

# **ADAS3XX FORTRAN**

# ABINEW

```
FUNCTION ABINEW(OA, YA, FA, A, B, N)
C
C   IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 FUNCTION: ABINEW *****
C-----
C FUNCTION TO EVALUATE INNER INTEGRALS FOR RATE COEFFICIENTS .ABINEW IS
C CALLED BY QH & QHE.  THE PROCEDURES ALLOW FOR PROJECTILE AND TARGET
C MASSES.
C INPUT
C   OA=VECTOR OF CROSS-SECTIONS (CM2)
C   YA=VECTOR OF REDUCED RELATIVE SPEEDS. 1ST VALUE IS AT THRESHOLD
C   FA=VECTOR OF ALPHAS (12TH VALUE IS FOR EXTRAPOLATION, PROVIDED
C     EXPLICITLY. EXTRAPOLATION BELOW YA(1) IS BASED ON FA(1))
C     N.B. OA(1) MUST BE NON-ZERO.
C       (OA, YA AND FA ARE OF FIXED LENGTH =24)
C
C   A=LOWER INTEGRAL LIMIT
C   B=UPPER INTEGRAL LIMIT
C   N=NUMBER OF CROSS-SECTIONS
C OUTPUT
C   ABINEW=DEFINITE INTEGRAL.
C
C ***** H.P. SUMMERS, JET          18 FEB 1987 *****
C *****                          COR. 31 JUL 1990 *****
C *****                          15 JUL 1991 REORDER EVAL AT
C                                         LABEL 50
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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   DIMENSION OA(24), YA(24), FA(24)
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# BNQCTB

```
SUBROUTINE BNQCTB(Z0, Z1, NMIN, NMAX, IMAX, NREP, NBEAM, BMENA, BMFRA,
&
& CXMEMB, IBLOCK, QTHREP, ALPHA)
C
C   IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: BNQCTB *****
C-----
C SUBROUTINE TO CALCULATE THEORETICAL CHARGE EXCHANGE RATE COEFFICIENTS
C FROM NEUTRAL HYDROGEN.
C
C RATE DATA IS RETURNED TO REPRESENTATIVE N-SHELLS FOR USE BY BUNDLE-N
C CODES.
C
C INPUT FROM ARCHIVED DATASET IS ON UNIT 11.
C
C THE NAME OF THE SELECTED DATASET IS CONTAINED IN: 'CXMEMB'
C
C AND IS OPENED IN THE SUBROUTINE.
C
C THIS VERSION USES '1989 RESTRUCTURED DATA' MEMBERS WITH THE
C CHANGED L-FITTING PARAMETERS
C THE NEW PARAMETERS ARE TRANSFERRED IN COMMON /LFIT89/
C
C 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
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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 *****
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
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.

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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      (R*8) ALPHAA() = EXTRAPOLATION PARAMETER ALPHA.
C                      DIMENSION: MXE
C      (R*8) XLCUTA() = PARAMETERS FOR CALCULATING L-RES X-SEC.
C                      DIMENSION: MXE
C      (R*8) PL2A() = PARAMETERS FOR CALCULATING L-RES X-SEC.
C                      DIMENSION: MXE
C      (R*8) PL3A() = PARAMETERS FOR CALCULATING L-RES X-SEC.
C                      DIMENSION: MXE
C      (R*8) XTOT() = TOTAL CHARGE EXCHANGE CROSS-SECTION.
C                      UNITS: CM2
C                      DIMENSION: MXE
C
C      (R*8) XSIGN(,) = N-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS.
C                      UNITS: CM2
C                      1ST DIMENSION: MXE
C                      2ND DIMENSION: MXN
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      (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
C
C-----
C
C      INTEGER      MXN      , MXE
C      PARAMETER( MXN = 20  , MXE = 40 )
C-----
C      INTEGER      IZR      , IZD      , INDD      , NBENG2      , NMINF      ,
C      &            NMAXF
C-----
C      LOGICAL      LPARMS      , LSETL      , LSETM
C-----
C      CHARACTER   TITLE*80      , SYMBR*2      , SYMBD*2
C-----
C      INTEGER      LFORMA(MXE)
C-----
C      REAL*8      BENGY(MXE)      , ALPHAA(MXE)      , XLCUTA(MXE)      ,
C      &            PL2A(MXE)      , PL3A(MXE)      , XTOT(MXE)
C-----
C      REAL*8      XSIGN(MXE,MXN)      ,
C      &            XSIGL(MXE,(MXN*(MXN+1))/2)      ,
C      &            XSIGM(MXE,(MXN*(MXN+1)*(MXN+2))/6)
C-----
C
C      CHARACTER   CXMEMB*80
C      DIMENSION  ZDATA(30),BMENA(6),BMFRA(6)
C      DIMENSION  NDATA(2),IEDATA(2)
C      DIMENSION  QTHREP(31),RATE(6,31),NREP(31)
C      DIMENSION  XSA(MXE),YSA(MXE),ZSA(MXE)
C      DIMENSION  WTS(MXE),B(MXE),A(MXE+4,4),DIAG(MXE+4)
C      DIMENSION  XKA(MXE+4),C(MXE+4),ZKA(MXE+4),ZC(MXE+4)
CX      DIMENSION  WRK(160)
C      DATA  LCK,LWRK/28,160/
C      DATA  ZDATA/1.00D+00,2.00D+00,0.00D+00,4.00D+00,5.00D+00,6.00D+00,
C      &          0.00D+00,8.00D+00,0.00D+00,1.00D+01,0.00D+00,0.00D+00,
C      &          0.00D+00,1.40D+01,0.00D+00,0.00D+00,0.00D+00,0.00D+00,
C      &          0.00D+00,0.00D+00,0.00D+00,0.00D+00,0.00D+00,0.00D+00,
C      &          0.00D+00,0.00D+00,0.00D+00,0.00D+00,0.00D+00,0.00D+00/

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## C1BSIG

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SUBROUTINE C1BSIG( NENRGY , NSHELL , NENER ,
&                INSEL , ILSEL , IMSEL ,
&                IEDATA , NDATA ,
&                XTOT , XSIGN , XSIGL , XSIGM ,
&                ALPHAA ,
&                SIGA
&                )
C
C      IMPLICIT NONE
C-----
C      ***** FORTRAN77 SUBROUTINE: C1BSIG *****
C
C      PURPOSE:  TO EXTRACT VALID CROSS-SECTIONS FROM INPUT CHARGE-EXCHANGE
C                FILE FOR A GIVEN SUB-BLOCK.
C
C      CALLING PROGRAM:  ADAS301
C
C      SUBROUTINE:
C
C      INPUT : (I*4) NENRGY = NUMBER OF TABULATED INPUT ENERGIES.
C      INPUT : (I*4) NSHELL = NO. OF TABULATED PRINCIPAL QUANTUM N-SHELLS

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C
C INPUT : (I*4)  NENER   = NUMBER OF VALID ENERGIES/VEL. FOR SUB-BLOCK
C INPUT : (I*4)  INSEL   = SELECTED INPUT PRINCIPAL QUANTUM N-SHELL
C                      ( 0 => TOTAL CROSS SECTION).
C INPUT : (I*4)  ILSEL   = SELECTED INPUT DATA L QUANTUM SHELL
C                      (-1 => TOTAL CROSS-SECTION FOR N SHELL)
C INPUT : (I*4)  IMSEL   = SELECTED INPUT DATA M QUANTUM SHELL
C                      (-1 => TOTAL CROSS-SECTION FOR NL SHELL)
C
C INPUT : (I*4)  IEDATA() = INDEX RANGE FOR VALID QUANTUM NUMBERS IN
C                      'XSIGN(,)'
C                      DIMENSION: 1 => LOWER INDEX BOUND
C                      DIMENSION: 2 => UPPER INDEX BOUND
C INPUT : (I*4)  NDATA() = INDEX RANGE FOR VALID INPUT ENERGIES/VELS.
C                      IN 'XTOT()', 'XSIGN(,)', 'ALPHAA()'
C                      DIMENSION: 1 => LOWER INDEX BOUND
C                      DIMENSION: 2 => UPPER INDEX BOUND
C
C INPUT : (R*8)  XTOT()   = TOTAL CROSS SECTIONS (UNITS: cm**2)
C                      1st DIMENSION: ENERGY INDEX
C INPUT : (R*8)  XSIGN(, ) = CROSS SECTIONS FOR EACH N-SHELL
C                      (UNITS: cm**2)
C                      1st DIMENSION: ENERGY INDEX
C                      2nd DIMENSION: QUANTUM N-SHELL INDEX
C INPUT : (R*8)  XSIGL(,,) = INPUT DATA FILE: L-RESOLVED CROSS-SECTIONS.
C                      1st DIMENSION: ENERGY INDEX
C                      2ND DIMENSION: INDEXED BY FUNCTION I4IDFL.
C                      3rd DIMENSION: DATA SUB-BLOCK INDEX
C INPUT : (R*8)  XSIGM(,,) = INPUT DATA FILE: M-RESOLVED CROSS-SECTIONS.
C                      1st DIMENSION: ENERGY INDEX
C                      2ND DIMENSION: INDEXED BY FUNCTION I4IDFM.
C                      3rd DIMENSION: DATA SUB-BLOCK INDEX
C INPUT : (R*8)  ALPHAA() =
C                      1st DIMENSION: ENERGY INDEX
C
C OUTPUT: (R*8)  SIGA()   = VALID CROSS SECTIONS READ FROM INPUT FILE
C                      FOR PRINCIPAL QUATUM NUMBER 'INSEL' AND
C                      GIVEN SUB-BLOCK. (UNITS: cm**2)
C                      1st DIMENSION: ENERGY INDEX
C
C          (I*4)  IE      = ARRAY INDEX: ENERGY INDEX
C          (I*4)  I1ST    = ARRAY INDEX: FIRST VALID ENERGY INDEX - 1
C          (I*4)  IN      = 'NDATA(2)' - IF 'INSEL > NDATA(2)'
C
C          (R*8)  AVAL    = 'NDATA(2)/INSEL' - IF 'INSEL > NDATA(2)'
C          (R*8)  ZERO    = PARAMETER = EFFECTIVE ZERO (1.0D-72)
C
C ROUTINES:
C          ROUTINE      SOURCE      BRIEF DESCRIPTION
C          -----
C          I4IDFL      ADAS          PROVIDES UNIQUE INDEX GIVEN N AND L
C          I4IDFM      ADAS          PROVIDES UNIQUE INDEX GIVEN N, L AND M
C
C AUTHOR:  PAUL E. BRIDEN (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/81
C          JET EXT. 4569
C
C DATE:    07/02/91
C
C UPDATE:  19/04/95  H P SUMMERS - EXTENSION TO INCLUDE L AND M
C          SUB-SHELL CROSS-SECTIONS
C
C-----
C          REAL*8      ZERO
C-----
C          PARAMETER ( ZERO = 1.0D-72 )
C-----
C          INTEGER     NENRGY      , NSHELL      ,
C          &           NENER      , INSEL      ,
C          &           ILSEL      , IMSEL      ,
C          INTEGER     IE          , I1ST      , IN
C          INTEGER     I4IDFL      , I4IDFM
C-----
C          REAL*8      AVAL
C-----
C          INTEGER     IEDATA(2)  , NDATA(2)
C-----
C          REAL*8      XTOT(NENRGY) , ALPHAA(NENRGY) ,
C          &           SIGA(NENRGY)  , XSIGN(NENRGY,NSHELL) ,
C          &           XSIGL(NENRGY,(NSHELL*(NSHELL+1))/2) ,
C          &           XSIGM(NENRGY,(NSHELL*(NSHELL+1))*(NSHELL+2))/6)
C-----

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## C1OUT0

```

SUBROUTINE C1OUT0( IWRITE , LSETL , LSETM ,
&                LOSEL , LFSEL , TITLF ,
&                TITLE , TITLX , TITLM , DATE ,
&                INSEL , ILSEL , IMSEL ,
&                IEVAL , LERNG , EOA , SIGOA ,
&                KPLUS1 , COEF
&                )
IMPLICIT NONE

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C
C ***** FORTRAN77 SUBROUTINE: C1OUT0 *****
C
C PURPOSE: TO PRINT DATA CONCERNING THE SELECTED CHEXDATA SUB-BLOCK
C AND SELECTED PRINCIPAL QUANTUM NUMBER.
C
C CALLING PROGRAM: ADAS301
C
C SUBROUTINE:
C
C INPUT : (I*4) IWRITE = OUTPUT UNIT FOR RESULTS
C INPUT : (L*4) LSETL() = .TRUE. => L-RESOLVED DATA READ
C .FALSE. => NO L-RESOLVED DATA READ
C INPUT : (L*4) LSETM() = .TRUE. => M-RESOLVED DATA READ
C .FALSE. => NO M-RESOLVED DATA READ
C INPUT : (L*4) LOSEL = .TRUE. => INTERPOLATED VALUES FOR ISPF
C PANEL INPUT VALUES CALCULATED
C .FALSE => INTERPOLATED VALUES FOR ISPF
C PANEL INPUT VALUES NOT CALCULATED
C INPUT : (L*4) LFSSEL = .TRUE. => MINIMAX POLYNOMIAL FITTED.
C .FALSE. => MINIMAX POLYNOMIAL NOT FITTED
C INPUT : (C*80) TITLF = INFORMATION STRING READ FROM CHEXDATA FILE
C FOR SELECTED SUB-BLOCK.
C
C INPUT : (C*40) TITLE = TITLE OF RUN (READ FROM ISPF PANEL)
C INPUT : (C*80) TITLX = INFORMATION STRING CONTAINING: INPUT DATA
C FILE-NAME, SELECTED SUB-BLOCK AND N-SHELL.
C INPUT : (C*80) TITLM = DIAGNOSTIC LINE INFORMATION FROM 'MINIMAX'
C INPUT : (C*8) DATE = CURRENT DATE (AS 'DD/MM/YY')
C
C INPUT : (I*4) INSEL = SELECTED PRINCIPAL QUANTUM NUMBER.
C (0 => TOTAL CROSS-SECTION).
C INPUT : (I*4) ILSEL = SELECTED INPUT DATA L QUANTUM SHELL
C (-1 => TOTAL CROSS-SECTION FOR N SHELL)
C INPUT : (I*4) IMSEL = SELECTED INPUT DATA M QUANTUM SHELL
C (-1 => TOTAL CROSS-SECTION FOR NL SHELL)
C
C INPUT : (I*4) IEVAL = NUMBER OF ISPF ENTERED ENERGY VALUES.
C INPUT : (L*4) LERNG() = .TRUE. => ENERGY 'EOA()' IN RANGE
C .FALSE. => ENERGY 'EOA()' OUT OF RANGE
C (RANGE = INPUT ENERGY RANGE FOR SUB-BLOCK)
C INPUT : (R*8) EOA() = ISPF ENTERED ENERGIES (eV/amu)
C INPUT : (R*8) SIGOA() = SPLINE INTEROPLATED X-SEC VALUE AT 'EOA()'
C
C INPUT : (I*4) KPLUS1 = NUMBER OF MINIMAX COEFFICIENTS
C INPUT : (R*8) COEF() = COEFFICIENTS OF FITTED MINIMAX POLYNOMIAL
C
C (I*4) L1 = PARAMETER = 1
C (I*4) L2 = PARAMETER = 2
C (I*4) L3 = PARAMETER = 3
C
C (I*4) I = GENERAL ARRAY ELEMENT INDEX
C
C (R*8) R8ECON = FUNCTION (SEE ROUTINE SECTION BELOW)
C (R*8) R8SCON = FUNCTION (SEE ROUTINE SECTION BELOW)
C (R*8) VAUNIT = VELOCITY (UNITS: at.units)
C (R*8) VCMS = VELOCITY (UNITS: cm/sec )
C (R*8) SIGAO2 = CROSS-SECTION (UNITS: pi*(a0**2) )
C (R*8) RCOEF = RATE-COEFFICIENT (UNITS: cm**3/sec )
C
C (C*80) CADAS = ADAS HEADER: INCLUDES RELEASE, PROGRAM, TIME
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C XXADAS ADAS GATHERS ADAS HEADER INFORMATION
C R8ECON ADAS REAL*8 FUNCTION: CONVERT ENGY/VEL. FORM
C R8SCON ADAS REAL*8 FUNCTION: CONVERT X-SECTION FORM
C
C AUTHOR : PAUL E. BRIDEN (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 4569
C
C DATE: 07/02/91
C
C UPDATE: 22/09/93 - J NASH - ADAS91:
C REMOVED PRINTING OF DATA SUB-BLOCK TITLE (COMMENTED OUT).
C
C UPDATE: 18/04/95 H P SUMMERS - ADDED L AND M RESOLUTION
C
C UNIX-IDL PORT:
C
C VERSION: 1.1 DATE: 24-04-95
C MODIFIED: TIM HAMMOND(TESSELLA SUPPORT SERVICES PLC)
C - FIRST VERSION
C
C VERSION: 1.2 DATE: 13-05-96
C MODIFIED: TIM HAMMOND
C - REMOVED HOLLERITH CONSTANTS FROM OUTPUT AND TIDIED UP
C HEADER
C
C -----
C INTEGER L1 , L2 , L3
C -----
C PARAMETER( L1 = 1 , L2 = 2 , L3 = 3 )
C -----
C INTEGER IWRITE , INSEL , ILSEL , IMSEL ,
C & IEVAL , KPLUS1

```

INTEGER	I				
REAL*8	R8ECON		R8SCON		
REAL*8	VAUNIT		VCMS	SIGAO2	RCOEF
LOGICAL	LSETL		LSETM	LOSEL	LFSEL
CHARACTER	TITLF*(*)		TITLE*(*)	TITLX*(*)	TITLM*(*)
&	DATE*8				
CHARACTER	CADAS*80				
REAL*8	EOA(IEVAL)		SIGOA(IEVAL)		
&	COEF(KPLUS1)				
LOGICAL	LERNG(IEVAL)				
SAVE	CADAS				
DATA	CADAS/' '/				

## C1OUTG

```

SUBROUTINE C1OUTG( LGHOST , TITLF ,
& TITLE , TITLX , TITLM , DATE ,
& ENERA , SIGA , NENER ,
& EOMA , SIGOMA , NMX ,
& EOSA , SIGOSA , NPSPL ,
& LGRD1 , LDEF1 , LFSEL ,
& XMIN , XMAX , YMIN , YMAX
& )
IMPLICIT NONE
-----
C
C ***** FORTRAN77 SUBROUTINE: C1OUTG *****
C
C PURPOSE: GRAPHIC ROUTINE FOR SELECTED TRANSITION USING GHOST80.
C (IDENTICAL TO: B1OUTG - EXCEPT SOME VARIABLES HAVE BEEN
C RENAMED AS HAVE THE MAIN TITLE 'ISPEC(1:48)' AND AXES.
C - ALSO ARGUMENT 'TITLF(C*80)' INTRODUCED.)
C
C PROVIDES COMPARATIVE GRAPH OF:
C ORIGINAL CHEXDATA.DATA (CROSSES )
C SPLINE INTERPOLATED DATA (FULL CURVE)
C MINIMAX FIT TO DATA (DASH CURVE)
C
C PLOT IS LOG10(X-SECT.(CM**2)) VERSUS LOG10(ENERGY(EV/AMU))
C
C CALLING PROGRAM: ADAS301
C
C SUBROUTINE:
C
C INPUT : (L*4) LGHOST = .TRUE. => GHOST80 INITIALISED
C .FALSE. => GHOST80 NOT INITIALISED
C INPUT : (C*80) TITLF = INFORMATION STRING READ FROM CHEXDATA FILE
C FOR SELECTED SUB-BLOCK.
C
C INPUT : (C*40) TITLE = TITLE OF RUN (READ FROM ISPF PANEL)
C INPUT : (C*120) TITLX = INFORMATION STRING CONTAINING: INPUT DATA
C FILE-NAME, SELECTED BLOCK and QUANTUM SHELL
C INPUT : (C*80) TITLM = DIAGNOSTIC LINE INFORMATION FROM 'MINIMAX'
C INPUT : (C*8) DATE = CURRENT DATE (AS 'DD/MM/YY')
C
C INPUT : (R*8) ENERA() = INPUT DATA FILE: SELECTED SUB-BLOCK -
C VALID ENERGIES (eV/amu)
C INPUT : (R*8) SIGA() = INPUT DATA FILE: SELECTED SUB-BLOCK/N-SHELL
C CROSS-SECTIONS (cm**2) AT 'ENERA()'
C INPUT : (I*4) NENER = INPUT DATA FILE: NUMBER OF ENERGY/X-SECTION
C PAIRS FOR THE SELECTED SUB-BLOCK.
C
C INPUT : (R*8) EOMA() = MINIMAX: SELECTED ENERGIES (eV/amu)
C INPUT : (R*8) SIGOMA() = N-SHELL CROSS-SECTIONS (cm**2) AT 'EOMA()'
C INPUT : (I*4) NMX = NUMBER OF MINIMAX GENERATED ENERGY/X-SECT.
C PAIRS FOR GRAPHICAL DISPLAY.
C
C INPUT : (R*8) EOSA() = SPLINE: SELECTED ENERGIES (eV/amu)
C INPUT : (R*8) SIGOSA() = N-SHELL CROSS-SECTIONS (cm**2) AT 'EOSA()'
C INPUT : (I*4) NPSPL = NUMBER OF SPLINE INTERPOLATED ENGY/X-SECT.
C PAIRS FOR GRAPHICAL DISPLAY.
C
C INPUT : (L*4) LGRD1 = .TRUE. => PUT GRAPH IN GRID FILE
C .FALSE. => DO NOT PUT GRAPH IN GRID FILE
C INPUT : (L*4) LDEF1 = .TRUE. => USE DEFAULT GRAPH SCALING
C .FALSE. => DO NOT USE DEFAULT GRAPH SCALING
C INPUT : (L*4) LFSEL = .TRUE. => CARRY OUT MINIMAX POLYNOMIAL
C FITTING
C .FALSE. => - DO NOT DO THE ABOVE -
C
C INPUT : (R*8) XMIN = GRAPH: LOWER LIMIT FOR ENERGY (eV/amu)
C INPUT : (R*8) XMAX = GRAPH: UPPER LIMIT FOR ENERGY (eV/amu)
C INPUT : (R*8) YMIN = GRAPH: LOWER LIMIT FOR CROSS-SECTION (cm**2)
C INPUT : (R*8) YMAX = GRAPH: UPPER LIMIT FOR CROSS-SECTION (cm**2)
C

```

```

C
C      (R*4) GHZERO = PARAMETER = VALUE BELOW WHICH GHOST80
C              TAKES NUMBERS AS BEING ZERO = 1.0E-36
C      (R*4) YDMIN  = PARAMETER = MINIMUM ALLOWED Y-VALUE FOR
C              PLOTTING. (USED FOR DEFAULT GRAPH SCALING)
C              (SET TO 'GHZERO'/ZERO TO REMOVE)
C
C      (I*4) I4UNIT = FUNCTION (SEE ROUTINE SECTION BELOW)
C      (I*4) I      = GENERAL USE - ARRAY INDEX
C      (I*4) IKEY   = NUMBER OF 'KEY()' VALUES TO BE OUTPUT
C      (I*4) ICOUNT = NUMBER OF POINTS PLOTTED FOR GRAPH CURVE
C
C      (R*4) XHIGH  = UPPER X-AXIS LIMIT FOR USE WITH GHOST80
C      (R*4) XLOW   = LOWER X-AXIS LIMIT FOR USE WITH GHOST80
C      (R*4) YHIGH  = UPPER Y-AXIS LIMIT FOR USE WITH GHOST80
C      (R*4) YLOW   = LOWER Y-AXIS LIMIT FOR USE WITH GHOST80
C      (R*4) XA4()  = X-AXIS COORDINATES FOR USE WITH GHOST80
C      (R*4) YA4()  = Y-AXIS COORDINATES FOR USE WITH GHOST80
C
C      (C*88) ISPEC = GRAPH TITLE (INCORPORATES 'TITLE')
C      (C*80) CADAS = ADAS HEADER: INCLUDES RELEASE, PROGRAM, TIME
C      (C*12) DNAME = '      DATE: '
C      (C*23) XTIT  = X-AXIS UNITS/TITLE
C      (C*23) YTIT  = Y-AXIS UNITS/TITLE
C      (C*9)  KEY0  = '      KEY: '
C      (C*9)  MNMX0 = 'MINIMAX: '
C      (C*8)  CINFO = 'TITLE  : '
C      (C*8)  ADAS0 = 'ADAS   : '
C      (C*22) KEY() = DESCRIPTIVE KEY FOR GRAPH (3 TYPES)
C
C      (C*1) GRID  = DUMMY NAME VARIABLE FOR USE WITH GHOST80
C      (C*1) PIC   = DUMMY NAME VARIABLE FOR USE WITH GHOST80
C      (C*3) C3BLNK = BLANK 3 BYTE STRING
C      (C*7) C7    = 7 BYTE STRING = 'TITLX(1:4)('//C3BLNK'
C
C
C ROUTINES:
C
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      XXADAS      ADAS        GATHERS ADAS HEADER INFORMATION
C      XXLIM8      ADAS        SETTING UP OF DEFAULT GRAPH AXES
C      XXGSEL      ADAS        SELECTS POINTS WHICH WILL FIT ON GRAPH
C      I4UNIT      ADAS        FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C                      GHOST80  NUMEROUS SUBROUTINES
C
C
C AUTHOR:  PAUL E. BRIDEN (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/81
C          JET EXT. 4569
C
C DATE:    07/02/91
C
C UPDATE:  07/08/91 - PE BRIDEN: INTRODUCED SUBROUTINE 'XXGSEL'
C
C UPDATE:  25/11/91 - PE BRIDEN: MADE FILNAM/PICSAV ARGUMENT LIST
C                      COMPATIBLE WITH GHOST VERSION 8.
C
C UPDATE:  23/04/93 - PE BRIDEN - ADAS91: ADDED I4UNIT FUNCTION TO WRITE
C                      STATEMENTS FOR SCREEN MESSAGES
C
C UPDATE:  24/05/93 - PE BRIDEN - ADAS91: CHANGED I4UNIT(0)-> I4UNIT(-1)
C
C UPDATE:  22/09/93 - J NASH      - ADAS91:
C                      REMOVED PRINTING OF DATA SUB-BLOCK TITLE (COMMENTED OUT).
C
C UPDATE:  01/05/95 - Tim Hammond - IDL-ADAS:
C                      UNIX conversion
C
C
C-----
C
C      REAL*4      GHZERO      , YDMIN
C
C      PARAMETER( GHZERO = 1.0E-36 , YDMIN = 1.0E-20 )
C
C-----
C
C      INTEGER    I4UNIT
C      INTEGER    NENER      , NMX      , NPSPL
C      INTEGER    I          , IKEY     , ICOUNT
C      INTEGER    PIPEOU     , ONE      , ZERO
C      PARAMETER ( PIPEOU = 6      , ONE=1 , ZERO=0)
C
C-----
C
C      REAL*8      ENERA(NENER) , SIGA(NENER) ,
C      &           EOMA(NMX)    , SIGOMA(NMX)  ,
C      &           EOSA(NPSPL)  , SIGOSA(NPSPL) ,
C      &           XMIN        , XMAX      ,
C      &           YMIN        , YMAX      ,
C
C-----
C
C      REAL*4      XHIGH      , XLOW      ,
C      &           YHIGH      , YLOW      ,
C      REAL*4      XA4(100)   , YA4(100)
C
C-----
C
C      CHARACTER  TITLE*40 , TITLF*80 , TITLX*120 , TITLM*80 ,
C      &          DATE*8
C      CHARACTER  CADAS*80 ,
C      &          ISPEC*88 , DNAME*12 , XTIT*23 , YTIT*23 ,
C      &          MNMX0*9 , KEY0*9 , ADAS0*8 , CINFO*8 ,
C      &          KEY(3)*22
C      CHARACTER  GRID*1 , PIC*1 , C3BLNK*3 , C7*7
C-----

```



```

LOGICAL  LHOST      , LGRD1      , LDEF1      , LFSEL
C-----
SAVE     ISPEC      , CADAS
C-----
DATA ISPEC(1:48)
& /'CHARGE-EXCHANGE CROSS-SECTION VERSUS ENERGY: '/
DATA DNAME/'      DATE: '/
DATA XTIT/'      ENERGY (eV/amu) '/
DATA YTIT/'      CROSS-SECTION (cm**2) '/
DATA ADAS0/'ADAS :'/
& CINFO/'TITLE  :'/,
& MNMX0/'MINIMAX: '/,
& KEY0 /'KEY    : '/,
& KEY(1)/'(CROSSES - INPUT DATA)'/,
& KEY(2)/' (FULL LINE - SPLINE) '/,
& KEY(3)/'(DASH LINE - MINIMAX) '/
DATA GRID /' '/ ,
& PIC /' '/ ,
& C3BLNK/' '/ ,
& CADAS /' '/
C-----

```

## C1SPLN

```

SUBROUTINE C1SPLN(      LOSEL ,
&                      NENER , IEVAL , NPSPL ,
&                      ENERA , EOA , EOSA ,
&                      SIGA , SIGOA , SIGOSA ,
&                      LERNG
&                      )
IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C1SPLN *****
C (IDENTICAL TO: B1SPLN (EXCEPT SOME VARIABLE NAMES ARE CHANGED))
C
C PURPOSE:
C 1) PERFORMS CUBIC SPLINE ON LOG(ENERGY) VERSUS LOG(X-SECTION)
C INPUT DATA, ('ENERA' VERSUS 'SIGA' , NENER DATA PAIRS),
C FOR A GIVEN SUB-BLOCK.
C
C 2) INTERPOLATES 'IEVAL' X-SECT. VALUES USING ABOVE SPLINES
C AT ENERGIES READ IN FROM ISPF PANELS FOR TABULAR OUTPUT.
C (ANY ENERGIES VALUES WHICH REQUIRED EXTRAPOLATION ARE SET
C TO ZERO).
C - THIS STEP ONLY TAKES PLACE IF 'LOSEL=.TRUE.' -
C
C 3) INTERPOLATES 'NPSPL' X-SECT VALUES USING ABOVE SPLINES AT
C ENERGIES EQUI-DISTANCE ON RANGE OF LOG(ENERGIES) STORED
C IN INPUT 'ENERA' ARRAY.
C
C CALLING PROGRAM: ADAS301
C
C SUBROUTINE:
C
C INPUT : (L*4) LOSEL = .TRUE. => CALCULATE X-SECS FOR INPUT ENGY.
C READ FROM ISPF PANEL.
C .FALSE. => - DO NOT DO THE ABOVE -
C
C INPUT : (I*4) NENER = INPUT DATA FILE: NO. OF VALID ENERGY/X-SECT.
C PAIRS READ FOR THE SUB-BLOCK BEING ASSESSED
C INPUT : (I*4) IEVAL = NUMBER OF ISPF ENTERED ENERGY VALUES AT
C WHICH INTERPOLATED X-SEC VALUES ARE REQUIRED
C FOR TABULAR OUTPUT.
C INPUT : (I*4) NPSPL = NUMBER OF SPLINE INTERPOLATED ENGY/X-SECT
C REQUIRED FOR GRAPHICAL DISPLAY.
C
C INPUT : (I*4) ENERA() = INPUT DATA FILE: ENERGIES (EV/AMU)
C INPUT : (I*4) EOA() = ISPF PANEL ENTERED ENERGIES (EV/AMU)
C OUTPUT: (I*4) EOSA() = 'NPSPL' ENERGIES FOR GRAPHICAL OUTPUT
C (EV/AMU).
C
C INPUT : (R*8) SIGA() = INPUT DATA FILE: SELECTED SUB-BLOCK -
C X-SECTION VALUES AT 'ENERA()'. (CM**2)
C OUTPUT: (I*4) SIGOA() = SPLINE INTERPOLATED X-SEC VALUES AT 'EOA()'
C (EXTRAPOLATED VALUES = 0.0).
C OUTPUT: (R*8) SIGOSA() = SPLINE INTERPOLATED X-SEC VALUES AT 'EOSA()'
C
C OUTPUT: (L*4) LERNG() = .TRUE. => OUTPUT SPLINE VALUE WAS
C INTERPOLATED FOR 'DLOG(EOA())'.
C .FALSE. => OUTPUT SPLINE VALUE WAS
C EXTRAPOLATED FOR 'DLOG(EOA())'.
C (NOTE: 'YOUT()=0' AS 'IOPT < 0').
C
C (I*4) NIN = PARAMETER = MAX. NO. OF INPUT ENGY/X-SEC
C PAIRS MUST BE >= 'NENER'
C (I*4) NOUT = PARAMETER = MAX. NO. OF 'OUTPUT ENGY/X-SEC
C PAIRS MUST BE >= 'IEVAL' &'NPSPL'
C
C (R*8) ZERO = PARAMETER = EFFECTIVE ZERO (1.0D-72)
C (R*8) ZEROL = PARAMETER = LN(ZERO) APPROX. = -165.7
C
C

```

```

C      (I*4) IARR = ARRAY SUBSCRIPT USED FOR ENGY/X-SEC PAIRS
C      (I*4) IOPT = DEFINES THE BOUNDARY DERIVATIVES FOR THE
C                  SPLINE ROUTINE 'XXSPLE', SEE 'XXSPLE'.
C                  (VALID VALUES = <0, 0, 1, 2, 3, 4)
C
C      (R*8) ESTEP = THE SIZE OF STEP BETWEEN 'XOUT()' VALUES FOR
C                  GRAPHICAL OUTPUT ENGY/X-SEC PAIRS TO BE
C                  CALCULATED USING SPLINES.
C
C      (L*4) LSETX = .TRUE. => SET UP SPLINE PARAMETERS RELATING
C                  TO 'XIN' AXIS.
C                  .FALSE. => DO NOT SET UP SPLINE PARAMETERS
C                  RELATING TO 'XIN' AXIS.
C                  (I.E. THEY WERE SET IN A PREVIOUS
C                   CALL )
C                  (VALUE SET TO .FALSE. BY 'XXSPLE')
C
C      (R*8) XIN() = LOG( 'ENERA()' )
C      (R*8) YIN() = LOG( 'SIGA()' )
C      (R*8) XOUT() = LOG(ENERGIES AT WHICH SPLINES REQUIRED)
C      (R*8) YOUT() = LOG(OUTPUT SPLINE INTERPOLATED X-SEC VALUES)
C      (R*8) DF() = SPLINE INTERPOLATED DERIVATIVES
C
C      (L*4) LDUMP() = .TRUE. => OUTPUT SPLINE VALUE INTRPOLATED
C                  FOR 'YOUT()'.
C                  .FALSE. => OUTPUT SPLINE VALUE EXTRAPOLATED
C                  FOR 'YOUT()'.
C                  (NOTE: USED AS A DUMMY ARGUMENT.
C                   ALL VALUES WILL BE TRUE.)
C
C NOTE:
C
C ROUTINES:
C
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      XXSPLE      ADAS          SPLINE SUBROUTINE (EXTENDED DIAGNOSTICS)
C      R8FUN1      ADAS          REAL*8 FUNCTION: ( X -> X )
C
C AUTHOR:  PAUL E. BRIDEN (TESSELLA SUPPORT SERVICES PLC)
C          KL/0/81
C          JET EXT. 4569
C
C DATE:    07/02/91
C
C UPDATE:  30/11/93 - J NASH      - ADAS91:
C          INCREASED MAX NUMBER OF INPUT ENERGIES ('NIN') FROM 24 TO 30.
C
C UPDATE:  19/04/95  H P SUMMERS - ADDED TRAP FOR ZERO INPUTS
C
C -----
C
C      INTEGER      NIN          , NOUT
C
C      REAL*8       ZERO         , ZEROL
C
C      PARAMETER(  NIN = 30      , NOUT = 100      )
C      PARAMETER(  ZERO = 1.0D-72 , ZEROL = -165.7D0 )
C
C      INTEGER      NENER        , IEVAL          , NPSPL
C      INTEGER      IOPT        , IARR
C
C      REAL*8       R8FUN1      , ESTEP
C
C      LOGICAL      LOSEL       , LSETX
C
C      REAL*8       ENERA(NENER) , SIGA(NENER)    ,
C      &            EOA(IEVAL)   , SIGOA(IEVAL)   ,
C      &            EOSA(NPSPL)  , SIGOSA(NPSPL)  ,
C      REAL*8       XIN(NIN)    , YIN(NIN)      ,
C      &            XOUT(NOUT)   , YOUT(NOUT)    ,
C      REAL*8       DF(NIN)
C
C      LOGICAL      LERNG(IEVAL) , LDUMP(NOUT)
C
C      EXTERNAL    R8FUN1
C
C -----

```

## C2CHKB

```

C      SUBROUTINE C2CHKB( IUNIT , NBSEL , IBSEL ,
C      &                  IZ0IN , IZO ,
C      &                  LOPEN , IRCODE
C      &                  )
C      IMPLICIT NONE
C
C -----
C ***** FORTRAN77 SUBROUTINE: C2CHKB *****
C
C PURPOSE: TO CHECK THE SELECTED BLOCK (IBSEL) OF DATA EXISTS IN THE
C          INPUT DATA SET AND IF SO IT REPRESENTS THE ENTERED VALUES OF
C          'IZ0IN' (NUCLEAR CHARGE OF SELECTED IONISING ION ELEMENT).
C
C

```

```

C          IT ALSO CLOSES THE INPUT DATA SET ALLOCATION IF OPEN.
C
C CALLING PROGRAM: SSIA
C
C SUBROUTINE:
C
C INPUT : (I*4)  IUNIT  = UNIT TO WHICH INPUT DATA SET IS ALLOCATED
C INPUT : (I*4)  NBSEL  = TOTAL NUMBER OF DATA-BLOCKS READ FROM INPUT
C                   DATA SET.
C INPUT : (I*4)  IBSEL  = INDEX OF DATA-BLOCK SELECTED FOR ANALYSIS
C
C INPUT : (I*4)  IZ0IN  = REQUESTED: NUCLEAR CHARGE OF ELEMENT
C INPUT : (I*4)  IZ0    = INPUT FILE: NUCLEAR CHARGE OF ELEMENT
C
C I/O   : (L*4)  LOPEN  = INPUT : .TRUE. => INPUT DATA SET OPEN.
C                   .FALSE. => INPUT DATA SET CLOSED.
C                   OUTPUT: ALWAYS RETURNED AS .FALSE.
C OUTPUT: (I*4)  IRCODE = RETURN CODE FROM SUBROUTINE:
C                   0 => NO ERROR DETECTED.
C                   2 => DISCREPANCY BETWEEN REQUESTED ELEMENT
C                   AND THAT IN INPUT DATA FILE.
C                   3 => SELECTED DATA-BLOCK OUT OF RANGE OR
C                   DOES NOT EXIST.
C
C          (I*4)  I4UNIT = FUNCTION (SEE ROUTINE SECTION BELOW)
C
C          (C*44) DSNAME = FULL MVS NAME OF DATA SET OPENED
C
C ROUTINES:
C          ROUTINE      SOURCE      BRIEF DESCRIPTION
C          -----
C          E2FILE      ADAS        OPEN DATA SET FOR SELECTED ELEMENT
C          I4UNIT      ADAS        FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C AUTHOR:  PAUL E. BRIDEN (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/37
C          JET EXT. 2520
C
C DATE:    06/06/91
C
C UPDATE:  23/04/93 - PE BRIDEN - ADAS91: ADDED I4UNIT FUNCTION TO WRITE
C          STATEMENTS FOR SCREEN MESSAGES
C
C UPDATE:  24/05/93 - PE BRIDEN - ADAS91: CHANGED I4UNIT(0)-> I4UNIT(-1)
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1                      DATE: 19-11-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C          - PUT UNDER S.C.C.S. CONTROL
C
C -----
C
C          INTEGER      I4UNIT
C          INTEGER      IUNIT          , IRCODE          ,
C          &            NBSEL          , IBSEL          ,
C          &            IZ0IN          , IZ0
C
C          LOGICAL      LOPEN
C
C          CHARACTER    DSNAME*44
C
C -----

```

## C2DATA

```

C          SUBROUTINE C2DATA( IUNIT , DSNAME ,
C          &                 NSTORE , NEDIM ,
C          &                 NBSEL , ISELA ,
C          &                 CPRIMY , CSECDY , CTYPE ,
C          &                 AMPA , AMSA , ALPHA , ETHRA ,
C          &                 IEA ,
C          &                 TEEA , SIA
C          &                 )
C          IMPLICIT NONE
C
C -----
C          ***** FORTRAN77 SUBROUTINE: C2DATA *****
C
C PURPOSE: TO FETCH DATA FROM INPUT ION/ATOM CROSS-SECTION
C          FILES OF TYPE ADF02.
C
C CALLING PROGRAM: ADAS302/SSIA
C
C DATA:
C
C          UP TO 'NSTORE' SETS (DATA-BLOCKS) OF DATA MAY BE READ FROM
C          THE FILE - EACH BLOCK FORMING A COMPLETE SET OF CROSS-
C          SECTION VALUES FOR GIVEN COLLISION ENERGIES.
C          EACH DATA-BLOCK IS ANALYSED INDEPENDENTLY OF ANY OTHER
C          DATA-BLOCK.
C
C -----

```

```

C      THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
C
C      COLLISION ENERGIES   : EV/AMU
C      CROSS-SECTION       : CM**2
C
C  SUBROUTINE:
C
C  INPUT : (I*4) IUNIT      = UNIT TO WHICH INPUT FILE IS ALLOCATED.
C  INPUT : (C*80) DSNAME    = MVS DATA SET NAME OF DATA SET BEING READ
C
C  INPUT : (I*4) NSTORE     = MAXIMUM NUMBER OF INPUT DATA-BLOCKS THAT
C                          CAN BE STORED.
C  INPUT : (I*4) NEDIM      = MAX NUMBER OF COLLISION ENERGIES ALLOWED
C
C  OUTPUT: (I*4) NBSEL      = NUMBER OF DATA-BLOCKS ACCEPTED & READ IN.
C  OUTPUT: (I*4) ISELA()    = READ - DATA-SET DATA-BLOCK ENTRY INDICES
C                          DIMENSION: DATA-BLOCK INDEX
C
C  OUTPUT: (C*5) CPRIMY()   = READ - PRIMARY SPECIES IDENTIFICATION
C                          DIMENSION: DATA-BLOCK INDEX
C  OUTPUT: (C*5) CSECDY()  = READ - SECONDARY SPECIES IDENTIFICATION
C                          DIMENSION: DATA-BLOCK INDEX
C  OUTPUT: (C*3) CTYPE()    = READ - CROSS-SECTION TYPE
C                          DIMENSION: DATA-BLOCK INDEX
C
C  OUTPUT: (R*8) AMPA()     = READ - PRIMARY SPECIES ATOMIC MASS NUMBER
C                          DIMENSION: DATA-BLOCK INDEX
C  OUTPUT: (R*8) AMSA()     = READ - SECONDARY SPECIES ATOMIC MASS NUMBER
C                          DIMENSION: DATA-BLOCK INDEX
C  OUTPUT: (R*8) ALPHA()   = READ - HIGH ENERGY EXTRAPOLATION PARM.
C                          DIMENSION: DATA-BLOCK INDEX
C  OUTPUT: (R*8) ETHRA()   = READ - ENERGY THRESHOLD (EV)
C                          DIMENSION: DATA-BLOCK INDEX
C
C  OUTPUT: (I*4) IEA()      = READ - NUMBER OF COLLISION ENERGIES
C                          DIMENSION: DATA-BLOCK INDEX
C
C  OUTPUT: (R*8) TEEA(,)    = READ - COLLISION ENERGIES (UNITS: eV/AMU)
C                          1st DIMENSION: COLLISION ENERGY INDEX
C                          2nd DIMENSION: DATA-BLOCK INDEX
C
C  OUTPUT: (R*8) SIA(,)    =READ - FULL SET OF COLLISION CROSS-
C                          SECTION VALUES (cm**2)
C                          1st DIMENSION: COLLISION ENERGY INDEX
C                          2nd DIMENSION: DATA-BLOCK INDEX
C
C  (I*4) I4EIZ0            = FUNCTION - (SEE ROUTINES SECTION BELOW)
C  (I*4) I4FCTN            = FUNCTION - (SEE ROUTINES SECTION BELOW)
C  (I*4) I4UNIT            = FUNCTION - (SEE ROUTINE SECTION BELOW)
C  (I*4) IBLK              = ARRAY INDEX: DATA-BLOCK INDEX
C  (I*4) ITT               = ARRAY INDEX: COLLISION ENERGY INDEX
C  (I*4) NENUM             = NUMBER OF COLLISION ENERGIES FOR CURRENT
C                          DATA-BLOCK
C  (I*4) IABT              = RETURN CODE FROM 'I4FCTN'
C  (I*4) IPOS2             = GENERAL USE STRING INDEX VARIABLE
C
C  (R*8) R8FCTN           = FUNCTION - (SEE ROUTINES SECTION BELOW)
C
C  (L*4) LBEND             = IDENTIFIES WHETHER THE LAST OF THE INPUT
C                          DATA SUB-BLOCKS HAS BEEN LOCATED.
C                          (.TRUE. => END OF SUB-BLOCKS REACHED)
C
C  (C*1) CSLASH            = '/' - DELIMITER FOR 'XXHKEY'
C  (C*2) C2                = GENERAL USE TWO BYTE CHARACTER STRING
C  (C*1) CKEY1             = 'P' - INPUT BLOCK HEADER KEY
C  (C*1) CKEY2             = 'S' - INPUT BLOCK HEADER KEY
C  (C*1) CKEY3             = 'A' - INPUT BLOCK HEADER KEY
C  (C*1) CKEY4             = 'E' - INPUT BLOCK HEADER KEY
C  (C*4) CKEY5             = 'T' - INPUT BLOCK HEADER KEY
C  (C*4) CKEY6             = 'ISEL' - INPUT BLOCK HEADER KEY
C  (C*3) C3                = GENERAL USE THREE BYTE CHARACTER STRING
C  (C*9) C10               = GENERAL USE NINE BYTE CHARACTER STRING
C  (C*80) C80              = GENERAL USE 80 BYTE CHARACTER STRING FOR
C                          THE INPUT OF DATA-SET RECORDS.
C
C  ROUTINES:
C  ROUTINE   SOURCE   BRIEF DESCRIPTION
C  -----
C  XXHKEY    ADAS     OBTAIN KEY/RESPONSE STRINGS FROM TEXT
C  I4FCTN    ADAS     INTEGER*4 FUNCTION -
C                          CONVERT CHARACTER STRING TO INTEGER
C  I4UNIT    ADAS     INTEGER*4 FUNCTION -
C                          FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C  R8FCTN    ADAS     REAL*8 FUNCTION -
C                          CONVERT CHARACTER STRING TO REAL*8
C
C  AUTHOR:   H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C           JA8.08
C           TEL. 0141-553-4196
C
C  DATE:    12/11/96
C
C  UNIX-IDL PORT: H.P.SUMMERS
C
C  VERSION: 1.1
C           DATE: 19-11-96
C  MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C           - PUT UNDER S.C.C.S. CONTROL
C

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```

C VERSION: 1.2                                DATE: 14-02-97
C MODIFIED: RICHARD MARTIN
C                                     - CHANGED INITIALISATION 'CKEY2 /'S '/' TO 'CKEY2 /'S'/'
C
C
C-----
C      INTEGER    I4FCTN                , I4UNIT
C      INTEGER    IUNIT                  , NSTORE
C      &          NEDIM                    , NBSEL
C      INTEGER    IBLK                    , ITF
C      &          NENUM                     , IABT
C      &          IPOS2
C-----
C      REAL*8     R8FCTN
C-----
C      LOGICAL    LBEND
C-----
C      CHARACTER  DSNAME*80
C      CHARACTER  CSLASH*1                , C2*2
C      &          CKEY1*1                  , CKEY2*1
C      &          CKEY3*1                  , CKEY4*1
C      &          CKEY5*3                  , CKEY6*4
C      &          C3*3                    , C9*9
C                                     , C80*80
C-----
C      INTEGER    ISELA(NSTORE)          , IEA(NSTORE)
C-----
C      CHARACTER  CPRIMY(NSTORE)*5       , CSECDY(NSTORE)*5
C      &          CTYPE(NSTORE)*3
C-----
C      REAL*8     AMPA(NSTORE)            , AMSA(NSTORE)
C      REAL*8     ALPHA(NSTORE)          , ETHRA(NSTORE)
C      REAL*8     TEEA(NEDIM,NSTORE)    , SIA(NEDIM,NSTORE)
C-----
C      SAVE      CSLASH
C      &        CKEY1
C      &        CKEY3
C      &        CKEY5
C-----
C      DATA     CSLASH / '/' /
C      DATA     CKEY1 / 'P' / , CKEY2 / 'S' / ,
C      &        CKEY3 / 'A' / , CKEY4 / 'E' / ,
C      &        CKEY5 / 'T' / , CKEY6 / 'ISEL' /
C-----
C *****

```

## C2ECON

```

SUBROUTINE C2ECON( INTYP, OUTTYP, AMD,AMR,IEVAL, EIN, EOUT )
IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C2ECON *****
C
C PURPOSE: TO CONVERT AN ARRAY OF COLLISION ENERGIES INTO A SPECIFIED
C          FORM.
C
C CALLING PROGRAM: GENERAL USE
C
C SUBROUTINE:
C
C INPUT :   (I*4) INTYP   = 1 => 'EIN(ARRAY)' UNITS: DONOR   EV
C           (I*4) OUTTYP  = 2 => 'EIN(ARRAY)' UNITS: RECVR   EV
C           (I*4) OUTTYP  = 3 => 'EIN(ARRAY)' UNITS: ENERGY EV/AMU
C INPUT :   (I*4) OUTTYP  = 1 => 'EOUT(ARRAY)' UNITS: DONOR   EV
C           (I*4) OUTTYP  = 2 => 'EOUT(ARRAY)' UNITS: RECVR   EV
C           (I*4) OUTTYP  = 3 => 'EOUT(ARRAY)' UNITS: ENERGY EV/AMU
C INPUT :   (R*8) AMD     = DONOR MASS NUMBER
C INPUT :   (R*8) AMR     = RECEIVER MASS NUMBER
C INPUT :   (I*4) IEVAL   = NO. OF ENERGIES IN EIN(ARRAY)
C INPUT :   (R*8) EIN()   = INPUT ENERGIES (STATED UNITS)
C OUTPUT:   (R*8) EOUT()  = OUTPUT ENERGIES (STATED UNITS)
C
C           (I*4) I       = GENERAL USE
C
C           (R*8) ECONV() = ENERGY/VELOCITY CONVERSION PARAMETERS
C
C ROUTINES: NONE
C
C AUTHOR:   H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C           JA8.08
C           TEL. 0141-553-4196
C
C DATE:    17/11/95
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1                                DATE: 19-11-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C          - PUT UNDER S.C.C.S. CONTROL

```

```

C
C-----
C
C
C      INTEGER      INTYP      , OUTTYP
C      &            IEVAL
C      INTEGER      I
C-----
C      REAL*8      AMD          , AMR
C      REAL*8      EIN(IEVAL)  , EOUT(IEVAL)
C      REAL*8      ECONV(3)
C-----

```

## C2OUT0

```

      SUBROUTINE C2OUT0( IWRITE , LFSSEL ,
& TITLE , TITLX , TITLM ,
& DATE , CADAS ,
& IBSEL , IEVAL ,
& ESYM , IZ0 , IZ , IZ1 ,
& CPRIMY , CSECDY ,
& CTYPE ,
& LERNG ,
& VCMS , VATU , EEVA ,
& SIAA ,
& KPLUS1 , COEF
& )
      IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C2OUT0 *****
C
C PURPOSE: TO PRINT DATA CONCERNING THE SELECTED CROSS-SECTION
C          DATA BLOCK UNDER ANALYSIS.
C
C CALLING PROGRAM: ADAS302
C
C SUBROUTINE:
C
C INPUT : (I*4) IWRITE = OUTPUT UNIT FOR RESULTS
C INPUT : (L*4) LFSSEL = .TRUE. => MINIMAX POLYNOMIAL FITTED.
C          .FALSE. => MINIMAX POLYNOMIAL NOT FITTED
C
C INPUT : (C*40) TITLE = TITLE OF RUN (READ FROM ISPF PANEL)
C INPUT : (C*120) TITLX = INFORMATION STRING CONTAINING INPUT DATA-
C          SET NAME IN BYTES 1->35.
C INPUT : (C*80) TITLM = DIAGNOSTIC LINE INFORMATION FROM 'MINIMAX'
C INPUT : (C*8) DATE = CURRENT DATE (AS 'DD/MM/YY')
C INPUT : (C*80) CADAS = ADAS HEADER
C
C INPUT : (I*4) IBSEL = DATA-BLOCK INDEX SELECTED FROM INPUT DATASET
C          FOR ANALYSIS.
C INPUT : (I*4) IEVAL = NUMBER OF USER ENTERED COLLISION ENERGIES
C
C INPUT : (C*2) ESYM = INPUT FILE: SECONDARY - ELEMENT SYMBOL
C INPUT : (I*4) IZ0 = INPUT FILE: SECONDARY - NUCLEAR CHARGE
C INPUT : (I*4) IZ = INPUT DATA FILE - SELECTED DATA-BLOCK:
C          SECONDARY SPECIES CHARGE
C INPUT : (I*4) IZ1 = INPUT DATA FILE - SELECTED DATA-BLOCK:
C          SECONDARY SPECIES EFFECTIVE CHARGE
C
C INPUT : (C*9) CPRIMY = INPUT DATA FILE - SELECTED DATA-BLOCK:
C          PRIMARY SPECIES IDENTIFICATION
C INPUT : (C*9) CSECDY = INPUT DATA FILE - SELECTED DATA-BLOCK:
C          SECONDARY SPECIES IDENTIFICATION
C INPUT : (C*2) CTYPE = INPUT DATA FILE - SELECTED DATA-BLOCK:
C          CROSS-SECTION TYPE
C
C INPUT : (L*4) LERNG() = .TRUE. => OUTPUT 'SIAA()' VALUE WAS INTER-
C          POLATED FOR THE USER ENTERED
C          COLLISION ENERGIES 'EEVA()'.
C          .FALSE. => OUTPUT 'SIAA()' VALUE WAS EXTRA-
C          POLATED FOR THE USER ENTERED
C          COLLISION ENERGIES 'EEVA()'.
C          DIMENSION: COLLISION ENERGY INDEX
C
C INPUT : (R*8) VCMS() = USER ENTERED: COLLISION VELOCITY (cm s-1)
C          DIMENSION: COLLISION ENERGY INDEX
C INPUT : (R*8) VATU() = USER ENTERED: COLLISION VELOCITY (At. Un.)
C          DIMENSION: COLLISION ENERGY INDEX
C INPUT : (R*8) EEVA() = USER ENTERED: COLLISION ENERGY (EV/AMU)
C          DIMENSION: COLLISION ENERGY INDEX
C
C INPUT : (R*8) SIAA() = SPLINE INTERPOLATED OR EXTRAPOLATED CX
C          COLLISION CROSS-SECTIONS FOR
C          THE USER ENTERED COLLISION ENERGIES.
C          DIMENSION: COLLISION ENERGY INDEX
C
C INPUT : (I*4) KPLUS1 = NUMBER OF MINIMAX COEFFICIENTS
C INPUT : (R*8) COEF() = COEFFICIENTS OF FITTED MINIMAX POLYNOMIAL
C
C          (I*4) I = GENERAL USE - ARRAY ELEMENT INDEX
C

```

```

C      (C*1) C1E      = '*' IF RATE-COEFFICIENT WAS EXTRAPOLATED FOR
C                      THE CURRENT COLLISION ENERGY. (IT EQUALS
C                      ' ' IF IT WAS INTERPOLATED.)
C      (C*12) XFELEM = FUNCTION - (SEE ROUTINES SECTION BELOW)
C      (C*12) CELEM  = RECEIVER ION  ELEMENT NAME
C
C  ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      XFELEM      ADAS          CHARACTER*12 FUNCTION -
C                      RETURNS ELEMENT NAME  FOR GIVEN Z0
C
C  AUTHOR   : H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C            JA8.08
C            TEL. 0141-553-4196
C
C  DATE:    12/11/96
C
C  UNIX-IDL PORT: H.P.SUMMERS
C
C  VERSION: 1.1                      DATE: 19-11-96
C  MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C            - PUT UNDER S.C.C.S. CONTROL
C
C  -----
C      INTEGER      IWRITE      , IBSEL      , IEVAL      ,
C      &            IZO          , IZ         , IZ1        , KPLUS1
C      INTEGER      I
C
C  -----
C      LOGICAL      LFSEL
C
C      CHARACTER    TITLE*(*)    , TITLX*(*)    , TITLM*(*)    , ESYM*2    ,
C      &            CPRIMY*5      , CSECDY*5      ,
C      &            CTYPE*3       , DATE*8
C      CHARACTER    XFELEM*12    ,
C      &            C1E*1         ,
C      &            CELEM*12      , CADAS*80
C
C  -----
C      REAL*8       VCMS(IEVAL)  , EEVA(IEVAL)  , VATU(IEVAL)  ,
C      &            SIAA(IEVAL)  ,
C      &            COEF(KPLUS1)
C
C  -----
C      LOGICAL      LERNG(IEVAL)
C  -----

```

## C2OUTG

```

C      SUBROUTINE C2OUTG( LGHOST ,
C      &                TITLE , TITLX , TITLM , DATE ,
C      &                ESYM , IZO , IZ ,
C      &                CPRIMY , CSECDY ,
C      &                CTYPE ,
C      &                EEVA , SIAA , IEVAL ,
C      &                EFITM , SIAM , NMX ,
C      &                LGRD1 , LDEF1 , LFSEL ,
C      &                XMIN , XMAX , YMIN , YMAX
C      &                )
C      IMPLICIT NONE
C
C  -----
C      ***** FORTRAN77 SUBROUTINE: C2OUTG *****
C
C  PURPOSE:  PIPE COMMUNICATION WITH IDL TO PLOT GRAPH
C
C            PROVIDES COMPARATIVE GRAPH OF:
C                SPLINE INTERPOLATED POINTS : CROSSES
C                CURVE THROUGH SPLINE POINTS: FULL CURVE
C                MINIMAX FIT TO SPLINE DATA : DASH CURVE
C
C            PLOT IS LOG10(CROSS-SECTION (cm**2))
C                VERSUS
C                LOG10(COLLISION ENERGY (eV/AMU))
C
C  CALLING PROGRAM: ADAS302
C
C  SUBROUTINE:
C
C  INPUT : (L*4) LGHOST = .TRUE. => GHOST80 INITIALISED
C          .FALSE. => GHOST80 NOT INITIALISED
C
C  INPUT : (C*40) TITLE = TITLE OF RUN (READ FROM ISPF PANEL)
C  INPUT : (C*120) TITLX = INFORMATION STRING CONTAINING: INPUT DATA
C          FILE-NAME, SELECTED BLOCK, ION INFORMATION
C  INPUT : (C*80) TITLM = DIAGNOSTIC LINE INFORMATION FROM 'MINIMAX'
C  INPUT : (C*8)  DATE  = CURRENT DATE (AS 'DD/MM/YY')
C
C  INPUT : (C*2)  ESYM  = INPUT FILE: SECONDARY - ELEMENT SYMBOL
C  INPUT : (I*4)  IZO   = INPUT FILE: SECONDARY - NUCLEAR CHARGE
C  INPUT : (I*4)  IZ    = INPUT DATA FILE - SELECTED DATA-BLOCK:
C          SECONDARY SPECIES CHARGE
C
C  INPUT : (C*5)  CPRIMY = INPUT DATA FILE - SELECTED DATA-BLOCK:
C          PRIMARY SPECIES IDENTIFICATION
C

```

```

C INPUT : (C*5) CSECDY = INPUT DATA FILE - SELECTED DATA-BLOCK:
C                   SECONDARY SPECIES IDENTIFICATION
C INPUT : (C*3) CTYPE  = INPUT DATA FILE - SELECTED DATA-BLOCK:
C                   CROSS-SECTION TYPE
C
C INPUT : (R*8) EEVA() = USER ENTERED: COLLISION ENERGIES (eV/AMU)
C                   DIMENSION: COLLISION ENERGY INDEX
C INPUT : (R*8) SIAA() = SPLINE INTERPOLATED OR EXTRAPOLATED
C                   I/A CROSS-SECTIONS FOR
C                   THE USER ENTERED COLLISION ENERGIES.
C                   DIMENSION: COLLISION ENERGY INDEX
C INPUT : (I*4) IEVAL  = NUMBER OF USER ENTERED ENERGY VALUES
C
C INPUT : (R*8) EFITM() = MINIMAX: SELECTED ENERGIES (eV/AMU)
C INPUT : (R*8) SIAM() = CROSS-SECTIONS AT 'EFITM()'
C INPUT : (I*4) NMX    = NUMBER OF MINIMAX GENERATED CX CROSS-
C                   SECTION VALUES FOR GRAPHICAL DISPLAY
C
C INPUT : (L*4) LGRD1  = .TRUE. => PUT GRAPH IN GRID FILE
C                   .FALSE. => DO NOT PUT GRAPH IN GRID FILE
C INPUT : (L*4) LDEF1  = .TRUE. => USE DEFAULT GRAPH SCALING
C                   .FALSE. => DO NOT USE DEFAULT GRAPH SCALING
C INPUT : (L*4) LFSEL  = .TRUE. => CARRY OUT MINIMAX POLYNOMIAL
C                   FITTING
C                   .FALSE. => - DO NOT DO THE ABOVE -
C
C INPUT : (R*8) XMIN   = GRAPH: LOWER LIMIT FOR ENERGY
C INPUT : (R*8) XMAX   = GRAPH: UPPER LIMIT FOR ENERGY
C INPUT : (R*8) YMIN   = GRAPH: LOWER LIMIT FOR CROSS-SECTION.
C INPUT : (R*8) YMAX   = GRAPH: UPPER LIMIT FOR CROSS-SECTION.
C
C                   (I*4) I      = GENERAL USE - ARRAY INDEX
C
C                   (C*28) STRG1 = DESCRIPTIVE STRING FOR ELEMENT SYMBOL
C                   (C*28) STRG2 = DESCRIPTIVE STRING FOR NUCLEAR CHARGE
C                   (C*28) STRG4 = DESCRIPTIVE STRING FOR STATE ION
C                   (C*28) STRG5 = DESCRIPTIVE STRING FOR STATE ION CHARGE
C                   (C*28) STRG6 = DESCRIPTIVE STRING FOR STATE META. INDEX
C                   (C*32) HEAD1 = HEADING FOR IONISING ION INFORMATION
C                   (C*16) HEAD2 = HEADING FOR INITIAL STATE INFORMATION
C                   (C*16) HEAD3 = HEADING FOR FINAL STATE INFORMATION
C
C ROUTINES:
C          ROUTINE      SOURCE      BRIEF DESCRIPTION
C -----
C          XXADAS      ADAS        GATHERS ADAS HEADER INFORMATION
C          XXFLSH      IDL-ADAS    CALLS FLUSH COMMAND TO CLEAR PIPE.
C
C AUTHOR:  H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C          JA8.08
C          TEL. 0141-553-4196
C
C DATE:    12/11/96
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1                      DATE: 19-11-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C           - PUT UNDER S.C.C.S. CONTROL
C
C -----
C          REAL*4      GHZERO      , YDMIN
C -----
C          PARAMETER( GHZERO = 1.0E-36 , YDMIN = 1.0E-20 )
C -----
C          INTEGER    IZ0          , IZ          ,
C          &          IEVAL        , NMX
C          INTEGER    I
C -----
C          REAL*8      XMIN        , XMAX        ,
C          &          YMIN        , YMAX
C -----
C          LOGICAL    LGHOST      ,
C          &          LGRD1      , LDEF1      , LFSEL
C -----
C          CHARACTER  TITLE*40    , TITLX*120   , TITLM*80 ,
C          &          DATE*8      , ESYM*2
C          &          CPRIMY*5    , CSECDY*5
C          &          CTYPE*3
C          CHARACTER  STRG1*28    , STRG2*28    ,
C          &          STRG3*28    , STRG4*28    ,
C          &          STRG5*28    , STRG6*28    ,
C          &          HEAD1*32    , HEAD2*16    , HEAD3*16
C -----
C          REAL*8      EEVA(IEVAL) , SIAA(IEVAL) ,
C          &          EFITM(NMX)   , SIAM(NMX)
C -----
C          DATA HEAD1 /'----- REACTION INFORMATION -----'/ ,
C          &          HEAD2 /' PRIMARY :      '/ ,
C          &          HEAD3 /' SECONDARY:      '/ ,
C          DATA STRG1 /' SECONDARY ELEMENT SYMBOL = '/ ,
C          &          STRG2 /' SECONDARY NUCLEAR CHARGE = '/ ,
C          &          STRG4 /' SECONDARY CHARGE = '/ ,
C          &          STRG5 /' TRANSITION TYPE = '/ ,
C          &          STRG6 /'

```



```

-----
C      INTEGER    PIPEIN    , PIPEOU , ONE    , ZERO
C      PARAMETER( PIPEIN=5 , PIPEOU=6 , ONE=1 , ZERO=0 )
-----

```

# C2SPLN

```

SUBROUTINE C2SPLN( NEDIM ,
&                IEA    , IEVAL  ,
&                TEEA   , EEVA   ,
&                SCX    , SCXA   ,
&                LERNG  )
&
IMPLICIT NONE
-----
C
C ***** FORTRAN77 SUBROUTINE: C2SPLN *****
C
C PURPOSE:
C PERFORMS CUBIC SPLINE ON LOG(ENERGY <EV/AMU> ) VERSUS
C LOG(CX CROSS-SECTION <CM2>).
C INPUT DATA FOR A GIVEN DONOR/RECEIVER COMBINATION DATA-BLOCK.
C
C USING ONE-WAY SPLINES IT CALCULATES THE CROSS-SECTIONS
C FOR 'IEVAL' COLLISION ENERGIES VALUES FROM
C THE LIST OF COLLISION ENERGIES READ IN FROM THE INPUT FILE
C
C IF A VALUE CANNOT BE INTERPOLATED USING SPLINES IT IS
C EXTRAPOLATED VIA 'XXSPLE'. (SEE NOTES BELOW).
C
C CALLING PROGRAM: ADAS302/SSIA
C
C SUBROUTINE:
C
C INPUT : (I*4) IEA    = INPUT DATA FILE: NUMBER OF COLLISION ENER-
C                   GIES READ FOR THE DATA-BLOCK BEING ASSESSED
C INPUT : (I*4) IEVAL  = NUMBER OF ISPF ENTERED COLLISION ENERGIES
C                   VALUES FOR WHICH CX CROSS-SECTIONS
C                   ARE REQUIRED FOR TABULAR/GRAPHICAL OUTPUT.
C
C INPUT : (R*8) TEEA() = INPUT DATA FILE: COLLISION ENERGIES (EV/AMU)
C                   FOR THE DATA-BLOCK BEING ASSESSED.
C                   DIMENSION: COLLISION ENERGY INDEX
C INPUT : (R*8) EEVA() = USER ENTERED: COLLISION ENERGIES (EV/AMU)
C                   DIMENSION: COLLISION ENERGY INDEX
C
C INPUT : (R*8) SCX()  =INPUT DATA FILE: FULL SET OF CX CROSS-
C                   SECTIONS FOR THE DATA-BLOCK BEING ANALYSED
C                   1ST DIMENSION: COLLISION ENERGY INDEX
C OUTPUT: (R*8) SCXA() = SPLINE INTERPOLATED OR EXTRAPOLATED
C                   CX CROSS-SECTIONS FOR
C                   THE USER ENTERED COLLISION ENERGIES.
C                   DIMENSION: COLLISION ENERGIES INDEX
C
C OUTPUT: (I*4) LERNG()= .TRUE.  => OUTPUT 'SCXA()' VALUE WAS INTER-
C                   POLATED FOR THE USER ENTERED
C                   COLLISION ENERGY 'EEVA()'.
C                   .FALSE. => OUTPUT 'SCXA()' VALUE WAS EXTRA-
C                   POLATED FOR THE USER ENTERED
C                   COLLISION ENERGY 'EEVA()'.
C                   DIMENSION: COLLISION ENERGY INDEX
C
C (I*4) NIN    = PARAMETER = MAX. NO. OF INPUT ENERGY
C                   VALUES. MUST BE >= 'IEA'
C (I*4) NOUT   = PARAMETER = MAX. NO. OF OUTPUT ENERGY
C                   VALUES. MUST BE >= 'IEVAL'
C (I*4) L1     = PARAMETER = 1
C
C (I*4) IET    = ARRAY SUBSCRIPT USED INPUT FILE COLLISION
C                   ENERGIES.
C (I*4) IT     = ARRAY SUBSCRIPT USED FOR USER ENTERED
C                   COLLISION ENERGIES.
C (I*4) IOPT   = DEFINES THE BOUNDARY DERIVATIVES FOR THE
C                   SPLINE ROUTINE 'XXSPLE', SEE 'XXSPLE'.
C                   (VALID VALUES = <0, 0, 1, 2, 3, 4)
C
C (L*4) LSETX  = .TRUE.  => SET UP SPLINE PARAMETERS RELATING
C                   TO 'XIN' AXIS.
C                   .FALSE. => DO NOT SET UP SPLINE PARAMETERS
C                   RELATING TO 'XIN' AXIS.
C                   (I.E. THEY WERE SET IN A PREVIOUS
C                   CALL )
C                   (VALUE SET TO .FALSE. BY 'XXSPLE')
C
C (R*8) R8FUN1 = FUNCTION - (SEE ROUTINES SECTION BELOW)
C
C (R*8) XIN()  = LOG( DATA FILE COLLISION ENERGIES )
C (R*8) YIN()  = LOG( DATA FILE CX CROSS-SECTIONS)
C (R*8) XOUT() = LOG( USER ENTERED COLLISION ENERGIES.)
C (R*8) YOUT() = LOG( OUTPUT GENERATED CX CROSS-SECTIONS)
C (R*8) DF()   = SPLINE INTERPOLATED DERIVATIVES

