

## ADAS Subroutine bnqctb

```
SUBROUTINE BNQCTB (Z0, Z1, NMIN, NMAX, IMAX, NREP, NBEAM, BMENA, BMFRA,  
&                  CXMEMB, IBLOCK, QTHREP, ALPHA)
```

C

```
    IMPLICIT REAL*8 (A-H, O-Z)
```

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```
***** FORTRAN77 SUBROUTINE: BNQCTB *****
```

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```
PURPOSE: CALCULATE THEORETICAL CHARGE EXCHANGE RATE COEFFICIENTS  
FROM NEUTRAL HYDROGEN.
```

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```
RATE DATA IS RETURNED TO REPRESENTATIVE N-SHELLS FOR USE BY BUNDLE-N  
CODES.
```

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```
INPUT FROM ARCHIVED DATASET IS ON UNIT 11.
```

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```
THE NAME OF THE SELECTED DATASET IS CONTAINED IN: 'CXMEMB'
```

C

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```
AND IS OPENED IN THE SUBROUTINE.
```

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```
THIS VERSION USES '1989 RESTRUCTURED DATA' MEMBERS WITH THE  
CHANGED L-FITTING PARAMETERS
```

C

```
THE NEW PARAMETERS ARE TRANSFERED IN COMMON /LFIT89/
```

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```
THE SUBROUTINE IS A DEVELOPMENT OF QCHEX, NEWCX2, NCHEX2 ETC.
```

