

## ADF09: direct resolved dielectronic recombination coefficients

Formatting conventions and variable storage are given below for transfer files from Nigel Badnell's dielectronic calculations. Data for an ion is specified by the isoelectronic sequence of the final (ie. recombined) ion and nuclear charge of the element. There are distinct blocks of data for LS-resolved low levels and bundle-n levels. The former is divided according to recombining ion metastable parents(including ground state) and the latter by both parents and recombined ion spin system. Representative bundle-n levels are used. In this organisation, recombination data is provided as a function of temperature. Up to 10 temperatures may be given with some preference for using the tmperature set  $T_e(k)=z1^{**2}*\theta(k)$  where  $z1$  is the recombining ion charge and  $\theta=1.0d3,2.0d3,5.0d3,1.0d4,2.0d4,5.0d4,1.0d5,2.0d5,5.0d5,1.0d6$ . The secondary Auger rate coefficient associated with metastable parent change is required.

**An extension to intermediate coupling is in progress as part of the DR Project. New IC and :LS specifications have to be added**

*Utilising subroutines :*

ADAS204      ADAS208      ADAS212

*Formatted files to ADF09 specification :*

Database Status	Date = January 12, 1999	Data type =drc files	Data root =/.../adas/adas/adf09/		
<i>Recombining seq.</i>	<i>Members</i>	<i>Library</i>	<i>n-n'</i>	<i>Comments</i>	<i>Quality</i>
H-like.	Ar,B,Be,C,Fe,He,Li, Mg,O,Sn,Y,	nrb93#h	1-2	LS resolution	medium
He-like	Ar,B,Be,C,Fe,Li,Mg, O,Sn,Y	nrb93#he	1-2, 2-2	LS resolution	medium
Li-like	Ar,B,Be,C,Fe,Mg, O,Sn,Y	nrb93#li	1-2, 2-2, 2-3	LS resolution	medium
Be-like	Ar,B,C,Fe,Mg, O,Sn,Y	nrb93#be	2-2, 2-3	LS resolution	medium
B-like	Ar,C,Fe,Mg,nrb93#b O,Sn,Y		2-2, 2-3	LS resolution	medium
C-like	Ar, Fe,Mg,O,Y	nrb93#c	2-2, 2-3	LS resolution	medium
N-like	Ar,Fe,Mg,O,Y	nrb93#n	2-2, 2-3	LS resolution	medium
O-like	Ar,Fe,Mg,Y	nrb93#o	2-2, 2-3	LS resolutiio	medium
F-like	Ar,Fe,Mg,Y	nrb93#f	2-2, 2-3	LS resolution	medium
Ne-like	Ar,Fe,Mg,Y	nrb93#ne	2-3	LS resolution	medium

H-like.	C, N, Ne	mom93#h	1-2	LS resolution	medium
He-like	C, N, Ne	mom93#he	1-2, 2-2	LS resolution	medium
Li-like	C, N, Ne	mom93#li	1-2, 2-2, 2-3	LS resolution	medium
Be-like	C, N, Ne	mom93#be	2-2, 2-3	LS resolution	medium
B-like	C, N, O, Ne	mom93#b	2-2, 2-3	LS resolution	medium
C-like	N, O, Ne	mom93#c	2-2, 2-3	LS resolution	medium
N-like	O, Ne	mom93#n	2-2, 2-3	LS resolution	medium
O-like	Ne, Mg	mom93#o	2-2, 2-3	LS resolution	medium
F-like	Ne, Mg	mom93#f	2-2, 2-3	LS resolution	medium

Notes: 1. The formerly named 'mom96' data have been renamed as 'mom93' since they are of the same calculation type as for the 'nrb93' data. The year number is therefore being used to mark the first year of a calculation type. A new year number will shortly be introduced for the intermediate coupling 'ic' dielectronic data now in preparation.

