

ADF39: Opacity project extension: photoionisation cross-sections

The basic process is inner shell photo-ionisation $(n_c l_c^q)nl + \gamma \rightarrow (n_c l_c^{q-1})nl + e$. A separate file is provided for each n . It is convenient at the production stage to separate the level list file (denoted by the postfix 'l') from the partial cross-section file (denoted by postfix 'px'). Separate files are given for term (LS) coupling and intermediate (IC) coupling. Outer shell photo-ionisation, $(n_c l_c^q)nl + \gamma \rightarrow (n_c l_c^q) + e$, is included for completeness. Where inner shell photo-ionisation is present, the atomic structure is optimised for the inner-shell processes

Utilising subroutines :

ADAS204? ADAS208? ADAS212?

Formatted files to ADF39 specification :

Database Status	Date = March 17, 2003	Data type =pea files	Data root =/.../adas/adas/adf39/			
<i>Recombining seq.</i>	<i>Library</i>	<i>Elements</i>	<i>Members</i>	<i>n</i>	<i>Comments</i>	<i>Quality</i>
Bare nucleus	nrb02##	He, C, O, S, Fe	<ion>lsK<n>l.dat	1,2,3,4,5,6	LS resolution	medium
		He, C, O, S, Fe	<ion>icK<n>l.dat	1,2,3,4,5,6	IC resolution	medium
		He, C, O, S, Fe	<ion>lsK<n>px.dat	1,2,3,4,5,6	LS resolution	medium
		He, C, O, S, Fe	<ion>icK<n>px.dat	1,2,3,4,5,6	IC resolution	medium
H-like.	nrb02#h	He, C, O, S, Fe	<ion>lsK<n>l.dat	1,2,3,4,5,6	LS resolution	medium
		He, C, O, S, Fe	<ion>icK<n>l.dat	1,2,3,4,5,6	IC resolution	medium
		He, C, O, S, Fe	<ion>lsK<n>px.dat	1,2,3,4,5,6	LS resolution	medium
		He, C, O, S, Fe	<ion>icK<n>px.dat	1,2,3,4,5,6	IC resolution	medium
He-like.	nrb02#he	C, O, S, Fe	<ion>lsK<n>l.dat	1,2,3,4,5,6	LS resolution	medium
		C, O, S, Fe	<ion>icK<n>l.dat	1,2,3,4,5,6	IC resolution	medium
		C, O, S, Fe	<ion>lsK<n>px.dat	1,2,3,4,5,6	LS resolution	medium
		C, O, S, Fe	<ion>icK<n>px.dat	1,2,3,4,5,6	IC resolution	medium
		C, O, S, Fe	<ion>lsL<n>l.dat	2,3,4	IC resolution	medium
		C, O, S, Fe	<ion>icL<n>l.dat	2,3,4	IC resolution	medium
		C, O, S, Fe	<ion>lsL<n>px.dat	2,3,4	LS resolution	medium
		C, O, S, Fe	<ion>icL<n>px.dat	2,3,4	IC resolution	medium
Li-like.	nrb02#li	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>px.dat	2,3,4,5,6	LS resolution	medium
C, O, S, Fe	<ion>icK<n>px.dat	2,3,4,5,6	IC resolution	medium
C, O, S, Fe	<ion>lsL<n>l.dat	2,3,4	LS resolution	medium
C, O, S, Fe	<ion>icL<n>l.dat	2,3,4	IC resolution	medium
C, O, S, Fe	<ion>lsL<n>px.dat	2,3,4	LS resolution	medium
C, O, S, Fe	<ion>icL<n>px.dat	2,3,4	IC resolution	medium

Notes:

Data lines for LS coupled 'l' 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
IND0, 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

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,f12.1,1a7,i5
1a28
1a56
1a56

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

i6,i6,4x,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 :

name

meaning

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)

IND0(INDP)

parent index as used in the 'px' file

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

(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 'px' 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 B39c – example – LS coupling level list (l) file.