C

```
ORIGINALLY WRITTEN BY J. SPENCE. THIS VERSION ECONOMISES ON
```

C

```
SUBROUTINES.
```

C

C INPUT

C

```
    Z0=TARGET ION NUCLEAR CHARGE
```

C

```
    Z1=RECOMBINING TARGET ION CHARGE
```

C

```
    NMIN=LOWEST REPRESENTATIVE N-LEVEL OF TARGET
```

C

```
    NMAX=HIGHEST REPRESENTATIVE N-LEVEL OF TARGET
```

C

```
    IMAX=NUMBER OF REPRESENTATIVE LEVELS
```

C

```
    NREP(I)=REPRESENTATIVE N-LEVELS
```

C

```
    NBEAM=NUMBER OF ENERGY COMPONENTS IN NEUTRAL HYDROGEN BEAM
```

C

```
    BMENA(J)=BEAM ENERGY COMPONENTS (EV/AMU)
```

C

```
    BMFRA(J)=BEAM FRACTIONS IN ENERGY COMPONENTS
```

C

```
    CXMEMB=DATA SET NAME OF CHARGE EXCHANGE DATA SET.
```

C

```
    IBLOCK=1 SELECT UDW METHOD OR 1ST DATA BLOCK
```

C

```
           =2 SELECT CCAO METHOD OR 2ND DATA BLOCK
```

C

```
           =3 SELECT CTMC METHOD OR 3RD DATA BLOCK
```

C

```
           =4 SELECT CCMO METHOD OR 4TH DATA BLOCK
```

C

C OUTPUT

C

```
    QTHREP(I)=MEAN RATE COEFFICIENTS FOR REPRESENTATIVE
```

C

```
        N-LEVELS (AVERAGED OVER BEAM FRACTIONS) (CM3 SEC-1)
```

C

```
    ALPHA=SIZE OF 1/N**ALPHA TAIL FOR CH.EXCH X-SECT.
```

C

C

```
***** H.P.SUMMERS, JET 13 DEC 1989 *****
```

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C -----
C
C -----
C
C UPDATE: 19/01/94 - JONATHAN NASH - TESSELLA SUPPORT SERVICES PLC
C
C THE FOLLOWING MODIFICATIONS HAVE BEEN MADE TO THE SUBROUTINE:
C
C 1) THE COMPLETE CHARGE EXCHANGE DATA SET NAME IS NOW PASSED
C INTO THE ROUTINE RATHER THAN JUST THE MEMBER NAME.
C
C 2) THE ROUTINE HAS BEEN UPGRADED TO READ NEW ADF01 FORMAT.
C
C NOTES: NO ATTEMPT HAS BEEN MADE TO RESTRUCTURE THE ROUTINE. RATHER
C THE MINIMUM AMOUNT OF WORK TO INTEGRATE THE ROUTINE INTO
C ADAS310 HAS BEEN COMPLETED.
C
C UNIX-IDL PORT:
C
C VERSION: 1.1 DATE: 16-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - FIRST VERSION
C
C VERSION: 1.2 DATE: 17-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - ADDED "STATUS='UNKNOWN'" TO OPEN STATEMENT
C
C VERSION: 1.3 DATE: 22-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - REPLACED CALLS TO NAG ROUTINE E02BBF WITH ADAS ROUTINE
C DXNBBF
C
C VERSION: 1.4 DATE: 23-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - REPLACED CALLS TO NAG ROUTINE E01BAF WITH ADAS ROUTINE
C DXNBAF
C
C VERSION: 1.5 DATE: 23-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - RELABELLED LOOP COUNTERS FOR LOOPS 176 AND 177
C
C VERSION: 1.6 DATE: 24-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - RENAMED NBENG TO NBENG2 TO AVOID CONFUSION WITH
C OTHER NBENG IN OTHER ROUTINES
C REMOVED SUPERFLUOUS VARIABLES
C
C VERSION: 1.7 DATE: 14-10-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C - CORRECTED SECOND CALL TO DXNBAF - IT WAS USING XSA AND
C YSA RATHER THAN XSA AND ZSA
C
C VERSION: 1.8 DATE: 09-04-98
```

C MODIFIED: HARVEY ANDERSON ( UNIVERSITY OF STRATHCLYDE )  
C - CHANGED VARIABLE MXE FROM 24 TO 40.  
C - INCREASED SIZE OF ARRAYS ASSOCIATED WITH THE  
C ROUTINES DXNBAF AND DXNBBF.  
C - REPLACED NUMERICAL VALUE WITH THE PARAMETER  
C MXE IN THE IF STATEMENT WHICH TESTS TO ENSURE  
C THAT THE NUMBER OF BEAM ENERGIES READ FROM  
C INPUT FILE IS NOT GREATER THE ARRAY DIMMENSIONS  
C OF THE RELEVANT ARRAYS.

C  
C VERSION: 1.9 DATE: 23-06-98

C MODIFIED: RICHARD MARTIN  
C -CORRECTED SCCS ERROR.

C  
C VERSION: 1.10 DATE: 07-07-2004

C MODIFIED: ALLAN WHITEFORD  
C -CHANGED CALLS FROM DXNB{A,B}F TO XXNB{A,B}F

C  
C VERSION: 1.11 DATE: 16-05-07

C MODIFIED: Allan Whiteford  
C - Updated comments as part of subroutine documentation  
C procedure.

C  
C VERSION : 1.12

C DATE : 22-05-2007

C MODIFIED : Martin O'Mullane

C - Remove unused m-subshell data possibility and  
C use xxdata\_01 to access adf01 data.

C-----  
C  
C (I\*4) MXE = MAXIMUM NO. OF ENERGIES.  
C (I\*4) MXN = MAXIMUM NO. OF N SHELLS.  
C (I\*4) IZR = ION CHARGE OF RECEIVER.  
C (I\*4) IZD = ION CHARGE OF DONOR.  
C (I\*4) INDD = DONOR STATE INDEX.  
C (I\*4) NBENG2 = NUMBER OF ENERGIES READ.  
C (I\*4) NMINF = LOWEST N-SHELL FOR WHICH DATA READ.  
C (I\*4) NMAXF = HIGHEST N-SHELL FOR WHICH DATA READ.  
C  
C (L\*4) LPARMS = FLAGS IF L-SPLITTING PARAMETERS PRESENT.  
C .TRUE. => L-SPLITTING PARAMETERS PRESENT.  
C .FALSE => L-SPLITTING PARAMETERS ABSENT.  
C (L\*4) LSETL = FLAGS IF L-RESOLVED DATA PRESENT.  
C .TRUE. => L-RESOLVED DATA PRESENT.  
C .FALSE => L-RESOLVED DATA ABSENT.  
C (L\*4) LSETM = FLAGS IF M-RESOLVED DATA PRESENT.  
C .TRUE. => M-RESOLVED DATA PRESENT.  
C .FALSE => M-RESOLVED DATA ABSENT.  
C  
C (C\*80) TITLE = NOT SET - TITLE FOR DATA SOURCE.  
C (C\*2) SYMBR = RECEIVER ION ELEMENT SYMBOL.  
C (C\*2) SYMBD = DONOR ION ELMENT SYMBOL.

```

C
C      (I*4)  LFORMA ( )  = PARAMETERS FOR CALCULATING L-RES X-SEC.
C                      DIMENSION: MXE
C
C      (R*8)  BENGY ( )   = COLLISION ENERGIES.
C                      UNITS: EV/AMU (READ AS KEV/AMU)
C                      DIMENSION: MXE
C
C      (R*8)  ALPHAA ( )  = EXTRAPOLATION PARAMETER ALPHA.
C                      DIMENSION: MXE
C
C      (R*8)  XLCUTA ( )  = PARAMETERS FOR CALCULATING L-RES X-SEC.
C                      DIMENSION: MXE
C
C      (R*8)  PL2A ( )    = PARAMETERS FOR CALCULATING L-RES X-SEC.
C                      DIMENSION: MXE
C
C      (R*8)  PL3A ( )    = PARAMETERS FOR CALCULATING L-RES X-SEC.
C                      DIMENSION: MXE
C
C      (R*8)  XTOT ( )    = TOTAL CHARGE EXCHANGE CROSS-SECTION.
C                      UNITS: CM2
C                      DIMENSION: MXE
C
C
C      (R*8)  XSIGN ( , ) = N-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS.
C                      UNITS: CM2
C                      1ST DIMENSION: MXE
C                      2ND DIMENSION: MXN
C
C      (R*8)  XSIGL ( , ) = L-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS.
C                      UNITS: CM2
C                      1ST DIMENSION: MXE
C                      2ND DIMENSION: (MXN*(MXN+1))/2
C
C      (R*8)  XSIGM ( , ) = M-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS.
C                      UNITS: CM2
C                      1ST DIMENSION: MXE
C                      2ND DIMENSION: (MXN*(MXN+1)*(MXN+2))/6

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CHARACTER*80	CXMEMB			
INTEGER	IBLOCK,	IMAX,	NBEAM,	NMAX
INTEGER	NMIN,	NREP (31)		
REAL*8	ALPHA,	BMENA (6) ,	BMFRA (6)	
REAL*8	QTHREP (31) ,	Z0,	Z1	