

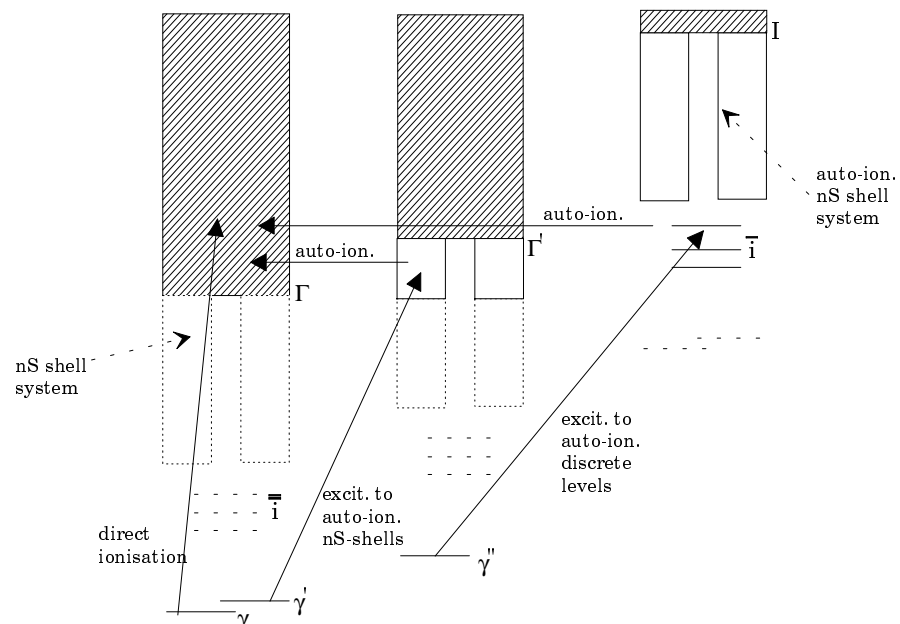
ADAS213: Collisional ionisation - process for specific ion file

The program adds state selective electron impact ionisation data to specific ion files of type *adf04* and electron impact excitation data to levels of the *adf04* file which are auto-ionising. To achieve this it, it opens the primary data archives for Maxwell averaged ionisation/excitation-autoionisation coefficient data of type *adf23*. The mapping of the data into the *adf04* files makes use of a cross-referencing file which must be set up prior to execution. Such cross-referencing files are archived in data format *adf18/a23_a04*. The result of the operation of the code is a fully specified *adf04* file ready for immediate inclusion in a personal database. The code includes an added capability for mapping LS-resolved ionisation data to J-resolved levels rather than terms. Also the code is internally set up for mapping from true J-resolved intermediate coupling *adf23* data archives to *adf04* files, when these become available.

Background theory:

The code and background theory is being extended to include planned new intermediate coupling ionisation data and *adf04* files at J-resolution. The following notes are incomplete.

Consider the electron impact ionisation reaction on a z times ionised ion \mathcal{A}^{+z} in state i , leaving the residual $z+1$ times ionised ion \mathcal{A}^{+z+1} in the state Γ . Let the states i be partitioned into true bound states \bar{i} and auto-ionising states \bar{i} and that the auto-ionising states of the ion \mathcal{A}^{+z} are the set of terms $\{S_i L_i : \bar{i} = 1, \dots, N_z\}$ and that the ion also has ground and metastable terms denoted by $\{S_\gamma L_\gamma : \gamma = 1, \dots, M_z\}$. Also let the final states of the ion \mathcal{A}^{+z+1} be the set of terms $\{S_I L_I : I = 1, \dots, N_{z+1}\}$ of which the subset $\{S_\Gamma L_\Gamma : \Gamma = 1, \dots, M_{z+1}\}$ constitutes the metastables. We use small letters for ionising ion term indices and capital letters for ionised ion term indices. The improvement of ionisation data linking the metastables is the main concern. We seek to map relevant collision data from state selective ionisation rate coefficient archives of type *adf23* onto a specific ion file of type *adf04*.



