ADF01: bundle-n and bundle-nl charge exchange cross-sections

The data sets provide total, nl-resolved and arbitrarily m-resolved charge exchange cross-sections up to high n-shells of an ion. Optionally parametrisations may be given for l-subshell cross-section dependence for asymptotic behaviour. Formatting conventions and variable storage are given below.

Some additional data for positive ion impact excitation of a target neutral has been included in this data class. The appropriate sub-libraries are of the form /qex#. This is a temporary decision at this time. Utilising subroutine ADAS301 interrogates such data but further processing is not meaningful at this stage.

Utilising subroutines :

ADAS301 ADAS306 ADAS307

ADAS308 ADAS309

Formatted files to ADF01 specification :

Database Status Date = March 17, 2003 Data type =qcx files Data root =/.../adas/adas/adf01/

Donor	*Prefix*	*Members*	*Library*	*Comments*	*Quality*
h0	e2p	h1	qcx#h0	2p donor	low
h0	e2s	h1	qcx#h0	2s donor	low
	en2_kvi	he2,li3,be4,b5,c6	qcx#h0	nlr, Hoekstra, Bliek, Olson,	medium
		ne10		H(n=2) donor	
	ex2	c6	qcx#h0	n=2 donor	low
	ex3	h1,c6	qcx#h0	n=3 donor	low
	ex4	c6	qcx#h0	n=4 donor	low
	exk	be2,be4,c4,c6,he2,o6	qcx#h0	n=2 donor, various	varied
	gyt	b5,be4,c6,h1,he2,li3,	qcx#h0	nlm, Gayet - high energy	medium
		n7,o8			
	ofr	c6,he2,o8	qcx#h0	nl, Fritsch - from l parms.	medium
	old	b5,be4,c6,h1,he2,	qcx#h0	nl, preferred - from l parms	medium/high
		n7,ne10,o8,si14			
	omo	c6,o8	qcx#h0	nl, CCMO - from l parms.	medium
	ool	c6,o8	qcx#h0	nl, Olson - from l parms.	medium
	ory	b5,be4,c6,h1,he2,	qcx#h0	nl, Ryufuku - from l parms.	medium

		ne10,o8,si14			
	tmp	ar18	qcx#h0	nl, Olson	low/incomplete
he0	2s-s_kvi	he2,c6	qcx#he0	nl, Hoekstra, Turkstra, Lubinski, Olson	medium
	2s-t_kvi	he2,c6	qcx#he0	nl, Hoekstra, Turkstra, Lubinski, Olson	medium
	gyt	b5,be4,c6,h1,he2,li3,	qcx#he0	nlm, Gayet - high energy	medium
		n7,o8			
	kvi	h1,he2	qcx#he0	nl, Hoekstra - assessed	high
	ofr	be4,c6,he2,o8	qcx#he0	nl, Fritsch - h0 transfer	low
	old	b5,be4, c6, he2,	qcx#he0	nl, preferred - h0 transfer	low/medium
		n7,ne10,o8			
	omo	c6,o8	qcx#he0	nl, CCMO - h0 transfer	low
	ool	c6,o8	qcx#he0	nl, Olson - h0 transfer	low
	ory	b5,be4,c6,he2,	qcx#he0	nl, Ryufuku - h0 transfer	low
		ne10,o8			
he0	1s-s_kvi	h1	qex#he0	nl, Hoekstra, Turkstra, Lubinski	medium
he1	gyt	b5,be4,c6,h1,he2,li3,	qcx#he1	nlm, Gayet - high energy	medium
		n7,o8			
li0	kvi	he2,li3,be4,b5,c6,n7,	qcx#li0	nl, Hoekstra,Bliek, Olson	medium
		o8,ne10			
na0	kvi	he2	qcx#na0	nl, Hoekstra/Shingal	high

Notes:

1. When the first letter of the prefix is ‘o’, it indicates that the data has been converted from the orginal JET prescription for this data class to the present prescription. The original prescription stored n-shell data with a fitted formula for the l-distribution. The formula has been used to reconstitue the explicit nl-shell data for the present prescription. .
2. h0 transfer indicates that there was no specific data for this donor. The data set has been created by formulaic conversion of the corresponding h0 donor data. Limited spot checks have indicated that this conversion is remarkably accurate.
3. The prefix ‘en..’ indicates charge transfer data from excited donor states.
4. The prefices `1s-s’, `2s-s’ and `2s-t’ indicate donation from the $1s^2\ ^1S$, $1s2s\ ^1S$ and $1s2s\ ^3S$ metastables respectively.

