

## ADF38: Opacity project extension: photoexcitation-autoionisation rate coefficients

The basic process is  $1s^2nl + \gamma \rightarrow 1slnl'n' \rightarrow 1sn''l'' + e$ . A separate file is provided for each  $n$ , which contains data for all  $n' \geq n$ . Note however that  $1slnl'n' \leftrightarrow 1s^2n'l' + \gamma$  has to be considered consistently at the same time to avoid multiple counting. It is convenient at the production stage to separate the level list file (denoted by the postfix 'l') from the rate file (denoted by postfix 'r'). Separate files are given for term (LS) coupling and intermediate (IC) coupling. Conventions used are (1) L=-1=> the outer electron is part of the core - ; (2) '\*' after L (>=0 only) means that the nl electron was active – otherwise it is assumed passive.

Utilising subroutines :

ADAS204?      ADAS208?      ADAS212?

Formatted files to ADF38 specification :

Database Status	Date = March 17, 2003	Data type =pea files	Data root =/.../adas/adas/adf38/			
<i>Recombining seq.</i>	<i>Library</i>	<i>Elements</i>	<i>Members</i>	<i>n'</i>	<i>Comments</i>	<i>Quality</i>
H-like.	nrb02#h	C, O, S, Fe	<ion>lsK<n>l.dat	2,3,4,5,6	LS resolution	medium
		C, O, S, Fe	<ion>icK<n>l.dat	2,3,4,5,6	IC resolution	medium
		C, O, S, Fe	<ion>lsK<n>r.dat	2,3,4,5,6	LS resolution	medium
		C, O, S, Fe	<ion>icK<n>r.dat	2,3,4,5,6	IC resolution	medium
He-like.	nrb02#he	C, O, S, Fe	<ion>lsK<n>l.dat	2,3,4,5,6	LS resolution	medium
		C, O, S, Fe	<ion>icK<n>l.dat	2,3,4,5,6	IC resolution	medium
		C, O, S, Fe	<ion>lsK<n>r.dat	2,3,4,5,6	LS resolution	medium
		C, O, S, Fe	<ion>icK<n>r.dat	2,3,4,5,6	IC resolution	medium
Li-like.	nrb02#li	C, O, S, Fe	<ion>lsK<n>l.dat	2,3,4,5	LS resolution	medium
		C, O, S, Fe	<ion>icK<n>l.dat	2,3,4,5	IC resolution	medium
		C, O, S, Fe	<ion>lsK<n>r.dat	2,3,4,5	LS resolution	medium
		C, O, S, Fe	<ion>icK<n>r.dat	2,3,4,5	IC resolution	medium
		C, O, S, Fe	<ion>lsL<n>l.dat	2,3,4,5	LS resolution	medium
		C, O, S, Fe	<ion>icL<n>l.dat	2,3,4,5	IC resolution	medium
		C, O, S, Fe	<ion>lsL<n>r.dat	2,3,4,5	LS resolution	medium
		C, O, S, Fe	<ion>icL<n>r.dat	2,3,4,5	IC resolution	medium

Notes:

*Data lines for LS coupled 'I' file:*

[prescribed text], SEQ, [prescribed text], IZ0, CCPLG

[blank line]

[prescribed text], BWNP, [prescribed text], NPRNT

[prescribed text field]

[prescribed text field]

[prescribed text field]

for indp=1, NPRNT

    INDP, CFGP, ISP, ILP, XJP, WNPI

repeat

[blank line]

[prescribed text], BWNR, [prescribed text], NTRM

[prescribed text field]

[prescribed text field]

[prescribed text field]

for indx=1, NTRM

    INDX, IRSL, CFGT, IS, IL, XJ, WNRT

repeat

[blank line]

[prescribed comment line]

[prescribed comment line]

[prescribed comment line]

[prescribed comment line]

*Format:*

1a5,1a2,1a11,i2,50x,1a4

1a80

1a45,f12.1,1a8,i4

1a23

1a56

1a56

i6,10x,1a20,1x,i1,1x,i1,1x,f4.1,1x,f11.1

1a80

1a45,f12.1,1a8,i4

1a28

1a56

1a56

2i6,4x,1a20,1x,i1,1x,i1,1x,f4.1,1x,f11.1

1a80

1a80

1a80

1a80

1a80

*variable identification :*

<i>name</i>	<i>meaning</i>
SEQ	sequence identifier (two characters)
IZO	nuclear charge
CCPLG	coupling scheme, '/LS/' => LS coupling
BWNP	binding wave number of lowest parent (cm-1)
NPRNT	number of metastable parents (including ground parent)
INDP	index of parent
CFGP	configuration (or Eissner code therefore) for parent.
ISP	multiplicity of parent ( $2S_p+1$ )
ILP	total orbital quantum number ( $L_p$ ) for parent
XJP	(statist. weight - 1)/2 of parent term
WNPI	energy of parent term relative to lowest parent (cm-1)
BWNR	binding wave number of lowest resolved term (cm-1)
NTRM	number of terms in LS-resolved set
INDX	index value for term
IRSL	initial term index as used in the 'r' file
CFGT	configuration (or Eissner code therefor) for level.
IS	multiplicity for level ( $2*S+1$ )
IL	total orbital quantum number for term
XJ	(statist. weight - 1)/2 for term
WNRI	energy of term relative to ground (cm-1)

Table B38c – example – LS coupling level list (l) file.