```

```

C
C
C NOTE:
C
C ONE-DIMENSIONAL SPLINE CARRIED OUT BY THIS SUBROUTINE:
C
C LOG( SCX ) vs. LOG( E )
C
C E = COLLISION ENERGY (units: eV/AMU)
C SCX = CX CROSS-SECTION (units: cm**2)
C
C Extrapolation criteria:
C
C Low E: zero gradient extrapolation (i.e. DY(1) = 0.0)
C High E: zero curvature extrapolation (i.e. DDY(N) = 0.0)
C
C (These criteria are met by calling XXSPLE with IOPT=4)
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C XXSPLE ADAS SPLINE SUBROUTINE (EXTENDED DIAGNOSTICS)
C R8FUN1 ADAS REAL*8 FUNCTION: ( X -> X )
C
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL. 0141-553-4196
C
C DATE: 16/11/95
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1 DATE: 19-11-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C - PUT UNDER S.C.C.S. CONTROL
C
C -----
C
C INTEGER NIN , NOUT , L1
C
C REAL*8 ZERO
C
C PARAMETER( NIN = 24 , NOUT = 24 , L1 = 1 )
C PARAMETER( ZERO = 1.0D-30 )
C
C INTEGER NEDIM , IEA , IEVAL
C INTEGER IET , IT , IOPT
C
C REAL*8 R8FUN1
C
C LOGICAL LSETX
C
C REAL*8 TEEA(NEDIM) , EEVA(IEVAL) ,
C & SCX(NEDIM) , SCXA(IEVAL)
C REAL*8 DF(NIN) ,
C & XIN(NIN) , YIN(NIN) ,
C & XOUT(NOUT) , YOUT(NOUT)
C
C LOGICAL LERNG(IEVAL)
C
C EXTERNAL R8FUN1
C
C -----

```

## C2TITL

```

SUBROUTINE C2TITL( IBSEL , DSFULL ,
& CPRIMARY , CSECDY ,
& CTYPE ,
& TITLX
& )
IMPLICIT NONE
C
C -----
C ***** FORTRAN77 SUBROUTINE: C2TITL *****
C
C PURPOSE: TO CREATE THE DESCRIPTIVE TITLE FOR SELECTED DATA-BLOCK.
C
C CALLING PROGRAM: ADAS302/SSIA
C
C SUBROUTINE:
C
C INPUT : (I*4) IBSEL = SELECTED DATA-BLOCK: INDEX
C INPUT : (C*80) DSFULL = FULL MVS INPUT DATA SET NAME
C
C INPUT : (C*5) CPRIMARY = SELECTED DATA-BLOCK: PRIMARY SPECIES
C IDENTIFICATION.
C INPUT : (C*5) CSECDY = SELECTED DATA-BLOCK: SECONDARY SPECIES
C IDENTIFICATION.
C
C INPUT : (C*3) CTYPE = SELECTED DATA-BLOCK: CROSS. SECT. TYPE
C
C

```

```

C OUTPUT: (C*120) TITLX = SELECTED DATA-BLOCK: DESCRIPTIVE TITLE
C
C (C*2) C2 = GENERAL USE 2 BYTE CHARACTER STRING
C (I*4) POS_NOW = CURRENT POSITION IN TITLE STRING
C (I*4) LEN_NAME = LENGTH OF FILENAME
C (I*4) IFIRST = POSITION OF FIRST CHARACTER IN FILENAME
C (I*4) ILAST = POSITION OF LAST CHARACTER IN FILENAME
C
C ROUTINES:
C XXSLEN = UTILITY ROUTINE WHICH FINDS FIRST AND LAST
C NON-BLANK CHARACTERS IN A STRING.
C
C AUTHOR: H. P. SUMMERS
C JA8.08
C TEL. 0141-553-4196
C
C DATE: 12/11/96
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1 DATE: 19-11-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C - PUT UNDER S.C.C.S. CONTROL
C
C-----
C
C INTEGER IBSEL
C INTEGER POS_NOW , LEN_NAME
C INTEGER IFIRST , ILAST
C-----
C CHARACTER DSFULL*80 ,
C & CPRIMARY*5 , CSECDY*5
C & CTYPE*3 , TITLX*120
C CHARACTER C2*2
C-----

```

## C2VRDC

```

SUBROUTINE C2VRDC( ICIND ,
& NBSEL ,
& CDONOR , CRECVR , CFSTAT , CTYPE ,
& SCI ,
& SDONOR , SRECVR , SFSTAT , STYPE
& )
IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C2VRDC *****
C
C PURPOSE: TO SETUP DONOR/RECVR CHARACTER STRINGS FOR USE WITH SETTING
C ISPF VARIABLES WHEN SELECTED CROSS-SECTIONS ARE DISPLAYED.
C
C CALLING PROGRAM: C2PAN2
C
C SUBROUTINE:
C
C INPUT : (I*4) ICIND = SELECTED/REQUESTED CROSS-SECTION DATA-BLOCK
C INDEX.
C
C INPUT : (I*4) NBSEL = NUMBER OF DATA-BLOCK CROSS-SECTIONS.
C
C INPUT : (C*9) CDONOR() = INPUT DATA FILE: DONOR ION IDENTIFICATION
C DIMENSION: DATA-BLOCK INDEX
C INPUT : (C*9) CRECVR() = INPUT DATA FILE: RECEIVER ION IDENTIFICATION
C DIMENSION: DATA-BLOCK INDEX
C INPUT : (C*10) CFSTAT() = INPUT DATA FILE: FINAL STATE SPECIFICATION
C DIMENSION: DATA-BLOCK INDEX
C INPUT : (C*2) CTYPE() = INPUT DATA FILE: CROSS-SECTION TYPE
C DIMENSION: DATA-BLOCK INDEX
C DIMENSION: DATA-BLOCK INDEX
C
C OUTPUT: (C*3) SCI = ISPF PANEL VARIABLE: DATA-BLOCK INDEX
C
C OUTPUT: (C*9) SDONOR = ISPF PANEL VARIABLE: DONOR ION IDENTIFICATION
C OUTPUT: (C*9) SRECVR = ISPF PANEL VARIABLE: RECEIVER ION IDENTIFICATION
C OUTPUT: (C*10) SFSTAT = ISPF PANEL VARIABLE: FINAL STATE SPECIFICATION
C OUTPUT: (C*2) STYPE = ISPF PANEL VARIABLE: CROSS-SECTION TYPE
C
C ROUTINES: NONE
C
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL. 0141-553-4196
C
C DATE: 15/11/95
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1 DATE: 19-11-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C - PUT UNDER S.C.C.S. CONTROL
C

```



```

C      (C*2) CEQUAL = PARAMETER = 'EQ'
C
C      (I*4) I4EIZ0 = FUNCTION - (SEE ROUTINES SECTION BELOW)
C      (I*4) I4FCTN = FUNCTION - (SEE ROUTINES SECTION BELOW)
C      (I*4) I4UNIT = FUNCTION - (SEE ROUTINE SECTION BELOW)
C      (I*4) IBLK  = ARRAY INDEX: DATA-BLOCK INDEX
C      (I*4) ITR   = ARRAY INDEX: SECONDARY TEMPERATURE INDEX
C      (I*4) ITD   = ARRAY INDEX: PRIMARY TEMPERATURE INDEX
C      (I*4) NTRNUM = NUMBER OF SECONDARY TEMPERATURES FOR CURRENT
C                      DATA-BLOCK
C      (I*4) NTDNUM = NUMBER OF PRIMARY TEMPERATURES FOR CURRENT
C                      DATA-BLOCK
C      (I*4) IABT  = RETURN CODE FROM 'I4FCTN'
C
C      (C*10) IONNAM = READ - PRIMARY SPECIES DESIGNATION STRING
C      (C*80) C80   = GENERAL USE 80 BYTE CHARACTER STRING FOR
C                      THE INPUT OF DATA-SET RECORDS.
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      I4UNIT      ADAS        INTEGER*4 FUNCTION -
C                      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C AUTHOR:  H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C          JA8.08
C          TEL. 0141-553-4196
C
C DATE:    18/11/96
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1                      DATE: 19-11-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C           - PUT UNDER S.C.C.S. CONTROL
C
C -----
C      INTEGER      I4UNIT
C      INTEGER      IUNIT          , NSTORE
C      &            NTDIM          , NBSEL
C      INTEGER      IBLK          , IT
C      &            ITR           , ITD
C
C -----
C      CHARACTER   UID*6          , DATE*8
C      CHARACTER   CEQUAL*10
C
C -----
C      INTEGER      ISELA(NSTORE)
C      &            ITA(NSTORE)
C
C -----
C      REAL*8      AMRA(NSTORE)   , AMDA(NSTORE)
C      REAL*8      TPA(NTDIM,NSTORE)
C      &            QFTEQA(NTDIM,NSTORE)
C      REAL*8      QFTIAA(NTDIM,NTDIM,NSTORE)
C
C -----
C      CHARACTER   DSFLLA(NSTORE)*80
C      CHARACTER   CPRMYA(NSTORE)*5 , CSCDYA(NSTORE)*5
C      &            CTYPEPA(NSTORE)*3
C
C -----
C      DATA      CEQUAL/' *EQUAL**'/
C -----

```

## C3ALRS

```

      SUBROUTINE C3ALRS( IORD , EM1 , EM2 ,
&                      EPRO , TTAR , ETHR ,
&                      YA , N , NS ,
&                      OA , SQEF
&                      )
      IMPLICIT NONE
C -----
C *****
C ***** FORTRAN77 SUBROUTINE : C3ALRS *****
C
C PURPOSE:  COMPUTES ALPHAS AND REDUCED SPEEDS. RETURNS AN EFFECTIVE
C           CHARGE-EXCHANGE RATE COEFFICIENT
C
C CALLING PROGRAM: SQEF
C
C SUBROUTINE:
C
C INPUT : (I*4) IORD = 1 FOR 1ST PARTICLE INCIDENT AND MONOENERGETIC
C           = 2 FOR 2ND PARTICLE INCIDENT AND MONOENERGETIC
C INPUT : (I*4) ISEL = SELECTOR FOR PARTICULAR RATE COEFFT.
C           CHOSEN FROM TABLE
C INPUT : (R*8) EM1  = ATOMIC MASS NUMBER FOR 1ST PARTICLE
C INPUT : (R*8) EM2  = ATOMIC MASS NUMBER FOR 2ND PARTICLE
C INPUT : (R*8) EPRO = INCIDENT PARTICLE ENERGY (EV/AMU)
C INPUT : (R*8) TTAR = MAXWELL TEMPERATURE OF TARGET PARTICLES (EV)
C INPUT : (R*8) ETHR = THRESHOLD ENERGY
C INPUT : (R*8) ZSEL = NUCLEAR CHARGE (REQUIRED ONLY
C           FOR PARTICULAR ISEL)
C INPUT : (I*4) NSEL = PRINC. QUANTUM NO. (REQUIRED ONLY

```

```

C                                     FOR PARTICULAR ISEL
C                                     NB. NSEL SHOULD BE ZERO ON ENTRY OTHERWISE)
C INPUT : (I*4)  N      = NUMBER OF SOURCE DATA VALUES
C
C OUTPUT: (R*8)  SQEF  = RATE COEFFICIENT (CM3 SEC-1)
C OUTPUT: (R*8)  OA()  = RATE COEFFTS.(CM**3 SEC-1) FOR SELECTED
C                                     SOURCE DATA
C OUTPUT: (R*8)  EA()  = SET OF ENERGIES (EV/AMU) FOR
C                                     SELECTED SOURCE DATA
C I/O   : (R*8)  YA()  = ENERGIES ON INPUT, SPEEDS ON OUTPUT
C
C (I*4)  ISWIT = ENERGY RANGE SWITCHING INDEX
C (I*4)  I      = GENERAL INDEX
C (I*4)  K      = GENERAL INDEX
C
C (R*8)  ABI    = FUNCTION - SEE BELOW
C (R*8)  EMT    = SELECTED MASS
C (R*8)  F      = GENERAL VARIABLE
C (R*8)  SUM    = GENERAL VARIABLE
C (R*8)  SXI    = GENERAL VARIABLE
C (R*8)  SXXI   = GENERAL VARIABLE
C (R*8)  U      = GENERAL VARIABLE
C (R*8)  V      = GENERAL VARIABLE
C (R*8)  VTHR   = THRESHOLD SPEED
C (R*8)  X      = GENERAL VARIABLE
C (R*8)  XI     = GENERAL VARIABLE
C (R*8)  XRMIN  = GENERAL VARIABLE
C (R*8)  XXI    = GENERAL VARIABLE
C (R*8)  XA()   = GAUSS-LAGUERRE NODES (9-POINT)
C (R*8)  WXA()  = GAUSS-LAGUERRE WEIGHTS (9-POINT)
C
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C -----
C      ABI          ADAS        COMPUTES INTEGRAL FOR RATE COEFFICIENT
C
C AUTHOR:  C J. WHITEHEAD, PAP, UNIVERSITY OF STRATHCLYDE
C          EXT 4205
C
C DATE:    14/11/94
C
C UPDATE:  09/12/94 - HP SUMMERS: ADJUST FORMATTING
C
C UPDATE:  03/05/95 - PE BRIDEN : ADD DATA DECLARATION FOR F AND EMT.
C                                     (STOPS COMPILATION WARNING OF
C                                     UNINITIALISED VARIABLES.)
C
C UPDATE:  15/05/95 - TIM HAMMOND: UNIX PORT - PUT INTO SCCS
C
C -----
C      INTEGER IORD , N , ISWIT , K , NS , I
C -----
C      REAL*8  EM1 , EM2 , EPRO , TTAR , ETHR ,
C      &      EMT , U , V , VTHR , ABI
C      REAL*8  XI , X , XRMIN , SUM , SXI , F , XXI ,
C      &      SQEF , SXXI
C -----
C      REAL*8  XA(9) , WXA(9)
C      REAL*8  YA(24) , FA(24) , OA(24)
C -----
C      GAUSS-LAGUERRE DATA (9PT)
C -----
C      DATA F / 0.0 / ,
C      &      EMT/ 0.0 / ,
C      DATA XA / 0.1523222277D0 , 0.8072200227D0 , 2.0051351556D0 ,
C      &      3.7834739733D0 , 6.2049567778D0 , 9.3729852516D0 ,
C      &      13.4662369110D0 , 18.8335977889D0 , 26.3740718909D0 /
C      DATA WXA/ 3.36126421798D-1 , 4.11213980424D-1 , 1.99287525371D-1 ,
C      &      4.74605627657D-2 , 5.59962661079D-3 , 3.05249767093D-4 ,
C      &      6.59212302608D-6 , 4.11076933035D-8 , 3.29087403035D-11/
C -----

```

## C3CORR

```

C      SUBROUTINE C3CORR( NVALS , IBSEL ,
C      &      QATOM , ATOM ,
C      &      QEFREF , ATMREF ,
C      &      NSTORE , NA ,
C      &      RION , SCALED
C      &      )
C      IMPLICIT NONE
C -----
C      ***** FORTRAN77 SUBROUTINE: C3CORR *****
C
C PURPOSE: APPLY A CORRECTION TO REFERENCE RATE COEFFICIENT TO ALLOW
C          FOR VARIATION OF PLASMA PARAMETERS ALONG ONE-DIMENSIONAL
C          SCANS
C
C CALLING PROGRAM: SQEF
C

```

```

C SUBROUTINE:
C
C INPUT : (I*4) NVALS( ) = NUMBER OF VALUES IN SELECTED DATA BLOCK
C 1ST. DIM: NSTORE
C INPUT : (I*4) IBSEL = SELECTED BLOCK INDEX
C INPUT : (R*8) QATOM( , ) = EFFECT. RATE COEFFT. TO SCALE WITH PARAM.
C 1ST. DIM: NA
C 2ND. DIM: NSTORE
C INPUT : (R*8) ATOM( , ) = PLASMA PARAM. VALUES TO BASE SCALING ON
C 1ST. DIM: NA
C 2ND. DIM: NSTORE
C INPUT : (R*8) QEFREF( ) = RATE COEFFICIENT REFERENCE VALUES
C 1ST. DIM: NSTORE
C INPUT : (R*8) ATMREF( ) = REFERENCE VALUES FOR PLASMA PARAM.
C 1ST. DIM: NSTORE
C INPUT : (R*8) RION = SPECIFIED PARM. VALUE FOR COEFFT. OUTPUT
C INPUT : (I*4) NSTORE = NUMBER OF DATA BLOCKS IN DATASET.
C INPUT : (I*4) NA = MAX. NO. OF PARAM. VALUES IN BLOCK
C
C OUTPUT: (R*8) SCALED = SCALED PLASMA PARAMETER
C
C PARAM : (I*4) MXIN = MAX. NO. OF INPUT DATA SET VALUES
C
C (I*4) MAXVAL = NUMBER OF DATA VALUES IN SELECTED SET
C (I*4) IOPT = DEFINES THE BOUNDARY DERIVATIVES FOR THE
C SPLINE ROUTINE 'XXSPLE'. SEE 'XXSPLE'.
C ( VALID VALUES = <0, 0, 1, 2, 3, 4 )
C (I*4) J = LOOP INDEX.
C
C (L*4) LSETX = FLAGS TO SPLINE ROUTINE 'XXSPLN' IF
C SPLINE PARAMETERS SHOULD BE SET UP.
C .TRUE. => SET UP SPLINE PARAMS.
C .FALSE. => DO NOT SET UP SPLINE PARAMS.
C
C (L*4) LINTRP = FLAGS TO IDENTIFY IF SCALED VALUE INTER-
C POLATED. (OUTPUT FROM XXSPLE).
C .TRUE. => SCALED VALUE INTERPOLATED
C .FALSE. => SCALED VALUE EXTRAPOLATED.
C
C (R*8) VL( ) = LN(INPUT VALUE/REF. VALUE) FOR PARAM.
C DIMENSION: 1
C (R*8) QVL( ) = LN(INPUT TABLE RATE COEF.) FOR PARAM.
C DIMENSION: 1
C (R*8) VECL( ) = LN(TABLE VALUE/REF. VALUE) FOR PARAM.
C DIMENSION: MXIN
C (R*8) QVECL( ) = LN(TABLE RATE COEF./REF. RATE COEF.)
C DIMENSION: MXIN
C (R*8) DY( ) = DERIVATIVES AT INPUT KNOTS TO XXSPLN.
C DIMENSION: MXIN
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C XXSPLE ADAS SPLINE SUBROUTINE (EXTENDED DIAGNOSTICS)
C R8FUN1 ADAS PERFORMS TRANSFORMATION ( X -> X )
C
C NOTES: THE QUANTITIES WHICH ARE SCALED BY THIS ROUTINE ARE : ION
C DENSITY, ION TEMPERATURE, EFFECTIVE Z AND MAGNETIC
C FIELD THIS CODE IS TAKEN FROM THE OLDER ADAS CODE
C 'QEFFH.FOR' BY H.P. SUMMERS
C
C AUTHOR: C.J. WHITEHEAD, PAP, UNIVERSITY OF STRATHCLYDE
C EXT 4205
C
C DATE: 24/11/94
C
C UPDATE: 19/12/94 - HP SUMMERS: ADJUST FORMATTING
C
C UPDATE: 21/04/95 - HP SUMMERS: REORDER TWO-DIMENSIONAL ARRAY INDICES
C
C UPDATE: 03/05/95 - PE BRIDEN : 1) REPLACED CALLS TO SPLINE NAG
C ROUTINES E01BAF/E02BBF WITH A
C CALL TO XXSPLE. (REQUIRED SOME
C RECODING). + CHECK FOR ATTEMPTED
C EXTRAPOLATION.
C 2) MADE CHANGES TO CODE TO MAKE IT
C ANSI STANDARD FORTRAN 77.
C 3) TIDIED UP CODE + ADDED CHECK TO
C MAKE SURE INTERNAL ARRAYS ARE
C LARGE ENOUGH.
C 4) GENERAL CHANGES TO FORMAT ETC.
C
C UPDATE: 15/05/95 - Tim Hammond: UNIX PORT
C Put under SCCS control
C
C -----
C
C INTEGER MXIN
C REAL*8 R8FUN1
C
C PARAMETER( MXIN = 24 )
C EXTERNAL R8FUN1
C
C -----
C
C INTEGER I4UNIT
C INTEGER IBSEL , NSTORE , NA

```

```

C-----
C      REAL*8      RION              , SCALED
C-----
C      INTEGER     NVALS(NSTORE)
C-----
C      REAL*8      QEFREF(NSTORE)   , ATMREF(NSTORE)   ,
&      QATOM(NA,NSTORE)   , ATOM(NA,NSTORE)
C-----
C
C-----
C      INTEGER     MAXVAL            , IOPT              , J
C-----
C      LOGICAL     LSETX             , LINTRP(1)
C-----
C      REAL*8      VL(1)             , QVL(1)         ,
&      VECL(MXIN)   , QVECL(MXIN)   ,
&      DY(MXIN)
C-----

```

## C3DATA

```

SUBROUTINE C3DATA( IUNIT , DSNAME ,
&                NSTORE ,
&                NBSEL , ISELA ,
&                CWAVEL , CDONOR , CRECVR ,
&                CFILE , CPCODE , CINDM ,
&                QEFREF ,
&                ENREF , TEREf , DEREf , ZEREf , BMREF ,
&                NENERA , NTEMPA , NDENSA , NZEFFA , NBMAGA ,
&                ENERA , TEMPA , DENSA , ZEFFA , BMAGA ,
&                QENERA , QTEMPA , QDENSA , QZEFFA , QBMAGA
&                )
IMPLICIT NONE
C-----
C
C ***** FORTRAN77 SUBROUTINE: C3DATA *****
C
C PURPOSE : TO FETCH DATA FROM INPUT QEF DATA SET.
C
C CALLING PROGRAM: ADAS303, SQEF
C
C SUBROUTINE:
C
C INPUT : (I*4) IUNIT = UNIT NUMBER TO READ FROM
C INPUT : (C*80) DSNAME = MVS DATA SET NAME OF DATA SET BEING READ
C INPUT : (I*4) NSTORE = MAXIMUM NUMBER OF DATA BLOCKS ALLOWED
C
C OUTPUT: (I*4) NBSEL = NUMBER OF BLOCKS PRESENT
C OUTPUT: (I*4) ISELA() = INDEX NUMBER OF DATA BLOCK
C
C OUTPUT: (C*5) CWAVEL()= INPUT DATA FILE: TRANSITION
C DIMENSION: DATA-BLOCK INDEX
C OUTPUT: (C*8) CDONOR()= INPUT DATA FILE: DONOR NEUTRAL ATOM
C DIMENSION: DATA-BLOCK INDEX
C OUTPUT: (C*5) CRECVR()= INPUT DATA FILE: RECEIVER NUCLEUS
C DIMENSION: DATA-BLOCK INDEX
C OUTPUT: (C*8) CFILE() = INPUT DATA FILE: SPECIFIC ION FILE SOURCE
C DIMENSION: DATA-BLOCK INDEX
C OUTPUT: (C*8) CPCODE()= INPUT DATA FILE: PROCESSING CODE
C DIMENSION: DATA-BLOCK INDEX
C OUTPUT: (C*6) CINDM() = FILE DATA FILE: EMISSION TYPE
C DIMENSION: DATA-BLOCK INDEX
C
C OUTPUT: (R*8) QEFREF() = REFERENCE VALUE OF RATE COEFFICIENT
C OUTPUT: (R*8) ENREF() = " " " ENERGY
C OUTPUT: (R*8) TEREf() = " " " TEMPERATURE
C OUTPUT: (R*8) DEREf() = " " " DENSITY
C OUTPUT: (R*8) ZEREf() = " " " EFFECTIVE Z
C OUTPUT: (R*8) BMREF() = " " " MAGNETIC FIELD
C OUTPUT: (I*4) NENERA() = NUMBER OF ENERGIES
C OUTPUT: (I*4) NTEMPA() = NUMBER OF TEMPERATURES
C OUTPUT: (I*4) NDENSA() = NUMBER OF DENSITIES
C OUTPUT: (I*4) NZEFFA() = NUMBER OF EFFECTIVE Z'S
C OUTPUT: (I*4) NBMAGA() = NUMBER OF MAGNETIC FIELD VALUES
C 1ST. DIM: NSTORE
C (FOR ABOVE ARRAYS)
C
C OUTPUT: (R*8) ENERA(,) = ENERGIES
C OUTPUT: (R*8) QENERA(,) = RATE COEFFICIENTS FOR ENERGY VALUE
C OUTPUT: (R*8) TEMPA(,) = TEMPERATURES
C OUTPUT: (R*8) QTEMPA(,) = RATE COEFFICIENTS FOR TEMPERATURES
C OUTPUT: (R*8) DENSA(,) = DENSITIES
C OUTPUT: (R*8) QDENSA(,) = RATE COEFFICIENTS FOR DESNITIES
C OUTPUT: (R*8) ZEFFA(,) = EFFECTIVE Z
C OUTPUT: (R*8) QZEFFA(,) = RATE COEFFICIENTS FOR EFFECTIVE Z
C OUTPUT: (R*8) BMAGA(,) = MAGNETIC FIELD
C OUTPUT: (R*8) QBMAGA(,) = RATE COEFFICIENTS FOR MAGNETIC FIELDS
C 1ST DIM: 12 OR 24 DEPENDING ON PARAMETER
C 2ND DIM: NSTORE
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C-----

```



```

C          I4UNIT      ADAS      FETCHES FILE HANDLE FOR ERROR MESSAGE
C
C  AUTHOR:  H P SUMMERS, UNIVERSITY OF STRATHCLDYE
C          JA 8.08
C          TEL. 0141-553-4196
C
C  DATE:    19/04/95
C
C  UPDATE:  04/05/95 TIM HAMMOND - UNIX PORT
C                                     Increased DSNAME from 44 -> 80
C
C  UPDATE:  15/05/95 TIM HAMMOND - UNIX PORT
C                                     Changed delimiter character from
C                                     '\' to '!' as otherwise will not
C                                     compile.
C
C-----
C          INTEGER IUNIT , ISTORE , NSTORE , NBSEL , J
C          INTEGER I4UNIT
C-----
C          CHARACTER DSNAME*80          , STRING*80
C          CHARACTER CINDM(NSTORE)*6    , CFILE(NSTORE)*8
C          &          CPCODE(NSTORE)*8   , CWAVEL(NSTORE)*5
C          &          CDONOR(NSTORE)*8   , CRECVR(NSTORE)*5
C-----
C          INTEGER ISELA(NSTORE)
C          INTEGER NENERA(NSTORE), NTEMPA(NSTORE), NDENSA(NSTORE)
C          INTEGER NZEFFA(NSTORE), NBMAGA(NSTORE)
C-----
C          REAL*8 QEFREF(NSTORE)
C          REAL*8 ENREF(NSTORE) , TEREf(NSTORE)
C          REAL*8 DEREf(NSTORE) , ZEREf(NSTORE)
C          REAL*8 BMREF(NSTORE)
C          REAL*8 ENERA(24,NSTORE), QENERA(24,NSTORE)
C          REAL*8 TEMPA(12,NSTORE), QTEMPA(12,NSTORE)
C          REAL*8 DENSA(24,NSTORE), QDENSA(24,NSTORE)
C          REAL*8 ZEFFA(12,NSTORE), QZEFFA(12,NSTORE)
C          REAL*8 BMAGA(12,NSTORE), QBMAGA(12,NSTORE)
C-----
C          EXTERNAL I4UNIT
C-----

```

## C3DATAO

```

SUBROUTINE C3DATAO( IUNIT , IBSEL ,
&                  NBSEL , NSTORE ,
&                  IPASS ,
&                  IONNAM , QEFREF ,
&                  TEREf , DEREf ,
&                  ZEREf , ENREF ,
&                  BMREF , NENERA ,
&                  NDENSA , NZEFFA ,
&                  NBMAGA , NTEMPA ,
&                  ENERA , QENERA ,
&                  TEMPA , QTEMPA ,
&                  DENSA , QDENSA ,
&                  ZEFFA , QZEFFA ,
&                  BMAGA , QBMAGA )
IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C3DATAO *****
C *****
C * WARNING - WARNING - WARNING - WARNING - WARNING - WARNING - WARNING*
C *-----*
C * OLD VERSION OF C3DATA - ONLY USED BY SQEF (UNTIL SQEF UPDATED) *
C *****
C
C PURPOSE : READ IN VALUES FROM AN 'IONATOM' DATA SET OPENED BY
C          C3FILE
C
C CALLING PROGRAM: SQEF
C
C SUBROUTINE:
C
C INPUT : (I*4) IUNIT      = UNIT NUMBER TO READ FROM
C                                     (OPENED BY C3FILE)
C INPUT : (I*4) NSTORE     = ARRAY DIMENSION
C INPUT : (I*4) ISEL      = INDEX NUMBER OF SELECTED BLOCK
C                                     FROM IONATOM FILE
C INPUT : (I*4) IPASS      = 0 IF DATA FILE TO BE READ IN AFRESH
C                                     = 1 IF DATA FILE IS NOT TO BE READ IN AGAIN
C                                     (IPASS IS SET TO 0 WHEN
C                                     ISEL IS NOT A VALID INDEX)
C OUTPUT: (I*4) NBSEL     = NUMBER OF BLOCKS PRESENT
C OUTPUT: (C*80) IONNAM   = NAME OF ION
C
C OUTPUT: (R*8) QEFREF()  = REFERENCE VALUE OF RATE COEFFICIENT
C OUTPUT: (R*8) ENREF()   = " " " " ENERGY
C OUTPUT: (R*8) TEREf()   = " " " " TEMPERATURE
C OUTPUT: (R*8) DEREf()   = " " " " DENSITY

```

```

C OUTPUT: (R*8) ZEREF() = " " " EFFECTIVE Z
C OUTPUT: (R*8) BMREF() = " " " MAGNETIC FIELD
C OUTPUT: (I*4) NENERA() = NUMBER OF ENERGIES
C OUTPUT: (I*4) NTEMPA() = NUMBER OF TEMPERATURES
C OUTPUT: (I*4) NDENSA() = NUMBER OF DENSITIES
C OUTPUT: (I*4) NZEFFA() = NUMBER OF EFFECTIVE Z'S
C OUTPUT: (I*4) NBMAGA() = NUMBER OF MAGNETIC FIELD VALUES
C
C 1ST. DIM: NSTORE
C (FOR ABOVE ARRAYS)
C OUTPUT: (R*8) ENERA(,) = ENERGIES
C OUTPUT: (R*8) QENERA(,) = RATE COEFFICIENTS FOR ENERGY VALUE
C OUTPUT: (R*8) TEMPA(,) = TEMPERATURES
C OUTPUT: (R*8) QTEMPA(,) = RATE COEFFICIENTS FOR TEMPERATURES
C OUTPUT: (R*8) DENSA(,) = DENSITIES
C OUTPUT: (R*8) QDENSA(,) = RATE COEFFICIENTS FOR DENSNITIES
C OUTPUT: (R*8) ZEFFA(,) = EFFECTIVE Z
C OUTPUT: (R*8) QZEFFA(,) = RATE COEFFICIENTS FOR EFFECTIVE Z
C OUTPUT: (R*8) BMAGA(,) = MAGNETIC FIELD
C OUTPUT: (R*8) QBMAGA(,) = RATE COEFFICIENTS FOR MAGNETIC FIELDS
C
C 1ST DIM: NSTORE
C 2ND DIM: 12 OR 24 DEPENDING ON PARAMETER
C
C
C ROUTINES:
C
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS FETCHES FILE HANDLE FOR ERROR MESSAGE
C
C UPDATE: 15/05/95 - Tim Hammond UNIX PORT
C Put under SCCS control
C -----
C
C INTEGER IUNIT , ISTORE , NBSEL , J ,
C & IBSEL , NSTORE , IPASS
C INTEGER I4UNIT
C -----
C CHARACTER STRING*80
C CHARACTER IONNAM*80(80)
C -----
C INTEGER NENERA(NSTORE) , NTEMPA(NSTORE) , NDENSA(NSTORE)
C INTEGER NZEFFA(NSTORE) , NBMAGA(NSTORE)
C -----
C REAL*8 QEFREF(NSTORE)
C REAL*8 ENREF(NSTORE) , TEREFF(NSTORE)
C REAL*8 DEREFF(NSTORE) , ZEREF(NSTORE)
C REAL*8 BMREF(NSTORE)
C REAL*8 ENERA(NSTORE,24) , QENERA(NSTORE,24)
C REAL*8 TEMPA(NSTORE,12) , QTEMPA(NSTORE,12)
C REAL*8 DENSA(NSTORE,24) , QDENSA(NSTORE,24)
C REAL*8 ZEFFA(NSTORE,12) , QZEFFA(NSTORE,12)
C REAL*8 BMAGA(NSTORE,12) , QBMAGA(NSTORE,12)
C -----
C EXTERNAL I4UNIT
C -----

```

## C3FILE

```

SUBROUTINE C3FILE(IUNIT, ATNAME, IRCODE, DSNAME)
IMPLICIT NONE
C -----
C ***** FORTRAN77 SUBROUTINE: C3FILE *****
C
C PURPOSE: TO OPEN AN 'IONATOM' DATA SET FOR ATOM 'ATNAME'
C CURRENTLY AVAILABLE ATOMS ARE : H, HE, LI
C
C
C DATA SET OPENED: 'JETUID.<GROUP>.<TYPE>'
C (<EXTENSION>#<ATOM SYMBOL>)'
C
C CALLING PROGRAM: SQEF
C
C SUBROUTINE:
C
C INPUT : (I*4) IUNIT = UNIT TO WHICH DATA SET WILL BE CONNECTED
C (C*2) ATNAME = NAME OF ATOM
C
C OUTPUT: (I*4) IRCODE = RETURN CODE FROM SUBROUTINE:
C 0 => DATA SET SUCCESSFULLY CONNECTED
C 1 => REQUESTED DATA SET MEMBER DOES NOT
C EXISTS - DATA SET NOT CONNECTED.
C 9 => REQUESTED DATA SET EXISTS BUT CANNOT
C BE OPENED.
C
C OUTPUT: (C*44) DSNAME = FULL MVS NAME OF OPENED DATA SET
C
C (I*4) LENF1 = FIRST NON-BLANK CHR OF 'DSNAME' GROUP PART
C (I*4) LENF2 = LAST NON-BLANK CHR OF 'DSNAME' GROUP PART
C (I*4) LENF3 = FIRST NON-BLANK CHR OF 'DSNAME' TYPE PART
C (I*4) LENF4 = LAST NON-BLANK CHR OF 'DSNAME' TYPE PART
C (I*4) LENF5 = FIRST NON-BLANK CHR OF 'DSNAME' EXT PART
C (I*4) LENF6 = LAST NON-BLANK CHR OF 'DSNAME' EXT PART
C (I*4) LENF7 = FIRST NON-BLANK CHR OF 'ATNAME'
C (I*4) LENF8 = LAST NON-BLANK CHR OF 'ATNAME'

```

```

C
C      (C*6)  USERID = ADAS SOURCE DATA USER ID
C      (C*8)  USRGRP  = ADAS SOURCE DATA GROUPNAME
C      (C*5)  USRTYP  = ADAS SOURCE DATA TYPENAME
C      (C*4)  USREXT  = ADAS SOURCE DATA EXTENSION
C
C      (L*4)  LEXIST  = .TRUE.  => REQUESTED DATA SET EXISTS.
C                      .FALSE. => REQUESTED DATA SET DOES NOT
C                      EXIST.
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      XXUID        ADAS        FETCHES/SETS ADAS SOURCE DATA USER ID
C      XXSQEF        ADAS        FETCHES/SETS ADAS SOURCE DATA FILENAME
C      XXSLEN        ADAS        OBTAINS FIRST AND LAST NON-BLANK
C                               CHARACTERS IN A STRING
C
C AUTHOR:  C.J. WHITEHEAD, STRATHCLYDE
C          EXT 4205
C          BASED ON CODE IN FIFILE.F
C
C DATE:    24/11/94
C
C UPDATE:  15/05/95 - Tim Hammond - UNIX PORT
C                               Added SCCS Header
C
C-----
C
C      INTEGER      IUNIT        , IRCODE        ,
C      &             LENF1        , LENF2          , LENF3          ,
C      &             LENF4        , LENF5          , LENF6          ,
C      &             LENF7        , LENF8
C-----
C      CHARACTER    USERID*6     , DSNAME*44     , ATNAME*2     ,
C      &            USRGRP*8     , USRTYP*5     , USREXT*4
C-----
C      LOGICAL      LEXIST
C-----

```

## C3OUT0

```

SUBROUTINE C3OUT0( IWRITE , LFSEL ,
&                TITLE , TITLX , TITLM , DATE ,
&                IBSEL , IEVAL ,
&                DIVAL , DEREf ,
&                TIVAL , TEREf ,
&                ZFVAL , ZEREf ,
&                BMVAL , BMREF ,
&                CWAVEL , CDONOR ,
&                CRECVR , CFILE ,
&                CPCODE , CINDM ,
&                LERNG ,
&                EAMU , EATM , ECMS ,
&                QEFA ,
&                KPLUS1 , COEF
&                )
IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C3OUT0 *****
C
C PURPOSE: TO PRINT DATA CONCERNING THE SELECTED TRANSITION DATA-
C          BLOCK UNDER ANALYSIS.
C
C CALLING PROGRAM: ADAS303
C
C SUBROUTINE:
C
C INPUT : (I*4) IWRITE = OUTPUT UNIT FOR RESULTS
C INPUT : (L*4) LFSEL  = .TRUE. => MINIMAX POLYNOMIAL FITTED.
C          .FALSE. => MINIMAX POLYNOMIAL NOT FITTED
C
C INPUT : (C*40) TITLE = TITLE OF RUN (READ FROM ISPF PANEL)
CX INPUT : (C*120) TITLX = INFORMATION STRING CONTAINING INPUT DATA-
C          SET NAME IN BYTES 1->35.
C INPUT : (C*80) TITLM = DIAGNOSTIC LINE INFORMATION FROM 'MINIMAX'
C INPUT : (C*8) DATE  = CURRENT DATE (AS 'DD/MM/YY')
C
C INPUT : (R*8) DIVAL = SELECTED OUTPUT VALUE: ION DENSITY (CM-3)
C INPUT : (R*8) DEREf = REFERENCE VALUE : ION DENSITY (CM-3)
C
C INPUT : (R*8) TIVAL = SELECTED OUTPUT VALUE: ION TEMPERATURE(EV)
C INPUT : (R*8) TEREf = REFERENCE VALUE : ION TEMPERATURE(EV)
C
C INPUT : (R*8) ZFVAL = SELECTED OUTPUT VALUE: Z-EFFECTIVE
C INPUT : (R*8) ZEREf = REFERENCE VALUE : Z-EFFECTIVE
C
C INPUT : (R*8) BMVAL = SELECTED OUTPUT VALUE: MAGNETIC FIELD (T)
C INPUT : (R*8) BMREF = REFERENCE VALUE : MAGNETIC FIELD (T)

```

```

C
C INPUT : (I*4) IBSEL = DATA-BLOCK INDEX SELECTED FROM INPUT DATASET
C FOR ANALYSIS.
C INPUT : (I*4) IEVAL = NUMBER OF USER ENTERED BEAM ENERGY VALUES
C
C INPUT : (C*5) CWAVEL = INPUT DATA FILE: TRANSITION
C INPUT : (C*8) CDONOR = INPUT DATA FILE: DONOR NEUTRAL ATOM
C INPUT : (C*5) CRECVR = INPUT DATA FILE: RECEIVER NUCLEUS
C INPUT : (C*8) CFILE = INPUT DATA FILE: SPECIFIC ION FILE SOURCE
C INPUT : (C*8) CPCODE = INPUT DATA FILE: PROCESSING CODE
C INPUT : (C*6) CINDM = FILE DATA FILE: EMISSION TYPE
C
C INPUT : (L*4) LERNG( ) = .TRUE. => OUTPUT 'QEFA()' VALUE WAS INTER-
C POLATED FOR THE USER ENTERED
C BEAM ENERGY 'EAMU()'.
C .FALSE. => OUTPUT 'QEFA()' VALUE WAS EXTRA-
C POLATED FOR THE USER ENTERED
C BEAM ENERGY 'EAMU()'.
C DIMENSION: BEAM ENERGY INDEX
C
C INPUT : (R*8) EAMU( ) = USER ENTERED: BEAM ENERGY (EV/AMU)
C DIMENSION: BEAM ENERGY INDEX
C INPUT : (R*8) EATM( ) = USER ENTERED: BEAM ENERGY (AT. UNITS)
C DIMENSION: BEAM ENERGY INDEX
C INPUT : (R*8) ECMS( ) = USER ENTERED: BEAM ENERGY (CM/SEC)
C DIMENSION: BEAM ENERGY INDEX
C
C INPUT : (R*8) QEFA( ) = SPLINE INTERPOLATED OR EXTRAPOLATED EFF.
C EMIS. COEFFTS. FOR THE USER ENTERED BEAM
C ENERGIES.
C DIMENSION: BEAM ENERGY INDEX
C
C INPUT : (I*4) KPLUS1 = NUMBER OF MINIMAX COEFFICIENTS
C INPUT : (R*8) COEF( ) = COEFFICIENTS OF FITTED MINIMAX POLYNOMIAL
C
C (I*4) I = GENERAL USE - ARRAY ELEMENT INDEX
C
C (C*1) C1E = '*' IF RATE-COEFFICIENT WAS EXTRAPOLATED FOR
C THE CURRENT BEAM ENERGY. (IT EQUALS
C ' ' IF IT WAS INTERPOLATED.)
C
C (C*80) CADAS = ADAS HEADER: INCLUDES RELEASE, PROGRAM, TIME
C (C*80) CSTRNG = MARKER TO USED TO FIND TITLE IN TITLX
C (I*4) IFIRST = FIRST POSITION OF MARKER CSTRNG IN TITLX
C (I*4) ILAST = LAST POSITION OF MARKER CSTRNG IN TITLX
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C XXADAS ADAS GATHERS ADAS HEADER INFORMATION
C
C AUTHOR : H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL. 0141-553-4196
C
C DATE: 23/04/95
C
C UPDATE: 03/05/95 PE BRIDEN - ADDED 1-D SCAN POSITIONS TABLE.
C - ADDED BEAM ENERGY COLUMN FOR CM/SEC.
C (REQD. UPDATE OF ARGUMENT LIST)
C + OTHER MINOR MODS.
C
C UNIX-IDL PORT:
C
C VERSION: 1.1 DATE: 15-05-95
C MODIFIED: TIM HAMMOND(TESSELLA SUPPORT SERVICES PLC)
C - FIRST VERSION
C
C VERSION: 1.2 DATE: 13-05-96
C MODIFIED: TIM HAMMOND
C - REMOVED HOLLERITH CONSTANTS FROM OUTPUT AND TIDIED UP
C HEADER
C
C -----
C INTEGER IWRITE , IBSEL , IEVAL ,
C & IZO , IZ , KPLUS1
C INTEGER I , IFIRST , ILAST
C
C -----
C LOGICAL LFSEL
C
C -----
C CHARACTER TITLE*(*) , TITLX*(*) , TITLM*(*) , DATE*8
C CHARACTER CINDM*6 , CFILE*8 ,
C & CPCODE*8 , CWAVEL*5 ,
C & CDONOR*8 , CRECVR*5
C CHARACTER C1E*1 ,
C & CADAS*80
C CHARACTER CSTRNG*80
C
C -----
C REAL*8 DIVAL , DEREf ,
C & TIVAL , TEREf ,
C & ZFVAL , ZEREf ,
C & BMVAL , BMREF
C
C -----
C REAL*8 EAMU(IEVAL) ,
C & EATM(IEVAL) ,
C & ECMS(IEVAL) ,
C & QEFA(IEVAL) ,
C & COEF(KPLUS1)
C
C -----
C LOGICAL LERNG(IEVAL)

```

```

-----
C          SAVE          CADAS
-----
C          DATA        CADAS /' '/ CSTRNG/'BLK'/
-----

```

## C3OUTG

```

SUBROUTINE C3OUTG( LGHOST ,
& TITLE , TITLX , TITLM , DATE ,
& DIVAL , DEREf ,
& TIVAL , TEREf ,
& ZFVAL , ZEREf ,
& BMVAL , BMREF ,
& CWAVEL , CDONOR ,
& CRECVR , CFILE ,
& CPCODE , CINDM ,
& EAMU , QEFA , IEVAL ,
& EFITM , QEFM , NMx ,
& LGRD1 , LDEF1 , LFSEL ,
& XMIN , XMAX , YMIN , YMAX
& )
IMPLICIT NONE
-----
C
C ***** FORTRAN77 SUBROUTINE: C3OUTG *****
C
C PURPOSE: PIPE COMMUNICATION WITH IDL TO PLOT GRAPH
C
C PROVIDES COMPARATIVE GRAPH OF:
C           SPLINE INTERPOLATED POINTS: CROSSES
C           CURVE THROUGH SPLINE POINTS: FULL CURVE
C           MINIMAX FIT TO SPLINE DATA : DASH CURVE
C
C PLOT IS LOG10(EFF. EMIS. COEF.) V LOG10(BM. ENRGY(EV/AMU))
C
C CALLING PROGRAM: ADAS303
C
C SUBROUTINE:
C
CX UNIX PORT - LGHOST RETAINED ONLY TO KEEP ARGUMENT LIST THE SAME.
C INPUT : (L*4) LGHOST = .TRUE. => GHOST80 INITIALISED
C           .FALSE. => GHOST80 NOT INITIALISED
C
C INPUT : (C*40) TITLE = TITLE OF RUN (READ FROM ISPF PANEL)
CX INPUT : (C*120)TITLX = INFORMATION STRING CONTAINING: INPUT DATA
C           FILE-NAME, SELECTED BLOCK,TYPE AND TRANSIT.
C INPUT : (C*80) TITLM = DIAGNOSTIC LINE INFORMATION FROM 'MINIMAX'
C INPUT : (C*8) DATE = CURRENT DATE (AS 'DD/MM/YY')
C
C INPUT : (R*8) DIVAL = SELECTED OUTPUT VALUE: ION DENSITY (CM-3)
C INPUT : (R*8) DEREf = REFERENCE VALUE : ION DENSITY (CM-3)
C
C INPUT : (R*8) TIVAL = SELECTED OUTPUT VALUE: ION TEMPERATURE(EV)
C INPUT : (R*8) TEREf = REFERENCE VALUE : ION TEMPERATURE(EV)
C
C INPUT : (R*8) ZFVAL = SELECTED OUTPUT VALUE: Z-EFFECTIVE
C INPUT : (R*8) ZEREf = REFERENCE VALUE : Z-EFFECTIVE
C
C INPUT : (R*8) BMVAL = SELECTED OUTPUT VALUE: MAGNETIC FIELD (T)
C INPUT : (R*8) BMREF = REFERENCE VALUE : MAGNETIC FIELD (T)
C
C INPUT : (C*5) CWAVEL = INPUT DATA FILE: TRANSITION
C INPUT : (C*8) CDONOR = INPUT DATA FILE: DONOR NEUTRAL ATOM
C INPUT : (C*5) CRECVR = INPUT DATA FILE: RECEIVER NUCLEUS
C INPUT : (C*8) CFILE = INPUT DATA FILE: SPECIFIC ION FILE SOURCE
C INPUT : (C*8) CPCODE = INPUT DATA FILE: PROCESSING CODE
C INPUT : (C*6) CINDM = FILE DATA FILE: EMISSION TYPE
C
C INPUT : (R*8) EAMU() = USER ENTERED: BEAM ENERGIES (EV/AMU)
C           DIMENSION: BEAM ENERGY INDEX
C INPUT : (R*8) QEFA() = SPLINE INTERPOLATED OR EXTRAPOLATED EFF.
C           EMIS. COEFFTS. FOR THE USER ENTERED BEAM
C           ENERGIES.
C           DIMENSION: BEAM ENERGY INDEX
C INPUT : (I*4) IEVAL = NUMBER OF USER ENTERED BEAM ENERGIES.
C
C INPUT : (R*8) EFITM() = MINIMAX: SELECTED BEAM ENERGIES(EV/AMU)
C INPUT : (R*8) QEFM() = EFF. EMISSION COEFFTS. AT 'EFITM()'
C INPUT : (I*4) NMx = NUMBER OF MINIMAX GENERATED EFF. EMIS. COEF.
C
C INPUT : (L*4) LGRD1 = .TRUE. => PUT GRAPH IN GRID FILE
C           .FALSE. => DO NOT PUT GRAPH IN GRID FILE
C INPUT : (L*4) LDEF1 = .TRUE. => USE DEFAULT GRAPH SCALING
C           .FALSE. => DO NOT USE DEFAULT GRAPH SCALING
C INPUT : (L*4) LFSEL = .TRUE. => CARRY OUT MINIMAX POLYNOMIAL
C           FITTING
C           .FALSE. => - DO NOT DO THE ABOVE -
C
C INPUT : (R*8) XMIN = GRAPH: LOWER LIMIT FOR BEAM ENERGY
C INPUT : (R*8) XMAX = GRAPH: UPPER LIMIT FOR BEAM ENERGY
C INPUT : (R*8) YMIN = GRAPH: LOWER LIMIT FOR EFF. EMIS. COEFFT.
C INPUT : (R*8) YMAX = GRAPH: UPPER LIMIT FOR EFF. EMIS. COEFFT.

```

```

C
C
C      (R*4) GHZERO = PARAMETER = VALUE BELOW WHICH GHOST80
C                    TAKES NUMBERS AS BEING ZERO = 1.0E-36
C      (R*4) YDMIN  = PARAMETER = MINIMUM ALLOWED Y-VALUE FOR
C                    PLOTTING. (USED FOR DEFAULT GRAPH SCALING)
C                    (SET TO 'GHZERO'/ZERO TO REMOVE)
C
C      (I*4) I4UNIT = FUNCTION (SEE ROUTINE SECTION BELOW)
C      (I*4) I      = GENERAL USE - ARRAY INDEX
C      (I*4) IKEY   = NUMBER OF 'KEY()' VALUES TO BE OUTPUT
C      (I*4) ICOUNT = NUMBER OF POINTS PLOTTED FOR GRAPH CURVE
C
C      (R*4) XHIGH  = UPPER X-AXIS LIMIT FOR USE WITH GHOST80
C      (R*4) XLOW   = LOWER X-AXIS LIMIT FOR USE WITH GHOST80
C      (R*4) YHIGH  = UPPER Y-AXIS LIMIT FOR USE WITH GHOST80
C      (R*4) YLOW   = LOWER Y-AXIS LIMIT FOR USE WITH GHOST80
C      (R*4) XA4( ) = X-AXIS CO-ORDINATES FOR USE WITH GHOST80
C      (R*4) YA4( ) = Y-AXIS CO-ORDINATES FOR USE WITH GHOST80
C
C      (R*8) R8VAL1( ) = 1-D SCAN POSITIONS - OUTPUT DATA VALUES
C                    DIMENSION: 4
C      (R*8) R8VAL2( ) = 1-D SCAN POSITIONS - OUTPUT REFERENCE VALUES
C                    DIMENSION: 4
C
C      (C*88) ISPEC = GRAPH TITLE (INCORPORATES 'TITLE')
C      (C*80) CADAS = ADAS HEADER: INCLUDES RELEASE, PROGRAM, TIME
C      (C*12) DNAME = '      DATE: '
C      (C*25) XTITE = X-AXIS UNITS/TITLE: NEUTRAL BEAM ENERGY
C      (C*22) YTIT  = Y-AXIS UNITS/TITLE
C      (C*9)  KEY0  = '      KEY: '
C      (C*9)  MNMX0 = 'MINIMAX: '
C      (C*8)  ADAS0 = 'ADAS   : '
C      (C*28) KEY( ) = DESCRIPTIVE KEY FOR GRAPH (2 TYPES)
C
C      (C*1) GRID  = DUMMY NAME VARIABLE FOR USE WITH GHOST80
C      (C*1) PIC   = DUMMY NAME VARIABLE FOR USE WITH GHOST80
C      (C*3) C3BLNK = BLANK 3 BYTE STRING
C      (C*7) C7    = 7 BYTE STRING = 'TITLX(1:4)''/'C3BLNK'
C
C      (C*28) STRG1 = DESCRIPTIVE STRING FOR ELEMENT SYMBOL
C      (C*28) STRG2 = DESCRIPTIVE STRING FOR NUCLEAR CHARGE
C      (C*28) STRG3 = DESCRIPTIVE STRING FOR CHARGE-STATE
C      (C*28) STRG4 = DESCRIPTIVE STRING TRANSITION
C      (C*28) STRG5 = DESCRIPTIVE STRING NEUTRAL DONOTOR ATOM
C      (C*28) STRG6 = DESCRIPTIVE STRING BARE NUCLEUS RECEIVER
C      (C*28) STRG7 = DESCRIPTIVE STRING QCX SOURCE FILE MEMBER
C      (C*28) STRG8 = DESCRIPTIVE STRING PROCESSING CODE
C      (C*28) STRG9 = DESCRIPTIVE STRING EMISSION TYPE
C      (C*13) STRG10( ) = DESCRIPTIVE STRINGS: 1-D SCAN POSITIONS
C                    DIMENSION: 4
C      (C*32) HEAD1 = HEADING FOR RECEIVER INFORMATION
C      (C*45) HEAD2A = FIRST HEADER FOR RECEIVER/DONOR ENER. INFO
C      (C*45) HEAD2B = SECOND HEADER FOR RECEIVER/DONOR ENER. INFO
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      XXADAS      ADAS        GATHERS ADAS HEADER INFORMATION
C      XXLIM8      ADAS        SETTING UP OF DEFAULT GRAPH AXES
C      XXGSEL      ADAS        SELECTS POINTS WHICH WILL FIT ON GRAPH
C      I4UNIT      ADAS        GET UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C AUTHOR:  H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C          JA 8.08
C          TEL. 0141-553-4196
C
C DATE:    23/04/95
C
C UPDATE:  03/05/95 PE BRIDEN - ADDED/MODIFIED 1-D SCAN POSITIONS TABLE.
C          (REQD. UPDATE OF ARGUMENT LIST)
C          + OTHER MINOR MODS.
C
C UPDATE:  15/05/95 TIM HAMMOND - UNIX PORT
C
C -----
C
C      REAL*4      GHZERO      , YDMIN
C
C      PARAMETER( GHZERO = 1.0E-36 , YDMIN = 1.0E-20 )
C
C      INTEGER    I4UNIT
C      INTEGER    IEVAL      , NMX
C      INTEGER    I          , IKEY      , ICOUNT
C
C      REAL*4      XHIGH      , XLOW      ,
C      &          YHIGH      , YLOW
C
C      REAL*8      XMIN      , XMAX      ,
C      &          YMIN      , YMAX
C
C      REAL*8      DIVAL      , DEREf      ,
C      &          TIVAL      , TEREf      ,
C      &          ZFVAL      , ZEREf      ,
C      &          BMVAL      , BMREF
C
C -----

```

```

LOGICAL      LGHOST
&           LGRD1      , LDEF1      , LFSEL
-----
CHARACTER    TITLE*40  , TITLX*120  , TITLM*80  ,
&           DATE*8
CHARACTER    CINDM*6   , CFILE*8   ,
&           CPCODE*8   , CWAVEL*5   ,
&           CDONOR*8   , CRECVR*5
CHARACTER    GRID*1    , PIC*1      , C3BLNK*3  , C7*7  ,
&           MNMX0*9    , KEY0*9      , ADAS0*8   ,
&           DNAME*12   ,
&           XTITE*25   , YTIT*32   ,
&           CADAS*80   , ISPEC*88
CHARACTER    STRG1*28  , STRG2*28  ,
&           STRG3*28  , STRG4*28  ,
&           STRG5*28  , STRG6*28  , STRG7*28  ,
&           STRG8*28  , STRG9*28  ,
&           HEAD1*32
CHARACTER    STRG10(4)*13 ,
&           HEAD2A*45  , HEAD2B*45
-----
REAL*4       XA4(100)  , YA4(100)
-----
REAL*8       R8VAL1(4) , R8VAL2(4)
-----
REAL*8       EAMU(IEVAL) , QEFA(IEVAL) ,
&           EFITM(NMX)  , QEFM(NMX)
-----
CHARACTER    KEY(2)*28
-----
SAVE        ISPEC      , CADAS
-----
DATA ISPEC(1:24)
&           /'EFF. EMISSION COEFFTS. '/
DATA DNAME  /'      DATE: '/
DATA XTITE  /'BEAM ENERGY (EV/AMU) '/
DATA YTIT   /'EFF. EMISSION COEFFT. (cm3/sec)'/
DATA ADAS0  /'ADAS      :'/
&           MNMX0 /'MINIMAX: '/
&           KEY0  /'KEY   : '/
&           KEY(1) /'(CROSSES/FULL LINE - SPLINE)'/ ,
&           KEY(2) /'(DASH LINE - MINIMAX)  '/
DATA GRID   /' '/ ,
&           PIC /' '/ ,
&           C3BLNK /' '/ ,
&           CADAS /' '/
DATA HEAD1  /'--- EMITTING ION INFORMATION ---'/
&           HEAD2A /'----- ONE DIMENSIONAL SCAN POSITIONS -----' / ,
&           HEAD2B /'  PARAMETER          VALUE          REFERENCE  '/
DATA STRG1  /' ELEMENT SYMBOL          = '/ ,
&           STRG2 /' NUCLEAR CHARGE      = '/ ,
&           STRG3 /' CHARGE STATE        = '/ ,
&           STRG4 /' TRANSITION (N-N')   = '/ ,
&           STRG5 /' NEUTRAL ATOM DONOR  = '/ ,
&           STRG6 /' BARE NUCLEUS RECEIVER = '/ ,
&           STRG7 /' QCX SOURCE FILE MEMBER = '/ ,
&           STRG8 /' PROCESSING CODE     = '/ ,
&           STRG9 /' EMISSION TYPE       = '/
DATA STRG10 /'DENSI (cm-3) ',
&           'TI (eV) ',
&           'ZEFF ',
&           'BMAG (T) '/
-----
INTEGER      PIPEIN    , PIPEOU    , ONE    , ZERO
PARAMETER(   PIPEIN=5  , PIPEOU=6  , ONE=1   , ZERO=0 )
INTEGER      J          , K          , L
-----

```

## C3SPLN

```

SUBROUTINE C3SPLN( NEIN  , NEOUT  ,
&               EIN    , EOUT    ,
&               QEF    , QEFA    ,
&               LERNG
&               )
IMPLICIT NONE
-----
C
C *****
C ***** FORTRAN77 SUBROUTINE: C3SPLN *****
C
C PURPOSE:
C PERFORMS CUBIC SPLINE ON LOG(BEAM ENERGY <EV/AMU> ) VERSUS
C LOG(EFF. EMISSION COEFFICIENTS).
C INPUT DATA FOR A GIVEN EMITTING ION EMISS. COEFF. DATA BLOCK
C
C USING ONE-WAY SPLINES IT CALCULATES THE EFF. EMISSION
C COEFFICIENT FOR 'NEOUT' BEAM ENERGY VALUES FROM
C THE LIST OF BEAM ENERGIES READ IN FROM THE INPUT FILE
C
C IF A VALUE CANNOT BE INTERPOLATED USING SPLINES IT IS
C EXTRAPOLATED VIA 'XXSPL'. (SEE NOTES BELOW).
C

```

```

C CALLING PROGRAM: ADAS303/SQEF
C
C SUBROUTINE:
C
C INPUT : (I*4) NEIN = INPUT DATA FILE: NUMBER OF BEAM ENERGIES
C READ FOR THE DATA-BLOCK BEING ASSESSED
C INPUT : (I*4) NEOUT = NUMBER OF ISPF ENTERED BEAM ENERGY
C VALUES FOR WHICH EFF. EMISS. COEFFTS.
C ARE REQUIRED FOR TABULAR/GRAPHICAL OUTPUT.
C
C INPUT : (R*8) EIN() = INPUT DATA FILE: BEAM ENERGIES (EV/AMU)
C FOR THE DATA-BLOCK BEING ASSESSED.
C DIMENSION: ELECTRON TEMPERATURE INDEX
C INPUT : (R*8) EOUT() = USER ENTERED: BEAM ENERGIES (EV/AMU)
C DIMENSION: BEAM ENERGY INDEX
C
C INPUT : (R*8) QEF() =INPUT DATA FILE: FULL SET OF EFF. EMISS.
C COEFFTS FOR THE DATA-BLOCK
C BEING ANALYSED.
C 1ST DIMENSION: BEAM ENERGY INDEX
C OUTPUT: (R*8) QEFA() = SPLINE INTERPOLATED OR EXTRAPOLATED EFF.
C EMISS. COEFFTS FOR
C THE USER ENTERED BEAM ENERGIES.
C DIMENSION: BEAM ENERGY INDEX
C
C OUTPUT: (L*4) LERNG()= .TRUE. => OUTPUT 'QEFA()' VALUE WAS INTER-
C POLATED FOR THE USER ENTERED
C BEAM ENERGY 'EOUT()'.
C .FALSE. => OUTPUT 'QEFA()' VALUE WAS EXTRA-
C POLATED FOR THE USER ENTERED
C BEAM ENERGY 'EOUT()'.
C DIMENSION: ELECTRON TEMPERATURE INDEX
C
C (I*4) NIN = PARAMETER = MAX. NO. OF INPUT BEAM ENERGIES
C VALUES. MUST BE >= 'NEIN'
C (I*4) NOUT = PARAMETER = MAX. NO. OF OUTPUT BEAM ENERGY
C VALUES MUST BE >= 'NEOUT'
C (I*4) L1 = PARAMETER = 1
C
C (I*4) IET = ARRAY SUBSCRIPT USED INPUT FILE BEAM
C ENERGIES.
C (I*4) IT = ARRAY SUBSCRIPT USED FOR USER ENTERED
C BEAM ENERGIES.
C (I*4) IOPT = DEFINES THE BOUNDARY DERIVATIVES FOR THE
C SPLINE ROUTINE 'XXSPLE', SEE 'XXSPLE'.
C (VALID VALUES = <0, 0, 1, 2, 3, 4)
C
C (L*4) LSETX = .TRUE. => SET UP SPLINE PARAMETERS RELATING
C TO 'XIN' AXIS.
C .FALSE. => DO NOT SET UP SPLINE PARAMETERS
C RELATING TO 'XIN' AXIS.
C (I.E. THEY WERE SET IN A PREVIOUS
C CALL )
C (VALUE SET TO .FALSE. BY 'XXSPLE')
C
C (R*8) R8FUN1 = FUNCTION - (SEE ROUTINES SECTION BELOW)
C
C (R*8) XIN() = LOG( DATA FILE ELECTRON TEMPERATURES )
C (R*8) YIN() = LOG( DATA FILE SCALED ION. RATE COEFFTS.)
C (R*8) XOUT() = LOG( USER ENTERED ELECTRON TEMPS.)
C (R*8) YOUT() = LOG( OUTPUT GENERATED SCALED ION. RATE COEF)
C (R*8) DF() = SPLINE INTERPOLATED DERIVATIVES
C
C NOTE:
C
C ONE-DIMENSIONAL SPLINE CARRIED OUT BY THIS SUBROUTINE:
C
C LOG( QEF ) VS. LOG( Te )
C
C TE = ELECTRON TEMPERATURE (UNITS: EV)
C QEF = ZERO DENSITY RADIATED POWER COEFFICIENT
C (UNITS: W CM**3)
C
C EXTRAPOLATION CRITERIA:
C
C LOW TE: ZERO GRADIENT EXTRAPOLATION (I.E. DY(1) = 0.0)
C HIGH TE: ZERO CURVATURE EXTRAPOLATION (I.E. DDY(N) = 0.0)
C
C (THESE CRITERIA ARE MET BY CALLING XXSPLE WITH IOPT=4)
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C XXSPLE ADAS SPLINE SUBROUTINE (EXTENDED DIAGNOSTICS)
C R8FUN1 ADAS REAL*8 FUNCTION: ( X -> X )
C
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL. 0141-553-4196
C
C DATE: 21/04/95
C
C UPDATE: 15/05/95 Tim Hammond UNIX PORT
C Put under SCCS control
C

```



```

C-----
C
C
C      INTEGER    NIN              , NOUT              , L1
C-----
C      PARAMETER( NIN    = 24      , NOUT = 24        , L1 = 1    )
C-----
C      INTEGER    NEIN              , NEOUT
C      INTEGER    IET              , IT              , IOPT
C-----
C      REAL*8     R8FUN1
C-----
C      LOGICAL    LSETX
C-----
C      REAL*8     EIN(NEIN)         , EOUT(NEOUT)   ,
C      &          QEF(NEIN)         , QEFA(NEOUT)   ,
C      REAL*8     DF(NIN)           ,
C      &          XIN(NIN)          , YIN(NIN)     ,
C      &          XOUT(NOUT)        , YOUT(NOUT)   ,
C-----
C      LOGICAL    LERNG(NEOUT)
C-----
C      EXTERNAL  R8FUN1
C-----

```

## C3TITL

```

      SUBROUTINE C3TITL( IBSEL , DSFULL ,
&                      CWAVEL , CDONOR ,
&                      CRECVR , CFILE ,
&                      CPCODE , CINDM ,
&                      TITLX
&                      )
      IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C3TITL *****
C
C PURPOSE: TO CREATE THE DESCRIPTIVE TITLE FOR SELECTED DATA-BLOCK.
C
C CALLING PROGRAM: ADAS303/SQEF
C
C SUBROUTINE:
C
C INPUT : (I*4) IBSEL = SELECTED DATA-BLOCK: INDEX
CX INPUT : (C*(*)) DSFULL = FULL MVS INPUT DATA SET NAME
C
C INPUT : (C*5) CWAVEL = INPUT DATA FILE: TRANSITION
C INPUT : (C*8) CDONOR = INPUT DATA FILE: DONOR NEUTRAL ATOM
C INPUT : (C*5) CRECVR = INPUT DATA FILE: RECEIVER NUCLEUS
C INPUT : (C*8) CFILE = INPUT DATA FILE: SPECIFIC ION FILE SOURCE
C INPUT : (C*8) CPCODE = INPUT DATA FILE: PROCESSING CODE
C INPUT : (C*6) CINDM = FILE DATA FILE: EMISSION TYPE
C
CX OUTPUT: (C*120)TITLX = SELECTED DATA-BLOCK: DESCRIPTIVE TITLE
C
C      (C*2) C2 = GENERAL USE 2 BYTE CHARACTER STRING
CX      (I*4) LEN_NAME = LENGTH OF FILENAME
CX      (I*4) POS_NOW = CURRENT POSITION IN TITLE STRING
C
C ROUTINES:
C      XXSLEN USED TO FIND LENGTH OF FILE NAME
C
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C      JA8.08
C      TEL. 0141-553-4196
C
C DATE: 23/04/95
C
C UPDATE: TIM HAMMOND 15/05/95 UNIX PORT UPDATES
C      Included call to xxslen to find
C      length of filename and edit if
C      required.
C-----
C
C      INTEGER    IBSEL      , LEN_NAME
C      INTEGER    IFIRST    , ILAST
C      INTEGER    POS_NOW
C-----
C      CHARACTER DSFULL*(*)  , TITLX*120
C      CHARACTER C2*2
C      CHARACTER CINDM*6    , CFILE*8    ,
C      &          CPCODE*8    , CWAVEL*5    ,
C      &          CDONOR*8    , CRECVR*5
C-----

```

# C4CHKZ

```
      SUBROUTINE C4CHKZ( DSNAME , TSYM , ITZ )
C
C      IMPLICIT NONE
C-----
C
C ***** FORTRAN77 SUBROUTINE: C4CHKZ *****
C
C PURPOSE: TO CHECK THAT THE STOPPING ION ELEMENT SYMBOL/CHARGE AS READ
C          FROM THE INPUT DATA SET AGREE WITH THOSE OBTAINED FROM THE
C          INPUT DATA SET MEMBER NAME.
C
C          NOTE THAT THE INFORMATION WHICH WAS PREVIOUSLY DETERMINED
C          FROM THE DATASET NAME IS NOW PASSED VIA UNIX PIPE FROM THE
C          IDL ROUTINE c4chkz.pro
C
C CALLING PROGRAM: ADAS304
C
C SUBROUTINE:
C
C INPUT : (C*) DSNAME = MVS DATA SET NAME - WHERE INPUT VALUES
C          ORIGINATE
C INPUT : (C2) TSYM   = INPUT FILE DATA:EMITTING ION ELEMENT SYMBOL
C INPUT : (I4) ITZ    = INPUT FILE DATA:EMITTING ION CHARGE
C
C          (I4) ITZM   = MEMBER NAME:EMITTING ION CHARGE
C
C          (C2) TSYMM  = MEMBER NAME:EMITTING ION ELEMENT SYMBOL
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C-----
C          I4UNIT    ADAS      RETURNS UNIT NO. FOR OUTPUT OF MESSAGES
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/87
C          JET EXT. 5183
C
C DATE:    16/12/93
C
C UNIX-IDL PORT:
C
C VERSION: 1.1                      DATE: 16-11-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - FIRST VERSION
C
C VERSION: 1.2                      DATE: 11-12-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - TIDIED UP COMMENTS AND CODE
C-----
C-----
C          INTEGER    I4UNIT
C          INTEGER    PIPEIN          , PIPEOU
C          PARAMETER( PIPEIN=5        , PIPEOU=6 )
C-----
C          INTEGER    ITZ
C          INTEGER    ITZM
C-----
C          CHARACTER DSNAME*(*)      , TSYM*2
C          CHARACTER TSYMM*2
C-----
```

# C4DATA

```
      SUBROUTINE C4DATA( IUNIT , MXBE , MXTD , MXTT ,
&                      ITZ , TSYM , BEREf , TDREF ,
&                      TTREF , SVREF , NBE , BE ,
&                      NTDENS , TDENS , NTTEMP , TTEMP ,
&                      SVT , SVED , DSNIN
&                      )
C
C      IMPLICIT NONE
C-----
C
C ***** FORTRAN77 SUBROUTINE: C4DATA *****
C
C PURPOSE: TO READ DATA FROM AN EFFECTIVE BEAM STOPPING DATA SET.
C          (ADAS FORMAT ADF21).
C
C CALLING PROGRAM: SBMS / ADAS304
C
C SUBROUTINE:
C
C INPUT : (I*4) IUNIT = UNIT TO WHICH DATA SET IS CONNECTED.
C INPUT : (I*4) MXBE  = MAXIMUM NUMBER OF BEAM ENERGIES WHICH CAN
C                     BE READ.
C
```

```

C INPUT : (I*4) MXTD = MAXIMUM NUMBER OF TARGET DENSITIES WHICH
C CAN BE READ.
C INPUT : (I*4) MXTT = MAXIMUM NUMBER OF TARGET TEMPERATURES
C WHICH CAN BE READ.
C INPUT : (C*80) DSNIN = NAME OF FILE TO BE READ.
C OUTPUT: (I*4) ITZ = TARGET ION CHARGE.
C OUTPUT: (C*2) TSYM = TARGET ION ELEMENT SYMBOL.
C OUTPUT: (R*8) BEREf = REFERENCE BEAM ENERGY.
C UNITS: EV/AMU
C OUTPUT: (R*8) TDREF = REFERENCE TARGET DENSITY.
C UNITS: CM-3
C OUTPUT: (R*8) TTREF = REFERENCE TARGET TEMPERATURE.
C UNITS: EV
C OUTPUT: (R*8) SVREF = STOPPING COEFFT. AT REFERENCE BEAM ENERGY,
C TARGET DENSITY AND TEMPERATURE.
C UNITS: CM3 S-1
C OUTPUT: (I*4) NBE = NUMBER OF BEAM ENERGIES.
C OUTPUT: (R*8) BE() = BEAM ENERGIES.
C UNITS: EV/AMU
C DIMENSION: MXBE
C OUTPUT: (I*4) NTDENS = NUMBER OF TARGET DENSITIES.
C OUTPUT: (R*8) TDENS() = TARGET DENSITIES.
C UNITS: CM-3
C DIMENSION: MXTD
C OUTPUT: (I*4) NTTEMP = NUMBER OF TARGET TEMPERATURES.
C OUTPUT: (R*8) TTEMP() = TARGET TEMPERATURES.
C UNITS: EV
C DIMENSION: MXTT
C OUTPUT: (R*8) SVT() = STOPPING COEFFT. AT REFERENCE BEAM ENERGY
C AND TARGET DENSITY.
C UNITS: CM3 S-1
C DIMENSION: MXTT
C OUTPUT: (R*8) SVED(,) = STOPPING COEFFT. AT REFERENCE TARGET
C TEMPERATURE.
C UNITS: CM3 S-1
C 1ST DIMENSION: MXBE
C 2ND DIMENSION: MXTD
C
C (I*4) I = ARRAY / LOOP INDEX.
C (I*4) J = ARRAY INDEX.
C
C (C*80) LINE = TEXT LINE IN DATA SET.
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C-----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/87
C JET EXT. 5183
C
C DATE: 07/12/93
C
C UNIX-IDL PORT:
C
C VERSION: 1.1 DATE: 16-11-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - FIRST VERSION
C
C-----
C
C INTEGER I4UNIT
C-----
C INTEGER IUNIT , MXBE , MXTD , MXTT , ITZ ,
C & NBE , NTDENS , NTTEMP
C INTEGER I , J
C-----
C REAL*8 BEREf , TDREF , TTREF , SVREF
C-----
C CHARACTER TSYM*2
C CHARACTER LINE*80 , DSNIN*80
C-----
C REAL*8 BE(MXBE) , TDENS(MXTD) , TTEMP(MXTT) ,
C & SVT(MXTT)
C-----
C REAL*8 SVED(MXBE,MXTD)
C-----

```

## C4MNMX

```

SUBROUTINE C4MNMX( NSITYP , MXA , NA , A , AMNMX )
C
C IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C4MNMX *****
C
C PURPOSE: GIVEN A 2D ARRAY 'A' IT RETURNS THE MINIMUM AND MAXIMUM OF
C BOTH 'A(1,I)' AND 'A(NA(I),I)', WHERE I=1,NSITYP. ITS MAIN
C USE IS TO FIND THE RANGE ON THE MINIMUM AND MAXIMUM

```

```

C          OF THE BEAM ENERGIES, AND TARGET DENSITIES AND TEMPERATURES
C          ACROSS THE DIFFERENT ION TYPES.
C
C          CALLING PROGRAM: ADAS304
C
C          SUBROUTINE:
C
C          INPUT : (I*4)  NSITYP   = NUMBER OF DIFFERENT ION TYPES.
C          INPUT : (I*4)  MXA      = SIZE OF FIRST DIMENSION OF 'A(,)' .
C          INPUT : (I*4)  NA( )    = NO. OF ENTRIES IN EACH COLUMN OF 'A(,)' .
C                                     DIMENSION: NSITYP
C          INPUT : (R*8)  A( , )   = INPUT ARRAY.
C                                     1ST DIMENSION: MXA
C                                     2ND DIMENSION: NSITYP
C
C          OUTPUT: (R*8)  AMNMX( ) = MINIMUM/MAXIMUM VALUES.
C                                     INDICES ARE AS FOLLOWS:
C                                     1 => MIN OF 'A(1,I)'
C                                     2 => MAX OF 'A(1,I)'
C                                     3 => MIN OF 'A(NA(I),I)'
C                                     4 => MAX OF 'A(NA(I),I)'
C                                     WHERE I=1,NSITYP.
C                                     DIMENSION: 4
C
C          (I*4)  I      = LOOP INDEX.
C          (I*4)  J      = ARRAY INDEX.
C
C          ROUTINES: NONE
C
C          AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C                   KL/0/87
C                   JET EXT. 5183
C
C          DATE:    17/12/93
C
C          UNIX-IDL PORT:
C
C          VERSION: 1.1                      DATE: 16-11-95
C          MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C                   - FIRST VERSION
C
C-----
C
C          INTEGER      NSITYP , MXA
C          INTEGER      I      , J
C
C-----
C          INTEGER      NA(NSITYP)
C
C-----
C          REAL*8       AMNMX(4)
C
C-----
C          REAL*8       A(MXA,NSITYP)
C-----

```

## C4OUT0

```

          SUBROUTINE C4OUT0( IWRITE , MXREQ , MXDEG , DATE ,
&                          TITLE , NSITYP , DSNIN , TSYM ,
&                          ITZ , SIFRAC , NREQ , UBMENG ,
&                          UTDENS , UTTEMP , BSTOT , LINTOT ,
&                          BSION , LINION , LFSEL , IFIT ,
&                          NCOEF , FCOEF , FINFO , CADAS ,
&                          LINE1 , DATASET, FACT1 , TFLAG )
C
C          IMPLICIT NONE
C
C-----
C          ***** FORTRAN77 SUBROUTINE: C4OUT0 *****
C
C          PURPOSE: WRITES TEXT OUTPUT TO FILE FOR ADAS304.
C
C          CALLING PROGRAM: ADAS304
C
C          INPUT : (I*4)  IWRITE   = UNIT NO. FOR OUTPUT OF TEXT RESULTS.
C          INPUT : (I*4)  MXREQ    = MAX NO. OF USER REQUESTED TRIPLETS OF
C                                     ENERGY, TEMPERATURE AND DENSITY.
C          INPUT : (I*4)  MXDEG    = MAX NO. DEGREES FOR MINIMAX FIT.
C          INPUT : (C*8)  DATE     = DATE STRING.
C          INPUT : (C*40) TITLE    = ISPF ENTERED GENERAL TITLE FOR PROGRAM RUN
C          INPUT : (I*4)  NSITYP   = NUMBER OF STOPPING IONS TYPES.
C          INPUT : (C*80) DSNIN( ) = INPUT DATA SET NAMES (FULL MVS DSN).
C                                     (IN FORM SUITABLE FOR DYNAMIC ALLOCATION)
C                                     DIMENSION: NSITYP
C          INPUT : (C*2)  TSYM( )  = TARGET ION ELEMENT SYMBOL.
C                                     DIMENSION: NSITYP
C          INPUT : (I*4)  ITZ( )   = TARGET ION CHARGE.
C                                     DIMENSION: NSITYP
C          INPUT : (R*8)  SIFRAC( ) = FRACTION OF EACH STOPPING ION.
C                                     DIMENSION: NSITYP
C          INPUT : (I*4)  NREQ     = NUMBER OF USER REQUESTED TRIPLETS OF
C                                     ENERGY, TEMPERATURE AND DENSITY.
C          INPUT : (R*8)  UBMENG( ) = USER REQUESTED BEAM ENERGIES.