*Data lines :*

*Format:*

```

seq='SEQ'  nucchg=IZ0                                ADFID
parent term indexing      bwnp= BWNP  nprnt= NPRNT
-----
indp code      wnp
-----
for indp=1,NPRNT
      INDP  CCPI      WNPI
repeat
ls resolved term indexing  bwnr= BWNR  nlev= NLEV
-----

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indx code      s l  xj      wnr
-----
for indx=1,NLEV
      INDX CCI      (M)L( WJ)      WNRI
repeat
n-shell indexing & Auger rates      nrep= NREP
-----
irep  n  m'-m = TRNS1  TRNS2  TRNS3
---- - -----
for irep=1,NREP
      IREP NR      AA21I  AA31I  AA32I
repeat
for IPRT=1,NPRNT
      -----
      prt=IP  trmprt= (TP)  spnprt= SP  nsys= NSYS
      indx Te=  TE1   TE2   TE3   TE4   TE5   TE6
      ---- ---
      for indx=1,NLEV
            INDX  ALT1I  ALT2I  ALT3I  ALT4I  ALT5I  ALT6I
      repeat
      for isys=1,NSYS
            -----
            sys= IS  spnsys= SS
            irep
            ----

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        for irep=1,NREP
            IREP  ANT1I ANT2I ANT3I ANT4I ANT5I ANT6I
        repeat
    repeat
repeat

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DESCRIPTIVE TEXT  
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*variable identification :*

<i>name</i>	<i>meaning</i>
SEQ	sequence identifier (two characters)
IZO	nuclear charge
ADFID	ADAS data file type code (ADF09)
BWNP	binding wave number of lowest parent(cm-1)
NPRNT	number of metastable parents
INDP	index of parent
CCPI	configuration (or Eissner code therefor) for parent.
WNPI	energy of parent relative to lowest parent (cm-1)
BWNR	binding wave number of lowest resolved level (cm-1)
NLEV	number of levels in LS-resolved set
INDX	index value for level
CCI	configuration (or Eissner code therefor) for level.
M	multiplicity for level ( $2*S+1$ )
L	total orbital quantum number for level

WJ	(statist. weight - 1)/2 in LS case or J quantum number in LSJ case.
WNRI	energy of level relative to ground (cm-1)
NREP	number of representative n-shells
TRNS1,--	specifies metastable to metastable secondary Auger path written as m'-m where m' and m are metastable parent indices.
IREP	index of representative n-shells
NR	principal quantum number
AA21I,--	Auger rate coefficients (sec-1)
IP	index of parent
TP	term specification of parent
SP	spin multiplicity of parent
NSYS	number of spin systems associated with recombination stating with this parent (1 or 2)
TE1,--	electron temperatures (K)
INDX	index of level
ALT1I,--	dielectronic coefficients for level
IS	index of spin system
SS	spin multiplicity of spin system