SEQ='HE'	NUCCHG= 6	/LS/		
PARENT TERM INDEXING		BWNP=	3950546.5	NPRNT= 3
-----				
INDP	CODE	S L	WI	WNP

1	1S1	(2)0( 0.5)	0.0
2	2P1	(2)1( 2.5)	2962909.9
3	2S1	(2)0( 0.5)	2962910.0
LS RESOLVED TERM INDEXING		BWNR=	4690709.4 NTRM= 40
INDX	IRSL	CODE	S L WJ WNR
1	3	1S1 2S1	(3)0( 1.0) 0.0
2	1	1S1 2P1	(3)1( 4.0) 49775.7
3	4	1S1 2S1	(1)0( 0.0) 57804.1
4	2	1S1 2P1	(1)1( 1.0) 94734.4
5	5	1S1 3S1	(3)0( 1.0) 414040.5
36	40	1S1 6H1	(1)5( 5.0) 663956.4
37	33	1S1 6F1	(3)3(10.0) 663956.7
38	34	1S1 6F1	(1)3( 3.0) 663957.6
39	28	1S1 6D1	(1)2( 2.0) 664007.7
40	20	1S1 6P1	(1)1( 1.0) 664687.2
C	-----		
C			
C			
C			
C	-----		

Data lines for IC coupled 'I' file:

[prescribed text], SEQ, [prescribed text], IZ0, CFGP

[blank line]

[prescribed text], BWNP, [prescribed text], NPRNT

[prescribed text field]

[prescribed text field]

[prescribed text field]

for indp=1, NPRNT

INDP, CFGP, ISP, ILP, XJP, WNPI

repeat

[blank line]

[prescribed text], BWNR, [prescribed text], NLVL

Format:

1a5,1a2,1a11,i2,50x,1a4

1a80

1a45,f12.1,1a8,i4

1a23

1a56

1a56

i6,10x,1a20,1x,i1,1x,i1,1x,f4.1,2x,f10.1

1a80

1a45,f12.1,1a8,i4

[prescribed text field]	1a28
[prescribed text field]	1a56
[prescribed text field]	1a56
for indx=1,NLVL	
INDX,ISRL,CFGL,IS, IL, XJ, WNRL	i6,10x,1a20,1x,i1,1x,i1,1x,f4.1,2x,f10.1
repeat	
[blank line]	1a80
[prescribed comment line]	1a80
[prescribed comment line]	1a80
[prescribed comment line]	1a80
[prescribed comment line]	1a80

*variable identification :*

<i>name</i>	<i>meaning</i>
SEQ	sequence identifier (two characters)
IZO	nuclear charge
CFGP	coupling scheme, '/IC/' => intermediate coupling
BWNP	binding wave number of lowest parent(cm-1)
NPRNT	number of metastable parents (including ground parent)
INDP	index of parent
CFGP	configuration (or Eissner code therefor) for parent.
ISP	multiplicity of parent ( $2S_p+1$ )
ILP	total orbital quantum number ( $L_p$ ) for parent
XJP	J quantum number of parent level.
WNPI	energy of parent relative to lowest parent (cm-1)
BWNR	binding wave number of lowest resolved level (cm-1)



*Data lines for LS coupled 'r' file:*

ELEM, IZ, CCPLG

[blank line]

[prescribed text field]

until <blank line for each upper state> do

    IRSL,G,N,L,CODEL,DEL,B,R,A,A1,A2,A3

for <all lower state with same upper state> do

    IRSL,G,N,L,CODEL,DEL,B

repeat

repeat

[blank line]

[prescribed text],NRSLMX, [prescribed text], NVMAX, [prescribed tex], LVMAX

[blank line]

[prescribed comment line]

[prescribed comment line]

[prescribed comment line]

[prescribed comment line]

*Format:*

1a2,i2,5x,1a4

1a80

1a56

3i5,i4,1a1,e15.6,6e12.3

3i5,i4,1a1,e15.6

1a80

1a10,i4,1a10,i4,1a10,i4

1a80

1a80

1a80

1a80

1a80

*variable identification :*

*name*

*meaning*

ELEM

sequence identifier (two characters)

IZ

nuclear charge

CCPLG

coupling scheme, '/LS/' => LS coupling

IRSL

initial term (see term list in 'l' file)

G	statistical weight of term
N	principal quantum number of outer electron of upper state
L	orbital quantum number of outer electron of upper state
CODEL	'*' => NL electron was active; ' ' => NL electron passive
DEL	photon energy (Rydberg)
B	Einstein absorption rate (sec-1)
R	total radiative width (sec-1)
A	total Auger width (sec-1)
A1	resolved Auger width to parent 1
A2	resolved Auger width to parent 2
.	.
An	resolved Auger width to parent n. (Note $\sum_n A_n \leq A$ in general since not all are necessarily resolved).
NRSLMX	maximum resolved n
NVMAX	maximum n' in data set
LVMAX	maximum l' in data set

Table B38d – example – LS coupling rate coefficient (r) file.

C 5		/LS/									
IRSL	G	N	L	DEL(RYD)	B(SEC)	R(SEC)	A(SEC):	1	2	3	
2	3	2	-1	2.535700E+01	1.015E+11	3.045E+11	3.603E+14	3.603E+14	0.000E+00	0.000E+00	
1	9	2	-1	2.626002E+01	1.495E+12	1.495E+12	0.000E+00	0.000E+00	0.000E+00	0.000E+00	
2	3	2	-1	2.610345E+01	2.447E+12	1.468E+12	3.904E+14	3.904E+14	0.000E+00	0.000E+00	
2	3	2	-1	2.681239E+01	4.104E+11	1.231E+12	2.293E+13	2.293E+13	0.000E+00	0.000E+00	
3	3	2	-1	2.633861E+01	2.262E+12	7.541E+11	1.984E+13	1.984E+13	0.000E+00	0.000E+00	
4	1	2	-1	2.651498E+01	2.308E+12	7.694E+11	1.914E+14	1.914E+14	0.000E+00	0.000E+00	
3	3	3	1	3.074555E+01	3.489E+11	1.304E+11	3.282E+12	3.282E+12	0.000E+00	0.000E+00	
4	1	3	1	3.026374E+01	3.328E+11	1.250E+11	2.961E+13	2.961E+13	0.000E+00	0.000E+00	
3	3	4	1	3.209593E+01	1.596E+11	5.925E+10	1.524E+12	1.524E+12	0.000E+00	0.000E+00	
4	1	4	1	3.158658E+01	1.521E+11	5.676E+10	1.347E+13	1.347E+13	0.000E+00	0.000E+00	