The general specification of the *adf23* file includes excitation rate coefficient data to autoionising levels and Auger yields as well as direct ionisation data. The *adf23* file marks the metastable terms of the ion \mathcal{A}^{+z} with a '*'. Also, the metastables of the \mathcal{A}^{+z+1} are marked by a '*'. Terms of the \mathcal{A}^{+z+1} ion which act as parents for building doubly excited

autoionising terms of the \mathcal{A}^{+z} ion are marked by a '#'. The '*' parent terms are therefore automatically included in the '#' parent set. Auto-ionising states are grouped into individually identified terms, \bar{i} (which include the most important auto-ionising terms and those participating in the formation of resolved satellite spectra) and bundle-nS sets. The latter can be identified with a parent. The *adf23* file includes Auger yields for these auto-ionising states to end up finally in labelled \mathcal{A}^{+z+1} ion terms (especially '*' metastables). The metastable terms of the ion \mathcal{A}^{+z} may be extended with additional true bound states, \bar{i} , if direct ionisation data is available for these from the *adf23* precursor collision calculations.

```

seq = 'b '      nucchg = 8                                ADF23
-----
final term indexing          bwnf = 918702.0      nprf = 6
-----
indf   code             S L   WJ           wnf
-----
1 *2s2                (1)0( 0.0)           0.0
2 *2s2p               (3)1( 4.0)          82564.1
3 #2s2p               (1)1( 1.0)          158798.0
4 #2p2                (3)1( 4.0)          214066.2
5 #2p2                (1)2( 2.0)          231722.0
6 2p2                 (1)0( 0.0)          287909.0

initial term indexing       bwni = 624383.8      nlev = 8
-----
indi   code             S L   WJ           wni
-----
1 *2s2 2p1            (2)1( 2.5)           0.0
2 *2s1 2p2            (4)2( 9.5)          71492.0
3 2p2 3p1            (2)3(13.5)          624882.0
4 2s1 3p1 5p1        (2)0(13.5)          628496.0
5 2p2 3d1            (2)1(13.5)          630095.0
6 2s1 2p1 5p1        (4)0(13.5)          630879.0
7 2p2 3d1            (2)2(13.5)          632594.0
8 2s1 2p1 5d1        (2)1(13.5)          633898.0

```

The mappings implemented by ADAS213 are only concerned with the individually labelled terms. The choice of excited or metastable terms, upon which doubly excited states are built, is determined at the point of production of the *adf23* file. For collisional-radiative ionisation calculations only doubly excited states built on metastables are of relevance. If the *adf23* file is restricted for this purpose, then indirect ionisation via autoionising levels built on true excited parents is grossed up with the direct ionisation. For spectral analysis of satellite lines however explicit entry of true excited parents in the *adf23* file production is relevant. The excitation rate coefficients to such levels may be mapped onto *adf04* files designed for modelling the collisional-radiative populations of doubly excited states (cf. ADAS series 7). The *adf04* files dedicated to such studies include explicit doubly excited states and data lines of resonance capture coefficients and Auger rates. Such data is included in *adf04* files by the dielectronic recombination mapping code ADAS212. Thus ADAS213 is only used for insertion of the additional data lines of electron impact excitation rate coefficients to auto-ionising levels.

In general the mapping from *adf23* to *adf04* requires an alteration of the temperatures at which the data are stored in the *adf23* file to those required in the *adf04* file by interpolation. The known energies of the terms assist in providing accurate interpolation and such data are available in both files. It is convenient to indicate values relating to the *adf04* file by the superscript ^{04} and to the *adf23* file by the superscript ^{23}. Thus the electron temperature set for the *adf04* file is $\{T_k^{\{04\}} : k = 1, \dots, N_T^{\{04\}}\}$.

Since *adf04* files and *adf23* files are prepared independently (often exploiting different atomic structure codes) there is no certainty that the indexing of terms for the same ion in two such data sets will be the same. Also choice and indexing of metastables is to a degree at the choice of the user and varies with physical scenario. Thus it is necessary to match terms between the two file types with a cross-referencing file which is set up explicitly by hand. Cross-referencing files for the present purpose are archived in ADAS data format *adf18/a23_a04*.