```

```

C
C INPUT : (R*8)  UTDENS( ) = DIMENSION: NREQ
C                               USER REQUESTED TARGET DENSITIES.
C                               DIMENSION: NREQ
C INPUT : (R*8)  UTTEMP( ) = USER REQUESTED TARGET TEMPERATURES.
C                               DIMENSION: NREQ
C INPUT : (R*8)  BSTOT( ) = TOTAL BEAM STOPPING COEFFICIENTS.
C                               DIMENSION: NREQ
C INPUT : (L*4)  LINTOT( ) = FLAGS IF INTERPOLATION OR EXTRAPOLATION
C                               USED IN SPLINING ROUTINE.
C                               .TRUE. => ONLY INTERPOLATION USED.
C                               .FALSE. => AT LEAST ONE OF ENERGY, DENISTY
C                               OR TEMPERATURE EXTRAPOLATED.
C                               DIMENSION: NREQ
C INPUT : (R*8)  BSION( , ) = BEAM STOPPING COEFFICIENTS FOR INDIVIDUAL
C                               IONS.
C                               1ST DIMENSION: MXREQ
C                               2ND DIMENSION: NSITYP
C INPUT : (L*4)  LINION( , ) = FLAGS IF INTERPOLATION OR EXTRAPOLATION
C                               USED IN SPLINING ROUTINE.
C                               .TRUE. => ONLY INTERPOLATION USED.
C                               .FALSE. => AT LEAST ONE OF ENERGY, DENISTY
C                               OR TEMPERATURE EXTRAPOLATED.
C                               1ST DIMENSION: MXREQ
C                               2ND DIMENSION: NSITYP
C INPUT : (L*4)  LFSEL      = FLAGS MINIMAX POLYNOMIAL FITTING.
C                               .TRUE. => FIT PERFORMED.
C                               .FALSE. => NO FIT.
C INPUT : (I*4)  IFIT       = QUANTITY TO FIT AND DISPLAY.
C                               1 => BEAM ENERGY.
C                               2 => TARGET DENSITY.
C                               3 => TARGET TEMPERATURE.
C INPUT : (I*4)  NCOEF( ) = NUMBER OF TAYLOR COEFFICIENTS FROM FIT.
C                               DIMENSION: NSITYP
C INPUT : (R*8)  FCOEF( , ) = TAYLOR COEFFICIENTS FROM FIT.
C                               1ST DIMENSION: MXDEG
C                               2ND DIMENSION: NSITYP
C INPUT : (C*80) FINFO( ) = INFORMATION STRING FROM FIT.
C                               INDICES 1 TO 'NSITYP' ARE FOR THE
C                               INDIVIDUAL IONS AND 'NSITYP+1' FOR THE
C                               TOTAL.
C                               DIMENSION: NSITYP+1
C INPUT : I*4    TFLAG      = DETERMINES TITLE TYPE IN OUTPUT
C                               0 => 'BEAM STOPPING ... '
C                               1 => 'BEAM EMISSION ... '
C
C (I*4)  LEN      = LENGTH OF ION NAME STRINGS.
C (I*4)  L1       = LENGTH OF 'LINE1' STRING.
C (I*4)  L2       = LENGTH OF 'LINE2' STRING.
C (I*4)  I        = LOOP / ARRAY INDEX.
C (I*4)  J        = LOOP / ARRAY INDEX.
C
C (C*80) CADAS    = ADAS HEADER: INCLUDES RELEASE, PROGRAM,
C                               TIME.
C (C*133) LINE1   = LINE OF TEXT.
C (C*133) LINE2   = LINE OF TEXT.
C (C*100) TITLG   = TITLE FOR GRAPH.
C (C*4)  SION     = ION NAME STRING.
C
C ROUTINES:
C
C ROUTINE      SOURCE      BRIEF DESCRIPTION
C -----
C XXSION      ADAS        RETURNS ION STRING.
C
C AUTHOR:     JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C             KL/0/87
C             JET EXT. 5183
C
C DATE:      23/12/93
C
C UNIX-IDL PORT:
C
C VERSION: 1.1                      DATE: 16-11-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C             - FIRST VERSION
C
C VERSION: 1.2                      DATE: 11-12-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C             - TIDIED UP COMMENTS AND CODE
C
C VERSION: 1.3                      DATE: 12-03-97
C MODIFIED: RICHARD MARTIN
C             - ADDED 'TFLAG' AND 'BEAMEVENT'
C -----
C
C INTEGER      IWRITE , MXREQ , MXDEG , NSITYP , NREQ ,
C &
C INTEGER      LEN , L1 , L2 , I , J
C -----
C LOGICAL      LFSEL
C -----
C CHARACTER    DATE*8 , TITLE*40 , BEAMEVENT*13
C CHARACTER    CADAS*80 , LINE1*133 , LINE2*133 , SION*4
C CHARACTER    DATASET*44
C -----
C INTEGER      ITZ(NSITYP) , NCOEF(NSITYP)
C -----
C REAL*8       SIFRAC(NSITYP) , UBMENG(NREQ) , UTDENS(NREQ) ,

```

&	UTTEMP(NREQ)	, BSTOT(NREQ)	, FACT1
C	-----		
	LOGICAL	LINTOT(NREQ)	
C	-----		
	CHARACTER	DSNIN(NSITYP)*80	, TSYM(NSITYP)*2
&		FINFO(NSITYP+1)*80	
C	-----		
	REAL*8	BSION(MXREQ,NSITYP)	, FCOEF(MXDEG+1,NSITYP+1)
C	-----		
	LOGICAL	LINION(MXREQ,NSITYP)	
C	-----		

## C4OUTG

```

SUBROUTINE C4OUTG( LGHOST , LGRD1 , TITLE , DATE ,
&                IFIT , NSITYP , DSNIN , TSYM ,
&                ITZ , SIFRAC , MXREQ , NREQ ,
&                UBMENG , UTDENS , UTTEMP , BSTOT ,
&                BSION , LFSEL , NFIT , XFIT ,
&                YFIT , FINFO , LDEF1 , XMIN ,
&                XMAX , YMIN , YMAX
&                )
C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C4OUTG *****
C
C PURPOSE:  COMMUNICATES GRAPHICS DATA TO IDL
C
C          PLOT IS LOG10(BEAM STOPPING COEFFT. (CM3 S-1) VERSUS
C          LOG10(BEAM ENERGY (EV)) OR
C          LOG10(TARGET DENSITY (CM-3)) OR
C          LOG10(TARGET TEMPERATURE (EV))
C
C          BOTH THE CONTRIBUTION OF THE INDIVIDUAL IONS AND THE
C          TOTAL STOPPING COEFFICIENTS ARE PLOTTED.
C
C          FOR EACH SET OF DATA POINTS THE FOLLOWING IS DRAWN:
C          SPLINE INTERPOLATED POINTS:  CROSSES
C          CURVE THROUGH SPLINE POINTS:  FULL CURVE
C          MINIMAX FIT TO SPLINE DATA :  DASH CURVE
C
C CALLING PROGRAM:  ADAS304
C
C I/O   : (L*4)  LGHOST   =  INITIALISATION FLAG FOR GHOST80.
C          .TRUE.  => GHOST80 INITIALISED.
C          .FALSE. => GHOST80 NOT INITIALISED.
C
C INPUT : (L*4)  LGRD1   =  FLAGS WHETHER TO PUT GRAPHS IN GRID FILE.
C          .TRUE.  => PUT GRAPHS IN GRID FILE
C          .FALSE. => DO NOT PUT GRAPHS IN GRID FILE
C
C INPUT : (C*40) TITLE    =  ISPF ENTERED GENERAL TITLE FOR PROGRAM RUN
C INPUT : (C*8)  DATE     =  DATE STRING.
C INPUT : (I*4)  IFIT     =  QUANTITY TO FIT AND DISPLAY.
C          1 => BEAM ENERGY.
C          2 => TARGET DENSITY.
C          3 => TARGET TEMPERATURE.
C
C INPUT : (I*4)  NSITYP   =  NUMBER OF STOPPING IONS TYPES.
C INPUT : (C*80) DSNIN()  =  INPUT DATA SET NAMES (FULL MVS DSN).
C          (IN FORM SUITABLE FOR DYNAMIC ALLOCATION)
C          DIMENSION: NSITYP
C
C INPUT : (C*2)  TSYM()   =  TARGET ION ELEMENT SYMBOL.
C          DIMENSION: NSITYP
C
C INPUT : (I*4)  ITZ()    =  TARGET ION CHARGE.
C          DIMENSION: NSITYP
C
C INPUT : (R*8)  SIFRAC() =  FRACTION OF EACH STOPPING ION.
C          DIMENSION: NSITYP
C
C INPUT : (I*4)  MXREQ    =  MAX NO. OF USER REQUESTED TRIPLETS OF
C          ENERGY, TEMPERATURE AND DENSITY.
C
C INPUT : (I*4)  NREQ     =  NUMBER OF USER REQUESTED TRIPLETS OF
C          ENERGY, TEMPERATURE AND DENSITY.
C
C INPUT : (R*8)  UBMENG() =  USER REQUESTED BEAM ENERGIES.
C          DIMENSION: NREQ
C
C INPUT : (R*8)  UTDENS() =  USER REQUESTED TARGET DENSITIES.
C          DIMENSION: NREQ
C
C INPUT : (R*8)  UTTEMP() =  USER REQUESTED TARGET TEMPERATURES.
C          DIMENSION: NREQ
C
C INPUT : (R*8)  BSTOT()  =  TOTAL BEAM STOPPING COEFFICIENTS.
C          DIMENSION: NREQ
C
C INPUT : (R*8)  BSION(,) =  BEAM STOPPING COEFFICIENTS FOR INDIVIDUAL
C          IONS.
C          1ST DIMENSION: MXREQ
C          2ND DIMENSION: NSITYP
C
C INPUT : (L*4)  LFSEL    =  FLAGS MINIMAX POLYNOMIAL FITTING.
C          .TRUE.  => FIT PERFORMED.
C          .FALSE. => NO FIT.
C
C INPUT : (I*4)  NFIT     =  NUMBER OF POINTS IN FIT.
C INPUT : (R*8)  XFIT(,)  =  X COORDINATES OF POINTS FROM FIT.
C          FOR THE 2ND INDEX INDICES 1 TO 'NSITYP'
C          ARE FOR THE INDIVIDUAL IONS AND 'NSITYP+1'

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```

C          FOR THE TOTAL.
C          1ST DIMENSION: NFIT
C          2ND DIMENSION: NSITYP+1
C INPUT : (R*8)  YFIT(,) = Y COORDINATES OF POINTS FROM FIT.
C          FOR THE 2ND INDEX INDICES 1 TO 'NSITYP'
C          ARE FOR THE INDIVIDUAL IONS AND 'NSITYP+1'
C          FOR THE TOTAL.
C          1ST DIMENSION: NFIT
C          2ND DIMENSION: NSITYP+1
C INPUT : (C*80) FINFO() = INFORMATION STRING FROM FIT.
C          INDICES 1 TO 'NSITYP' ARE FOR THE
C          INDIVIDUAL IONS AND 'NSITYP+1' FOR THE
C          TOTAL.
C          DIMENSION: NSITYP+1
C INPUT : (L*4)  LDEF1  = FLAGS DEFAULT GRAPH SCALING.
C          .TRUE. => USE DEFAULT GRAPH SCALING.
C          .FALSE. => DO NOT USE DEFAULT SCALING.
C INPUT : (R*8)  XMIN   = LOWER LIMIT FOR X-AXIS OF GRAPH.
C INPUT : (R*8)  XMAX   = UPPER LIMIT FOR X-AXIS OF GRAPH.
C INPUT : (R*8)  YMIN   = LOWER LIMIT FOR Y-AXIS OF GRAPH.
C INPUT : (R*8)  YMAX   = UPPER LIMIT FOR Y-AXIS OF GRAPH.
C
C PARAM : (R*8)  GHZERO = VALUE BELOW WHICH GHOST80 TAKES NUMBERS AS
C          BEING ZERO = 1.0E-36.
C PARAM : (R*8)  YDMIN  = MINIMUM ALLOWED Y-VALUE FOR PLOTTING.
C          (USED FOR DEFAULT GRAPH SCALING)
C          (SET TO 'GHZERO'/ZERO TO REMOVE)
C
C          (I*4)  I      = LOOP / ARRAY INDEX.
C          (I*4)  J      = ARRAY INDEX.
C
C
C
C ROUTINES:
C          ROUTINE    SOURCE    BRIEF DESCRIPTION
C          -----
C          XXFLSH     IDL_ADAS  FLUSHES OUT THE UNIX PIPE
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/87
C          JET EXT. 5183
C
C DATE:    22/12/93
C
C UNIX-IDL PORT:
C
C VERSION: 1.1          DATE: 16-11-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - FIRST VERSION
C
C VERSION: 1.2          DATE: 11-12-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - TIDIED UP COMMENTS AND CODE
C
C
C-----
C          REAL*4      GHZERO      , YDMIN
C          PARAMETER( GHZERO = 1.0E-36 , YDMIN = 1.0E-20 )
C-----
C          INTEGER    IFIT      , NSITYP , MXREQ , NREQ , NFIT
C          INTEGER    I        , J
C-----
C          REAL*8      XMIN      , XMAX , YMIN , YMAX
C-----
C          LOGICAL    LGHOST , LGRD1 , LFSEL , LDEF1
C-----
C          CHARACTER  TITLE*40 , DATE*8
C-----
C          INTEGER    ITZ(NSITYP)
C          INTEGER    PIPEIN , PIPEOU
C          PARAMETER( PIPEIN=5 , PIPEOU=6 )
C-----
C          REAL*8      SIFRAC(NSITYP) , UBMENG(NREQ) , UTDENS(NREQ) ,
C          &          UTEMP(NREQ) , BSTOT(NREQ)
C-----
C          CHARACTER  DSNIN(NSITYP)*80 , TSYM(NSITYP)*2 ,
C          &          FINFO(NSITYP+1)*80
C-----
C          REAL*8      BSION(MXREQ,NSITYP) , XFIT(NFIT,NSITYP+1) ,
C          &          YFIT(NFIT,NSITYP+1)
C-----

```

## C4SPLN

```

C          SUBROUTINE C4SPLN( MXBE , MXTD , MXTT , MXREQ ,
C          &          NREQ , BMENGA , DENSA , TIA ,
C          &          NSITYP , SVREF , NBE , BE ,
C          &          NTDENS , TDENS , NTTEMP , TTEMP ,
C          &          SVT , SVED , SVREQ , LIBMA ,
C          &          LIDNA , LITIA , FACT1 , ITZ , FACT2 )
C
C          IMPLICIT NONE
C-----

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C ***** FORTRAN77 SUBROUTINE: C4SPLN *****
C
C PURPOSE: CALCULATES THE BEAM STOPPING COEFFICIENT FOR EACH TRIPLET
C OF BEAM ENERGY, ION DENSITY AND ION TEMPERATURE. IT USES
C A ONE-WAY CUBIC SPLINE FOR THE TEMPERATURE AND A TWO-WAY
C CUBIC SPLINE FOR THE ENERGY/DENSITY PAIR TO DETERMINE THE
C STOPPING COEFFICIENT FROM THE INPUT DATA SET. IF A VALUE
C CANNOT BE INTERPOLATED USING SLPINES THEN IT IS
C EXTRAPOLATED BY 'XXSPLN'.
C
C CALLING PROGRAM: SBMS / ADAS304
C
C SUBROUTINE:
C
C INPUT : (I*4) MXBE      = MAXIMUM NUMBER OF BEAM ENERGIES WHICH CAN
C                        BE READ.
C INPUT : (I*4) MXTD      = MAXIMUM NUMBER OF TARGET DENSITIES WHICH
C                        CAN BE READ.
C INPUT : (I*4) MXTT      = MAXIMUM NUMBER OF TARGET TEMPERATURES
C                        WHICH CAN BE READ.
C INPUT : (I*4) MXREQ      = MAXIMUM NUMBER OF REQUESTED TRIPLETS OF
C                        BEAM ENERGY, ION DENSITY AND ION TEMP.
C INPUT : (I*4) NREQ       = NUMBER OF REQUESTED TRIPLETS OF BEAM
C                        ENERGY, ION DENSITY AND ION TEMP.
C INPUT : (R*8) BMENGA()  = REQUESTED BEAM ENERGIES.
C                        UNITS: EV/AMU
C                        DIMENSION: NREQ
C INPUT : (R*8) DENSA()   = REQUESTED ION DENSITIES.
C                        UNITS: CM-3
C                        DIMENSION: NREQ
C INPUT : (R*8) TIA()     = REQUESTED ION TEMPERATURES.
C                        UNITS: EV
C                        DIMENSION: NREQ
C INPUT : (I*4) NSITYP    = NUMBER OF STOPPING ION TYPES.
C INPUT : (R*8) SVREF()   = STOPPING COEFFT. AT REFERENCE BEAM ENERGY,
C                        TARGET DENSITY AND TEMPERATURE.
C                        UNITS: CM3 S-1
C                        DIMENSION: NSITYP
C INPUT : (I*4) NBE()     = NUMBER OF BEAM ENERGIES.
C                        DIMENSION: NSITYP
C INPUT : (R*8) BE(,)     = BEAM ENERGIES.
C                        UNITS: EV/AMU
C                        1ST DIMENSION: MXBE
C                        2ND DIMENSION: NSITYP
C INPUT : (I*4) NTDENS()  = NUMBER OF TARGET DENSITIES.
C                        DIMENSION: NSITYP
C INPUT : (R*8) TDENS(,)  = TARGET DENSITIES.
C                        UNITS: CM-3
C                        1ST DIMENSION: MXTD
C                        2ND DIMENSION: NSITYP
C INPUT : (I*4) NTTEMP()  = NUMBER OF TARGET TEMPERATURES.
C                        DIMENSION: NSITYP
C INPUT : (R*8) TTEMP(,)  = TARGET TEMPERATURES.
C                        UNITS: EV
C                        1ST DIMENSION: MXTT
C                        2ND DIMENSION: NSITYP
C INPUT : (R*8) SVT(,)    = STOPPING COEFFT. AT REFERENCE BEAM ENERGY
C                        AND TARGET DENSITY.
C                        UNITS: CM3 S-1
C                        1ST DIMENSION: MXTT
C                        2ND DIMENSION: NSITYP
C INPUT : (R*8) SVED(,,)  = STOPPING COEFFT. AT REFERENCE TARGET
C                        TEMPERATURE.
C                        UNITS: CM3 S-1
C                        1ST DIMENSION: MXBE
C                        2ND DIMENSION: MXTD
C                        3RD DIMENSION: NSITYP
C OUTPUT: (R*8) SVREQ(,)  = STOPPING COEFFT. AT REQUESTED BEAM ENERGY,
C                        ION DENSITY AND ION TEMPERATURE.
C                        UNITS: CM3 S-1
C                        1ST DIMENSION: MXREQ
C                        2ND DIMENSION: NSITYP
C OUTPUT: (L*4) LIBMA(,)  = FLAGS IF INTERPOLATION OR EXTRAPOLATION
C                        USED FOR REQUESTED BEAM ENERGIES.
C                        .TRUE. => INTERPOLATION USED.
C                        .FALSE. => EXTRAPOLATION USED.
C                        1ST DIMENSION: MXREQ
C                        2ND DIMENSION: NSITYP
C OUTPUT: (L*4) LIDNA(,)  = FLAGS IF INTERPOLATION OR EXTRAPOLATION
C                        USED FOR REQUESTED ION DENSITIES.
C                        .TRUE. => INTERPOLATION USED.
C                        .FALSE. => EXTRAPOLATION USED.
C                        1ST DIMENSION: MXREQ
C                        2ND DIMENSION: NSITYP
C OUTPUT: (L*4) LITIA(,)  = FLAGS IF INTERPOLATION OR EXTRAPOLATION
C                        USED FOR REQUESTED ION TEMPERATURES.
C                        .TRUE. => INTERPOLATION USED.
C                        .FALSE. => EXTRAPOLATION USED.
C                        1ST DIMENSION: MXREQ
C                        2ND DIMENSION: NSITYP
C
C PARAM : (I*4) MXI       = MAX. NO. OF STOPPING ION TYPES >= NSITYP.
C PARAM : (I*4) MXIN      = MAX. NO. OF INPUT DATA SET VALUES
C                        >= MXBE , MXTD , MXTT.
C PARAM : (I*4) MXOUT     = MAX. NO. OF OUTPUT VALUES >= NREQ.
C
C (I*4) IOPT             = DEFINES THE BOUNDARY DERIVATIVES FOR THE

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C          SPLINE ROUTINE 'XXSPLE'. SEE 'XXSPLE'.
C          ( VALID VALUES = <0, 0, 1, 2, 3, 4 )
C          (I*4) NOUT      = NUMBER OF OUTPUT VALUES FOR SPLINE.
C          (I*4) I        = LOOP INDEX.
C          (I*4) J        = LOOP INDEX.
C          (I*4) K        = LOOP INDEX.
C
C          (I*4) LSETX    = FLAGS TO SPLINE ROUTINE 'XXSPLE' IF
C          SPLINE PARAMETERS SHOULD BE SET UP.
C          .TRUE. => SET UP SPLINE PARAMS.
C          .FALSE. => DO NOT SET UP SPLINE PARAMS.
C
C          (R*8) DY()     = SPLINE INTERPOLATED DERIVATIVES.
C          DIMENSION: MXIN
C          (R*8) YOUT()   = Y OUTPUT ARRAY FROM SPLINE ROUTINE.
C          DIMENSION: MXOUT
C
C          (R*8) SVTO(,)  = STOPPING COEFFICIENTS AT REQUESTED ION
C          TEMPERATURES.
C          1ST DIMENSION: MXOUT
C          2ND DIMENSION: MXI
C          (R*8) SVEDO(,) = STOPPING COEFFICIENTS AT REQUESTED BEAM
C          ENERGIES AND ION DENSITY.
C          1ST DIMENSION: MXOUT
C          2ND DIMENSION: MXI
C          (R*8) YPASS(,) = STOPPING COEFFICIENTS AT REQUESTED BEAM
C          ENERGIES.
C          1ST DIMENSION: MXIN
C          2ND DIMENSION: MXOUT
C          (R*8) FACT1    = WEIGHTING FACTOR ASSOCIATED WITH THE
C          EVALUATION OF AN EFFECTIVE DENSITY.
C          (R*8) FACT2    = SIMILAR TO THAT OF FACT1.
C          (I*4) ITZ()    = ARRAY CONTAINING THE NUCLEAR CHARGE OF
C          EACH IMPURITY CONSIDERED.
C
C ROUTINES:
C          ROUTINE      SOURCE      BRIEF DESCRIPTION
C          -----
C          I4UNIT      ADAS        RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C          XXSPLE      ADAS        SPLINE SUBROUTINE (EXTENDED DIAGNOSTICS)
C          R8FUN1      ADAS        PERFORMS TRANSFORMATION ( X -> X )
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/87
C          JET EXT. 5183
C
C DATE:    10/12/93
C
C UNIX-IDL PORT:
C
C VERSION: 1.1          DATE: 16-11-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - FIRST VERSION
C
C VERSION: 1.2
C MODIFIED: HARVEY ANDERSON
C          - THE BEAM STOPPING COEFFICIENT FOR EACH
C          INDIVIDUAL IMPURITY WAS BEING EVALUATED
C          AT THE WRONG DENSITY. THE BEAM STOPPING
C          COEFFICIENT SHOULD BE EVALUATED AT AN
C          EFFECTIVE DENSITY. THIS HAS BEEN CORRECTED.
C          - THE TARGET DENSITY READ FROM ADF21 FILE IS THE
C          ELECTRON DENSITY. THE CORRECTION TO THE EVALUATION
C          OF THE EFFECTIVE DENSITY WAS DONE IN TERMS OF THE
C          ION DENSITY. THIS WAS CORRECTED SO THAT THE EFFECTIVE
C          DENSITY IS EVALUATED IN TERMS OF THE ELECTRON DENSITY.
C          20/12/96
C          - INTRODUCED THE PARAMETER FACT2, TO ENABLE THE
C          EFFECTIVE ELECTRON DENSITY TO BE EVALUATED. ORIGINALLY
C          THE USER WOULD ENTER THE TOTAL ION DENSITY AND
C          THE STOPPING COEFFICIENTS WOULD BE EVALUATED AT AN
C          EFFECTIVE ELECTRON DENSITY. NOW THE CODE HAS BEEN
C          CHANGED TO ALLOW THE USER TO ENTER THE TOTAL ELECTRON
C          DENSITY.
C
C -----
C
C          INTEGER      I4UNIT
C
C          EXTERNAL     R8FUN1
C          REAL*8        R8FUN1
C
C          INTEGER      MXI      , MXIN      , MXOUT
C          PARAMETER( MXI = 10 , MXIN = 25 , MXOUT = 25 )
C
C          INTEGER      MXBE      , MXTD      , MXTT      , MXREQ      ,
C          &            NREQ      , NSITYP
C          INTEGER      IOPT      , NOUT      , I          , J          , K
C
C          LOGICAL      LSETX
C
C          INTEGER      NBE(NSITYP) , NTDENS(NSITYP) , NTEMP(NSITYP) ,
C          &            ITZ(10)
C
C          REAL*8       BMENGA(NREQ) , DENSA(NREQ) , TIA(NREQ) ,
C          &            SVREF(NSITYP)
C          REAL*8       DY(MXIN) , YOUT(MXOUT) , FACT1
C
C -----

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REAL*8    BE(MXBE,NSITYP) , TDENS(MXTD,NSITYP) ,
&         TTEMP(MXTT,NSITYP) , SVT(MXTT,NSITYP) ,
&         SVREQ(MXREQ,NSITYP)
REAL*8    SVTO(MXOUT,MXI) , SVEDO(MXOUT,MXI) ,
&         YPASS(MXIN,MXOUT)
-----
LOGICAL   LIBMA(MXREQ,NSITYP) , LIDNA(MXREQ,NSITYP) ,
&         LITIA(MXREQ,NSITYP)
-----
REAL*8    SVED(MXBE,MXTD,NSITYP) , FACT2
-----

```

## C6AJTB

```

SUBROUTINE C6AJTB( MXJSHL , IZ1 , NU , LU , NL , LL , AA )
C
C   IMPLICIT NONE
C
C-----
C ***** FORTRAN77 SUBROUTINE: C6AJTB *****
C
C PURPOSE:  CALCULATES HYDRONIC LJ RESOLVED A-VALUES.
C
C           THE SUBROUTINE CHECKS TO SEE IF A-VALUE IS POSSIBLE AND
C           DIPOLE ALLOWED AND RETURNS ZEROES IF NOT.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) IZ1    = ION CHARGE.
C INPUT : (I*4) NU    = UPPER PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) LU    = ORBITAL QUANTUM NUMBER FOR NU.
C INPUT : (I*4) NL    = LOWER PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) LL    = ORBITAL QUANTUM NUMBER FOR NL.
C
C OUTPUT: (R*8) AA()  = LJ RESOLVED A-VALUE.
C                   DIMENSION: TRANSITION INDEX WHERE:
C                   1 GIVES LU+0.5 --> LL+0.5
C                   2 GIVES LU+0.5 --> LL-0.5
C                   3 GIVES LU-0.5 --> LL+0.5
C                   4 GIVES LU-0.5 --> LL-0.5
C
C (I*4) I          = LOOP INDEX.
C
C (R*8) A          = L RESOLVED A VALUE.
C (R*8) XLU        = REAL VALUE = LU.
C
C ROUTINES:
C   ROUTINE   SOURCE   BRIEF DESCRIPTION
C-----
C   R8ATAB    ADAS     RETURNS L RESOLVED HYDRONIC A-VALUE.
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C         K1/0/81
C         JET EXT. 5183
C
C DATE:    08/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR:  WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:    22ND MAY 1996
C
C VERSION: 1.1                      DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C           - FIRST VERSION. IBM VERSION NOT CHANGED
C
C-----
C
C   REAL*8    R8ATAB
C-----
C   INTEGER   MXJSHL , IZ1 , NU , LU , NL ,
&           LL
C   INTEGER   I
C-----
C   REAL*8    A , XL
C-----
C   REAL*8    AA(2*MXJSHL)
C-----

```

## C6CHRG

```

SUBROUTINE C6CHRG( SYMBD , IZD , SYMBR , IZR , IDZ0 ,
&               IRZ0 , IRZ1 , IRZ2 , NGRND , NBOT

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```

C      &      )
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C6CHRG *****
C
C PURPOSE:  SETS UP NUCLEAR CHARGE OF DONOR AND NULEAR, INITIAL AND
C           FINAL CHARGES OF RECEIVER. CHECKS VALIDITY OF RECEIVER
C           CHARGES. ALSO SETS GROUND STATE N LEVEL AND LOWEST N LEVEL
C           FOR TABULAR OUTPUTS.
C
C CALLING PROGRAM: ADAS306
C
C INPUT  : (C*2)  SYMBD  = DONOR ELEMENT SYMBOL.
C INPUT  : (I*4)  IZD    = DONOR ION CHARGE.
C INPUT  : (C*2)  SYMBR  = RECEIVER ELEMENT SYMBOL.
C INPUT  : (I*4)  IZR    = RECEIVER ION CHARGE.
C
C OUTPUT: (I*4)  IDZ0   = DONOR NUCLEAR CHARGE.
C OUTPUT: (I*4)  IRZ0   = RECEIVER NUCLEAR CHARGE.
C OUTPUT: (I*4)  IRZ1   = RECEIVER ION INITIAL CHARGE.
C OUTPUT: (I*4)  IRZ2   = RECEIVER ION FINAL CHARGE.
C OUTPUT: (I*4)  NGRND  = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C OUTPUT: (I*4)  NBOT   = MINIMUM PRINCIPAL QUANTUM NUMBER.
C
C ROUTINES:
C           ROUTINE      SOURCE      BRIEF DESCRIPTION
C-----
C           I4UNIT      ADAS        RETURNS UNIT NO. FOR OUTPUT MESSAGES
C           CXCHRG      ADAS        RETURNS DONOR NUCLEAR CHARGE AND
C                                     RECEIVER NULEAR, INITIAL AND FINAL
C                                     CHARGES.
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/81
C          JET EXT. 5183
C
C DATE:    11/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR:  WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:    22ND MAY 1996
C
C VERSION: 1.1                      DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C          - FIRST VERSION. NO CHANGES FROM IBM VERSION.
C-----
C-----
C           INTEGER      I4UNIT
C-----
C           INTEGER      IZR      , IZD      , IDZ0      , IRZ0      , IRZ1      ,
C           &            IRZ2      , NGRND      , NBOT
C-----
C           CHARACTER    SYMBD*2  , SYMBR*2
C-----

```

## C6EMIS

```

      SUBROUTINE C6EMIS( MXNSHL , MXJSHL , MXOBSL , MXPRSL ,
&                      IZ0      , IZ1      , NGRND  , NTOT   ,
&                      NBOT    , DENSZ    , DENS    , NOLINE  ,
&                      NU      , NL      , EMISA   , NPLINE  ,
&                      NPU     , NPL     , QTHEOR  , FTHEOR  ,
&                      QTHIN   , TBQMEEP , TBQMEMP , TBQMIP  ,
&                      TBQMIM  , TBFMP   , TBFM    , TBFMM   ,
&                      NUMIN   , NUMAX   , EM      , QEX    ,
&                      TOTPOP  , TOTEMI  , AVRGWL  , QEFF   ,
&                      TBLPOP  , TBLEMI  , TBLWLN
&                      )
C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C6EMIS *****
C
C PURPOSE:  PREDICTS THE J-RESOLVED EMMISIVITY FOR REQUESTED
C           TRANSITIONS.
C
C CALLING PROGRAM: ADAS306
C
C INPUT  : (I*4)  MXNSHL  = MAXIMUM NUMBER OF N SHELLS.
C INPUT  : (I*4)  MXJSHL  = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT  : (I*4)  MXOBSL  = MAXIMUM NUMBER OF OBSERVED SPECTRUM
C                           LINES.
C INPUT  : (I*4)  MXPRSL  = MAXIMUM NUMBER OF SPECTRUM LINES TO
C                           PREDICT.
C

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```

C INPUT : (I*4) IZ0 = NUCLEAR CHARGE.
C INPUT : (I*4) IZ1 = ION CHARGE.
C INPUT : (I*4) NGRND = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) NTOT = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND
C STATE.
C INPUT : (I*4) NBOT = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) DENSZ = PLASMA ION DENSITY.
C UNITS: CM-3
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C UNITS: CM-3
C INPUT : (I*4) NOLINE = NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8) EMISA() = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NPLINE = NUMBER OF SPECTRUM LINES TO PREDICT.
C INPUT : (I*4) NPU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (I*4) NPL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) QTHEOR() = MEAN CHARGE EXCHANGE, EXCITATION RATE OR
C RECOMBINATION RATE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) FTHEOR(,) = FRACTION OF N-LEVEL MEAN CHARGE EXCHANGE,
C EXCITATION RATE OR RECOMBINATION RATE
C COEFFICIENTS IN NL-LEVEL.
C 1ST DIMENSION: J SHELL INDEX WHERE:
C 1 GIVES J=L+0.5
C 2 GIVES J=L-0.5
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) QTHIN() = IONISATION RATE COEFFICIENT.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) TBQMEP(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMEM(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIP(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIM(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMP(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NLJ'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C OUTPUT: (I*4) NUMIN = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER
C FOR OBSERVED SPECTRUM LINES.
C OUTPUT: (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER
C FOR OBSERVED SPECTRUM LINES.
C OUTPUT: (R*8) EM = EMISSION MEASURE.
C OUTPUT: (R*8) QEX() =
C DIMENSION: MXNSHL.
C OUTPUT: (R*8) TOTPOP() = TOTAL COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TOTEMI() = TOTAL COLLISION EMISSIVITIES FOR PREDICTED
C SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) AVRGWL() = AVERAGE AIR WAVELENGTH FOR PREDICTED
C SPECTRUM LINE.
C UNITS: A
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) QEFF() = EFF. RATE COEFFICIENT FOR PREDICTED
C SPECTRUM LINE.
C UNITS:
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TBLPOP(,,) = TABLE OF COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C 1ST DIMENSION: J->J' TRANSITION INDEX.

```

```

C
C OUTPUT: (R*8) TBLEMI(,,) = 2ND DIMENSION: REFERENCED BY I4IDLI().
C TABLE OF COLLISION EMISSIVITIES FOR
C PREDICTED SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDLI().
C 3RD DIMENSION: PREDICTED LINE INDEX.
C
C OUTPUT: (R*8) TBLWLN(,,) = TABLE OF WAVELENGTHS FOR PREDICTED
C SPECTRUM LINE.
C UNITS: A
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDLI().
C 3RD DIMENSION: PREDICTED LINE INDEX.
C
C PARAM : (I*4) MXN = MXNSHL.
C PARAM : (I*4) MXJ = MXJSHL.
C PARAM : (I*4) MXOB = MXOBSL.
C
C (I*4) NREP =
C (I*4) IC = LOOP INDEX.
C
C (I*4) ICREP() =
C DIMENSION: MXOB.
C
C (R*8) WHICH(,) =
C 1ST DIMENSION: J SHELL INDEX.
C 2ND DIMENSION: REFERENCED BY L+1.
C
C (R*8) WLOW(,,) =
C 1ST DIMENSION: J SHELL INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C 3RD DIMENSION: REFERENCED BY L+1.
C
C ROUTINES:
C
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C C6WFIL ADAS
C C6EMQX
C C6PRSL ADAS PREDICTS REQUESTED SPECTRUM LINES.
C
C NOTES:
C 1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C 1 : J=L+0.5 -> J'=L'+0.5
C 2 : J=L+0.5 -> J'=L'-0.5
C 3 : J=L-0.5 -> J'=L'+0.5
C 4 : J=L-0.5 -> J'=L'-0.5
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 10/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. IBM VERSION NOT CHANGED
C
C -----
C
C INTEGER I4UNIT
C
C -----
C INTEGER MXN , MXJ , MXOB
C PARAMETER( MXN = 20 , MXJ = 2 , MXOB = 10 )
C
C -----
C INTEGER MXNSHL , MXJSHL ,
C & MXOBSL , MXPRSL , IZO , IZ1 ,
C & NGRND , NTOT , NBOT , NOLINE ,
C & NPLINE , NUMIN , NUMAX
C INTEGER NREP , IC
C
C -----
C REAL*8 DENSZ , DENS , EM
C
C -----
C INTEGER NU(MXOBSL) , NL(MXOBSL) , NPU(MXPRSL) ,
C & NPL(MXPRSL)
C INTEGER ICREP(MXOB)
C
C -----
C REAL*8 EMISA(MXOBSL) , QTHEOR(MXNSHL) , QTHIN(MXNSHL) ,
C & QEX(MXNSHL) , TOTPOP(MXPRSL) , TOTEMI(MXPRSL) ,
C & AVRGWL(MXPRSL) , QEFF(MXPRSL)
C
C -----
C REAL*8 FTHEOR(MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBQMEP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBQMEM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBFMP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBFM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBFMM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2)
C REAL*8 WHICH(MXJ, (MXN*(MXN+1))/2)
C
C -----
C REAL*8 TBLPOP(2*MXJSHL, 2*MXNSHL-3, MXPRSL) ,

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&          TBLEMI(2*MXJSHL,2*MXNSHL-3,MXPRSL)
&          TBLWLN(2*MXJSHL,2*MXNSHL-3,MXPRSL)
REAL*8     WLOW(MXJ,(MXN*(MXN+1))/2,MXN)
C-----

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## C6EMQX

```

SUBROUTINE C6EMQX( MXNSHL , MXJSHL , MXOBSL , IZ1 ,
&                NBOT , NUMIN , NUMAX , NU ,
&                NL , EMISA , NREP , ICREP ,
&                QTHEOR , WLOW , EM , QEX
&                )
C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C6EMQX *****
C
C PURPOSE:
C
C CALLING PROGRAM: C6EMIS
C
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) MXOBSL = MAXIMUM NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) IZ1    = ION CHARGE.
C INPUT : (I*4) NBOT   = MINIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NUMIN  = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                      OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NUMAX  = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                      OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NU( )  = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF
C                      OBSERVED SPECTRUM LINES.
C                      DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NL( )  = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF
C                      OBSERVED SPECTRUM LINES.
C                      DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8) EMISA( ) = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C                      LINES.
C                      DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NREP   =
C INPUT : (I*4) ICREP( ) =
C                      DIMENSION: MXOBSL.
C INPUT : (R*8) QTHEOR( ) = MEAN CHARGE EXCHANGE, EXCITATION RATE OR
C                      RECOMBINATION RATE COEFFICIENTS FOR
C                      N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C                      UNITS: CM3 SEC-1
C                      DIMENSION: N SHELL INDEX.
C INPUT : (R*8) WLOW( , , ) =
C                      1ST DIMENSION: J SHELL INDEX.
C                      2ND DIMENSION: REFERENCED BY I4IDPL(N,L).
C                      3RD DIMENSION: REFERENCED BY L+1.
C
C OUTPUT: (R*8) EM     = EMISSION MEASURE.
C OUTPUT: (R*8) QEX( ) =
C                      DIMENSION: MXNSHL.
C
C PARAM : (I*4) MXN    = MXNSHL.
C PARAM : (I*4) MXJ    = MXJSHL.
C PARAM : (I*4) MXOB   = MXOBSL.
C
C      (I*4) N        = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C      (I*4) L        = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C      (I*4) N1       = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C      (I*4) L1       = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C      (I*4) IDL      = TABLE INDEX.
C      (I*4) IC       = ARRAY INDEX.
C      (I*4) IC1      = ARRAY INDEX.
C      (I*4) IC2      = ARRAY INDEX.
C      (I*4) IFAIL    = RETURN FLAG FROM NAG ROUTINE.
C      (I*4) M        = LOOP INDEX.
C      (I*4) I        = LOOP INDEX.
C      (I*4) J        = ARRAY INDEX.
C
C      (R*8) XM       = REAL VALUE = M.
C      (R*8) X1       =
C      (R*8) X2       =
C      (R*8) T1       =
C      (R*8) T2       =
C      (R*8) SUM      =
C      (R*8) SUMEX    =
C      (R*8) SUMTH    =
C
C      (I*4) JLIST( ) =
C                      DIMENSION: MXN.
C
C      (R*8) AA( )    = LJ RESOLVED A-VALUE.
C                      DIMENSION: TRANSITION INDEX WHERE:
C                      1 GIVES LU+0.5 --> LL+0.5
C                      2 GIVES LU+0.5 --> LL-0.5
C                      3 GIVES LU-0.5 --> LL+0.5
C                      4 GIVES LU-0.5 --> LL-0.5

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C
C      (R*8)  REMISA( ) =
C              DIMENSION: MXOB.
C
C      (R*8)  REMQ( ) =
C              DIMENSION: MXOB.
C
C      (R*8)  WKSPACE( ) = WORKSPACE FOR NAG ROUTINE.
C              DIMENSION: MXOB.
C
C      (R*8)  EMQ( ) =
C              DIMENSION: MXNSHL.
C
C      (R*8)  CNDSA( , ) = CONDENSED MATRIX.
C              1ST DIMENSION: MXN.
C              2ND DIMENSION: 2.
C
C      (R*8)  ARED( , ) = LINEAR CONDENSATION TRANSFORMATION ARRAY.
C              1ST DIMENSION: MXN.
C              2ND DIMENSION: MXN.
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      I4UNIT      ADAS      RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C      I4IDFL      ADAS      RETURNS UNIQUE INDEX GIVEN QUANTUM
C      C6AJTB      ADAS      CALCULATES LJ RESOLVED A-VALUES.
CX      F04ARF      NAG      FINDS SOLUTION TO A SET OF REAL LINEAR
CX      EQUATIONS.
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/81
C          JET EXT. 5183
C
C DATE:    09/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR:  WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:    22ND MAY 1996
C
C VERSION: 1.1                      DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C          - FIRST VERSION. IBM VERSION NOT CHANGED
C
C VERSION: 1.2                      DATE: 29-05-96
C MODIFIED: WILLIAM OSBORN
C          - REMOVED UNUSED VARIABLES
C
C-----
C
C      INTEGER      I4UNIT      , I4IDFL
C-----
C      INTEGER      MXN          , MXJ          , MXOB
C      PARAMETER(  MXN = 20      , MXJ = 2       , MXOB = 10 )
C-----
C      INTEGER      MXNSHL      , MXJSHL      , MXOBSL      , IZ1          , NBOT          ,
C      &            NUMIN      , NUMAX      , NREP          ,
C      INTEGER      N          , L          , N1          , L1          , IDL          ,
C      &            IC          , IC1         , IC2         , M          ,
C      &            I          , J
C-----
C      REAL*8      EM
C      REAL*8      XM          , X1          , X2          , T1          , T2          ,
C      &            SUM          , SUMEX          , SUMTH
C-----
C      INTEGER      ICREP(MXOBSL) , NU(MXOBSL)   , NL(MXOBSL)
C      INTEGER      JLIST(MXN)
C-----
C      REAL*8      EMISA(MXOBSL) , QTHEOR(MXNSHL) , QEX(MXNSHL)
C      REAL*8      AA(2*MXJ)    , REMISA(MXOB)   , REMQ(MXOB)   ,
C      &            EMQ(MXN)
C      REAL*8      CNDSA(MXN,2)
C      &            ARED(MXOB,MXOB)
C      REAL*8      WLOW(MXJSHL,(MXNSHL*(MXNSHL+1))/2,MXNSHL)
C-----
C      INTEGER      PIPEIN      , PIPEOU
C      PARAMETER(  PIPEIN=5     , PIPEOU=6 )
C-----

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## C6OUT0

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SUBROUTINE C6OUT0( IWRITE , MXNSHL , MXJSHL , MXBEAM ,
&                MXOBSL , MXPRSL , MXTAB , NRTABS ,
&                NUMIN , NUMAX , NBOT , NTOP ,
&                NTAB , IDTAB , LRTTB , LRTABS ,
&                DATE , TITLE , DSFULL , SYMBD ,
&                IDZ0 , SYMBR , IRZ0 , IRZ1 ,
&                IRZ2 , RAMSNO , TEV , TIEV ,
&                DENS , DENSZ , ZEFF , BMAG ,
&                NBEAM , BMFRA , BMENA , NOLINE ,
&                NU , NL , EMISA , ITHEOR ,
&                IBSTAT , IEMMS , EM , QEX ,
&                TBLF , QTHEX , FTHEXJ , QTHCH ,

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&          FTHCHJ , QTHRC , FTHRCJ , QTHIN ,
&          TBQMFP , TBQMFM , TBQMIP , TBQMIM ,
&          TBFMP , TBFM , TBFMM , NPLINE ,
&          NPL , NPU , TOTPOP , TOTEMI ,
&          AVRGWL , QEFF , TBLPOP , TBLEMI ,
&          TBLWLN
&      )
C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C6OUT0 *****
C
C PURPOSE: WRITES TEXT OUTPUT TO FILE FOR ADAS306.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4) IWRITE = UNIT NUMBER FOR OUTPUT.
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) MXBEAM = MAXIMUM NUMBER OF BEAM COMPONENTS.
C INPUT : (I*4) MXOBSL = MAXIMUM NUMBER OF OBSERVED SPECTRUM
C                   LINES.
C INPUT : (I*4) MXPRSL = MAXIMUM NUMBER OF SPECTRUM LINES TO
C                   PREDICT.
C INPUT : (I*4) MXTAB = MAXIMUM NUMBER OF TABLES FOR OUTPUT.
C INPUT : (I*4) NRTABS = NUMBER OF INDIVIDUAL RATE TABLES.
C INPUT : (I*4) NUMIN = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER
C                   FOR OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER
C                   FOR OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NBOT = MINIMUM PRINCIPAL QUANTUM NUMBER FOR
C                   TABLES.
C INPUT : (I*4) NTOP = MAXIMUM PRINCIPAL QUANTUM NUMBER FOR
C                   TABLES.
C INPUT : (I*4) NTAB = NUMBER OF TABLES FOR OUTPUT.
C INPUT : (I*4) IDTAB() = LIST OF INDEXES OF TABLES FOR OUTPUT.
C                   DIMENSION: MXTAB
C INPUT : (L*4) LRTTB = FLAG FOR RATE TABLE PRINTING.
C                   .TRUE. = PRINT RATE TABLES.
C                   .FALSE. = DO NOT PRINT RATE TABLES.
C INPUT : (L*4) LRTABS() = FLAGS FOR INDIVIDUAL TABLES.
C                   INDEX: 1 = DIRECT CAPTURE TABLE.
C                   2 = FIELD DYNAMIC TABLE.
C                   3 = FIELD STATIC TABLE.
C                   4 = ION IMPACT TABLE.
C                   5 = ELECTRON IMPACT TABLE.
C INPUT : (C*8) DATE = DATE.
C INPUT : (C*40) TITLE = ISPF ENTERED GENERAL TITLE FOR RUN.
C INPUT : (C*80) DSFULL = FILE NAME OF INPUT DATA SET.
C INPUT : (C*2) SYMBD = DONOR ELEMENT SYMBOL.
C INPUT : (I*4) IDZ0 = DONOR NUCLEAR CHARGE.
C INPUT : (C*2) SYMBR = RECEIVER ELEMENT SYMBOL.
C INPUT : (I*4) IRZ0 = RECEIVER NUCLEAR CHARGE.
C INPUT : (I*4) IRZ1 = RECEIVER ION INITIAL CHARGE.
C INPUT : (I*4) IRZ2 = RECEIVER ION FINAL CHARGE.
C INPUT : (R*8) RAMSNO = RECEIVER ATOMIC MASS.
C INPUT : (R*8) TEV = ELECTRON TEMPERATURE.
C                   UNITS: EV
C INPUT : (R*8) TIEV = ION TEMPERATURE.
C                   UNITS: EV
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C                   UNITS: CM-3
C INPUT : (R*8) DENSZ = PLASMA ION DENSITY.
C                   UNITS: CM-3
C INPUT : (R*8) ZEFF = EFFECTIVE ION CHARGE.
C INPUT : (R*8) BMAG = PLASMA MAGNETIC INDUCTION.
C                   UNITS: TESLA
C INPUT : (I*4) NBEAM = NUMBER OF BEAM ENERGIES.
C INPUT : (R*8) BMFRA() = BEAM COMPONENT FRACTIONS.
C                   DIMENSION: COMPONENT INDEX.
C INPUT : (R*8) BMENA() = BEAM ENERGY COMPONENTS.
C                   UNITS: EV/AMU
C                   DIMENSION: COMPONENT INDEX.
C INPUT : (I*4) NOLINE = NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C                   OF OBSERVED SPECTRUM LINES.
C                   DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C                   OF OBSERVED SPECTRUM LINES.
C                   DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8) EMISA() = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C                   LINES.
C                   DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) ITHEOR = CHARGE EXCHANGE MODEL OPTION.
C                   1 => USE INPUT DATA SET.
C                   2 => USE EIKONAL MODEL.
C INPUT : (I*4) IBSTAT = DONOR STATE FOR EIKONAL MODEL.
C                   1 => H(1S)
C                   2 => H(2S)
C                   3 => H(2P)
C                   4 => HE(1S2)
C                   5 => HE(1S2S)
C INPUT : (I*4) IEMMS = EMISSION MEASURE MODEL OPTION.
C                   1 => CHARGE EXCHANGE.
C                   2 => ELECTRON IMPACT EXCITATION.
C                   3 => RADIATIVE RECOMBINATION.

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```

C INPUT : (R*8) EM = EMISSION MEASURE.
C UNITS: CM-5
C INPUT : (R*8) QEX() =
C DIMENSION: MXNSHL.
C INPUT : (R*8) TBLF() = TABLE OF RADIATIVE LIFETIMES.
C UNITS: SECS
C DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) QTHEX() = MEAN EXCITATION RATE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) FTHEXJ(,) = FRACTION OF N-LEVEL MEAN EXCITATION RATE
C COEFFICIENTS IN NLJ-LEVEL.
C 1ST DIMENSION: J SHELL INDEX WHERE:
C 1 GIVES J=L+0.5
C 2 GIVES J=L-0.5
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) QTHCH() = MEAN CHARGE EXCHANGE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) FTHCHJ(,) = FRACTION OF N-LEVEL MEAN CHARGE EXCHANGE
C COEFFICIENTS IN NLJ-LEVEL.
C 1ST DIMENSION: J SHELL INDEX WHERE:
C 1 GIVES J=L+0.5
C 2 GIVES J=L-0.5
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) QTHRC() = MEAN RECOMBINATION RATE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) FTHRCJ(,) = FRACTION OF N-LEVEL MEAN RECOMBINATION
C RATE COEFFICIENTS IN NLJ-LEVEL.
C 1ST DIMENSION: J SHELL INDEX WHERE:
C 1 GIVES J=L+0.5
C 2 GIVES J=L-0.5
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) QTHIN() = IONISATION RATE COEFFICIENT.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) TBQMEP(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMEM(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIP(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIM(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMP(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NLJ'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (I*4) NPLINE = NUMBER OF SPECTRUM LINES TO PREDICT.
C INPUT : (I*4) NPU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (I*4) NPL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) TOTPOP() = TOTAL COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) TOTEMI() = TOTAL COLLISION EMISSIVITIES FOR PREDICTED
C SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) AVRGWL() = AVERAGE AIR WAVELENGTH FOR PREDICTED
C SPECTRUM LINE.
C UNITS: A
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) QEFF() = EFF. RATE COEFFICIENT FOR PREDICTED
C SPECTRUM LINE.
C UNITS:
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) TBLPOP(,,) = TABLE OF COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDLI().
C 3RD DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) TBLEMI(,,) = TABLE OF COLLISION EMISSIVITIES FOR

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C          PREDICTED SPECTRUM LINE.
C          UNITS: PH CM-2 SEC-1
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDLI().
C          3RD DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8)  TBLWLN(,,)= TABLE OF WAVELENGTHS FOR PREDICTED
C          SPECTRUM LINE.
C          UNITS: A
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDLI().
C          3RD DIMENSION: PREDICTED LINE INDEX.
C
C          (I*4)  N      = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C          (I*4)  L      = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C          (I*4)  J      = LOOP INDEX FOR J QUANTUM NUMBER INDEX.
C          (I*4)  JMX    = UPPER LIMIT ON 'J' LOOP.
C          (I*4)  N1     = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C          (I*4)  L1     = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C          (I*4)  J1     = LOOP INDEX FOR J QUANTUM NUMBER INDEX.
C          (I*4)  J1MX   = UPPER LIMIT ON 'J' LOOP.
C          (I*4)  IDL    = L-RESOLVED TABLE INDEX.
C          (I*4)  ID     = SPECTRUM LINE TABLE INDEX.
C          (I*4)  I      = LOOP INDEX.
C          (I*4)  K      = ARRAY INDEX.
C
C          (R*8)  XJ     = J QUANTUM NUMBER.
C          (R*8)  XJ1    = J QUANTUM NUMBER.
C
C          (C*80)  CADAS  = ADAS HEADER: INCLUDES RELEASE, PROGRAM,
C                       TIME.
C
C ROUTINES:
C ROUTINE      SOURCE      BRIEF DESCRIPTION
C -----
C I4IDFL       ADAS        RETURNS UNIQUE INDEX GIVEN QUANTUM
C                       NUMBERS N AND L.
C I4IDLI       ADAS        RETURNS INDEX FOR PREDICTED SPECTRUM
C                       LINE TABLES.
C
C NOTES:
C 1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C   1 : J=L+0.5 -> J'=L'+0.5
C   2 : J=L+0.5 -> J'=L'-0.5
C   3 : J=L-0.5 -> J'=L'+0.5
C   4 : J=L-0.5 -> J'=L'-0.5
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          KL/0/87
C          JET EXT. 5183
C
C DATE:    19/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR:  WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:    22ND MAY 1996
C
C VERSION: 1.1                      DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C          - FIRST VERSION. IBM VERSION NOT CHANGED
C
C VERSION: 1.2                      DATE: 24-11-98
C MODIFIED: RICHARD MARTIN & MARTIN OMULLANE
C          - CORRECTED WRITING OF ELECTRON & ION TEMPS. FROM
C          BEING WRITTED WRONG WAY ROUND.
C
C -----
C          INTEGER      I4IDFL      , I4IDLI
C -----
C          INTEGER      IWRITE      , MXNSHL      , MXJSHL      , MXBEAM      , MXOBSL      ,
C          &            MXPRSL      , MXTAB      , NRTABS      , NUMIN      , NUMAX      ,
C          &            NBOT      , NTOP      , NTAB      , IDZ0      , IRZ0      ,
C          &            IRZ1      , IRZ2      , NBEAM      , NOLINE      , ITHEOR      ,
C          &            IBSTAT      , IEMMS      , NPLINE
C          INTEGER      N      , L      , J      , JMX      , N1      ,
C          &            L1      , J1      , J1MX      , IDL      , ID      ,
C          &            I      , K
C -----
C          REAL*8      RAMSNO      , TEV      , TIEV      , DENS      , DENSZ      ,
C          &            ZEFF      , BMAG      , EM
C          REAL*8      XJ      , XJ1
C -----
C          LOGICAL      LRTTB
C -----
C          CHARACTER   DATE*8      , TITLE*40      , DSFULL*80      , SYMBR*2      ,
C          &            SYMBD*2
C          CHARACTER   CADAS*80
C -----
C          INTEGER      IDTAB(MXTAB)      , NU(MXOBSL)      , NL(MXOBSL)      ,
C          &            NPU(MXPRSL)      , NPL(MXPRSL)
C -----
C          REAL*8      BMFRA(MXBEAM)      , BMENA(MXBEAM)      , QEX(MXNSHL)      ,
C          &            QTHCH(MXNSHL)      , QTHX(MXNSHL)      , QTHIN(MXNSHL)      ,
C          &            QTHRC(MXNSHL)      , EMISA(MXOBSL)      , TOTPOP(MXPRSL)      ,
C          &            TOTEMI(MXPRSL)      , AVRGWL(MXPRSL)      , QEFF(MXPRSL)      ,

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&          TBLF((MXNSHL*(MXNSHL+1))/2)
C-----
LOGICAL    LRTABS(NRTABS)
C-----
REAL*8     FTHCHJ(MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          FTHEXJ(MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          FTHRCJ(MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          TBQMEP(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          TBQMEM(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          TBQMIP(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          TBQMIM(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          TBFMP(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          TBFMM(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
&          TBFM(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C-----
REAL*8     TBLPOP(2*MXJSHL,2*MXNSHL-3,MXPRSL) ,
&          TBLEMI(2*MXJSHL,2*MXNSHL-3,MXPRSL) ,
&          TBLWLN(2*MXJSHL,2*MXNSHL-3,MXPRSL)
C-----
SAVE       CADAS
C-----
DATA       CADAS / ' ' /
C-----

```

## C6OUTG

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SUBROUTINE C6OUTG( MXNSHL , MXJSHL , MXBEAM , MXOBSL ,
&                MXPRSL , MXGRF , NGFPLN , NGRF ,
&                IDGRF , LPLT1 , LGRD1 , LDEF1 ,
&                DATE , TITLE , DSFULL , SYMBD ,
&                IDZ0 , SYMBR , IRZ0 , IRZ1 ,
&                IRZ2 , RAMSNO , TEV , TIEV ,
&                DENS , DENSZ , ZEFF , BMAG ,
&                NBEAM , BMFRA , BMENA , NOLINE ,
&                NU , NL , EMISA , ITHEOR ,
&                IBSTAT , IEMMS , NPLINE , NPU ,
&                NPL , XLG , XUG , YLG ,
&                YUG , QEFF , TBLEMI , TBLWLN ,
&                LGHOST
)
C
C      IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C6OUTG *****
C
C PURPOSE: PLOTS EMISSIVITY GRAPHS FOR ADAS306.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) MXBEAM = MAXIMUM NUMBER OF BEAM COMPONENTS.
C INPUT : (I*4) MXOBSL = MAXIMUM NUMBER OF OBSERVED SPECTRUM
C                   LINES.
C INPUT : (I*4) MXPRSL = MAXIMUM NUMBER OF SPECTRUM LINES TO
C                   PREDICT.
C INPUT : (I*4) MXGRF = MAXIMUM NUMBER OF GRAPHS FOR OUTPUT.
C INPUT : (I*4) NGFPLN = NUMBER OF GRAPHS PER PREDICTED SPECTRUM
C                   LINE.
C INPUT : (I*4) NGRF = NUMBER OF GRAPHS FOR OUTPUT.
C INPUT : (I*4) IDGRF( ) = LIST OF INDEXES OF GRAPHS FOR OUTPUT.
C                   DIMENSION: MXGRF
C INPUT : (L*4) LPLT1 = FLAGS WHETHER TO PLOT GRAPHS ON SCREEN.
C                   .TRUE. => PLOT GRAPHS ON SCREEN.
C                   .FALSE. => DO NOT PLOT GRAPHS ON SCREEN.
C INPUT : (L*4) LGRD1 = FLAGS WHETHER TO PUT GRAPHS IN GRID FILE.
C                   .TRUE. => PUT GRAPHS IN GRID FILE
C                   .FALSE. => DO NOT PUT GRAPHS IN GRID FILE
C INPUT : (L*4) LDEF1 = FLAGS DEFAULT GRAPH SCALING
C                   .TRUE. => USE DEFAULT GRAPH SCALING.
C                   .FALSE. => DO NOT USE DEFAULT SCALING.
C INPUT : (C*8) DATE = DATE.
C INPUT : (C*40) TITLE = ISPF ENTERED GENERAL TITLE FOR RUN.
C INPUT : (C*80) DSFULL = FILE NAME OF INPUT DATA SET.
C INPUT : (C*2) SYMBD = DONOR ELEMENT SYMBOL.
C INPUT : (I*4) IDZ0 = DONOR NUCLEAR CHARGE.
C INPUT : (C*2) SYMBR = RECEIVER ELEMENT SYMBOL.
C INPUT : (I*4) IRZ0 = RECEIVER NUCLEAR CHARGE.
C INPUT : (I*4) IRZ1 = RECEIVER ION INITIAL CHARGE.
C INPUT : (I*4) IRZ2 = RECEIVER ION FINAL CHARGE.
C INPUT : (R*8) RAMSNO = RECEIVER ATOMIC MASS.
C INPUT : (R*8) TEV = ELECTRON TEMPERATURE.
C                   UNITS: EV
C INPUT : (R*8) TIEV = ION TEMPERATURE.
C                   UNITS: EV
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C                   UNITS: CM-3
C INPUT : (R*8) DENSZ = PLASMA ION DENSITY.
C                   UNITS: CM-3
C INPUT : (R*8) ZEFF = EFFECTIVE ION CHARGE.
C INPUT : (R*8) BMAG = PLASMA MAGNETIC INDUCTION.

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C
C INPUT : (I*4) NBEAM = UNITS: TESLA
C INPUT : (R*8) BMFRA() = NUMBER OF BEAM ENERGIES.
C = BEAM COMPONENT FRACTIONS.
C DIMENSION: COMPONENT INDEX.
C INPUT : (R*8) BMENA() = BEAM ENERGY COMPONENTS.
C UNITS: EV/AMU
C DIMENSION: COMPONENT INDEX.
C INPUT : (I*4) NOLINE = NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8) EMISA() = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) ITHEOR = CHARGE EXCHANGE MODEL OPTION.
C 1 => USE INPUT DATA SET.
C 2 => USE EIKONAL MODEL.
C INPUT : (I*4) IBSTAT = DONOR STATE FOR EIKONAL MODEL.
C 1 => H(1S)
C 2 => H(2S)
C 3 => H(2P)
C 4 => HE(1S2)
C 5 => HE(1S2S)
C INPUT : (I*4) IEMMS = EMISSION MEASURE MODEL OPTION.
C 1 => CHARGE EXCHANGE.
C 2 => ELECTRON IMPACT EXCITATION.
C 3 => RADIATIVE RECOMBINATION.
C INPUT : (I*4) NPLINE = NUMBER OF SPECTRUM LINES TO PREDICT.
C INPUT : (I*4) NPU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (I*4) NPL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) XLG() = LOWER LIMIT FOR X-AXIS OF GRAPHS.
C DIMENSION: NGFPLN
C INPUT : (R*8) XUG() = UPPER LIMIT FOR X-AXIS OF GRAPHS.
C DIMENSION: NGFPLN
C INPUT : (R*8) YLG() = LOWER LIMIT FOR Y-AXIS OF GRAPHS.
C DIMENSION: NGFPLN
C INPUT : (R*8) YUG() = UPPER LIMIT FOR Y-AXIS OF GRAPHS.
C DIMENSION: NGFPLN
C INPUT : (R*8) QEFF() = EFF. RATE COEFFICIENT FOR PREDICTED
C SPECTRUM LINE.
C UNITS:
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) TBLEMI(,,) = TABLE OF COLLISION EMISSIVITIES FOR
C PREDICTED SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDLI().
C 3RD DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) TBLWLN(,,) = TABLE OF WAVELENGTHS FOR PREDICTED
C SPECTRUM LINE.
C UNITS: A
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDLI().
C 3RD DIMENSION: PREDICTED LINE INDEX.
C
C I/O : (L*4) LGHOST = INITIALISATION FLAG FOR GHOST80.
C .TRUE. => GHOST80 INITIALISED.
C .FALSE. => GHOST80 NOT INITIALISED.
C
C PARAM : (I*4) NDIV = NUMBER OF DIVISIONS ON X AXIS.
C PARAM : (I*4) MXA = MAXIMUM NUMBER OF DATA POINTS FOR GRAPH A.
C PARAM : (I*4) MXB = MAXIMUM NUMBER OF DATA POINTS FOR GRAPH B.
C
C PARAM : (R*8) ANGDIV = NO. OF ANGSTROMS PER DIVISION.
C
C (I*4) N = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) J = LOOP INDEX FOR J QUANTUM NUMBER INDEX.
C (I*4) JMX = UPPER LIMIT ON 'J' LOOP.
C (I*4) N1 = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L1 = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) J1 = LOOP INDEX FOR J QUANTUM NUMBER INDEX.
C (I*4) JIMX = UPPER LIMIT ON 'J' LOOP.
CX (I*4) IDL = L-RESOLVED TABLE INDEX.
C (I*4) NPTS = NO. OF EMISSIVITY AND WAVELENGTH VALUES.
C (I*4) ID = SPECTRUM LINE TABLE INDEX.
C (I*4) I = LOOP INDEX.
C (I*4) K = ARRAY INDEX.
C
C (R*8) CWLN = CENTRAL WAVELENGTH ON GRAPH.
C UNITS: A
C (R*8) ERATE = EFFECTIVE RATE COEFFICIENT.
C UNITS:
C
C (C*1) GRID = DUMMY NAME VARIABLE FOR USE WITH GHOST80.
C (C*1) PIC = DUMMY NAME VARIABLE FOR USE WITH GHOST80.
C
C (R*8) CEMIS() = COLUMN EMISSIVITIES.
C UNITS: PHOT CM-2 SEC-1
C DIMENSION: MXA
C (R*8) WAVLN() = WAVELENGTHS.

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```

C
C
C          UNITS: A
C          DIMENSION: MXA
C          (R*8) XA() = X DATA POINTS FOR GRAPH A.
C          DIMENSION: MXA
C          (R*8) YA() = Y DATA POINTS FOR GRAPH A.
C          DIMENSION: MXA
C          (R*8) XB() = X DATA POINTS FOR GRAPH B.
C          DIMENSION: MXB
C          (R*8) YB() = Y DATA POINTS FOR GRAPH B.
C          DIMENSION: MXB
C
C
C ROUTINES:
C
C          ROUTINE      SOURCE      BRIEF DESCRIPTION
C-----
C          I4UNIT      ADAS          RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C          I4IDFL      ADAS          RETURNS UNIQUE INDEX GIVEN QUANTUM
CX          NUMBERS N AND L.
CX          I4IDLI      ADAS          RETURNS INDEX FOR PREDICTED SPECTRUM
C          LINE TABLES.
C          CXGFIL      ADAS          FILLS ADAS306 / 308 GRAPH ARRAYS.
C          CXGEMI      ADAS          PLOTS ADAS306 / 308 EMISSIVITY GRAPHS.
C          GHOST80     VARIOUS SUBROUTINES.
C
C
C NOTES:
C
C          1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C
C              1 : J=L+0.5 -> J'=L'+0.5
C              2 : J=L+0.5 -> J'=L'-0.5
C              3 : J=L-0.5 -> J'=L'+0.5
C              4 : J=L-0.5 -> J'=L'-0.5
C
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/87
C          JET EXT. 5183
C
C
C DATE:    24/11/93
C
C
C UNIX-IDL PORT:
C
C AUTHOR:  WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C
C DATE:    22ND MAY 1996
C
C
C
C VERSION: 1.1                      DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C          - FIRST VERSION. IBM VERSION NOT CHANGED
C
C
C VERSION: 1.2                      DATE: 29-05-96
C MODIFIED: WILLIAM OSBORN
C          - REMOVED UNUSED VARIABLES
C
C
C VERSION: 1.3                      DATE: 29-05-96
C MODIFIED: WILLIAM OSBORN
C          - S.C.C.S. MISTAKE
C
C-----
C
C          INTEGER      I4UNIT      , I4IDLI
C-----
C          INTEGER      MXN          , MXJ          , NDIV
C          PARAMETER( MXN = 20      , MXJ = 2      , NDIV = 600 )
C          INTEGER      MXA          , MXB
C          PARAMETER( MXA = (2*MXJ-1)*(2*MXN-3) , MXB = NDIV )
C-----
C          REAL*8      ANGDIV
C          PARAMETER( ANGDIV = 0.096D0 )
C-----
C          INTEGER      MXNSHL      , MXJSHL      , MXBEAM      , MXOBSL      , MXPRSL      ,
C          &             MXGRF      , NGFPLN      , NGRF          , IDZ0          , IRZ0          ,
C          &             IRZ1          , IRZ2          , NBEAM          , NOLINE          , ITHEOR          ,
C          &             IBSTAT      , IEMMS          , NPLINE
C          INTEGER      N          , L          , J          , JMX          , N1          ,
C          &             L1          , J1          , J1MX          , NPTS          ,
C          &             ID          , I          , K
C-----
C          REAL*8      RAMSNO      , TEV          , TIEV          , DENS          , DENSZ          ,
C          &             ZEFF          , BMAG
C          REAL*8      CWLN          , ERATE
C-----
C          LOGICAL      LPLT1      , LGRD1          , LDEF1          , LGHOST
C-----
C          CHARACTER   DATE*8      , TITLE*40      , DSFULL*80      , SYMBD*2      ,
C          &             SYMBR*2
C          CHARACTER   GRID*1      , PIC*1
C-----
C          INTEGER      IDGRF(MXGRF) , NU(MXOBSL)      , NL(MXOBSL)      ,
C          &             NPU(MXPRSL)    , NPL(MXPRSL)
C-----
C          REAL*8      BMFRA(MXBEAM) , BMENA(MXBEAM) , EMISA(MXOBSL) ,
C          &             XLG(NGFPLN)    , XUG(NGFPLN) , YLG(NGFPLN) ,
C          &             YUG(NGFPLN)    , QEFF(MXPRSL)
C          REAL*8      CEMIS(MXA)   , WAVLN(MXA)   , XA(MXA)      ,
C          &             YA(MXA)        , XB(MXB)      , YB(MXB)
C-----
C          REAL*8      TBLEMI(2*MXJSHL,2*MXNSHL-3,MXPRSL) ,
C          &             TBLWLN(2*MXJSHL,2*MXNSHL-3,MXPRSL)
C-----
C          INTEGER      PIPEIN      , PIPEOU