4	1	5	1	3.218374E+01	7.917E+10	2.948E+10	6.997E+12	6.997E+12	0.000E+00	0.000E+00
3	3	6	1	3.302605E+01	4.827E+10	1.788E+10	4.673E+11	4.673E+11	0.000E+00	0.000E+00
4	1	6	1	3.250406E+01	4.601E+10	1.713E+10	4.064E+12	4.064E+12	0.000E+00	0.000E+00
5	3	0*	0*	3.690884E+01	8.408E+10	8.070E+10	8.000E+12	8.000E+12	0.000E+00	0.000E+00
6	1	0	0	2.689336E+01	2.407E+12	8.062E+11	2.541E+13	2.541E+13	0.000E+00	0.000E+00
7	3	4	0*	2.696852E+01	2.426E+12	8.104E+11	8.012E+11	8.012E+11	0.000E+00	0.000E+00
8	1	4	0*	2.695150E+01	2.424E+12	8.095E+11	1.066E+13	1.066E+13	0.000E+00	0.000E+00
9	3	5	0*	2.698407E+01	2.432E+12	8.114E+11	3.822E+11	3.822E+11	0.000E+00	0.000E+00
10	1	5	0*	2.697485E+01	2.430E+12	8.109E+11	5.341E+12	5.341E+12	0.000E+00	0.000E+00
11	3	6	0*	2.699088E+01	2.434E+12	8.118E+11	2.120E+11	2.120E+11	0.000E+00	0.000E+00
12	1	6	0*	2.698542E+01	2.433E+12	8.115E+11	3.043E+12	3.043E+12	0.000E+00	0.000E+00
13	2	3	1	2.995127E+01	2.748E+11	9.517E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
14	3	3	1*	2.664283E+01	6.628E+11	9.550E+11	1.901E+11	1.901E+11	0.000E+00	0.000E+00
1	9	3	1	3.033454E+01	3.747E+11	9.550E+11	1.901E+11	1.901E+11	0.000E+00	0.000E+00
13	3	1	1*	2.679611E+01	1.194E+12	9.601E+11	3.293E+11	3.293E+11	0.000E+00	0.000E+00
13	9	3	1*	3.038418E+01	7.532E+10	9.601E+11	3.293E+11	3.293E+11	0.000E+00	0.000E+00
13	9	3	1*	2.684574E+01	2.400E+11	9.045E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	1	9	3	3.041892E+01	3.577E+10	9.045E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
13	9	3	1*	2.688048E+01	8.547E+11	8.932E+11	1.027E+14	1.027E+14	0.000E+00	0.000E+00
2	3	3	1	3.014300E+01	2.421E+10	8.932E+11	1.027E+14	1.027E+14	0.000E+00	0.000E+00
14	3	3	1*	2.683457E+01	1.441E+12	9.042E+11	5.222E+13	5.222E+13	0.000E+00	0.000E+00
2	3	3	1	3.025440E+01	4.896E+09	9.042E+11	5.222E+13	5.222E+13	0.000E+00	0.000E+00
14	3	3	1*	2.694597E+01	2.918E+11	8.750E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	3	4	1	3.124824E+01	1.021E+11	8.750E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
16	3	4	1*	2.686828E+01	7.668E+11	8.762E+11	1.307E+11	1.307E+11	0.000E+00	0.000E+00
1	1	9	4	3.165341E+01	1.433E+11	8.762E+11	1.307E+11	1.307E+11	0.000E+00	0.000E+00
15	9	4	1*	2.692594E+01	1.307E+12	8.781E+11	2.228E+11	2.228E+11	0.000E+00	0.000E+00
1	1	9	4	3.167280E+01	2.871E+10	8.781E+11	2.228E+11	2.228E+11	0.000E+00	0.000E+00
15	9	4	1*	2.694533E+01	2.620E+11	8.556E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	1	9	4	3.168338E+01	2.498E+10	8.556E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
15	9	4	1*	2.695591E+01	8.245E+11	8.500E+11	4.443E+13	4.443E+13	0.000E+00	0.000E+00
2	3	4	1	3.132051E+01	2.492E+10	8.500E+11	4.443E+13	4.443E+13	0.000E+00	0.000E+00
16	3	4	1*	2.694056E+01	1.382E+12	8.541E+11	2.326E+13	2.326E+13	0.000E+00	0.000E+00
2	3	4	1	3.136459E+01	5.004E+09	8.541E+11	2.326E+13	2.326E+13	0.000E+00	0.000E+00
16	3	4	1*	2.698463E+01	2.777E+11	8.448E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	3	5	1	3.184484E+01	4.952E+10	8.448E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
18	3	5	1*	2.693645E+01	7.922E+11	8.453E+11	7.926E+10	7.926E+10	0.000E+00	0.000E+00
1	1	9	5	3.225316E+01	7.037E+10	8.453E+11	7.926E+10	7.926E+10	0.000E+00	0.000E+00
17	9	5	1*	2.696442E+01	1.333E+12	8.462E+11	1.342E+11	1.342E+11	0.000E+00	0.000E+00
1	1	9	5	3.226253E+01	1.409E+10	8.462E+11	1.342E+11	1.342E+11	0.000E+00	0.000E+00
17	9	5	1*	2.697379E+01	2.669E+11	8.351E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	1	9	5	3.226727E+01	1.448E+10	8.351E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
17	9	5	1*	2.697854E+01	8.175E+11	8.321E+11	2.257E+13	2.257E+13	0.000E+00	0.000E+00
2	3	5	1	3.187955E+01	1.566E+10	8.321E+11	2.257E+13	2.257E+13	0.000E+00	0.000E+00
18	3	5	1*	2.697116E+01	1.366E+12	8.341E+11	1.196E+13	1.196E+13	0.000E+00	0.000E+00
2	3	5	1	3.190108E+01	3.139E+09	8.341E+11	1.196E+13	1.196E+13	0.000E+00	0.000E+00
18	3	5	1*	2.699269E+01	2.739E+11	8.311E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
20	3	6	1*	3.216585E+01	2.783E+10	8.311E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	3	6	1	2.696439E+01	8.015E+11	8.315E+11	4.968E+10	4.968E+10	0.000E+00	0.000E+00
1	1	9	6	3.257497E+01	3.981E+10	8.315E+11	4.968E+10	4.968E+10	0.000E+00	0.000E+00
19	9	6	1*	2.698010E+01	1.343E+12	8.319E+11	8.388E+10	8.388E+10	0.000E+00	0.000E+00
1	1	9	6	3.258019E+01	7.966E+09	8.319E+11	8.388E+10	8.388E+10	0.000E+00	0.000E+00
19	9	6	1*	2.698532E+01	2.687E+11	8.257E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	1	9	6	3.258277E+01	8.181E+09	8.257E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00
19	9	6	1*	2.698790E+01	8.151E+11	8.239E+11	1.295E+13	1.295E+13	0.000E+00	0.000E+00
2	3	6	1	3.218519E+01	9.858E+09	8.239E+11	1.295E+13	1.295E+13	0.000E+00	0.000E+00
2	3	6	1*	2.698374E+01	1.360E+12	8.250E+11	6.908E+12	6.908E+12	0.000E+00	0.000E+00
2	3	6	1	3.219729E+01	1.974E+09	8.250E+11	6.908E+12	6.908E+12	0.000E+00	0.000E+00
20	3	6	1*	2.699583E+01	2.724E+11	9.550E+11	1.901E+11	1.901E+11	0.000E+00	0.000E+00