Formally, *adf04* files and *adf23* files make almost no distinction between term and level resolution. The J-quantum number in level resolution data sets is written and handled as the (statistical weight-1)/2. It is only in the leading line of the *adf04* file (where a

classification string for parents is written) that any difference occurs. Thus the above discussion applies equally to J-resolved level resolution. The cross-referencing file is where term/level distinction is made and steering of cross-transcription (term \rightarrow level) may be set up.

Direct Ionisation The *adf23* tabulation is of the rate coefficient $q_{i \rightarrow \Gamma}^{(23)}(T)$. The rate coefficient is strongly varying with temperature at low temperatures and may be zero for sufficiently low temperatures at machine precision in numerical tabulations. Let rate coefficients be zero at temperatures up to index number k_0 . The code computes the quantities $\{Y_{i \rightarrow \Gamma}^{(23)}(T_k^{(23)}): k = 1, N_T^{(23)}\}$ with $Y_{i \rightarrow \Gamma}^{(23)}(T_k^{(23)}) = Y_{i \rightarrow \Gamma}^{(23)}(T_{k_0+1}^{(23)})$ for $k = 1, \dots, k_0$ and with

$$Y_{i \rightarrow \Gamma}^{(23)}(T_k^{(23)}) = \exp(\Delta E_{i\Gamma}^{(23)}) q_{i \rightarrow \Gamma}^{(23)}(T_k^{(23)}) \quad 3.13.1$$

to regularise and smooth the rate coefficients. It is these latter forms which are interpolated in the log/log plane by cubic splines and then converted back to rate coefficients to provide data at the *adf04* file temperature set as $\{q_{i \rightarrow \Gamma}^{(04)}(T_k^{(04)}): k = 1, N_T^{(04)}\}$. The spline is constructed to have zero gradient at the first node with zero gradient extrapolation and zero curvature at the last node with constant gradient extrapolation. As pointed out above, indexing of terms may not be identical in *adf04* and *adf23* files. A cross-reference table defines the one-to-one mapping $i^{(04)} \leftrightarrow i^{(23)}$ and the mapping $\Gamma^{(23)} \rightarrow \Gamma^{(04)}$. The latter may not be one-to-one. This is because excited final ionised states may be delivered by the ionisation cross-section calculations which generate the *adf23* files or the working metastable set for the ionised ion in the *adf04* file may be actively reduced by the user over that of the *adf23* file. An assumption must be made by the user in setting up the cross-referencing about which excited final states of the ionised system cascade to which metastables. Thus terms labelled by different indices $\Gamma^{(23)}$ in the *adf23* file may map to the same term $\Gamma^{(04)}$ in the *adf04* file and the code in these circumstances simply adds up the different *adf23* contributions.

Resolution detection and switching For term-term or level-level mappings, keywords in the *adf18/a23_a04* cross-reference file identify the working resolution for the mapping. These are ‘Term/parent’, ‘*adf04-trm adf23-trm*’ and ‘*adf04-ptrm adf23-ptrm*’ for LS resolution and ‘Levl/parent’, ‘*adf04-lvl adf23-lvl*’ and ‘*adf04-plvl adf23-plvl*’ for J resolution.

Term/parent cross-reference lists for specific ion and ionisation file	
adf04-trm	adf23-trm
1	1
2	2
.	.
10	7
11	9
12	11
*	13
adf04-ptrm	adf23-ptrm
+1	+1
+2	+2
+3	+3
+3	+4
+1	+5

The first keyword sets the code’s internal switches and inconsistency between it and the later ones generates warning messages. The code only supports resolution switching from LS-resolved in the *adf23* file to J-resolved in the *adf04* file. This is because most *adf23* data sets in the ADAS database at this time are for LS-resolved terms however many *adf04* files are for J-resolved levels. For mapping to such levels, additional information is provided in the *adf18/123_a04* cross-reference file on the fractional splitting, $F(SLJ) / F(SL)$ of terms into levels (normally proportional to statistical weight), where $F(SL) = \sum_J F(SLJ)$. Thus

$$q_{S_i L_i J_i \rightarrow S_\Gamma L_\Gamma J_\Gamma} = \frac{F(S_i L_i)}{F(S_i L_i J_i)} \frac{F(S_\Gamma L_\Gamma J_\Gamma)}{F(S_\Gamma L_\Gamma)} q_{S_i L_i \rightarrow S_\Gamma L_\Gamma} \quad 3.13.2$$

and

$$q_{S_i L_i J_i \rightarrow S_\Gamma L_\Gamma} = \frac{F(S_i L_i)}{F(S_i L_i J_i)} q_{S_i L_i \rightarrow S_\Gamma L_\Gamma} \quad 3.13.3$$