```

```

PARAMETER( PIPEIN=5 , PIPEOU=6)
C-----
C DATA GRID / ' ' / ,
& PIC / ' ' /
C-----

```

## C6PMIN

```

SUBROUTINE C6PMIN( MXNSHL , MXJSHL , N , VD , VDS , VDI , RHS )
C
C IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C6PMIN *****
C
C PURPOSE: CALCULATES THE SOLUTION OF A TRIDIAGONAL PARTITIONED MATRIX
C ORGANISED SET OF SIMULTANEOUS EQUATIONS.
C
C THE PARTITIONS ARE 2X2 IN THE PRESENT IMPLEMENTATION. A
C VARIANT OF OF THE DOUBLE PASS ALGORITHM (IN A PARTITIONED
C MATRIX SENSE) IS USED WITH RECURRENCE IN TWO DIRECTIONS TO
C THE CENTRE AND BACK. THIS IS ANALOGOUS TO THE NAG ROUTINE
C F04EAF FOR AN ORDINARY TRIDAGONAL MATRIX THE INDEXING OF
C THE DIAG, SUPRADIAG AND INFRADIAG ELEMENTS FOLLOWS THAT OF
C THE NAG ROUTINE F04EAF.
C
C CALLING PROGRAM: C6WSOL
C
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) N = NUMBER OF PARTIONS ALONG THE DIAGONAL.
C INPUT : (R*8) VD( , ) = DIAGONAL PARTITION.
C 1ST DIMENSION: 2 * MXJSHL
C 2ND DIMENSION: N SHELL INDEX.
C INPUT : (R*8) VDS( , ) = SUPRADIAGONAL PARTITION.
C 1ST DIMENSION: 2 * MXJSHL
C 2ND DIMENSION: N SHELL INDEX.
C INPUT : (R*8) VDI( , ) = INFRADIAGONAL PARTITION.
C 1ST DIMENSION: 2 * MXJSHL
C 2ND DIMENSION: N SHELL INDEX.
C
C I/O : (R*8) RHS( , ) = INPUT: RIGHT HAND SIDE OF VECTOR PARTITION.
C OUTPUT: SOLUTION OF VECTOR PARTITION.
C 1ST DIMENSION: 2 * MXJSHL
C 2ND DIMENSION: N SHELL INDEX.
C
C PARAM : (I*4) MXJ = MXJSHL.
C (I*4) I = LOOP INDEX.
C (I*4) K =
C (R*8) UNIT( ) =
C DIMENSION: 4
C (R*8) W1( ) =
C DIMENSION: 4
C (R*8) W2( ) =
C DIMENSION: 4
CX (R*8) W3( ) =
CX DIMENSION: 4
C (R*8) VW1( ) =
C DIMENSION: 2
C (R*8) VW2( ) =
C DIMENSION: 2
C (R*8) TEMP( ) = TEMPORARY STORE.
C DIMENSION: 4
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C-----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C
C NOTES:
C 1) THE 2X2 PARTITIONS ARE STORED AS LINEAR VECTORS BY COLUMN
C IN THE 1ST DIMENSIONS OF VD( , ) , VDS( , ) , VDI( , ) .
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 11/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. IBM VERSION NOT CHANGED
C

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C VERSION: 1.2 DATE: 29-05-96
C MODIFIED: WILLIAM OSBORN
C - REMOVED UNUSED VARIABLES
C
C
C VERSION: 1.3 DATE: 29-05-96
C MODIFIED: WILLIAM OSBORN
C - S.C.C.S. MISTAKE
C
C
C-----
C
C INTEGER I4UNIT
C-----
C INTEGER MXJ
C PARAMETER( MXJ = 2 )
C-----
C INTEGER MXNSHL , MXJSHL , N
C INTEGER I , K
C-----
C REAL*8 VD(2*MXJSHL,MXNSHL) , VDS(2*MXJSHL,MXNSHL) ,
& VDI(2*MXJSHL,MXNSHL) , RHS(MXJSHL,MXNSHL)
C REAL*8 UNIT(2*MXJ) , W1(2*MXJ) , W2(2*MXJ) ,
& VW1(MXJ) , VW2(MXJ) ,
& TEMP(2*MXJ)
C-----
C DATA UNIT / 1.0D0 , 0.0D0 , 0.0D0 , 1.0D0 /
C-----

```

## C6PRSL

```

SUBROUTINE C6PRSL( MXNSHL , MXJSHL , MXPRSL , IZ0 ,
& IZ1 , NPLINE , NPU , NPL ,
& NUMAX , WHIGH , WLOW , EM ,
& QEX , TOTPOP , TOTEMI , AVRGWL ,
& QEFF , TBLPOP , TBLEMI , TBLWLN
& )
C
C IMPLICIT NONE
C
C-----
C ***** FORTRAN77 SUBROUTINE: C6PRSL *****
C
C PURPOSE: FILLS TABLES FOR REQUESTED PREDICTIONS OF SPECTRUM LINES.
C
C CALLING PROGRAM: C6EMIS
C
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) MXPRSL = MAXIMUM NUMBER OF SPECTRUM LINES TO
C PREDICT.
C INPUT : (R*8) IZ0 = NUCLEAR CHARGE.
C INPUT : (R*8) IZ1 = ION CHARGE.
C INPUT : (I*4) NPLINE = NUMBER OF SPECTRUM LINES TO PREDICT.
C INPUT : (I*4) NPU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (I*4) NPL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER
C FOR OBSERVED SPECTRUM LINES.
C INPUT : (R*8) WHIGH( , ) =
C 1ST DIMENSION: J SHELL INDEX.
C 2ND DIMENSION: REFERENCED BY L+1.
C INPUT : (R*8) WLOW( , , ) =
C 1ST DIMENSION: J SHELL INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C 3RD DIMENSION: REFERENCED BY L+1.
C INPUT : (R*8) EM = EMISSION MEASURE.
C INPUT : (R*8) QEX() =
C DIMENSION: MXNSHL.
C
C OUTPUT: (R*8) TOTPOP() = TOTAL COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TOTEMI() = TOTAL COLLISION EMISSIONS FOR
C PREDICTED
C SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) AVRGWL() = AVERAGE AIR WAVELENGTH FOR PREDICTED
C SPECTRUM LINE.
C UNITS: A
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) QEFF() = EFF. RATE COEFFICIENT FOR PREDICTED
C SPECTRUM LINE.
C UNITS:
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TBLPOP( , , ) = TABLE OF COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2

```

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C      1ST DIMENSION: J->J' TRANSITION INDEX.
C      2ND DIMENSION: REFERENCED BY I4IDLI().
C      OUTPUT: (R*8)  TBLEMI(,,) = TABLE OF COLLISION EMISSIVITIES FOR
C      PREDICTED SPECTRUM LINE.
C      UNITS: PH CM-2 SEC-1
C      1ST DIMENSION: J->J' TRANSITION INDEX.
C      2ND DIMENSION: REFERENCED BY I4IDLI().
C      3RD DIMENSION: PREDICTED LINE INDEX.
C      OUTPUT: (R*8)  TBLWLN(,,) = TABLE OF WAVELENGTHS FOR PREDICTED
C      SPECTRUM LINE.
C      UNITS: A
C      1ST DIMENSION: J->J' TRANSITION INDEX.
C      2ND DIMENSION: REFERENCED BY I4IDLI().
C      3RD DIMENSION: PREDICTED LINE INDEX.
C
C      PARAM : (I*4)  C1      = PRECISION AIR WAVELENGTH PARAM.
C      PARAM : (I*4)  C2      = PRECISION AIR WAVELENGTH PARAM.
C      PARAM : (I*4)  C3      = PRECISION AIR WAVELENGTH PARAM.
C      PARAM : (I*4)  C4      = PRECISION AIR WAVELENGTH PARAM.
C      PARAM : (I*4)  C5      = PRECISION AIR WAVELENGTH PARAM.
C      PARAM : (I*4)  RZ      = PRECISION AIR WAVELENGTH PARAM.
C
C      (I*4)  IN      = LOOP INDEX FOR SPECTRUM LINES.
C      (I*4)  N       = PRINCIPAL QUANTUM NUMBER OF INITIAL
C      STATE.
C      (I*4)  L       = LOOP INDEX FOR ORBITAL QUANTUM NUMBER OF
C      (I*4)  J       = LOOP INDEX FOR J QUANTUM NUMBER OF
C      INITIAL STATE.
C      (I*4)  N1      = PRINCIPAL QUANTUM NUMBER OF FINAL STATE.
C      (I*4)  L1      = LOOP INDEX FOR ORBITAL QUANTUM NUMBER OF
C      FINAL STATE.
C      (I*4)  J1      = LOOP INDEX FOR J QUANTUM NUMBER OF
C      FINAL STATE.
C      (I*4)  NP      = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C      (I*4)  IDL     = TABLE INDEX.
C      (I*4)  ID      = TABLE INDEX.
C
C      (R*8)  Z1      = REAL VALUE = IZ1.
C      (R*8)  ZEFF1   = EFFECTIVE ION CHARGE.
C      (R*8)  ZEFF2   = EFFECTIVE ION CHARGE.
C      (R*8)  ZEFF3   = EFFECTIVE ION CHARGE.
C      (R*8)  SUM1    = SUM OF COL. POP. FOR PREDICTED LINE.
C      UNITS: CM-2
C      (R*8)  SUM2    = SUM OF COL. EMIS. FOR PREDICTED LINE.
C      UNITS: PH CM-2 SEC-1
C      (R*8)  SUM3    = SUM OF WAVELENGTHS FOR PREDICTED LINE.
C      UNITS: A
C      (R*8)  EU0     = BINDING ENERGY
C      UNITS: RYD
C      (R*8)  T1      = COL. POP. FOR PREDICTED SPECTRUM LINE.
C      UNITS: CM-2
C      (R*8)  T2      = COL. EMIS. FOR PREDICTED SPECTRUM LINE.
C      UNITS: PH CM-2 SEC-1
C      (R*8)  DELTA   =
C      (R*8)  SIG2    =
C      (R*8)  RF      =
C      (R*8)  WAVAIR  = WAVELENGTH FOR PREDICTED SPECTRUM LINE.
C      UNITS: A
C
C      (R*8)  EL()    = BINDING ENERGY.
C      UNITS: RYD
C      DIMENSION: J SHELL INDEX WHERE:
C      1 => L+0.5
C      2 => L-0.5
C      (R*8)  EUJ()   = INITIAL STATE J RESOLVED ENERGY.
C      DIMENSION: J SHELL INDEX WHERE:
C      1 => L+0.5
C      2 => L-0.5
C      (R*8)  AA()    = LJ RESOLVED A-VALUE.
C      DIMENSION: TRANSITION INDEX WHERE:
C      1 => L+0.5 --> L'+0.5
C      2 => L+0.5 --> L'-0.5
C      3 => L-0.5 --> L'+0.5
C      4 => L-0.5 --> L'-0.5
C
C      (R*8)  ELJ(,)  = FINAL STATE J RESOLVED ENERGY.
C      1ST DIMENSION: L SHELL INDEX WHERE:
C      1 => L'=L+1
C      2 => L'=L-1
C      2ND DIMENSION: J SHELL INDEX WHERE:
C      1 => J'=L'+0.5
C      2 => J'=L'-0.5
C
C      ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      I4UNIT       ADAS        RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C      I4IDFL       ADAS        RETURNS UNIQUE INDEX GIVEN QUANTUM
C      NUMBERS N AND L.
C      I4IDLI       ADAS        RETURNS INDEX FOR PREDICTED SPECTRUM
C      LINE TABLES.
C      R8ZETA       ADAS
C      C6AJTB       ADAS        RETURNS LJ RESOLVED A-VALUES.
C
C      NOTES:
C      1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C      1 : J=L+0.5 -> J'=L'+0.5
C      2 : J=L+0.5 -> J'=L'-0.5

```



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C          3 : J=L-0.5 -> J'=L'+0.5
C          4 : J=L-0.5 -> J'=L'-0.5
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/81
C          JET EXT. 5183
C
C DATE:    09/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR:  WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:    22ND MAY 1996
C
C VERSION: 1.1                                DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C          - FIRST VERSION. IBM VERSION NOT CHANGED
C
C-----
C
C          INTEGER      I4UNIT      , I4IDFL      , I4IDLI
C          REAL*8        R8ZETA
C-----
C          INTEGER      MXJ
C          PARAMETER( MXJ = 2 )
C-----
C          REAL*8        C1            , C2            ,
C          &             C3            , C4            ,
C          &             C5            , RZ            ,
C          PARAMETER( C1 = 6432.8D0    , C2 = 2949810.0D0 ,
C          &             C3 = 25540.0D0 , C4 = 176.0D0    ,
C          &             C5 = 41.0D0    , RZ = 109737.2D0 )
C-----
C          INTEGER      MXNSHL      , MXJSHL      , MXPRSL      , IZ0      , IZ1      ,
C          &             NPLINE      , NUMAX
C          INTEGER      IN          , N          , L          , J          , N1         ,
C          &             L1          , J1          , NP          , IDL         , ID
C-----
C          REAL*8        EM
C          REAL*8        Z1          , ZEFF1      , ZEFF2      , ZEFF3      , SUM1      ,
C          &             SUM2      , SUM3      , EU0          , T1          , T2          ,
C          &             DELTA      , SIG2      , RF          , WAVAIR
C-----
C          INTEGER      NPU(MXPRSL)  , NPL(MXPRSL)
C-----
C          REAL*8        QEX(MXNSHL)  , TOTPOP(MXPRSL) , TOTEMI(MXPRSL) ,
C          &             AVRGWL(MXPRSL) , QEFF(MXPRSL)
C          REAL*8        EL(MXJ)      , EUJ(MXJ)      , AA(2*MXJ)
C-----
C          REAL*8        WHIGH(MXJSHL, (MXNSHL*(MXNSHL+1))/2)
C          REAL*8        ELJ(MXJ, MXJ)
C-----
C          REAL*8        WLOW(MXJSHL, (MXNSHL*(MXNSHL+1))/2, MXNSHL) ,
C          &             TBLPOP(2*MXJSHL, 2*MXNSHL-3, MXPRSL) ,
C          &             TBLEMI(2*MXJSHL, 2*MXNSHL-3, MXPRSL) ,
C          &             TBLWLN(2*MXJSHL, 2*MXNSHL-3, MXPRSL)
C-----

```

## C6QEIK(

```

SUBROUTINE C6QEIK( MXNSHL , MXJSHL , MXBEAM , IZ1 ,
&                 IDONOR , NBOT , NTOP , NBEAM ,
&                 BMENA , BMFRA , QTHCH , PTHCHJ
&                 )
C
C      IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C6QEIK *****
C
C PURPOSE:  USES THE EIKONIAL APPROXIMATION TO CALCULATE THE
C           THEORETICAL CHARGE EXCHANGE RATE COEFFICIENTS TO N SHELLS
C           AND THE NLJ FRACTIONS FROM NEUTRAL HYDROGEN OR HELLIUM IN
C           GROUND OR EXCITED STATE TO A BARE NUCLEUS TARGET.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4) MXNSHL = MAXIMUM NO. OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NO. OF J SUB-SHELLS.
C INPUT : (I*4) MXBEAM = MAXIMUM NO. OF BEAM ENERGIES.
C INPUT : (R*8) IZ1    = CHARGE OF TARGET ION.
C INPUT : (I*4) IDONOR = DONOR STATE FOR EIKONAL MODEL.
C           1 = H(1S)   DONOR
C           2 = H(2S)   DONOR
C           3 = H(2P)   DONOR
C           4 = H(1S2)  DONOR
C           5 = HE(1S2S) DONOR
C INPUT : (I*4) NBOT   = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NTOP   = MAXIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NBEAM  = NUMBER OF BEAM ENERGIES.

```

```

C INPUT : (R*8) BMENA() = BEAM ENERGY COMPONENTS.
C UNITS: EV/AMU
C DIMENSION: COMPONENT INDEX.
C INPUT : (R*8) BMFRA() = BEAM COMPONENT FRACTIONS.
C DIMENSION: COMPONENT INDEX.
C
C OUTPUT: (R*8) QTHCH() = MEAN RATE COEFFICIENTS FOR N-LEVELS
C AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: REFERENCED BY N QUANTUM NUMBER.
C OUTPUT: (R*8) FTHCHJ(,) = MEAN RATE COEFFICIENTS FOR NLJ-LEVELS
C AVERAGED OVER BEAM FRACTIONS. EXPRESSED AS
C FRACTIONS OF CORRESPONDING N-LEVELS.
C 1ST DIMENSION: J SUB-SHELL
C 1 => J=L+0.5
C 2 => J=L-0.5
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L)
C
C PARAM : (I*4) MXN = 'MXNSHL'.
C
C (I*4) N = N-SHELL INDEX.
C (I*4) L = L-SHELL INDEX.
C (I*4) J = J-SHELL INDEX.
C (I*4) IDL = L-RESOLVED INDEX.
C
C (R*8) XL = REAL VALUE = L.
C (R*8) WL =
C
C (R*8) FTHCH() = MEAN RATE COEFFICIENTS FOR NL-LEVELS
C AVERAGED OVER BEAM FRACTIONS. EXPRESSED AS
C FRACTIONS OF CORRESPONDING N-LEVELS.
C DIMENSION: REFERENCED BY I4IDFL(N,L)
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C NUMBERS N AND L.
C CXQEIK ADAS CALCULATES N-LEVEL AND NL-LEVEL CHARGE
C EXCHANGE RATE COEFFICIENTS USING EIKONAL
C APPROX. NL RATES ARE GIVEN AS FRACTION
C OF CORRESPONDING N RATE.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 22/10/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. IBM VERSION NOT CHANGED
C
C -----
C
C INTEGER I4UNIT , I4IDFL
C -----
C INTEGER MXN
C PARAMETER( MXN = 20 )
C -----
C INTEGER MXNSHL , MXJSHL , MXBEAM , IZ1 , IDONOR ,
C & NBOT , NTOP , NBEAM
C INTEGER N , L , J , IDL
C -----
C REAL*8 XL , WL
C -----
C REAL*8 BMENA(MXBEAM) ,
C & BMFRA(MXBEAM) ,
C & QTHCH(MXNSHL)
C REAL*8 FTHCH((MXN*(MXN+1))/2)
C REAL*8 FTHCHJ(MXJSHL,(MXNSHL*(MXNSHL+1))/2)
C -----

```

## C6QXCH

```

C SUBROUTINE C6QXCH ( MXNENG , MXNSHL , MXJSHL , MXBEAM ,
C & NBEAM , BMENA , BMFRA , NBOT ,
C & NTOP , NMINF , NMAXF , NENRGY ,
C & ENRGYA , ALPHAA , XSECNA , FRACLA ,
C & QTHCH , FTHCHJ
C )
C
C IMPLICIT NONE
C
C -----

```

```

C ***** FORTRAN77 SUBROUTINE: C6QXCH *****
C
C PURPOSE:  USES THE INPUT DATASET TO CALCULATE THE CHARGE EXCHANGE
C           RATE COEFFICIENTS FOR BOTH N-LEVELS AND NLJ-LEVELS AVERAGED
C           OVER THE BEAM FRACTIONS. NLJ-LEVEL RATES ARE EXPRESSED AS A
C           FRACTION OF CORRESPONDING N-LEVEL.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4)  MXNENG   = MAXIMUM NO. OF ENERGIES.
C INPUT : (I*4)  MXNSHL   = MAXIMUM NO. OF N SHELLS.
C INPUT : (I*4)  MXJSHL   = MAXIMUM NO. OF J SUB-SHELLS.
C INPUT : (I*4)  MXBEAM   = MAXIMUM NO. OF BEAM ENERGIES.
C INPUT : (I*4)  NBEAM    = NUMBER OF BEAM ENERGIES.
C INPUT : (R*8)  BMENA()  = BEAM ENERGY COMPONENTS.
C                       UNITS: EV/AMU
C                       DIMENSION: COMPONENT INDEX.
C INPUT : (R*8)  BMFRA()  = BEAM COMPONENT FRACTIONS.
C                       DIMENSION: COMPONENT INDEX.
C INPUT : (I*4)  NBOT     = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4)  NTOP     = MAXIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4)  NMINF    = MINIMUM PRINCIPAL QUANTUM NUMBER OF INPUT
C                       DATASET.
C INPUT : (I*4)  NMAXF    = MAXIMUM PRINCIPAL QUANTUM NUMBER OF INPUT
C                       DATASET.
C INPUT : (I*4)  NENRGY   = NUMBER OF ENERGIES IN DATASET.
C INPUT : (R*8)  ENRGYA() = COLLISION ENERGIES.
C                       UNITS: EV/AMU
C                       DIMENSION: ENERGY INDEX
C INPUT : (R*8)  ALPHAA() = EXTRAPOLATION PARAMETER ALPHA.
C                       DIMENSION: ENERGY INDEX
C INPUT : (R*8)  XSECNA(,) = N-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS.
C                       UNITS: CM2
C                       1ST DIMENSION: ENERGY INDEX
C                       2ND DIMENSION: N-SHELL
C INPUT : (R*8)  FRACLA(,) = L-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS
C                       EXPRESSED AS FRACTION OF CORRESPONDING
C                       N-RESOLVED CROSS-SECTION.
C                       1ST DIMENSION: ENERGY INDEX
C                       2ND DIMENSION: REFERENCED BY I4IDFL(N,L)
C
C OUTPUT: (R*8)  QTHCH()  = MEAN RATE COEFFICIENTS FOR N-LEVELS
C                       AVERAGED OVER BEAM FRACTIONS.
C                       UNITS: CM3 SEC-1
C                       DIMENSION: REFERENCED BY N QUANTUM NUMBER.
C OUTPUT: (R*8)  FTHCHJ(,) = MEAN RATE COEFFICIENTS FOR NLJ-LEVELS
C                       AVERAGED OVER BEAM FRACTIONS. EXPRESSED AS
C                       FRACTIONS OF CORRESPONDING N-LEVELS.
C                       1ST DIMENSION: J SUB-SHELL
C                               1 => J=L+0.5
C                               2 => J=L-0.5
C                       2ND DIMENSION: REFERENCED BY I4IDFL(N,L)
C
C PARAM : (I*4)  MXN      = 'MXNSHL'.
C
C           (I*4)  N       = N-SHELL INDEX.
C           (I*4)  L       = L-SHELL INDEX.
C           (I*4)  J       = J-SHELL INDEX.
C           (I*4)  IDL     = L-RESOLVED INDEX.
C
C           (R*8)  XL      = REAL VALUE = L.
C           (R*8)  WL      =
C
C           (R*8)  FTHCH() = MEAN RATE COEFFICIENTS FOR NL-LEVELS
C                       AVERAGED OVER BEAM FRACTIONS. EXPRESSED AS
C                       FRACTIONS OF CORRESPONDING N-LEVELS.
C                       DIMENSION: REFERENCED BY I4IDFL(N,L)
C
C ROUTINES:
C
C           ROUTINE   SOURCE   BRIEF DESCRIPTION
C -----
C           I4UNIT    ADAS     RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C           I4IDFL    ADAS     RETURNS UNIQUE INDEX GIVEN QUANTUM
C                               NUMBERS N AND L.
C           CXQXCH    ADAS     CALCULATES N-LEVEL AND NL-LEVEL CHARGE
C                               EXCHANGE RATE COEFFICIENTS USING INPUT
C                               DATASET. NL RATES ARE GIVEN AS FRACTION
C                               OF CORRESPONDING N RATE.
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          KL/0/81
C          JET EXT. 5183
C
C DATE:    22/10/93
C
C UNIX-IDL PORT:
C
C AUTHOR:  WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:    22ND MAY 1996
C
C VERSION: 1.1                      DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C          - FIRST VERSION. IBM VERSION NOT CHANGED
C
C -----

```

```

C-----
C      INTEGER      I4UNIT      , I4IDFL
C-----
C      INTEGER      MXN
C      PARAMETER( MXN = 20 )
C-----
C      INTEGER      MXNENG      , MXNSHL      , MXJSHL      , MXBEAM      , NBEAM      ,
&      NBOT        , NTOP        , NMINF        , NMAXF        , NENRGY
C      INTEGER      N          , L          , J          , IDL
C-----
C      REAL*8       XL          , WL
C-----
C      REAL*8       BMENA(MXBEAM)          ,
&      BMFRA(MXBEAM)          ,
&      ENRGYA(MXNENG)          ,
&      ALPHAA(MXNENG)          ,
&      QTHCH(MXNSHL)
C      REAL*8       FTHCH( (MXN*(MXN+1))/2 )
C      REAL*8       XSECNA(MXNENG,MXNSHL)
&      FRACLA(MXNENG, (MXNSHL*(MXNSHL+1))/2) ,
&      FTHCHJ(MXJSHL, (MXNSHL*(MXNSHL+1))/2)
C-----

```

## C6TBEX

```

SUBROUTINE C6TBEX( MXNSHL , MXJSHL , IZ1      , NBOT      ,
&      NTOP      , NGRND      , TEV      , QTHEX      ,
&      FTHEXJ
&      )
C
C      IMPLICIT NONE
C-----
C
C ***** FORTRAN77 SUBROUTINE: C6TBEX *****
C
C PURPOSE: SETS UP A TABLE OF ELECTRON IMPACT EXCITATION RATE
C          COEFFICIENTS FOR A HYDROGENIC ION FROM THE GROUND STATE
C          TO EXCITED NL LEVELS.
C
C CALLING PROGRAM: ADAS306.
C
C INPUT : (I*4) MXNSHL      = MAXIMUM NO. OF N SHELLS.
C INPUT : (I*4) MXJSHL      = MAXIMUM NO. J SUB-SHELLS.
C INPUT : (I*4) IZ1         = ION CHARGE.
C INPUT : (I*4) NBOT        = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NTOP        = MAXIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NGRND       =
C INPUT : (R*8) TEV         = ELECTRON TEMPERATURE.
C                               UNITS: EV
C
C OUTPUT: (R*8) QTHEX( )   = TABLE OF N-LEVEL EXCITATION RATE
C                               COEFFICIENTS.
C                               UNITS:
C                               DIMENSION: N-SHELL
C OUTPUT: (R*8) FTHEXJ( , ) = TABLE OF NLJ-LEVEL EXCITATION RATE
C                               COEFFICIENTS EXPRESSED AS FRACTION OF
C                               CORRESPONDING N-LEVEL RATE.
C                               1ST DIMENSION: J SUB-SHELL
C                               1 => J=L+0.5
C                               2 => J=L-0.5
C                               2ND DIMENSION: REFERENCED BY I4IDFL(N,L)
C
C PARAM : (I*4) MXN        = 'MXNSHL'.
C
C          (I*4) N          = N-SHELL INDEX.
C          (I*4) L          = L-SHELL INDEX.
C          (I*4) J          = J-SHELL INDEX.
C          (I*4) IDL        = L-RESOLVED INDEX.
C
C          (R*8) XL         = REAL VALUE = L.
C          (R*8) WL         =
C
C          (R*8) TBQEX( )   = TABLE OF NL-LEVEL EXCITATION RATE
C                               COEFFICIENTS.
C                               UNITS:
C                               DIMENSION: REFERENCED BY I4IDFL(N,L).
C          (R*8) FTHEX( )   = TABLE OF NL-LEVEL EXCITATION RATE
C                               COEFFICIENTS EXPRESSED AS FRACTION OF
C                               CORRESPONDING N-LEVEL RATE.
C                               DIMENSION: REFERENCED BY I4IDFL(N,L).
C
C ROUTINES:
C
C          ROUTINE      SOURCE      BRIEF DESCRIPTION
C-----
C          I4UNIT      ADAS          RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C          I4IDFL      ADAS          RETURNS UNIQUE INDEX GIVEN QUANTUM
C                                     NUMBERS N AND L.
C          CXTBEX      ADAS          CALCULATES N-LEVEL AND NL-LEVEL
C                                     EXCITATION RATE COEFFICIENTS. NL RATES
C                                     ARE GIVEN AS FRACTION OF CORRESPONDING
C                                     N RATE.
C

```

```

C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 22/10/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. IBM VERSION NOT CHANGED
C
C-----
C
C INTEGER I4UNIT , I4IDFL
C-----
C INTEGER MXN
C PARAMETER( MXN = 20 )
C-----
C INTEGER MXNSHL , MXJSHL , IZ1 , NBOT , NTOP ,
C & NGRND
C INTEGER N , L , J , IDL
C-----
C REAL*8 TEV
C REAL*8 XL , WL
C-----
C REAL*8 QTHEX(MXNSHL)
C REAL*8 TBQEX((MXN*(MXN+1))/2) ,
C & FTHEX((MXN*(MXN+1))/2)
C REAL*8 FTHEXJ(MXJSHL,(MXNSHL*(MXNSHL+1))/2)
C-----

```

## C6TBFM

```

SUBROUTINE C6TBFM( MXNSHL , MXJSHL , IZ0 , IZ1 ,
& AMSSNO , NBOT , NTOP , BMAG ,
& TIEV , TBLF , TBFMP , TBFM ,
& TBFMM
& )
C
C IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C6TBFM *****
C
C PURPOSE: FILLS TABLES OF MAGNETIC FIELD DEPENDENT MIXING RATE
C COEFFICIENTS BETWEEN NEARLY DEGENERATE LEVELS FOR
C HYDROGEN-LIKE, LITHIUM-LIKE AND SODIUM-LIKE IONS. RATES
C ARE CALCULATED FOR THE SEPARATE NLJ->NL+1J' , NLJ->NLJ'
C AND NLJ->NL-1J' TRANSITIONS.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) IZ0 = TARGET NUCLEAR CHARGE.
C INPUT : (I*4) IZ1 = ION CHARGE.
C INPUT : (R*8) AMSSNO = ATOMIC MASS NO.
C INPUT : (I*4) NBOT = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NTOP = MAXIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) BMAG = MAGNETIC INDUCTION.
C UNITS: TESLA
C INPUT : (R*8) TIEV = TEMPERATURE (ION DISTRIBUTION).
C UNITS: EV
C INPUT : (R*8) TBLF( ) = TABLE OF RADIATIVE LIFETIMES.
C UNITS: SECS
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C OUTPUT: (R*8) TBFMP( , ) = RATE COEFFT. FOR NLJ->NL+1J' .
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C OUTPUT: (R*8) TBFM( , ) = RATE COEFFT. FOR NLJ->NL+1J' .
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C OUTPUT: (R*8) TBFMM( , ) = RATE COEFFT. FOR NLJ->NLJ' FOR STATE I.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C
C PARAM : (I*4) MXJ = 'MXJSHL'.
C
C (I*4) NI = VALENCE ELECTRON PRINCIPAL QUANTUM NUMBER
C IN STATE I.
C (I*4) NJ = VALENCE ELECTRON PRINCIPAL QUANTUM NUMBER
C IN STATE J.
C (I*4) LI = VALENCE ELECTRON ORBITAL QUANTUM NUMBER IN
C STATE I.
C (I*4) LJ = VALENCE ELECTRON ORBITAL QUANTUM NUMBER IN

```

```

C
C      (I*4) IDLI = STATE J.
C      (I*4) IDLJ = TABLE INDEX.
C      (I*4) I    = TABLE INDEX.
C      (I*4) J    = LOOP INDEX.
C
C      (R*8) FMP( ) = RATE COEFFT. FOR NLJ->NL+1J'.
C      DIMENSION: J->J' TRANSITION INDEX.
C      (R*8) FMM( ) = RATE COEFFT. FOR NLJ->NL+1J'.
C      DIMENSION: J->J' TRANSITION INDEX.
C      (R*8) FMI( ) = RATE COEFFT. FOR NLJ->NLJ' FOR STATE I.
C      DIMENSION: J->J' TRANSITION INDEX.
C      (R*8) FMJ( ) = RATE COEFFT. FOR NLJ->NLJ' FOR STATE J.
C      DIMENSION: J->J' TRANSITION INDEX.
C
C NOTES:
C      1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C          1 : J=L+0.5 -> J'=L'+0.5
C          2 : J=L+0.5 -> J'=L'-0.5
C          3 : J=L-0.5 -> J'=L'+0.5
C          4 : J=L-0.5 -> J'=L'-0.5
C
C      2) BEFORE CALLING C6TBQM THE LIFETIME TABLE MUST BE FILLED
C          WITH A CALL TO C6TBLF.
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      I4UNIT      ADAS      RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C      I4IDFL      ADAS      RETURNS UNIQUE INDEX GIVEN QUANTUM
C      NUMBERS N AND L.
C      CXMRDG      ADAS      CALCULATES MIXING RATE COEFFICIENTS
C      BETWEEN NEARLY DEGENERATE LEVELS OF
C      H-, LI- OR NA-LIKE IONS.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C      K1/0/81
C      JET EXT. 5183
C
C DATE: 04/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C      - FIRST VERSION. IBM VERSION NOT CHANGED
C
C
C
C
C      INTEGER      I4UNIT , I4IDFL
C
C      INTEGER      MXJ
C      PARAMETER( MXJ = 2 )
C
C      INTEGER      MXNSHL , MXJSHL , IZ0 , IZ1 , NTOP ,
C      & NBOT
C      INTEGER      NI , NJ , LI , LJ , IDLI ,
C      & IDLJ , I , J
C
C      REAL*8      AMSSNO , BMAG , TIEV
C
C      REAL*8      TBLF( (MXNSHL*(MXNSHL+1))/2) ,
C      & TBFMP( 2*MXJSHL , (MXNSHL*(MXNSHL+1))/2) ,
C      & TBFM( 2*MXJSHL , (MXNSHL*(MXNSHL+1))/2) ,
C      & TBFMM( 2*MXJSHL , (MXNSHL*(MXNSHL+1))/2)
C      REAL*8      FMP( 2*MXJ ) , FMM( 2*MXJ ) , FMI( 2*MXJ ) ,
C      & FMJ( 2*MXJ )
C
C

```

## C6TBIN

```

C      SUBROUTINE C6TBIN( MXNSHL , IZ1 , NBOT , NTOP , TEV , QTHIN )
C
C      IMPLICIT NONE
C
C      -----
C
C      ***** FORTRAN77 SUBROUTINE: C6TBIN *****
C
C      PURPOSE: SETS UP AN ELECTRON IMPACT IONISATION RATE COEFFICIENT
C      TABLE FOR N-LEVELS BASED ON THE ECIP APPROXIMATION. ENERGY
C      LEVELS ARE ASSUMED HYDROGENIC IN THE EFFECTIVE ION CHARGE.
C
C      CALLING PROGRAM: ADAS306
C
C      INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C      INPUT : (I*4) IZ1   = ION CHARGE.
C      INPUT : (I*4) NBOT  = MINIMUM PRINCIPAL QUANTUM NUMBER.

```

```

C INPUT : (I*4) NTOP = MAXIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) TEV = ELECTRON TEMPERATURE.
C UNITS: EV
C
C OUTPUT: (R*8) QTHIN() = IONISATION RATE COEFFICIENT.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C
C PARAM : (R*8) P1 =
C
C (I*4) N = LOOP INDEX.
C (I*4) IZC = IZ1-1.
C
C (R*8) ZETA = EFFECTIVE NUMBER OF EQUIVALENT ELECTRONS FOR
C SHELL.
C (R*8) TE = ELECTRON TEMPERATURE.
C UNITS: K
C (R*8) XI =
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C R8ECIP ADAS
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 03/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. IBM VERSION NOT CHANGED
C
C -----
C REAL*8 R8ECIP
C -----
C REAL*8 P1
C PARAMETER( P1 = 1.16054D4 )
C -----
C INTEGER MXNSHL , IZ1 , NBOT , NTOP
C INTEGER N , IZC
C -----
C REAL*8 TEV
C REAL*8 ZETA , TE , XI
C -----
C REAL*8 QTHIN(MXNSHL)
C -----

```

## C6TBQM

```

SUBROUTINE C6TBQM( MXNSHL , MXJSHL , IZ0 , IZ1 ,
& NBOT , NTOP , TEV , DENS ,
& ZP , TPV , EMP , TBLF ,
& TBQMEP , TBQMEM , TBQMIP , TBQMIM
& )
C
C IMPLICIT NONE
C
C ***** FORTRAN77 SUBROUTINE: C6TBQM *****
C
C PURPOSE: SETS UP TABLES OF ELECTRON AND POSITIVE ION COLLISIONAL
C RATE COEFFICIENTS BETWEEN NEARLY DEGENERATE LEVELS FOR
C H-, LI-, AND NA-LIKE IONS. THE RATES FOR THE SEPARATE
C TRANSITIONS NLJ->NL+1J' AND NLJ->NL-1J' ARE OBTAINED.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) IZ0 = NUCLEAR CHARGE OF TARGET ION.
C INPUT : (I*4) IZ1 = ION CHARGE.
C INPUT : (I*4) NBOT = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NTOP = MAXIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) TEV = ELECTRON TEMPERATURE.
C UNITS: EV
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C UNITS: CM-3
C INPUT : (R*8) ZP = CHARGE OF COLLIDING POSITIVE ION.
C INPUT : (R*8) TPV = TEMPERATURE (COLLIDING POSITIVE ION
C DISTRIBUTION).
C UNITS: EV
C INPUT : (R*8) EMP = REDUCED MASS FOR COLLIDING POSITIVE ION.

```

```

C
C INPUT : (R*8) ZP      = CHARGE OF COLLIDING POSITIVE ION.
C INPUT : (R*8) TPV     = POSITIVE ION TEMPERATURE.
C
C UNITS: EV
C INPUT : (R*8) EMP     = REDUCED MASS FOR COLLIDING POSITIVE ION.
C UNITS: ELECTRON MASSES
C INPUT : (R*8) TBLF( ) = TABLE OF RADIATIVE LIFETIMES.
C UNITS: SECS
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C OUTPUT: (R*8) TBQMEP(,) = ELECTRON RATE COEFFT. FOR NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C OUTPUT: (R*8) TBQMEM(,) = ELECTRON RATE COEFFT. FOR NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C OUTPUT: (R*8) TBQMIP(,) = POSITIVE ION RATE COEFFT. FOR NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C OUTPUT: (R*8) TBQMIM(,) = POSITIVE ION RATE COEFFT. FOR NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C
C PARAM : (I*4) MXJ     = 'MXJSHL'.
C
C (I*4) NI      = VALENCE ELECTRON PRINCIPAL QUANTUM NUMBER
C IN STATE I.
C (I*4) NJ      = VALENCE ELECTRON PRINCIPAL QUANTUM NUMBER
C IN STATE J.
C (I*4) LI      = VALENCE ELECTRON ORBITAL QUANTUM NUMBER IN
C STATE I.
C (I*4) LJ      = VALENCE ELECTRON ORBITAL QUANTUM NUMBER IN
C STATE J.
C (I*4) IDLI    = TABLE INDEX.
C (I*4) IDLJ    = TABLE INDEX.
C (I*4) I       = LOOP INDEX.
C (I*4) J       = LOOP INDEX.
C
C (R*8) GAE     = GAMA RATE PARAMETER FOR ELECTRON COLLISIONS.
C (R*8) GAP     = GAMA RATE PARAMETER FOR POSITIVE ION
C COLLISIONS.
C
C (R*8) QEP( )  = ELECTRON RATE COEFFT. FOR NLJ->NL+1J'
C DIMENSION: J->J' TRANSITION INDEX.
C (R*8) QEM( )  = ELECTRON RATE COEFFT. FOR NLJ->NL-1J'
C DIMENSION: J->J' TRANSITION INDEX.
C (R*8) QIP( )  = POSITIVE ION RATE COEFFT. FOR NLJ->NL+1J'
C DIMENSION: J->J' TRANSITION INDEX.
C (R*8) QIM( )  = POSITIVE ION RATE COEFFT. FOR NLJ->NL-1J'
C DIMENSION: J->J' TRANSITION INDEX.
C
C NOTES:
C 1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C 1 : J=L+0.5 -> J'=L'+0.5
C 2 : J=L+0.5 -> J'=L'-0.5
C 3 : J=L-0.5 -> J'=L'+0.5
C 4 : J=L-0.5 -> J'=L'-0.5
C
C 2) BEFORE CALLING C6TBQM THE LIFETIME TABLE MUST BE FILLED
C WITH A CALL TO C6TBLF.
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C NUMBERS N AND L.
C CXCRDG ADAS CALCULATES COLLISIONAL RATE COEFFICIENTS
C BETWEEN NEARLY DEGENERATE LEVELS OF
C H-, LI- OR NA-LIKE IONS.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 02/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. IBM VERSION NOT CHANGED
C
C -----
C INTEGER I4UNIT , I4IDFL
C -----
C INTEGER MXJ
C PARAMETER( MXJ = 2 )
C -----
C INTEGER MXNSHL , MXJSHL , IZO , IZ1 , NTOP ,
C & NBOT
C INTEGER NI , NJ , LI , LJ , IDLI ,

```



&	IDLJ	, I	, J
REAL*8	TEV	, DENS	, ZP
REAL*8	GAE	, GAP	, TPV
REAL*8	TBLF((MXNSHL*(MXNSHL+1))/2)		
&	TBQMEP(2*MJSHL, (MXNSHL*(MXNSHL+1))/2)		
&	TBQMEM(2*MJSHL, (MXNSHL*(MXNSHL+1))/2)		
&	TBQMIP(2*MJSHL, (MXNSHL*(MXNSHL+1))/2)		
&	TBQMIM(2*MJSHL, (MXNSHL*(MXNSHL+1))/2)		
REAL*8	QEP(2*MJ)	, QEM(2*MJ)	, QIP(2*MJ)
&	QIM(2*MJ)		

## C6TBRC

```

SUBROUTINE C6TBRC( MXNSHL , MXJSHL , IZ1 , NBOT ,
& NTOP , TEV , QTHRC , FTHRCJ ,
& )
C
C   IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C6TBRC *****
C
C PURPOSE: SETS UP A TABLE OF RADIATIVE RECOMBINATION RATE
C           COEFFICIENTS FOR A BARE NUCLEUS, HELIUM-LIKE OR NEON-LIKE
C           ION TO EXCITED NLJ LEVELS.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) IZ1    = ION CHARGE.
C INPUT : (I*4) NBOT   = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NTOP   = MAXIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) TEV    = ELECTRON TEMPERATURE.
C                       UNITS: EV
C
C OUTPUT: (R*8) QTHRC() = RECOMBINATION RATE COEFFICIENT TO LEVEL N.
C                       UNITS: CM3 SEC-1
C                       DIMENSION: N-SHELL
C OUTPUT: (R*8) FTHRCJ(, ) = FRACTION OF RECOMBINATION RATE OF LEVEL N
C                           TO STATE NLJ.
C                           1ST DIMENSION: J-SHELL INDEX WHERE
C                               1 GIVES J=L+0.5
C                               2 GIVES J=L-0.5
C                           2ND DIMENSION: REFERENCED BY I4IDFL().
C
C PARAM : (R*8) P1     = BOLTZMANN CONSTANT.
C                       UNITS: EV K-1
C PARAM : (R*8) P2     =
C
C (I*4) N             = PRINCIPAL QUANTUM NUMBER OF BOUND ELECTRON.
C (I*4) L             = ORBITAL QUANTUM NUMBER OF BOUND ELECTRON.
C (I*4) L1            = ORBITAL QUANTUM NUMBER OF FREE ELECTRON.
C (I*4) LP            = TOTAL ORBITAL ANGULAR MOMENTUM QUANTUM
C                       NUMBER OF PARENT STATE.
C (I*4) ISP           = 2*SP+1 WHERE SP IS TOTAL SPIN OF PAREN T
C                       STATE.
C (I*4) LT            = TOTAL ORBITAL ANGULAR MOMENTUM QUANTUM
C                       NUMBER OF BOUND SYSTEM.
C (I*4) LT1           = TOTAL ORBITAL ANGULAR MOMENTUM QUANTUM
C                       NUMBER OF FREE SYSTEM.
C (I*4) IS            = 2*S+1 WHERE S IS TOTAL SPIN OF SYSTEM.
C (I*4) IRES          = LEVEL OF RESOLUTION.
C                       = 1 :
C                       = 2 : ABOVE LT1 SUM.
C                       = 3 : ABOVE LT SUM.
C                       = 4 : ABOVE S SUM.
C                       = 5 : UNRESOLVED GBF.
C (I*4) I             = LOOP INDEX.
C (I*4) J             = LOOP INDEX.
C (I*4) IDL           = TABLE INDEX.
C
C (R*8) Z1            = REAL VALUE = IZ1.
C (R*8) TE            = ELECTRON TEMPERATURE.
C                       UNITS: K
C (R*8) V             = EFFECTIVE PRINCIPAL QUANTUM NUMBER OF BOUND
C                       ELECTRON.
C (R*8) FACT          =
C (R*8) SUM            =
C (R*8) XL            = REAL VALUE = L.
C (R*8) WL            =
C (R*8) T             =
C (R*8) PREC1         = RADIATIVE RECOMBINATION INTEGRAL.
C (R*8) PION1         = PHOTOIONISATION INTEGRAL.
C (R*8) PSTIM1        = STIMULATED RECOMBINATION INTEGRAL.
C (R*8) PREC2         = RADIATIVE RECOMBINATION INTEGRAL.
C (R*8) PION2         = PHOTOIONISATION INTEGRAL.
C (R*8) PSTIM2        = STIMULATED RECOMBINATION INTEGRAL.
C

```

```

C PARAM : (R*8) P1 = BOLTZMANN CONSTANT.
C UNITS: EV K-1
C PARAM : (R*8) P2 =
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C NUMBERS N AND L.
C CXPHOT ADAS CALCULATES PHOTO INTEGRALS USING GIIH
C BOUND-FREE GAUNT-FACTORS.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 05/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. IBM VERSION NOT CHANGED
C
C VERSION: 1.2 DATE: 29-05-96
C MODIFIED: WILLIAM OSBORN
C - REMOVED UNUSED VARIABLES
C
C -----
C
C INTEGER I4IDFL
C
C REAL*8 P1 , P2
C PARAMETER( P1 = 8.61663D-5 , P2 = 1.5789D5 )
C
C INTEGER MXNSHL , MXJSHL , IZ1 , NBOT , NTOT
C INTEGER N , L , L1 , LP , ISP ,
C & LT , LT1 , IS , IRES , I ,
C & J , IDL
C
C REAL*8 TEV
C REAL*8 Z1 , TE , V , FACT ,
C & SUM , XL , WL , T , PREC1 ,
C & PION1 , PSTIM1 , PREC2 , PION2 , PSTIM2
C
C REAL*8 QTHRC(MXNSHL)
C
C REAL*8 FTHRCJ(MXJSHL, (MXNSHL*(MXNSHL+1))/2)
C
C -----

```

## C6WFIL

```

SUBROUTINE C6WFIL( MXNSHL , MXJSHL , IZ1 , NGRND ,
& NTOT , NBOT , NUMAX , DENSZ ,
& DENS , QTHEOR , FTHEOR , QTHIN ,
& TBQMFP , TBQMFM , TBQMIP , TBQMIM ,
& TBFMP , TBFM , TBFMM , WHIGH ,
& WLOW
& )
C
C IMPLICIT NONE
C
C -----
C
C ***** FORTRAN77 SUBROUTINE: C6WFIL *****
C
C PURPOSE:
C
C CALLING PROGRAM: C6EMIS
C
C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) IZ1 = ION CHARGE.
C INPUT : (I*4) NGRND = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) NTOT = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND
C STATE.
C INPUT : (I*4) NBOT = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C OBSERVED SPECTRUM LINES.
C INPUT : (R*8) DENSZ = PLASMA ION DENSITY.
C UNITS: CM-3
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C UNITS: CM-3
C INPUT : (R*8) QTHEOR( ) = MEAN CHARGE EXCHANGE, EXCITATION RATE OR
C RECOMBINATION RATE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: REFERENCED BY N QUANTUM NUMBER.

```

```

C INPUT : (R*8) FTHEOR(,) = FRACTION OF N-LEVEL MEAN CHARGE EXCHANGE,
C EXCITATION RATE OR RECOMBINATION RATE
C COEFFICIENTS IN NL-LEVEL.
C 1ST DIMENSION: J SHELL INDEX WHERE:
C 1 GIVES J=L+0.5
C 2 GIVES J=L-0.5
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) QTHIN(,) = IONISATION RATE COEFFICIENT.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) TBQMEP(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMEM(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIP(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIM(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMP(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NLJ'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C OUTPUT: (R*8) WHIGH(,) =
C 1ST DIMENSION: J SHELL INDEX.
C 2ND DIMENSION: REFERENCED BY L+1.
C OUTPUT: (R*8) WLOW(,,) =
C 1ST DIMENSION: J SHELL INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C 3RD DIMENSION: REFERENCED BY L+1.
C PARAM : (I*4) MXN = MXNSHL.
C PARAM : (I*4) MXJ = MXJSHL.
C
C (I*4) N = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) J = LOOP INDEX FOR J QUANTUM NUMBER.
C (I*4) N1 = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L1 = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) N2 = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L2 = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) LP = ARRAY INDEX = L+1.
C (I*4) IDL = ARRAY INDEX.
C
C (R*8) AA(,) = LJ RESOLVED A-VALUE.
C DIMENSION: TRANSITION INDEX WHERE:
C 1 GIVES LU+0.5 --> LL+0.5
C 2 GIVES LU+0.5 --> LL-0.5
C 3 GIVES LU-0.5 --> LL+0.5
C 4 GIVES LU-0.5 --> LL-0.5
C
C (R*8) RHS(,) = RIGHT HAND SIDE OF N LEVEL EQUATION.
C 1ST DIMENSION: MXJ.
C 2ND DIMENSION: MXN.
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C NUMBERS N AND L.
C C6WSOL ADAS
C
C NOTES:
C 1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C 1 : J=L+0.5 -> J'=L'+0.5
C 2 : J=L+0.5 -> J'=L'-0.5
C 3 : J=L-0.5 -> J'=L'+0.5
C 4 : J=L-0.5 -> J'=L'-0.5
C
C 2) FOR MATRIX HANDLING PURPOSES, L=0 STATES ARE TREATED AS TWO
C STATES OF J=0.5. RATES INTO EACH OF THESE ARE SET EQUAL TO
C HALF THE TOTAL INTO A TRUE L=0,J=0.5 STATE. RATES OUT OF
C EACH STATE ARE SET EQUAL TO THE TOTAL OUT OF A TRUE L=0,J=0.5
C STATE. THUS EACH ARTIFICIAL STATE HAS THE SAME POPULATION
C WHICH IS HALF THE TOTAL OF THE TRUE L=0,J=0.5 STATE. THE
C POPULATIONS ARE RECOMBINED AT THE END OF THE MATRIX
C MANIPULATIONS.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183

```

```

C
C DATE:      08/10/93
C
C UNIX-IDL PORT:
C
C AUTHOR:    WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:      22ND MAY 1996
C
C VERSION: 1.1                      DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C           - FIRST VERSION.  IBM VERSION NOT CHANGED
C
C-----
C
C           INTEGER      I4UNIT      , I4IDFL
C-----
C           INTEGER      MXN          , MXJ
C           PARAMETER(  MXN = 20    , MXJ = 2 )
C-----
C           INTEGER      MXNSHL      , MXJSHL      , IZ1          , NGRND      , NTOT      ,
C           &            NBOT          , NUMAX
C           INTEGER      N            , L            , J            , N1          , L1          ,
C           &            N2            , L2            , LP            , IDL
C-----
C           REAL*8       DENSZ        , DENS
C-----
C           REAL*8       QTHEOR(MXNSHL) , QTHIN(MXNSHL)
C           REAL*8       AA(2*MXJ)
C-----
C           REAL*8       FTHEOR(MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C           &            TBQMEP(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C           &            TBQMEM(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C           &            TBQMIP(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C           &            TBQMIM(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C           &            TBFMM(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C           &            TBFM(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C           &            TBFMP(2*MXJSHL,(MXNSHL*(MXNSHL+1))/2) ,
C           &            WHIGH(MXJSHL,(MXNSHL*(MXNSHL+1))/2)
C           REAL*8       RHS(MXJ,MXN)
C-----
C           REAL*8       WLOW(MXJSHL,(MXNSHL*(MXNSHL+1))/2,MXNSHL)
C-----

```

## C6WSOL

```

SUBROUTINE C6WSOL( MXNSHL , MXJSHL , IZ1      , NGRND      ,
&                N        , DENSZ      , DENS      , QTHIN      ,
&                TBQMEP   , TBQMEM     , TBQMIP    , TBQMIM    ,
&                TBFMM    , TBFM       , TBFMP     , RHS
&                )
C
C IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C6WSOL *****
C
C PURPOSE:
C
C CALLING PROGRAM: C6WFIL
C
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) IZ1    = ION CHARGE.
C INPUT : (I*4) NGRND = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) N      = PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) DENSZ  = PLASMA ION DENSITY.
C                   UNITS: CM-3
C INPUT : (R*8) DENS   = ELECTRON DENSITY.
C                   UNITS: CM-3
C INPUT : (R*8) QTHIN() = IONISATION RATE COEFFICIENT.
C                   UNITS: CM3 SEC-1
C                   DIMENSION: N SHELL INDEX.
C INPUT : (R*8) TBQMEP(,) = ELECTRON RATE COEFFTT. FOR NLJ->NL+1J'.
C                   1ST DIMENSION: J->J' TRANSITION INDEX.
C                   2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMEM(,) = ELECTRON RATE COEFFTT. FOR NLJ->NL-1J'.
C                   1ST DIMENSION: J->J' TRANSITION INDEX.
C                   2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIP(,) = POSITIVE ION RATE COEFFTT. FOR NLJ->NL+1J'.
C                   1ST DIMENSION: J->J' TRANSITION INDEX.
C                   2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIM(,) = POSITIVE ION RATE COEFFTT. FOR NLJ->NL-1J'.
C                   1ST DIMENSION: J->J' TRANSITION INDEX.
C                   2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMP(,) = RATE COEFFTT. FOR NLJ->NL+1J'.
C                   1ST DIMENSION: J->J' TRANSITION INDEX.
C                   2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFM(,) = RATE COEFFTT. FOR NLJ->NL+1J'.
C                   1ST DIMENSION: J->J' TRANSITION INDEX.
C                   2ND DIMENSION: REFERENCED BY I4IDFL(N,L).

```

```

C INPUT : (R*8) TBFMM(, ) = RATE COEFFT. FOR NLJ->NLJ' FOR STATE I.
C                               1ST DIMENSION: J->J' TRANSITION INDEX.
C                               2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C
C I/O : (R*8) RHS( ) =
C                               DIMENSION: REFERENCED BY L+1.
C
C PARAM : (I*4) MXN = MXNSHL.
C PARAM : (I*4) MXJ = MXJSHL.
C
C (I*4) L = ORBITAL QUANTUM NUMBER.
C (I*4) L1 = ORBITAL QUANTUM NUMBER.
C (I*4) J = J->J' TRANSITION INDEX.
C (I*4) IDL = TABLE INDEX.
C (I*4) N1 = PRINCIPAL QUANTUM NUMBER.
C (I*4) LP = ARRAY INDEX = L+1.
C
C (R*8) AA( ) = LJ RESOLVED A-VALUE.
C                               DIMENSION: TRANSITION INDEX WHERE:
C                               1 GIVES LU+0.5 --> LL+0.5
C                               2 GIVES LU+0.5 --> LL-0.5
C                               3 GIVES LU-0.5 --> LL+0.5
C                               4 GIVES LU-0.5 --> LL-0.5
C
C (R*8) VDS(, ) =
C (R*8) VDI(, ) =
C (R*8) VD(, ) =
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C NUMBERS N AND L.
C
C NOTES:
C 1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C 1 : J=L+0.5 -> J'=L'+0.5
C 2 : J=L+0.5 -> J'=L'-0.5
C 3 : J=L-0.5 -> J'=L'+0.5
C 4 : J=L-0.5 -> J'=L'-0.5
C
C 2) FOR MATRIX HANDLING PURPOSES, L=0 STATES ARE TREATED AS TWO
C STATES OF J=0.5. RATES INTO EACH OF THESE ARE SET EQUAL TO
C HALF THE TOTAL INTO A TRUE L=0,J=0.5 STATE. RATES OUT OF
C EACH STATE ARE SET EQUAL TO THE TOTAL OUT OF A TRUE L=0,J=0.5
C STATE. THUS EACH ARTIFICIAL STATE HAS THE SAME POPULATION
C WHICH IS HALF THE TOTAL OF THE TRUE L=0,J=0.5 STATE.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 08/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 22ND MAY 1996
C
C VERSION: 1.1 DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. IBM VERSION NOT CHANGED
C
C -----
C INTEGER I4UNIT , I4IDFL
C -----
C INTEGER MXN , MXJ
C PARAMETER( MXN = 20 , MXJ = 2 )
C -----
C INTEGER MXNSHL , MXJSHL , NGRND , N , IZ1
C INTEGER L , L1 , J , IDL , N1 ,
C & LP
C -----
C REAL*8 DENSZ , DENS
C -----
C REAL*8 QTHIN(MXNSHL)
C REAL*8 AA(2*MXJ)
C -----
C REAL*8 TBQMEP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBQMEM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBFMM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBFM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & TBFMP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C & RHS(MXJSHL, MXNSHL)
C REAL*8 VDS(2*MXJ, MXN) , VDI(2*MXJ, MXN) , VD(2*MXJ, MXN)
C -----