21	15	3	2*	2.687149E+01	1.121E+12	8.413E+11	2.949E+12	2.949E+12	0.000E+00	0.000E+00	0.000E+00
21	15	3	2*	2.694845E+01	8.077E+11	8.482E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
21	15	3	2*	2.697359E+01	4.976E+11	8.697E+11	2.977E+11	2.977E+11	0.000E+00	0.000E+00	0.000E+00
22	5	3	3*	2.700899E+01	5.486E+11	8.801E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
22	5	3	2*	2.710388E+01	1.151E+12	8.622E+11	1.364E+13	1.364E+13	0.000E+00	0.000E+00	0.000E+00
23	5	4	2*	2.694422E+01	8.073E+11	8.202E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
23	15	4	2*	2.694841E+01	1.131E+12	8.206E+11	1.561E+12	1.561E+12	0.000E+00	0.000E+00	0.000E+00
23	15	4	2*	2.697789E+01	8.104E+11	8.233E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
23	15	4	2*	2.698553E+01	4.989E+11	8.295E+11	1.564E+11	1.564E+11	0.000E+00	0.000E+00	0.000E+00
24	5	4	2*	2.703179E+01	4.948E+11	8.375E+11	4.222E+10	4.222E+10	0.000E+00	0.000E+00	0.000E+00
24	5	4	2*	2.703470E+01	1.142E+12	8.284E+11	7.242E+12	7.242E+12	0.000E+00	0.000E+00	0.000E+00
26	5	2	2*	2.697237E+01	8.099E+11	8.158E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
25	15	5	2*	2.697437E+01	1.134E+12	8.160E+11	8.651E+11	8.651E+11	0.000E+00	0.000E+00	0.000E+00
25	15	5	2*	2.698861E+01	8.113E+11	8.172E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
25	15	5	2*	2.699205E+01	4.884E+11	8.199E+11	8.640E+10	8.640E+10	0.000E+00	0.000E+00	0.000E+00
26	5	5	2*	2.701439E+01	4.907E+11	8.237E+11	2.457E+10	2.457E+10	0.000E+00	0.000E+00	0.000E+00
26	5	5	2*	2.701573E+01	1.139E+12	8.197E+11	4.009E+12	4.009E+12	0.000E+00	0.000E+00	0.000E+00
28	5	6	2*	2.698431E+01	8.110E+11	8.142E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
27	15	6	2*	2.698542E+01	1.135E+12	8.143E+11	5.197E+11	5.197E+11	0.000E+00	0.000E+00	0.000E+00
27	15	6	2*	2.699340E+01	8.118E+11	8.150E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
27	15	6	2*	2.699526E+01	4.879E+11	8.164E+11	5.184E+10	5.184E+10	0.000E+00	0.000E+00	0.000E+00
28	5	6	2*	2.700776E+01	4.892E+11	8.185E+11	1.515E+10	1.515E+10	0.000E+00	0.000E+00	0.000E+00
28	5	6	2*	2.700849E+01	1.138E+12	8.164E+11	2.407E+12	2.407E+12	0.000E+00	0.000E+00	0.000E+00
30	7	4	3*	2.698373E+01	8.109E+11	8.109E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
29	21	4	3*	2.698538E+01	8.111E+11	8.111E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
29	21	4	3*	2.700007E+01	1.044E+12	8.124E+11	1.158E+11	1.158E+11	0.000E+00	0.000E+00	0.000E+00
30	7	4	3*	2.700785E+01	1.045E+12	8.131E+11	2.041E+11	2.041E+11	0.000E+00	0.000E+00	0.000E+00
29	21	4	3*	2.700864E+01	5.808E+11	8.132E+11	6.692E+08	6.692E+08	0.000E+00	0.000E+00	0.000E+00
30	7	4	3*	2.701285E+01	5.811E+11	8.135E+11	2.117E+09	2.117E+09	0.000E+00	0.000E+00	0.000E+00
32	7	5	3*	2.699156E+01	8.116E+11	8.116E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