PARENT TERM INDEXING		BWNP= 3952439.9		NPRNT= 4
INDP	CODE	S L	WI	WNP
1	1S1	(2)0	(0.5)	0.0
2	3S1	(2)0	(0.5)	3513280.1
3	3P1	(2)1	(2.5)	3513373.4
4	3D1	(2)2	(4.5)	3513448.2

LS RESOLVED TERM INDEXING		BWNR= 4268185.4		NTRM= 6	
INDX	IRSL	CODE	S L	WJ	WNR
1	1	1S1 3S1	(3)0	(1.0)	0.0
2	2	1S1 3P1	(3)1	(4.0)	14018.3
3	3	1S1 3S1	(1)0	(0.0)	15190.7
4	4	1S1 3D1	(3)2	(7.0)	22628.8
5	5	1S1 3D1	(1)2	(2.0)	23279.9
6	6	1S1 3P1	(1)1	(1.0)	25953.9

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

Data lines for IC coupled 'l' 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]

Format:

1a5,1a2,1a11,i2,50x,1a4
 1a80
 1a45,f12.1,1a8,i4
 1a23
 1a56
 1a56

for indp=1,NPRNT	
IND0, CFGP, ISP, ILP ,XJP,WNPI	i6,10x,1a20,1x,i1,1x,i1,1x,f4.1,2x,f10.1
repeat	
[blank line]	1a80
[prescribed text], BWNR, [prescribed text], NLVL	1a45,f12.1,1a7,i5
[prescribed text field]	1a28
[prescribed text field]	1a56
[prescribed text field]	1a56
for indx=1,NLVL	
INDX,ISRL,CFGL,IS, IL, XJ, WNRL	i6,i6,4x,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)
IND0 (INDP)	parent index as used in the 'px' file.
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)
NLVL	number of levels in IC coupled set
INDX	index value for level
CFGL	configuration (or Eissner code therefor) for level.
IS	multiplicity for level ($2*S+1$)
IL	total orbital quantum number for level (L)
XJ	J quantum number of level.
WNRL	energy of level relative to ground (cm-1)

Table B39d – example – intermediate coupling level list (I) file.

PARENT LEVEL INDEXING		BWNP= 3952439.9		NPRNT= 6	
INDP	CODE	S L	WI	WNP	
1	1S1	(2)0	(0.5)	0.0	
2	3P1	(2)1	(0.5)	3513279.9	
3	3S1	(2)0	(0.5)	3513280.1	
4	3D1	(2)2	(1.5)	3513420.2	
5	3P1	(2)1	(1.5)	3513420.2	
6	3D1	(2)2	(2.5)	3513466.9	

IC RESOLVED LEVEL INDEXING			BWNR= 4268185.4		NLVL= 10	
INDX	IRSL	CODE	S L	WJ	WNR	
1	1	1S1 3S1	(3)0	(1.0)	0.0	
2	2	1S1 3P1	(3)1	(0.0)	13924.8	
3	3	1S1 3P1	(3)1	(1.0)	13971.2	
4	4	1S1 3P1	(3)1	(2.0)	14065.1	
5	5	1S1 3S1	(1)0	(0.0)	15190.7	
6	6	1S1 3D1	(3)2	(1.0)	22600.8	
7	7	1S1 3D1	(3)2	(2.0)	22618.7	
8	8	1S1 3D1	(3)2	(3.0)	22647.5	
9	9	1S1 3D1	(1)2	(2.0)	23280.7	
10	10	1S1 3P1	(1)1	(1.0)	25954.2	



Data lines for LS coupled 'px' file:

Format:

ELEM, IZ, CCPLG,NENG	1a2,i2,5x,1a4,26x,i2
IENG(I),I=1,NENG	39x,10(i2,10x)
ENG(I),I=1,NENG	31x,10e12.3
[blank line]	1a80
IPCS(I),I=1,NENG	39x,10(i2,10x)
until <blank line for each initial state> do	
IRSL,G,IND0,(PCS(I),I=1,NENG)	3i5, e15.6,10e12.3
repeat	
[blank line]	1a80
[prescribed text],NRSLMX	1a10,i4
[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>
ELEM	sequence identifier (two characters)