J-resolved		
adf04-lvl	frac.split	adf04-trm
1	1.0	1
2	0.5	2
3	0.5	2
4	0.2	3
5	0.4	3
6	0.6	3
adf04-plvl	frac.split	adf04-ptrm
1	1.0	1
2	0.5	2
3	0.5	2

In the future true intermediate coupling J-resolved *adf23* data will be provided. Mapping in this case to a J-resolved *adf04* file will follow exactly the pattern of the first part of this section.

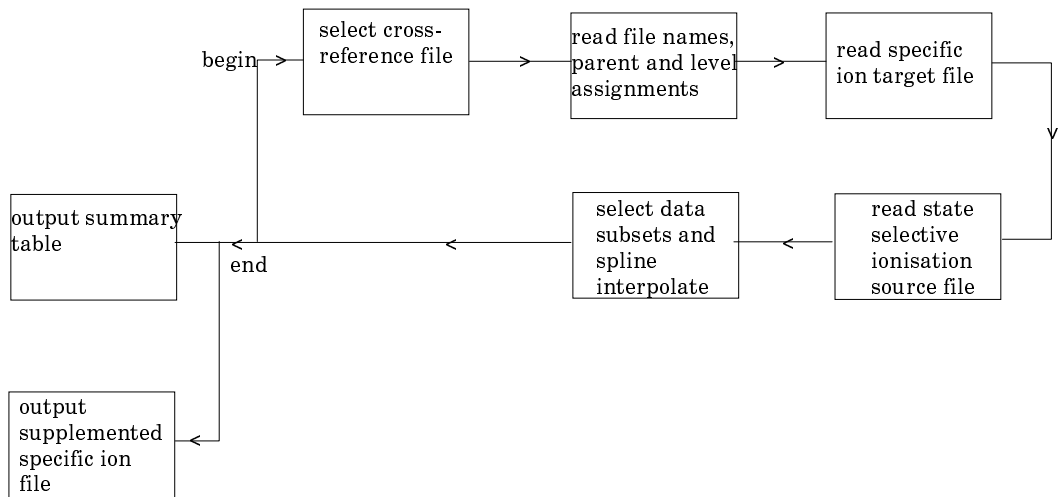
Indirect Ionisation Indirect ionisation via implicit doubly excited states built on excited parents are included in the *adf23* file as an addition to the direct rate coefficient. Indirect ionisation via explicit doubly excited states, tabulated excitation rate coefficients and Auger yields in the *adf23* file are handled as excitation below. However the excitation rate coefficients are multiplied by their Auger yields, summed up allocated to the appropriate final state and combined with the direct rate coefficient. This is only done for individually identified auto-ionising terms of the \mathcal{A}^{+z} ion. Bundle-nS contributions are not included even if present in the *adf23* file.

Excitation The *adf23* tabulation is of the rate coefficient $q_{i \rightarrow \Gamma}^{\{23\}}(T)$. The rate coefficient is regularised and smoothed by converting to the usual maxwell averaged collision strength, $Y_{i \rightarrow \Gamma}^{\{23\}}(T)$ and low temperature zeroes filled in as for the ionisation rate coefficient. Spline interpolation and extrapolation are carried out to convert to the *adf04* file temperatures as for the ionisation coefficient. There is no implementation of transition type dependent interpolation (cf. ADAS215) since the temperature spread of the *adf23* file is normally very wide. The term indexing already set up in the cross-reference file is sufficient to locate and place the excitation data correctly in the *adf04* file. Note that only \bar{i} terms included explicitly in the cross-referencing will be handled even if more such terms are present in the *adf23* file.