31	21	5	3*	2.699268E+01	8.117E+11	8.117E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
31	21	5	3*	2.699907E+01	1.044E+12	8.123E+11	9.283E+10	9.283E+10	0.000E+00	0.000E+00	0.000E+00
31	21	5	3*	2.700364E+01	5.805E+11	8.127E+11	5.340E+08	5.340E+08	0.000E+00	0.000E+00	0.000E+00
32	7	5	3*	2.700438E+01	1.045E+12	8.128E+11	1.643E+11	1.643E+11	0.000E+00	0.000E+00	0.000E+00
32	7	5	3*	2.700653E+01	5.807E+11	8.130E+11	1.696E+09	1.696E+09	0.000E+00	0.000E+00	0.000E+00
34	7	6	3*	2.699509E+01	8.119E+11	8.119E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
33	21	6	3*	2.699581E+01	8.120E+11	8.120E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
33	21	6	3*	2.699919E+01	1.044E+12	8.123E+11	6.500E+10	6.500E+10	0.000E+00	0.000E+00	0.000E+00
33	21	6	3*	2.700188E+01	5.804E+11	8.125E+11	3.727E+08	3.727E+08	0.000E+00	0.000E+00	0.000E+00
34	7	6	3*	2.700262E+01	1.045E+12	8.126E+11	1.153E+11	1.153E+11	0.000E+00	0.000E+00	0.000E+00
34	7	6	3*	2.700375E+01	5.805E+11	8.127E+11	1.187E+09	1.187E+09	0.000E+00	0.000E+00	0.000E+00
36	9	5	4*	2.699629E+01	8.120E+11	8.120E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
35	27	5	4*	2.699631E+01	8.120E+11	8.120E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
35	27	5	4*	2.700124E+01	9.930E+11	8.125E+11	2.010E+09	2.010E+09	0.000E+00	0.000E+00	0.000E+00
36	9	5	4*	2.700141E+01	9.931E+11	8.125E+11	2.477E+09	2.477E+09	0.000E+00	0.000E+00	0.000E+00
35	27	5	4*	2.700257E+01	6.320E+11	8.126E+11	1.590E+06	1.590E+06	0.000E+00	0.000E+00	0.000E+00
36	9	5	4*	2.700267E+01	6.320E+11	8.126E+11	3.973E+07	3.973E+07	0.000E+00	0.000E+00	0.000E+00
38	9	6	4*	2.699785E+01	8.122E+11	8.122E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
37	27	6	4*	2.699787E+01	8.122E+11	8.122E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
37	27	6	4*	2.700068E+01	9.930E+11	8.124E+11	2.155E+09	2.155E+09	0.000E+00	0.000E+00	0.000E+00
38	9	6	4*	2.700084E+01	9.930E+11	8.124E+11	2.660E+09	2.660E+09	0.000E+00	0.000E+00	0.000E+00
37	27	6	4*	2.700145E+01	6.319E+11	8.125E+11	1.747E+06	1.747E+06	0.000E+00	0.000E+00	0.000E+00
38	9	6	4*	2.700155E+01	6.320E+11	8.125E+11	4.299E+07	4.299E+07	0.000E+00	0.000E+00	0.000E+00
40	11	6	5*	2.699883E+01	8.123E+11	8.123E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
39	33	6	5*	2.69983E+01	8.123E+11	8.123E+11	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
39	33	6	5*	2.700045E+01	9.601E+11	8.124E+11	2.207E+07	2.207E+07	0.000E+00	0.000E+00	0.000E+00
40	11	6	5*	2.700045E+01	9.601E+11	8.124E+11	2.377E+07	2.377E+07	0.000E+00	0.000E+00	0.000E+00
39	33	6	5*	2.700078E+01	6.647E+11	8.124E+11	9.698E+04	9.698E+04	0.000E+00	0.000E+00	0.000E+00
40	11	6	5*	2.700078E+01	6.647E+11	8.124E+11	2.925E+05	2.925E+05	0.000E+00	0.000E+00	0.000E+00