Data lines :

RELEM, IZR, DELEM, IZD, LVLD, ... /LPARMS/

Format:

1a2,1x,1a2,5x,1a2,1x,1a2,2x,1a1

```
do until NENER.eq.-1
        NENER                                                   1x,1i4
        NMIN                                                    1x,1i4
        NMAX                                                    1x,1i4
        (ENER(IE), IE = 1, NENER)                               10x,9f9.2
        (BETA(IE), I = 1, NENER)                                10x,9f9.2
        if LPARMS is set
                (LTYP(IE), I = 1, NENER)                        10,9i9
                (XLCR(IE), I = 1, NENER)                        10x,9f9.2
                (PL2A(IE), I = 1, NENER)                        10x,9f9.2
                (PL3A(IE), I = 1, NENER)                        10x,9f9.2
        endif
        (OMTOT(IE), IE = 1, NENER)                              10x,1p,9d9.2
        for IN = NMIN to NMAX
                (OMN(IN,IE), IE = 1, NENER)                     10x,1p,9d9.2
                for IL = 0 to IN-1
                        (OMNL(IN,IL,IE), IE=1,NENER)            10x,1p,9d9.2
[                       for IM= 0 to IL
                                (OMNLM(IN,IL,IM,IE,IE=1,NENER)  10x,1p,9d9.2
                        repeat                                  ]
                repeat
        repeat
repeat
-1     -1
```

variable identification :

name	*meaning*
RELEM	receiving element symbol
IZR	receiving ion charge
DELEM	donor element symbol
IZD	donor atom (ion) charge
LVLD	donor atom (ion) state index
NENER	number of beam energies in subtable block
NMIN	lowest n-shell for which data is included
NMAX	largest n-shell for which data is included
ENER()	beam energy (ev/amu)
BETA()	power for n-shell xsect. extrapolation
LTYP()	type of fitting for l-shell distribution
XLCR()	critical l for the fitting (non-integral)
PL2A()	parameter of l-shell fitting
PL3A()	parameter of l-shell fitting
OMTOT()	total charge transfer cross-section (cm**2)
OMN(,)	charge transfer cross-section for n-shell 1st parameter - n-shell index 2nd parameter - energy index
OMNL(,,)	charge transfer cross-section for nl-shell 1st parameter - n-shell index 2nd parameter - l-shell index 3rd parameter - energy index
OMNLM(,,,)	charge transfer cross-section for nlm-shell