```

# C7CXEE

```
      SUBROUTINE C7CXEE( MXNENG , MXNSHL , NGRND , NTOT ,
&                      NBOT , NTOP , IRZ0 , IRZ1 ,
&                      RAMSNO , TEV , TIEV , DENS ,
&                      DENSZ , ZEFF , BMAG , BMENG ,
&                      ITHEOR , IBSTAT , IEMMS , NTU ,
&                      NTL , NMINF , NMAXF , NENRGY ,
&                      ENRGYA , ALPHA , XSECNA , FRACLA ,
&                      ERATE
&                      )
C
C      IMPLICIT NONE
C
C-----
C
C***** FORTRAN77 SUBROUTINE: C7CXEE *****
C
C PURPOSE: CALCULATES THE J-RESOLVED EFFECTIVE EMISSIVITY RATE
C           COEFFICIENT FOR THE GIVEN TRANSITION.
C
C           IT IS APPLICABLE TO IMPURITIES IN PLASMA TRAVERSED BY
C           NEUTRAL BEAMS OF H OR HE. THE RECOMBINED TARGET ION MAY BE
C           H, LI OR NA-LIKE.
C
C           THE MODEL INCLUDES CAPTURE, N-N' LEVEL CASCADE, AND MIXING
C           AMONG L,J LEVELS OF SAME N BY COLLISIONS OR MAGNETIC
C           FIELDS.
C
C           ELECTRON IMPACT IONISATION IS INCLUDED TO GIVE COLLISION
C           LIMIT EFFECT.
C
C           AN INTERNAL EIKONAL APPROXIMATION IS USED FOR CAPTURE FROM
C           EXCITED H OR HE STATES, ALTHOUGH NORMALLY THE EXTERNAL DATA
C           SET SHOULD BE USED.
C
C CALLING PROGRAM: ADAS307
C
C INPUT : (I*4) MXNENG = MAXIMUM NO. OF ENERGIES IN DATA SET.
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) NGRND  = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) NTOT   = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND
C                      STATE.
C INPUT : (I*4) NBOT   = MINIMUM PRINCIPAL QUANTUM NUMBER FOR
C                      RATE TABLES.
C INPUT : (I*4) NTOP   = MAXIMUM PRINCIPAL QUANTUM NUMBER FOR
C                      RATE TABLES.
C INPUT : (I*4) IRZ0   = RECEIVER NUCLEAR CHARGE.
C INPUT : (I*4) IRZ1   = RECEIVER ION INITIAL CHARGE.
C INPUT : (R*8) RAMSNO = RECEIVER ATOMIC MASS.
C INPUT : (R*8) TEV    = ELECTRON TEMPERATURE.
C                      UNITS: EV
C INPUT : (R*8) TIEV   = ION TEMPERATURE.
C                      UNITS: EV
C INPUT : (R*8) DENS    = ELECTRON DENSITY.
C                      UNITS: CM-3
C INPUT : (R*8) DENSZ  = PLASMA ION DENSITY.
C                      UNITS: CM-3
C INPUT : (R*8) ZEFF   = EFFECTIVE ION CHARGE.
C INPUT : (R*8) BMAG   = PLASMA MAGNETIC INDUCTION.
C                      UNITS: TESLA
C INPUT : (R*8) BMENG  = BEAM ENERGY.
C                      UNITS: EV/AMU
C INPUT : (I*4) ITHEOR = CHARGE EXCHANGE MODEL OPTION.
C                      1 => USE INPUT DATA SET.
C                      2 => USE EIKONAL MODEL.
C INPUT : (I*4) IBSTAT = DONOR STATE FOR EIKONAL MODEL.
C                      1 => H(1S)
C                      2 => H(2S)
C                      3 => H(2P)
C                      4 => HE(1S2)
C                      5 => HE(1S2S)
C INPUT : (I*4) IEMMS  = EMISSION MEASURE MODEL OPTION.
C                      1 => CHARGE EXCHANGE.
C                      2 => ELECTRON IMPACT EXCITATION.
C                      3 => RADIATIVE RECOMBINATION.
C INPUT : (I*4) NTL    = LOWER PRINCIPAL QUANTUM NUMBER OF
C                      TRANSITION.
C INPUT : (I*4) NTU    = UPPER PRINCIPAL QUANTUM NUMBER OF
C                      TRANSITION.
C INPUT : (I*4) NMINF  = LOWEST N-SHELL FOR WHICH DATA READ.
C INPUT : (I*4) NMAXF  = HIGHEST N-SHELL FOR WHICH DATA READ.
C INPUT : (I*4) NENRGY = NUMBER OF ENERGIES READ FROM DATA SET.
C INPUT : (R*8) ENRGYA() = COLLISION ENERGIES READ FROM INPUT DATA
C                      SET.
C                      UNITS: EV/AMU
C                      DIMENSION: ENERGY INDEX
C INPUT : (R*8) ALPHA() = EXTRAPOLATION PARAMETER ALPHA READ FROM
C                      INPUT DATA SET.
C                      DIMENSION: ENERGY INDEX
C INPUT : (R*8) XSECNA(,) = N-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS
C                      READ FROM INPUT DATA SET.
C                      UNITS: CM2
C                      1ST DIMENSION: ENERGY INDEX
C                      2ND DIMENSION: N-SHELL
C INPUT : (R*8) FRACLA(,) = L-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS.
```

```

C AFTER CXDATA: ABSOLUTE VALUES (CM2).
C AFTER CXFRAC: FRACTION OF N-RESOLVED
C DATA.
C 1ST DIMENSION: ENERGY INDEX
C 2ND DIMENSION: INDEXED BY I4IDFL(N,L)
C
C OUTPUT: (R*8) ERATE = EFFECTIVE EMISSIVITY RATE COEFFICIENT FOR
C REQUESTED TRANSITION
C SPECTRUM LINE.
C UNITS: CM3 SEC-1
C
C PARAM : (I*4) MXN = MXNSHL.
C PARAM : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C PARAM : (I*4) MXBEAM = MAXIMUM NUMBER OF BEAM COMPONENTS.
C PARAM : (I*4) MXOBSL = MAXIMUM NUMBER OF OBSERVED SPECTRUM
C LINES.
C PARAM : (I*4) MXPRSL = MAXIMUM NUMBER OF SPECTRUM LINES TO
C PREDICT.
C
C PARAM : (R*8) EMP = REDUCED MASS FOR POSITIVE ION.
C UNITS: ELECTRON MASSES
C
C (I*4) NBEAM = NUMBER OF BEAM ENERGIES.
C (I*4) NOLINE = NUMBER OF OBSERVED SPECTRUM LINES.
C (I*4) NPLINE = NUMBER OF SPECTRUM LINES TO PREDICT.
C (I*4) NUMIN = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER
C FOR OBSERVED SPECTRUM LINES.
C (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER
C FOR OBSERVED SPECTRUM LINES.
C
C (R*8) EM = EMISSION MEASURE.
C UNITS: CM-5
C
C (I*4) NL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C (I*4) NU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C (I*4) NPL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: SPECTRUM LINE INDEX.
C (I*4) NPU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: SPECTRUM LINE INDEX.
C
C (R*8) BMFRA() = BEAM COMPONENT FRACTIONS.
C DIMENSION: COMPONENT INDEX.
C (R*8) BMENA() = BEAM ENERGY COMPONENTS.
C UNITS: EV/AMU
C (R*8) EMISA() = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C LINES.
C UNITS: PH CM-2 SEC-1
C DIMENSION: SPECTRUM LINE INDEX.
C (R*8) TBLF() = TABLE OF RADIATIVE LIFETIMES.
C UNITS: SECS
C DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) QTHIN() = IONISATION RATE COEFFICIENT.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C (R*8) QTHEX() = MEAN EXCITATION RATE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C (R*8) QTHCH() = MEAN CHARGE EXCHANGE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C (R*8) QTHRC() = MEAN RECOMBINATION RATE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C (R*8) QEX() =
C DIMENSION: N SHELL INDEX.
C (R*8) TOTPOP() = TOTAL COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C DIMENSION: PREDICTED LINE INDEX.
C (R*8) TOTEMI() = TOTAL COLLISION EMISSIVITIES FOR PREDICTED
C SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C DIMENSION: PREDICTED LINE INDEX.
C (R*8) AVRGWL() = AVERAGE AIR WAVELENGTH FOR PREDICTED
C SPECTRUM LINE.
C UNITS: A
C DIMENSION: PREDICTED LINE INDEX.
C (R*8) QEFF() = EFF. RATE COEFFICIENT FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM3 SEC-1
C DIMENSION: PREDICTED LINE INDEX.
C
C (R*8) FTHEXJ(,) = FRACTION OF N-LEVEL MEAN EXCITATION RATE
C COEFFICIENTS IN NLJ-LEVEL.
C 1ST DIMENSION: J SHELL INDEX WHERE:
C 1 GIVES J=L+0.5
C 2 GIVES J=L-0.5
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) FTHCHJ(,) = FRACTION OF N-LEVEL MEAN CHARGE EXCHANGE

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C          COEFFICIENTS IN NLJ-LEVEL.
C          1ST DIMENSION: J SHELL INDEX WHERE:
C              1 GIVES J=L+0.5
C              2 GIVES J=L-0.5
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) FTHRCJ(,) = FRACTION OF N-LEVEL MEAN RECOMBINATION
C          RATE COEFFICIENTS IN NLJ-LEVEL.
C          1ST DIMENSION: J SHELL INDEX WHERE:
C              1 GIVES J=L+0.5
C              2 GIVES J=L-0.5
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) TBQMEP(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C          NLJ->NL+1J'.
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) TBQMEM(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C          NLJ->NL-1J'.
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) TBQMIP(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C          NLJ->NL+1J'.
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) TBQMIM(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C          NLJ->NL-1J'.
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) TBFMP(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C          NLJ->NL+1J'.
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) TBFM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C          NLJ->NLJ'.
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C (R*8) TBFMM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C          NLJ->NL-1J'.
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C
C (R*8) TBLPOP(,,) = TABLE OF COLLISION POP. FOR PREDICTED
C          SPECTRUM LINE.
C          UNITS: CM-2
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDL1().
C          3RD DIMENSION: PREDICTED LINE INDEX.
C (R*8) TBLEMI(,,) = TABLE OF COLLISION EMISSIVITIES FOR
C          PREDICTED SPECTRUM LINE.
C          UNITS: PH CM-2 SEC-1
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDL1().
C          3RD DIMENSION: PREDICTED LINE INDEX.
C (R*8) TBLWLN(,,) = TABLE OF WAVELENGTHS FOR PREDICTED
C          SPECTRUM LINE.
C          UNITS: A
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDL1().
C          3RD DIMENSION: PREDICTED LINE INDEX.
C
C ROUTINES:
C
C ROUTINE   SOURCE   BRIEF DESCRIPTION
C -----
C I4UNIT    ADAS     RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C CXTBLF    ADAS     FILLS L-RESOLVED RADIATIVE LIFETIME
C          TABLE.
C C6TBIN    ADAS     FILLS N-RESOLVED ELECTRON IMPACT
C          IONISATION RATE TABLE.
C C6TBEX    ADAS     FILLS N AND J-RESOLVED ELECTRON IMPACT
C          EXCITATION RATE TABLES.
C C6QEIK    ADAS     FILLS N AND J-RESOLVED CHARGE EXCHANGE
C          RATE TABLES USING EIKONAL APPROXIMATION.
C C6QXCH    ADAS     FILLS N AND J-RESOLVED CHARGE EXCHANGE
C          RATE TABLES USING INPUT DATA SET.
C C6TBRC    ADAS     FILLS N AND J-RESOLVED RADIATIVE
C          RECOMBINATION RATE TABLES.
C C6TBQM    ADAS     FILLS N AND J-RESOLVED COLLISIONAL RATE
C          TABLES.
C C6TBFM    ADAS     FILLS N AND J-RESOLVED B-FIELD
C          DEPENDENT MIXING RATE TABLES.
C C7EMIS    ADAS     PREDICTS THE J-RESOLVED EMISSIVITY FOR
C          REQUESTED TRANSITIONS.
C
C NOTES:
C 1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C   1 : J=L+0.5 -> J'=L'+0.5
C   2 : J=L+0.5 -> J'=L'-0.5
C   3 : J=L-0.5 -> J'=L'+0.5
C   4 : J=L-0.5 -> J'=L'-0.5
C
C AUTHOR:   JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C           K1/0/87
C           JET EXT. 5183
C
C DATE:    26/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR:   WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)

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C DATE: 24TH MAY 1996
C
C VERSION: 1.1 DATE: 24-05-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION
C
C-----
C
C INTEGER I4UNIT
C-----
C INTEGER MXN , MXJSHL , MXBEAM ,
& MXOBSL , MXPRSL
PARAMETER( MXN = 20 , MXJSHL = 2 , MXBEAM = 1 ,
& MXOBSL = 1 , MXPRSL = 1 )
C-----
C REAL*8 EMP
PARAMETER( EMP = 1836.0D0 )
C-----
C INTEGER MXNENG , MXNSHL , NGRND , NTOT , NBOT ,
& NTOP , IRZ0 , IRZ1 , ITHEOR , IBSTAT ,
& IEMMS , NTU , NTL , NMINF , NMAXF ,
& NENRGY
INTEGER NBEAM , NOLINE , NPLINE , NUMIN , NUMAX
C-----
C REAL*8 RAMSNO , TEV , TIEV , DENS , DENSZ ,
& ZEFF , BMAG , BMENG , ERATE
REAL*8 EM
C-----
C INTEGER NL(MXOBSL) , NU(MXOBSL) , NPL(MXPRSL) ,
& NPU(MXPRSL)
C-----
C REAL*8 ENRGYA(MXNENG) , ALPHAA(MXNENG)
REAL*8 BMENA(MXBEAM) , BMFRA(MXBEAM) , EMISA(MXOBSL) ,
& QTHIN(MXN) , QTHEX(MXN) , QTHCH(MXN) ,
& QTHRC(MXN) , QEX(MXN) , TOTPOP(MXPRSL) ,
& TOTEMI(MXPRSL) , AVRGWL(MXPRSL) , QEFF(MXPRSL) ,
& TBLF((MXN*(MXN+1))/2)
C-----
C REAL*8 XSECNA(MXNENG,MXNSHL)
& FRACLA(MXNENG,(MXNSHL*(MXNSHL+1))/2)
REAL*8 FTHEXJ(MXJSHL,(MXN*(MXN+1))/2)
& FTCHCJ(MXJSHL,(MXN*(MXN+1))/2)
& FTJRCJ(MXJSHL,(MXN*(MXN+1))/2)
& TBQMCP(2*MXJSHL,(MXN*(MXN+1))/2)
& TBQMCP(2*MXJSHL,(MXN*(MXN+1))/2)
& TBQMIP(2*MXJSHL,(MXN*(MXN+1))/2)
& TBQMIP(2*MXJSHL,(MXN*(MXN+1))/2)
& TBQMIM(2*MXJSHL,(MXN*(MXN+1))/2)
& TBQMIM(2*MXJSHL,(MXN*(MXN+1))/2)
& TBFMP(2*MXJSHL,(MXN*(MXN+1))/2)
& TBFMM(2*MXJSHL,(MXN*(MXN+1))/2)
& TBFMM(2*MXJSHL,(MXN*(MXN+1))/2)
C-----
C REAL*8 TBLPOP(2*MXJSHL,2*MXN-3,MXPRSL)
& TBLEMI(2*MXJSHL,2*MXN-3,MXPRSL)
& TBLWLN(2*MXJSHL,2*MXN-3,MXPRSL)
C-----

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## C7EMIS

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SUBROUTINE C7EMIS( MXNSHL , MXJSHL , MXOBSL , MXPRSL ,
& IZ0 , IZ1 , NGRND , NTOT ,
& NBOT , DENSZ , DENS , NOLINE ,
& NU , NL , EMISA , NPLINE ,
& NPU , NPL , QTHEOR , FTHEOR ,
& QTHIN , TBQMCP , TBQMCP , TBQMIP ,
& TBQMIM , TBFMP , TBFM , TBFMM ,
& NUMIN , NUMAX , EM , QEX ,
& TOTPOP , TOTEMI , AVRGWL , QEFF ,
& TBLPOP , TBLEMI , TBLWLN
& )
C
C IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: C6EMIS *****
C
C PURPOSE: PREDICTS THE J-RESOLVED EMMISIVITY FOR REQUESTED
C TRANSITIONS.
C
C CALLING PROGRAM: ADAS306
C
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) MXOBSL = MAXIMUM NUMBER OF OBSERVED SPECTRUM
C LINES.
C INPUT : (I*4) MXPRSL = MAXIMUM NUMBER OF SPECTRUM LINES TO
C PREDICT.
C INPUT : (I*4) IZ0 = NUCLEAR CHARGE.
C INPUT : (I*4) IZ1 = ION CHARGE.
C INPUT : (I*4) NGRND = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) NTOT = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND

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C STATE.
C INPUT : (I*4) NBOT = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) DENSZ = PLASMA ION DENSITY.
C UNITS: CM-3
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C UNITS: CM-3
C INPUT : (I*4) NOLINE = NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8) EMISA() = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NPLINE = NUMBER OF SPECTRUM LINES TO PREDICT.
C INPUT : (I*4) NPU() = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (I*4) NPL() = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS
C OF SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) QTHEOR() = MEAN CHARGE EXCHANGE, EXCITATION RATE OR
C RECOMBINATION RATE COEFFICIENTS FOR
C N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) FTHEOR(,) = FRACTION OF N-LEVEL MEAN CHARGE EXCHANGE,
C EXCITATION RATE OR RECOMBINATION RATE
C COEFFICIENTS IN NL-LEVEL.
C 1ST DIMENSION: J SHELL INDEX WHERE:
C 1 GIVES J=L+0.5
C 2 GIVES J=L-0.5
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) QTHIN() = IONISATION RATE COEFFICIENT.
C UNITS: CM3 SEC-1
C DIMENSION: N SHELL INDEX.
C INPUT : (R*8) TBQMEP(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMEM(,) = ELECTRON COLLISIONAL RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIP(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBQMIM(,) = POSITIVE ION COLLISIONAL RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMP(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NL+1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NLJ'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C INPUT : (R*8) TBFMM(,) = B-FIELD DEPENDENT MIXING RATE COEFFT. FOR
C NLJ->NL-1J'.
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C OUTPUT: (I*4) NUMIN = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER
C FOR OBSERVED SPECTRUM LINES.
C OUTPUT: (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER
C FOR OBSERVED SPECTRUM LINES.
C OUTPUT: (R*8) EM = EMISSION MEASURE.
C OUTPUT: (R*8) QEX() =
C DIMENSION: MXNSHL.
C OUTPUT: (R*8) TOTPOP() = TOTAL COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TOTEMI() = TOTAL COLLISION EMISSIVITIES FOR PREDICTED
C SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) AVRGWL() = AVERAGE AIR WAVELENGTH FOR PREDICTED
C SPECTRUM LINE.
C UNITS: A
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) QEFF() = EFF. RATE COEFFICIENT FOR PREDICTED
C SPECTRUM LINE.
C UNITS:
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TBLPOP(,,) = TABLE OF COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C 1ST DIMENSION: J->J' TRANSITION INDEX.
C 2ND DIMENSION: REFERENCED BY I4IDLI().
C OUTPUT: (R*8) TBLEMI(,,) = TABLE OF COLLISION EMISSIVITIES FOR
C PREDICTED SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1

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C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDLI().
C          3RD DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TBLWLN(,,) = TABLE OF WAVELENGTHS FOR PREDICTED
C          SPECTRUM LINE.
C          UNITS: A
C          1ST DIMENSION: J->J' TRANSITION INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDLI().
C          3RD DIMENSION: PREDICTED LINE INDEX.
C
C PARAM : (I*4) MXN      = MXNSHL.
C PARAM : (I*4) MXJ      = MXJSHL.
C PARAM : (I*4) MXOB     = MXOBSL.
C
C          (I*4) NREP     =
C          (I*4) IC       = LOOP INDEX.
C
C          (I*4) ICREP()  =
C                      DIMENSION: MXOB.
C
C          (R*8) WHIGH(,) =
C                      1ST DIMENSION: J SHELL INDEX.
C                      2ND DIMENSION: REFERENCED BY L+1.
C
C          (R*8) WLOW(,,) =
C                      1ST DIMENSION: J SHELL INDEX.
C                      2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C                      3RD DIMENSION: REFERENCED BY L+1.
C
C ROUTINES:
C ROUTINE   SOURCE   BRIEF DESCRIPTION
C -----
C I4UNIT    ADAS     RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C C6WFIL    ADAS
C C7EMQX    ADAS
C C6PRSL    ADAS     PREDICTS REQUESTED SPECTRUM LINES.
C
C NOTES:
C 1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C   1 : J=L+0.5 -> J'=L'+0.5
C   2 : J=L+0.5 -> J'=L'-0.5
C   3 : J=L-0.5 -> J'=L'+0.5
C   4 : J=L-0.5 -> J'=L'-0.5
C
C AUTHOR:   JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C           K1/0/81
C           JET EXT. 5183
C
C DATE:    10/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR:   WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:    22ND MAY 1996
C
C VERSION: 1.1                               DATE: 22-05-96
C MODIFIED: WILLIAM OSBORN
C           - FIRST VERSION. COPIED FROM C6EMIS. CALL TO C6EMQX
C           REPLACED BY CALL TO C7EMQX
C
C -----
C          INTEGER   I4UNIT
C -----
C          INTEGER   MXN      , MXJ      , MXOB
C PARAMETER( MXN = 20 , MXJ = 2 , MXOB = 10 )
C -----
C          INTEGER   MXNSHL , MXJSHL ,
C          &        MXOBSL , MXPRSL , IZ0 , IZ1 ,
C          &        NGRND , NTOT , NBOT , NOLINE ,
C          &        NPLINE , NUMIN , NUMAX
C          INTEGER   NREP , IC
C -----
C          REAL*8    DENSZ , DENS , EM
C -----
C          INTEGER   NU(MXOBSL) , NL(MXOBSL) , NPU(MXPRSL) ,
C          &        NPL(MXPRSL)
C          INTEGER   ICREP(MXOB)
C -----
C          REAL*8    EMISA(MXOBSL) , QTHEOR(MXNSHL) , QTHIN(MXNSHL) ,
C          &        QEX(MXNSHL) , TOTPOP(MXPRSL) , TOTEMI(MXPRSL) ,
C          &        AVRGWL(MXPRSL) , QEFF(MXPRSL)
C -----
C          REAL*8    FTHEOR(MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C          &        TBQMEP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C          &        TBQMEM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C          &        TBQMIP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C          &        TBQMIM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C          &        TBFMP(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C          &        TBFM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2) ,
C          &        TBFMM(2*MXJSHL, (MXNSHL*(MXNSHL+1))/2)
C          REAL*8    WHIGH(MXJ, (MXN*(MXN+1))/2)
C -----
C          REAL*8    TBLPOP(2*MXJSHL, 2*MXNSHL-3, MXPRSL) ,
C          &        TBLEMI(2*MXJSHL, 2*MXNSHL-3, MXPRSL) ,
C          &        TBLWLN(2*MXJSHL, 2*MXNSHL-3, MXPRSL)
C          REAL*8    WLOW(MXJ, (MXN*(MXN+1))/2, MXN)

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# C7EMQX

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SUBROUTINE C7EMQX( MXNSHL , MXJSHL , MXOBSL , IZ1 ,
&                NBOT , NUMIN , NUMAX , NU ,
&                NL , EMISA , NREP , ICREP ,
&                QTHEOR , WLOW , EM , QEX
&                )
C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C6EMQX *****
C
C PURPOSE:
C
C CALLING PROGRAM: C6EMIS
C
C INPUT : (I*4) MXNSHL = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4) MXJSHL = MAXIMUM NUMBER OF J SUB-SHELLS.
C INPUT : (I*4) MXOBSL = MAXIMUM NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) IZ1    = ION CHARGE.
C INPUT : (I*4) NBOT  = MINIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NUMIN = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                   OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                   OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NU( ) = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF
C                   OBSERVED SPECTRUM LINES.
C                   DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NL( ) = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF
C                   OBSERVED SPECTRUM LINES.
C                   DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8) EMISA( ) = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C                   LINES.
C                   DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NREP    =
C INPUT : (I*4) ICREP( ) =
C                   DIMENSION: MXOBSL.
C INPUT : (R*8) QTHEOR( ) = MEAN CHARGE EXCHANGE, EXCITATION RATE OR
C                   RECOMBINATION RATE COEFFICIENTS FOR
C                   N-LEVELS AVERAGED OVER BEAM FRACTIONS.
C                   UNITS: CM3 SEC-1
C                   DIMENSION: N SHELL INDEX.
C INPUT : (R*8) WLOW( , , ) =
C                   1ST DIMENSION: J SHELL INDEX.
C                   2ND DIMENSION: REFERENCED BY I4IDFL(N,L).
C                   3RD DIMENSION: REFERENCED BY L+1.
C
C OUTPUT: (R*8) EM      = EMISSION MEASURE.
C OUTPUT: (R*8) QEX( ) =
C                   DIMENSION: MXNSHL.
C
C PARAM : (I*4) MXN     = MXNSHL.
C PARAM : (I*4) MXJ     = MXJSHL.
C PARAM : (I*4) MXOB    = MXOBSL.
C
C (I*4) N      = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L      = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) N1     = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L1     = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) IDL    = TABLE INDEX.
C (I*4) IC     = ARRAY INDEX.
C (I*4) IC1    = ARRAY INDEX.
C (I*4) IC2    = ARRAY INDEX.
C (I*4) IFAIL  = RETURN FLAG FROM NAG ROUTINE.
C (I*4) M      = LOOP INDEX.
C (I*4) I      = LOOP INDEX.
C (I*4) J      = ARRAY INDEX.
C
C (R*8) XM     = REAL VALUE = M.
C (R*8) X1     =
C (R*8) X2     =
C (R*8) T1     =
C (R*8) T2     =
C (R*8) SUM    =
C (R*8) SUMEX  =
C (R*8) SUMTH  =
C
C (I*4) JLIST( ) =
C                   DIMENSION: MXN.
C
C (R*8) AA( )   = LJ RESOLVED A-VALUE.
C                   DIMENSION: TRANSITION INDEX WHERE:
C                   1 GIVES LU+0.5 --> LL+0.5
C                   2 GIVES LU+0.5 --> LL-0.5
C                   3 GIVES LU-0.5 --> LL+0.5
C                   4 GIVES LU-0.5 --> LL-0.5
C
C (R*8) REMISA( ) =
C                   DIMENSION: MXOB.

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C      (R*8) REMQ( ) = DIMENSION: MXOB.
C
C      (R*8) EMQ( ) = DIMENSION: MXNSHL.
C
C      (R*8) CNDSA( , ) = CONDENSED MATRIX.
C                        1ST DIMENSION: MXN.
C                        2ND DIMENSION: 2.
C      (R*8) ARED( , ) = LINEAR CONDENSATION TRANSFORMATION ARRAY.
C                        1ST DIMENSION: MXN.
C                        2ND DIMENSION: MXN.
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      I4UNIT      ADAS      RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C      I4IDFL      ADAS      RETURNS UNIQUE INDEX GIVEN QUANTUM
C                        NUMBERS N AND L.
C      C6AJTB      ADAS      CALCULATES LJ RESOLVED A-VALUES.
C      XXMINV      ADAS      MATRIX SOLUTION REPLACING NAG ROUTINE F04ARF
CX      F04ARF      NAG      FINDS SOLUTION TO A SET OF REAL LINEAR
CX                        EQUATIONS.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C        K1/0/81
C        JET EXT. 5183
C
C DATE: 09/11/93
C
C UNIX-IDL PORT:
C
C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE: 28ND MAY 1996
C
C VERSION: 1.1 DATE: 28-05-96
C MODIFIED: WILLIAM OSBORN
C           - FIRST VERSION. COPIED FROM C6EMQX BUT WITH NAG ROUTINE
C           REPLACED BY XXMINV.
C
C-----
C      INTEGER      I4UNIT , I4IDFL
C-----
C      INTEGER      MXN , MXJ , MXOB
C      PARAMETER( MXN = 20 , MXJ = 2 , MXOB = 10 )
C-----
C      INTEGER      MXNSHL , MXJSHL , MXOBSL , IZ1 , NBOT ,
C      &            NUMIN , NUMAX , NREP
C      INTEGER      N , L , N1 , L1 , IDL ,
C      &            IC , IC1 , IC2 , IFAIL , M ,
C      &            I , J
C-----
C      REAL*8      EM
C      REAL*8      XM , X1 , X2 , T1 , T2 ,
C      &            SUM , SUMEX , SUMTH
C-----
C      INTEGER      ICREP(MXOBSL) , NU(MXOBSL) , NL(MXOBSL)
C      INTEGER      JLIST(MXN)
C-----
C      REAL*8      EMISA(MXOBSL) , QTHEOR(MXNSHL) , QEX(MXNSHL)
C      REAL*8      AA(2*MXJ) , REMISA(MXOB) , REMQ(MXOB) ,
C      &            EMQ(MXN)
C      REAL*8      CNDSA(MXN,2)
C      &            ARED(MXOB,MXOB)
C      REAL*8      WLOW(MXJSHL, (MXNSHL*(MXNSHL+1))/2, MXNSHL)
C-----
C      INTEGER      PIPEIN , PIPEOU
C      PARAMETER( PIPEIN=5 , PIPEOU=6)
C-----

```

## C8CHRG

```

SUBROUTINE C8CHRG( SYMBD , IZD , SYMBR , IZR , IDZ0 ,
&                IRZ0 , IRZ1 , IRZ2
&                )
C
C      IMPLICIT NONE
C-----
C *****
C      PURPOSE: SETS UP NUCLEAR CHARGE OF DONOR AND NUCLEAR, INITIAL AND
C              FINAL CHARGES OF RECEIVER. CHECKS VALIDITY OF RECEIVER
C              CHARGES.
C
C      CALLING PROGRAM: ADAS308
C
C      INPUT : (C*2) SYMBD = DONOR ELEMENT SYMBOL.
C      INPUT : (I*4) IZD   = DONOR ION CHARGE.
C      INPUT : (C*2) SYMBR = RECEIVER ELEMENT SYMBOL.

```

```

C INPUT : (I*4) IZR = RECEIVER ION CHARGE.
C
C OUTPUT: (I*4) IDZ0 = DONOR NUCLEAR CHARGE.
C OUTPUT: (I*4) IRZ0 = RECEIVER NUCLEAR CHARGE.
C OUTPUT: (I*4) IRZ1 = RECEIVER ION INITIAL CHARGE.
C OUTPUT: (I*4) IRZ2 = RECEIVER ION FINAL CHARGE.
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT MESSAGES
C CXCHRG ADAS RETURNS DONOR NUCLEAR CHARGE AND
C RECEIVER NUCLEAR, INITIAL AND FINAL
C CHARGES.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 26/11/93
C
C -----
C
C INTEGER I4UNIT
C -----
C INTEGER IZR , IZD , IDZ0 , IRZ0 , IRZ1 ,
C & IRZ2
C -----
C CHARACTER SYMBD*2 , SYMBR*2
C -----

```

## C8EMIS

```

SUBROUTINE C8EMIS( MXNSHL , MXOBSL , MXPRSL , IZ0 ,
& IZ1 , NGRND , NTOT , NBOT ,
& DENSZ , DENS , NOLINE , NU ,
& NL , EMISA , NPLINE , NPU ,
& NPL , QTHEOR , FTHEOR , TBQMEMP ,
& TBQMEMP , TBQMIP , TBQMIM , NUMIN ,
& NUMAX , EM , QEX , TOTPOP ,
& TOTEMI , AVRGWL , QEFF , TBLPOP ,
& TBLEMI , TBLWLN
& )
C
C IMPLICIT NONE
C
C -----
C ***** FORTRAN77 SUBROUTINE: C8EMIS *****
C
C PURPOSE: PREDICTS THE L-RESOLVED EMISSIVITY FOR REQUESTED
C TRANSITIONS.
C
C CALLING PROGRAM: ADAS308
C
C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) MXOBSL = MAXIMUM NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) MXPRSL = MAXIMUM NUMBER OF SPECTRUM LINES TO
C PREDICT.
C INPUT : (I*4) IZ0 = NUCLEAR CHARGE.
C INPUT : (I*4) IZ1 = ION CHARGE.
C INPUT : (I*4) NGRND = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) NTOT = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND
C STATE.
C INPUT : (I*4) NBOT = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) DENSZ = PLASMA ION DENSITY.
C UNITS: CM-3
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C UNITS: CM-3
C INPUT : (I*4) NOLINE = NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NU( ) = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF
C OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NL( ) = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF
C OBSERVED SPECTRUM LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8) EMISA( ) = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C LINES.
C DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NPLINES = NUMBER OF SPECTRUM LINES TO PREDICT.
C INPUT : (I*4) NPU( ) = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF
C SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (I*4) NPL( ) = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF
C SPECTRUM LINES TO PREDICT.
C DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8) QTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE
C COEFFICIENTS FOR N-LEVELS AVERAGED OVER
C BEAM FRACTIONS.
C UNITS: CM3 SEC-1
C DIMENSION: REFERENCED BY N QUANTUM NUMBER.
C INPUT : (R*8) FTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE

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C
C FOR NL-LEVELS AS A FRACTION OF
C CORRESPONDING N-LEVEL.
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMEP( ) = ELECTRON RATE COEFFT. FOR NL->NL+1.
C INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C I4IDFL(N,L).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMEM( ) = ELECTRON RATE COEFFT. FOR NL+1->NL.
C INDEX FOR NL+1->NL TRANSITION GIVEN BY
C I4IDFL(N,L+1).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMIP( ) = POSITIVE ION RATE COEFFT. FOR NL->NL+1.
C INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C I4IDFL(N,L).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMIM( ) = POSITIVE ION RATE COEFFT. FOR NL+1->NL.
C INDEX FOR NL+1->NL TRANSITION GIVEN BY
C I4IDFL(N,L+1).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C OUTPUT: (I*4) NUMIN = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C OBSERVED SPECTRUM LINES.
C OUTPUT: (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C OBSERVED SPECTRUM LINES.
C OUTPUT: (R*8) EM = EMISSION MEASURE.
C OUTPUT: (R*8) QEX( ) =
C DIMENSION: MXNSHL.
C OUTPUT: (R*8) TOTPOP( ) = TOTAL COLLISION POP. FOR PREDICTED SPECTRUM
C LINE.
C UNITS: CM-2
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TOTEMI( ) = TOTAL COLLISION EMISSIVITIES FOR PREDICTED
C SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) AVRGWL( ) = AVERAGE AIR WAVELENGTH FOR PREDICTED
C SPECTRUM LINE.
C UNITS: A
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) QEFF( ) = EFF. RATE COEFFICIENT FOR PREDICTED
C SPECTRUM LINE.
C UNITS:
C DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8) TBLPOP( , ) = TABLE OF COLLISION POP. FOR PREDICTED
C SPECTRUM LINE.
C UNITS: CM-2
C 1ST DIMENSION: PREDICTED LINE INDEX.
C 2ND DIMENSION: REFERENCED BY FUNC I4IDL( ).
C OUTPUT: (R*8) TBLEMI( , ) = TABLE OF COLLISION EMISSIVITIES FOR
C PREDICTED SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C 1ST DIMENSION: PREDICTED LINE INDEX.
C 2ND DIMENSION: REFERENCED BY FUNC I4IDL( ).
C OUTPUT: (R*8) TBLWLN( , ) = TABLE OF WAVELENGTHS FOR PREDICTED SPECTRUM
C LINE.
C UNITS: A
C 1ST DIMENSION: PREDICTED LINE INDEX.
C 2ND DIMENSION: REFERENCED BY FUNC I4IDL( ).
C
C PARAM : (I*4) MXN = MXNSHL.
C PARAM : (I*4) MXOB = MXOBSL.
C
C (I*4) NREP =
C (I*4) IC = LOOP INDEX.
C
C (I*4) ICREP( ) =
C DIMENSION: MXOB.
C
C (R*8) WHIGH( ) =
C DIMENSION: REFERENCED BY L+1.
C
C (R*8) WLOW( , ) =
C 1ST DIMENSION: REFERENCED BY I4IDFL(N,L).
C 2ND DIMENSION: REFERENCED BY L+1.
C
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C CXWFIL ADAS
C CXEMQX
C CXPRSL ADAS PREDICTS REQUESTED SPECTRUM LINES.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 15/10/93
C
C -----
C
C INTEGER I4UNIT
C -----
C INTEGER MXN , MXOB
C PARAMETER( MXN = 20 , MXOB = 10 )
C -----
C INTEGER MXNSHL , MXOBSL , MXPRSL , IZ0 , IZ1 ,

```





```

C      (I*4)  J      = ARRAY INDEX.
C
C      (R*8)  XM      = REAL VALUE = M.
C      (R*8)  X1      =
C      (R*8)  X2      =
C      (R*8)  T1      =
C      (R*8)  T2      =
C      (R*8)  SUM      =
C      (R*8)  SUMEX    =
C      (R*8)  SUMTH    =
C
C      (I*4)  JLIST() =
C                      DIMENSION: MXN.
C
C      (R*8)  REMISA() =
C                      DIMENSION: MXOB.
C      (R*8)  REMQ()  =
C                      DIMENSION: MXOB.
C      (R*8)  WKSPACE() = WORKSPACE FOR NAG ROUTINE.
C                      DIMENSION: MXOB.
C      (R*8)  EMQ()   =
C                      DIMENSION: MXNSHL.
C
C      (R*8)  CNDSA(, ) = CONDENSED MATRIX.
C                      1ST DIMENSION: MXN.
C                      2ND DIMENSION: 2.
C      (R*8)  ARED(, ) = LINEAR CONDENSATION TRANSFORMATION ARRAY.
C                      1ST DIMENSION: MXN.
C                      2ND DIMENSION: MXN.
C      (I*4)  PIPEIN - PARAMETER = UNIT NUMBER FOR OUTPUT TO PIPE
C      (I*4)  PIPEOU - PARAMETER = UNIT NUMBER FOR INPUT FROM PIPE
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C -----
C      I4UNIT      ADAS      RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C      I4IDFL      ADAS      RETURNS UNIQUE INDEX GIVEN QUANTUM
C                      NUMBERS N AND L.
C      R8ATAB      ADAS      RETURNS HYDRONIC L-RESOLVED A-VALUES.
C                      IF INPUT QUANTUM NUMBERS ARE INVALID
C                      THEN RETURNS ZERO.
C      XXFLSH      ADAS      FLUSHES UNIX PIPE.
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          K1/0/81
C          JET EXT. 5183
C
C DATE:    14/10/93
C
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C           CHANGED ...J.EQ.NREP... TO ...J.NE.NREP... IN THE IF
C           STATEMENT AFTER LINE 2.
C           GENERAL UNIX PORT.
C
C DATE:    20/6/95
C
C -----
C
C      INTEGER      I4UNIT , I4IDFL
C      REAL*8       R8ATAB
C
C -----
C
C      INTEGER      MXN , MXOB
C      PARAMETER( MXN = 20 , MXOB = 10 )
C
C -----
C
C      INTEGER      MXNSHL , MXOBSL , IZ1 , NBOT , NUMIN ,
C      &            NUMAX , NREP
C      INTEGER      N , L , N1 , L1 , IC ,
C      &            IC1 , IC2 , IFAIL , M , I ,
C      &            J
C      INTEGER      PIPEOU , PIPEIN
C      PARAMETER ( PIPEOU=6, PIPEIN=5)
C
C -----
C
C      REAL*8       EM
C      REAL*8       XM , X1 , X2 , T1 , T2 ,
C      &            SUM , SUMEX , SUMTH
C
C -----
C
C      INTEGER      ICREP(MXOBSL) , NU(MXOBSL) , NL(MXOBSL)
C      INTEGER      JLIST(MXN)
C
C -----
C
C      REAL*8       EMISA(MXOBSL) , QTHEOR(MXNSHL) , QEX(MXNSHL)
C      REAL*8       REMISA(MXOB) , REMQ(MXOB) , WKSPACE(MXOB) ,
C      &            EMQ(MXN)
C      REAL*8       WLOW((MXNSHL*(MXNSHL+1))/2,MXNSHL)
C      REAL*8       CNDSA(MXN,2)
C      &            ARED(MXOB,MXOB)
C
C -----

```

## C8PRSL

```

SUBROUTINE C8PRSL( MXNSHL , MXPRSL , IZ0 , IZ1 ,
&                NPLINE , NPU , NPL , NUMAX ,
&                WHIGH , WLOW , EM , QEX ,

```



```

C      (R*8) RF =
C      (R*8) WAVAIR = WAVELENGTH FOR PREDICTED SPECTRUM LINE.
C                      UNITS: A
C      (R*8) SUM1 = SUM OF COL. POP. FOR PREDICTED LINE.
C                      UNITS: CM-2
C      (R*8) SUM2 = SUM OF COL. EMIS. FOR PREDICTED LINE.
C                      UNITS: PH CM-2 SEC-1
C      (R*8) SUM3 = SUM OF WAVELENGTHS FOR PREDICTED LINE.
C                      UNITS: A
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C-----
C      I4UNIT      ADAS      RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C      I4IDFL      ADAS      RETURNS UNIQUE INDEX GIVEN QUANTUM
C                      NUMBERS N AND L.
C      I4IDLI      ADAS      RETURNS INDEX FOR PREDICTED SPECTRUM
C                      LINE TABLES.
C      R8ATAB      ADAS      RETURNS HYDRONIC L-RESOLVED A-VALUES.
C                      IF INPUT QUANTUM NUMBERS ARE INVALID
C                      THEN RETURNS ZERO.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C      K1/0/81
C      JET EXT. 5183
C
C DATE: 14/10/93
C
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      ADDED ERROR MESSAGE FOR NUMERICAL ERRORS INTRODUCED
C      BY BAD VALUES FOR THE OBSERVED SPECTRUM LINES
C      ALSO GENERAL UNIX PORT.
C
C DATE: 20/6/95
C
C-----
C      INTEGER      I4IDFL , I4IDLI, I4UNIT
C      REAL*8      R8ATAB
C-----
C      REAL*8      C1 , C2 ,
C      &          C3 , C4 ,
C      &          C5 , RZ ,
C      PARAMETER( C1 = 6432.8D0 , C2 = 2949810.0D0 ,
C      &          C3 = 25540.0D0 , C4 = 176.0D0 ,
C      &          C5 = 41.0D0 , RZ = 109737.2D0 )
C-----
C      INTEGER      MXNSHL , MXPRSL , IZ0 , IZ1 , NPLINE ,
C      &          NUMAX
C      INTEGER      IN , N , L , N1 , L1 ,
C      &          NP , IDL , ID
C-----
C      REAL*8      EM
C      REAL*8      Z1 , T1 , T2 , E0 , E10 ,
C      &          DELTA , SIG2 , RF , WAVAIR , SUM1 ,
C      &          SUM2 , SUM3
C-----
C      INTEGER      NPU(MXPRSL) , NPL(MXPRSL)
C-----
C      REAL*8      WHIGH((MXNSHL*(MXNSHL+1))/2) ,
C      &          QEX(MXNSHL) ,
C      &          TOTPOP(MXPRSL) ,
C      &          TOTEMI(MXPRSL) ,
C      &          AVRGWL(MXPRSL) ,
C      &          QEFF(MXPRSL)
C      REAL*8      WLOW((MXNSHL*(MXNSHL+1))/2,MXNSHL) ,
C      &          TBLPOP(MXPRSL,2*MXNSHL-3) ,
C      &          TBLEMI(MXPRSL,2*MXNSHL-3) ,
C      &          TBLWLN(MXPRSL,2*MXNSHL-3)
C-----

```

## C8TBQM

```

C      SUBROUTINE C8TBQM( MXNSHL , IZ0 , IZ1 , NBOT ,
C      &          NTOP , TEV , DENS , ZP ,
C      &          TFPV , EMP , TBLF , TBQMEP ,
C      &          TBQMEMP , TBQMIP , TBQMIM
C      &          )
C
C      IMPLICIT NONE
C-----
C      ***** FORTRAN77 SUBROUTINE: C8TBQM *****
C
C PURPOSE: SETS UP TABLES OF ELECTRON AND POSITIVE ION IMPACT RATE
C          COEFFICIENTS BETWEEN NEARLY DEGENERATE L STATES OF THE
C          SAME N FOR HYDROGENIC IONS.
C
C CALLING PROGRAM: ADAS308
C

```

```

C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) IZ0 = NUCLEAR CHARGE OF TARGET ION.
C INPUT : (I*4) IZ1 = ION CHARGE.
C INPUT : (I*4) NBOT = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NTOP = MAXIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) TEV = ELECTRON TEMPERATURE.
C UNITS: EV
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C UNITS: CM-3
C INPUT : (R*8) ZP = CHARGE OF COLLIDING POSITIVE ION.
C INPUT : (R*8) TPV = TEMPERATURE (COLLIDING POSITIVE ION
C DISTRIBUTION).
C UNITS: EV
C INPUT : (R*8) EMP = REDUCED MASS FOR COLLIDING POSITIVE ION.
C UNITS: ELECTRON MASSES
C INPUT : (R*8) ZP = CHARGE OF COLLIDING POSITIVE ION.
C INPUT : (R*8) TPV = POSITIVE ION TEMPERATURE.
C UNITS: EV
C INPUT : (R*8) EMP = REDUCED MASS FOR COLLIDING POSITIVE ION.
C UNITS: ELECTRON MASSES
C INPUT : (R*8) TBLF() = TABLE OF RADIATIVE LIFETIMES.
C UNITS: SECS
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C OUTPUT: (R*8) TBQMEP() = ELECTRON RATE COEFFT. FOR NL->NL+1.
C INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C I4IDFL(N,L).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C OUTPUT: (R*8) TBQMEM() = ELECTRON RATE COEFFT. FOR NL+1->NL.
C INDEX FOR NL+1->NL TRANSITION GIVEN BY
C I4IDFL(N,L+1).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C OUTPUT: (R*8) TBQMIP() = POSITIVE ION RATE COEFFT. FOR NL->NL+1.
C INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C I4IDFL(N,L).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C OUTPUT: (R*8) TBQMIM() = POSITIVE ION RATE COEFFT. FOR NL+1->NL.
C INDEX FOR NL+1->NL TRANSITION GIVEN BY
C I4IDFL(N,L+1).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C PARAM : (I*4) MXJ = MAXIMUM NUMBER OF J SUB-SHELLS.
C PARAM : (R*8) P1 =
C PARAM : (R*8) P2 =
C
C (I*4) NI = VALENCE ELECTRON PRINCIPAL QUANTUM NUMBER
C IN STATE I.
C (I*4) NJ = VALENCE ELECTRON PRINCIPAL QUANTUM NUMBER
C IN STATE J.
C (I*4) LI = VALENCE ELECTRON ORBITAL QUANTUM NUMBER IN
C STATE I.
C (I*4) LJ = VALENCE ELECTRON ORBITAL QUANTUM NUMBER IN
C STATE J.
C (I*4) IDLI = TABLE INDEX.
C (I*4) IDLJ = TABLE INDEX.
C (I*4) I = LOOP INDEX.
C
C (R*8) FACE =
C (R*8) FACI =
C (R*8) WI = STATISTICAL WEIGHT OF STATE I.
C (R*8) WJ = STATISTICAL WEIGHT OF STATE J.
C (R*8) GAE = GAMA RATE PARAMETER FOR ELECTRON COLLISIONS.
C (R*8) GAP = GAMA RATE PARAMETER FOR POSITIVE ION
C COLLISIONS.
C (R*8) QEP() = ELECTRON RATE COEFFT. FOR NLJ->NL+1J'
C DIMENSION: J->J' TRANSITION INDEX.
C (R*8) QEM() = ELECTRON RATE COEFFT. FOR NLJ->NL-1J'
C DIMENSION: J->J' TRANSITION INDEX.
C (R*8) QIP() = POSITIVE ION RATE COEFFT. FOR NLJ->NL+1J'
C DIMENSION: J->J' TRANSITION INDEX.
C (R*8) QIM() = POSITIVE ION RATE COEFFT. FOR NLJ->NL-1J'
C DIMENSION: J->J' TRANSITION INDEX.
C
C NOTES:
C 1) THE J->J' TRANSITION INDEX IS AS FOLLOWS:
C 1 : J=L+0.5 -> J'=L'+0.5
C 2 : J=L+0.5 -> J'=L'-0.5
C 3 : J=L-0.5 -> J'=L'+0.5
C 4 : J=L-0.5 -> J'=L'-0.5
C
C 2) BEFORE CALLING C8TBQM THE LIFETIME TABLE MUST BE FILLED
C WITH A CALL TO CXTBLF.
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C NUMBERS N AND L.
C CXCRDG ADAS CALCULATES COLLISIONAL RATE COEFFICIENTS
C BETWEEN NEARLY DEGENERATE LEVELS OF
C H-, LI- OR NA-LIKE IONS.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 12/10/93
C

```

```

C-----
C
C-----
C      INTEGER      I4IDFL
C-----
C      INTEGER      MXJ
C      PARAMETER( MXJ = 2 )
C-----
C      REAL*8       P1          , P2
C      PARAMETER( P1 = 2.17161D-8 , P2 = 13.6048D0 )
C-----
C      INTEGER      MXNSHL , IZ0 , IZ1 , NTOP , NBOT
C      INTEGER      NI      , NJ   , LI   , LJ   , IDLI ,
C      &            IDLJ   , I
C-----
C      REAL*8       TEV      , DENS  , ZP   , TPV  , EMP
C      REAL*8       FACE    , FACI  , WI   , WJ   , GAE
C      &            GAP
C-----
C      REAL*8       TBLF( (MXNSHL*(MXNSHL+1))/2 ) ,
C      &            TBQMEP( (MXNSHL*(MXNSHL+1))/2 ) ,
C      &            TBQMEM( (MXNSHL*(MXNSHL+1))/2 ) ,
C      &            TBQMIP( (MXNSHL*(MXNSHL+1))/2 ) ,
C      &            TBQMIM( (MXNSHL*(MXNSHL+1))/2 )
C      REAL*8       QEP(2*MXJ) , QEM(2*MXJ) , QIP(2*MXJ) ,
C      &            QIM(2*MXJ)
C-----

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## C8WFIL

```

      SUBROUTINE C8WFIL( MXNSHL , IZ1 , NGRND , NTOT ,
&                      NBOT , NUMAX , DENSZ , DENS ,
&                      QTHEOR , FTHEOR , TBQMEP , TBQMEM ,
&                      TBQMIP , TBQMIM , WHICH , WLOW
&                      )
C
C      IMPLICIT NONE
C-----
C *****
C ***** FORTRAN77 SUBROUTINE: C8WFIL *****
C-----
C PURPOSE:
C
C CALLING PROGRAM: C8EMIS
C
C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) IZ1    = ION CHARGE.
C INPUT : (I*4) NGRND  = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) NTOT   = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND
C                      STATE.
C INPUT : (I*4) NBOT   = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NUMAX  = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                      OBSERVED SPECTRUM LINES.
C INPUT : (R*8) DENSZ  = PLASMA ION DENSITY.
C                      UNITS: CM-3
C INPUT : (R*8) DENS   = ELECTRON DENSITY.
C                      UNITS: CM-3
C INPUT : (R*8) QTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE
C                      COEFFICIENTS FOR N-LEVELS AVERAGED OVER
C                      BEAM FRACTIONS.
C                      UNITS: CM3 SEC-1
C                      DIMENSION: REFERENCED BY N QUANTUM NUMBER.
C INPUT : (R*8) FTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE
C                      FOR NL-LEVELS AS A FRACTION OF
C                      CORRESPONDING N-LEVEL.
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMEP( ) = ELECTRON RATE COEFFT. FOR NL->NL+1.
C                      INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C                      I4IDFL(N,L).
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMEM( ) = ELECTRON RATE COEFFT. FOR NL+1->NL.
C                      INDEX FOR NL+1->NL TRANSITION GIVEN BY
C                      I4IDFL(N,L+1).
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMIP( ) = POSITIVE ION RATE COEFFT. FOR NL->NL+1.
C                      INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C                      I4IDFL(N,L).
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMIM( ) = POSITIVE ION RATE COEFFT. FOR NL+1->NL.
C                      INDEX FOR NL+1->NL TRANSITION GIVEN BY
C                      I4IDFL(N,L+1).
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C OUTPUT: (R*8) WHICH( ) =
C                      DIMENSION: REFERENCED BY L+1.
C OUTPUT: (R*8) WLOW( , ) =
C                      1ST DIMENSION: REFERENCED BY I4IDFL(N,L).
C                      2ND DIMENSION: REFERENCED BY L+1.
C
C PARAM : (I*4) MXN    = MXNSHL.
C
C      (I*4) N          = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.

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C      (I*4) L      = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C      (I*4) N1     = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C      (I*4) L1     = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C      (I*4) N2     = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C      (I*4) L2     = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C      (I*4) LP     = ARRAY INDEX = L+1.
C      (I*4) IDL    = ARRAY INDEX.
C
C      (R*8) A1     = LOCAL STORE FOR RETURN VALUE OF FUNC R8ATAB.
C
C      (R*8) RHS()  = RIGHT HAND SIDE OF N LEVEL EQUATION.
C                    DIMENSION: MXN.
C      (I*4) PIPEIN - PARAMETER = UNIT NUMBER FOR OUTPUT TO PIPE
C      (I*4) PIPEOU - PARAMETER = UNIT NUMBER FOR INPUT FROM PIPE
C
C ROUTINES:
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C      -----
C      I4UNIT       ADAS        RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C      I4IDFL       ADAS        RETURNS UNIQUE INDEX GIVEN QUANTUM
C                                NUMBERS N AND L.
C      R8ATAB       ADAS        RETURNS HYDRONIC L-RESOLVED A-VALUES.
C                                IF INPUT QUANTUM NUMBERS ARE INVALID
C                                THEN RETURNS ZERO.
C      CXWSOL       ADAS
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C         K1/0/81
C         JET EXT. 5183
C
C DATE:    13/10/93
C
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C           UNIX PORT
C
C DATE:    20/6/95
C
C-----
C
C      INTEGER      I4UNIT , I4IDFL
C      REAL*8       R8ATAB
C-----
C
C      INTEGER      MXN
C      PARAMETER( MXN = 20 )
C-----
C
C      INTEGER      MXNSHL , IZ1 , NGRND , NTOT , NBOT ,
C      &            NUMAX
C      INTEGER      N , L , N1 , L1 , N2 ,
C      &            L2 , LP , IDL
C      INTEGER      NTIMES
C      INTEGER      PIPEOU , PIPEIN
C      PARAMETER ( PIPEOU=6, PIPEIN=5)
C-----
C
C      REAL*8       DENSZ , DENS
C      REAL*8       A1
C-----
C
C      REAL*8       QTHEOR(MXNSHL)
C      &            FTHEOR((MXNSHL*(MXNSHL+1))/2) ,
C      &            TBQMEP((MXNSHL*(MXNSHL+1))/2) ,
C      &            TBQMEM((MXNSHL*(MXNSHL+1))/2) ,
C      &            TBQMIP((MXNSHL*(MXNSHL+1))/2) ,
C      &            TBQMIM((MXNSHL*(MXNSHL+1))/2) ,
C      &            WHIGH((MXNSHL*(MXNSHL+1))/2)
C      REAL*8       RHS(MXN)
C-----
C
C      REAL*8       WLOW((MXNSHL*(MXNSHL+1))/2,MXNSHL)
C-----

```

## C8WSOL

```

SUBROUTINE C8WSOL( MXNSHL , IZ1 , NGRND , N
&                DENSZ , DENS , TBQMEP , TBQMEM ,
&                TBQMIP , TBQMIM , RHS
&                )
C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C8WSOL *****
C
C PURPOSE:
C
C CALLING PROGRAM: C8WFIL
C
C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) IZ1    = ION CHARGE.
C INPUT : (I*4) NGRND  = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) N      = PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) DENSZ  = PLASMA ION DENSITY.
C                    UNITS: CM-3
C INPUT : (R*8) DENS   = ELECTRON DENSITY.

```

```

C
C INPUT : (R*8) TBQMEP() = UNITS: CM-3
                        ELECTRON RATE COEFFT. FOR NL->NL+1.
                        INDEX FOR NL->NL+1 TRANSITION GIVEN BY
                        I4IDFL(N,L).
                        DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMEM() = ELECTRON RATE COEFFT. FOR NL+1->NL.
                        INDEX FOR NL+1->NL TRANSITION GIVEN BY
                        I4IDFL(N,L+1).
                        DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMIP() = POSITIVE ION RATE COEFFT. FOR NL->NL+1.
                        INDEX FOR NL->NL+1 TRANSITION GIVEN BY
                        I4IDFL(N,L).
                        DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMIM() = POSITIVE ION RATE COEFFT. FOR NL+1->NL.
                        INDEX FOR NL+1->NL TRANSITION GIVEN BY
                        I4IDFL(N,L+1).
                        DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C I/O : (R*8) RHS() =
                        DIMENSION: REFERENCED BY L+1.
C
C PARAM : (I*4) MXN = MXNSHL.
C
C (I*4) L = ORBITAL QUANTUM NUMBER.
C (I*4) IDL = ARRAY INDEX.
C (I*4) N1 = PRINCIPAL QUANTUM NUMBER.
C (I*4) LP = ARRAY INDEX = L+1.
C (I*4) IFAIL = RETURN FLAG FROM NAG ROUTINE.
C
C (R*8) VDS() =
C (R*8) VDI() =
C (R*8) VD() =
C (I*4) PIPEIN - PARAMETER = UNIT NUMBER FOR OUTPUT TO PIPE
C (I*4) PIPEOU - PARAMETER = UNIT NUMBER FOR INPUT FROM PIPE
C
C ROUTINES:
C
C ROUTINE SOURCE BRIEF DESCRIPTION
C-----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C NUMBERS N AND L.
C R8ATAB ADAS RETURNS HYDRONIC L-RESOLVED A-VALUES.
C IF INPUT QUANTUM NUMBERS ARE INVALID
C THEN RETURNS ZERO.
C XXFLSH ADAS FLUSHES UNIX PIPE.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 12/10/93
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C UNIX PORT - ROUTINE NOW USES AN IDL ROUTINE TO SOLVE
C EQUATIONS RATHER THAN NAG
C
C DATE: 20/6/95
C-----
C
C INTEGER I4UNIT , I4IDFL
C REAL*8 R8ATAB
C-----
C INTEGER MXN
C PARAMETER( MXN = 20 )
C-----
C INTEGER MXNSHL , NGRND , N , IZ1
C INTEGER L , IDL , N1 , LP , IFAIL
C INTEGER I
C INTEGER PIPEOU , PIPEIN
C PARAMETER (PIPEOU=6, PIPEIN=5)
C-----
C REAL*8 DENSZ , DENS
C-----
C REAL*8 TBQMEP((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMEM((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIP((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIM((MXNSHL*(MXNSHL+1))/2) ,
C & RHS(MXNSHL)
C REAL*8 VDS(MXN) , VDI(MXN) , VD(MXN)
C-----

```

## C9CXEE

```

SUBROUTINE C9CXEE( MXNENG , MXNSHL , NGRND , NTOT ,
& NBOT , NTOP , IRZ0 , IRZ1 ,
& RAMSNO , TEV , TIEV , DENS ,
& DENSZ , ZEFF , BMAG , BMENG ,
& ITHEOR , IBSTAT , IEMMS , NTU ,
& NTL , NMINF , NMAXF , NENRGY ,
& ENRGYA , ALPHAA , XSECNA , FRACLA ,
& ERATE
& )

```

```

C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C9CXEE *****
C
C PURPOSE:  CALCULATES THE L-RESOLVED EFFECTIVE EMISSIVITY RATE
C            COEFFICIENT FOR THE GIVEN TRANSITION.
C
C            IT IS APPLICABLE TO IMPURITIES IN PLASMA TRAVERSED BY
C            NEUTRAL BEAMS OF H OR HE.
C
C            THE RECOMBINED TARGET ION IS TREATED AS H-LIKE.
C
C            THE MODEL INCLUDES CAPTURE, N-N' LEVEL CASCADE, AND MIXING
C            AMONG L LEVELS OF SAME N BY COLLISIONS.
C
C            AN INTERNAL EIKONAL APPROXIMATION IS USED FOR CAPTURE FROM
C            EXCITED H OR HE STATES, ALTHOUGH NORMALLY THE EXTERNAL DATA
C            SET SHOULD BE USED.
C
C CALLING PROGRAM: ADAS309
C
C INPUT : (I*4)  MXNENG      = MAXIMUM NO. OF ENERGIES IN DATA SET.
C INPUT : (I*4)  MXNSHL     = MAXIMUM NUMBER OF N SHELLS.
C INPUT : (I*4)  NGRND      = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4)  NTOT       = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND
C                           STATE.
C INPUT : (I*4)  NBOT       = MINIMUM PRINCIPAL QUANTUM NUMBER FOR
C                           RATE TABLES.
C INPUT : (I*4)  NTOP       = MAXIMUM PRINCIPAL QUANTUM NUMBER FOR
C                           RATE TABLES.
C INPUT : (I*4)  IRZ0       = RECEIVER NUCLEAR CHARGE.
C INPUT : (I*4)  IRZ1       = RECEIVER ION INITIAL CHARGE.
C INPUT : (R*8)  RAMSNO     = RECEIVER ATOMIC MASS.
C INPUT : (R*8)  TEV        = ELECTRON TEMPERATURE.
C                           UNITS: EV
C INPUT : (R*8)  TIEV      = ION TEMPERATURE.
C                           UNITS: EV
C INPUT : (R*8)  DENS       = ELECTRON DENSITY.
C                           UNITS: CM-3
C INPUT : (R*8)  DENSZ     = PLASMA ION DENSITY.
C                           UNITS: CM-3
C INPUT : (R*8)  ZEFF       = EFFECTIVE ION CHARGE.
C INPUT : (R*8)  BMAG       = PLASMA MAGNETIC INDUCTION.
C                           UNITS: TESLA
C INPUT : (R*8)  BMENG      = BEAM ENERGY.
C                           UNITS: EV/AMU
C INPUT : (I*4)  ITHEOR     = CHARGE EXCHANGE MODEL OPTION.
C                           1 => USE INPUT DATA SET.
C                           2 => USE EIKONAL MODEL.
C INPUT : (I*4)  IBSTAT     = DONOR STATE FOR EIKONAL MODEL.
C                           1 => H(1S)
C                           2 => H(2S)
C                           3 => H(2P)
C                           4 => HE(1S2)
C                           5 => HE(1S2S)
C INPUT : (I*4)  IEMMS     = EMISSION MEASURE MODEL OPTION.
C                           1 => CHARGE EXCHANGE.
C                           2 => ELECTRON IMPACT EXCITATION.
C INPUT : (I*4)  NTL       = LOWER PRINCIPAL QUANTUM NUMBER OF
C                           TRANSITION.
C INPUT : (I*4)  NTU       = UPPER PRINCIPAL QUANTUM NUMBER OF
C                           TRANSITION.
C INPUT : (I*4)  NMINF     = LOWEST N-SHELL FOR WHICH DATA READ.
C INPUT : (I*4)  NMAXF     = HIGHEST N-SHELL FOR WHICH DATA READ.
C INPUT : (I*4)  NENRGY    = NUMBER OF ENERGIES READ FROM DATA SET.
C INPUT : (R*8)  ENRGYA( ) = COLLISION ENERGIES READ FROM INPUT DATA
C                           SET.
C                           UNITS: EV/AMU
C                           DIMENSION: ENERGY INDEX
C INPUT : (R*8)  ALPHA( )  = EXTRAPOLATION PARAMETER ALPHA READ FROM
C                           INPUT DATA SET.
C                           DIMENSION: ENERGY INDEX
C INPUT : (R*8)  XSECNA( , ) = N-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS
C                           READ FROM INPUT DATA SET.
C                           UNITS: CM2
C                           1ST DIMENSION: ENERGY INDEX
C                           2ND DIMENSION: N-SHELL
C INPUT : (R*8)  FRACLA( , ) = L-RESOLVED CHARGE EXCHANGE CROSS-SECTIONS.
C                           AFTER CXDATA: ABSOLUTE VALUES (CM2).
C                           AFTER CXFRAC: FRACTION OF N-RESOLVED
C                           DATA.
C                           1ST DIMENSION: ENERGY INDEX
C                           2ND DIMENSION: INDEXED BY I4IDFL(N,L)
C
C OUTPUT: (R*8)  ERATE     = EFFECTIVE EMISSIVITY RATE COEFFICIENT FOR
C                           REQUESTED TRANSITION
C                           SPECTRUM LINE.
C                           UNITS: CM3 SEC-1
C
C PARAM : (I*4)  MXN        = MXNSHL.
C PARAM : (I*4)  MXJSHL    = MAXIMUM NUMBER OF J SUB-SHELLS.
C PARAM : (I*4)  MXBEAM    = MAXIMUM NUMBER OF BEAM COMPONENTS.
C PARAM : (I*4)  MXOBSL    = MAXIMUM NUMBER OF OBSERVED SPECTRUM
C                           LINES.
C
C

```



C	PARAM : (I*4)	MXPRSL	= MAXIMUM NUMBER OF SPECTRUM LINES TO PREDICT.
C			
C	PARAM : (R*8)	EMP	= REDUCED MASS FOR POSITIVE ION. UNITS: ELECTRON MASSES
C			
C	(I*4)	NBEAM	= NUMBER OF BEAM ENERGIES.
C	(I*4)	NOLINE	= NUMBER OF OBSERVED SPECTRUM LINES.
C	(I*4)	NPLINE	= NUMBER OF SPECTRUM LINES TO PREDICT.
C	(I*4)	NUMIN	= MINIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR OBSERVED SPECTRUM LINES.
C	(I*4)	NUMAX	= MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR OBSERVED SPECTRUM LINES.
C			
C	(R*8)	EM	= EMISSION MEASURE. UNITS: CM-5
C			
C	(I*4)	NL()	= LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF OBSERVED SPECTRUM LINES. DIMENSION: SPECTRUM LINE INDEX.
C	(I*4)	NU()	= LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF OBSERVED SPECTRUM LINES. DIMENSION: SPECTRUM LINE INDEX.
C	(I*4)	NPL()	= LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF SPECTRUM LINES TO PREDICT. DIMENSION: SPECTRUM LINE INDEX.
C	(I*4)	NPU()	= LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF SPECTRUM LINES TO PREDICT. DIMENSION: SPECTRUM LINE INDEX.
C			
C	(R*8)	BMFRA()	= BEAM COMPONENT FRACTIONS. DIMENSION: COMPONENT INDEX.
C	(R*8)	BMENA()	= BEAM ENERGY COMPONENTS. UNITS: EV/AMU
C	(R*8)	EMISA()	= LIST OF EMISSIONS OF OBSERVED SPECTRUM LINES. UNITS: PH CM-2 SEC-1 DIMENSION: SPECTRUM LINE INDEX.
C	(R*8)	TBLF()	= TABLE OF RADIATIVE LIFETIMES. UNITS: SECS DIMENSION: REFERENCED BY I4IDFL(N,L).
C	(R*8)	TBQEX()	= MEAN EXCITATION RATE COEFFICIENTS FOR NL-LEVELS AVERAGED OVER BEAM FRACTIONS. UNITS: CM3 SEC-1 DIMENSION: REFERENCED BY I4IDFL(N,L).
C	(R*8)	QTHEX()	= MEAN EXCITATION RATE COEFFICIENTS FOR N-LEVELS AVERAGED OVER BEAM FRACTIONS. UNITS: CM3 SEC-1 DIMENSION: N SHELL INDEX.
C	(R*8)	FTHEX()	= FRACTION OF N-LEVEL MEAN EXCITATION RATE COEFFICIENTS IN NL-LEVEL. DIMENSION: REFERENCED BY I4IDFL(N,L).
C	(R*8)	QTHCH()	= MEAN CHARGE EXCHANGE COEFFICIENTS FOR N-LEVELS AVERAGED OVER BEAM FRACTIONS. UNITS: CM3 SEC-1 DIMENSION: N SHELL INDEX.
C	(R*8)	FTHCH()	= FRACTION OF N-LEVEL MEAN CHARGE EXCHANGE COEFFICIENTS IN NL-LEVEL. DIMENSION: REFERENCED BY I4IDFL(N,L).
C	(R*8)	TBQMEP()	= ELECTRON COLLISIONAL RATE COEFFT. FOR NL->NL+1. DIMENSION: REFERENCED BY I4IDFL(N,L).
C	(R*8)	TBQMEM()	= ELECTRON COLLISIONAL RATE COEFFT. FOR NL->NL-1. DIMENSION: REFERENCED BY I4IDFL(N,L).
C	(R*8)	TBQMIP()	= POSITIVE ION COLLISIONAL RATE COEFFT. FOR NL->NL+1. DIMENSION: REFERENCED BY I4IDFL(N,L).
C	(R*8)	TBQMIM()	= POSITIVE ION COLLISIONAL RATE COEFFT. FOR NL->NL-1. DIMENSION: REFERENCED BY I4IDFL(N,L).
C	(R*8)	QEX()	= DIMENSION: N SHELL INDEX.
C	(R*8)	TOTPOP()	= TOTAL COLLISION POP. FOR PREDICTED SPECTRUM LINE. UNITS: CM-2 DIMENSION: PREDICTED LINE INDEX.
C	(R*8)	TOTEMI()	= TOTAL COLLISION EMISSIONS FOR PREDICTED SPECTRUM LINE. UNITS: PH CM-2 SEC-1 DIMENSION: PREDICTED LINE INDEX.
C	(R*8)	AVRGWL()	= AVERAGE AIR WAVELENGTH FOR PREDICTED SPECTRUM LINE. UNITS: A DIMENSION: PREDICTED LINE INDEX.
C	(R*8)	QEFF()	= EFF. RATE COEFFICIENT FOR PREDICTED SPECTRUM LINE. UNITS: CM3 SEC-1 DIMENSION: PREDICTED LINE INDEX.
C	(R*8)	TBLPOP(,)	= TABLE OF COLLISION POP. FOR PREDICTED SPECTRUM LINE. UNITS: CM-2 1ST DIMENSION: PREDICTED LINE INDEX. 2ND DIMENSION: REFERENCED BY I4IDLI().
C	(R*8)	TBLEMI(,)	= TABLE OF COLLISION EMISSIONS FOR PREDICTED SPECTRUM LINE. UNITS: PH CM-2 SEC-1

```

C          1ST DIMENSION: PREDICTED LINE INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDL1().
C      (R*8) TBLWLN(, ) = TABLE OF WAVELENGTHS FOR PREDICTED
C          SPECTRUM LINE.
C          UNITS: A
C          1ST DIMENSION: PREDICTED LINE INDEX.
C          2ND DIMENSION: REFERENCED BY I4IDL1().
C
C ROUTINES:
C
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C-----
C      I4UNIT      ADAS      RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C      CXTBLF      ADAS      FILLS L-RESOLVED RADIATIVE LIFETIME
C          TABLE.
C      CXTBEX      ADAS      FILLS N AND L-RESOLVED ELECTRON IMPACT
C          EXCITATION RATE TABLES.
C      CXQEIK      ADAS      FILLS N AND L-RESOLVED CHARGE EXCHANGE
C          RATE TABLES USING EIKONAL APPROXIMATION.
C      CXQXCH      ADAS      FILLS N AND L-RESOLVED CHARGE EXCHANGE
C          RATE TABLES USING INPUT DATA SET.
C      C8TBQM      ADAS      FILLS N AND L-RESOLVED COLLISIONAL RATE
C          TABLES.
C      C9EMIS      ADAS      PREDICTS THE L-RESOLVED EMISSIVITY FOR
C          REQUESTED TRANSITIONS.
C
C AUTHOR:  JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          KL/0/87
C          JET EXT. 5183
C
C DATE:    03/12/93
C
C UNIX PORT: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          DATE:    10/07/95          VERSION 1.1
C-----
C
C      INTEGER      I4UNIT
C-----
C      INTEGER      MXN          , MXBEAM          , MXOBSL          ,
C      &            MXPRSL
C      PARAMETER(  MXN   = 20  , MXBEAM = 1  , MXOBSL = 1  ,
C      &            MXPRSL = 1  )
C-----
C      REAL*8      EMP
C      PARAMETER(  EMP = 1836.0D0  )
C-----
C      INTEGER      MXNENG      , MXNSHL      , NGRND      , NTOT      , NBOT      ,
C      &            NTOP      , IRZ0      , IRZ1      , ITHEOR      , IBSTAT      ,
C      &            IEMMS      , NTU      , NTL      , NMINF      , NMAXF      ,
C      &            NENRGY
C      INTEGER      NBEAM      , NOLINE      , NPLINE      , NUMIN      , NUMAX
C-----
C      REAL*8      RAMSNO      , TEV      , TIEV      , DENS      , DENSZ      ,
C      &            ZEFF      , BMAG      , BMENG      , ERATE
C      REAL*8      EM
C-----
C      INTEGER      NL(MXOBSL)      , NU(MXOBSL)      , NPL(MXPRSL)      ,
C      &            NPU(MXPRSL)
C-----
C      REAL*8      ENRGYA(MXNENG)      , ALPHAA(MXNENG)
C      REAL*8      BMENA(MXBEAM)      , BMFRA(MXBEAM)      , EMISA(MXOBSL)      ,
C      &            QTHEX(MXN)      , QTHCH(MXN)      , QEX(MXN)      ,
C      &            TOTPOP(MXPRSL)      , TOTEMI(MXPRSL)      , AVRGWL(MXPRSL)      ,
C      &            QEFF(MXPRSL)
C      &            TBLF((MXN*(MXN+1))/2)      ,
C      &            TBQEX((MXN*(MXN+1))/2)      ,
C      &            FTHEX((MXN*(MXN+1))/2)      ,
C      &            FTHCH((MXN*(MXN+1))/2)      ,
C      &            TBQMEP((MXN*(MXN+1))/2)      ,
C      &            TBQMEMP((MXN*(MXN+1))/2)      ,
C      &            TBQMIP((MXN*(MXN+1))/2)      ,
C      &            TBQMIM((MXN*(MXN+1))/2)
C-----
C      REAL*8      XSECNA(MXNENG, MXNSHL)      ,
C      &            FRACLA(MXNENG, (MXNSHL*(MXNSHL+1))/2)      ,
C      REAL*8      TBLPOP(MXPRSL, 2*MXN-3)      ,
C      &            TBLEMI(MXPRSL, 2*MXN-3)      ,
C      &            TBLWLN(MXPRSL, 2*MXN-3)
C-----

```

## C9EMIS

```

SUBROUTINE C9EMIS( MXNSHL , MXOBSL , MXPRSL , IZ0
&                IZ1 , NGRND , NTOT , NBOT
&                DENSZ , DENS , NOLINE , NU
&                NL , EMISA , NPLINE , NPU
&                NPL , QTHEOR , FTHEOR , TBQMEMP
&                TBQMEMP , TBQMIP , TBQMIM , NUMIN
&                NUMAX , EM , QEX , TOTPOP
&                TOTEMI , AVRGWL , QEFF , TBLPOP
&                TBLEMI , TBLWLN
&                )

```

```

C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C9EMIS *****
C
C PURPOSE:  PREDICTS THE L-RESOLVED EMISSIVITY FOR REQUESTED
C           TRANSITIONS.
C
C CALLING PROGRAM: C9CXEE
C
C INPUT : (I*4)  MXNSHL  = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4)  MXOBSL  = MAXIMUM NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4)  MXPRSL  = MAXIMUM NUMBER OF SPECTRUM LINES TO
C                       PREDICT.
C INPUT : (I*4)  IZ0     = NUCLEAR CHARGE.
C INPUT : (I*4)  IZ1     = ION CHARGE.
C INPUT : (I*4)  NGRND   = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4)  NTOT    = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND
C                       STATE.
C INPUT : (I*4)  NBOT    = MINIMUM PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8)  DENSZ    = PLASMA ION DENSITY.
C                       UNITS: CM-3
C INPUT : (R*8)  DENS     = ELECTRON DENSITY.
C                       UNITS: CM-3
C INPUT : (I*4)  NOLINE  = NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4)  NU( )   = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF
C                       OBSERVED SPECTRUM LINES.
C                       DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4)  NL( )   = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF
C                       OBSERVED SPECTRUM LINES.
C                       DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8)  EMISA( ) = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C                       LINES.
C                       DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4)  NPLINES = NUMBER OF SPECTRUM LINES TO PREDICT.
C INPUT : (I*4)  NPU( )   = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF
C                       SPECTRUM LINES TO PREDICT.
C                       DIMENSION: PREDICTED LINE INDEX.
C INPUT : (I*4)  NPL( )   = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF
C                       SPECTRUM LINES TO PREDICT.
C                       DIMENSION: PREDICTED LINE INDEX.
C INPUT : (R*8)  QTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE
C                       COEFFICIENTS FOR N-LEVELS AVERAGED OVER
C                       BEAM FRACTIONS.
C                       UNITS: CM3 SEC-1
C                       DIMENSION: REFERENCED BY N QUANTUM NUMBER.
C INPUT : (R*8)  FTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE
C                       FOR NL-LEVELS AS A FRACTION OF
C                       CORRESPONDING N-LEVEL.
C                       DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8)  TBQMEP( ) = ELECTRON RATE COEFFT. FOR NL->NL+1.
C                       INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C                       I4IDFL(N,L).
C                       DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8)  TBQMEM( ) = ELECTRON RATE COEFFT. FOR NL+1->NL.
C                       INDEX FOR NL+1->NL TRANSITION GIVEN BY
C                       I4IDFL(N,L+1).
C                       DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8)  TBQMIP( ) = POSITIVE ION RATE COEFFT. FOR NL->NL+1.
C                       INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C                       I4IDFL(N,L).
C                       DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8)  TBQMIM( ) = POSITIVE ION RATE COEFFT. FOR NL+1->NL.
C                       INDEX FOR NL+1->NL TRANSITION GIVEN BY
C                       I4IDFL(N,L+1).
C                       DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C OUTPUT: (I*4)  NUMIN   = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                       OBSERVED SPECTRUM LINES.
C OUTPUT: (I*4)  NUMAX   = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                       OBSERVED SPECTRUM LINES.
C OUTPUT: (R*8)  EM      = EMISSION MEASURE.
C OUTPUT: (R*8)  QEX( )  =
C                       DIMENSION: MXNSHL.
C OUTPUT: (R*8)  TOTPOP( ) = TOTAL COLLISION POP. FOR PREDICTED SPECTRUM
C                       LINE.
C                       UNITS: CM-2
C                       DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8)  TOTEMI( ) = TOTAL COLLISION EMISSIVITIES FOR PREDICTED
C                       SPECTRUM LINE.
C                       UNITS: PH CM-2 SEC-1
C                       DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8)  AVRGWL( ) = AVERAGE AIR WAVELENGTH FOR PREDICTED
C                       SPECTRUM LINE.
C                       UNITS: A
C                       DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8)  QEFF( )  = EFF. RATE COEFFICIENT FOR PREDICTED
C                       SPECTRUM LINE.
C                       UNITS:
C                       DIMENSION: PREDICTED LINE INDEX.
C OUTPUT: (R*8)  TBLPOP( , ) = TABLE OF COLLISION POP. FOR PREDICTED
C                       SPECTRUM LINE.
C                       UNITS: CM-2
C                       1ST DIMENSION: PREDICTED LINE INDEX.
C                       2ND DIMENSION: REFERENCED BY FUNC I4IDL( ).
C OUTPUT: (R*8)  TBLEMI( , ) = TABLE OF COLLISION EMISSIVITIES FOR

```