NRSLMX= 6 NVMAX= 6 LVMAX= 5

C-----  
C  
C  
C  
C-----

*Data lines for IC coupled 'r' file:*

*Format:*

ELEM, IZ, CCPLG

1a2,i2,5x,1a4

[blank line]

1a80

[prescribed text field]

1a56

until <blank line for each upper state> do

IRSL,G,N,L,CODEL,DEL,B,R,A,A1,A2,A3

3i5,i4,1a1,e15.6,6e12.3

for <all lower state with same upper state> do

IRSL,G,N,L,CODEL,DEL,B

3i5,i4,1a1,e15.6

repeat

repeat

[blank line]

1a80

[prescribed text],NRSLMX, [prescribed text], NVMAX, [prescribed text], LVMAX

1a10,i4,1a10,i4,1a10,i4

[blank line]

1a80

[prescribed comment line]

1a80

[prescribed comment line]

1a80

[prescribed comment line]

1a80

[prescribed comment line]

1a80

*variable identification :*

*name*

*meaning*

ELEM	sequence identifier (two characters)
IZ	nuclear charge
CCPLG	coupling scheme, '/IC/' => intermediate coupling
IRSL	initial level (see level list in 'l' file)
G	statistical weight of level
N	principal quantum number of outer electron of upper state
L	orbital quantum number of outer electron of upper state
CODEL	'*' => NL electron was active; ' ' => NL electron passive
DEL	photon energy (Rydberg)
B	Einstein absorption rate (sec-1)
R	total radiative width (sec-1)
A	total Auger width (sec-1)
A1	resolved Auger width to parent 1
A2	resolved Auger width to parent 2
.	.
An	resolved Auger width to parent n (Note $\sum_n A_n \leq A$ in general since not all are necessarily resolved).
NRSLMX	maximum resolved n
NVMAX	maximum n' in data set
LVMAX	maximum l' in data set

Table B38e – example – intermediate coupling rate coefficient (r) file.

c 5 /IC/

IRSL	G	N	L	DEL(RYD)	B(SEC)	R(SEC)	A(SEC):	1	2	3	4
2	3	2	-1	2.577842E+01	1.836E+07	3.030E+11	3.600E+14	3.600E+14	0.000E+00	0.000E+00	0.000E+00
4	3	2	-1	2.536727E+01	1.010E+11	1.497E+12	2.986E+09	2.986E+09	0.000E+00	0.000E+00	0.000E+00
2	3	2	-1	2.627332E+01	4.990E+11	1.497E+12	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
4	3	2	-1	2.586217E+01	5.904E+06	1.497E+12	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
1	1	2	-1	2.627619E+01	1.498E+12	1.497E+12	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
2	3	2	-1	2.627476E+01	3.743E+11	1.497E+12	2.574E+10	2.574E+10	0.000E+00	0.000E+00	0.000E+00
3	5	2	-1	2.627188E+01	3.742E+11	1.497E+12	3.899E+14	3.899E+14	0.000E+00	0.000E+00	0.000E+00
4	3	2	-1	2.586361E+01	8.732E+06	1.497E+12	2.574E+10	2.574E+10	0.000E+00	0.000E+00	0.000E+00
2	3	2	-1	2.627762E+01	6.241E+11	1.471E+12	3.899E+14	3.899E+14	0.000E+00	0.000E+00	0.000E+00
3	5	2	-1	2.627474E+01	1.123E+12	1.471E+12	3.899E+14	3.899E+14	0.000E+00	0.000E+00	0.000E+00
4	3	2	-1	2.586647E+01	7.481E+07	1.471E+12	2.317E+13	2.317E+13	0.000E+00	0.000E+00	0.000E+00
2	3	2	-1	2.652934E+01	2.110E+06	1.471E+12	2.317E+13	2.317E+13	0.000E+00	0.000E+00	0.000E+00
3	5	2	-1	2.652646E+01	7.541E+07	1.471E+12	2.317E+13	2.317E+13	0.000E+00	0.000E+00	0.000E+00
4	3	2	-1	2.611819E+01	2.451E+12	1.235E+12	2.317E+13	2.317E+13	0.000E+00	0.000E+00	0.000E+00
2	3	2	-1	2.723699E+01	2.269E+05	1.235E+12	1.987E+13	1.987E+13	0.000E+00	0.000E+00	0.000E+00
4	3	2	-1	2.682584E+01	4.117E+11	7.551E+11	1.987E+13	1.987E+13	0.000E+00	0.000E+00	0.000E+00
5	3	2	-1	2.635047E+01	2.517E+11	7.553E+11	1.987E+13	1.987E+13	0.000E+00	0.000E+00	0.000E+00
6	1	2	-1	2.635190E+01	7.553E+11	7.553E+11	1.987E+13	1.987E+13	0.000E+00	0.000E+00	0.000E+00
5	3	2	-1	2.582515E+01	1.776E+07	7.555E+11	1.986E+13	1.986E+13	0.000E+00	0.000E+00	0.000E+00