2	9	3	3.476573E+01	1.749E-19	1.699E-19	1.648E-19	1.502E-19	1.358E-19	1.005E-19	6.948E-20	5.629E-20	4.622E-20	1.744E-20
				8.317E-21	4.569E-21								
6	3	3	3.465696E+01	1.744E-19	1.694E-19	1.643E-19	1.498E-19	1.354E-19	1.002E-19	6.933E-20	5.618E-20	4.614E-20	1.742E-20
				8.309E-21	4.565E-21								
4	15	4	3.468794E+01	1.745E-19	1.696E-19	1.644E-19	1.499E-19	1.355E-19	1.003E-19	6.938E-20	5.621E-20	4.616E-20	1.743E-20
				8.311E-21	4.566E-21								
5	5	4	3.468201E+01	1.745E-19	1.695E-19	1.644E-19	1.499E-19	1.355E-19	1.003E-19	6.937E-20	5.621E-20	4.616E-20	1.743E-20
				8.311E-21	4.566E-21								
NRSLMX=			6										
C-----													
C													
C													
C													
C-----													

Data lines for IC coupled 'px' file:

Format:

ELEM, IZ, CCPLG, NENG	1a2, i2, 5x, 1a4, 26x, i2
IENG(I), I=1, NENG	39x, 10(i2, 10x)
ENG(I), I=1, NENG	31x, 10e12.3
[blank line]	1a80
IPCS(I), I=1, NENG	39x, 10(i2, 10x)
until <blank line for each initial state> do	
IRSL, G, IND0, DELI, (PCS(I), I=1, NENG)	3i5, e15.6, 10e12.3/30x, 10e12.3
repeat	
[blank line]	1a80
[prescribed text], NRSLMX	1a10, i4
[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>
ELEM	sequence identifier (two characters)
IZ	ionised ion charge
CCPLG	coupling scheme, '/IC/' => IC coupling
NENG	number of energies for tabulation
IENG()	indexing for energy tabulation
ENG()	ejected electron energies (Ryd)
IPCS()	indexing for photoionisation cross-section tabulation
IRSL	initial level (see level list in 'l' file)
G	statistical weight of level
IND0	index of parent to which photoionisation occurs
DELI	photon ionisation energy (Rydberg)
PCS()	photoionisation cross-section (cm ²)
NRSLMX	maximum resolved n

Table B39f – example – intermediate coupling rate coefficient (px) file.

C	5	/IC/	NENG=12											
			E: 1	2	3	4	5	6	7	8	9	10		
			11	12										
			0.000E+00	9.600E-01	1.600E+00	3.200E+00	4.800E+00	9.600E+00	1.600E+01	2.000E+01	2.400E+01	4.800E+01		
			7.200E+01	9.600E+01										
IRSL	G	IND0	DELI (RYD)	PCS: 1										
				11	12	3	4	5	6	7	8	9	10	
1	3	1	2.877282E+00	1.164E-18	7.741E-19	6.003E-19	3.397E-19	2.087E-19	6.833E-20	2.472E-20	1.529E-20	1.019E-20	1.969E-21	
6	3	1	2.671329E+00	1.360E-18	6.444E-19	4.093E-19	1.503E-19	6.422E-20	9.133E-21	1.539E-21	6.639E-22	3.274E-22	1.926E-23	
3	3	1	2.749967E+00	1.375E-18	8.384E-19	6.132E-19	3.017E-19	1.631E-19	3.888E-20	1.031E-20	5.470E-21	3.199E-21	3.604E-22	
10	3	1	2.640770E+00	1.321E-18	8.137E-19	5.979E-19	2.961E-19	1.608E-19	3.853E-20	1.025E-20	5.444E-21	3.186E-21	3.596E-22	