```

C
C PREDICTED SPECTRUM LINE.
C UNITS: PH CM-2 SEC-1
C 1ST DIMENSION: PREDICTED LINE INDEX.
C 2ND DIMENSION: REFERENCED BY FUNC I4IDLI().
C OUTPUT: (R*8) TBLWLN(,) = TABLE OF WAVELENGTHS FOR PREDICTED SPECTRUM
C LINE.
C UNITS: A
C 1ST DIMENSION: PREDICTED LINE INDEX.
C 2ND DIMENSION: REFERENCED BY FUNC I4IDLI().
C
C PARAM : (I*4) MXN = MXNSHL.
C PARAM : (I*4) MXOB = MXOBSL.
C
C (I*4) NREP =
C (I*4) IC = LOOP INDEX.
C
C (I*4) ICREP() =
C DIMENSION: MXOB.
C
C (R*8) WHIGH() =
C DIMENSION: REFERENCED BY L+1.
C
C (R*8) WLOW(,) =
C 1ST DIMENSION: REFERENCED BY I4IDFL(N,L).
C 2ND DIMENSION: REFERENCED BY L+1.
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C C9WFIL ADAS
C C9EMQX
C CXPRSL ADAS PREDICTS REQUESTED SPECTRUM LINES.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 15/10/93
C
C DATE: 30/06/95 VERSION:1.1
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - UNIX PORT FOR ADAS309, CREATED C9EMIS FROM C8EMIS
C ONLY DIFFERENCE IS IT CALLS C9WFIL RATHER THAN C8WFIL
C
C DATE: 10/07/95 VERSION:1.2
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - CHANGED CALL FROM C8EMQX TO C9EMQX
C
C -----
C INTEGER I4UNIT
C -----
C INTEGER MXN , MXOB
C PARAMETER( MXN = 20 , MXOB = 10 )
C -----
C INTEGER MXNSHL , MXOBSL , MXPRSL , IZ0 , IZ1 ,
C & NGRND , NTOT , NBOT , NOLINE , NPLINE
C INTEGER NREP , NUMIN , NUMAX , IC
C -----
C REAL*8 DENSZ , DENS , EM
C -----
C INTEGER NU(MXOBSL) , NL(MXOBSL) , NPU(MXPRSL) ,
C & NPL(MXPRSL)
C INTEGER ICREP(MXOB)
C -----
C REAL*8 EMISA(MXOBSL) ,
C & QTHEOR(MXNSHL) ,
C & QEX(MXNSHL) ,
C & TOTPOP(MXPRSL) ,
C & TOTEMI(MXPRSL) ,
C & AVRGWL(MXPRSL) ,
C & QEFF(MXPRSL) ,
C & FTHEOR((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMEP((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMEM((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIP((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIM((MXNSHL*(MXNSHL+1))/2)
C REAL*8 WHIGH((MXN*(MXN+1))/2)
C -----
C REAL*8 TBLPOP(MXPRSL,2*MXNSHL-3) ,
C & TBLEMI(MXPRSL,2*MXNSHL-3) ,
C & TBLWLN(MXPRSL,2*MXNSHL-3)
C REAL*8 WLOW((MXN*(MXN+1))/2,MXN)
C -----

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## C9EMQX

```

SUBROUTINE C9EMQX( MXNSHL , MXOBSL , IZ1 , NBOT ,
& NUMIN , NUMAX , NU , NL ,
& EMISA , NREP , ICREP , QTHEOR ,
& WLOW , EM , QEX

```

```

C      &      )
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C9EMQX *****
C
C PURPOSE:
C
C CALLING PROGRAM: C8EMIS
C
C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) MXOBSL = MAXIMUM NUMBER OF OBSERVED SPECTRUM LINES.
C INPUT : (I*4) IZ1    = ION CHARGE.
C INPUT : (I*4) NBOT   = MINIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) NUMIN  = MINIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                     OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NUMAX  = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                     OBSERVED SPECTRUM LINES.
C INPUT : (I*4) NU( )  = LIST OF UPPER PRINCIPAL QUANTUM NUMBERS OF
C                     OBSERVED SPECTRUM LINES.
C                     DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NL( )  = LIST OF LOWER PRINCIPAL QUANTUM NUMBERS OF
C                     OBSERVED SPECTRUM LINES.
C                     DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (R*8) EMISA( ) = LIST OF EMISSIVITIES OF OBSERVED SPECTRUM
C                     LINES.
C                     DIMENSION: SPECTRUM LINE INDEX.
C INPUT : (I*4) NREP   =
C INPUT : (I*4) ICREP( ) =
C                     DIMENSION: MXOBSL.
C INPUT : (R*8) QTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE
C                     COEFFICIENTS FOR N-LEVELS AVERAGED OVER
C                     BEAM FRACTIONS.
C                     UNITS: CM3 SEC-1
C                     DIMENSION: PRINCIPAL QUANTUM NUMBER INDEX.
C INPUT : (R*8) WLOW( , ) =
C                     1ST DIMENSION: REFERENCED BY I4IDFL(N,L).
C                     2ND DIMENSION: REFERENCED BY L+1.
C
C OUTPUT: (R*8) EM     = EMISSION MEASURE.
C OUTPUT: (R*8) QEX( ) =
C                     DIMENSION: MXNSHL.
C
C PARAM : (I*4) MXN    = MXNSHL.
C PARAM : (I*4) MXOB   = MXOBSL.
C
C      (I*4) N        = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C      (I*4) L        = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C      (I*4) N1       = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C      (I*4) L1       = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C      (I*4) IC       = ARRAY INDEX.
C      (I*4) IC1      = ARRAY INDEX.
C      (I*4) IC2      = ARRAY INDEX.
C      (I*4) IFAIL    = RETURN FLAG FROM NAG ROUTINE.
C      (I*4) M        = LOOP INDEX.
C      (I*4) I        = LOOP INDEX.
C      (I*4) J        = ARRAY INDEX.
C
C      (R*8) XM       = REAL VALUE = M.
C      (R*8) X1       =
C      (R*8) X2       =
C      (R*8) T1       =
C      (R*8) T2       =
C      (R*8) SUM      =
C      (R*8) SUMEX    =
C      (R*8) SUMTH    =
C
C      (I*4) JLIST( ) =
C                     DIMENSION: MXN.
C
C      (R*8) REMISA( ) =
C                     DIMENSION: MXOB.
C      (R*8) REMQ( )  =
C                     DIMENSION: MXOB.
C      (R*8) WKSPACE( ) = WORKSPACE FOR NAG ROUTINE.
C                     DIMENSION: MXOB.
C      (R*8) EMQ( )   =
C                     DIMENSION: MXNSHL.
C
C      (R*8) CNDSA( , ) = CONDENSED MATRIX.
C                     1ST DIMENSION: MXN.
C                     2ND DIMENSION: 2.
C      (R*8) ARED( , ) = LINEAR CONDENSATION TRANSFORMATION ARRAY.
C                     1ST DIMENSION: MXN.
C                     2ND DIMENSION: MXN.
C
C ROUTINES:
C
C ROUTINE   SOURCE   BRIEF DESCRIPTION
C-----
C I4UNIT    ADAS     RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C I4IDFL    ADAS     RETURNS UNIQUE INDEX GIVEN QUANTUM
C                   NUMBERS N AND L.
C R8ATAB    ADAS     RETURNS HYDRONIC L-RESOLVED A-VALUES.
C                   IF INPUT QUANTUM NUMBERS ARE INVALID
C                   THEN RETURNS ZERO.
C F04ARF    NAG      FINDS SOLUTION TO A SET OF REAL LINEAR

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CX      EQUATIONS.
C      XXMINV      ADAS      MATRIX SOLUTION - REPLACES ABOVE NAG
C      ROUTINE
C
C      AUTHOR:    JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C      KL/0/81
C      JET EXT. 5183
C
C      DATE:      14/10/93
C
C      DATE:      10/07/95      VERSION 1.1
C      MODIFIED:  TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - CREATED C9EMQX FROM C8EMQX - ONLY DIFFERENCE IS CALL TO
C      FORTRAN ROUTINE F04ARF IS REPLACED WITH CALL TO XXMINV
C
C-----
C
C      INTEGER      I4UNIT      , I4IDFL
C      REAL*8      R8ATAB
C
C-----
C      INTEGER      MXN      , MXOB
C      PARAMETER(  MXN = 20      , MXOB = 10 )
C
C-----
C      INTEGER      MXNSHL      , MXOBSL      , IZ1      , NBOT      , NUMIN      ,
C      &      NUMAX      , NREP
C      INTEGER      N      , L      , N1      , L1      , IC      ,
C      &      IC1      , IC2      , IFAIL      , M      , I      ,
C      &      J
C
C-----
C      REAL*8      EM
C      REAL*8      XM      , X1      , X2      , T1      , T2      ,
C      &      SUM      , SUMEX      , SUMTH
C
C-----
C      INTEGER      ICREP(MXOBSL)      , NU(MXOBSL)      , NL(MXOBSL)
C      INTEGER      JLIST(MXN)
C
C-----
C      REAL*8      EMISA(MXOBSL)      , QTHEOR(MXNSHL)      , QEX(MXNSHL)
C      REAL*8      REMISA(MXOB)      , REMQ(MXOB)      , WKSPCE(MXOB)      ,
C      &      EMQ(MXN)
C      REAL*8      WLOW((MXNSHL*(MXNSHL+1))/2,MXNSHL)
C      REAL*8      CNDSA(MXN,2)
C      &      ARED(MXOB,MXOB)
C
C-----

```

## C9OUT0

```

SUBROUTINE C9OUT0( IWRITE , MXSCAN , DATE , DSNIN ,
&
&      DSNPAS , IPSET , TITLE , SYMBD ,
&      IDZ0 , SYMBR , IRZ0 , IRZ1 ,
&      IRZ2 , RAMSNO , TEV , TIEV ,
&      DENS , DENSZ , ZEFF , BMAG ,
&      BMENG , NTU , NTL , ITHEOR ,
&      IBSTAT , IEMMS , NBMENG , BMENGA ,
&      NTIEV , TIEVA , NDENSZ , DENSZA ,
&      NZEFF , ZEFFA , NBMAG , BMAGA ,
&      CADAS
&
)
C
C      IMPLICIT NONE
C
C-----
C
C      ***** FORTRAN77 SUBROUTINE: C9OUT0 *****
C
C      PURPOSE:  WRITES TEXT OUTPUT TO FILE FOR ADAS309.
C
C      CALLING PROGRAM:  ADAS309
C
C      INPUT : (I*4)  IWRITE      = UNIT NUMBER FOR OUTPUT.
C      INPUT : (I*4)  MXSCAN      = MAXIMUM NUMBER OF VALUES IN A SCAN.
C      INPUT : (C*8)  DATE        = DATE STRING.
C      INPUT : (C*80) DSNIN       = FULL INPUT DATA SET NAME.
C      INPUT : (C*80) DSNPAS      = FULL OUTPUT PASSING DATA SET NAME.
C      INPUT : (I*4)  IPSET       = INPUT PARAMETER SET NUMBER FOR CURRENT.
C      INPUT : (C*40) TITLE       = ISPF ENTERED GENERAL TITLE FOR RUN.
C      INPUT : (C*2)  SYMBD       = DONOR ELEMENT SYMBOL.
C      INPUT : (I*4)  IDZ0        = DONOR NUCLEAR CHARGE.
C      INPUT : (C*2)  SYMBR       = RECEIVER ELEMENT SYMBOL.
C      INPUT : (I*4)  IRZ0        = RECEIVER NUCLEAR CHARGE.
C      INPUT : (I*4)  IRZ1        = RECEIVER ION INITIAL CHARGE.
C      INPUT : (I*4)  IRZ2        = RECEIVER ION FINAL CHARGE.
C      INPUT : (R*8)  RAMSNO      = RECEIVER ATOMIC MASS.
C      INPUT : (R*8)  TEV         = ELECTRON TEMPERATURE.
C      UNITS:  EV
C      INPUT : (R*8)  TIEV        = ION TEMPERATURE.
C      UNITS:  EV
C      INPUT : (R*8)  DENS        = ELECTRON DENSITY.
C      UNITS:  CM-3
C      INPUT : (R*8)  DENSZ       = PLASMA ION DENSITY.
C      UNITS:  CM-3
C      INPUT : (R*8)  ZEFF        = EFFECTIVE ION CHARGE.
C      INPUT : (R*8)  BMAG        = PLASMA MAGNETIC INDUCTION.

```

```

C
C INPUT : (R*8) BMENG = UNITS: TESLA
C                      = REFERENCE VALUE FOR BEAM ENERGY.
C                      UNITS: EV/AMU
C INPUT : (I*4) NTU = UPPER PRINCIPAL QUANTUM NUMBER OF
C                      TRANSITION.
C INPUT : (I*4) NTL = LOWER PRINCIPAL QUANTUM NUMBER OF
C                      TRANSITION.
C INPUT : (I*4) ITHEOR = CHARGE EXCHANGE MODEL OPTION.
C                      1 => USE INPUT DATA SET.
C                      2 => USE EIKONAL MODEL.
C INPUT : (I*4) IBSTAT = DONOR STATE FOR EIKONAL MODEL.
C                      1 => H(1S)
C                      2 => H(2S)
C                      3 => H(2P)
C                      4 => HE(1S2)
C                      5 => HE(1S2S)
C INPUT : (I*4) IEMMS = EMISSION MEASURE MODEL OPTION.
C                      1 => CHARGE EXCHANGE.
C                      2 => ELECTRON IMPACT EXCITATION.
C INPUT : (I*4) NBMENG = NUMBER OF BEAM ENERGIES IN SCAN.
C INPUT : (R*8) BMENGA() = BEAM ENERGIES FOR SCAN.
C                      UNITS: EV/AMU
C                      DIMENSION: MXSCAN
C INPUT : (I*4) NTIEV = NUMBER OF ION TEMPERATURES IN SCAN.
C INPUT : (R*8) TIEVA() = ION TEMPERATURES FOR SCAN.
C                      UNITS: EV
C                      DIMENSION: MXSCAN
C INPUT : (I*4) NDENSZ = NUMBER OF ION DENSZTIES IN SCAN.
C INPUT : (R*8) DENSZA() = ION DENSZTIES FOR SCAN.
C                      UNITS: CM-3
C                      DIMENSION: MXSCAN
C INPUT : (I*4) NZEFF = NUMBER OF PLASMA EFFECTIVE Z IN SCAN.
C INPUT : (R*8) ZEFFA() = PLASMA EFFECTIVE Z FOR SCAN.
C                      DIMENSION: MXSCAN
C INPUT : (I*4) NBMAG = NUMBER OF PLASMA MAGNETIC FIELDS IN SCAN.
C INPUT : (R*8) BMAGA() = PLASMA MAGNETIC FIELDS FOR SCAN.
C                      UNITS: TESLA
C                      DIMENSION: MXSCAN
C
C I/O : (C*80) CADAS = ADAS HEADER: INCLUDES RELEASE, PROGRAM,
C                      TIME.
C
C          (I*4) I = ARRAY INDEX.
C
C          (L*4) LFIRST = FLAGS IF FIRST CALL OF SUBROUTINE.
C                      .TRUE. => FIRST CALL.
C                      .FALSE. => NOT FIRST CALL.
C
C ROUTINES: NONE
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C          KL/0/87
C          JET EXT. 5183
C
C DATE: 03/12/93
C
C UNIX PORT: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C DATE: 10/07/95 VERSION 1.1
C
C-----
C
C INTEGER IWRITE , MXSCAN , IDZ0 , IRZ0 ,
C & IRZ1 , IRZ2 , NTU , NTL , ITHEOR ,
C & IBSTAT , IEMMS , NBMENG , NTIEV , NDENSZ ,
C & NZEFF , NBMAG
C INTEGER I , IPSET
C-----
C REAL*8 RAMSNO , TEV , TIEV , DENS , DENSZ ,
C & ZEFF , BMAG , BMENG
C-----
C LOGICAL LFIRST
C-----
C CHARACTER DATE*8 , DSNIN*80 , DSNPAS*80 , TITLE*40 ,
C & SYMBR*2 , SYMBD*2
C CHARACTER CADAS*80
C-----
C REAL*8 BMENGA(MXSCAN) , DENSZA(MXSCAN) , TIEVA(MXSCAN) ,
C & ZEFFA(MXSCAN) , BMAGA(MXSCAN)
C-----
C SAVE LFIRST
C-----
C DATA LFIRST / .TRUE. /
C-----

```

## C9OUT1

```

SUBROUTINE C9OUT1( IWRITE , MXSCAN , DATE , DSNIN ,
& IPSET , SYMBD , SYMBR , IRZ1 ,
& NTU , NTL , ITHEOR , IBSTAT ,
& IEMMS , BMENG , TIEV , DENSZ ,
& ZEFF , BMAG , QEFREF , NBMENG ,
& BMENGA , QEFBEA , NTIEV , TIEVA ,

```

```

&          QEFTIA , NDENSZ , DENSZA , QEFDZA ,
&          NZEFF , ZEFFA , QEFZEA , NBMAG ,
&          BMAGA , QEFBMA
&          )
C
C      IMPLICIT NONE
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: C9OUT0 *****
C
C PURPOSE: WRITES DATA OUTPUT TO FILE FOR ADAS309.
C
C CALLING PROGRAM: ADAS309
C
C INPUT : (I*4) IWRITE = UNIT NUMBER FOR OUTPUT.
C INPUT : (I*4) MXSCAN = MAXIMUM NUMBER OF VALUES IN A SCAN.
C INPUT : (C*8) DATE = DATE STRING.
C INPUT : (C*80) DSNIN = FULL INPUT DATA SET NAME.
C INPUT : (I*4) IPSET = INPUT PARAMETER SET NUMBER FOR CURRENT
C                   RUN.
C INPUT : (C*2) SYMBD = DONOR ELEMENT SYMBOL.
C INPUT : (C*2) SYMBR = RECEIVER ELEMENT SYMBOL.
C INPUT : (I*4) IRZ1 = ION CHARGE OF RECEIVER.
C INPUT : (I*4) NTU = UPPER PRINCIPAL QUANTUM NUMBER OF
C                   TRANSITION.
C INPUT : (I*4) NTL = LOWER PRINCIPAL QUANTUM NUMBER OF
C                   TRANSITION.
C INPUT : (I*4) ITHEOR = CHARGE EXCHANGE MODEL OPTION.
C                   1 => USE INPUT DATA SET.
C                   2 => USE EIKONAL MODEL.
C INPUT : (I*4) IBSTAT = DONOR STATE FOR EIKONAL MODEL.
C                   1 => H(1S)
C                   2 => H(2S)
C                   3 => H(2P)
C                   4 => HE(1S2)
C                   5 => HE(1S2S)
C INPUT : (I*4) IEMMS = EMISSION MEASURE MODEL OPTION.
C                   1 => CHARGE EXCHANGE.
C                   2 => ELECTRON IMPACT EXCITATION.
C INPUT : (R*8) BMENG = REFERENCE VALUE FOR BEAM ENERGY.
C                   UNITS: EV/AMU
C INPUT : (R*8) TIEV = REFERENCE VALUE FOR ION TEMPERATURE.
C                   UNITS: EV
C INPUT : (R*8) DENSZ = REFERENCE VALUE FOR PLASMA ION DENSITY.
C                   UNITS: CM-3
C INPUT : (R*8) ZEFF = REFERENCE VALUE FOR EFFECTIVE ION CHARGE.
C INPUT : (R*8) BMAG = REFERENCE VALUE FOR PLASMA MAGNETIC
C                   FIELD.
C                   UNITS: TESLA
C INPUT : (R*8) QEFREF = REFERENCE VALUE FOR EFFECTIVE RATE COEFFT.
C                   UNITS: CM3 SEC-1
C INPUT : (I*4) NBMENG = NUMBER OF BEAM ENERGIES IN SCAN.
C INPUT : (R*8) BMENGA() = BEAM ENERGIES FOR SCAN.
C                   UNITS: EV/AMU
C                   DIMENSION: MXSCAN
C INPUT : (R*8) QEFBEA() = EFFECTIVE RATE COEFFICIENTS FOR BEAM
C                   ENERGY SCAN.
C                   UNITS: CM3 SEC-1
C                   DIMENSION: MXSCAN
C INPUT : (I*4) NTIEV = NUMBER OF ION TEMPERATURES IN SCAN.
C INPUT : (R*8) TIEVA() = ION TEMPERATURES FOR SCAN.
C                   UNITS: EV
C                   DIMENSION: MXSCAN
C INPUT : (R*8) QEFTIA() = EFFECTIVE RATE COEFFICIENTS FOR ION
C                   TEMPERATURE SCAN.
C                   UNITS: CM3 SEC-1
C                   DIMENSION: MXSCAN
C INPUT : (I*4) NDENSZ = NUMBER OF ION DENSZTIES IN SCAN.
C INPUT : (R*8) DENSZA() = ION DENSZTIES FOR SCAN.
C                   UNITS: CM-3
C                   DIMENSION: MXSCAN
C INPUT : (R*8) QEFDZA() = EFFECTIVE RATE COEFFICIENTS FOR ION
C                   DENSITY SCAN.
C                   UNITS: CM3 SEC-1
C                   DIMENSION: MXSCAN
C INPUT : (I*4) NZEFF = NUMBER OF PLASMA EFFECTIVE Z IN SCAN.
C INPUT : (R*8) ZEFFA() = PLASMA EFFECTIVE Z FOR SCAN.
C                   DIMENSION: MXSCAN
C INPUT : (R*8) QEFZEA() = EFFECTIVE RATE COEFFICIENTS FOR PLASMA
C                   EFFECTIVE Z SCAN.
C                   UNITS: CM3 SEC-1
C                   DIMENSION: MXSCAN
C INPUT : (I*4) NBMAG = NUMBER OF PLASMA MAGNETIC FIELDS IN SCAN.
C INPUT : (R*8) BMAGA() = PLASMA MAGNETIC FIELDS FOR SCAN.
C                   UNITS: TESLA
C                   DIMENSION: MXSCAN
C INPUT : (R*8) QEFBMA() = EFFECTIVE RATE COEFFICIENTS FOR PLASMA
C                   MAGNETIC FIELD SCAN.
C                   UNITS: CM3 SEC-1
C                   DIMENSION: MXSCAN
C
C (I*4) I = ARRAY INDEX.
C (I*4) I1 = ARRAY INDEX.
C (I*4) I2 = ARRAY INDEX.
C
C (C*8) DONOR = DONOR SYMBOL AND ION CHARGE (OR STATE IF
C              EIKONAL MODEL.

```



```

C      (C*5)  RECVR   = RECEIVER SYMBOL AND ION CHARGE.
C      (C*5)  TRANS  = N LEVELS OF TRANSITION.
C      (C*7)  FILE   = INPUT DATA SET MEMBER NAME.
C      (C*2)  MODEL  = EMISSION MEASURE MODEL.
C
C  ROUTINES:  NONE
C
C  AUTHOR:   JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C            K1/0/87
C            JET EXT. 5183
C
C  DATE:    03/12/93
C
C  UNIX PORT: TIM HAMMOND(TESSELLA SUPPORT SERVICES PLC)
C  DATE:    10/07/95          VERSION 1.1
C
C-----
C
C
C      INTEGER  IWRITE , MXSCAN , IZD , IRZ1 , NTU ,
C      &        NTL , ITHEOR , IBSTAT , IEMMS , IPSET ,
C      &        NBMENG , NTIEV , NDENSZ , NZEFF , NBMAG
C      INTEGER  I , I1 , I2
C-----
C
C      REAL*8   BMENG , TIEV , DENSZ , ZEFF , BMAG ,
C      &       QEFREF
C-----
C
C      CHARACTER DATE*8 , DSNIN*80 , SYMBD*2 , SYMBR*2
C      CHARACTER DONOR*8 , RECVR*5 , TRANS*5 , FILE*7 ,
C      &       MODEL*2
C-----
C
C      REAL*8   BMENGA(MXSCAN) , DENSZA(MXSCAN) , TIEVA(MXSCAN) ,
C      &       ZEFFA(MXSCAN) , BMAGA(MXSCAN) , QEFBEA(MXSCAN) ,
C      &       QEFTIA(MXSCAN) , QEFDZA(MXSCAN) , QEFZEA(MXSCAN) ,
C      &       QEFBMA(MXSCAN)
C-----

```

## C9WFIL

```

C      SUBROUTINE C9WFIL( MXNSHL , IZ1 , NGRND , NTOT ,
C      &                  NBOT , NUMAX , DENSZ , DENS ,
C      &                  QTHEOR , FTHEOR , TBQMEP , TBQMEM ,
C      &                  TBQMIP , TBQMIM , WHIGH , WLOW
C      &                  )
C
C      IMPLICIT NONE
C
C-----
C
C      ***** FORTRAN77 SUBROUTINE: C9WFIL *****
C
C  PURPOSE:
C
C  CALLING PROGRAM: C9EMIS
C
C  INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C  INPUT : (I*4) IZ1   = ION CHARGE.
C  INPUT : (I*4) NGRND = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C  INPUT : (I*4) NTOT  = PRINCIPAL QUANTUM NUMBER OF HIGHEST BOUND
C                      STATE.
C  INPUT : (I*4) NBOT  = MINIMUM PRINCIPAL QUANTUM NUMBER.
C  INPUT : (I*4) NUMAX = MAXIMUM UPPER PRINCIPAL QUANTUM NUMBER FOR
C                      OBSERVED SPECTRUM LINES.
C  INPUT : (R*8) DENSZ = PLASMA ION DENSITY.
C                      UNITS: CM-3
C  INPUT : (R*8) DENS  = ELECTRON DENSITY.
C                      UNITS: CM-3
C  INPUT : (R*8) QTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE
C                      COEFFICIENTS FOR N-LEVELS AVERAGED OVER
C                      BEAM FRACTIONS.
C                      UNITS: CM3 SEC-1
C                      DIMENSION: REFERENCED BY N QUANTUM NUMBER.
C  INPUT : (R*8) FTHEOR( ) = MEAN CHARGE EXCHANGE OR EXCITATION RATE
C                      FOR NL-LEVELS AS A FRACTION OF
C                      CORRESPONDING N-LEVEL.
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C  INPUT : (R*8) TBQMEP( ) = ELECTRON RATE COEFFT. FOR NL->NL+1.
C                      INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C                      I4IDFL(N,L).
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C  INPUT : (R*8) TBQMEM( ) = ELECTRON RATE COEFFT. FOR NL+1->NL.
C                      INDEX FOR NL+1->NL TRANSITION GIVEN BY
C                      I4IDFL(N,L+1).
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C  INPUT : (R*8) TBQMIP( ) = POSITIVE ION RATE COEFFT. FOR NL->NL+1.
C                      INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C                      I4IDFL(N,L).
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C  INPUT : (R*8) TBQMIM( ) = POSITIVE ION RATE COEFFT. FOR NL+1->NL.
C                      INDEX FOR NL+1->NL TRANSITION GIVEN BY
C                      I4IDFL(N,L+1).
C                      DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C
C
C
C

```

```

C OUTPUT: (R*8) WHIGH() = DIMENSION: REFERENCED BY L+1.
C OUTPUT: (R*8) WLOW(, ) = 1ST DIMENSION: REFERENCED BY I4IDFL(N,L).
C 2ND DIMENSION: REFERENCED BY L+1.
C
C PARAM : (I*4) MXN = MXNSHL.
C
C (I*4) N = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) N1 = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L1 = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) N2 = LOOP INDEX FOR PRINCIPAL QUANTUM NUMBER.
C (I*4) L2 = LOOP INDEX FOR ORBITAL QUANTUM NUMBER.
C (I*4) LP = ARRAY INDEX = L+1.
C (I*4) IDL = ARRAY INDEX.
C
C (R*8) A1 = LOCAL STORE FOR RETURN VALUE OF FUNC R8ATAB.
C
C (R*8) RHS() = RIGHT HAND SIDE OF N LEVEL EQUATION.
C DIMENSION: MXN.
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C R8ATAB ADAS RETURNS HYDRONIC L-RESOLVED A-VALUES.
C IF INPUT QUANTUM NUMBERS ARE INVALID
C THEN RETURNS ZERO.
C
C CXWSOL ADAS
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 13/10/93
C
C DATE: 30/06/95 VERSION:1.1
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - UNIX PORT FOR ADAS309, CREATED THIS C9WFIL FROM C8WFIL
C WHICH COMMUNICATED VIA UNIX PIPE WITH IDL. REMOVED THIS.
C
C DATE: 10/07/95 VERSION:1.2
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - TIDIED CODE AND COMMENTS UP.
C
C -----
C INTEGER I4UNIT , I4IDFL
C REAL*8 R8ATAB
C -----
C INTEGER MXN
C PARAMETER( MXN = 20 )
C -----
C INTEGER MXNSHL , IZ1 , NGRND , NTOT , NBOT ,
C & NUMAX
C INTEGER N , L , N1 , L1 , N2 ,
C & L2 , LP , IDL
C -----
C REAL*8 DENSZ , DENS
C REAL*8 A1
C -----
C REAL*8 QTHEOR(MXNSHL)
C & FTHEOR((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMPEP((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMEM((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIP((MXNSHL*(MXNSHL+1))/2) ,
C & TBQMIM((MXNSHL*(MXNSHL+1))/2) ,
C & WHIGH((MXNSHL*(MXNSHL+1))/2)
C REAL*8 RHS(MXN)
C -----
C REAL*8 WLOW((MXNSHL*(MXNSHL+1))/2,MXNSHL)
C -----

```

## C9WSOL

```

SUBROUTINE C9WSOL( MXNSHL , IZ1 , NGRND , N
& DENSZ , DENS , TBQMPEP , TBQMEM ,
& TBQMIP , TBQMIM , RHS
& )
C
C IMPLICIT NONE
C
C -----
C *****
C ***** FORTRAN77 SUBROUTINE: C9WSOL *****
C
C PURPOSE:
C
C CALLING PROGRAM: C8WFIL

```

```

C INPUT : (I*4) MXNSHL = MAXIMUM VALUE OF PRINCIPAL QUANTUM NUMBER.
C INPUT : (I*4) IZ1 = ION CHARGE.
C INPUT : (I*4) NGRND = PRINCIPAL QUANTUM NUMBER OF GROUND STATE.
C INPUT : (I*4) N = PRINCIPAL QUANTUM NUMBER.
C INPUT : (R*8) DENSZ = PLASMA ION DENSITY.
C UNITS: CM-3
C INPUT : (R*8) DENS = ELECTRON DENSITY.
C UNITS: CM-3
C INPUT : (R*8) TBQMEP( ) = ELECTRON RATE COEFFT. FOR NL->NL+1.
C INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C I4IDFL(N,L).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMEM( ) = ELECTRON RATE COEFFT. FOR NL+1->NL.
C INDEX FOR NL+1->NL TRANSITION GIVEN BY
C I4IDFL(N,L+1).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMIP( ) = POSITIVE ION RATE COEFFT. FOR NL->NL+1.
C INDEX FOR NL->NL+1 TRANSITION GIVEN BY
C I4IDFL(N,L).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C INPUT : (R*8) TBQMIM( ) = POSITIVE ION RATE COEFFT. FOR NL+1->NL.
C INDEX FOR NL+1->NL TRANSITION GIVEN BY
C I4IDFL(N,L+1).
C DIMENSION: REFERENCED BY FUNC I4IDFL(N,L).
C I/O : (R*8) RHS( ) =
C DIMENSION: REFERENCED BY L+1.
C PARAM : (I*4) MXN = MXNSHL.
C (I*4) L = ORBITAL QUANTUM NUMBER.
C (I*4) IDL = ARRAY INDEX.
C (I*4) N1 = PRINCIPAL QUANTUM NUMBER.
C (I*4) LP = ARRAY INDEX = L+1.
C (I*4) IFAIL = RETURN FLAG FROM NAG ROUTINE.
C (R*8) VDS( ) =
C (R*8) VDI( ) =
C (R*8) VD( ) =
C (R*8) VDNEW( , ) = NEW (TEMPORARY?) VARIABLE WHICH IS
C USED TO HOLD THE FULL MATRIX BUILT FROM
C ZEROES AND THE THREE DIAGONALS VDS, VDI
C AND VD
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS RETURNS UNIT NO. FOR OUTPUT OF MESSAGES.
C I4IDFL ADAS RETURNS UNIQUE INDEX GIVEN QUANTUM
C NUMBERS N AND L.
C R8ATAB ADAS RETURNS HYDRONIC L-RESOLVED A-VALUES.
C IF INPUT QUANTUM NUMBERS ARE INVALID
C THEN RETURNS ZERO.
C XXGTSL IDL_ADAS TRIDIAGONAL MATRIX SOLVER.
C
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C
C DATE: 12/10/93
C
C DATE: 10/07/95 VERSION 1.1
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - UNIX PORT OF ADAS309 - HAVE CREATED C9WSOL FROM C8WSOL
C THE ORIGINAL C8WSOL CALLED A NAG ROUTINE TO SOLVE LINEAR
C EQUATIONS AND THE UPDATED C8WSOL USED PIPE COMMUNICATIONS
C WITH IDL. THIS VERSION OF C9WSOL CALLS THE FORTRAN
C ROUTINE XXGTSL INSTEAD.
C
C -----
C INTEGER I4UNIT , I4IDFL
C REAL*8 R8ATAB
C
C INTEGER MXN
C PARAMETER( MXN = 20 )
C
C INTEGER MXNSHL , NGRND , N , IZ1
C INTEGER L , IDL , N1 , LP , IFAIL
C INTEGER I , J
C
C REAL*8 DENSZ , DENS
C
C REAL*8 TBQMEP( (MXNSHL*(MXNSHL+1))/2 ) ,
C & TBQMEM( (MXNSHL*(MXNSHL+1))/2 ) ,
C & TBQMIP( (MXNSHL*(MXNSHL+1))/2 ) ,
C & TBQMIM( (MXNSHL*(MXNSHL+1))/2 ) ,
C & RHS(MXNSHL)
C REAL*8 VDS(MXN) , VDI(MXN) , VD(MXN)
C REAL*8 VDNEW(MXN,MXN)
C -----

```

# CACHKB

```
      SUBROUTINE CACHKB( IUNIT , NBSEL , IBSEL ,
&                      IZ0IN , IZ0 ,
&                      LOPEN , IRCODE , DLPATH
&                      )
C
C      IMPLICIT NONE
C-----
C
C ***** FORTRAN77 SUBROUTINE: CACHKB *****
C
C PURPOSE: TO CHECK THE SELECTED BLOCK (IBSEL) OF DATA EXISTS IN THE
C INPUT DATA SET AND IF SO IT REPRESENTS THE ENTERED VALUES OF
C 'IZ0IN' (NUCLEAR CHARGE OF SELECTED IONISING ION ELEMENT).
C
C IT ALSO CLOSES THE INPUT DATA SET ALLOCATION IF OPEN.
C
C CALLING PROGRAM: CASSZD
C
C SUBROUTINE:
C
C INPUT : (I*4)  IUNIT  = UNIT TO WHICH INPUT DATA SET IS ALLOCATED
C INPUT : (I*4)  NBSEL  = TOTAL NUMBER OF DATA-BLOCKS READ FROM INPUT
C                   DATA SET.
C INPUT : (I*4)  IBSEL  = INDEX OF DATA-BLOCK SELECTED FOR ANALYSIS
C
C INPUT : (I*4)  IZ0IN  = REQUESTED: NUCLEAR CHARGE OF ELEMENT
C INPUT : (I*4)  IZ0    = INPUT FILE: NUCLEAR CHARGE OF ELEMENT
C
C I/O   : (L*4)  LOPEN  = INPUT : .TRUE.  => INPUT DATA SET OPEN.
C                   .FALSE. => INPUT DATA SET CLOSED.
C                   OUTPUT: ALWAYS RETURNED AS .FALSE.
C OUTPUT: (I*4)  IRCODE = RETURN CODE FROM SUBROUTINE:
C                   0 => NO ERROR DETECTED.
C                   2 => DISCREPANCY BETWEEN REQUESTED ELEMENT
C                       AND THAT IN INPUT DATA FILE.
C                   3 => SELECTED DATA-BLOCK OUT OF RANGE OR
C                       DOES NOT EXIST.
C
C                   (I*4)  I4UNIT = FUNCTION (SEE ROUTINE SECTION BELOW)
C
C (C*44) DSNAME  = FULL MVS NAME OF DATA SET OPENED
CA (C*80) DSNAME  = DATA FILE NAME UNDER UNIX, INCLUDING PATH.
C
C ROUTINES:
C ROUTINE   SOURCE   BRIEF DESCRIPTION
C-----
C E2FILE    ADAS     OPEN DATA SET FOR SELECTED ELEMENT
C I4UNIT    ADAS     FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C
C AUTHOR:   PAUL E. BRIDEN (TESSELLA SUPPORT SERVICES PLC)
C           K1/0/37
C           JET EXT. 2620
C
C DATE:    06/06/91
C
C UNIX-IDL PORT:
C
C VERSION: 1.1                      DATE: 25-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C           - CREATED FROM E2CHKB TO WHICH IT IS ESSENTIALLY
C           IDENTICAL EXCEPT IT CALLS CAFILE RATHER THAN E2FILE
C           AND HAS THE EXTRA PATHNAME VARIABLE DLPATH INCLUDED
C           IN THE ARGUMENT LIST.
C-----
C-----
C
C INTEGER   I4UNIT
C INTEGER   IUNIT      , IRCODE
C &         NBSEL      , IBSEL
C &         IZ0IN      , IZ0
C-----
C LOGICAL   LOPEN
C-----
CX CHARACTER DSNAME*44
CA CHARACTER DSNAME*80 , DLPATH*80
C-----
```

# CAFILE

```
      SUBROUTINE CAFILE( IUNIT , IZ0 , IRCODE , DSNAME , DLPATH )
C
C      IMPLICIT NONE
C-----
C
C ***** FORTRAN77 SUBROUTINE: CAFILE *****
C
C PURPOSE: TO OPEN AN IONIZATION RATE-COEFFT 'IONELEC' DATA SET
```

```

C          BY DEFAULT, OR AN ALTERNATIVE DATA SET IF REQUIRED, FOR
C          IONIZING ION WITH NUCLEAR CHARGE 'IZ0'
C          THIS WILL BE CONNECTED TO UNIT 'IUNIT'.
C
C          DATA SET OPENED: DLPATH/adf07/<DEFADF>/<GROUP>(OPTIONAL)/<TYPE>/
C          <GROUP_EXT>#<ELEMENT SYMBOL>'
C
C          CALLING PROGRAM: CASSZD
C
C          SUBROUTINE:
C
C          INPUT : (I*4)   IUNIT   = UNIT TO WHICH DATA SET WILL BE CONNECTED
C          INPUT : (I*4)   IZ0     = NUCLEAR CHARGE OF EMITTING ION REQUESTED
C          INPUT : (C*80)  DLPATH  = PATH NAME TO THE RELEVANT DATA FILES
C
C          OUTPUT: (I*4)   IRCODE  = RETURN CODE FROM SUBROUTINE:
C                                0 => DATA SET SUCCESSFULLY CONNECTED
C                                1 => REQUESTED DATA SET MEMBER DOES NOT
C                                    EXISTS - DATA SET NOT CONNECTED.
C                                9 => REQUESTED DATA SET EXISTS BUT CANNOT
C                                    BE OPENED.
CX OUTPUT: (C*44)  DSNAME  = FULL MVS NAME OF OPENED DATA SET
C OUTPUT: (C*80)  DSNAME  = NAME OF OPENED DATA SET UNDER UNIX
C
C          (I*4)   IDLEN   = LENGTH, IN BYTES, OF FIXED 'DSNAME' PREFIX
C          (I*4)   LENF1  = FIRST NON-BLANK CHR OF 'DSNAME' GROUP PART
C          (I*4)   LENF2  = LAST  NON-BLANK CHR OF 'DSNAME' GROUP PART
C          (I*4)   LENF3  = FIRST NON-BLANK CHR OF 'DSNAME' TYPE PART
C          (I*4)   LENF4  = LAST  NON-BLANK CHR OF 'DSNAME' TYPE PART
C          (I*4)   LENF5  = LAST  NON-BLANK CHR OF 'DSNAME' USERID PART
C          (I*4)   LENF6  = LAST  NON-BLANK CHR OF 'DSNAME' USERID PART
C          (I*4)   LENF7  = LAST  NON-BLANK CHR OF 'DSNAME' EXTENSION PART
C          (I*4)   LENF8  = LAST  NON-BLANK CHR OF 'DSNAME' EXTENSION PART
CA          (C*1)   HASH   = '#'   IF NON-BLANK EXT, ELSE ' '.
C          (C*2)   XFESYM = FUNCTION - (SEE ROUTINES SECTION BELOW)
C          (C*2)   ESYM   = ELEMENT SYMBOL FOR NUCLEAR CHARGE 'IZ0'
C          (C*3)   USREXT = ADAS SOURCE DATA FILE EXTENSION
CA          (C*80)  USERID = ADAS SOURCE DATA USER ID
C          (C*8)   USRGRP = ADAS SOURCE DATA GROUPNAME
CA          (C*80)  USRTYP = ADAS SOURCE DATA TYPENAME
C          (C*5)   DEFADF = DEFAULT DATA DIRECTORY, I.E. ADF13
C
C          (L*4)   LEXIST = .TRUE. => REQUESTED DATA SET EXISTS.
C                                .FALSE. => REQUESTED DATA SET DOES NOT
C                                EXIST.
C
C          ROUTINES:
C          ROUTINE   SOURCE   BRIEF DESCRIPTION
C          -----
C          XXUID     ADAS     FETCHES/SETS ADAS SOURCE DATA USER ID
C          XXSSZD    ADAS     FETCHES/SETS ADAS SOURCE DATA FILENAME
C                                AND FILE EXTENSION
C          XFESYM    ADAS     CHARACTER*2 FUNCTION -
C                                GATHERS ELEMENT SYMBOL FOR NUC. CHARGE
C          XXSLEN    ADAS     FINDS FIRST AND LAST NON-BLANK
C                                CHARACTERS IN STRING.
C
C          AUTHOR:   H.P. SUMMERS
C                   K1/1/57
C                   JET EXT. 4941
C          DATE:     11/10/91
C
C          UPDATE:   10/03/93 - PE BRIDEN: ADDED CALL TO XXUID AND USERID VARIABLE
C                                - NOW ALLOWS ANY INPUT DATASET USER ID.
C          UPDATE:   2/09/93 - HPS       : ADDED CALL TO XXSSZD AND USRGRP, USRTYP
C                                AND USREXT NAMES
C                                - NOW ALLOWS ANY INPUT DATASET FILENAME
C                                AND EXTENSION
C          UPDATE:   23/11/93 - PEB       : CORRECT ERROR - A '.' HAD MISTAKENLY
C                                BEEN PLACED BEFORE THE MEMBER NAME IN
C                                VARIABLE DSNAME.
C
C          UPDATE:   10/11/94 - L. JALOTA: MODIFIED CODE FOR RUNNING UNDER UNIX
C                                USING NEW FILE NAMING CONVENTION.
C                                "ACTION" KEYWORD IN OPEN COMMAND IS IBM
C                                SO REMOVED HERE.
C                                ADDED DEFADF
C          UPDATE:   22/11/94 - L. JALOTA: TIDIED UP CHARACTER LENGTH DEFINITIONS
C
C          UPDATE:   24/03/95 - HPS       : INTRODUCED HASH TO ELIMINATE # IN FILE IF
C                                THERE IS NO EXTENSION PART OF THE FILE NAME
C                                ALTER LOGIC TO ALLOW USRTYP, USREXT TO BE A
C                                SINGLE CHARACTER.
C
C          VERSION:  1.1                               DATE: 08-02-96
C          MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C                   - FIRST VERSION
C
C          -----
C          INTEGER   IUNIT       , IZ0           ,
C          &         IRCODE      , IDLEN        ,
C          &         LENF1       , LENF2      ,
C          &         LENF3       , LENF4      ,
C          &         LENF5       , LENF6      ,
C          &         LENF7       , LENF8      ,
C          INTEGER   IF1         ,
C          &         IL1
C          -----

```

```

CHARACTER  XFESYM*2      , ESYM*2      ,
&          USERID*80   , DSNNAME*80   , DEFADF*5   ,
&          USRGRP*8    , USRTYP*80   , USREXT*3   ,
&          HASH*1      , DLPATH*80
C-----
LOGICAL    LEXIST
C-----
C SET DEFAULT DIRECTORY.
PARAMETER (DEFADF = 'adf07')
C-----
C-----

```

## CAPASF

```

SUBROUTINE CAPASF( IUPS1 , IUPS2 , IUPS3 , IUPS4 , IURUN ,
&                DSNPS1 , DSNPS2 , DSNPS3 , DSNPS4 , DSNRUN ,
&                LPASS1 , LPASS2 , LPASS3 , LPASS4 , LRUN ,
&                IRCODE )
C
C IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: CAPASF *****
C
C PURPOSE: HANDLES OPENING OF OUTPUT PASSING FILES.
C
C CALLING PROGRAM: ADAS310
C
C SUBROUTINE:
C
C INPUT : (I*4) IUPS1 = UNIT NO. FOR FIRST PASSING FILE.
C INPUT : (I*4) IUPS2 = UNIT NO. FOR SECOND PASSING FILE.
C INPUT : (I*4) IUPS3 = UNIT NO. FOR THIRD PASSING FILE.
C INPUT : (I*4) IUPS4 = UNIT NO. FOR FOURTH PASSING FILE.
C INPUT : (I*4) IURUN = UNIT NO. FOR RUN SUMMARY FILE.
C INPUT : (C*80) DSNPS1 = FIRST PASSING FILE DATA SET NAME.
C INPUT : (C*80) DSNPS2 = SECOND PASSING FILE DATA SET NAME.
C INPUT : (C*80) DSNPS3 = THIRD PASSING FILE DATA SET NAME.
C INPUT : (C*80) DSNPS4 = FOURTH PASSING FILE DATA SET NAME.
C INPUT : (C*80) DSNRUN = RUN SUMMARY FILE DATA SET NAME.
C INPUT : (L*4) LPASS1 = FLAG FOR WHETHER OR NOT 1ST PASSING FILE
C                   HAS BEEN REQUESTED
C INPUT : (L*4) LPASS2 = FLAG FOR WHETHER OR NOT 2ND PASSING FILE
C                   HAS BEEN REQUESTED
C INPUT : (L*4) LPASS3 = FLAG FOR WHETHER OR NOT 3RD PASSING FILE
C                   HAS BEEN REQUESTED
C INPUT : (L*4) LPASS4 = FLAG FOR WHETHER OR NOT 4TH PASSING FILE
C                   HAS BEEN REQUESTED
C
C OUTPUT: (I*4) IRCODE = RETURN CODE AFTER ATTEMPTING TO OPEN FILES.
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C-----
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C        KL/0/81
C        JET EXT. 5183
C
C DATE: 17/01/94
C
C UNIX-IDL PORT:
C
C VERSION: 1.1 DATE: 08-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - FIRST VERSION
C
C VERSION: 1.2 DATE: 02-04-96
C MODIFIED: TIM HAMMOND/PAUL BRIDEN
C          - REMOVED FILE= ARGUMENT FROM SCRATCH FILE OPEN
C            STATEMENTS AS IT CAN CAUSE A COMPILATION ERROR OF
C            WARNING MESSAGE UNDER AIX.
C-----
C
C INTEGER IUPS1 , IUPS2 , IUPS3 , IUPS4 , IURUN
C INTEGER IRCODE
C-----
C CHARACTER DSNPS1*80 , DSNPS2*80 , DSNPS3*80 , DSNPS4*80 ,
&          DSNRUN*80
C-----
C LOGICAL LPASS1 , LPASS2 , LPASS3 , LPASS4 , LRUN
C-----

```

## CASSZD

```

SUBROUTINE CASSZD( IBSEL , IZ0IN ,
& ITVAL , TVAL ,
& BWNO , IZ , IZ1 ,
& METI , METF ,
& SZDA , LTRNG ,
& TITLX , IRCODE , DLPATH
& )
C
C      IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: CASSZD *****
C
C PURPOSE: TO EXTRACT AND INTERPOLATE ZERO-DENSITY IONIZATION RATE-
C COEFFICIENTS FOR GIVEN ELEMENT NUCLEAR CHARGE AND DATA-BLOCK
C FOR AN INPUT SET OF ELECTRON TEMPERATURES (eV).
C - USES THE SAME ROUTINES USED BY SSZD, EXCEPT FOR:
C
C 'CAFILE' - WHICH OPENS THE REQUESTED FILE.
C 'CACHKB' - WHICH CHECKS INPUT VALUES ARE CONSISTENT WITH
C THE SELECTED DATA-BLOCK 'IBSEL' AND 'IBSEL' IS
C IN RANGE.
C
C THE FIRST OF THESE FUNCTIONS IS CARRIED OUT IN 'ADAS502'
C VIA ISPF PANELS USING THE ROUTINE 'E2SPF0' - ADAS502 DOES
C NOT REQUIRE THE ROUTINE 'CACHKB' AS THE USER CANNOT SELECT
C AN INVALID VALUE FOR 'IBSEL' OR 'IBSEL'/ELEMENT COMBINATION
C
C CALLING PROGRAM: NSUPH1
C
C SUBROUTINE:
C
C INPUT : (I*4) IBSEL = INDEX OF DATA-BLOCK SELECTED FOR ANALYSIS
C INPUT : (I*4) IZ0IN = NUCLEAR CHARGE OF REQUIRED ELEMENT
C
C INPUT : (I*4) ITVAL = NUMBER OF ELECTRON TEMPERATURE VALUES
C INPUT : (R*8) TVAL() = ELECTRON TEMPERATURES (UNITS: EV)
C DIMENSION: ELECTRON TEMPERATURE INDEX
C INPUT : (C*80) DLPATH = PATH NAME TO THE RELEVANT DATA FILES
C (PASSED THROUGH TO CAFILE TO BUILD FILENAME)
C
C OUTPUT: (R*8) BWNO = INPUT FILE - SELECTED DATA-BLOCK:
C EFFECTIVE IONIZATION POTENTIAL (cm-1).
C OUTPUT: (I*4) IZ = INPUT FILE - SELECTED DATA BLOCK:
C IONIZING ION - INITIAL CHARGE
C OUTPUT: (I*4) IZ1 = INPUT FILE - SELECTED DATA BLOCK:
C IONIZING ION - FINAL CHARGE
C
C OUTPUT: (I*4) METI = INPUT FILE - SELECTED DATA-BLOCK:
C INITIAL STATE METSTABLE INDEX
C OUTPUT: (I*4) METF = INPUT FILE - SELECTED DATA-BLOCK:
C FINAL STATE METSTABLE INDEX
C
C OUTPUT: (R*8) SZDA() = ZERO-DENSITY IONIZATION RATE-COEFFICIENTS
C DIMENSION: ELECTRON TEMPERATURE INDEX
C OUTPUT: (L*4) LTRNG() = .TRUE. => OUTPUT 'SZDA()' VALUE WAS INTER-
C POLATED FOR THE USER ENTERED
C ELECTRON TEMPERATURE 'TVAL()'.
C .FALSE. => OUTPUT 'SZDA()' VALUE WAS EXTRA-
C POLATED FOR THE USER ENTERED
C ELECTRON TEMPERATURE 'TVAL()'.
C DIMENSION: ELECTRON TEMPERATURE INDEX
C
C OUTPUT: (C*80) TITLX = INFORMATION STRING (DSN ETC.)
C OUTPUT: (I*4) IRCODE = RETURN CODE FROM SUBROUTINE:
C 0 => NORMAL COMPLETION - NO ERROR DETECTED
C 1 => DATA SET MEMBER FOR IONIZING ION WITH
C NUCLEAR CHARGE 'IZ0IN' CAN NOT BE
C FOUND/DOES NOT EXIST.
C 2 => DISCREPANCY BETWEEN REQUESTED CHARGES
C AND THOSE IN INPUT FILE.
C 3 => THE SELECTED DATA-BLOCK 'IBSEL' IS OUT
C OF RANGE OR DOES NOT EXIST.
C 4 => INVALID VALUE FOR 'IZ0IN' ENTERED.
C ('IZ0MIN' <= 'IZ0IN' <= 'IZ0MAX')
C 9 => ERROR ENCOUNTERED WHEN TRYING TO OPEN
C INPUT DATA-SET.
C
C (I*4) NSTORE = PARAMETER= MAXIMUM NUMBER OF DATA-BLOCKS
C WHICH CAN BE READ FROM THE INPUT
C DATA-SET.
C (I*4) NTDIM = PARAMETER= MAXIMUM NUMBER OF ELECTRON TEMP-
C ERATURES THAT CAN BE READ FROM
C AN INPUT DATA-SET DATA-BLOCK.
C (I*4) IZ0MIN = PARAMETER: MIN. ALLOWED VALUE FOR 'IZ0IN'
C (I*4) IZ0MAX = PARAMETER: MAX. ALLOWED VALUE FOR 'IZ0IN'
C
C (I*4) IZ0LST = LAST VALUE OF 'IZ0IN' FOR WHICH INPUT
C DATA WAS READ.
C (I*4) IUNIT = UNIT TO WHICH INPUT DATA SET IS ALLOCATED
C (I*4) NBSSEL = TOTAL NUMBER OF DATA-BLOCKS READ FROM INPUT
C DATA SET.
C (I*4) IZ0 = INPUT FILE - EMITTING ION - NUCLEAR CHARGE
C
C (L*4) LOPEN = .TRUE. => INPUT DATA SET OPEN.
C .FALSE. => INPUT DATA SET CLOSED.
C

```





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C VERSION: 1.1 DATE: 25-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - CREATED FROM SSZD.FOR WITH SPECIFIC USE IN ADAS 310
C AS GOAL. ALL FUNCTIONALITY IS MAINTAINED, BUT
C ROUTINE CALLS A NEW FILE CAFILE.FOR TO OPEN
C THE REQUESTED FILE IF IT IS AVAILABLE, THIS
C HAS ALSO NECESSITATED BRINGING IN THE VARIABLE
C DLPATH WHICH HOLDS THE PATH TO THE DATA FILES.
C
C-----
C
C
C-----
C
C INTEGER NSTORE , NTDIM
C INTEGER IZOMIN , IZOMAX
C-----
C PARAMETER( NSTORE = 160 , NTDIM = 24 )
C PARAMETER( IZOMIN = 1 , IZOMAX = 60 )
C-----
C INTEGER IBSEL , IZ0IN , ITVAL ,
C & IZ , IZ1 ,
C & METI , METF ,
C & IRCODE
C INTEGER IZ0LST , IUNIT , NBSEL ,
C & IZ0
C-----
C REAL*8 BWNO
C-----
C LOGICAL LOPEN
C-----
C CHARACTER ESYM*2 , EXTIN*3 , EXTLST*3 ,
CX & UIDIN*6 , UIDLST*6 ,
C & UIDIN*80 , UIDLST*80 ,
C & GRPIN*8 , GRPLST*8 ,
C & TYPIN*80 , TYPLST*80 ,
CX & DSNREQ*44 , DSNAME*44 , TITLX*80 ,
C & DSNREQ*80 , DSNAME*80 , TITLX*80 ,
C & DLPATH*80
C-----
C INTEGER ISELA(NSTORE) , ITA(NSTORE) ,
C & IZOUT(NSTORE) , IZ1OUT(NSTORE)
C-----
C REAL*8 TVAL(ITVAL) , SZDA(ITVAL) ,
C & BWNOUT(NSTORE)
C-----
C LOGICAL LTRNG(ITVAL)
C-----
C CHARACTER CICODE(NSTORE)*2 , CFCODE(NSTORE)*2 ,
C & CIION(NSTORE)*6 , CFION(NSTORE)*6
C-----
C REAL*8 TETA(NTDIM,NSTORE) , SZD(NTDIM,NSTORE)
C-----
C SAVE DSNAME , UIDLST , GRPLST , TYPLST ,
C & EXTLST , IZ0LST ,
C & IUNIT
C-----
C DATA DSNAME /' '/ , UIDLST /' '/ , GRPLST /' '/ ,
C & TYPLST /' '/ ,
C & EXTLST /' '/ , IZ0LST /0/ ,
C & IUNIT /16/
C-----

```

## CATMPF

```

SUBROUTINE CATMPF( IUTMP , NUCCHG , DSNEK , DSNCX ,
C & JDENSM , JTEM , TS , W ,
C & Z , CION , CPY , W1 ,
C & NIP , INTD , IPRS , ILOW ,
C & IONIP , NIONIP , ILPRS , IVDISP ,
C & ZEFF , NOSCAN , NIMP , ZIMPA ,
C & AMIMPA , FRIMPA , DENSA , TEA ,
C & DENPA , TPA , BMENER , DENSH ,
C & NMN , NMAX , IMAX , NREP ,
C & WBREP , JCOR , COR , JMAX ,
C & EPSIL , FIJ , WIJ , JDEF ,
C & DEFECT
C )
C
C IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: CATMPF *****
C
C PURPOSE: TO WRITE TEMPORARY FILE CONTAINING PARAMETERS TO BE READ BY
C SUBROUTINE 'V2BNDLN'. THIS ROUTINE IS A TEMPORARY MEASURE TO
C ALLOW 'V2BNDLN' TO RUN WITHIN THE FRAMEWORK OF ADAS WITHOUT
C HAVING TO EDIT 'V2BNDLN'. THE PARAMETERS SHOULD REALLY BE
C PASSED INTO 'V2BNDLN' THROUGH ITS ARGUMENT LIST.
C
C CALLING PROGRAM: ADAS310
C
C INPUT : (I*4) IUTMP = UNIT NUMBER OF TEMPORARY FILE.

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```

C INPUT : (I*4)  NUCCHG = NUCLEAR CHARGE.
C INPUT : (C*80) DSNEX  = FULL MVS DATA SET NAME FOR EXPANSION FILE
C                               (SUITABLE FOR DYNAMIC ALLOCATION).
C INPUT : (C*80) DSNCX  = FULL MVS DATA SET NAME FOR CHARGE EXCHANGE
C                               DATA SET (SUITABLE FOR DYNAMIC ALLOCATION)
C INPUT : (I*4)  JDENSM = NUMBER OF DENSITIES.
C INPUT : (I*4)  JTEM   = NUMBER OF TEMPERATURES.
C INPUT : (R*8)  TS     = EXTERNAL RADIATION FIELD TEMPERATURE.
C                               UNITS: K
C INPUT : (R*8)  W      = EXTERNAL RADIATION FIELD DILUTION FACTOR
C                               (HIGHER LEVELS).
C INPUT : (R*8)  Z      = RECOMBINING ION CHARGE.
C INPUT : (R*8)  CION   = MULTIPLIER OF GROUND LEVEL ELECTRON IMPACT
C                               IONISATION RATE COEFFICIENT.
C INPUT : (R*8)  CPY    = MULTIPLIER OF ELECTRON EXCITATION RATE
C                               COEFFICIENT FROM THE GOUND LEVEL.
C INPUT : (R*8)  W1     = EXTERNAL RADIATION FIELD DILUTION FACTOR
C                               FOR PHOTO-IONISATION FROM THE GROUND
C                               LEVEL.
C INPUT : (R*8)  NIP    = RANGE OF DELTA N FOR IMPACT PARAMETER
C                               XSECTS. (.LE. 4)
C INPUT : (R*8)  INTD   = ORDER OF MAXWELL QUADRATURE FOR XSECTS.
C                               (.LE. 3)
C INPUT : (R*8)  IPRS   = CONTROLS XSECTS BEYOND NIP RANGE.
C                               0 => DEFAULT TO VAN REGEMORTER XSECTS.
C                               1 => USE PERCIVAL-RICHARDS XSECTS.
C INPUT : (R*8)  ILOW   = CONTROLS ACCESS OF SPECIAL LOW LEVEL DATA.
C                               0 => NO SPECIAL LOW LEVEL DATA ACCESSED.
C                               1 => SPECIAL LOW LEVEL DATA ACCESSED.
C INPUT : (R*8)  IONIP  = CONTROLS INCLUSION OF ION IMPACT
C                               COLLISIONS.
C                               0 => NO ION IMPACT COLLISIONS INCLUDED.
C                               1 => ION IMPACT EXCITATION AND IONISATION
C                               INCLUDED.
C INPUT : (R*8)  NIONIP = RANGE OF DELTA N FOR ION IMPACT EXCITATION
C                               XSECTS.
C INPUT : (R*8)  ILPRS  = CONTROLS USE OF LODGE-PERCIVAL-RICHARDS
C                               XSECTS.
C                               0 => DEFAULT TO VAINSHTEIN XSECTS.
C                               1 => USE LODGE-PERCIVAL-RICHARDS XSECTS.
C INPUT : (R*8)  IVDISP = CONTROLS USE OF BEAM ENERGY IN CALCULATION
C                               OF XSECTS.
C                               0 => ION IMPACT AT THERMAL MAXWELLIAN
C                               ENERGIES.
C                               1 => ION IMPACT AT DISPLACED THERMAL
C                               ENERGIES ACCORDING TO THE NEUTRAL
C                               BEAM ENERGY PARAMETER.
C                               NB: IF IVDISP=0 THEN SPECIAL LOW LEVEL
C                               DATA FOR ION IMPACT IS NOT
C                               SUBSTITUTED - ONLY VAINSHTEIN AND
C                               LODGE ET AL. OPTIONS ARE OPEN.
C                               ELECTRON IMPACT DATA SUBSTITUTION
C                               DOES OCCUR.
C INPUT : (R*8)  ZEFF   = NUCLEAR CHARGE OF IMPURITY.
C                               (ONLY SET IF 'NOSCAN'=0 )
C INPUT : (I*4)  NOSCAN = CONTROLS MODE OF OPERATION.
C                               0 => SINGLE IMPURITY.
C                               1 => MULTIPLE IMPURITIES.
C INPUT : (I*4)  NIMP   = NUMBER OF IMPURITY SPECIES
C                               (ONLY SET IF 'NOSCAN'=1 )
C INPUT : (R*8)  ZIMPA() = NUCLEAR CHARGE OF IMPURITIES.
C                               (ONLY SET IF 'NOSCAN'=1 )
C                               DIMENSION: NIMP
C INPUT : (R*8)  AMIMPA() = ATOMIC MASS NUMBERS OF IMPURITIES.
C                               (ONLY SET IF 'NOSCAN'=1 )
C                               DIMENSION: NIMP
C INPUT : (R*8)  FRIMPA() = IMPURITY FRACTIONS.
C                               (ONLY SET IF 'NOSCAN'=1 )
C                               DIMENSION: NIMP
C INPUT : (R*8)  DENSA() = ELECTRON DENSITIES.
C                               UNITS: CM-3
C                               DIMENSION: JDENSM
C INPUT : (R*8)  TEA()  = ELECTRON TEMPERATURES.
C                               UNITS: K
C                               DIMENSION: JTEM
C INPUT : (R*8)  DENPA() = PROTON DENSITIES.
C                               UNITS: CM-3
C                               DIMENSION: JDENSM
C INPUT : (R*8)  TPA()  = PROTON TEMPERATURES.
C                               UNITS: K
C                               DIMENSION: JTEM
C INPUT : (R*8)  BMENER = NEUTRAL BEAM PARTICLE ENERGY.
C                               UNITS: EV / AMU
C INPUT : (R*8)  DENSH  = NEUTRAL HYDROGEN DENSITY IN BEAM.
C                               UNITS: CM-3
C INPUT : (I*4)  NMIN   = LOWEST N-SHELL.
C INPUT : (I*4)  NMAX   = HIGHEST N-SHELL.
C INPUT : (I*4)  IMAX   = NUMBER OF REPRESENTATIVE N-SHELL LEVELS.
C INPUT : (I*4)  NREP() = SET OF REPRESENTATIVE N-SHELL LEVELS.
C                               DIMENSION: IMAX
C INPUT : (R*8)  WBREP() =
C                               DIMENSION: IMAX
C INPUT : (I*4)  JCOR   =
C INPUT : (R*8)  COR()  =
C                               DIMENSION: JCOR
C INPUT : (I*4)  JMAX   =
C INPUT : (R*8)  EPSIL() =
C                               DIMENSION: JMAX

```

```

C INPUT : (R*8) FIJ() = DIMENSION: JMAX
C INPUT : (R*8) WIJ() = DIMENSION: JMAX
C INPUT : (I*4) JDEF = NUMBER OF QUANTUM DEFECTS.
C INPUT : (R*8) DEFECT() = SET OF QUANTUM DEFECT.
C DIMENSION: JDEF
C (I*4) I = ARRAY INDEX.
C (L*4) LOPEN = FLAGS IF SCRATCH FILE OPEN.
C .TRUE. => SCRATCH FILE OPEN.
C .FALSE. => SCRATCH FILE CLOSED.
C AUTHOR: JONATHAN NASH (TESSELLA SUPPORT SERVICES PLC)
C K1/0/81
C JET EXT. 5183
C DATE: 17/01/94
C UNIX-IDL PORT:
C VERSION: 1.1 DATE: 08-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - FIRST VERSION
C -----
C
C INTEGER IUTMP , NUCCHG , JDENSM , JTEM , NIP ,
C & INTD , IPRS , ILOW , IONIP , NIONIP ,
C & ILPRS , IVDISP , NOSCAN , NIMP , NMIN ,
C & NMAX , IMAX , JCOR , JMAX , JDEF
C INTEGER I
C -----
C REAL*8 TS , W , Z , CION , CPY ,
C & W1 , ZEFF , BMENER , DENSH
C -----
C LOGICAL LOPEN
C -----
C CHARACTER DSNE*80 , DSN*80
C -----
C INTEGER NREP(IMAX)
C -----
C REAL*8 ZIMPA(NIMP) , AMIMPA(NIMP) , FRIMPA(NIMP) ,
C & DENSA(JDENSM) , TEA(JTEM) , DENPA(JDENSM) ,
C & TPA(JTEM) , WBREP(IMAX) , COR(JCOR) ,
C & EPSIL(JMAX) , FIJ(JMAX) , WIJ(JMAX) ,
C & DEFECT(JDEF)
C -----

```

## CCDATA

```

SUBROUTINE CCDATA( TERAY , NERAY , EBRAY , N1N , SRAY ,
& F1 , F2 , F3 , BN ,
& NN , IZ , INFILE , INUNIT ,
& MAXNE , MAXTE , MAXEB ,
& INCOUNT , ITCOUNT , IECOUNT , LEVEL ,
& EBREF , TERE , NERE ,
& INA , IEA , ITA , NLEVEL
& )
IMPLICIT NONE
C -----
C ***** PORTRAN77 SUBROUTINE: CCDATA *****
C
C PURPOSE: TO FETCH DATA FROM BUNDLE-N POPULATION
C FILES OF TYPE ADF26.
C
C CALLING PROGRAM: ADAS312
C
C SUBROUTINE:
C
C INPUT : (C*80) INFILE = MVS DATA SET NAME OF DATA SET BEING READ
C INPUT : (I*4) INUNIT = UNIT TO WHICH INPUT FILE IS ALLOCATED.
C INPUT : (I*4) MAXNE = MAXIMUM NUMBER OF DENSITIES
C INPUT : (I*4) MAXTE = MAXIMUM NUMBER OF TEMPERATURES
C INPUT : (I*4) MAXEB = MAXIMUM NUMBER OF BEAM ENERGIES
C
C OUTPUT: (R*8) TERAY() = TEMPERATURE SET (EV)
C 1ST. DIM.: TEMPERATURE INDEX
C OUTPUT: (R*8) NERAY() = DENSITY SET (CM-3)
C 1ST. DIM.: DENSITY INDEX
C OUTPUT: (R*8) EBRAY() = BEAM ENERGY SET (EV/AMU)
C 1ST. DIM.: BEAM ENERGY INDEX
C OUTPUT: (R*8) N1N(,,) = ???
C 1ST. DIM.: BEAM ENERGY INDEX
C 2ND. DIM.: DENSITY INDEX
C 3RD. DIM.: TEMPERATURE INDEX
C OUTPUT: (R*8) SRAY(,,) = COLL. RAD. IONIS COEFFT. (CM3 S-1)
C 1ST. DIM.: BEAM ENERGY INDEX
C 2ND. DIM.: DENSITY INDEX
C 3RD. DIM.: TEMPERATURE INDEX

```