IREP	index of representative n-shell
ANT1I,--	dielectronic coefficients for n-shell

Table B9c - example.

SEQ= 'HE '	NUCHG=18			
PARENT TERM INDEXING	BWNP= 35554796.2	NPRNTI= 1	NPRNTF= 1	

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-----
INDP  CODE          S  L  WI  WNP
-----
  1  1S1          (2)0( 0.5)  -----  0.0

LS RESOLVED TERM INDEXING          BWNR= 43705714.3  NTRM= 58
-----
INDX  CODE          S  L  WJ  WNR
-----
  1  1S1 2S1      (3)0( 1.0)  -----  0.0
  2  1S1 2P1      (3)1( 4.0)  146281.7
  3  1S1 2S1      (1)0( 0.0)  167385.9
  4  1S1 2P1      (1)1( 1.0)  275729.5
  5  1S1 3S1      (3)0( 1.0)  4563528.2
  6  1S1 3P1      (3)1( 4.0)  4603478.8
  7  1S1 3S1      (1)0( 0.0)  4607252.5
  8  1S1 3D1      (3)2( 7.0)  4626143.8
  9  1S1 3D1      (1)2( 2.0)  4627702.9
 10  1S1 3P1      (1)1( 1.0)  4637801.3

 50  1S1 8P1      (3)1( 4.0)  7649624.1
 51  1S1 8S1      (1)0( 0.0)  7649703.9
 52  1S1 8D1      (3)2( 7.0)  7650756.2
 53  1S1 8F1      (3)3(10.0)  7650833.7
 54  1S1 8G1      (3)4(13.0)  7650835.2
 55  1S1 8G1      (1)4( 4.0)  7650835.2
 56  1S1 8F1      (1)3( 3.0)  7650836.9
 57  1S1 8D1      (1)2( 2.0)  7650879.5
 58  1S1 8P1      (1)1( 1.0)  7651271.0

N-SHELL INDEXING & AUGER RATES          NREP= 42
-----
IREP  N
-----
  1  1
  2  2
  3  3
  4  4
  5  5
  6  6
  7  7
  8  8
  9  9
 10 10

 40 700
 41 811
 42 999

-----
PRTI= 1  TEMPRT= (2S)  SPNPR= 2
-----
INDX TE= 2.89E+05  5.78E+05  1.44E+06  2.89E+06  5.78E+06  1.45E+07  2.89E+07  5.78E+07  1.44E+08  2.89E+08

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1	0.00E+00	3.99E-31	7.48E-20	2.41E-16	8.24E-15	3.30E-14	2.94E-14	1.66E-14	5.54E-15	2.15E-15
2	0.00E+00	1.49E-37	3.78E-23	1.40E-18	1.65E-16	1.38E-15	1.57E-15	9.96E-16	3.58E-16	1.42E-16
3	0.00E+00	3.08E-31	8.11E-20	2.92E-16	1.06E-14	4.36E-14	3.93E-14	2.22E-14	7.44E-15	2.89E-15
4	0.00E+00	1.20E-30	2.98E-19	1.06E-15	3.80E-13	1.57E-13	1.42E-13	8.03E-14	2.69E-14	1.05E-14
5	0.00E+00	1.10E-36	2.41E-22	8.11E-18	8.86E-16	6.99E-15	7.78E-15	4.88E-15	1.74E-15	6.90E-16
6	0.00E+00	5.96E-37	1.44E-22	5.04E-18	1.59E-16	4.46E-15	4.98E-15	3.13E-15	1.12E-15	4.43E-16
7	0.00E+00	1.46E-36	3.72E-22	1.32E-17	1.47E-15	1.18E-14	1.32E-14	8.30E-15	2.97E-15	1.18E-15
8	0.00E+00	2.35E-36	5.56E-22	1.92E-17	2.13E-15	1.69E-14	1.89E-14	1.18E-14	4.23E-15	1.68E-15
9	0.00E+00	3.00E-36	8.26E-22	3.01E-17	3.41E-15	2.75E-14	3.09E-14	1.94E-14	6.95E-15	2.76E-15
10	0.00E+00	5.76E-36	1.42E-21	5.00E-17	5.58E-15	4.45E-14	4.98E-14	3.13E-14	1.12E-14	4.43E-15
50	0.00E+00	2.38E-41	5.67E-25	9.12E-20	2.17E-17	2.74E-16	3.57E-16	2.42E-16	9.04E-17	3.64E-17