5	1	1	2.738854E+00	9.027E-23 1.108E-18 6.990E-22	3.167E-23 7.462E-19 3.227E-22	5.818E-19	3.320E-19	2.050E-19	6.761E-20	2.456E-20	1.521E-20	1.014E-20	1.967E-21
7	5	1	2.671166E+00	1.360E-18 3.283E-24	6.444E-19 7.807E-25	4.093E-19	1.503E-19	6.422E-20	9.133E-21	1.539E-21	6.639E-22	3.274E-22	1.926E-23
9	5	1	2.665133E+00	1.357E-18 3.282E-24	6.433E-19 7.807E-25	4.087E-19	1.501E-19	6.417E-20	9.129E-21	1.538E-21	6.637E-22	3.273E-22	1.926E-23
2	1	1	2.750390E+00	1.376E-18 9.041E-23	8.385E-19 3.171E-23	6.133E-19	3.017E-19	1.631E-19	3.888E-20	1.031E-20	5.471E-21	3.199E-21	3.604E-22
4	5	1	2.749112E+00	1.375E-18 9.040E-23	8.382E-19 3.171E-23	6.131E-19	3.016E-19	1.631E-19	3.888E-20	1.030E-20	5.470E-21	3.199E-21	3.604E-22
8	7	1	2.670903E+00	1.360E-18 3.283E-24	6.443E-19 7.807E-25	4.092E-19	1.503E-19	6.422E-20	9.133E-21	1.539E-21	6.639E-22	3.274E-22	1.926E-23
3	3	2	3.476531E+01	1.175E-19 5.588E-21	1.142E-19 3.070E-21	1.107E-19	1.009E-19	9.123E-20	6.749E-20	4.668E-20	3.782E-20	3.105E-20	1.172E-20
4	5	2	3.476445E+01	2.446E-42 1.163E-43	2.376E-42 6.390E-44	2.305E-42	2.101E-42	1.899E-42	1.405E-42	9.717E-43	7.873E-43	6.464E-43	2.440E-43
10	3	2	3.465611E+01	5.722E-20 2.726E-21	5.559E-20 1.498E-21	5.392E-20	4.915E-20	4.444E-20	3.288E-20	2.275E-20	1.844E-20	1.514E-20	5.717E-21
2	1	2	3.476573E+01	1.749E-19 8.317E-21	1.699E-19 4.569E-21	1.648E-19	1.502E-19	1.358E-19	1.005E-19	6.948E-20	5.629E-20	4.622E-20	1.744E-20
5	1	3	3.475419E+01	1.743E-19 8.315E-21	1.695E-19 4.568E-21	1.644E-19	1.500E-19	1.356E-19	1.004E-19	6.944E-20	5.627E-20	4.620E-20	1.744E-20
7	5	3	3.468650E+01	5.818E-25 1.545E-31	2.084E-25 3.406E-32	1.145E-25	3.194E-26	1.118E-26	1.086E-27	1.376E-28	5.276E-29	2.373E-29	1.035E-30
9	5	3	3.468047E+01	5.817E-25 1.545E-31	2.084E-25 3.406E-32	1.145E-25	3.194E-26	1.118E-26	1.086E-27	1.376E-28	5.275E-29	2.373E-29	1.035E-30
1	3	3	3.489262E+01	1.761E-19 8.328E-21	1.709E-19 4.574E-21	1.657E-19	1.509E-19	1.364E-19	1.008E-19	6.968E-20	5.644E-20	4.633E-20	1.747E-20
6	3	3	3.468667E+01	5.818E-25 1.545E-31	2.084E-25 3.406E-32	1.145E-25	3.194E-26	1.118E-26	1.086E-27	1.376E-28	5.276E-29	2.373E-29	1.035E-30
3	3	3	3.476531E+01	5.728E-25 4.254E-30	2.660E-25 1.383E-30	1.689E-25	6.341E-26	2.816E-26	4.601E-27	9.192E-28	4.338E-28	2.315E-28	1.936E-29
