbitals ($n=90-98$, only) must have their angular momenta kept synchronised with that of the valence orbital. Let *l_c* denote the continuum angular momenta and *l_v* the valence angular momentum. Then the internal assignment is $l_c=l_v-(LCON-1)/2$, $l_v-(LCON-1)/2+1$, ..., $l_v+LCON/2$. Generally, LCON should be set (and the appropriate orbitals and configurations defined) to $2*LAMAX+1$ where LAMAX is the largest target multipole transition required. Thus, LCON=3 for dipole, and =5 for quadrupole core transitions as well.

Example 6.

(Si¹¹⁺ DR via 2s-2p core transition).

```
S.S.
123456789 12515 13515
           12517 12518 12519
           13517 13518 13519
           22 12513 23
                10 20 21 801 900901902
&SALGEB RUN='DR' RAD='E1' CUP='IC' TITLE='2-2,n' KCOR1=1 KCOR2=1 &END
&DRR NMIN=8 NMAX=15 JND=14 LMIN=0 LMAX=13 LCON=3 &END
      16 20 25 35 45 55 70 100 140 200 300 450 700 999
&SMINIM NZION=-14 PRINT='UNFORM' MCFMX=7 &END
      3 1 2 0 1 0 3
&SRADCON MENG=-7 &END
      0.00 2.50
```

- Notes
1. The angular momenta of the valence and continuum orbitals in the orbital redefinition list is arbitrary, although in the case of the continuum they should be distinct. The choice of $n=80$ is arbitrary, any value between 80 and 89 would suffice. Similarly, for the continuum any value between 90 and 98 would suffice (but NOT 99).
 2. Only outer electron radiation into the core is specified. Outer electron radiation into higher states will be added-in (hydrogenically) during post-processing.

Example 7.

(Si¹¹⁺ DR via an inner-shell transition, 1-3).

```
S.S.
123456789 11512514517 11512515517 11512516517
           11513514517 11513515517 11513516517
           21512518 21512519 2151251A 2151251B 2151251C
           21513518 21513519 2151351A 2151351B 2151351C
           11522518 11522519 1152251A 1152251B 1152251C
           11512513518 11512513519 1151251351A 1151251351B 1151251351C
           11523518 11523519 1152351A 1152351B 1152351C
           2151751D 2151751E 2151751F
           2151751G
           21514518 21515518 21516518
           21514519 21515519 21516519
           2151451A 2151551A 2151651A
           2151451B 2151551B 2151651B
           2151451C 2151551C 2151651C
           21513514 21513515 21513516 21513517
           21512514 21512515 21512516 21512517
           10 20 21 30 31 32802900901902903904990991992 X
           993
&SALGEB RUN='DR' RAD='E1' CUP='IC' TITLE='1-3,n'
           KORB1=0 KORB2=0 &END
&DRR NMIN=4 NMAX=10 JND=0 LMIN=0 LMAX=2 LCON=5 &END
&SMINIM NZION=-14 PRINT='UNFORM' MCFMX=8 &END
      7 7 12 1 2 3 1 7
&SRADCON MENG=-15 &END
      0.0000 200.0000
```

- Notes
1. The D, E, F and G continuum orbital angular momenta do not get redefined.
 2. We allow for quadrupole transitions (LCON=5).
 3. It is safest to define only those continuum orbitals that are used in the configuration list.
 4. The target + continuum configurations $1s^22s$, $1s^22p$, $1s2s2p$, $1s2s^2$, $1s2p^2$, $1s^23s$, $1s^23p$, $1s^23d$ +e⁻ should have the same continuum expansion attached to them. If the $1s2s^2$ had orbitals 8,9,A,B,C attached but the $1s2p^2$ 8,A,C only, say, then there would be no mixing between the $1s2s^2$ and $1s2p^2$ ¹S terms for the $1s2s^2$ 9 and B configurations. This will cause the post processor some problems.
 5. The orbital definition list was extended to a second line using a non-blank character in column 63. The orbital definition list is formatted (T16,15(I2,A1)). Hence the continuation mark is two spaces past the last (15th) orbital.