51	0.00E+00	8.73E-41	2.08E-24	3.35E-19	8.00E-17	1.01E-15	1.31E-15	8.90E-16	3.33E-16	1.34E-16
52	0.00E+00	6.61E-41	2.05E-24	3.30E-19	7.86E-17	9.91E-16	1.29E-15	8.74E-16	3.27E-16	1.32E-16
53	0.00E+00	3.19E-41	7.61E-25	1.22E-19	2.92E-17	3.68E-16	4.79E-16	3.25E-16	1.22E-16	4.90E-17
54	0.00E+00	4.13E-42	9.87E-26	1.59E-20	3.79E-18	4.78E-17	6.22E-17	4.22E-17	1.58E-17	6.36E-18
55	0.00E+00	7.77E-43	1.86E-26	2.99E-21	7.14E-19	9.01E-18	1.17E-17	7.95E-18	2.97E-18	1.20E-18
56	0.00E+00	1.09E-40	2.61E-24	4.20E-19	1.00E-16	1.26E-15	1.64E-15	1.12E-15	4.17E-16	1.68E-16
57	0.00E+00	1.78E-40	4.26E-24	6.87E-19	1.64E-16	2.07E-15	2.69E-15	1.82E-15	6.82E-16	2.75E-16
58	0.00E+00	3.49E-40	8.31E-24	1.34E-18	3.19E-16	4.01E-15	5.22E-15	3.54E-15	1.32E-15	5.33E-16
-----										
PRTP= 1 TRMPRT= (2S) SPNPR= 2 NSYS= 2										
-----										
IREP	-----									
1	0.00E+00	1.51E-30	3.79E-19	1.35E-15	4.86E-14	2.01E-13	1.81E-13	1.02E-13	3.44E-14	1.34E-14
2	0.00E+00	1.02E-35	2.62E-21	9.33E-17	1.05E-14	8.39E-14	9.38E-14	5.90E-14	2.11E-14	8.37E-15
3	0.00E+00	1.52E-37	3.92E-22	3.00E-17	4.94E-15	4.99E-14	6.03E-14	3.94E-14	1.44E-14	5.76E-15
4	0.00E+00	1.64E-38	1.23E-22	1.35E-17	2.65E-15	2.98E-14	3.72E-14	2.48E-14	9.16E-15	3.67E-15
5	0.00E+00	1.64E-38	1.23E-22	1.35E-17	2.65E-15	2.98E-14	3.72E-14	2.48E-14	9.16E-15	3.67E-15
6	0.00E+00	4.05E-39	5.43E-23	7.21E-18	1.86E-14	2.37E-14	1.59E-14	5.92E-15	2.38E-15	2.38E-15
7	0.00E+00	1.52E-39	2.89E-23	4.31E-18	9.89E-16	1.22E-14	1.57E-14	1.06E-14	3.97E-15	1.60E-15
8	0.00E+00	7.24E-40	1.73E-23	2.78E-18	6.63E-16	8.36E-15	1.09E-14	7.38E-15	2.76E-15	1.11E-15
9	0.00E+00	4.02E-40	1.12E-23	1.90E-18	4.65E-16	5.96E-15	7.79E-15	5.30E-15	1.98E-15	8.00E-16
10	0.00E+00	2.47E-40	7.71E-24	1.36E-18	3.38E-16	4.38E-15	5.75E-15	3.92E-15	1.47E-15	5.92E-16
30	0.00E+00	1.18E-43	5.88E-27	1.21E-21	3.27E-19	4.43E-18	5.91E-18	4.06E-18	1.53E-18	6.17E-19
31	0.00E+00	7.74E-44	3.87E-27	7.96E-22	2.15E-19	2.91E-18	3.88E-18	2.67E-18	1.00E-18	4.06E-19
32	0.00E+00	4.28E-44	2.14E-27	4.41E-22	1.19E-19	1.61E-18	2.15E-18	1.48E-18	5.57E-19	2.25E-19
33	0.00E+00	2.76E-44	1.38E-27	2.84E-22	7.68E-20	1.04E-18	1.39E-18	9.54E-19	3.59E-19	1.45E-19
34	0.00E+00	1.47E-44	7.34E-28	1.51E-22	4.08E-20	5.54E-19	7.38E-19	5.07E-19	1.91E-19	7.71E-20
35	0.00E+00	9.03E-45	4.52E-28	9.32E-23	2.51E-20	3.41E-19	4.55E-19	3.13E-19	1.18E-19	4.75E-20
36	0.00E+00	4.34E-45	2.17E-28	4.48E-23	1.21E-20	1.64E-19	2.19E-19	1.50E-19	5.66E-20	2.28E-20
37	0.00E+00	2.66E-45	1.33E-28	2.75E-23	7.42E-21	1.01E-19	1.34E-19	9.22E-20	3.47E-20	1.40E-20
38	0.00E+00	1.28E-45	6.43E-29	1.33E-23	3.58E-21	4.86E-20	6.48E-20	4.45E-20	1.68E-20	6.77E-21