10	3	3	3.465611E+01	5.710E-25 4.249E-30	2.652E-25 1.382E-30	1.684E-25	6.323E-26	2.808E-26	4.590E-27	9.172E-28	4.330E-28	2.311E-28	1.934E-29
2	1	3	3.476573E+01	5.728E-25 4.254E-30	2.660E-25 1.383E-30	1.689E-25	6.342E-26	2.816E-26	4.601E-27	9.192E-28	4.338E-28	2.315E-28	1.936E-29
4	5	3	3.476445E+01	5.728E-25 4.254E-30	2.660E-25 1.383E-30	1.689E-25	6.341E-26	2.816E-26	4.601E-27	9.191E-28	4.338E-28	2.315E-28	1.936E-29
8	7	3	3.468624E+01	5.818E-25 1.545E-31	2.084E-25 3.406E-32	1.145E-25	3.194E-26	1.118E-26	1.086E-27	1.376E-28	5.276E-29	2.373E-29	1.035E-30
7	5	4	3.468778E+01	1.106E-19 5.267E-21	1.074E-19 2.894E-21	1.042E-19	9.498E-20	8.588E-20	6.354E-20	4.396E-20	3.562E-20	2.925E-20	1.104E-20
8	7	4	3.468752E+01	1.606E-33 7.647E-35	1.560E-33 4.201E-35	1.513E-33	1.379E-33	1.247E-33	9.226E-34	6.383E-34	5.172E-34	4.247E-34	1.603E-34
9	5	4	3.468175E+01	6.393E-20 3.045E-21	6.211E-20 1.673E-21	6.023E-20	5.491E-20	4.964E-20	3.673E-20	2.541E-20	2.059E-20	1.691E-20	6.384E-21
6	3	4	3.468794E+01	1.745E-19 8.311E-21	1.696E-19 4.566E-21	1.644E-19	1.499E-19	1.355E-19	1.003E-19	6.938E-20	5.621E-20	4.616E-20	1.743E-20
3	3	5	3.476658E+01	5.740E-20 2.729E-21	5.576E-20 1.499E-21	5.408E-20	4.929E-20	4.456E-20	3.296E-20	2.280E-20	1.847E-20	1.517E-20	5.724E-21
10	3	5	3.465739E+01	1.172E-19 5.582E-21	1.138E-19 3.067E-21	1.104E-19	1.006E-19	9.098E-20	6.733E-20	4.658E-20	3.775E-20	3.100E-20	1.170E-20
4	5	5	3.476573E+01	1.749E-19 8.317E-21	1.699E-19 4.569E-21	1.648E-19	1.502E-19	1.358E-19	1.005E-19	6.948E-20	5.629E-20	4.622E-20	1.744E-20

2	1	5	3.476701E+01	1.600E-42	1.554E-42	1.507E-42	1.373E-42	1.242E-42	9.185E-43	6.353E-43	5.147E-43	4.226E-43	1.595E-43
				7.605E-44	4.178E-44								
6	3	6	3.468837E+01	4.298E-33	4.175E-33	4.049E-33	3.691E-33	3.337E-33	2.469E-33	1.708E-33	1.384E-33	1.137E-33	4.291E-34
				2.047E-34	1.124E-34								
7	5	6	3.468821E+01	6.394E-20	6.212E-20	6.024E-20	5.491E-20	4.965E-20	3.674E-20	2.542E-20	2.059E-20	1.691E-20	6.385E-21
				3.045E-21	1.673E-21								
9	5	6	3.468218E+01	1.106E-19	1.074E-19	1.042E-19	9.497E-20	8.586E-20	6.353E-20	4.396E-20	3.562E-20	2.925E-20	1.104E-20
				5.266E-21	2.893E-21								
8	7	6	3.468794E+01	1.745E-19	1.696E-19	1.644E-19	1.499E-19	1.355E-19	1.003E-19	6.938E-20	5.621E-20	4.616E-20	1.743E-20
				8.311E-21	4.566E-21								

NRSLMX= 6

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