Example 8.

(Si¹¹⁺ LMn with *l*-mixing within the complex).

```
S.S.
```

```

123456789 14517 15517 16517
          14518 15518 16518
          14519 15519 16519
          1451A 1551A 1651A
          1251B 1251C 1251D 1251E 1251F 1251G
          1351B 1351C 1351D 1351E 1351F 1351G
          12514 12515 12516 12517 12518 12519 1251A
          13514 13515 13516 13517 13518 13519 1351A
              10 20 21 30 31 32800801802803900901902903904 X
              905
&SALGEB RUN='DR' RAD='E1' CUP='IC' KCOR1=1 KCOR2=1 TITLE='2-3,n' &END
&DRR NMIN=4 NMAX=9 JND=0 LMIN=0 LMAX=-5 &END
&SMINIM NZION=14 PRINT='UNFORM' MCFMX=0 &END
&SRADCON MENG=-15 &END
          00.0000 25.0000

```

Note Only *l*-mixing for 0,1,2,3 is investigated here. Also we cannot start with *n*. Je. 3 the maximum *l*-mixing investigated. Thus the lowest few *n* must be run separately. LCON is not required.

n=70-79: An orbital to be replaced in SR.RADWIN. If there exists an orbital tagged for replacement SR.RADWIN is entered and a namelist is read.

SRADWIN

KEY=-9, default.

If the input file (radwin) is in Opacity Project format (approx. the old IMPACT format) nothing need be entered here. See code for details of alternative formats i.e. different KEY values.

Example 9.

(Cr yet again).

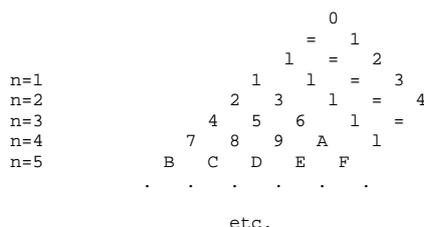
```

A.S. Cr MCHF
&SALGEB RUN=' ' RAD='E1' CUP='LS' MXVORB=7 MXCONF=8
          KCOR1=1 KCOR2=-5 NAST=2 &END
71 0 72 0 72 1 73 0 73 1 73 2 74 0 74 1 74 2 74 3 75 0 75 1
4 0 1 1 0 0 0
4 1 0 1 0 0 0
5 0 1 0 0 0 0
4 1 1 0 0 0 0
4 1 0 0 0 0 1
4 0 1 0 0 1 0
5 1 0 0 0 0 0
4 0 0 0 0 1 1
5 0 0
5 1 1
&SMINIM NZION=24 PRINT='FORM' &END
&SRADWIN &END

```

- Notes
1. The use of negative KCOR2 to read ALL *nl* definitions (as we must if we want to replace the core orbitals as well as the valence) but valence occupation numbers only for the configurations.
 2. All of the orbitals are tagged for replacement so SMINIM requires little input. Although the use of 71 0 72 0 is suggestive of 1s and 2s replacement (and helpful) it should be noted that the 1st orbital (71 0) will be replaced by the first s-orbital in the file radwin. We could have written 72 0 71 0 and the same result would be obtained, if somewhat confusing - the 1s orbital (assuming it was in front of the 2s on radwin) would be in 72 0.

Appendix: Eissner configurations are defined by occupation numbers and orbital numbers. Each occupation/orbital-number pair is separated from the next by a '5'. Each configuration is separated from the next by a blank. They do not have to fill the line, but a new line of configurations must start with column 11. Unless redefined after the configuration list (see example 1, where the "redefinition" is actually a specification of the default) the orbital numbers (actually alphanumeric) are associated with *nl* pairs as follows:

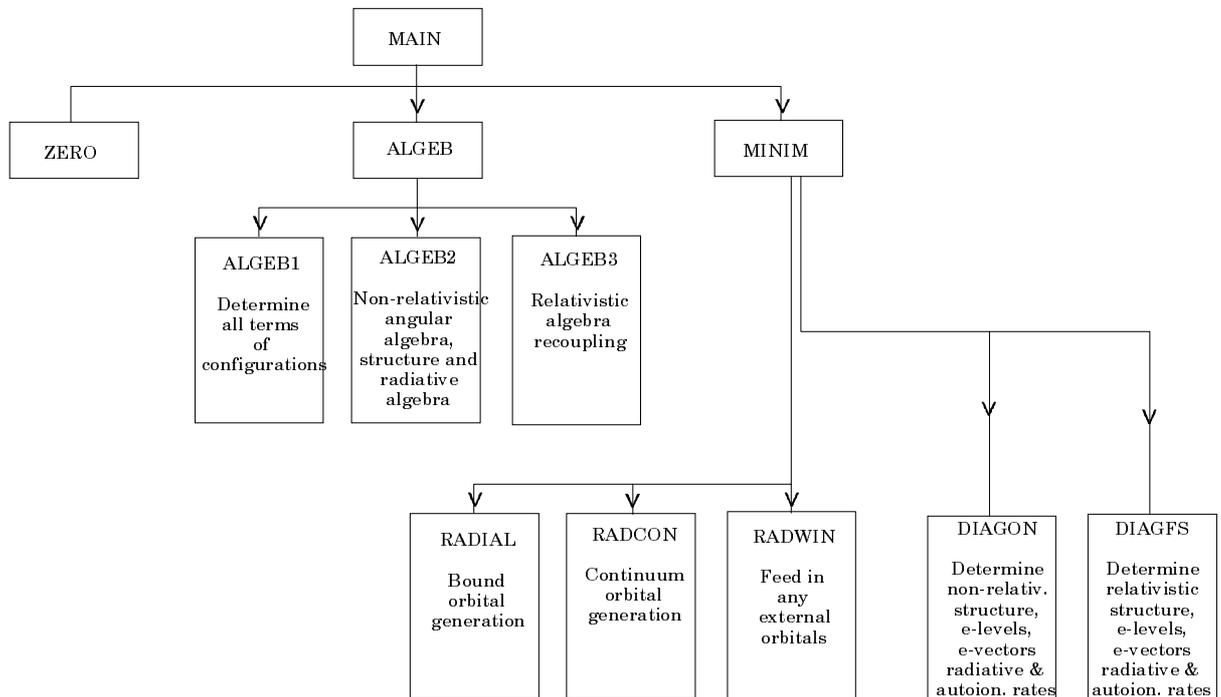


The horizontals of the triangle of numbers are of constant *n* and the upward (positive gradient) diagonals are of constant *l*. After 9 the numbers become UPPER CASE letters and eventually lower case letters (you shouldn't need them!). E.G. the configuration 2s 2p² 3d is rendered as 12523516.

Program steps:

These are summarised in the schematic below.

Figure 7.1



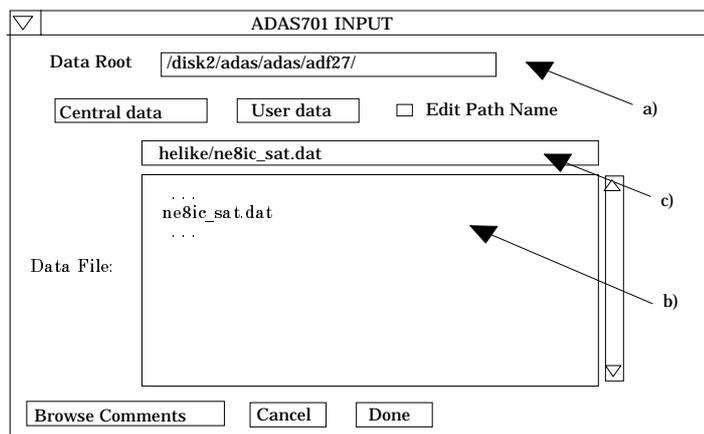
Interactive parameter comments:

Move to the sub-directory in which you wish text output from this program to appear. Initiate ADAS701 from the program selection menus in the usual manner.