```

C OUTPUT: (R*8) F1(,,, ) = F1 EXPANSION FACTOR OF BN
C 1ST. DIM.: BEAM ENERGY INDEX
C 2ND. DIM.: DENSITY INDEX
C 3RD. DIM.: TEMPERATURE INDEX
C 4TH. DIM.: REPRES. PRINC. QUANTUM SHELL INDEX
C OUTPUT: (R*8) F2(,,, ) = F2 EXPANSION FACTOR OF BN
C 1ST. DIM.: BEAM ENERGY INDEX
C 2ND. DIM.: DENSITY INDEX
C 3RD. DIM.: TEMPERATURE INDEX
C 4TH. DIM.: REPRES. PRINC. QUANTUM SHELL INDEX
C OUTPUT: (R*8) F3(,,, ) = F3 EXPANSION FACTOR OF BN
C 1ST. DIM.: BEAM ENERGY INDEX
C 2ND. DIM.: DENSITY INDEX
C 3RD. DIM.: TEMPERATURE INDEX
C 4TH. DIM.: REPRES. PRINC. QUANTUM SHELL INDEX
C OUTPUT: (R*8) BN(,,, ) = BN FACTOR
C 1ST. DIM.: BEAM ENERGY INDEX
C 2ND. DIM.: DENSITY INDEX
C 3RD. DIM.: TEMPERATURE INDEX
C 4TH. DIM.: REPRES. PRINC. QUANTUM SHELL INDEX
C OUTPUT: (R*8) NN(,,, ) = POPULATION CONVERSION FACTOR
C 1ST. DIM.: BEAM ENERGY INDEX
C 2ND. DIM.: DENSITY INDEX
C 3RD. DIM.: TEMPERATURE INDEX
C 4TH. DIM.: REPRES. PRINC. QUANTUM SHELL INDEX
C OUTPUT: (I*4) IZ = IMPURITY ION CHARGE
C OUTPUT: (I*4) INCOUNT = NUMBER OF DENSITIES
C OUTPUT: (I*4) ITCOUNT = NUMBER OF TEMPERATURES
C OUTPUT: (I*4) IECOUNT = NUMBER OF BEAM ENERGIES
C OUTPUT: (I*4) LEVEL = ??? APPEARS UNUSED ???
C OUTPUT: (R*8) EBREF = REFERENCE BEAM ENERGY (EV/AMU)
C OUTPUT: (R*8) TEREf = REFERENCE TEMPERATURE (EV)
C OUTPUT: (R*8) NEREf = REFERENCE DENSITY (CM-3)
C OUTPUT: (I*4) INA() = NUMBER OF LEVELS
C 1ST. DIM.: DENSITY INDEX
C OUTPUT: (I*4) ITA() = NUMBER OF LEVELS
C 1ST. DIM.: TEMPERATURE INDEX
C OUTPUT: (I*4) IEA() = NUMBER OF LEVELS
C 1ST. DIM.: BEAM ENERGY INDEX
C OUTPUT: (I*4) NLEVEL = NUMBER OF LEVELS
C
C (I*4) IT = GENERAL INDEX
C (I*4) IN = GENERAL INDEX
C (I*4) IE = GENERAL INDEX
C (R*8) TE = GENERAL REAL VARIABLE
C (R*8) NE = GENERAL REAL VARIABLE
C (R*8) EB = GENERAL REAL VARIABLE
C (C*132)LINE = GENERAL STRING
C (C*2) LEVELS() = PRINC. QU. SHELL STRINGS
C
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C I4UNIT ADAS FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C CCFIND ADAS ???
C
C
C AUTHOR: HARVEY ANDERSON, UNIVERSITY OF STRATHCLYDE/JET
C JA8.08
C TEL. 0141-553-4196
C
C
C DATE: 16/05/97
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1 DATE: 10-07-97
C MODIFIED: HUGH SUMMERS, UNIVERSITY OF STRATHCLYDE
C - PUT UNDER S.C.C.S. CONTROL
C
C
C -----
C INTEGER MAXTE , MAXNE , MAXEB ,
C & INUNIT , ITCOUNT , INCOUNT ,
C & IECOUNT , IZ , IT ,
C & IN , IE , LEVEL , NLEVEL
C -----
C INTEGER INA(MAXNE) , IEA(MAXEB) , ITA(MAXTE)
C -----
C REAL*8 TE , EB , Z ,
C & EBREF , NEREf , TEREf , NE
C -----
C REAL*8 NERAY(MAXNE) , TERAY(MAXTE) , EBRAy(MAXEB) ,
C & SRAY(MAXEB,MAXNE,MAXTE) , N1N(MAXEB,MAXNE,MAXTE) ,
C & F1(MAXEB,MAXNE,MAXTE,NLEVEL) ,
C & F2(MAXEB,MAXNE,MAXTE,NLEVEL) ,
C & F3(MAXEB,MAXNE,MAXTE,NLEVEL) ,
C & BN(MAXEB,MAXNE,MAXTE,NLEVEL) ,
C & NN(MAXEB,MAXNE,MAXTE,NLEVEL)
C -----
C CHARACTER LINE*132 , INFILE*80 , LEVELS(20)*2
C -----
C DATA LEVELS/' 1',' 2',' 3',' 4',' 5',' 6',' 7',' 8',' 9','10',
C & '11','12','13','14','15','16','17','18','19','20'/
C -----

```

## CCFILL

```
      SUBROUTINE CCFILL( NTA      , M )
      IMPLICIT NONE
-----
C
C ***** FORTRAN77 SUBROUTINE: CCFILL *****
C
C PURPOSE:  TO FILL AN INTEGER ARRAY WITH ITS OWN INDEX.
C
C CALLING PROGRAM: ADAS312
C
C SUBROUTINE:
C
C I/O      : (I*4)  NTA()   = ARRAY TO BE FILLED
C INPUT    : (I*4)  M       = NUMBER OF ELEMENTS TO BE FILLED
C
C           (I*4)  I       = GENERAL INTEGER
C
C ROUTINES:
C           NONE
C
C AUTHOR:   HARVEY ANDERSON, UNIVERSITY OF STRATHCLYDE/JET
C           JA8.08
C           TEL. 0141-553-4196
C
C DATE:    16/05/97
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1                      DATE: 10-07-97
C MODIFIED: HUGH SUMMERS, UNIVERSITY OF STRATHCLYDE
C           - PUT UNDER S.C.C.S. CONTROL
C
-----
C           INTEGER      M      , I
-----
C           INTEGER      NTA(*)
-----
C
```

## CCFIND

```
      SUBROUTINE CCFIND( ARR      , VALUE , IMAX , INDEX )
      IMPLICIT NONE
-----
C
C ***** FORTRAN77 SUBROUTINE: CCFIND *****
C
C PURPOSE:  TO ISOLATE DATA FROM ADF26 DATASET
C
C CALLING PROGRAM: CCDATA
C
C SUBROUTINE:
C
C INPUT    : (R*8)  ARR()   = ARRAY TO BE SEARCHED
C           1ST. DIM.:
C INPUT    : (R*8)  VALUE   = ???
C INPUT    : (I*4)  IMAX    = NUMBER OF VALUES IN ARR
C
C OUTPUT   : (I*4)  INDEX   = LOCATED POSITION
C
C           (L*4)  FOUND   = ???
C           (C*2)  OVER    = ???
C
C ROUTINES:
C           NONE
C
C AUTHOR:   HARVEY ANDERSON, UNIVERSITY OF STRATHCLYDE/JET
C           JA8.08
C           TEL. 0141-553-4196
C
C DATE:    16/05/97
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1                      DATE: 10-07-97
C MODIFIED: HUGH SUMMERS, UNIVERSITY OF STRATHCLYDE
C           - PUT UNDER S.C.C.S. CONTROL
C
-----
C
```

```

C-----
C
C      INTEGER  IMAX      , INDEX
C-----
C      REAL*8   VALUE
C-----
C      REAL*8   ARR(99)
C-----
C      LOGICAL  OVER     , FOUND
C-----

```

## CCINTP

```

      SUBROUTINE CCINTP( ZDATA , YDATA , XDATA , SRAY ,
&                      ITREF , IEREF , INREF ,
&                      TVAL , MAXEB , MAXNE , MAXTE ,
&                      EBRAY , NERAY , BMSTOP , BMEMIS ,
&                      IECOUNT , INCOUNT ,
&                      F1 , NN , AVALUE , LEVEL ,
&                      NLEVEL , IEA , INA , ITA
&                      )
      IMPLICIT NONE
C-----
C
C ***** FORTRAN77 SUBROUTINE: CCDATA *****
C
C PURPOSE: TO INTERPOLATE BETWEEN THE EFFECTIVE STOPPING
C          OR EMISSION COEFFICIENTS.
C
C CALLING PROGRAM: ADAS312
C
C SUBROUTINE:
C
C INPUT : (R*8) ZDATA( , ) =
C INPUT : (R*8) YDATA( ) =
C INPUT : (R*8) XDATA( ) =
C INPUT : (R*8) SRAY( , , ) =
C INPUT : (I*4) ITREF =
C INPUT : (I*4) IEREF =
C INPUT : (I*4) INREF =
C INPUT : (I*4) TVAL =
C INPUT : (I*4) MAXEB =
C INPUT : (I*4) MAXNE = MAXIMUM NUMBER OF DENSITIES
C INPUT : (I*4) MAXTE =
C INPUT : (R*8) EBRAY( ) =
C INPUT : (R*8) NERAY( ) =
C INPUT : (I*4) BMSTOP =
C INPUT : (I*4) BMEMIS =
C INPUT : (I*4) IECOUNT =
C INPUT : (I*4) INCOUNT =
C INPUT : (R*8) F1( , , , ) =
C INPUT : (R*8) NN( , , , ) =
C INPUT : (R*8) AVALUE =
C INPUT : (I*4) LEVEL =
C INPUT : (I*4) NLEVEL =
C INPUT : (I*4) IEA( ) =
C INPUT : (I*4) INA( ) =
C INPUT : (I*4) ITA( ) =
C
C      (I*4) I = GENERAL INTEGER VARIABLE
C      (I*4) J = GENERAL INTEGER VARIABLE
C
C
C ROUTINES:
C
C      ROUTINE      SOURCE      BRIEF DESCRIPTION
C-----
C      I4UNIT      ADAS      FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C-----
C
C AUTHOR: HARVEY ANDERSON, UNIVERSITY OF STRATHCLYDE/JET
C        JA8.08
C        TEL. 0141-553-4196
C
C DATE: 16/05/97
C
C UNIX-IDL PORT: H.P.SUMMERS
C
C VERSION: 1.1 DATE: 10-07-97
C MODIFIED: HUGH SUMMERS, UNIVERSITY OF STRATHCLYDE
C          - PUT UNDER S.C.C.S. CONTROL
C-----
C
C      INTEGER  MAXEB      , MAXNE      , MAXTE      ,
&              IECOUNT    , INCOUNT    , IEREF      ,
&              INREF      , ITREF      , I          ,
&              J          , BMSTOP     , BMEMIS     ,
&              TVAL       , NLEVEL     , LEVEL
C-----

```

```

      INTEGER IEA(MAXBEB) , INA(MAXNE) , ITA(MAXTE)
C-----
      REAL*8 AVALUE
C-----
      REAL*8 NERAY(MAXNE) , EBRAY(MAXBEB) ,
&           XDATA(MAXBEB) , YDATA(MAXNE) ,
&           ZDATA(MAXBEB,MAXNE) ,
&           SRAY(MAXBEB,MAXNE,MAXTE) ,
&           F1(MAXBEB,MAXNE,MAXTE,NLEVEL) ,
&           NN(MAXBEB,MAXNE,MAXTE,NLEVEL)
C-----

```

## CCOUTO

```

      SUBROUTINE CCOUTO( OFILE , OUNIT , IZ , IECOUNT , INCOUNT ,
&                     TEREf , EBRAY , NERAY , XRAY ,
&                     IEA , INA , ITREF ,
&                     ITCOUNT ,
&                     EBREF , NEREF , TERAY ,
&                     MAXTE , MAXNE , MAXEB ,
&                     ITA , IEREF , INREF ,
&                     DATE , TITLE , BMSTOP , BMEMIS ,
&                     F1 , NN , AVALUE , NLEVEL , LEVEL ,
&                     INFILE )
      IMPLICIT NONE
C-----
C
C ***** FORTRAN77 SUBROUTINE: CCOUTO *****
C
C PURPOSE: TO WRITE OUTPUT TO DATA FORMAT ADF21/22 SPECIFICATIONS.
C
C CALLING PROGRAM: ADAS312
C
C SUBROUTINE:
C
C INPUT : (R*8) TEREf = THE REFERENCE TARGET TEMPERATURE (eV).
C INPUT : (R*8) EBREF = THE REFERENCE NEUTRAL BEAM ENERGY
C                   (eV/amu).
C INPUT : (R*8) NEREF = THE REFERENCE TARGET ELECTRON DENSITY.
C                   (CM-**3)
C INPUT : (R*8) TERAY() = ARRAY CONTAINING THE TARGET TEMPERATURE.
C INPUT : (R*8) EBRAY() = ARRAY CONTAINING THE NEUTRAL BEAM
C                   ENERGY ( eV/amu ).
C INPUT : (R*8) NERAY() = ARRAY CONTAINING THE TARGET DENSITY.
C INPUT : (R*8) XRAY() = ARRAY CONTAINING EITHER THE BEAM STOPPING
C                   OR EMISSION COEFFICIENTS (CM**3/S).
C
C INPUT : (R*8) IZ = THE EFFECTIVE NUCLEAR CHARGE OF THE
C                   TARGET PLASMA.
C INPUT : (I*4) ITCOUNT = THE NUMBER OF TARGET TEMPERATURES.
C INPUT : (I*4) IECOUNT = THE NUMBER OF BEAM ENERGIES.
C INPUT : (I*4) INCOUNT = THE NUMBER OF TARGET DENSITIES.
C INPUT : (I*4) ITA() = ARRAY CONTAINING THE INDEX VALUES
C                   OF THE TEMPERATURE ARRAY TERAY().
C INPUT : (I*4) ITREF = THE INDEX VALUE AT WHICH THE REFERENCE
C                   TEMPERATURE CORRESPONDS TO IN THE ARRAY
C                   TERAY.
C INPUT : (I*4) IEA() = ARRAY CONTAINING THE INDEX VALUES
C                   OF THE ENERGY ARRAY EBRAY().
C INPUT : (I*4) IEREF = THE INDEX VALUE AT WHICH THE REFERENCE
C                   ENERGY CORRESPONDS TO IN THE ARRAY
C                   EBRAY().
C INPUT : (I*4) INA() = ARRAY CONTAINING THE INDEX VALUES
C                   OF THE DENSITY ARRAY NERAY().
C INPUT : (I*4) INREF = THE INDEX VALUE AT WHICH THE REFERENCE
C                   DENSITY CORRESPONDS TO IN THE ARRAY
C                   NERAY.
C INPUT : (I*4) MAXTE = THE MAXIMUM NUMBER OF TARGET TEMPERATURES.
C INPUT : (I*4) MAXNE = THE MAXIMUM NUMBER OF TARGET DENSITIES.
C INPUT : (I*4) MAXEB = THE MAXIMUM NUMBER OF BEAM ENERGIES.
C INPUT : (I*4) NUM = THE NUMBER OF ELEMENT SYMBOLS CONTAINED
C                   IN THE ARRAY SPEC().
C
C (CHR) OFILE = OUTPUT FILENAME.
C (CHR) SPEC() = ARRAY CONTAINING THE CHEMICAL SYMBOLS
C                   OF THE ELEMENTS UP TO THE FIRST
C                   PERIOD.
C (CHR) HEADER = STRING CONTAINING THE ADAS VERSION,
C                   THE EXECUTING PROGRAM AND DATE.
C (C*2) LEVELS() = PRINC. QU. SHELL STRINGS
C
C ROUTINES:
C
C ROUTINE SOURCE BRIEF DESCRIPTION
C-----
C I4UNIT ADAS FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C CCFIND ADAS ???
C
C AUTHOR: HARVEY ANDERSON, UNIVERSITY OF STRATHCLYDE/JET
C JA8.08

```

```

C      TEL. 0141-553-4196
C
C      DATE: 16/05/97
C
C      UNIX-IDL PORT: H.P.SUMMERS
C
C      VERSION: 1.1                      DATE: 10-07-97
C      MODIFIED: HUGH SUMMERS, UNIVERSITY OF STRATHCLYDE
C                - PUT UNDER S.C.C.S. CONTROL
C      VERSION: 1.2                      DATE: 28-07-97
C      MODIFIED: HARVEY ANDERSON, UNIVERSITY OF STRATHCLYDE
C                - INCLUDED PROGRAM NAME IN THE OUTPUT FILE.
C                - ADDED ADDITIONAL INFORMATION AT THE BOTTOM OF
C                  THE ADF21/22 TYPE FILE.
C      VERSION: 1.3 RICHARD MARTIN       DATE: 1-11-97
C                CORRECTED SYNTAX ERROR IN GETENV COMMAND.
C
C-----
C      INTEGER  MAXTE      , MAXNE      , MAXEB
C-----
C      INTEGER  IEA(MAXEB) , ITA(MAXTE) , INA(MAXNE) ,
C      &        IREF      , INREF      , ITREF      ,
C      &        ITCOUNT , INCOUNT    , IECOUNT    ,
C      &        OUNIT    , IZ          , BMSTOP     ,
C      &        BMEMIS   , J           , I          ,
C      &        NLEVEL   , LEVEL      ,
C-----
C      REAL*8   EBREF
C-----
C      REAL*8   EBRAY(MAXNE), NERAY(MAXNE), TERAY(MAXTE) ,
C      &        TREF      , NEREF      ,
C      &        XRAY(MAXEB,MAXNE,MAXTE)
C      &        F1(MAXEB,MAXNE,MAXTE,NLEVEL)
C      &        NN(MAXEB,MAXNE,MAXTE,NLEVEL), AVALUE
C      &        F1REF     , NNREF     , ECREF
C-----
C      CHARACTER*2 SPEC(10), DATE*24 ,TITLE*24
C      CHARACTER OFILE*80 , INFILE*80 , USERID*16
C-----
C      DATA SPEC/'H ','HE','LI','BE','B ','C ','N ','O ','F ','NE'/
C-----

```

## CCSORT

```

SUBROUTINE CCSORT( XA , IA , N )
IMPLICIT NONE
C-----
C      ***** FORTRAN77 SUBROUTINE: CCSORT *****
C
C      PURPOSE: TO SORT AN ARRAY SO THAT XA IS INCREASING ORDER.
C
C      CALLING PROGRAM: ADAS312
C
C      SUBROUTINE:
C
C      I/O : (R*8) XA() = X-VALUES INITIAL THEN SORTED
C      I/O : (I*4) IA() = I-VALUES INITIAL THEN SORTED
C      INPUT : (I*4) N = NUMBER OF VALUES
C
C      (I*4) N1 = GENERAL INTEGER VARIABLE
C      (I*4) I = GENERAL INTEGER VARIABLE
C      (I*4) I1 = GENERAL INTEGER VARIABLE
C      (I*4) J = GENERAL INTEGER VARIABLE
C      (I*4) ISWAP = GENERAL INTEGER VARIABLE
C      (R*8) SWAP = GENERAL REAL VARIABLE
C
C      ROUTINES:
C      NONE
C
C      AUTHOR: HARVEY ANDERSON, UNIVERSITY OF STRATHCLYDE/JET
C             JA8.08
C             TEL. 0141-553-4196
C
C      DATE: 16/05/97
C
C      UNIX-IDL PORT: H.P.SUMMERS
C
C      VERSION: 1.1                      DATE: 10-07-97
C      MODIFIED: HUGH SUMMERS, UNIVERSITY OF STRATHCLYDE
C                - PUT UNDER S.C.C.S. CONTROL
C-----
C      INTEGER  ISWAP , N , I , J , I1 , N1

```



```

C-----
C      INTEGER   IA(*)
C-----
C      REAL*8    SWAP
C-----
C      REAL*8    XA(*)
C-----

```

## CEECON

```

SUBROUTINE CEECON( INTYP , OUTTYP, IEVAL, EIN,
&                AMDON , AMREC , EOUT
&                )
IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: CEECON *****
C PURPOSE: TO CONVERT AN ARRAY OF ENERGIES INTO A SPECIFIED form.
C CALLING PROGRAM: ADAS314
C SUBROUTINE:
C INPUT : (I*4) INTYP = 1 => 'EIN(array)' UNITS: eV (Donor temp.)
C          = 2 => 'EIN(array)' UNITS: eV (Recvr temp.)
C          = 3 => 'EIN(array)' UNITS: eV/AMU (ENERGY)
C INPUT : (I*4) OUTTYP = 1 => 'EOUT(array)' UNITS: eV (Donor temp)
C          = 2 => 'EOUT(array)' UNITS: eV (Recvr temp)
C          = 3 => 'EOUT(array)' UNITS: EV/AMU (ENERGY)
C INPUT : (I*4) IEVAL = NO. OF ENERGIES IN EIN(array)
C INPUT : (R*8) EIN() = INPUT ENERGIES (STATED UNITS)
C INPUT : (R*8) AMDON = DONOR MASS NUMBER
C INPUT : (R*8) AMREC = RECEIVER MASS NUMBER
C OUTPUT: (R*8) EOUT() = OUTPUT ENERGIES (STATED UNITS)
C        (I*4) I = GENERAL USE
C        (R*8) ECONV() = ENERGY CONVERSION PARAMETERS
C ROUTINES: NONE
C NOTE:
C       ENERGY CONVERSION PARAMETERS:
C       INTYP = 1 ; ECONV(1) => ENERGY : EV      -> OUTPUT FORM
C       INTYP = 2 ; ECONV(2) => ENERGY : EV      -> OUTPUT FORM
C       INTYP = 3 ; ECONV(3) => ENERGY : EV/AMU  -> OUTPUT FORM
C AUTHOR:  H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C         JA8.08
C         TEL. 0141-553-4196
C DATE:    19/09/95
C UPDATE:  27/08/97 HP SUMMERS - CHANGED NAME FROM CEECON TO CDECON
C MODIFIED: Martin O'Mullane
C DATE:    9-07-98
C VERSION: 1.0 - ported to IDL
C
C VERSION: 1.1                                DATE: 01-12-98
C MODIFIED: RICHARD MARTIN
C          - PUT UNDER SCCS CONTROL
C-----
C      REAL*8    AMDON                , AMREC
C-----
C      INTEGER   INTYP                , OUTTYP
C      &         IEVAL
C      INTEGER   I
C-----
C      REAL*8    EIN(IEVAL)           , EOUT(IEVAL)
C      REAL*8    ECONV(3)
C-----

```

## CEEVTH

```

SUBROUTINE CEEVTH ( NDENR ,
&                 LSETX , LPASS ,
&                 AMDON , AMREC , CATYP , DREN , ILTYP ,
&                 NENIN , ENIN , NENOUT , ENOUT ,
&                 SGIN , RCOU
&                 )
IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: CEEVTH *****
C VERSION: 1.0
C PURPOSE: OBTAINS RATE COEFFICIENTS FOR DONOR/RECEIVER CHARGE
C          EXCHANGE COLLISIONS FOR CASES OF
C          MONOENERGETIC DONOR/THERMAL RECEIVER, THERMAL
C          DONOR/MONOENERGETIC RECEIVER, THERMAL DONOR/THERMAL
C          RECEIVER (SAME TEMPERATURE) FROM CROSS-SECTION TABULATIONS.
C          A MONO-ENERGETIC CASE IS ALLOWED WHICH CONVERTS INPUT
C          CROSS-SECTIONS TABULATED AT A SET OF ENERGIES/AMU TO
C          OUTPUT CROSS-SECTIONS TABULATED A DIFFERENT SET OF
C          ENERGIES/AMU.
C CALLING PROGRAM: ADAS314
C SUBROUTINE:
C INPUT : (I*4) NDENR = MAX. NUMBER OF ENERGIES/TEMPERATURES

```

```

C      IN INPUT/OUTPUT ENERGY/TEMPERATURE
C      VECTORS
C INPUT : (L*4) LSETX = .TRUE. => SPLINE PRESET FOR THESE KNOTS
C      .FLSE. => SPLINE NOT SET FOR THESE KNOTS
C INPUT : (L*4) LPASS = .TRUE. => DO NOT CONVERT INTO LOG10 FOR
C      ENERGIES AND X-SECTS. FOR SPLINE
C      .FLSE. => CONVERT INTO LOG10 FOR
C      ENERGIES AND X-SECTS. FOR SPLINE
C INPUT : (R*8) AMDON = DONOR MASS NUMBER
C INPUT : (R*8) AMREC = RECEIVER MASS NUMBER
C INPUT : (C2) CATYP = 'TT' THERMAL/THERMAL (EQUAL TEMPERATURES
C      FOR DONOR AND RECEIVER ONLY)
C      'TR' THERMAL RECEIVER, MONOENERGETIC DONOR
C      'TD' THERMAL DONOR, MONOENERGETIC RECEIVER
C      'ME' SPECIAL MONOENERGETIC CASE
C INPUT : (R*8) DREN = DONOR ENERGY ( 'TR' CASE )
C      RECEIVER ENERGY ( 'TD' CASE )
C INPUT : (I*4) ILTYP = TYPE FOR LOW AND HIGH ENERGY CROSS-
C      SECTION EXTRAPOLATION
C INPUT : (I*4) NENIN = NUMBER OF ENERGIES IN INPUT DATA SET
C INPUT : (R*8) ENIN() = ENERGIES (EV/AMU) IN INPUT DATA SET
C INPUT : (I*4) NENOUT = NUMBER OF TEMPERATURES FOR OUTPUT DATA SET
C INPUT : (R*8) ENOUT() = TEMPERATURES (EV) FOR OUTPUT DATA SET FOR
C      'TT', 'TD', 'TR' CASES.
C      = ENERGY/AMU FOR OUTPUT DATA SET FOR
C      'ME' CASE.
C INPUT : (R*8) SGIN() = INPUT X-SECTIONS (CM2) FROM INPUT DATA SET
C      1ST.DIM: ENERGY INDEX
C OUTPUT: (R*8) RCOUT() = RATE COEFF. (CM3 S-1) IN OUTPUT DATA SET
C      1ST.DIM: TEMPERATURE INDEX
C      (I*4) I = GENERAL INDEX
C      (I*4) IT = GENERAL INDEX
C      (I*4) ITHETA = GENERAL INDEX
C      (I*4) IOPT = SPLINE END POINT CURVATURE/GRADIENT OPTION
C      1 => DDY1 = 0, DDYN = 0
C      4 => DY1 = 0, DDYN = 0
C      (I*4) IXD = DONOR GAUSSIAN QUADRATURE INDEX
C      (I*4) IXR = RECEIVER GAUSSIAN QUADRATURE INDEX
C      (I*4) NGS = GAUSSIAN QUADRATURE DIMENSION
C      (I*4) NTHETA = NUMBER OF ANGLE VALUES FOR QUADRATURE
C      (I*4) LTHETA = NTHETA+1
C      (I*4) L1 = PARAMETER = 1
C      (R*8) ETHD = THERMAL ENERGY OF DONOR (JOULES)
C      (R*8) ETHR = THERMAL ENERGY RECEIVER (JOULES)
C      (R*8) HSIMP = SIMPSON'S RULE STEP INTERVAL
C      (R*8) THETA = ANGLE BETWEEN PARTICLE VELOCITIES (RAD)
C      (R*8) FAC = GENERAL VARIABLE
C      (R*8) FLAG = GENERAL VARIABLE
C      (R*8) XMRKG = DONOR MASS (KG)
C      (R*8) XMRKG = RECEIVER MASS (KG)
C      (R*8) VD = DONOR SPEED (M S-1)
C      (R*8) VR = RECEIVER SPEED (M S-1)
C      (R*8) RATE = EVALUATED RATE COEFFICIENT (CM3 S-1)
C      (R*8) PART1 = GENERAL VARIABLE
C      (R*8) PART2 = GENERAL VARIABLE
C      (R*8) PART3 = GENERAL VARIABLE
C      (R*8) PART12 = GENERAL VARIABLE
C      (R*8) PART23 = GENERAL VARIABLE
C      (R*8) PART123 = GENERAL VARIABLE
C      (R*8) VREL1 = GENERAL RELATIVE SPEED VARIABLE
C      (R*8) XSEC1 = GENERAL CROSS-SECTION VARIABLE
C      (R*8) VAL = GENERAL VARIABLE
C      (R*8) XGS() = GAUSSIAN QUADRATURE NODES
C      (R*8) WGS() = GAUSSIAN QUADRATURE WEIGHTS
C      (R*8) VREL() = RELATIVE SPEED OF PARTICLES FOR DIFFERENT
C      ANGLES (CM S-1)
C      (R*8) XSEC() = CHARGE EXCHANGE CROSS-SECTIONS FOR
C      RELATIVE SPEEDS AT DIFFERENT ANGLES (CM2)
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C SIGCX ADAS INTERPOLATES CX CROSS-SECTION TABLES
C
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL. 0141-553-4196
C DATE: 02/11/95
C
C UPDATE: 09/07/98 Martin O'Mullane
C CHANGED NAME FROM CXTHER TO CDEVTH. SIMILAR FUNCTIONALITY
C BUT IS EXTENDED TO DEAL WITH EXTRA AVERAGING METHODS.
C
C VERSION: 1.1 DATE: 01-12-98
C MODIFIED: RICHARD MARTIN
C - PUT UNDER SCCS CONTROL
C
C -----
C INTEGER NGS , NTHETA , LTHETA
C INTEGER IOPT , L1
C -----
C REAL*8 CMSAMU , PI
C -----
C PARAMETER ( NGS = 8 , NTHETA = 180 , LTHETA =NTHETA+1 )
C PARAMETER ( IOPT = 4 , L1 = 1 )
C PARAMETER ( CMSAMU = 1.389209D6 , PI = 3.141592654 )
C -----
C INTEGER NDENR
C INTEGER NENIN , NENOUT

```

```

      INTEGER      IXD      , IXR      , I      ,
&               IT      , ITHETA
      INTEGER      ILTYP
-----
      REAL*8      AMDON      , AMREC      , DREN
      REAL*8      ETHD      , ETHR      , HSIMP
      REAL*8      RATE
      REAL*8      THETA      , FAC      , FLAG
      REAL*8      XMDKG      , XMRKG      , VD      , VR
      REAL*8      PART1      , PART2      , PART3
      REAL*8      PART12      , PART23      , PART123
      REAL*8      VREL1      , XSEC1      , VAL
-----
      REAL*8      XGS(NGS)      , WGS(NGS)
      REAL*8      ENIN(NDENR)      , SGIN(NDENR)      ,
&               ENOUT(NDENR)      , RCOUT(NDENR)
      REAL*8      VREL(LTHETA)      , XSEC(LTHETA)
-----
      LOGICAL      LSETX      , LPASS
-----
      CHARACTER      CATYP*2
-----
      DATA XGS/ 0.170279632305      , 0.903701776799      , 2.251086629866,
&              4.266700170288      , 7.045905402393      , 10.758516010181,
&              15.740678641278      , 22.863131736889      /
      DATA WGS/ 3.69188589342D-01, 4.18786780814D-01,
&              1.75794986637D-01, 3.33434922612D-02,
&              2.79453623523D-03, 9.07650877336D-05,
&              8.48574671627D-07, 1.04800117487D-09 /
-----

```

## CEFILL

```

      SUBROUTINE CEFILL( MXNENG , MXNSHL , TITLED ,
&                     SYMBR , SYMBD , IZR , IZD ,
&                     INDD , NENRGY , NMIN , NMAX ,
&                     LPARMS , LSETL , LSETM , ENRGYA ,
&                     ALPHAA , LFORMA , XLCUTA , PL2A ,
&                     PL3A , SIGTA , SIGNA , SIGLA ,
&                     SIGMA
&                     )
      IMPLICIT NONE
-----
C ***** FORTRAN77 SUBROUTINE: CDFILL *****
C PURPOSE:  FILL HIGH N ZEROES IN AN ADF01 IF PRESENT.
C CALLING PROGRAM: ADAS314
C DATA:
C          THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
C          COLLISION ENERGIES      : KEV/AMU
C          ALPHA                    :
C          TOTAL XSECTS.            : CM2
C          N-SHELL XSECTS.          : CM2
C          NL-SHELL DATA           : CM2
C          NLM-SHELL DATA          : CM2
C SUBROUTINE:
C INPUT : (I*4) MXNENG      = MAXIMUM NO. OF ENERGIES.
C INPUT : (I*4) MXNSHL     = MAXIMUM NO. OF N SHELLS.
C INPUT : (C*80) TITLED    = NOT SET - TITLE FOR DATA SOURCE.
C INPUT : (C*2) SYMBR      = READ - RECEIVER ION ELEMENT SYMBOL.
C INPUT : (C*2) SYMBD      = READ - DONOR ION ELEMENT SYMBOL.
C INPUT : (I*4) IZR        = READ - ION CHARGE OF RECEIVER.
C INPUT : (I*4) IZD        = READ - ION CHARGE OF DONOR.
C INPUT : (I*4) INDD       = READ - DONOR STATE INDEX.
C INPUT : (I*4) NENRGY     = NUMBER OF ENERGIES READ.
C INPUT : (I*4) NMIN       = LOWEST N-SHELL FOR WHICH DATA READ.
C INPUT : (I*4) NMAX       = HIGHEST N-SHELL FOR WHICH DATA READ.
C INPUT : (L*4) LPARMS     = FLAGS IF L-SPLITTING PARAMETERS PRESENT.
C                          .TRUE. => L-SPLITTING PARAMETERS PRESENT.
C                          .FALSE => L-SPLITTING PARAMETERS ABSENT.
C INPUT : (L*4) LSETL      = FLAGS IF L-RESOLVED DATA PRESENT.
C                          .TRUE. => L-RESOLVED DATA PRESENT.
C                          .FALSE => L-RESOLVED DATA ABSENT.
C INPUT : (L*4) LSETM      = FLAGS IF M-RESOLVED DATA PRESENT.
C                          .TRUE. => M-RESOLVED DATA PRESENT.
C                          .FALSE => M-RESOLVED DATA ABSENT.
C INPUT : (R*8) ENRGYA()   = READ - COLLISION ENERGIES.
C                          UNITS: EV/AMU (READ AS KEV/AMU)
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) ALPHAA()   = READ - EXTRAPOLATION PARAMETER ALPHA.
C                          DIMENSION: ENERGY INDEX
C INPUT : (I*4) LFORMA()   = READ - PARAMETERS FOR CALCULATING L-RES
C                          X-SEC.
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) XLCUTA()   = READ - PARAMETERS FOR CALCULATING L-RES
C                          X-SEC.
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) PL2A()     = READ - PARAMETERS FOR CALCULATING L-RES
C                          X-SEC.
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) PL3A()     = READ - PARAMETERS FOR CALCULATING L-RES
C                          X-SEC.
C                          DIMENSION: ENERGY INDEX
C I/O   : (R*8) SIGTA()    = READ - TOTAL CHARGE EXCHANGE

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C                                     CROSS-SECTION.
C                                     UNITS: CM2
C                                     DIMENSION: ENERGY INDEX
C I/O : (R*8)  SIGNA(,) = READ - N-RESOLVED CHARGE EXCHANGE
C                                     CROSS-SECTIONS.
C                                     UNITS: CM2
C                                     1ST DIMENSION: ENERGY INDEX
C                                     2ND DIMENSION: N-SHELL
C I/O : (R*8)  SIGLA(,) = READ - L-RESOLVED CHARGE EXCHANGE
C                                     CROSS-SECTIONS.
C                                     UNITS: CM2
C                                     1ST DIMENSION: ENERGY INDEX
C                                     2ND DIMENSION: INDEXED BY I4IDFL(N,L)
C I/O : (R*8)  SIGMA(,) = READ - M-RESOLVED CHARGE EXCHANGE
C                                     CROSS-SECTIONS.
C                                     UNITS: CM2
C                                     1ST DIMENSION: ENERGY INDEX
C                                     2ND DIMENSION: INDEXED BY I4IDFM(N,L,M)
C                                     WITH M >= 0 ONLY
C (I*4) I      = N QUANTUM NUMBER.
C (I*4) J      = L QUANTUM NUMBER.
C (I*4) K      = M QUANTUM NUMBER.
C (I*4) N      = N QUANTUM NUMBER.
C (I*4) L1     = L QUANTUM NUMBER + 1
C (I*4) M1     = M QUANTUM NUMBER + 1
C
C ROUTINES:
C ROUTINE      SOURCE      BRIEF DESCRIPTION
C -----
C I4IDFL       ADAS        RETURNS UNIQUE INDEX FROM QUANTUM
C                                     NUMBERS N AND L.
C I4IDFM       ADAS        RETURNS UNIQUE INDEX FROM QUANTUM
C                                     NUMBERS N, L AND M.
C
C AUTHOR:      H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL 0141-553-4196
C DATE:        21/09/95
C UPDATE:      27/08/97 HP SUMMERS - CHANGED NAME FROM CCFILL TO CDFILL
C
C VERSION:     1.1
C MODIFIED:    RICHARD MARTIN
C              - PUT UNDER SCCS CONTROL
C
C -----
C
C INTEGER      I4FCTN , I4UNIT , I4IDFL , I4IDFM
C -----
C INTEGER      IUNIT , MXNSHL , MXNENG ,
C &            IZR , IZD , INDD ,
C &            NENRGY , NMIN , NMAX
C INTEGER      I , J , K ,
C &            N , L1 , M1
C -----
C REAL*8       FACTN
C -----
C LOGICAL      LPARMS , LSETL , LSETM
C -----
C CHARACTER    TITLED*80 , SYMBR*2 , SYMBD*2
C CHARACTER    CLINE*133 , CIZR*2 , CIZD*2 , CINDD*1
C -----
C INTEGER      LFORMA(MXNENG)
C -----
C REAL*8       ENRGYA(MXNENG) , ALPHAA(MXNENG) , XLCUTA(MXNENG) ,
C &            PL2A(MXNENG) , PL3A(MXNENG) , SIGTA(MXNENG)
C REAL*8       SIGMA(MXNENG,MXNSHL) ,
C &            SIGLA(MXNENG,(MXNSHL*(MXNSHL+1))/2) ,
C &            SIGMA(MXNENG,(MXNSHL*(MXNSHL+1)*(MXNSHL+2))/6)
C -----

```

## CEPARM

```

SUBROUTINE CEPARM ( NDENR ,
&                 LPARMS ,
&                 NENIN , ENIN , NENOUT , ENOUT ,
&                 ALFIN , XLCIN , PL2IN , PL3IN , LFMIN ,
&                 ALFOUT , XLCOUT , PL2OUT , PL3OUT , LFMOUT
&                 )
IMPLICIT NONE
C -----
C ***** FORTRAN77 SUBROUTINE: CEPARM *****
C VERSION: 1.0
C PURPOSE: CONVERTS ALPHA, PL2, PL3 AND LFORM CHARGE EXCHANGE
C           PARAMETER VALUES AT INPUT ENERGIES TO VALUES AT OUTPUT
C           ENERGIES
C CALLING PROGRAM: ADAS314
C SUBROUTINE:
C INPUT : (I*4) NDENR = MAX. NUMBER OF ENERGIES
C           ALLOWED IN CROSS-SECTION FILE
C           OR TEMPERATURES IN THERMAL
C           AVERAGED RATE COEFFT. OUTPUT FILE.
C INPUT : (I*4) LPARMS = .TRUE. => INPUT DATA HAS L-FIT PARAMETERS
C           .FALSE. => INPUT DATA HAS L-FIT PARAMETERS
C INPUT : (I*4) NENIN = NUMBER OF ENERGIES IN INPUT DATA SET
C INPUT : (R*8) ENIN( ) = ENERGIES (EV/AMU) IN INPUT DATA SET

```

```

C INPUT : (I*4) NENOUT = NUMBER OF ENERGIES FOR OUTPUT DATA SET
C INPUT : (R*8) ENOUT() = TEMPERATURES (EV/AMU) FOR OUTPUT DATA SET
C INPUT : (R*8) ALFIN() = ALPHA PARAMETER IN INPUT DATA SET
C                   1ST.DIM: ENERGY INDEX
C INPUT : (R*8) XLCIN() = NON-INTEGGER L-CUT-OFF PARAMETER
C                   1ST.DIM: ENERGY INDEX
C INPUT : (R*8) PL2IN(,) = P2 L-FIT PARAMETER IN INPUT DATA SET
C                   1ST.DIM: ENERGY INDEX
C INPUT : (R*8) PL3IN(,) = P3 L-FIT PARAMETER IN INPUT DATA SET
C                   1ST.DIM: ENERGY INDEX
C INPUT : (I*4) LFMIN(,) = L-FIT FORM TYPE INDEX IN INPUT DATA SET
C                   1ST.DIM: ENERGY INDEX
C OUTPUT: (R*8) ALFOUT() = ALPHA PARAMETER IN INPUT DATA SET
C                   1ST.DIM: ENERGY INDEX
C OUTPUT: (R*8) XLCOUT() = NON-INTEGGER L-CUT-OFF PARAMETER
C                   1ST.DIM: ENERGY INDEX
C OUTPUT: (R*8) PL2OUT() = P2 L-FIT PARAMETER IN INPUT DATA SET
C                   1ST.DIM: ENERGY INDEX
C OUTPUT: (R*8) PL3OUT() = P3 L-FIT PARAMETER IN INPUT DATA SET
C                   1ST.DIM: ENERGY INDEX
C OUTPUT: (I*4) LFMOUT() = L-FIT FORM TYPE INDEX IN INPUT DATA SET
C                   1ST.DIM: ENERGY INDEX
C (L*4) LSETX = .TRUE. => SPLINE PRESET FOR THESE KNOTS
C             .FLSE. => SPLINE NOT SET FOR THESE KNOTS
C (L*4) LPASS = .TRUE. => DO NOT CONVERT INTO LOG10 FOR
C             ENERGIES AND X-SECTS. FOR SPLINE
C             .FLSE. => CONVERT INTO LOG10 FOR
C             ENERGIES AND X-SECTS. FOR SPLINE
C (I*4) IOPT = SPLINE END POINT CURVATURE/GRADIENT OPTION
C           1 => DDY1 = 0, DDYN = 0
C           4 => DY1 = 0, DDYN = 0
C (R*8) CMSAMU = PARAMETER = CONVERSION FACTOR FOR ENERGY
C             (AMU) TO VELOCITY (CM S-1)
C (I*4) I = GENERAL INDEX
C (I*4) IT = GENERAL INDEX
C (R*8) XIN() = INTERNAL SPLINE INDEPENDENT VARIABLE
C (R*8) YIN() = INTERNAL SPLINE DEPENDENT VARIABLE
C (R*8) VIN() = INTERNAL VECTOR
C (R*8) DY() = DERIVATIVES AT SPLINE KNOTS
C (R*8) XOUT() = INTERNAL OUTPUT INDEPENDENT VARIABLE
C (R*8) YOUT() = INTERNAL OUTPUT DEPENDENT VARIABLE
C (L*4) LINTRP() = .TRUE. => POINT INTERPOLATED
C              = .FALSE. => POINT EXTRAPOLATED
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C XXSPLE ADAS INTERPOLATES USING CUBIC SPLINES
C R8FUN1 ADAS EXTERNAL FUNCTION FOR XXSPLE
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C         JA8.08
C         TEL. 0141-553-4196
C DATE: 13/11/95
C UPDATE: 27/08/97 HP SUMMERS - CHANGED NAME FROM CCPARM TO CDPARM
C
C VERSION: 1.1 DATE: 01-12-98
C MODIFIED: RICHARD MARTIN
C           - PUT UNDER SCCS CONTROL
C
C -----
C INTEGER MAXENS
C -----
C REAL*8 CMSAMU , ZERO
C -----
C PARAMETER ( MAXENS = 50 )
C PARAMETER ( CMSAMU = 1.389209D+06 , ZERO = 1.0D-30 )
C -----
C INTEGER NDENR
C INTEGER NENIN , NENOUT
C INTEGER IT , I , IOPT
C -----
C REAL*8 R8FUN1
C -----
C LOGICAL LPARMS , LSETX , LPASS
C -----
C INTEGER LFMIN(NDENR)
C INTEGER LFMOUT(NDENR)
C -----
C REAL*8 ENIN(NDENR) , XLCIN(NDENR)
C REAL*8 ENOUT(NDENR) , XLCOUT(NDENR)
C REAL*8 ALFIN(NDENR) , PL2IN(NDENR) , PL3IN(NDENR)
C REAL*8 ALFOUT(NDENR) , PL2OUT(NDENR) , PL3OUT(NDENR)
C REAL*8 XOUT(MAXENS) , YOUT(MAXENS)
C REAL*8 DY(MAXENS)
C REAL*8 XIN(MAXENS) , YIN(MAXENS)
C -----
C LOGICAL LINTRP(MAXENS)
C -----
C EXTERNAL R8FUN1
C -----

```

```

SUBROUTINE CETHER ( NDENR , NDSHL ,
& AMDON , AMREC , CATYP , DREN , ILTYP ,
& LSETL , LSETM , NMIN , NMAX ,
& NENIN , ENIN , NENOUT , ENOUT ,
& SGTIN , SGNIN , SGLIN , SGMIN ,
& RCTOUT , RCNOUT , RCLOUT , RCMOUT
& )
IMPLICIT NONE
-----
C *****
C ***** FORTRAN77 SUBROUTINE: CETHER *****
C VERSION: 1.0
C PURPOSE: OBTAINS RATE COEFFICIENTS FOR DONOR/RECEIVER CHARGE
C EXCHANGE COLLISIONS FOR CASES OF
C MONOENERGETIC DONOR/THERMAL RECEIVER, THERMAL
C DONOR/MONOENERGETIC RECEIVER, THERMAL DONOR/THERMAL
C RECEIVER (SAME TEMPERATURE) FROM CROSS-SECTION TABULATIONS
C CALLING PROGRAM: ADAS314
C SUBROUTINE:
C INPUT : (I*4) NDENR = MAX. NUMBER OF ENERGIES
C ALLOWED IN CROSS-SECTION FILE
C OR TEMPERATURES IN THERMAL
C AVERAGED RATE COEFFT. OUTPUT FILE.
C INPUT : (I*4) NDSHL = PARAMETER = MAX. NUMBER OF N-SHELLS
C ALLOWED IN CROSS-SECTION FILE
C INPUT : (R*8) AMDON = DONOR MASS NUMBER
C INPUT : (R*8) AMREC = RECEIVER MASS NUMBER
C INPUT : (C2) CATYP = 'TT' THERMAL/THERMAL (EQUAL TEMP. CASE)
C 'TR' THERMAL RECEIVER, MONOENERGETIC DONOR
C 'TD' THERMAL DONOR, MONOENERGETIC RECEIVER
C INPUT : (R*8) DREN = DONOR ENERGY ( 'TR' CASE )
C RECEIVER ENERGY ( 'TD' CASE )
C INPUT : (I*4) ILTYP = TYPE FOR LOW ENERGY CROSS-SECTION EXTRAPOL
C INPUT : (L*4) LSETL = .TRUE. => L-RESOLVED DATA READ
C .FALSE. => NO L-RESOLVED DATA READ
C INPUT : (L*4) LSETM = .TRUE. => M-RESOLVED DATA READ
C .FALSE. => NO M-RESOLVED DATA READ
C INPUT : (I*4) NMIN = LOWEST N-SHELL IN DATA SET
C INPUT : (I*4) NMAX = HIGHEST N-SHELL IN DATA SET
C INPUT : (I*4) NENIN = NUMBER OF ENERGIES IN INPUT DATA SET
C INPUT : (R*8) ENIN() = ENERGIES (EV/AMU) IN INPUT DATA SET
C INPUT : (I*4) NENOUT = NUMBER OF ENERGIES FOR OUTPUT DATA SET
C INPUT : (R*8) ENOUT() = TEMPERATURES (EV/AMU) FOR OUTPUT DATA SET
C INPUT : (R*8) SGTIN() = TOTAL X-SECTIONS (CM2) IN INPUT DATA SET
C 1ST.DIM: ENERGY INDEX
C INPUT : (R*8) SGNIN(,) = N-SHELL X-SECTIONS (CM2) IN INPUT DATA SET
C 1ST.DIM: ENERGY INDEX
C 2ND.DIM: PRINCIPAL QUANTUM NUMBER
C INPUT : (R*8) SGLIN(,) = L-SHELL X-SECTIONS (CM2) IN INPUT DATA SET
C 1ST.DIM: ENERGY INDEX
C 2ND.DIM: NL REFERENCE INDEX
C INPUT : (R*8) SGMIN(,) = M-SHELL X-SECTIONS (CM2) IN INPUT DATA SET
C 1ST.DIM: ENERGY INDEX
C 2ND.DIM: NLM REFERENCE INDEX
C OUTPUT: (R*8) RCTOUT() = TOTAL RATE COEFFT. (CM3 S-1) FOR OUTPUT
C 1ST.DIM: TEMPERATURE INDEX
C OUTPUT: (R*8) RCNOUT(,) = N-SHELL RATE COEFFT. (CM3 S-1) FOR OUTPUT
C 1ST.DIM: TEMPERATURE INDEX
C 2ND.DIM: PRINCIPAL QUANTUM NUMBER
C OUTPUT: (R*8) RCLOUT(,) = L-SHELL RATE COEFFT. (CM3 S-1) FOR OUTPUT
C 1ST.DIM: TEMPERATURE INDEX
C 2ND.DIM: NL REFERENCE INDEX
C OUTPUT: (R*8) RCMOUT(,) = M-SHELL RATE COEFFT. (CM3 S-1) FOR OUTPUT
C 1ST.DIM: TEMPERATURE INDEX
C 2ND.DIM: NLM REFERENCE INDEX
C LSETX = .TRUE. => SPLINE PRESET FOR THESE KNOTS
C .FLSE. => SPLINE NOT SET FOR THESE KNOTS
C LPASS = .TRUE. => DO NOT CONVERT INTO LOG10 FOR
C ENERGIES AND X-SECTS. FOR SPLINE
C .FLSE. => CONVERT INTO LOG10 FOR
C ENERGIES AND X-SECTS. FOR SPLINE
C (I*4) PIPEOU = STANDARD OUTPUT
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C CDEVTH ADAS EVALUATES THERMAL AVERAGE RATE COEFFTS.
C I4FCTN ADAS RETURNS CHARACTER STRING AS AN INTEGER.
C I4UNIT ADAS FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C I4IDFL ADAS RETURNS UNIQUE INDEX FROM QUANTUM
C NUMBERS N AND L.
C I4IDFM ADAS RETURNS UNIQUE INDEX FROM QUANTUM
C NUMBERS N, L AND M.
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL. 0141-553-4196
C DATE: 10/10/95
C UPDATE: 27/08/97 HP SUMMERS - CHANGED NAME FROM CCTHER TO CDOTHER
C
C VERSION: 1.1 DATE: 01-12-98
C MODIFIED: RICHARD MARTIN
C - PUT UNDER SCCS CONTROL
C
-----
C INTEGER PIPEOU , ONE
C
-----
C PARAMETER ( PIPEOU = 6 , ONE = 1)
C
-----
C INTEGER NDENR , NDSHL ,

```

&	INTEGER	ILTYP	, NMIN	, NMAX
&	INTEGER	NENIN	, NENOUT	
&	INTEGER	I4FCTN	, I4UNIT	, I4IDFL
&	INTEGER	I4IDFM		
C	-----	INTEGER	N	, L
				, M
				, IREF
C	-----	REAL*8	AMDON	, AMREC
				, DREN
C	-----	REAL*8	ENIN(NDENR)	, SGTIN(NDENR)
&			ENOUT(NDENR)	, RCTOUT(NDENR)
&	REAL*8	SGNIN(NDENR,NDSHL)		
&		SGLIN(NDENR,(NDSHL*(NDSHL+1))/2)		
&		SGMIN(NDENR,(NDSHL*(NDSHL+1)*(NDSHL+2))/6)		
REAL*8		RCNOUT(NDENR,NDSHL)		
&		RCLOUT(NDENR,(NDSHL*(NDSHL+1))/2)		
&		RCMOUT(NDENR,(NDSHL*(NDSHL+1)*(NDSHL+2))/6)		
C	-----	CHARACTER	CATYP*2	
C	-----	LOGICAL	LSETL	, LSETM
				, LSETX
				, LPASS
C	-----			

## CEWR11

```

SUBROUTINE CEWR11( DSFULL , DATE ,
& IUNIT , MXNENG , MXNSHL , TITLED ,
& CATYP , AMDON , AMREC , DREN ,
& SYMBR , SYMBD , IZR , IZD ,
& INDD , NENRGY , NMIN , NMAX ,
& LPARMS , LSETL , LSETM , ENRGYA ,
& ALPHAA , LFORMA , XLCUTA , PL2A ,
& PL3A , SIGTA , SIGNA , SIGLA ,
& SIGMA
& )
IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: CEWR11 *****
C PURPOSE: TO OUTPUT DATA TO MODIFIED ADF01 FILE. IF THE ADF01 FILE
C IS FOR THERMAL/THERMAL THERMAL/DONOR OR THERMAL/RECEIVER
C THEN THE RATE (PASSED AS SIGMA) IS DIVIDED BY
C 1.384D4 * 100 * DSQRT(TE)
C IN ORDER TO ALLOW THE FILE TO BE USED WITH UNMODIFIED
C SERIES 3 PROGRAMS.
C CALLING PROGRAM: ADAS314
C DATA:
C THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
C COLLISION ENERGIES : KEV/AMU
C ALPHA :
C TOTAL XSECTS. : CM2
C N-SHELL XSECTS. : CM2
C NL-SHELL DATA : CM2
C NLM-SHELL DATA : CM2
C SUBROUTINE:
C INPUT : (I*4) IUNIT = INPUT UNIT NUMBER FOR RESULTS
C INPUT : (I*4) MXNENG = MAXIMUM NO. OF ENERGIES.
C INPUT : (I*4) MXNSHL = MAXIMUM NO. OF N SHELLS.
C INPUT : (C*80) TITLED = NOT SET - TITLE FOR DATA SOURCE.
C INPUT : (C*80) DSFULL = SOURCE DATASET
C INPUT : (C2) CATYP = 'TT' THERMAL/THERMAL (EQUAL TEMPERATURES
C FOR DONOR AND RECEIVER ONLY)
C 'TR' THERMAL RECEIVER, MONOENERGETIC DONOR
C 'TD' THERMAL DONOR, MONOENERGETIC RECEIVER
C 'ME' SPECIAL MONOENERGETIC CASE
C INPUT : (R*8) AMDON = DONOR MASS NUMBER
C INPUT : (R*8) AMREC = RECEIVER MASS NUMBER
C INPUT : (R*8) DREN = DONOR ENERGY ( 'TR' CASE )
C RECEIVER ENERGY ( 'TD' CASE )
C INPUT : (C*2) SYMBR = READ - RECEIVER ION ELEMENT SYMBOL.
C INPUT : (C*2) SYMBD = READ - DONOR ION ELMENT SYMBOL.
C INPUT : (I*4) IZR = READ - ION CHARGE OF RECEIVER.
C INPUT : (I*4) IZD = READ - ION CHARGE OF DONOR.
C INPUT : (I*4) INDD = READ - DONOR STATE INDEX.
C INPUT : (I*4) NENRGY = NUMBER OF ENERGIES READ.
C INPUT : (I*4) NMIN = LOWEST N-SHELL FOR WHICH DATA READ.
C INPUT : (I*4) NMAX = HIGHEST N-SHELL FOR WHICH DATA READ.
C INPUT : (L*4) LPARMS = FLAGS IF L-SPLITTING PARAMETERS PRESENT.
C .TRUE. => L-SPLITTING PARAMETERS PRESENT.
C .FALSE => L-SPLITTING PARAMETERS ABSENT.
C INPUT : (L*4) LSETL = FLAGS IF L-RESOLVED DATA PRESENT.
C .TRUE. => L-RESOLVED DATA PRESENT.
C .FALSE => L-RESOLVED DATA ABSENT.
C INPUT : (L*4) LSETM = FLAGS IF M-RESOLVED DATA PRESENT.
C .TRUE. => M-RESOLVED DATA PRESENT.
C .FALSE => M-RESOLVED DATA ABSENT.
C INPUT : (R*8) ENRGYA() = READ - COLLISION ENERGIES.
C UNITS: EV/AMU (READ AS KEV/AMU)
C DIMENSION: ENERGY INDEX
C INPUT : (R*8) ALPHAA() = READ - EXTRAPOLATION PARAMETER ALPHA.
C DIMENSION: ENERGY INDEX
C INPUT : (I*4) LFORMA() = READ - PARAMETERS FOR CALCULATING L-RES
C X-SEC.
C DIMENSION: ENERGY INDEX
C INPUT : (R*8) XLCUTA() = READ - PARAMETERS FOR CALCULATING L-RES

```





&	SIGMA(MXNENG, (MXNSHL*(MXNSHL+1)*(MXNSHL+2))/6)
C-----	
DATA	BLANKS /' '/
C-----	

# CEWR12

```

SUBROUTINE CEWR12( IUNIT , MXNENG , MXNSHL , ILTYP ,
&                TITLED , DSFULL , DATE ,
&                CATYP ,
&                SYMBR , SYMBD , IZR , IZD ,
&                INDD , NENRGY , NMIN , NMAX ,
&                LPARMS , LSETL , LSETM , ENRGYA ,
&                ALPHAA , LFORMA , XLCUTA , PL2A ,
&                PL3A , SIGTA , SIGNA , SIGLA ,
&                SIGMA
&                )
      IMPLICIT NONE
C-----
C ***** FORTRAN77 SUBROUTINE: CEWR12 *****
C PURPOSE: TO OUTPUT DATA TO ADF24 FILE.
C CALLING PROGRAM: ADAS314
C DATA:
C       THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
C       COLLISION ENERGIES : KEV/AMU
C       ALPHA              :
C       TOTAL XSECTS.      : CM2
C       N-SHELL XSECTS.    : CM2
C       NL-SHELL DATA     : CM2
C       NLM-SHELL DATA    : CM2
C SUBROUTINE:
C INPUT : (I*4) IUNIT      = INPUT UNIT NUMBER FOR RESULTS
C INPUT : (I*4) MXNENG     = MAXIMUM NO. OF ENERGIES.
C INPUT : (I*4) MXNSHL     = MAXIMUM NO. OF N SHELLS.
C INPUT : (I*4) ILTYPL     = TYPE FOR LOW ENERGY X-SECT. EXTRAPOLATION
C INPUT : (C*80) TITLED    = NOT SET - TITLE FOR DATA SOURCE.
C INPUT : (C*44) DSFULL    = SOURCE DATASET
C INPUT : (C2) CATYP       = 'TT' THERMAL/THERMAL (EQUAL TEMPERATURES
C                          FOR DONOR AND RECEIVER ONLY)
C                          'TR' THERMAL RECEIVER, MONOENERGETIC DONOR
C                          'TD' THERMAL DONOR, MONOENERGETIC RECEIVER
C                          'ME' SPECIAL MONOENERGETIC CASE
C INPUT : (C*2) SYMBR      = READ - RECEIVER ION ELEMENT SYMBOL.
C INPUT : (C*2) SYMBD      = READ - DONOR ION ELEMENT SYMBOL.
C INPUT : (I*4) IZR        = READ - ION CHARGE OF RECEIVER.
C INPUT : (I*4) IZD        = READ - ION CHARGE OF DONOR.
C INPUT : (I*4) INDD       = READ - DONOR STATE INDEX.
C INPUT : (I*4) NENRGY     = NUMBER OF ENERGIES READ.
C INPUT : (I*4) NMIN       = LOWEST N-SHELL FOR WHICH DATA READ.
C INPUT : (I*4) NMAX       = HIGHEST N-SHELL FOR WHICH DATA READ.
C INPUT : (L*4) LPARMS     = FLAGS IF L-SPLITTING PARAMETERS PRESENT.
C                          .TRUE. => L-SPLITTING PARAMETERS PRESENT.
C                          .FALSE => L-SPLITTING PARAMETERS ABSENT.
C INPUT : (L*4) LSETL      = FLAGS IF L-RESOLVED DATA PRESENT.
C                          .TRUE.  => L-RESOLVED DATA PRESENT.
C                          .FALSE => L-RESOLVED DATA ABSENT.
C INPUT : (L*4) LSETM      = FLAGS IF M-RESOLVED DATA PRESENT.
C                          .TRUE.  => M-RESOLVED DATA PRESENT.
C                          .FALSE => M-RESOLVED DATA ABSENT.
C INPUT : (R*8) ENRGYA( )  = READ - COLLISION ENERGIES.
C                          UNITS: EV/AMU (READ AS KEV/AMU)
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) ALPHAA( )  = READ - EXTRAPOLATION PARAMETER ALPHA.
C                          DIMENSION: ENERGY INDEX
C INPUT : (I*4) LFORMA( )  = READ - PARAMETERS FOR CALCULATING L-RES
C                          X-SEC.
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) XLCUTA( )  = READ - PARAMETERS FOR CALCULATING L-RES
C                          X-SEC.
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) PL2A( )    = READ - PARAMETERS FOR CALCULATING L-RES
C                          X-SEC.
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) PL3A( )    = READ - PARAMETERS FOR CALCULATING L-RES
C                          X-SEC.
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) SIGTA( )   = READ - TOTAL CHARGE EXCHANGE
C                          CROSS-SECTION.
C                          UNITS: CM2
C                          DIMENSION: ENERGY INDEX
C INPUT : (R*8) SIGNA( , ) = READ - N-RESOLVED CHARGE EXCHANGE
C                          CROSS-SECTIONS.
C                          UNITS: CM2
C                          1ST DIMENSION: ENERGY INDEX
C                          2ND DIMENSION: N-SHELL
C INPUT : (R*8) SIGLA( , ) = READ - L-RESOLVED CHARGE EXCHANGE
C                          CROSS-SECTIONS.
C                          UNITS: CM2
C                          1ST DIMENSION: ENERGY INDEX
C                          2ND DIMENSION: INDEXED BY I4IDFL(N,L)
C INPUT : (R*8) SIGMA( , ) = READ - M-RESOLVED CHARGE EXCHANGE
C                          CROSS-SECTIONS.
C                          UNITS: CM2

```

```

C          1ST DIMENSION: ENERGY INDEX
C          2ND DIMENSION: INDEXED BY I4IDFM(N,L,M)
C                      WITH M >= 0 ONLY
C          (I*4) NWIDTH = NUMBER OF ENERGY VALUES PER LINE
C          (I*4) IBLK   = CURRENT DATA BLOCK.
C          (I*4) IVALUE = USED TO PARSE FOR END OF DATA FLAG (-1).
C          (I*4) N     = N QUANTUM NUMBER.
C          (I*4) L     = L QUANTUM NUMBER.
C          (I*4) M     = M QUANTUM NUMBER.
C          (I*4) I     = LOOP COUNTER.
C          (I*4) K     = LOOP COUNTER.
C          (I*4) IERR  = ERROR RETURN CODE.
C          (R*8) ALPH0 = LOW ENERGY PARAMETER FOR ILTYP = 1
C          (C*1) INDD  = DONOR STATE INDEX.
C          (C*9) FST   = FINAL STATE NAME.
C          (C*9) BLK9  = BLANK STRING OF LENGTH 9.
C          (C*1) LCHRA() = CHARACTER FOR L ANG.MOM.INDEXED BY L+1
C ROUTINES:
C          ROUTINE      SOURCE      BRIEF DESCRIPTION
C          -----
C          I4FCTN      ADAS        RETURNS CHARACTER STRING AS AN INTEGER.
C          I4UNIT      ADAS        FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C          I4IDFL      ADAS        RETURNS UNIQUE INDEX FROM QUANTUM
C          I4IDFM      ADAS        RETURNS UNIQUE INDEX FROM QUANTUM
C          I4IDFM      ADAS        NUMBERS N AND L.
C          I4IDFM      ADAS        RETURNS UNIQUE INDEX FROM QUANTUM
C          I4IDFM      ADAS        NUMBERS N, L AND M.
C          XXIDTL      ADAS        INVERSE OF I4IDFL. RETURNS QUANTUM
C          XXIDTL      ADAS        NUMBERS N AND L FROM INDEX.
C          XXIDTM      ADAS        INVERSE OF I4IDFM. RETURNS QUANTUM
C          XXIDTM      ADAS        NUMBERS N, L AND M FROM INDEX.
C          XXNAME      ADAS        FINDS REAL NAME OF USER
C          XXSLEN      ADAS        FINDS NON BLANK PART OF STRING
C AUTHOR:  H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C          JA8.08
C          TEL. 0141-553-4196
C DATE:    13/11/95
C UPDATE:  27/08/97 HP SUMMERS - CHANGED NAME FROM CCWR12 TO CDWR12
C UPDATE:  09/07/98 Martin O'Mullane - added DATE to input list and
C                      removed call to xxuid
C
C VERSION:      1.1                      DATE: 01-12-98
C MODIFIED: RICHARD MARTIN
C          - PUT UNDER SCCS CONTROL
C
C-----
C          INTEGER      NDSEL
C
C          PARAMETER ( NDSEL = 300 )
C-----
C          INTEGER      I4FCTN , I4UNIT , I4IDFL , I4IDFM
C-----
C          INTEGER      IUNIT , MXNSHL , MXNENG , ILTYP ,
C          &            IZR , IZD , INDD ,
C          &            NENRGY , NMIN , NMAX
C          INTEGER      NEMORE , NWIDTH , IBLK , IVALUE ,
C          &            N , L , M , I , K ,
C          &            ISEL , IERR
C          INTEGER      L1 , L2
C-----
C          REAL*8      ALPH0
C-----
C          LOGICAL      LPARMS , LSETL , LSETM
C-----
C          CHARACTER   TITLED*80 , SYMBR*2 , SYMBD*2 , CATYP*2
C          CHARACTER   CLINE*80 , CIZR*2 , CIZD*2 , CINDD*1
C          CHARACTER   BLANKS*80 , DSFULL*80 , UID*28 , DATE*8
C          CHARACTER   FST*9 , BLK9*9 , REALNAME*30
C-----
C          INTEGER      LFORMA(MXNENG)
C-----
C          REAL*8      ENRGYA(NENRGY) , ALPHAA(MXNENG) , XLCUTA(MXNENG) ,
C          &            PL2A(MXNENG) , PL3A(MXNENG) , SIGTA(MXNENG)
C          REAL*8      SIGNA(MXNENG,MXNSHL)
C          &            SIGLA(MXNENG,(MXNSHL*(MXNSHL+1))/2)
C          &            SIGMA(MXNENG,(MXNSHL*(MXNSHL+1)*(MXNSHL+2))/6)
C-----
C          CHARACTER   CINFO(NDSEL)*80 , LCHR(16)*1
C-----
C          DATA      BLANKS /' '/
C          DATA      BLK9 /' '/
C          DATA      LCHR /'s' , 'p' , 'd' , 'f' , 'g' , 'h' , 'i' , 'k' ,
C          &            'l' , 'm' , 'n' , 'o' , 'q' , 'r' , 't' , 'u' /
C-----

```

## CLDLBN2

```

C          SUBROUTINE CLDLBN2(EXMEMB,Z0,Z1,ZEFF,DENS,TE,DENSP,TP,BMENER,
C          &            DENSH,W1,NMIN,NMAX,NREP,IMAX,ARED,
C          &            RHS,SIONPT,DRECPT,RRECPT,XRECPT,IECION,
C          &            IEDREC,IERREC,IEXREC,DVEC,ACNST,A1CNST)
C
C          IMPLICIT REAL*8(A-H,O-Z)

```

```

C-----
C
C ***** FORTRAN77 SUBROUTINE: CLDLBN2 *****
C-----
C SUBROUTINE TO ESTABLISH THE PROJECTED INFLUENCE OF HIGH N-SHELLS IN
C THE BUNDLE-N COLLISIONAL DIELECTRONIC MODEL ON A SET OF LS OR LSJ
C RESOLVED LOW LEVEL POPULATION EQUATIONS
C
C BOTH THE RECOMBINATION AND IONISATION PATHWAYS THROUGH THE HIGH
C LEVELS ARE TAKEN INTO ACCOUNT AS WELL AS THE INDIRECT COUPLINGS OF
C LOW RESOLVED LEVELS VIA THE HIGH BUNDLE-N LEVELS.
C
C THE SUBROUTINE IS USED AS AN ARBITRARY CALL FROM WITHIN THE
C CONVENTIONAL BNDLEN ROUTINE FOLLOWING ESTABLISHMENT OF THE
C CONDENSED COLLISIONAL-DIELECTRONIC MATRIX AND RIGHT-HAND SIDE
C
C THE EXPANSION OF THE PROJECTED MATRICES OVER THE RESOLVED LOWER
C LEVELS IS DEFINED THROUGH RESOLVED - BUNDLEN INDEXING AND
C WEIGHTING FRACTION TABLES STORED IN DATA STATEMENTS.
C THESE ARE HELD FOR COMBINATIONS BASED ON THE A-D-A-S DATA BASE
C MEMBERS.
C
C THE ROUTINE PROVIDES TABULAR OUTPUT AND FOR THE MOMENT PREPARES A
C PASSING FILE FOR FURTHER PROCESSING IN THE A-D-A-S STRUCTURE
C
C PROCESSING CONTINUES WITH EXECUTION OF THE LOW LEVEL POPULATION
C CALCULATION PROVIDED THE LOW LEVEL DATA FILE 'REFMEM' IS NON-BLANK
C OTHERWISE ONLY THE PASSING FILE IS PRODUCED
C
C INPUT
C   EXMEMB   = DATA SET NAME OF EXPANSION FILE
C   Z0       = NUCLEAR CHARGE
C   Z1       = RECOMBINING ION CHARGE
C   ZEFF     = PLASMA Z EFFECTIVE
C   DENS     = ELECTRON DENSITY (CM-3)
C   TE      = ELECTRON TEMPERATURE (K)
C   DENSP    = PROTON DENSITY (CM-3)
C   TP      = PROTON TEMPERATURE (K)
C   BMENER   = NEUTRAL HYDROGEN BEAM ENERGY (EV/AMU)
C   DENSH    = NEUTRAL BEAM HYDROGEN DENSITY (CM-3)
C   W1       = GROUND STATE RADIATION DILUTION FACTOR
C   NMIN     = LOWEST N-SHELL
C   NMAX     = HIGHEST N-SHELL
C   NREP(I)  = SET OF REPRESENTATIVE LEVELS
C   IMAX     = NUMBER OF REPRESENTATIVE LEVELS
C   ARED(I,J)= CONDENSED COLLISIONAL-DIELECTRONIC MATRIX (CN SOLUTION)
C   RHS(I)   = CONDENSED RIGHT-HAND-SIDE (CN SOLUTION)
C   CIONPT(I)= COLLISIONAL IONISATION CONTRIBUTION TO ARED(I,I)
C   DRECPT(I)= DIELECTRONIC RECOMBINATION CONTRIBUTION TO RHS(I)
C   RRECPT(I)= RADIATIVE RECOMBINATION CONTRIBUTION TO RHS(I)
C   XRECPT(I)= CHARGE EXCHANGE RECOMB. CONTRIBUTION TO RHS(I)
C   IECION   = 0 ELIMINATE CIONPT FOR LOW LEVELS IN PROJECTION
C             1 DO NOT ELIMINATE CIONPT.
C   IEDREC   = 0 ELIMINATE DRECPT FOR LOW LEVEL PROJECTION
C             1 DO NOT ELIMINATE DRECPT.
C   IERREC   = 0 ELIMINATE RRECPT FOR LOW LEVEL PROJECTION
C             1 DO NOT ELIMINATE RRECPT.
C   IEXREC   = 0 ELIMINATE XRECPT FOR LOW LEVEL PROJECTION
C             1 DO NOT ELIMINATE XRECPT.
C   DVEC(I)  = CONVERSION FACTOR FOR BN --> POPULATION
C   ACNST    = 1.03928D-13*Z*ATE*DSQRT(ATE)
C   ALCNST   = 6.60074D-24*DENS*(157890.0/TE)**1.5
C
C OUTPUT
C
C ***** H.P. SUMMERS, JET                8 FEB 1990 *****
C *****                                24 APR 1990 *****
C *****                                18 JUL 1991 *****
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 EXPANSION FILE DATA SET NAME IS NOW PASSED
C INTO THE ROUTINE RATHER THAN JUST THE MEMBER NAME.
C
C 2) THE OUTPUT FILE (UNIT 18) IS NOW OPENED EXTERNAL TO THIS
C ROUTINE.
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
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

