

ADAS Subroutine d7datr

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C
      SUBROUTINE D7DATR( IUNIT  , NDLEV  , NDTRN  , NDQDN  ,
&                      TITLED  , IZ     , IZ0    , IZ1    , BWNO   ,
&                      IL     , QDORB  , LQDORB , QDN    ,
&                      IA     , CSTRGA , ISA    , ILA    , XJA    , WA    ,
&                      NV     , SCEF   ,
&                      ITRAN  , MAXLEV ,
&                      TCODE  , I1A    , I2A    , AVAL   , SCOM
&                      )
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C-----
C
C ***** FORTRAN77 SUBROUTINE: D7DATR *****
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C PURPOSE:  TO FETCH DATA FROM INPUT COPASE DATA SET.  THE SUBROUTINE
C           IS AN EXTENSION TO BXDATA TO OBTAIN ORBITAL QUANTUM
C           DEFECTS.  IN ALL OTHER RESPECTS IT IS IDENTICAL TO BXDATA.
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C CALLING PROGRAM: ADAS407
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C DATA:
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C THE 'REAL' DATA IN THE FILE IS REPRESENTED IN AN ABBREVIATED
C FORM WHICH OMITTS THE "D" OR "E" EXPONENT SPECIFIER.
C e.g. 1.23D-06 or 1.23E-06 IS REPRESENTED AS 1.23-06
C      6.75D+07 or 6.75E+07 IS REPRESENTED AS 6.75+07
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C THEREFORE THE FORM OF EACH 'REAL' NUMBER IN THE DATA SET IS:
C           N.NN+NN or N.NN-NN
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C THE UNITS USED IN THE DATA FILE ARE TAKEN AS FOLLOWS:
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C IONISATION POTENTIAL: WAVE NUMBER (CM-1)
C INDEX LEVEL ENERGIES: WAVE NUMBER (CM-1)
C TEMPERATURES          : KELVIN
C A-VALUES              : SEC-1
C GAMMA-VALUES          :
C RATE COEFFT.          : CM3 SEC-1
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C SUBROUTINE:
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C INPUT : (I*4)  IUNIT  = UNIT TO WHICH INPUT FILE IS ALLOCATED
C INPUT : (I*4)  NDLEV  = MAXIMUM NUMBER OF LEVELS THAT CAN BE READ
C INPUT : (I*4)  NDTRN  = MAX. NUMBER OF TRANSITIONS THAT CAN BE READ
C INPUT : (I*4)  NDQDN  = MAX. NUMBER OF N-SHELLS FOR QUANTUM DEFECTS
C
C OUTPUT: (C*3)  TITLED  = ELEMENT SYMBOL.
C OUTPUT: (I*4)  IZ     = RECOMBINED ION CHARGE READ
C OUTPUT: (I*4)  IZ0    =          NUCLEAR CHARGE READ
C OUTPUT: (I*4)  IZ1    = RECOMBINING ION CHARGE READ
C                   (NOTE: IZ1 SHOULD EQUAL IZ+1)
C OUTPUT: (R*8)  BWNO   = IONISATION POTENTIAL (CM-1)
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C
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C OUTPUT: (I*4) IL = INPUT DATA FILE: NUMBER OF ENERGY LEVELS
C OUTPUT: (R*8) QDORB() = QUANTUM DEFECTS FOR ORBITALS
C
C 1ST DIM: INDEX FOR NL ORBITAL (CF INDX)
C OUTPUT: (L*4) LQDORB() = .TRUE. => SOURCE DATA AVAILABLE FOR QD.
C
C = .FALSE. => SOURCE DATA NOT AVAILABE QD.=0.0
C OUTPUT: (R*8) QDN() = QUANTUM DEFECT FOR N-SHELLS. NON-ZERO ONLY
C
C FOR ADF04 FILES WITH ORBITAL ENERGY DATA
C
C 1ST. DIM: N-SHELL (1<=N<=NDQDN)
C
C OUTPUT: (I*4) IA() = ENERGY LEVEL INDEX NUMBER
C OUTPUT: (C*18) CSTRGA() = NOMENCLATURE/CONFIGURATION FOR LEVEL 'IA()'
C OUTPUT: (I*4) ISA() = MULTIPLICITY FOR LEVEL 'IA()'
C
C NOTE: (ISA-1)/2 = QUANTUM NUMBER (S)
C OUTPUT: (I*4) ILA() = QUANTUM NUMBER (L) FOR LEVEL 'IA()'
C OUTPUT: (R*8) XJA() = QUANTUM NUMBER (J-VALUE) FOR LEVEL 'IA()'
C
C NOTE: (2*XJA)+1 = STATISTICAL WEIGHT
C OUTPUT: (R*8) WA() = ENERGY RELATIVE TO LEVEL 1 (CM-1) FOR LEVEL
C
C 'IA()'
C
C OUTPUT: (I*4) NV = INPUT DATA FILE: NUMBER OF GAMMA/TEMPERATURE
C
C PAIRS FOR A GIVEN TRANSITION.
C OUTPUT: (R*8) SCEF() = INPUT DATA FILE: ELECTRON TEMPERATURES (K)
C
C (INITIALLY JUST THE MANTISSA. SEE 'ITPOW()')
C
C (NOTE: TE=TP=TH IS ASSUMED)
C
C OUTPUT: (I*4) ITRAN = INPUT DATA FILE: NUMBER OF TRANSITIONS
C OUTPUT: (I*4) MAXLEV = HIGHEST INDEX LEVEL IN READ TRANSITIONS
C
C OUTPUT: (C*1) TCODE() = TRANSITION: DATA TYPE POINTER:
C
C ' ' => Electron Impact Transition
C
C 'P' => Proton Impact Transition
C
C 'H' => Charge Exchange Recombination
C
C 'R' => Free Electron Recombination
C OUTPUT: (I*4) I1A() = TRANSITION:
C
C LOWER ENERGY LEVEL INDEX (CASE ' ' & 'P')
C
C SIGNED PARENT INDEX (CASE 'H' & 'R')
C OUTPUT: (I*4) I2A() = TRANSITION:
C
C UPPER ENERGY LEVEL INDEX (CASE ' ' & 'P')
C
C CAPTURING LEVEL INDEX (CASE 'H' & 'R')
C OUTPUT: (R*8) AVAL() = TRANSITION:
C
C A-VALUE (SEC-1) (CASE ' ')
C
C NEUTRAL BEAM ENERGY (CASE 'H')
C
C NOT USED (CASE 'P' & 'R')
C OUTPUT: (R*8) SCOM(,) = TRANSITION:
C
C GAMMA VALUES (CASE ' ' & 'P')
C
C RATE COEFFT. (CM3 SEC-1) (CASE 'H' & 'R')
C
C 1ST DIMENSION - TEMPERATURE 'SCEF()'
C
C 2ND DIMENSION - TRANSITION NUMBER
C
C
C (I*4) NVMAX = PARAMETER = MAX. NUMBER OF TEMPERATURES
C
C THAT CAN BE READ IN.
C
C (I*4) MTIED = PARAMETER = MUST BE GREATER THAN OR EQUAL TO
C
C THE MAX. NO. OF LEVELS.