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

1. Data root a) shows the full pathway to the appropriate data sub-directories. Click the *Central Data* button to insert the default central ADAS pathway to the correct data type. The appropriate ADAS data format for input to this program is *adf27* ('AUTOSTRUCTURE drivers'). Click the *User Data* button to insert the pathway to your own data. *User Data* is the default. Central ADAS contains samples from which the user can build his/her own driver. 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.
2. The Data root can be edited directly. Click the *Edit Path Name* button first to permit editing.

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. The practice in ADAS is to store drivers in sub-directories according to iso-electronic sequence of the recombining ion (eg. */belike*).



- 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. The individual data files all have the termination *.dat*. The purpose of the driver data set is indicated by the pattern of the file name as

$$/ <ion> <coupling> \{ <prt-trans> \} \{ - <n-shell> \} \{ _ <task> \} .dat$$

where *<ion>* denotes the recombining ion (eg. 'o4' for O⁺⁴)

<coupling> denotes the coupling scheme ('ls' for LS-coupling, 'ic'

for intermediate coupling)

<prt-trans> denotes the parent n-n' shell transition (eg. '23').

This

name portion does not appear for task 'sat' below '

<n-shell> denotes the outer n-shells treated, which may be a single shell (as eg. '3') or all n-shells (as eg. 'n')

This name portion does not appear for tasks '*str*' and '*sat*' below.

<task> denotes the objective ('*str*' for the baseline structure calculation, '*sat*' for satellite line data preparation) If the field is blank then the main Auger and radiative rate calculations for dielectronic rates take place.

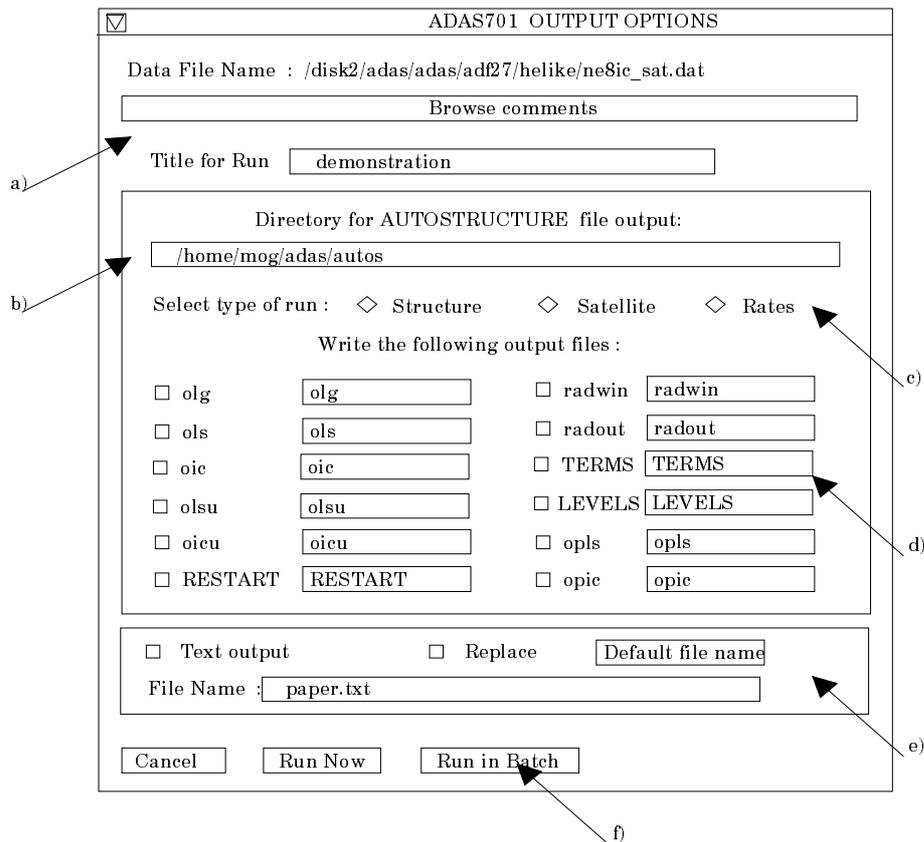
Thus '*o4ls23_str.dat*' is a driver for the n=2-3 parent transition related LS-coupled term structure calculation used to establish the resonance positions. '*o4ls23-3.dat*' and '*o4ls23-n.dat*' are for the dielectronic rate calculations with only the n=3 outer electron present and for all outer n-shells respectively. '*o4ls_sat.dat*' is for the preparation of Auger/radiative data for satellite line modelling.