Program steps:

These are summarised in figure 3.13.

Figure 3.13

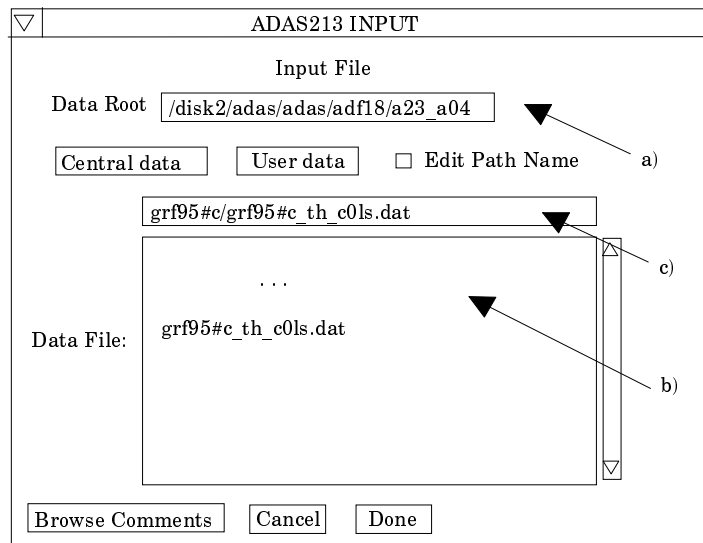


Interactive parameter comments:

Move to the directory in which you wish the output text file produced after executing any ADAS program (*paper.txt* is the default) to appear. There is no graphical output from this code. Initiate ADAS213 from the program selection menus in the usual manner.

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

1. An *adf18/a23_a04* format cross-referencing file is the appropriate input file for use by the program ADAS212. Your cross-referencing data should be held in such a file, in the same directory structure as central ADAS, but with your identifier replacing the first *adas*.



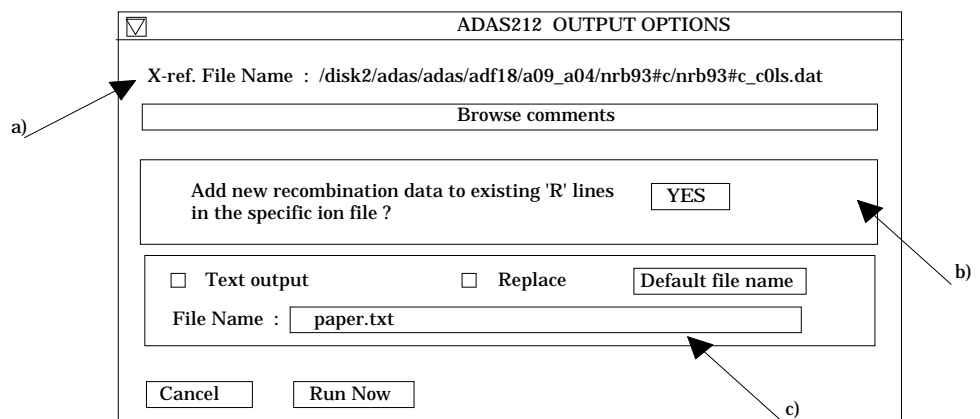
2. Available sub-directories are shown in the large file display window at b). Scroll bars appear if the number of entries exceed the file display window size. There are a large number of these. They are usually stored in sub-directories by isoelectronic sequence of the recombined ion with a prefix which identifies the primary author of the actual dielectronic data accessed. It is useful to use a naming convention for the final part of the file name which includes the ion and 'LS' (eg. *grf95#c/grf95#c_th_c0ls.dat*) to indicate that the data is for terms.
3. Click on a name to select it. The selected name appears in the smaller selection window c) above the file display window. Then the individual datafiles are presented for selection. Datafiles all have the termination *.dat*.
4. Once a data file is selected, the set of buttons at the bottom of the main window become active.

5. Clicking on the *Browse Comments* button displays any information stored with the selected datafile. It is important to use this facility to find out what has gone into the dataset and the attribution of the dataset. The possibility of browsing the comments appears in the subsequent main window also.
6. 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 for ADAS213.