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C (R*8) DZERO = PARAMETER = MINIMUM VALUE FOR 'AVAL()' AND
C 'SCOM()' ARRAYS = 1.0D-30
C
C (I*4) I4UNIT = FUNCTION (SEE ROUTINE SECTION BELOW)
C (I*4) IQS = X-SECT DATA FORMAT SELECTOR
C NOTE: IQS=3 ONLY ALLOWED IN THIS PROGRAM
C (I*4) I = GENERAL USE.
C (I*4) IABT = RETURN CODE FROM 'R8FCTN' (0 => NO ERROR)
C OR FROM INTERROGATION OF 'C7'
C (I*4) IFIRST = BYTE POSITION OF START OF NUMBER IN BUFFER
C (I*4) ILAST = BYTE POSITION OF END OF NUMBER IN BUFFER
C (I*4) INDX = INDEXING FUNCTION FOR NL ORBITALS IN
C QDORB() AS INDX(N,L)
C (I*4) IORB = ORBITAL INDEX
C (I*4) IWORD = THE WORD POSITION OF THE REQUIRED DATA IN
C A STRING TO BE INTERROGATED BY XXWORD.
C (I*4) J = GENERAL USE.
C (I*4) J1 = INPUT DATA FILE - SELECTED TRANSITION:
C LOWER ENERGY LEVEL INDEX (CASE ' ' & 'P')
C (I*4) J2 = INPUT DATA FILE - SELECTED TRANSITION:
C UPPER ENERGY LEVEL INDEX (CASE ' ' & 'P')
C CAPTURING LEVEL INDEX (CASE 'H' & 'R')
C (I*4) K = GENERAL USE
C (I*4) L = GENERAL USE FOR ORBITAL L
C (I*4) L1 = GENERAL USE
C (I*4) LENCST = BYTE LENGTH OF STRING CSTRGA()
C (R*8) NLAST = N-SHELL MARKER FOR ORBITALS
C (I*4) NWORDS = NUMBER OF NUMBERS STORED IN BUFFER
C (I*4) ILINE = ENERGY LEVEL INDEX FOR CURRENT LINE
C (I*4) IAPOW = EXPONENT OF 'AVALM'
C (I*4) IGPOW() = EXPONENT OF 'GAMMA()'
C (I*4) ITPOW() = TEMPERATURES - EXPONENT
C NOTE: MANTISSA INITIALLY KEPT IN 'SCEF()'
C
C (R*4) ZF = SHOULD BE EQUIVALENT TO 'IZ1'
C
C (R*8) AVALM = INPUT DATA FILE - SELECTED TRANSITION:
C MANTISSA OF: ('IAPOW' => EXPONENT)
C A-VALUE (SEC-1) (CASE ' ')
C NEUTRAL BEAM ENERGY (CASE 'H')
C NOT USED (CASE 'P' & 'R')
C (R*8) GAMMA() = INPUT DATA FILE - SELECTED TRANSITION:
C MANTISSA OF: ('IGPOW()') => EXPONENT)
C GAMMA VALUES (CASE ' ' & 'P')
C RATE COEFFT. (CM3 SEC-1) (CASE 'H' & 'R')
C DIMENSION => TEMPERATURE 'SCEF()'
C (R*8) QDORB() = QUANTUM DEFECTS FOR ORBITALS
C 1ST DIM: INDEX FOR NL ORBITAL (CF INDX)
C
C (C*7) C7 = USED TO PARSE VALUE FOR XJA()
C (C*7) CDELIM = DELIMITERS FOR INPUT OF DATA FROM HEADERS
C (C*18) C18 = USED TO PARSE VALUE TO CSTRGA()
C (C*80) CLINE = CURRENT ENERGY LEVEL INDEX PARAMETER LINE