39	0.00E+00	7.64E-46	3.83E-29	7.89E-24	2.13E-21	2.89E-20	3.85E-20	2.65E-20	9.97E-21	4.03E-21
40	0.00E+00	3.41E-46	1.71E-29	3.52E-24	9.50E-22	1.29E-20	1.72E-20	1.18E-20	4.45E-21	1.80E-21
41	0.00E+00	2.19E-46	1.10E-29	2.26E-24	6.11E-22	8.30E-21	1.11E-20	7.60E-21	2.86E-21	1.16E-21
42	0.00E+00	1.17E-46	5.88E-30	1.21E-24	3.27E-22	4.44E-21	5.92E-21	4.06E-21	1.53E-21	6.18E-22
-----										
IREP										
-----										
SYS= 1 SPNSYS= 1										
-----										
SYS= 2 SPNSYS= 3										
-----										

2	0.00E+00	3.99E-31	7.48E-20	2.42E-16	8.41E-15	3.44E-14	3.10E-14	1.76E-14	5.90E-15	2.29E-15
3	0.00E+00	4.04E-36	9.41E-22	3.24E-17	3.57E-15	2.83E-14	3.16E-14	1.98E-14	7.09E-15	2.81E-15
4	0.00E+00	4.64E-38	1.16E-22	8.80E-18	1.44E-15	1.45E-14	1.75E-14	1.14E-14	4.18E-15	1.67E-15
5	0.00E+00	4.44E-39	3.29E-23	3.58E-18	7.03E-16	7.88E-15	9.86E-15	6.56E-15	2.42E-15	9.73E-16
6	0.00E+00	1.03E-39	1.37E-23	1.82E-18	3.94E-16	4.68E-15	5.97E-15	4.01E-15	1.49E-15	5.99E-16
7	0.00E+00	3.74E-40	7.08E-24	1.06E-18	2.42E-16	2.98E-15	3.85E-15	2.60E-15	9.71E-16	3.91E-16
8	0.00E+00	1.75E-40	4.17E-24	6.70E-19	1.60E-16	2.01E-15	2.62E-15	1.78E-15	6.64E-16	2.68E-16
9	0.00E+00	9.61E-41	2.68E-24	4.53E-19	1.11E-16	1.42E-15	1.86E-15	1.26E-15	4.73E-16	1.91E-16
10	0.00E+00	5.87E-41	1.83E-24	3.22E-19	8.02E-17	1.04E-15	1.36E-15	9.28E-16	3.48E-16	1.40E-16
30	0.00E+00	2.78E-44	1.39E-27	2.85E-22	7.69E-20	1.04E-18	1.39E-18	9.56E-19	3.60E-19	1.45E-19
31	0.00E+00	1.82E-44	9.11E-28	1.87E-22	5.06E-20	6.86E-19	9.15E-19	6.28E-19	2.37E-19	9.56E-20
32	0.00E+00	1.01E-44	5.04E-28	1.04E-22	2.80E-20	3.80E-19	5.07E-19	3.48E-19	1.31E-19	5.30E-20
33	0.00E+00	6.51E-45	3.25E-28	6.70E-23	1.81E-20	2.45E-19	3.27E-19	2.25E-19	8.47E-20	3.42E-20
34	0.00E+00	3.45E-45	1.73E-28	3.56E-23	9.61E-21	1.30E-19	1.74E-19	1.19E-19	4.50E-20	1.82E-20
35	0.00E+00	2.13E-45	1.07E-28	2.20E-23	5.93E-21	8.04E-20	1.07E-19	7.36E-20	2.77E-20	1.12E-20
36	0.00E+00	1.02E-45	5.12E-29	1.06E-23	2.85E-21	3.87E-20	5.16E-20	3.54E-20	1.33E-20	5.39E-21
37	0.00E+00	6.27E-46	3.14E-29	6.48E-24	1.75E-21	2.37E-20	3.16E-20	2.17E-20	8.19E-21	3.31E-21
38	0.00E+00	3.03E-46	1.52E-29	3.13E-24	8.44E-22	1.15E-20	1.53E-20	1.05E-20	3.95E-21	1.60E-21
39	0.00E+00	1.80E-46	9.03E-30	1.86E-24	5.02E-22	6.82E-21	9.09E-21	6.24E-21	2.35E-21	9.49E-22
40	0.00E+00	8.04E-47	4.03E-30	8.30E-25	2.24E-22	3.04E-21	4.06E-21	2.79E-21	1.05E-21	4.24E-22
41	0.00E+00	5.17E-47	2.59E-30	5.34E-25	1.44E-22	1.96E-21	2.61E-21	1.79E-21	6.75E-22	2.73E-22
42	0.00E+00	2.77E-47	1.39E-30	2.86E-25	7.71E-23	1.05E-21	1.40E-21	9.59E-22	3.61E-22	1.46E-22