- Once a data file is selected, the set of buttons at the bottom of the main window become active.
- Clicking on the *Browse Comments* button displays any information stored with the selected data file. It is important to use this facility to find out what is broadly available in the data set. The possibility of browsing the comments appears in the subsequent main window also.
- Clicking the *Done* button moves you forward to the next window. Clicking the *Cancel* button takes you back to the previous window

There is no **processing options window**

The **output options window** appearance is shown below. Note that there is no graphical output in this case

- The full pathway to the driver data set to be used is shown for information at the top of the window and at a) the *Browse comments* button is available. A title for the run may also be entered in the text widget just below.



8. The sub-window at b) allows selection of which output files from ADAS701 are to be kept and the names to be assigned to them. Up to twelve output files are available in principle. The default file names are shown and their contents are as follow:

olg detailed (diagnostic) output.
ols energies & radiative and autoionisation rates between terms (formatted).
oic energies & radiative and autoionisation rates between levels (formatted).
olsu energies & radiative and autoionisation rates between terms (unformatted).
oicu energies & radiative and autoionisation rates between levels (unformatted).
RESTART restart file
radwin input file of externally prepared radial orbitals.
radout output file of internally calculated radial orbitals.
TERMS term labelling.
LEVELS level labelling.
opls LS-coupling photo-ionisation cross-sections.
opic intermediate coupling photo-ionisation cross-sections.

9. The pathway to the directory where you wish to place the saved files in entered at b). The default is to the sub-directory './.../<user>/adas/autos'. This is a sub-directory like the usual */pass* sub-directory but is dedicated to ADAS7 series. The output may be quite substantial and exceed small workstation capacities. The text widget is editable, so an alternative path may be substituted for the default.
10. At c) , the button for the type of run is clicked. This matches the driver data set names '*str*', '*sat*' and '' described above. According to your choice, various of the temporary output files are selected for saving. The text widgets are editable and you can replace default names by names of your choice. Warnings may be issued below the file names if a file already exists and will be over-written. This is simply a warning for the user to take action before proceeding if desired. There is no further protection. Note that the same standard names are always used by default and so the user must rename if he wishes to keep data.

Deselected output files will be eliminated in a clean-up after the code has completed. For dielectronic rate production, it is usual to do the calculation in a number of stages (cf. the drivers *o4ls23-3.dat* and *o4ls23-n.dat*). The Auger & radiative rate coefficient files, 'ols' - for LS coupling or 'oic' for intermediate coupling, should be renamed for each stage successively as 'o1', 'o2', etc. This is the responsibility of the user. Note that both formatted (eg. 'oic') and unformatted (eg. 'oicu') forms of the files can be produced. For large runs it is much more economical to use the unformatted forms and they are similarly renamed (eg. 'o1u').

11. At d) the *Text Output* button activates writing to a text output file. The file name may be entered in the editable File name box when *Text Output* is on. The default file name 'paper.txt' may be set by pressing the button *Default file name*. A 'pop-up' window issues a warning if the file already exists and the *Replace* button has not been activated.
12. At the base of the graph window, buttons are available for selection of foreground execution (*Run Now*), or batch submission (*Run in Batch*). Click *Cancel* to return to the input driver selection window without execution.

Notes:

1. The code can use substantial computer resources in complex ion cases. It has been compiled with dimensions set for medium-sized cases compatible with average workstation capacity. Abnormal termination of the code may result from exceeding these dimensions. Failure diagnostic information and recommendations are given at the end of the *olg* file. Please notify ADAS support if re-dimensioning is required.
2. The code requires IDL version 4 or later. If this is not available on your machine, ADAS support (University of Strathclyde) has some capacity for executing tasks on your behalf.