C (C*128) BUFFER = GENERAL STRING BUFFER STORAGE
 C (C*3) CITPOW() = USED TO PARSE VALUES TO ITPOW()
 C (C*5) CSCEF() = USED TO PARSE VALUES TO SCEF()
 C (C*7) CFORM7 = FORMAT FOR INTERNAL READING OF REAL NUMBER
 C
 C (L*4) LDATA = IDENTIFIES WHETHER THE END OF AN INPUT
 C SECTION IN THE DATA SET HAS BEEN LOCATED.
 C (.TRUE. => END OF SECTION REACHED)
 C (L*4) LTCHR = .TRUE. => CURRENT 'TCODE()' = 'H' OR 'R'.
 C = .FALSE. => CURRENT 'TCODE()' .NE.'H' OR 'R'.
 C (L*4) LTCPR = .TRUE. => CURRENT 'TCODE()' = 'P' OR 'R'.
 C = .FALSE. => CURRENT 'TCODE()' .NE.'P' OR 'R'.
 C (L*4) LERROR = .TRUE. => UNTIED LEVEL FOUND
 C = .FALSE. => ALL LEVELS TIED
 C (L*4) LTIED() = .TRUE. => SPECIFIED LEVEL TIED
 C = .FALSE. => SPECIFIED LEVEL IS UNTIED
 C DIMENSION => LEVEL INDEX
 C (L*4) LQDORB() = .TRUE. => SOURCE DATA AVAILABLE FOR QD.
 C = .FALSE. => SOURCE DATA NOT AVAILABE QD.=0.0
 C

C ROUTINES:

ROUTINE	SOURCE	BRIEF DESCRIPTION
XXWORD	ADAS	EXTRACT POSITION OF NUMBER IN BUFFER
I4UNIT	ADAS	FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
R8FCTN	ADAS	CONVERTS FROM CHARACTER TO REAL VARIABLE
INDX	INTRINSIC	INDEXES NL ORBITAL IN QDORB() ARRAY

NOTE:	LTCHR	LTCPR	TCODE()
	.TRUE.	.TRUE.	=> 'R'
	.TRUE.	.FALSE.	=> 'H'
	.FALSE.	.TRUE.	=> 'P'
	.FALSE.	.FALSE.	=> ' '

C FOR A-VALUES & GAMMA-VALUES ENTRIES LESS THAN 'DZERO' ARE TAKEN
 C AS BEING EQUAL TO DZERO. THIS AFFECTS THE 'AVAL()' AND 'SCOM()'
 C ARRAYS.
 C
 C

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C - PUT UNDER SCCS CONTROL.

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C

CHARACTER* (*)	CSTRGA (NDLEV)			
CHARACTER	TCODE (NDTRN)			
CHARACTER*3	TITLED			
INTEGER	I1A (NDTRN) ,	I2A (NDTRN) ,	IA (NDLEV) ,	IL
INTEGER	ILA (NDLEV) ,	ISA (NDLEV) ,	ITRAN ,	IUNIT
INTEGER	IZ ,	IZ0 ,	IZ1 ,	MAXLEV
INTEGER	NDLEV ,	NDQDN ,	NDTRN ,	NV
LOGICAL	LQDORB ((NDQDN* (NDQDN+1)) /2)			
REAL*8	AVAL (NDTRN) ,	BWNO ,	QDN (NDQDN)	
REAL*8	QDORB ((NDQDN* (NDQDN+1)) /2)			
REAL*8	SCEF (NVMAX) ,	SCOM (NVMAX , NDTRN)		
REAL*8	WA (NDLEV) ,	XJA (NDLEV)		