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C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - CHANGED ACTION=READ TO STATUS=UNKNOWN IN OPEN
C STATEMENT
C
C
C VERSION: 1.3 DATE: 24-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - COMMENTED OUT CALL TO USINFO AS NO LONGER NEEDED
C
C VERSION: 1.4 DATE: 08-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - REMOVED SUPERFLUOUS VARIABLES
C
C
C-----
C
C PARAMETER (NDIM=30,NLDIM=30,NDMAX=550,NDMET=5)
C CHARACTER SEQ*2,SYMBA*2,REFMEM*8
C CHARACTER EXMEMB*80
C CHARACTER STRING*80,STRNG1*80,PTSYMA*11,SUBSTRG*11,LVSYMA*26
C CHARACTER LSTRING*133,STRNG2*60
C
C
C DIMENSION NREP(NDIM+1),ARED(NDIM,NDIM),RHS(NDIM),DVEC(NDIM)
CX DIMENSION ARE2(NDIM,NDIM),RHS2(NDIM)
C DIMENSION CIONPT(NDIM),DRECPT(NDIM),RRECPT(NDIM),XRECPT(NDIM)
C DIMENSION AREDL(NDIM,NDIM),AREDH(NDIM,NDIM),RHSL(NDIM),RHS(NDIM)
C DIMENSION BREDL(NDIM,NDIM),VEC(NDIM)
C DIMENSION IPOINTA(NDMAX)
C DIMENSION PCRMAT(NDIM,NDIM),PCRRHS(NDIM),LVSYMA(NDIM)
C DIMENSION PEXMAT(NLDIM,NLDIM),PEXRHS(NLDIM)
C DIMENSION AMAT(NDIM,NDIM),RS(NDIM),CHMAT(NDIM,5),RH(NDIM)
C DIMENSION PCION(NDIM),PDREC(NDIM),PRREC(NDIM),PXREC(NDIM)
C DIMENSION PECION(NLDIM),PEDREC(NLDIM),PERREC(NLDIM),PEXREC(NLDIM)
C DIMENSION LSPA(NLDIM),LSHA(NLDIM),LPTA(NLDIM),WGHTA(NLDIM,5)
C DIMENSION SYMBA(30),PTSYMA(5),NSHELA(5),NSPNA(5,5),NLWSTA(5,5)
C DIMENSION PLWSTA(5,5),NPTSPA(5),NSPSYS(5),NCUTP(5),DEPA(5)
C DIMENSION IMETR(NDMET+1)
C NAMELIST /SEQINF/SEQ,REFMEM,NPARNT,NSHEL,NLEV
C DATA LSTRING/'
C
C &
C & ' /
C DATA IPASS/0/
C DATA SYMBA/'H ','HE','LE','BE','B ','C ','N ','O ','F ','NE',
C & 'NA','MG','AL','SI','P ','S ','CL','AR','K ','CA',
C & 'SC','TI','V ','CR','MN','FE','CO','NI','CU','ZN'/
C-----

```

## CMPRSS

```

SUBROUTINE CMPRSS(IUIN,IUOUT,DATE,IECOUNT,INCOUNT,ITCOUNT)
C
C-----
C ***** FORTRAN77 SUBROUTINE: CMPRSS *****
C
C PURPOSE:
C READ OUTPUT FROM V2BNLDN1 AND PRODUCE TABLES OF BEAM STOPPING RATES
C AS A FUNCTION OF PLASMA DENSITY AND TEMPERATURE AND OF BEAM ENERGY
C (FOR USE IN KS4FIT BY QHIOCH)
C
C-----
C
C UPDATE: 20/01/94 - JONATHAN NASH - TESSELLA SUPPORT SERVICES PLC
C
C THIS SUBROUTINE WAS ADAPTED FROM THE PROGRAM
C 'JETXJS.BMSTOP.FORT(COMPRESS)'.
C
C THE FOLLOWING MODIFICATIONS HAVE BEEN MADE:
C
C 1) THE MAXIMUM NUMBER OF BEAM ENERGIES HAS BEEN INCREASED
C FROM 13 TO 20.
C
C 2) THE UNIT NUMBERS OF THE INPUT AND OUTPUT FILES ARE PASSED
C INTO THE ROUTINE AS ARGUMENTS.
C
C 3) THE REFERENCE ELECTRON DENSITY AND TEMPERATURE AND BEAM
C ENERGY ARE DETERMINED RATHER THAN BEING DECLARED AS
C PARAMETERS. THESE ASSIGNMENTS ARE BASED ON KNOWING THE
C ORDER OF THE DATA IN THE INPUT FILE.
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: 01-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - PUT UNDER SCCS CONTROL
C
C VERSION: 1.2 DATE: 01-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)

```

```

C          - ALLOWED FOR CASE WHERE ZEFF=0.0
C
C VERSION: 1.3                      DATE: 05-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - ADDED NUMBER OF ENERGIES, TEMPS. AND DENSITIES
C          AS OUTPUT.
C
C VERSION: 1.4                      DATE: 05-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - CORRECTED SCCS KEYWORDS.
C
C VERSION: 1.5                      DATE: 08-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - REMOVED SUPERFLUOUS VARIABLES
C
C VERSION: 1.6                      DATE: 14-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - CHANGED FORMAT 1004 TO READ 97X RATHER THAN
C          98X AS THIS WAS NOT BEING READ CORRECTLY
C
C VERSION: 1.7                      DATE: 23-09-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C          - CHANGED FORMAT 1004 TO READ E12.5 RATHER THAN
C          E11.5 AS THIS WAS NOT BEING READ CORRECTLY
C
C VERSION: 1.8
C MODIFIED: HARVEY ANDERSON
C DATE: 23/01/96
C          - MODIFIED THE VALUE OF MAXTE, MAXNE, AND MAXEB FROM 10
C          TO 25.
C
C-----
C INPUT:  (I*4)  IUIN      = UNIT NO. OF INPUT FILE.
C INPUT:  (I*4)  IUOUT     = UNIT NO. OF OUTPUT FILE.
C INPUT:  (C*8)  DATE      = DATE STRING.
C OUTPUT: (I*4)  IECOUNT   = NUMBER OF BEAM ENERGIES
C OUTPUT: (I*4)  INCOUNT   = NUMBER OF DENSITIES
C OUTPUT: (I*4)  ITCOUNT   = NUMBER OF TEMPERATURES
C
C-----
C          INTEGER      IUIN      , IUOUT
C
C          CHARACTER    DATE*8
C
C-----
C          PARAMETER( MAXTE=25, MAXNE=25, MAXEB=25)
C
C          CHARACTER LINE*132
C          REAL  NERAY(MAXNE), TERAY(MAXTE), EBRAY(MAXEB)
C          REAL  SRAY(MAXEB,MAXNE,MAXTE)
C          INTEGER IEA(MAXEB), ITA(MAXTE), INA(MAXNE)
C          REAL  TEREf, NEREf, SREf
C          REAL  NE, TE, EB
C          INTEGER IZ
C          REAL  Z
C          CHARACTER*2 SPEC(11)
C          DATA SPEC/'H ', 'HE', 'LI', 'BE', 'B ', 'C ', 'N ', 'O ', 'F ', 'NE', 'NA'/
C-----
C          S = IONISATION COEFFICIENT
C          NE = ELECTRON DENSITY (CM -3)
C          TE = ELECTRON TEMPERATURE (EV)
C          EB = BEAM ENERGY (EV/AMU)
C          TEREf = REFERENCE TEMPERATURE FOR NE/EB MATRIX
C          NEREf = REFERENCE DENSITY FOR TE VECTOR
C          EBREf = REFERENCE BEAM ENERGY FOR TE VECTOR
C          SREf = RATE COEFFICIENT ASSOCIATED WITH THESE REFERENCE VALUES
C
C
C          C.F. MAGGI 22 JULY 1991
C          L.D. HORTON 31 JULY 91
C-----

```

## COLINT

```

SUBROUTINE COLINT(Y,Z,EN,AI)
C
C          IMPLICIT REAL*8 (A-H,O-Z)
C
C-----
C          ***** FORTRAN77 SUBROUTINE: COLINT *****
C
C          PURPOSE UNKNOWN
C
C          NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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: 08-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - REPLACED 0.0 ARGUMENT IN CALL TO YIP
C          WITH A DUMMY VARIABLE INSTEAD.
C
C-----
C
C          DIMENSION X(5),W(5)

```

---

## DIEL

```

SUBROUTINE DIEL(Z,EIJ,F,T,COR,JCORN,AD)
IMPLICIT REAL*8 (A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 PROGRAM: DIEL *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
C
C          DIMENSION THETA(1000),COR(20)

```

---

## EIQIP

```

SUBROUTINE EIQIP(EI,EIJ,EM,Z,PHI,SC,WI,WJ,R,EIQ,FLAG)
C
C          IMPLICIT REAL*8 (A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: EIQIP *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----

```

---

## FIND

```

SUBROUTINE FIND(ARR,VALUE,IMAX,INDEX)
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: FIND *****
C
C PURPOSE:
C SUBROUTINE TO FIND VALUES FROM LINE AND STORE ONLY NOT REPEATED
C VALUES
C
C
C INPUT
C ARR = NAME OF ARRAY TO STORE ELEMENTS
C VALUE = VALUE TO BE FOUND IN LINE
C IMAX = TOTAL NUMBER OF NOT REPEATED ELEMENTS IN ARRAY
C INDEX = COUNTER OF ELEMENT POSITION IN ARRAY
C
C OUTPUT
C ARR = ARRAY CONTAINING NOT REPEATED VALUES READ FROM LINE
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
C
C UNIX-IDL PORT:
C
C VERSION: 1.1                      DATE: 01-02-96

```

```
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - PUT UNDER SCCS CONTROL
C
C-----
C LOGICAL OVER,FOUND
C REAL ARR(*),VALUE
C INTEGER IMAX,INDEX
C
```

---

## FINTER

```
FUNCTION FINTER(EN)
IMPLICIT REAL*8 (A-H,O-Z)
C
C-----
C ***** FORTRAN77 FUNCTION: FINTER *****
C
C PURPOSE: UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
```

---

## FITSP

```
SUBROUTINE FITSP(X,XA,N,YAA,Y,DY,I0,C1,C2,C3,C4,ISW)
IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C ***** FORTRAN77 SUBROUTINE: FITSP *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
C
C UNIX-IDL PORT:
C
C VERSION: 1.1 DATE: 18-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - PUT UNDER SCCS CONTROL
C
C-----
C
C DIMENSION YAA(10),TA(10),XA(10)
C DIMENSION C1(10,9),C2(10,9),C3(10,9),C4(10,9)
C DIMENSION CT1(9),CT2(9),CT3(9),CT4(9)
```

---

## GBB

```
FUNCTION GBB(EN,EN1,X2,X)
IMPLICIT REAL*8 (A-H,O-Z)
C
C-----
C ***** FORTRAN77 FUNCTION: GBB *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
```

---

## GBF

```
      FUNCTION GBF(EN,U)
      IMPLICIT REAL*8 (A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 FUNCTION: GBF *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
C
```

---

## GENTAB

```
      SUBROUTINE GENTAB(NREP,IMAX,DENS,TE,BMENER,F1,F2,F3)
C
C      IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: GENTAB *****
C
C PURPOSE : SEND DATA TO STREAM '10' FOR SUBSEQUENT TABLE PRODUCTION
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
C
C UNIX-IDL PORT:
C
C VERSION: 1.1                      DATE: 25-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C           - FIRST VERSION
C
C-----
C
C      DIMENSION NREP(31),F1(30),F2(30),F3(30)
C
```

---

## GSPC

```
      SUBROUTINE GSPC(XA,N,C1,C2,C3,C4)
C
C      IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: GSPC *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
C
C UNIX-IDL PORT:
C
C VERSION: 1.1                      DATE: 18-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C           - PUT UNDER SCCS CONTROL
C
C-----
C
C      DIMENSION HA(10),XA(10),W(10,10),C1(10,9)
C      DIMENSION C2(10,9),C3(10,9),C4(10,9)
C
```

---

## INITPOS

```
      SUBROUTINE INITPOS(NTA,M)
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: INITPOS *****
C
C PURPOSE UNKNOWN
C
```



```

C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
C
C UNIX-IDL PORT:
C
C VERSION: 1.1 DATE: 01-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - PUT UNDER SCCS CONTROL
C
C -----
C
C INTEGER NTA(*)

```

# LOWPOP

```

C
C SUBROUTINE LOWPOP(SEQ,REFMEM,Z0,Z1,ZEFF,NMET,IMETR,TE,DENS,TP,
C & DENSP,DENSH,NPARNT,DEPA,LPTA,
C & PEXMAT,PEXRHS,PECION,PEDREC,PERREC,
C & PEXREC,IECION,IEDREC,IERREC,IEXREC)
C IMPLICIT REAL*8(A-H,O-Z)
C PARAMETER (NDLEV=30,NDTEM=20,NDDEN=20,NDMET=5,NDTRN=300)
C PARAMETER (NDSPL=10)
C PARAMETER (ICODE=0)
C -----
C SUBROUTINE TO CALCULATE POPULATIONS OF LOW EXCITED POPULATIONS OF
C IONS INCLUDING
C
C (A) COUPLING TO HIGH LEVELS AND CONTINUUM VIA PRELIMINARY
C BUNDLE-N CALCULATION (V2BNDLN) AND PROJECTION/EXPANSION
C MATRIX CALCULATION (CLDLBN2)
C
C (B) DEPENDENCE ON METASTABLES.
C
C PROCESSES CAN INCLUDE ELECTRON & PROTON IMPACT, SPONTANEOUS EMISSION,
C FREE ELECTRON RECOMBINATION AND CHARGE EXCHANGE RECOMBINATION
C DEPENDING ON THE INPUT DATA SET
C
C THE BASIC LOW LEVEL ATOMIC DATA IS ENTERED FROM COMPILATION
C DATA SETS OF THE FORM
C
C 'JETSHP.<SE>LIKE.DATA(<TITLE><EL>)'
C
C WHERE <SE> DENOTES THE ISOLELECTRONIC SEQUENCE, <TITLE> IS AN
C ARBITRARY IDENTIFIER FOR THE SOURCE AND YEAR, <EL> IS THE
C ELEMENT SYMBOL. <SE> AND <TITLE><EL> ARE PRESENTED TO THE
C SUBROUTINE AS PARAMETERS FROM CLDLBN2
C
C MAIN OUTPUT TABLES ARE GENERATED ON STREAM 7
C POPULATION DATA FOR DIAGNOSTIC USE ON STREAM 19
C
C THE SUBROUTINE WAS DEVELOPED FROM THE ORIGINAL PROGRAM SPMETPOP
C
C INPUT
C Z0 = NUCLEAR CHARGE
C Z1 = RECOMBINING ION CHARGE
C ZEFF = PLASMA Z EFFECTIVE
C NMET = NUMBER OF METASTABLES (1.LE.NMET.LE.5)
C IMETR(I) = INDEX OF METASTABLE I IN COMPLETE LEVEL LIST
C TE = ELECTRON TEMPERATURE (K)
C DENS = ELECTRON DENSITY (CM-3)
C TP = PROTON TEMPERATURE (K)
C DENSP = PROTON DENSITY (CM-3)
C DENSH = NEUTRAL HYDROGEN DENSITY(IN BEAMS) (CM-3)
C PEXMAT(I,J) = EXPANDED PROJECTION MATRIX FOR LOW LEVELS
C PEXRHS(I) = EXPANDED PROJECTED RIGHT HAND SIDE VECTOR
C PECION(I) = DENS*IONISATION RATE COEFFT FOR LOW LEVEL I
C PEDREC(I) = DIELECTRONIC RECOMB. COEFFT. FOR LOW LEVEL I
C PERREC(I) = RADIATIVE RECOMB. COEFFT. FOR LOW LEVEL I
C PEXREC(I) = DENSH*(CX RATE COEFFT)/DENS FOR LOW LEVEL I
C IECION = 0 IONISATION ELIMINATED FROM LEVEL I
C = 1 IONISATION NOT ELIMINATED FROM LEVEL I
C IEDREC = 0 DIEL. RECOMB. ELIMINATED FOR LEVEL I
C = 1 DIEL. RECOMB. NOT ELIMINATED FOR LEVEL I
C IERREC = 0 RAD. RECOMB. ELIMINATED FOR LEVEL I
C = 1 RAD. RECOMB. NOT ELIMINATED FOR LEVEL I
C IEXREC = 0 CX. RECOMB. ELIMINATED FOR LEVEL I
C = 1 CX. RECOMB. NOT ELIMINATED FOR LEVEL I
C
C ***** H.P. SUMMERS, JET 26 APR 1990 *****
C OPEN FILE ON STREAM 9 UNDER DIVUID 19 FEB 1991
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 INPUT UNIT NUMBER WAS CHANGE FROM 10 TO 9 AND THE
C      DIAGNOSTIC OUTPUT UNIT FROM 11 TO 19.
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: 18-1-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - PUT UNDER SCCS CONTROL
C
C      VERSION: 1.2                      DATE: 18-1-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - COMMENTED OUT LINE 'EXTERNAL GAMMA' AS IT APPEARS
C      TO SERVE NO PURPOSE AND THERE IS NO CORRESPONDING
C      GAMMA ROUTINE.
C
C      VERSION: 1.3                      DATE: 18-1-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - COMMENTED OUT LINE 'CALL ERRSET'
C
C-----
C
C      CHARACTER*40 TITLE,GTIT1,STRG1
C      CHARACTER*20 TIT2
C      CHARACTER*1 LCODE,GRAPH,TEXT,TCODE
C      CHARACTER ANS*3,CSTRGA*12,STRGA*22,ITITLE*3
C      CHARACTER SEQ*2,REFMEM*8,DSNAME*30
C      CHARACTER STRGB*36,STRGC*36,STRGD*36,BLANKS*36
C
C      CHARACTER JOBNAME*8,DIVUID*6,ACCT*4,POINT*2,SECLEV*2
C      DOUBLE PRECISION LOGTEA,LOGTPA,LOGTHA
C      REAL*4 XL14,XU14,YL14,YU14,SDENSA,STK4,STEV
C
C      DIMENSION IA (NDLEV) , ISA (NDLEV) , ILA (NDLEV) , XJA (NDLEV) , WA (NDLEV)
C      DIMENSION ER (NDLEV) , RHS (NDLEV) , XIA (NDLEV) , CIE (NDLEV)
C      DIMENSION CRHS (NDLEV,5) , LPTA (NDLEV) , DEPA (5)
C      DIMENSION CRA (NDLEV,NDLEV) , CRCE (NDLEV,NDLEV) , CRCP (NDLEV,NDLEV)
C      DIMENSION IORDR (NDLEV) , CC (NDLEV,NDLEV) , CMAT (NDLEV,NDLEV)
C      DIMENSION POPAR (NDLEV) , CSTRGA (NDLEV)
C      DIMENSION TEA (NDTEM) , TPA (NDTEM) , TEVA (NDTEM) , TPVA (NDTEM)
C      DIMENSION THA (NDTEM) , THVA (NDTEM)
C      DIMENSION ATEA (NDTEM) , ATPA (NDTEM) , ATHA (NDTEM)
C      DIMENSION LOGTEA (NDTEM) , LOGTPA (NDTEM) , LOGTHA (NDTEM)
C      DIMENSION SQATEA (NDTEM) , SQATPA (NDTEM) , SQATHA (NDTEM)
C      DIMENSION EXPTE (NDLEV,NDTEM) , EXPTP (NDLEV,NDTEM)
C      DIMENSION VECH (NDTEM,NDLEV) , VECP (NDTEM,NDLEV)
C      DIMENSION DENSA (NDDEN) , DENSPA (NDDEN) , RATHA (NDDEN) , RATIA (NDDEN)
C      DIMENSION SDENSA (NDDEN) , STK4 (NDLEV,NDMET,NDDEN)
C      DIMENSION SIONA (NDMET) , STVRH (NDMET,5) , ALFG (5)
C      DIMENSION IMETR (NDMET+1) , VRHRED (NDMET,5)
C      DIMENSION CRED (NDMET,NDMET)
C      DIMENSION IE1A (NDTRN) , IE2A (NDTRN) , IP1A (NDTRN) , IP2A (NDTRN)
C      DIMENSION AA (NDTRN)
C      DIMENSION DEXCRA (NDTEM,NDTRN) , DEXCRP (NDTEM,NDTRN)
C      DIMENSION STACK (NDLEV,NDMET,NDTEM,NDDEN)
C      DIMENSION STCKM (NDMET,NDTEM,NDDEN)
C      DIMENSION STVRHM (NDMET,5)
C      DIMENSION C1 (NDSPL,NDSPL-1) , C2 (NDSPL,NDSPL-1)
C      DIMENSION C3 (NDSPL,NDSPL-1) , C4 (NDSPL,NDSPL-1)
C      DIMENSION XA (NDSPL)
C      DIMENSION SCEF (8) , SCOM (8) , ERG (4) , OM (4)
C      DIMENSION PAR (18,17)
C      DIMENSION STRGA (NDLEV)
C      DIMENSION PEXMAT (NDLEV,NDLEV) , PEXRHS (NDLEV) , PECION (NDLEV)
C      DIMENSION PEDREC (NDLEV) , PERREC (NDLEV) , PEXREC (NDLEV)
C
CX     EXTERNAL GAMMA
C
C      DATA TIT2/'SPDFGHIJK'           '/'
C      DATA BLANKS/'                '/'
C
CX     CALL ERRSET(208,256,-1)
C-----

```

## NSUPH1

```

C      SUBROUTINE NSUPH1 (TEV,EBEAM,TIEV,NIMP ,ZIMPA ,FRIMPA,AMIMPA,
C      &                    ITYP1 ,ITYP2 ,ITYP3 ,ITYP4 ,ITYP5 ,ITYP6 ,
C      &                    XTBE ,XTBP ,XTBZ ,STBE ,STBP ,STBZ ,
C      &                    LXTBE ,LXTBP ,LXTBZ ,LSTBE ,LSTBP ,LSTBZ ,
C      &                    PXTBE ,PXTBP ,PXTBZ ,PSTBE ,PSTBP ,PSTBZ ,
C      &                    LPXTBE ,LPXTBP ,LPXTBZ ,LPSTBE ,LPSTBP ,LPSTBZ ,
C      &                    DSLPATH)
C
C      IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C      ***** FORTRAN77 SUBROUTINE: NSUPH1 *****
C-----

```

```

C SUBROUTINE TO ACCESS SPECIFIC HIGHER QUALITY DATA FOR
C
C H
C
C POPULATION STRUCTURE CALCULATION IN THE BUNDLE-N APPROXIMATION.
C
C DATA TYPES ARE:
C
C (1) ELECTRON IMPACT EXCITATION - SPECIFIC ION FILE IS OPENED.
C (2) ELECTRON IMPACT IONISATION - SPECIFIC FIT IS USED.
C (3) H+ IMPACT EXCITATION - QHIEXDAT FILE IS OPENED.
C (4) H+ IMPACT IONIS + CX - QHIEXDAT FILE IS OPENED.
C (5) ZIMP ION IMPACT EXCITATION - QHIEXDAT FILE IS OPENED.
C (6) ZIMP ION IMPACT IONIS + CX - QHIEXDAT FILE IS OPENED.
C
C INPUT
C TEV = ELECTRON TEMPERATURE (EV)
C EBEAM = BEAM ENERGY (EV/AMU) USED AS A UNIFORM VELOCITY SHIFT
C FOR ION COLLISIONS
C TIEV = ION TEMPERATURE (EV)
C NIMP = NUMBER OF IMPURITY IONS (EXCLUDING H+)
C ZIMPA() = Z OF EFFECTIVE IMPURITY FOR ION COLLISIONS(EXCEPT H+)
C FRIMPA() = FRACTION OF TOTAL IMPURITY NUMBER DENSITY (EXCL H+)
C AMIMPA() = ATOMIC MASS NUMBER OF IMPURITY
C ITYP1 = 0 DO NOT OBTAIN TYPE 1 DATA
C = 1 OBTAIN TYPE 1 DATA
C ITYP2 = 0 DO NOT OBTAIN TYPE 2 DATA
C = 1 OBTAIN TYPE 2 DATA
C ITYP3 = 0 DO NOT OBTAIN TYPE 3 DATA
C = 1 OBTAIN TYPE 3 DATA
C ITYP4 = 0 DO NOT OBTAIN TYPE 4 DATA
C = 1 OBTAIN TYPE 1 DATA
C ITYP5 = 0 DO NOT OBTAIN TYPE 5 DATA
C = 1 OBTAIN TYPE 2 DATA
C ITYP6 = 0 DO NOT OBTAIN TYPE 6 DATA
C = 1 OBTAIN TYPE 3 DATA
C DSLPATH = STRING CONTAINING PATH FOR INPUT FILE FOR UNIT 15
C
C OUTPUT
C XTBE(N,N'') = TYPE 1 RATE COEFFICIENT
C XTBP(N,N'') = TYPE 3 RATE COEFFICIENT
C XTBE(N,N'') = TYPE 5 RATE COEFFICIENT
C STBE(N) = TYPE 2 RATE COEFFICIENT
C STBP(N) = TYPE 4 RATE COEFFICIENT
C STBZ(N) = TYPE 6 RATE COEFFICIENT
C LXTBE(N,N'') = TYPE 1 MARKER (0 =NO VALUE, 1=VALUE)
C LXTBP(N,N'') = TYPE 3 MARKER
C LXTBZ(N,N'') = TYPE 5 MARKER
C LSTBE(N) = TYPE 2 MARKER
C LSTBP(N) = TYPE 4 MARKER
C LSTBZ(N) = TYPE 6 MARKER
C PXTBE(N) = TYPE 1 PROJECTION MULTIPLIER
C PXTBP(N) = TYPE 3 PROJECTION MULTIPLIER
C PXTBZ(N) = TYPE 5 PROJECTION MULTIPLIER
C PSTBE = TYPE 2 PROJECTION MULTIPLIER
C PSTBP = TYPE 4 PROJECTION MULTIPLIER
C PSTBZ = TYPE 6 PROJECTION MULTIPLIER
C LPXTBE(N) = TYPE 1 PROJECTION MULTIPLIER USED ABOVE THIS N'
C LPXTBP(N) = TYPE 3 PROJECTION MULTIPLIER USED ABOVE THIS N'
C LPXTBZ(N) = TYPE 5 PROJECTION MULTIPLIER USED ABOVE THIS N'
C LPSTBE = TYPE 2 PROJECTION MULTIPLIER USED ABOVE THIS N
C LPSTBP = TYPE 4 PROJECTION MULTIPLIER USED ABOVE THIS N
C LPSTBZ = TYPE 6 PROJECTION MULTIPLIER USED ABOVE THIS N
C
C ***** H.P. SUMMERS, JET 9 MAY 1990 *****
C ***** 20 JUL 1990 *****
C ***** 13 AUG 1990 *****
C ***** NEW ELECTRON EXCIT. DATA 22 JAN 1991 *****
C ***** NEW ION IMPACT EXCIT. DATA 3 JUL 1991 *****
C ***** NEW ELEC. IMPACT ION. DATA 3 JUL 1991 *****
C ***** DATA EXTENSION BY ADDING 1 MAR 1992 *****
C ***** SOME INTERMEDIATE VALUES +
C ***** ADDITION OF B, N, NE ION. +
C ***** CHARGE EXCHANGE.
C ***** MULTIPLE, SIMULTANEOUS 11 JAN 1994 *****
C ***** IMPURITY EXTENSION
C ***** ERROR CORRECTED IN IMPURITY
C ***** REDUCED MASSES
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) A PARAMETER FLAG HAS BEEN ADDED TO SWITCH ON/OFF
C DIAGNOSTIC PRINTING (UNIT 6).
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: 18-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - ADDED VARIABLE DSLPATH AND CHANGED NAME OF INPUT FILE
C
C VERSION: 1.3 DATE: 18-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - CORRECTED STRING HANDLING SYNTAX IN CONSTRUCTION OF
C DSNAME, COMMENTED OUT REFERENCES TO DEBUG LOGICAL
C VARIABLE AND INSERTED 'CALL' BEFORE XXSLEN.
C
C VERSION: 1.4 DATE: 18-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - MODIFIED CONSTRUCTION OF DSNAME
C
C VERSION: 1.5 DATE: 18-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - ADDED DSLPATH IN CALL TO QH.FOR
C
C VERSION: 1.6 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: 1.7 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: 1.8 DATE: 08-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - REMOVED SUPERFLUOUS VARIABLES
C
C VERSION: 1.9 DATE: 03-04-97
C MODIFIED: H.ANDERSON
C - ALTERED TO USE RESTRUCTURED ADF02 DATASET sia#h_rfm.dat
C
C VERSION: 1.10 DATE: 03/04/97
C MODIFIED: HARVEY ANDERSON.
C ALTERED TO USE NEW PREFERRED ADF02 DATASET sia#h_j97.dat
C
C VERSION: 1.11 DATE: 08-04-97
C MODIFIED: RICHARD MARTIN
C CHANGED NAME OF ADF02 FILE FROM sia#h_j97.dat TO
C sia#h_j97#h.dat
C
C-----
C PARAM : (L*4) DEBUG = FLAGS DIAGNOSTIC PRINTING.
C .TRUE. => PRINT DIAGNOSTICS.
C .FALSE. => DO NOT PRINT DIAGNOSTICS.
C-----
C
C-----
CX LOGICAL DEBUG
CX PARAMETER( DEBUG = .FALSE. )
CX PARAMETER (NCDIM=30,NDLOW=10)
C-----
C
C CHARACTER DSNAME*80,TITLF*80,TITLX*80,DSLPATH*80,
C & DSTEMP2*80
C
C LOGICAL LTRNG(1)
C
C DIMENSION NA(NCDIM),N1A(NCDIM),ICODEA(NCDIM)
C DIMENSION COEFFA(NCDIM),COEFFB(NCDIM)
C DIMENSION EA(24),OA(24)
C DIMENSION TEA(8),TEALG(24),GAMA(24)
CX DIMENSION XKA(28),C(28)
CX DIMENSION WRK(160)
CX DIMENSION WTS(24),B(24),A(28,4),DIAG(28)
CX DIMENSION TVAL(1),SZDA(1)
CX DIMENSION ZIMPA(10),FRIMPA(10),AMIMPA(10)
C
C DIMENSION XTBE(NDLOW,NDLOW),LXTBE(NDLOW,NDLOW)
C DIMENSION XTBP(NDLOW,NDLOW),LXTBP(NDLOW,NDLOW)
C DIMENSION XTbz(NDLOW,NDLOW),LXTbz(NDLOW,NDLOW)
C DIMENSION PXTBE(NDLOW),LPXTBE(NDLOW)
C DIMENSION PXTBP(NDLOW),LPXTBP(NDLOW)
C DIMENSION PXTbz(NDLOW),LPXTbz(NDLOW)
C DIMENSION STBE(NDLOW),LSTBE(NDLOW)
C DIMENSION STBP(NDLOW),LSTBP(NDLOW)
C DIMENSION STbz(NDLOW),LSTbz(NDLOW)
C
C DATA LCK,LWRK/28,160/
C-----

```

**PYPR**

SUBROUTINE PYPR(E,E11,N,N11,EM,Z1,PHI,WI,WJ,TE,INTD,PY,RDEXC)

```

C
C      IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: PYPR *****
C
C CALCULATES PY FACTOR (CF. VAN REGEMORTER,1962) USING PERCIVAL,RICHARD
C AND COWORKER CROSS-SECTIONS.
C VALID ONLY FOR ELECTRON INDUCED TRANSITIONS BETWEEN WHOLE PRINCIPAL
C QUANTUM SHELLS IN HYDROGEN AND HYDROGENIC IONS, FOR N,N11>4
C HOWEVER ADJUSTMENTS MADE TO ALLOW USE OF FORMULAE FOR N<4
C ***** H.P.SUMMERS, JET 12 NOVEMBER 1984 *****
C
C INPUT
C      E=1/V**2 WITH V THE INITIAL EFFECTIVE PRINCIPAL QUANTUM NUMBER
C      E11=1/V11**2 WITH V11 THE FINAL EFFECTIVE PRINCIPAL QUANTUM NUMBE
C      N=INITIAL PRINCIPAL QUANTUM NUMBER
C      N11=FINAL PRINCIPAL QUANTUM NUMBER (REQUIRE N11>N AND V11>V)
C      EM=REDUCED MASS OF COLLIDING PARTICLE (MUST BE 1.0 IN THIS CASE)
C      Z1=TARGET ION CHARGE +1
C      PHI=(IH/EIJ)F WITH EIJ=TRANSITION ENERGY, F=ABS. OSCILL. STRENGTH
C      WI=STATISTICAL WEIGHT OF INITIAL LEVEL
C      WJ=STATISTICAL WEIGHT OF FINAL LEVEL
C      TE=ELECTRON TEMPERATURE(K)
C      INTD=<3 FOR TWO POINT GAUSSIAN QUADRATURE.
C           = 3 FOR THREE POINT GAUSSIAN QUADRATURE
C           =>3 FOR FOUR POINT GAUSSIAN QUADRATURE
C
C OUTPUT
C      PY=P FACTOR
C      RDEXC=DEXCITATION RATE COEFFICIENT (CM+3 SEC-1)
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
C
C      DIMENSION A(4),H(4)

```

## PYVR

```

C      SUBROUTINE PYVR(Y,Z1,PY)
C
C      IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: PYVR *****
C
C CALCULATES VAN REGEMORTER'S P FACTOR FOR ELECTRON COLLISIONS WITH
C ATOMS AND IONS.
C INPUT
C      Y=ATE*(1/V1**2+1/V2**2) WHERE
C           ATE=1.5789D5*Z1*Z1/TE
C           TE=ELECTRON TEMPERATURE (K)
C           V1=INITIAL EFFECTIVE PRINCIPAL QUANTUM NUMBER
C           V2=FINAL EFFECTIVE PRINCIPAL QUANTUM NUMBER
C      Z1=TARGET ION CHARGE+1
C      PY=P-FACTOR
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----

```

## QH

```

C      FUNCTION QH(EPRO,TTAR,ISEL,ZSEL,NSEL,IORD,EA,OA,N,IPASS,
C      &          TITLF,DSLPTH)
C
C      IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 FUNCTION: QH *****
C
C-----

```

```

C      WARNING: DO NOT USE THIS PROGRAM WITH ADAS, IT HAS BEEN
C      ALTERED TO ACCOMADATE THE COMPARATIVE ADF02 FILE
C      AS WELL AS THE TOSHIMA & TAWARA ADF02 FILE.
C
C      14/3/97 HARVEY ANDERSON.
C
C      FUNCTION TO EVALUATE MAXWELL AVERAGED TOTAL IONISATION, EXCITATION
C      AND CHARGE EXCHANGE RATE COEFFICIENTS.
C
C      THE FUNCTION ALSO RETURNS THE RAW CROSS-SECTION DATA FOR VERIFICATION
C      AND GRAPHING PURPOSES.
C
C      THE INCIDENT PARTICLE IS A MONOENERGETIC BEAM AND THE TARGET IS A
C      MAXWELL DISTRIBUTION. THE TARGET AND PROJECTILE ROLES MAY BE
C      REVERSED. ARBITRARY RELATIVE SPEEDS ARE ALLOWED.
C
C      THE RATE COEFFICIENT REQUIRED IS SELECTED FROM A LIST. THERE IS SOME
C      SCALED DATA. ALL X-SECTS INVOLVE HYDROGEN AS ONE OF THE SPECIES.
C
C      NB. QH IS DESIGNED TO TAKE HYDROGEN XSECT DATA FROM
C
C      'JETSHP.IONATOM.DATA(H)'
C
C      INPUT
C      EPRO = INCIDENT PARTICLE ENERGY (EV/AMU)
C      TTAR = MAXWELL TEMPERATURE OF TARGET PARTICLES (EV)
C      IF (TTAR.LE.0) THEN ONLY RAW SOURCE VALUES ARE RETURNED
C      IN ARRAYS (EA(I),OA(I), I=1,N)
C      ISEL = SELECTOR FOR PARTICULAR RATE COEFFTT. CHOSEN FROM TABLE
C      BELOW (SEE ALSO NOTES ON DATA)
C      ZSEL = NUCLEAR CHARGE (REQUIRED ONLY FOR PARTICULAR ISEL)
C      NSEL = PRINC. QUANTUM NO. (REQUIRED ONLY FOR PARTICULAR ISEL
C      NB. NSEL SHOULD BE ZERO ON ENTRY OTHERWISE)
C      IORD = 1 FOR 1ST PARTICLE INCIDENT AND MONOENERGETIC
C      = 2 FOR 2ND PARTICLE INCIDENT AND MONOENERGETIC
C      IPASS = 0 IF DATA FILE TO BE READ IN AFRESH
C      = 1 IF DATA FILE IS NOT TO BE READ IN AGAIN
C
C      OUTPUT
C      QH = RATE COEFFICIENT (CM3 SEC-1)
C      EA(I) = SET OF ENERGIES (EV/AMU) FOR SELECTED SOURCE DATA
C      OA(I) = CROSS-SECTIONS (CM**2) FOR SELECTED SOURCE DATA
C      N = NUMBER OF SOURCE DATA VALUES
C      TITLF = INFORMATION STRING
C
C      ***** H.P.SUMMERS,JET          20 JUL 1990 *****
C      *****                          COR  31 JUL 1990 *****
C      *****                          ADD   3 JUL 1991 *****
C
C      NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
C
C      UNIX-IDL PORT:
C
C      VERSION: 1.1          DATE: 18-1-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - PUT UNDER SCCS CONTROL
C      - MODIFIED NAME OF INPUT FILE BY ADDING INPUT
C      PARAMETER DSLPATH CONTAINING THE PATH TO THE
C      FILE AND INCREASING THE LENGTH OF THE VARIABLE DSNAME
C
C      VERSION: 1.2          DATE: 18-1-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - MODIFIED CONSTRUCTION OF DSLPATH
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 CALL
C      TO ADAS REPLACEMENT ROUTINE DXNBBF
C
C      VERSION: 1.4          DATE: 23-1-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - REPLACED CALL TO NAG ROUTINE E01BAF WITH CALL
C      TO ADAS REPLACEMENT ROUTINE DXNBAF (NOTE THAT
C      THIS IS NOT A DIRECT REPLACEMENT ROUTINE BUT
C      HOPEFULLY IT WILL NOW GIVE THE SAME RESULTS)
C
C      VERSION: 1.5          DATE: 08-02-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - REMOVED SUPERFLUOUS VARIABLES
C
C      VERSION: 1.6          DATE: 08-02-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C      - CORRECTED NAME "TRING" TO "STRING"
C
C      VERSION: 1.7          DATE: 26/11/96
C      MODIFIED: HARVEY ANDERSON
C      MODIFIED FORMAT STATEMENT 1001 AND THE READ
C      STATEMENT BEGINING ON LINE 146 TO ACCOMODATE
C      FOR THE NEW FORMAT OF THE ADF02 FILE
C      /SIA#H/SIA#H_RFM#H.DAT. ALSO MODIFIED THE
C      DSNAME ON LINE 143. ALSO SLIGHTLY MODIFIED
C      LINE 152 AND 153 DUE TO THE NEW FORMAT OF
C      THE FILE. ALSO MODIFIED THE SELECT NUMBERS
C      ASSOCIATED WITH THE SCALING.
C
C      VERSION: 1.8          DATE: 03-04-97

```

```

C MODIFIED: HARVEY ANDERSON
C MODIFIED TO USE NEW PREFERRED ADF02 FILE sia#h_j97.dat
C
C VERSION: 1.9 DATE: 08-04-97
C MODIFIED: RICHARD MARTIN
C CHANGED NAME OF ADF02 FILE FROM sia#h_j97.dat TO
C sia#h_j97h.dat
C
C VERSION: 1.10 DATE: 08-04-97
C MODIFIED: RICHARD MARTIN
C CORRECTED MISTAKE MADE IN PREVIOUS MODIFICATION
C
C-----
C PARAMETER (NSTORE=80)
C DIMENSION XA(9),WXA(9),NA(NSTORE)
C DIMENSION SIGA(24,NSTORE),ERELA(24,NSTORE)
C DIMENSION EM1A(NSTORE),EM2A(NSTORE),ALFA(NSTORE)
C DIMENSION ETHRA(NSTORE),EA(24),OA(24),YA(24),FA(24)
C DIMENSION XSA(24),YSA(24),XKA(28),C(28),WTS(24)
CX DIMENSION WRK(160)
C CHARACTER DSNAM*80, STRING*80, TITLF*80, DSLPATH*80
C DIMENSION B(24),A(28,4),DIAG(28)
C-----
C GAUSS-LAGUERRE DATA (9PT)
C-----
C DATA XA/0.1523222277D0,0.8072200227D0,2.0051351556D0,
C & 3.7834739733D0,6.2049567778D0,9.3729852516D0,
C & 13.4662369110D0,18.8335977889D0,26.3740718909D0/
C DATA WXA/3.36126421798D-1,4.11213980424D-1,1.99287525371D-1,
C & 4.74605627657D-2,5.59962661079D-3,3.05249767093D-4,
C & 6.59212302608D-6,4.11076933035D-8,3.29087403035D-11/
C-----
C XSECT STORAGE - NA(ISEL),EM1A(ISEL),EM2A(ISEL),ALFA(ISEL),
C ETHRA(ISEL),ISEL
C ERELA(IVAL,ISEL), SIGA(IVAL,ISEL) WHERE
C NA=NUMBER OF ENERGIES FOR CROSS-SECTION
C EM1=1ST PARTICLE MASS (AT.MASS UNITS)
C EM2=2ND PARTICLE MASS (AT.MASS UNITS)
C ALF=HIGH ENERGY SLOPE (AS EREL**ALF)
C ETHR=THRESHOLD ENERGY FOR REACTION (EV)
C EREL=RELATIVE ENERGY (EV/AMU)
C SIG=X-SECT (CM2)
C WHERE THERE ARE UP TO 24 VALUES FOR EACH X-SECT
C
C N.B. IT ASSUMED FOR POWER LAW INTERPOLATION PURPOSES THAT THE
C CROSS-SECTION AT ERELA(1) IS FINITE.
C-----
C DATA LCK,LWRK/28,160/
C

```

# QLPR

```

C FUNCTION QLPR(Z1,N1,N2,E1,ZP,ATMSSP)
C IMPLICIT REAL*8(A-H,O-Z)
C-----
C ***** FORTRAN77 FUNCTION: QLPR *****
C-----
C LODGE-PERCIVAL-RICHARDS ION IMPACT EXCITATION CROSS-SECTIONS IN
C ORIGINAL FORM (J.PHYS.B. (1976)9,239).
C
C EXCITATION CROSS-SECTION IS EVALUATED AND DE-EXCITATION CROSS-SECTION
C OBTAINED BY DETAILED BALANCE
C
C SCALING TO ARBITRARY PROJECTILE CHARGE FOLLOWS RECOMMENDATIONS
C OF RIENHOLD,, OLSEN & FRITSCH (1990)PHYS.REV.A 41,4837
C
C INPUT
C Z1=TARGET ION CHARGE +1
C N1=INITIAL PRINCIPAL QUANTUM NUMBER
C N2=FINAL PRINCIPAL QUANTUM NUMBER
C E1=ENERGY OF EQUIVALENT ELECTRON IN RYDBERGS
C (CORRESPONDS TO ACTUAL PROJECTILE ENERGY/25KEV)
C ZP=PROJECTILE CHARGE
C ATMSSP= PROJECTILE MASS IN PROTON UNITS
C OUTPUT
C QLPR=CROSS-SECTION IN PI*A0**2 UNITS
C
C ***** H.P.SUMMERS, JET 16/ 7/90 *****
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
```

## QPR78

```
FUNCTION QPR78(Z1,N1,N2,E1,PHI)
C
C   IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 FUNCTION: QPR78 *****
C-----
C PERCIVAL AND RICHARDS-MNRAS(1978)183,329.
C ELECTRON COLLISION CROSS-SECTIONS FOR TRANSITIONS BETWEEN PRINCIPAL
C QUANTUM SHELLS IN HYDROGEN AND HYDROGENIC IONS.
C VALID FOR INCIDENT ELECTRON ENERGIES IN RANGE (Z1/N1)**2<E1<137**2
C AND FOR N1,N2>4.
C ANOMALIES DEVELOP IN ORIGINAL SPECIFICATION OF PERCIVAL RICHARDS FOR
C S=N2-N1 LARGE OR IF N1 IS <5. HENCE A MODIFIED PRESCRIPTION IS USED
C IN THESE CASES CONSISTENT WITH BANKS ET AL (1973) ASTR. LETT 14,161
C
C
C INPUT
C   Z1=TARGET ION CHARGE +1
C   N1=INITIAL PRINCIPAL QUANTUM NUMBER
C   N2=FINAL PRINCIPAL QUANTUM NUMBER
C   E1=ENERGY OF INCIDENT ELECTRON IN RYDBERGS
C
C OUTPUT
C   QPR78=CROSS-SECTION IN PI*A0**2 UNITS
C
C ***** H.P.SUMMERS, JET          12 NOV 1984          *****
C *****                          COR  28 FEB 1990          ****
C-----
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
```

## QVAIN

```
FUNCTION QVAIN(Z1,N1,N2,VION,PHI,ZP)
C
C   IMPLICIT REAL*8(A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 FUNCTION: QVAIN *****
C-----
C ION COLLISION CROSS-SECTIONS FOR TRANSITIONS BETWEEN PRINCIPAL
C QUANTUM SHELLS IN HYDROGEN AND HYDROGENIC IONS.
C INPUT
C   Z1 = TARGET ION CHARGE +1
C   N1 = INITIAL PRINCIPAL QUANTUM NUMBER
C   N2 = FINAL PRINCIPAL QUANTUM NUMBER
C   VION = VELOCITY OF INCIDENT ION (CM/SEC)
C   ZP = PROJECTILE CHARGE
C OUTPUT
C   QVAIN=CROSS-SECTION IN PI*A0**2 UNITS
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
```

## RQLNEW

```
FUNCTION RQLNEW(Z,N11,N,PHI,ZP, AMSIMP,TP,VDISP)
C
C   IMPLICIT REAL*8(A-H,O-Z)
```



```

C-----
C
C ***** FORTRAN77 FUNCTION: RQLNEW *****
C-----
C EVALUATES ION IMPACT RATE COEFFICIENTS OF LODGE, PERCIVAL & RICHARDS
C (ALTERNATIVE TO RQLPR WITH BETTER MAXWELL AVERAGING BUT SLOWER)
C
C ROUTINE MUST RETURN EXCITATION RATE COEFFICIENT IF N11.LT.N AND
C DEXCITATION RATE COEFFICIENT IF N11.GT.N
C
C NOTE THAT THE RELATION BETWEEN INVERSE PROCESSES IS DETERMINED BY THE
C TEMPERATURE TP AND THE SPEED VDISP
C THE TREATMENT GIVEN IS APPROXIMATE EXCEPT IN THE LIMITS VDISP=0 OR
C VDISP >> DSQRT(2*TP/AMSIMP)
C
C INPUT
C   Z           = TARGET ION CHARGE+1
C   N11        = PRINCIPAL QUANTUM NUMBER OF INITIAL LEVEL
C   N          = PRINCIPAL QUANTUM NUMBER OF FINAL LEVEL
C   PHI        = (IH/EIJ)F(N ---> N')
C   ZP         = PROJECTILE CHARGE
C   AMSIMP     = PROJECTILE MASS (PROTON UNITS)
C   TP         = PROJECTILE ION TEMPERATURE (K)
C   VDISP      = CONSTANT MEAN SPEED SHIFT FOR THE COLLISION (CM/SEC)
C               (DESCRIBES BEAM PLASMA SITUATIONS)
C
C OUTPUT
C   RQLNEW     = RATE COEFFICIENT (CM**3 SEC-1)
C
C ***** H.P. SUMMERS, JET                2 JUL 1991 *****
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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: 08-02-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C           - REMOVED SUPERFLUOUS VARIABLES
C-----
C
C   DIMENSION XA(9),WXA(9)
C   DIMENSION EA(24),OA(24),YA(24),FA(24)
C-----
C GAUSS-LAGUERRE DATA (9PT)
C-----
C   DATA XA/0.1523222277D0,0.8072200227D0,2.0051351556D0,
C   &      3.7834739733D0,6.2049567778D0,9.3729852516D0,
C   &      13.4662369110D0,18.8335977889D0,26.3740718909D0/
C   DATA WXA/3.36126421798D-1,4.11213980424D-1,1.99287525371D-1,
C   &      4.74605627657D-2,5.59962661079D-3,3.05249767093D-4,
C   &      6.59212302608D-6,4.11076933035D-8,3.29087403035D-11/
C-----
C   DATA LCK,LWRK/28,160/
C-----
C   DATA NN/22/
C   DATA (EA(I),I=1,24)/1.00D3,1.50D3,2.00D3,3.00D3,5.00D3,7.00D3,
C   &      1.00D4,1.50D4,2.00D4,3.00D4,4.00D4,5.00D4,
C   &      6.00D4,7.00D4,8.00D4,1.00D5,1.50D5,2.00D5,
C   &      3.00D5,5.00D5,7.00D5,1.00D6,0.00D0,0.00D0/
C   DATA IORD,EM1,ALFA /1,2.0D0,1.0D0/
C-----

```

## RQVNEW

```

FUNCTION RQVNEW(Z,N11,N,PHI,ZP, AMSIMP,TP,VDISP)
C
C IMPLICIT REAL*8(A-H,O-Z)
C-----
C ***** FORTRAN77 FUNCTION: RQVNEW *****
C-----
C EVALUATES ION IMPACT RATE COEFFICIENTS OF VAINSHTEIN ET AL 1981
C (ALTERNATIVE TO RQVAIN WITH BETTER MAXWELL AVERAGING BUT SLOWER)
C
C ROUTINE MUST RETURN EXCITATION RATE COEFFICIENT IF N11.LT.N AND
C DEXCITATION RATE COEFFICIENT IF N11.GT.N
C
C NOTE THAT THE RELATION BETWEEN INVERSE PROCESSES IS DETERMINED BY THE
C TEMPERATURE TP AND THE SPEED VDISP
C THE TREATMENT GIVEN IS APPROXIMATE EXCEPT IN THE LIMITS VDISP=0 OR
C VDISP >> DSQRT(2*TP/AMSIMP)
C
C INPUT

```

```

C      Z      = TARGET ION CHARGE+1
C      N11    = PRINCIPAL QUANTUM NUMBER OF INITIAL LEVEL
C      N      = PRINCIPAL QUANTUM NUMBER OF FINAL LEVEL
C      PHI    = (IH/EIJ)F(N ----> N'')
C      ZP     = PROJECTILE CHARGE
C      AMSIMP = PROJECTILE MASS (PROTON UNITS)
C      TP     = PROJECTILE ION TEMPERATURE (K)
C      VDISP  = CONSTANT MEAN SPEED SHIFT FOR THE COLLISION (CM/SEC)
C              (DESCRIBES BEAM PLASMA SITUATIONS)
C
C      OUTPUT
C      RQVNEW = RATE COEFFICIENT (CM**3 SEC-1)
C
C      ***** H.P. SUMMERS, JET                2 JUL 1991      *****
C
C      NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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: 08-02-96
C      MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C              - REMOVED SUPERFLUOUS VARIABLES
C
C-----
C
C      DIMENSION XA(9),WXA(9)
C      DIMENSION EA(24),OA(24),YA(24),FA(24)
C-----
C      GAUSS-LAGUERRE DATA (9PT)
C-----
C      DATA XA/0.1523222277D0,0.8072200227D0,2.0051351556D0,
C      &      3.7834739733D0,6.2049567778D0,9.3729852516D0,
C      &      13.4662369110D0,18.8335977889D0,26.3740718909D0/
C      DATA WXA/3.36126421798D-1,4.11213980424D-1,1.99287525371D-1,
C      &      4.74605627657D-2,5.59962661079D-3,3.05249767093D-4,
C      &      6.59212302608D-6,4.11076933035D-8,3.29087403035D-11/
C-----
C      DATA LCK,LWRK/28,160/
C-----
C      DATA NN/22/
C      DATA (EA(I),I=1,24)/1.00D3,1.50D3,2.00D3,3.00D3,5.00D3,7.00D3,
C      &      1.00D4,1.50D4,2.00D4,3.00D4,4.00D4,5.00D4,
C      &      6.00D4,7.00D4,8.00D4,1.00D5,1.50D5,2.00D5,
C      &      3.00D5,5.00D5,7.00D5,1.00D6,0.00D0,0.00D0/
C      DATA IORD,EML,ALFA /1,2.0D0,1.0D0/
C-----

```

## SIGIA

```

      SUBROUTINE SIGIA ( LSETX , LPASS ,
C      &      ALPH , ETH , ILTYP , IOPT ,
C      &      NENIN , ENIN , SGIN ,
C      &      LTHETA , VREL , XSEC
C      &      )
C      IMPLICIT NONE
C-----
C      ***** FORTRAN77 SUBROUTINE: SIGIA *****
C
C      VERSION: 1.0 (ADAS91)
C
C      PURPOSE: INTERPOLATES CROSS-SECTION DATA FROM AN INPUT VECTOR OF
C      VALUES USING CUBIC SPLINES.  EXTRAPOLATES FOR RELATIVE
C      SPEEDS OUT OF DATA RANGE ACCORDING TO VARIOUS TYPES
C      (ILTYP).  LOGARITHMIC INTERPOLATION MAY BE USED (LPASS).
C      SPEED ECONOMY IS POSSIBLE FOR REPEATS WITH THE SAME
C      SPLINE KNOTS (LSETX).
C
C      CALLING PROGRAM: CXTHER
C
C      NOTES:
C      (1) FOR ILTYP.EQ.0, EXTRAPOLATION IS AS FOLLOWS:
C
C      SUBROUTINE:
C
C      INPUT : (L*4) LSETX = .TRUE. => SPLINE NOT SET FOR THESE KNOTS
C      .FLSE. => SPLINE NOT FOR THESE KNOTS
C      INPUT : (L*4) LPASS = .TRUE. => DO NOT CONVERT INTO LOG10 FOR
C      ENERGIES AND X-SECTS. FOR SPLINE
C      .FLSE. => CONVERT INTO LOG10 FOR
C      ENERGIES AND X-SECTS. FOR SPLINE
C      INPUT : (R*8) ALPH = HIGH ENERGY EXTRAPOLATION PARAMETER
C      INPUT : (R*8) ETH = THRESHOLD ENERGY (RYD.)
C      INPUT : (I*4) ILTYP = TYPE FOR LOW AND HIGH ENERGY CROSS-
C      -SECTION EXTRAPOLATION.

```

```

C INPUT : (I*4) IOPT = SPLINE END POINT CURVATURE/GRADIENT OPTION
C 1 => DDY1 = 0, DDYN = 0
C 4 => DY1 = 0 , DDYN = 0
C
C INPUT : (I*4) NENIN = NUMBER OF ENERGIES IN INPUT DATA SET
C INPUT : (R*8) ENIN() = ENERGIES (EV/AMU) IN INPUT DATA SET
C INPUT : (R*8) SGIN() = INPUT X-SECTIONS (CM2) FROM INPUT DATA SET
C 1ST.DIM: ENERGY INDEX
C INPUT : (I*4) LTHETA = NUMBER OF VALUES IN VREL VECTOR
C INPUT : (R*8) VREL() = RELATIVE SPEEDS FOR OUTPUT (CM S-1)
C
C OUTPUT: (R*8) XSEC() = OUTPUT CROSS-SECTION (CM2)
C
C (I*4) MAXENS = PARAMETER = MAX. LENGTH OF TABULAR XSECT.
C VECTOR
C (I*4) LDTHET = PARAMETER = MAX. LENGTH OF INTERNAL
C VECTORS
C (R*8) CMSAMU = PARAMETER = CONVERSION FACTOR FOR ENERGY
C (AMU) TO VELOCITY (CM S-1)
C
C (I*4) I = GENERAL INDEX
C (I*4) N = GENERAL INDEX
C (R*8) ALPH0 = LOW VELOCITY EXTRAPOLATION PARAMETER
C (R*8) EXPON = EXPONENT OF EXPONENTIAL
C (R*8) VSLOPE = HIGH VELOCITY EXTRAPOLATION PARAMETER
C (R*8) XIN() = INTERNAL SPLINE INDEPENDENT VARIABLE
C (R*8) YIN() = INTERNAL SPLINE DEPENDENT VARIABLE
C (R*8) VIN() = INTERNAL VECTOR
C (R*8) DY() = DERIVATIVES AT SPLINE KNOTS
C (R*8) XOUT() = INTERNAL OUTPUT INDEPENDENT VARIABLE
C (R*8) YOUT() = INTERNAL OUTPUT DEPENDENT VARIABLE
C (L*4) LINTRP() = .TRUE. => POINT INTERPOLATED
C = .FALSE. => POINT EXTRAPOLATED
C
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C XXSPLE ADAS INTERPOLATES USING CUBIC SPLINES
C R8FUN1 ADAS EXTERNAL FUNCTION FOR XXSPLE
C
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL. 0141-553-4196
C
C DATE: 18/11/96
C
C VERSION: 1.1 DATE: 18-11-96
C MODIFIED: HUGH P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C - FIRST EDITION
C
C -----
C INTEGER MAXENS , LDTHET
C -----
C REAL*8 CMSAMU , ZERO
C -----
C PARAMETER ( MAXENS = 50 , LDTHET = 181 )
C PARAMETER ( CMSAMU = 1.389209D+06 , ZERO = 1.0D-30 )
C -----
C INTEGER I , N , NENIN
C INTEGER IOPT , LTHETA , ILTYP , I4UNIT
C -----
C REAL*8 ALPH0 , VSLOPE , EXPON
C REAL*8 R8FUN1 , ALPH , ETH
C -----
C LOGICAL LSETX , LPASS
C -----
C REAL*8 VREL(LTHETA) , XSEC(LTHETA)
C REAL*8 XOUT(LDTHET) , YOUT(LDTHET)
C REAL*8 ENIN(NENIN) , SGIN(NENIN) , DY(MAXENS)
C REAL*8 XIN(MAXENS) , YIN(MAXENS) , VIN(MAXENS)
C -----
C LOGICAL LINTRP(LDTHET)
C -----
C EXTERNAL R8FUN1
C -----

```

## V2BNMOD

```

C SUBROUTINE V2BNMOD(IPOSNT , JDENS , JTE , NREP , F1 ,
C & F2 , F3 , BNCALC , BNACT , XPOP ,
C & IMAX , DENSH , DENS , DENSP , TE ,
C & TP , BMENER , FLUX , DEXPTE , ALFA ,
C & S , DSLPATH , NIMP , ZIMPA , ZEFF ,
C & DNIMPA)
C
C IMPLICIT REAL*8 (A-H,O-Z)
C
C -----
C ***** FORTRAN77 SUBROUTINE: V2BNMOD *****

```

```

C
C VERSION: (ADAS91) - SEE SC CS COMMENTS FOR VERSION NO.
C
C PURPOSE: THIS CODE PERFORMS THE ACTUAL CALCULATIONS FOR ADAS 310
C IT IS IN AN INCOMPLETE VERSION AND THESE COMMENTS DO NOT
C YET FOLLOW THE STANDARD ADAS PATTERN.
C-----
C CALCULATION OF BN -1 CASE A,B
C
C EXCIT. XSECT. OPTIONS:
C-----
C (A) VAN REGEMORTER - ELECTRONS
C (B) IMPACT PARAMETER - ELECTRONS
C PROTONS
C (C) PERCIVAL-RICHARDS - ELECTRONS
C - PROTONS & ZIMP IONS
C (D) VAINSHTEIN - PROTONS & ZIMP IONS
C (E) SPECIAL LOW LEVEL - ELECTRONS
C - PROTONS & ZIMP IONS
C
C IONIS. XSECT. OPTIONS:
C-----
C (A) ECIP - ELECTRONS
C (B) PERCIVAL-RICHARDS - PROTONS & ZIMP IONS
C (C) SPECIAL LOW LEVEL - ELECTRONS
C - PROTONS & ZIMP IONS
C
C CX RECOM. XSECT. OPTIONS:
C-----
C (A) SPECIAL - H(1S) DONOR
C
C
C NOTES
C-----
C (A) SPECIAL LOW LEVEL DATA ACCESSED BY SPECIFIC ION ROUTINE
C
C ION ROUTINE ACCESSED FILE ACQUIS. ROUTINE
C-----
C H0 NSUPH1 IONATOM.DATA(H) QH
C HLIKE.DATA(AGG1984) -
C
C (B) SPECIAL CHARGE EXCHANGE DATA FROM CHEXDATA.DATA
C
C ION DONOR ROUTINE DATA MEMBER ACQUIS. ROUTINE
C-----
C H0 H(1S) BNQCTB H1NEW1 BNQCTB
C
C
C INPUT
C
C IPOSNT = 0 BYPASS
C = 1 LEAVE W1.NE.0 AND FORCE DENS.H.EQ.0
C = 2 FORCE W1.EQ.0 AND FORCE DENS.H.EQ.0
C = 3 LEAVE W1.NE.0 AND LEAVE DENS.H.NE.0
C = 4 FORCE W1.EQ.0 AND LEAVE DENS.H.NE.0
C = 5 BYPASS
C
C JDENS = DENSITY SELECTOR
C JTE = TEMPERATURE SELECTOR
C NREP(I) = PRINCIPAL QUANTUM NUMBER OF ITH REPRESENTATIVE LEVEL
C XPOP(I) = POPULATIONS OF REPRESENTATIVE LEVELS
C IMAX = NUMBER OF REPRESENTATIVE LEVELS
C DENS.H = NEUTRAL HYDROGEN DENSITY IN BEAM (CM-3)
C DENS = ELECTRON DENSITY (CM-3)
C DENSP = PROTON/DEUTERON DENSITY (CM-3)
C TE = ELECTRON TEMPERATURE (K)
C TP = PROTON/DEUTERON TEMPERATURE (K) (SAME FOR ZIMP IONS)
C BMENER = NEUTRAL BEAM PARTICLE ENERGY (EV/AMU)
C FLUX = NEUTRAL BEAM FLUX (CM-2 SEC-1)
C DEXPTE(I) = EXP(ATE/NREP(I)**2) FOR I THE REPRESENTATIVE LEVEL
C DSLPATH = STRING CONTAINING PATH TO THE REQUIRED INPUT FILES
C CALLED BY NSUPH1.FOR
C
C OUTPUT
C
C F1 =
C F2 =
C F3 =
C BNCALC =
C BNACT =
C ALPHA =
C S =
C
C INPUT SPECIFICATION FOR STREAM 51 DATA FILE
C
C NUCCHG = NUCLEAR CHARGE
C EXMEMB = DATA SET NAME OF EXPANSION FILE USED BY CLLDLBN2
C CXMEMB = DATA SET NAME FOR CHARGE EXCHANGE DATA TO BE USED BY
C BNQCTB
C IBLOCK = SUB-BLOCK SELECTOR FOR CXMEMB
C
C JDENSM = NUMBER OF DENSITIES
C JTEM = NUMBER OF TEMPERATURES
C TS = EXTERNAL RADIATION FIELD TEMPERATURE (K)
C W = EXTERNAL RADIATION FIELD DILUTION FACTOR (HIGH LEVELS)
C Z = RECOMBINING ION CHARGE (Z1 IN USUAL NOTATION)
C CION = MULTIPLIER OF GROUND LEVEL ELECTRON IMPACT IONISATION
C RATE COEFFICIENT
C CPY = MULTIPLIER ON ELECTRON IMPACT EXCITATION RATE COEFFICIENT
C FORM THE GROUND LEVEL

```

```

C      W1      = EXTERNAL RADIATION FIELD DILUTION FACTOR FOR PHOTO-IONI
C              SATION FORM THE GROUND LEVEL.
C
C      NIP      = RANGE OF DELTA N FOR IMPACT PARAMETER XSECTS. (LE.4)
C      INTD     = ORDER OF MAXWELL QUADRATURE FOR XSECTS. (LE.3)
C      IPRS     = 0  DEFAULT TO VAN REGEMORTER XSECTS. BEYOND NIP RANGE
C              1  USE PERCIVAL-RICHARDS XSECTS. BEYOND NIP RANGE
C      ILOW     = 0  NO SPECIAL LOW LEVEL DATA ACCESSED
C              1  SPECIAL LOW LEVEL DATA ACCESSED
C      IONIP    = 0  NO ION IMPACT COLLISIONS INCLUDED
C              1  ION IMPACT EXCITATION AND IONISATION INCLUDED
C      NIONIP   = RANGE OF DELTA N FOR ION IMPACT EXCITATION XSECTS.
C      ILPRS    = 0  DEFAULT TO VAINSHTEIN XSECTS.
C              1  USE LODGE-PERCIVAL-RICHARDS XSECTS.
C      IVDISP   = 0  ION IMPACT AT THERMAL MAXWELLIAN ENERGIES
C              1  ION IMPACT AT DISPLACED THERMAL ENERGIES ACCORDING
C                  TO THE NEUTRAL BEAM ENERGY PARAMETER
C                  * IF(IVDISP=0 THEN SPECIAL LOW LEVEL DATA FOR ION
C                    IMPACT IS NOT SUBSTITUTED - ONLY VAINSHTEIN AND
C                    LODGE ET AL. OPTIONS ARE OPEN. ELECTRON IMPACT
C                    DATA SUBSTITUTION DOES OCCUR.
C
C      1        = PLASMA Z EFFECTIVE
C      NOSCAN   = 0  EXECUTE SCANNING VERSION OF CODE
C              1  EXECUTE SIMULTANEOUS IMPURITY NO SCAN RUN
C      NIMP     = NUMBER OF IMPURITIES (EXCL.H+) IN NO SCAN CASE
C
C  ROUTINES:
C      ROUTINE   SOURCE   BRIEF DESCRIPTION
C      -----
C      MATINV    ADAS     MATRIX INVERSION WITH ACCOMPANYING
C                  SOLUTION OF LINEAR EQUATIONS
C      DIEL      ?????
C
C ***** H.P.SUMMERS, JET                11 APR 1990 *****
C *****                                ALT. 17 JUL 1991 SUB. RQINEW,
C *****                                RQLNEW, RQVNEW
C *****                                ALT. 10 JAN 1994 ALLOW MULTIPLE
C *****                                SIMULT.IMPURITY
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 INPUT FILE UNIT NUMBER HAS BEEN CHANGED FROM 5 TO 51.
C
C 2) THE SIZES OF 'EXMEMB' AND 'CXMEMB' HAVE BEEN INCREASED
C AS THEY NOW CONTAIN THE FULL DATA SET NAMES RATHER THAN
C JUST THE MEMBER NAMES.
C
C 3) A PARAMETER FLAG HAS BEEN ADDED TO SWITCH ON/OFF
C DIAGNOSTIC PRINTING (UNIT 6).
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: 12-12-95
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - FIRST VERSION
C - REPLACED ALL HOLLERITH CONSTANTS H0 ANF H1 WITH
C H<SPACE>
C - REPLACED HOLLERITH CONSTANTS WITH STANDARD STRINGS
C IN FORMAT STATEMENTS 117, 128 AND 129.
C - TIDIED UP PARTS OF THE COMMENTS AND CODE
C - ADDED STRING DSLPATH TO BE USED TO CONSTRUCT UNIX
C STYLE FILENAMES IN NSUPH1.FOR
C
C VERSION: 1.2 DATE: 24-01-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - ADDED NBENG TO INPUT LIST AND CALL TO BNQCTB
C
C VERSION: 1.3 DATE: 24-01-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - REVERSED ABOVE CHANGE
C
C VERSION: 1.4 DATE: 27-09-96
C MODIFIED: WILLIAM OSBORN + HUGH SUMMERS
C - REMOVED MISTAKEN TEST FOR 1.LE.0.0D0 IN
C THE CASE OF MULTIPLE IMPURITIES.
C
C VERSION: 1.5
C MODIFIED: HARVEY ANDERSON
C - IMPROVED THE HANDLING OF MULTIPLE IMPURITIES TO
C INCLUDE HYDROGEN.
C - ALTERED THE CALLING STRUCTURE OF THIS ROUTINE TO
C ALLOW ADDITIONAL VARIABLES TO BE PASSED TO RUN310.
C - INCREASED THE SIZE OF THE ARRAYS DENSA, DENPA, TEA
C AND TPA FROM 10 TO 25.
C -----
C
C PARAMETER (NDLOW=10)
C CHARACTER ELSYMB*2,SYMBA*2,EXMEMB*80,CXMEMB*80
C CHARACTER DSLPATH*80

```

```

DIMENSION EN2(550),EN3(550),DEXPTE(550),DEXPTS(550),OGARL(1100)
DIMENSION A(550),ARED(30,30),AGRL(550,3),NREP(31),INTER(550)
DIMENSION RHS(30),BREP(30),DEXPBN(30),EN23(550),FLAG(550)
DIMENSION COR(20),EPSIL(10),FIJ(10),POP(30),DEFECT(10)
DIMENSION DENSA(25),TEA(25),DENPA(25),TPA(25)
DIMENSION WIJ(10),EIJ(10),WEIJ(10)
DIMENSION PYMAT(550,4,2),DELCN(30),WBREP(30),WB(550),WBLOG(30)
DIMENSION BNCALC(30),BNACT(30),F1(30),F2(30),F3(30),XPOP(2)
DIMENSION SYMBA(30),QTHREP(31)
DIMENSION BMENA(6),BMFRA(6)
DIMENSION DVEC(30),CIONPT(30),DRECPT(30),RRECPT(30),XRECPT(30)
DIMENSION IMPA(10),ZIMPA(10),AMIMPA(10),FRIMPA(10),DNIMPA(10)

```

C

```

DIMENSION XTBE(NDLOW,NDLOW),LXTBE(NDLOW,NDLOW)
DIMENSION XTBP(NDLOW,NDLOW),LXTBP(NDLOW,NDLOW)
DIMENSION XTBZ(NDLOW,NDLOW),LXTBZ(NDLOW,NDLOW)
DIMENSION PXTBE(NDLOW),LPXTBE(NDLOW)
DIMENSION PXTBP(NDLOW),LPXTBP(NDLOW)
DIMENSION PXTBZ(NDLOW),LPXTBZ(NDLOW)
DIMENSION STBE(NDLOW),LSTBE(NDLOW)
DIMENSION STBP(NDLOW),LSTBP(NDLOW)
DIMENSION STBZ(NDLOW),LSTBZ(NDLOW)
LOGICAL  DEBUG

```

C

```

DATA SYMBA/'H ','HE','LI','BE','B ','C ','N ','O ','F ','NE',
&          'NA','MG','AL','SI','P ','S ','CL','AR','K ','CA',
&          'SC','TI','V ','CR','MN','FE','CO','NI','CU','ZN'/
NAMELIST /FILINFO/NUCCHG,EXMEMB,CXMEMB,IBLOCK

```

## XIP

```

FUNCTION XIP(XI,DELTA)
C
C   IMPLICIT REAL*8 (A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 FUNCTION: XIP *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----

```

## YIP

```

FUNCTION YIP(XI,DELTA)
C
C   IMPLICIT REAL*8 (A-H,O-Z)
C
C-----
C
C ***** FORTRAN77 FUNCTION: YIP *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
C
C   DIMENSION A(20),B(20)

```

## ZERO1

```

SUBROUTINE ZERO1(A,B,VA,VB,D1,X,XI,Z,E,TIF,T2)
C
C   IMPLICIT REAL*8 (A-H,O-Z)
C
C-----

```

```
C ***** FORTRAN77 SUBROUTINE: ZERO1 *****
C
C PURPOSE UNKNOWN
C
C NOTES: THIS ROUTINE IS NOT YET PROPERLY ANNOTATED
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-----
```