5	3	2	-1	2.635478E+01	1.259E+12	7.707E+11	1.913E+14	1.913E+14	0.000E+00	0.000E+00	0.000E+00
6	1	2	-1	2.705647E+01	6.808E+06	7.707E+11	3.274E+12	3.274E+12	0.000E+00	0.000E+00	0.000E+00
5	3	2	-1	2.652973E+01	2.312E+12	1.305E+11	3.274E+12	3.274E+12	0.000E+00	0.000E+00	0.000E+00
5	3	3	1	3.076177E+01	3.883E+10	1.305E+11	3.275E+12	3.275E+12	0.000E+00	0.000E+00	0.000E+00
5	3	3	1	3.076201E+01	1.655E+11	1.305E+11	3.275E+12	3.275E+12	0.000E+00	0.000E+00	0.000E+00
6	1	3	1	3.023526E+01	1.821E+07	1.305E+11	3.274E+12	3.274E+12	0.000E+00	0.000E+00	0.000E+00
5	3	3	1	3.076248E+01	1.942E+11	1.252E+11	2.958E+13	2.958E+13	0.000E+00	0.000E+00	0.000E+00
5	3	3	1	3.080719E+01	6.422E+06	1.252E+11	2.958E+13	2.958E+13	0.000E+00	0.000E+00	0.000E+00
6	1	3	1	3.028044E+01	3.333E+11	5.934E+10	1.521E+12	1.521E+12	0.000E+00	0.000E+00	0.000E+00
5	3	4	1	3.211268E+01	1.776E+10	5.934E+10	1.522E+12	1.522E+12	0.000E+00	0.000E+00	0.000E+00
5	3	4	1	3.211279E+01	5.329E+10	5.934E+10	1.522E+12	1.522E+12	0.000E+00	0.000E+00	0.000E+00
6	1	4	1	3.158604E+01	1.161E+07	5.934E+10	1.521E+12	1.521E+12	0.000E+00	0.000E+00	0.000E+00
5	3	4	1	3.211301E+01	8.882E+10	5.934E+10	1.521E+12	1.521E+12	0.000E+00	0.000E+00	0.000E+00
5	3	4	1	3.213030E+01	4.072E+06	5.684E+10	1.346E+13	1.346E+13	0.000E+00	0.000E+00	0.000E+00
6	1	4	1	3.160355E+01	1.524E+11	3.082E+10	7.985E+11	7.985E+11	0.000E+00	0.000E+00	0.000E+00
5	3	5	1	3.271900E+01	9.243E+09	3.082E+10	7.990E+11	7.990E+11	0.000E+00	0.000E+00	0.000E+00
5	3	5	1	3.271905E+01	2.773E+10	3.082E+10	7.990E+11	7.990E+11	0.000E+00	0.000E+00	0.000E+00
6	1	5	1	3.219230E+01	6.917E+06	3.082E+10	7.985E+11	7.985E+11	0.000E+00	0.000E+00	0.000E+00
5	3	5	1	3.271917E+01	4.622E+10	2.953E+10	6.993E+12	6.993E+12	0.000E+00	0.000E+00	0.000E+00
5	3	5	1	3.272758E+01	2.423E+06	2.953E+10	6.993E+12	6.993E+12	0.000E+00	0.000E+00	0.000E+00
6	1	5	1	3.220083E+01	7.929E+10	1.790E+10	4.664E+11	4.664E+11	0.000E+00	0.000E+00	0.000E+00
5	3	6	1	3.304313E+01	5.371E+09	1.790E+10	4.668E+11	4.668E+11	0.000E+00	0.000E+00	0.000E+00
5	3	6	1	3.251642E+01	4.310E+06	1.790E+10	4.668E+11	4.668E+11	0.000E+00	0.000E+00	0.000E+00
5	3	6	1	3.304323E+01	2.686E+10	1.715E+10	4.664E+11	4.664E+11	0.000E+00	0.000E+00	0.000E+00
6	1	6	1	3.304796E+01	1.088E+06	1.715E+10	4.061E+12	4.061E+12	0.000E+00	0.000E+00	0.000E+00
6	1	6	1	3.252121E+01	4.608E+10	8.082E+11	2.120E+12	2.120E+12	0.000E+00	0.000E+00	0.000E+00
7	3	3	0*	2.693778E+01	2.681E+11	8.082E+11	2.156E+12	2.156E+12	0.000E+00	0.000E+00	0.000E+00
7	3	3	0*	2.694210E+01	1.341E+12	8.082E+11	2.156E+12	2.156E+12	0.000E+00	0.000E+00	0.000E+00
7	3	3	0*	2.690198E+01	1.285E+09	8.076E+11	2.527E+13	2.527E+13	0.000E+00	0.000E+00	0.000E+00
8	1	3	0*	2.685713E+01	3.808E+09	8.076E+11	2.527E+13	2.527E+13	0.000E+00	0.000E+00	0.000E+00
8	1	3	0*	2.690818E+01	2.407E+12	8.031E+11	2.119E+12	2.119E+12	0.000E+00	0.000E+00	0.000E+00
9	3	4	0*	2.698037E+01	7.700E+11	8.115E+11	7.973E+11	7.973E+11	0.000E+00	0.000E+00	0.000E+00
10	1	4	0*	2.698161E+01	8.022E+11	8.116E+11	8.915E+11	8.915E+11	0.000E+00	0.000E+00	0.000E+00
9	3	4	0*	2.694560E+01	3.328E+10	8.116E+11	8.915E+11	8.915E+11	0.000E+00	0.000E+00	0.000E+00
9	3	4	0*	2.698469E+01	1.350E+12	8.119E+11	7.969E+11	7.969E+11	0.000E+00	0.000E+00	0.000E+00
9	3	4	0*	2.700245E+01	7.804E+09	8.108E+11	1.052E+13	1.052E+13	0.000E+00	0.000E+00	0.000E+00
10	1	4	0*	2.696644E+01	2.404E+12	8.108E+11	1.052E+13	1.052E+13	0.000E+00	0.000E+00	0.000E+00