The **output options window** is shown below. There is no graphical output possibility but in addition to the usual text file, an output data file is always produced

7. The data output file is of specific ion file form, that is *adf04* and is sent to your pass directory as *adas213.pass*. It comprises the *adf04* file for which the cross-referencing was prepared but includes dielectronic data. It is the normal practice to use ADAS211 to put radiative recombination data in the specific ion file and then use ADAS212 to add the dielectronic data. The button at b) allows the choice of whether the dielectronic data should be added on to the radiative recombination 'R-lines' or replace them.
8. By pressing *Run Now*, you can wait for the output to be generated before continuing. When this option is taken a small information box opens showing the progress the program has made. Once this has been done the calculations cannot be halted, but an execution time of less than 30 seconds can usually be expected.



9. Since the code operates rapidly, we have removed the background execution operation available in the sister program ADAS211.

Illustration:

A sample cross-reference file, */.../adas/adf18/a23_a04/grf95#be/grf95#be_th_c2ls.dat*, is shown in Table 3.13a below. The target specific ion file is of LS coupled type and so the cross-reference file does not include a J-splitting definition section. The file naming for the cross-reference file is chosen to match the primary ionisation data file of type *adf23* which is accessed. The example is one of simple direct ionisation only.

Table 3.13a

Specific ion input file	

"ADASCENT"/adf04/belike/belike_jll1990c.dat	: specific ion file for supplementation
Ionisation file (Griffin)	

"ADASUSER"/adf23/grf95#be/grf95#be_th_c2ls.dat	: file of ionis. & excit/auto. data
Output files	

"ADASUSER"/pass/adas213_adf04.pass	: supplemented specific ion file
Term/parent cross-reference lists for specific ion and ionisation file	

adf04-trm	adf23-trm

1	1
2	2
adf04-ptrm	adf23-ptrm
-----	-----
+1	+1
+2	+2
C-----	
C	
C	Note
C	-----
C	(a) For ionisation, different adf23-lvls referenced to the same adf04-lvl
C	implies summing over the multiple adf23-lvls and accumulating in the
C	adf04-lvl.
C	(b) For excitation, no radiative A-value is entered in the first column
C	following the transition indexing. This must be added separately if
C	the excitation line is not present in the original data set. If there
C	is already an excitation transition line, then the radiative A-value is
C	kept and the collisional-data is substituted.
C	(c) '+' signs are used for parent indices.
C	(d) Term coupling datas sets have 'trm' in the headings. Intermediate
C	coupling datasets have 'lvl' in the headings.
C	-----

The target *adf04* file is shown in Table 3.13b below and the state selective ionisation data *adf23* file in Table 3.13c. Note that there are two metastables identified on the first line of the *adf04* data which match the two entries under *adf04-ptrm* in the cross-reference file.

Table 3.13b

C + 2	6	3	386214.(2S)	450770.(2P)
1	2S2(1S)	(1)0(0.0)	0.	{1}2.000
2	2S2P(3P)	(3)1(4.0)	52419.	{1}1.000 {2}1.000
11	2S3P(3P)	(3)1(4.0)	259718.	{1}1.000
12	2S3D(3D)	(3)2(7.0)	270013.	{1}1.000
-1				
3.00	3	9.00+03 1.80+04 4.50+04 9.00+04 1.80+05 4.50+05 9.00+05 1.80+06		
2	1 3.20+01 1.07+00 1.02+00 9.70-01 8.56-01 7.03-01 4.89-01 3.45-01 2.20-01			
R 12	+2	1.35-19 1.37-16 8.90-15 2.37-14 2.51-14 1.30-14 6.94-15 4.68-15		
-1				
-1	-1			
C-----				
C	Energy levels			
C	Dielectronic data added to 14 existing rad. recom. level sets			
C				
C	15/07/92			
C	-----			

Correspondingly, there are two final state metastables identified in the *adf23* file under *Final term indexing*. The supplemented *adf04* file is shown in Table 3.13d. Three *S-lines* have been added. Note that lines of zeroes present in the *adf23* file are eliminated. The final part of the comments section of the output file summarises the files accessed.