1st parameter - n-shell index

2nd parameter - l-shell index

3rd parameter - m-shell index

4th parameter - energy index

Table B1c.

```
He+ 2     H + 0 (2) / receiver, donor (donor state n=2)       /        /
    9               / number of energies
    2               / nmin
    5               / nmax
             0.01     0.02     0.05     0.10     0.20     0.50     1.00     2.00     5.00 / energies         (keV/amu)
            17.00    16.20    15.00    13.86    12.68    11.00     9.65     8.30     5.85 / alpha
         1.11E-14 1.18E-14 1.18E-14 1.16E-14 1.16E-14 1.29E-14 1.30E-14 1.34E-14 1.34E-14 / total xsects.    (cm2)
  n  l  m                                                                                 / partial xsects.  (cm2)
  2        0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.75E-18 1.01E-17 1.77E-17 4.81E-17 9.32E-17
  2  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 2.20E-18 5.07E-18 7.60E-18 1.22E-17 3.09E-17
  2  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 5.50E-19 5.07E-18 1.01E-17 3.60E-17 6.23E-17

                         .        .        .

  5        1.50E-17 2.60E-17 5.30E-17 9.00E-17 1.60E-16 3.09E-16 5.50E-16 9.00E-16 1.55E-15
  5  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  2     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  3     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  4     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
    9               / number of energies
    2               / nmin
    5               / nmax
            10.00    15.00    20.00    25.00    30.00    35.00    40.00    45.00    50.00 / energies         (keV/amu)
             2.60     1.75     1.52     1.62     1.73     1.82     1.90     1.98     2.05 / alpha
         9.47E-15 4.87E-15 2.29E-15 1.14E-15 6.06E-16 3.37E-16 2.05E-16 1.28E-16 8.48E-17 / total xsects.    (cm2)
  n  l  m                                                                                 / partial xsects.  (cm2)
  2        1.79E-16 1.91E-16 1.31E-16 8.95E-17 6.40E-17 4.49E-17 3.15E-17 2.35E-17 1.69E-17
  2  0     6.08E-17 4.28E-17 2.56E-17 1.48E-17 9.78E-18 6.86E-18 4.61E-18 3.55E-18 2.47E-18
  2  1     1.18E-16 1.48E-16 1.05E-16 7.47E-17 5.42E-17 3.80E-17 2.69E-17 1.99E-17 1.44E-17



  5        1.58E-15 7.44E-16 3.37E-16 1.57E-16 7.75E-17 4.14E-17 2.36E-17 1.45E-17 9.05E-18
  5  0     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  1     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  2     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  3     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
  5  4     0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00 0.00E+00
    2               / number of energies
    2               / nmin
    5               / nmax
            75.00   100.00                                                           / energies         (keV/amu)
             2.25     2.40                                                           / alpha
         1.60E-17 5.03E-18                                                           / total xsects.    (cm2)
  n  l  m                                                                            / partial xsects.  (cm2)
```

```
  2        4.50E-18 1.68E-18
  2  0     7.43E-19 3.36E-19
  2  1     3.76E-18 1.34E-18

                          .       .       .

  5        1.42E-18 3.69E-19
  5  0     0.00E+00 0.00E+00
  5  1     0.00E+00 0.00E+00
  5  2     0.00E+00 0.00E+00
  5  3     0.00E+00 0.00E+00
  5  4     0.00E+00 0.00E+00
C-----------------------------------------------------------------------------------------------
C  Source:  The data consists of results of CTMC calculations made at the University of Missouri over
C              the period 1995-97.
C
C  Comments:  At this time, no direct comparison with other results is available for checking the
C             quality of the nl selective cross-sections except for Li+3 for which results are given
C             in a recent hidden curve crossing calculation by Janev et al. (1996).  Large differences
C             are observed in both the magnitude and energy dependence.  From inspection of the total
C             cross-sections, we have the strong impression that the CTMC data should be preferred.
C             In a plot of the scaled total one-electron capture cross-sections (sigma_tot(16q)^-1)
C             versus scaled energy (4Eq^-1/2), the total cross-sections should be approximately the
C             same for all systems (Janev, 1991) at least for q>3.  In these scaled units, a
C             recommendation by Janev and Smith (1995) has been presented.  The CTMC data are all close
C             to this curve except at lower energies.  The hidden curve crossing data for Li+3 deviate
C             from this curve.  Molecular orbital calculations by Errea et al. (1996) for B+5 are in
C             good agreement with the corresponding CTMC data.  For He+2, the recommendation of Janev
C             and Smith is based on the calculations of Harel and Jouin (1990) and it is completely
C             different from the CTMC results for He+2, especially at the lower energies.  A reason
C             for this huge difference is hard to see.  It may be the extremely strong resonant
C             nature of the electron capture at low collision energies.  Resonant transfer from H(n=2)
C             in collsions with He+2 would necessarily mean that the electron ends up exactly between
C             the n=3 and n=4 levels of He+1.  Therefore electron capture may be blocked. To what extent
C             this is well described by the CTMC method is still a point of discussion.  For higher
C             charged receiver ions, levels are resonantly present.  Except for He+2 at low energies,
C             we recommend use of the present CTMC data.
C
C             The data was assembled as ADAS data files of type adf01 at JET Joint Undertaking in the
C             period 2-3 June 1997.
C
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C                 # University of Missouri, Rolla, USA.
C
C  Date:  9 June 1997.
C
C  Updates:
C
C-----------------------------------------------------------------------------------------------
```