11	3	5	0*	2.699699E+01	7.851E+11	8.126E+11	5.429E+11	5.429E+11	0.000E+00	0.000E+00	0.000E+00
12	1	5	0*	2.697857E+01	8.004E+10	8.129E+11	3.801E+11	3.801E+11	0.000E+00	0.000E+00	0.000E+00
11	3	5	0*	2.700024E+01	1.353E+12	8.129E+11	3.801E+11	3.801E+11	0.000E+00	0.000E+00	0.000E+00
11	3	5	0*	2.700024E+01	2.698997E+01	8.129E+11	3.801E+11	3.801E+11	0.000E+00	0.000E+00	0.000E+00
12	1	5	0*	2.698997E+01	2.354E+12	8.129E+11	3.801E+11	3.801E+11	0.000E+00	0.000E+00	0.000E+00
13	3	6	0*	2.700274E+01	2.708E+11	8.129E+11	2.109E+11	2.109E+11	0.000E+00	0.000E+00	0.000E+00
13	3	6	0*	2.700360E+01	7.521E+11	8.129E+11	4.207E+11	4.207E+11	0.000E+00	0.000E+00	0.000E+00
14	1	6	0*	2.699299E+01	1.812E+11	8.129E+11	2.108E+11	2.108E+11	0.000E+00	0.000E+00	0.000E+00
13	3	6	0*	2.700705E+01	1.355E+12	8.129E+11	2.108E+11	2.108E+11	0.000E+00	0.000E+00	0.000E+00
13	3	6	0*	2.701134E+01	6.052E+10	8.129E+11	2.821E+12	2.821E+12	0.000E+00	0.000E+00	0.000E+00
14	1	6	0*	2.700074E+01	2.256E+12	8.129E+11	2.821E+12	2.821E+12	0.000E+00	0.000E+00	0.000E+00
1	1	3	1	3.032053E+01	5.957E+08	9.531E+11	5.565E+08	5.565E+08	0.000E+00	0.000E+00	0.000E+00
2	3	3	1	3.031913E+01	5.416E+08	9.531E+11	5.565E+08	5.565E+08	0.000E+00	0.000E+00	0.000E+00
3	5	3	1	3.031629E+01	6.986E+05	9.531E+11	5.565E+08	5.565E+08	0.000E+00	0.000E+00	0.000E+00
4	4	3	1	2.996734E+01	2.739E+11	9.531E+11	5.565E+08	5.565E+08	0.000E+00	0.000E+00	0.000E+00
15	1	3	1*	2.677850E+01	2.763E+09	9.531E+11	5.565E+08	5.565E+08	0.000E+00	0.000E+00	0.000E+00
16	3	3	1*	2.677825E+01	1.189E+09	9.531E+11	5.565E+08	5.565E+08	0.000E+00	0.000E+00	0.000E+00
17	5	3	1*	2.677773E+01	3.567E+07	9.531E+11	5.565E+08	5.565E+08	0.000E+00	0.000E+00	0.000E+00
18	3	3	1*	2.665797E+01	6.622E+11	9.531E+11	5.565E+08	5.565E+08	0.000E+00	0.000E+00	0.000E+00
1	1	3	1	3.035129E+01	3.764E+11	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
2	3	3	1	3.034988E+01	9.251E+10	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
3	5	3	1	3.034704E+01	3.679E+09	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
4	4	3	1	2.999809E+01	7.678E+08	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
15	1	3	1*	2.680926E+01	1.175E+12	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
16	3	3	1*	2.680900E+01	3.020E+11	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
17	5	3	1*	2.680848E+01	1.307E+10	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
18	3	3	1*	2.668872E+01	1.771E+09	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
2	3	3	1	3.035146E+01	2.825E+11	9.531E+11	1.887E+11	1.887E+11	0.000E+00	0.000E+00	0.000E+00
68	11	6	5*	2.701560E+01	1.989E+10	8.138E+11	1.050E+07	1.050E+07	0.000E+00	0.000E+00	0.000E+00
69	13	6	5*	2.701560E+01	3.337E+11	8.138E+11	1.050E+07	1.050E+07	0.000E+00	0.000E+00	0.000E+00
70	11	6	5*	2.701560E+01	5.475E+11	8.138E+11	1.050E+07	1.050E+07	0.000E+00	0.000E+00	0.000E+00
67	9	6	5*	2.701601E+01	4.058E+11	8.138E+11	1.281E+05	1.281E+05	0.000E+00	0.000E+00	0.000E+00
68	11	6	5*	2.701601E+01	3.151E+11	8.138E+11	1.281E+05	1.281E+05	0.000E+00	0.000E+00	0.000E+00
70	11	6	5*	2.701600E+01	1.879E+10	8.138E+11	1.281E+05	1.281E+05	0.000E+00	0.000E+00	0.000E+00
67	9	6	5*	2.701601E+01	8.885E+09	8.138E+11	6.079E+04	6.079E+04	0.000E+00	0.000E+00	0.000E+00
68	11	6	5*	2.701601E+01	1.798E+10	8.138E+11	6.079E+04	6.079E+04	0.000E+00	0.000E+00	0.000E+00
69	13	6	5*	2.701600E+01	3.327E+11	8.138E+11	6.079E+04	6.079E+04	0.000E+00	0.000E+00	0.000E+00
70	11	6	5*	2.701663E+01	3.953E+11	8.138E+11	6.079E+04	6.079E+04	0.000E+00	0.000E+00	0.000E+00
68	11	6	5*	2.701662E+01	9.412E+11	8.138E+11	2.289E+07	2.289E+07	0.000E+00	0.000E+00	0.000E+00
69	13	6	5*	2.701662E+01	1.061E+10	8.138E+11	2.289E+07	2.289E+07	0.000E+00	0.000E+00	0.000E+00
70	11	6	5*	2.701662E+01	8.079E+09	8.138E+11	2.289E+07	2.289E+07	0.000E+00	0.000E+00	0.000E+00
69	13	6	5*	2.701662E+01	9.391E+11	8.138E+11	2.200E+07	2.200E+07	0.000E+00	0.000E+00	0.000E+00
67	9	6	5*	2.701695E+01	6.330E+11	8.138E+11	9.728E+04	9.728E+04	0.000E+00	0.000E+00	0.000E+00
67	9	6	5*	2.701696E+01	1.781E+10	8.138E+11	1.842E+05	1.842E+05	0.000E+00	0.000E+00	0.000E+00
68	11	6	5*	2.701696E+01	5.241E+09	8.138E+11	1.842E+05	1.842E+05	0.000E+00	0.000E+00	0.000E+00
70	11	6	5*	2.701695E+01	6.461E+11	8.138E+11	1.842E+05	1.842E+05	0.000E+00	0.000E+00	0.000E+00

NRSIMX= 6 NVMAX= 6 LVMAX= 5

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