Table 3.13c

seq = 'Be'		nucchl = 6		ADF23									
final term indexing		bwnf = 520158.9		nprf = 2									
indf	code	S L	WJ	wnf									
1	2s12p0	(2)0(0.5)		0.0									
2	2s02p1	(2)1(2.5)		64556.1									
initial term indexing		bwni = 386231.6		nlev = 2									
indi	code	S L	WJ	wni									
1	2s22p0	(1)0(0.0)		0.0									
2	2s12p1	(3)1(4.0)		52369.2									

meti* = 1													
ionis rates													
indf	Te =	1.80D+04	4.50D+04	9.00D+04	1.80D+05	4.50D+05	9.00D+05	1.80D+06	4.50D+06	9.00D+06	1.80D+07	4.50D+07	9.00D+07
1	8.26D-23	1.55D-14	1.02D-11	2.91D-10	2.43D-09	5.10D-09	7.28D-09	8.32D-09	7.91D-09	6.94D-09	5.40D-09	4.30D-09	
2	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

meti* = 2													
ionis rates													
indf	Te =	1.80D+04	4.50D+04	9.00D+04	1.80D+05	4.50D+05	9.00D+05	1.80D+06	4.50D+06	9.00D+06	1.80D+07	4.50D+07	9.00D+07
1	6.17D-21	9.04D-14	2.49D-11	4.52D-10	2.76D-09	5.10D-09	6.69D-09	7.14D-09	6.56D-09	5.62D-09	4.29D-09	3.38D-09	
2	1.51D-23	5.13D-15	4.10D-12	1.29D-10	1.15D-09	2.47D-09	3.58D-09	4.13D-09	3.95D-09	3.47D-09	2.71D-09	2.16D-09	
C-----													
C	Data generated by Donald C. Griffin on 04/21/95												

```

C
C The rates were calculated using configuration-average ionization cross
C sections, with non-relativistic wavefunctions , using the
C frozen-core approximation, the prior form for the scattering
C potentials, and the natural-phase approximation.
C They were then multiplied by the appropriate angular coefficients.
C -----

```

Table 3.13d

C	+	2		6		3	386214.	(2S)	450770.	(2P)										
		1	2S2(1S)				(1)0(.0)	0.	{1}2.000										
		2	2S2P(3P)				(3)1(4.0)	52419.	{1}1.000	{2}1.000									
		11	2S3P(3P)				(3)1(4.0)	259718.	{1}1.000										
		12	2S3D(3D)				(3)2(7.0)	270013.	{1}1.000										
		-1																		
		3.00		3	9.00+03	1.80+04	4.50+04	9.00+04	9.00+04	1.80+05	4.50+05	9.00+05	1.80+06							
		2	1	3.20+01	1.07+00	1.02+00	9.70-01	8.56-01	7.03-01	4.89-01	3.45-01	2.20-01								
R		12	+2		1.35-19	1.37-16	8.90-15	2.37-14	2.51-14	1.30-14	6.94-15	4.68-15								
S		1	+1		1.00-30	8.26-23	1.55-14	1.02-11	2.91-10	2.43-09	5.10-09	7.28-09								
S		2	+1		1.00-30	6.17-21	9.04-14	2.49-11	4.52-10	2.76-09	5.10-09	6.69-09								
S		2	+2		1.00-30	1.51-23	5.13-15	4.10-12	1.29-10	1.15-09	2.47-09	3.58-09								
C	-----																			
C	Energy levels																			
C	Taken from NSRDS NBS 3 Sect 3.																			
C	.																			
C																15/07/92				
C	-----																			
C	Ionisation data is post-processed from file																			
C	/u/hps/adas/adf23/grf95#be/belike_th_c2ls.dat																			
C	The cross-referencing file is																			
C	/u/hps/adas/adf18/a23_a04/grf95#be/belike_th_c2ls.dat																			
C	The source specific ion file is																			
C	/u/adas/adas/adf04/belike/belike_jl1990c.dat																			
C	Producer: hps																			
C	Date: 14/04/98																			
C	-----																			

Notes: