

ADAS Subroutine xxdata_09

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SUBROUTINE xxdata_09( IUNIT , NDPRT , NDREP , NDLEV ,
&
&                      NDAUG , NDT ,
&                      SEQSYM , IZ , IZ0 , IZ1 ,
&                      NPRNT , NPRNTI , NPRNTF , BWNP ,
&                      IPA , CSTRPA , ISPA , ILPA , XJPA ,
&                      WPA ,
&                      IL , BWRN ,
&                      IA , CSTRGA , ISA , ILA , XJA ,
&                      WA ,
&                      NREP , IAPRS , CAPRS , IPAUG ,
&                      IREPA , NREPA , AUGA , LAUGA ,
&                      IPRTI , TPRTI , ISPRTI , DIELR , LDIELR ,
&                      IPRTF , TPRTF , ISPRTF ,
&                      NSYSF , ISYS , ISPSYS , DIELN , LDIELN ,
&                      DIELT ,
&                      NTE , TEA , AATP , DTOT
&                      )

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C
C ***** FORTRAN77 SUBROUTINE: DADATA *****
C
C PURPOSE: TO FETCH DATA FROM INPUT ADF09 DATA SET.
C
C CALLING PROGRAM:
C
C
C SUBROUTINE:
C
C INPUT : (I*4) IUNIT = UNIT TO WHICH INPUT FILE IS ALLOCATED
C
C INPUT : (I*4) NDPRT = MAXIMUM NUMBER OF PARENT STATES
C INPUT : (I*4) NDREP = MAX. NUMBER OF REPRESENTATIVE N-SHELLS
C INPUT : (I*4) NDLEV = MAXIMUM NUMBER OF RESOLVED LEVELS
C INPUT : (I*4) NDAUG = MAXIMUM NUMBER OF AUGER RATE INITIAL AND
C                      FINAL PARENT PAIRS
C INPUT : (I*4) NDT = MAX. NUMBER OF ELECTRON TEMPERATURES
C
C OUTPUT: (C*2) SEQSYM = RECOMBINED ION SEQ
C OUTPUT: (I*4) IZ = RECOMBINED ION CHARGE
C OUTPUT: (I*4) IZ0 = NUCLEAR CHARGE
C OUTPUT: (I*4) IZ1 = RECOMBINING ION CHARGE
C OUTPUT: (I*4) NPRNT = TOTAL NUMBER OF PARENTS
C OUTPUT: (I*4) NPRNTI = NUMBER OF PARENTS WHICH ARE INITIAL PARENTS
C OUTPUT: (I*4) NPRNTF = NUMBER OF PARENTS WHICH ARE FINAL PARENTS
C OUTPUT: (R*8) BWNP = BINDING WAVE NO. OF GROUND PARENT (CM-1)
C OUTPUT: (I*4) IPA() = NUMBER OF PARENT ENERGY LEVELS
C OUTPUT: (C*18) CSTRPA() = NOMENCL./CONFIG. FOR PARENT LEVEL 'IPA()'
C OUTPUT: (I*4) ISPA() = MULTIPLICITY FOR PARENT LEVEL 'IPA()'
C                      NOTE: (ISPA-1)/2 = QUANTUM NUMBER (SP)
C OUTPUT: (I*4) ILPA() = QUANTUM NUMBER (LP) FOR PARENT LEVEL 'IPA()'
C OUTPUT: (R*8) XJPA() = QUANTUM NUMBER (JP) FOR PARENT LEVEL 'IPA()'
C                      NOTE: (2*XJPA)+1 = STATISTICAL WEIGHT
C

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C OUTPUT: (R*8) WPA() = ENERGY RELATIVE TO PARENT LEVEL 1 (CM-1)
C FOR PARENT LEVEL 'IPA()'
C
C OUTPUT: (I*4) IL = NUMBER OF ENERGY LEVELS (TERMS) OF
C RECOMBINED ION
C OUTPUT: (R*8) BWNR = IONISATION POTENTIAL (CM-1) OF LOWEST LEVEL
C OF RECOMBINED ION
C OUTPUT: (I*4) IA() = RECOMBINED ION ENERGY LEVEL INDEX NUMBER
C OUTPUT: (I*4) IP() = ???
C OUTPUT: (C*18) CSTRGA() = NOMENCL./CONFIG. FOR RECOMBINED ION LEVEL
C 'IA()'
C OUTPUT: (I*4) ISA() = MULTIPLICITY FOR RECOMBINED LEVEL 'IA()'
C NOTE: (ISA-1)/2 = QUANTUM NUMBER (S)
C OUTPUT: (I*4) ILA() = QUANTUM NUMBER (L) FOR RECOMBINED LEVEL
C 'IA()'
C OUTPUT: (R*8) XJA() = QUANTUM NUMBER (J) FOR RECOMBINED LEVEL
C 'IA()'
C NOTE: (2*XJA)+1 = STATISTICAL WEIGHT
C OUTPUT: (R*8) WA() = ENERGY RELATIVE TO RECOMBINED LEVEL 1 (CM-1)
C FOR RECOMBINED LEVEL 'IA()'
C OUTPUT: (I*4) NREP = NUMBER OF REPRESENTATIVE N-SHELLS
C OUTPUT: (I*4) IREPA() = REPRESENTATIVE N-SHELL INDEX NUMBER
C OUTPUT: (I*4) NREPA() = REPRESENTATIVE N-SHELLS
C OUTPUT: (I*4) IAPRS = NUMBER OF AUGER RATE INITIAL AND FINAL
C PARENT PAIRS
C OUTPUT: (C*10) CAPRS() = AUGER RATE PARENT PAIR STRING
C 1ST.DIM: PARENT PAIR INDEX
C OUTPUT: (I*40) IPAUG(,) = INITIAL AND FINAL PARENTS FOR AUGER BREAKUPS
C 1ST.DIM: PARENT PAIR INDEX
C 2ND.DIM: INITIAL AND FINAL PARENT INDICES
C OUTPUT: (R*8) AUGA(,) = AUGER RATES (SEC-1)
C 1ST.DIM: REPRESENTATIVE N-SHELL INDEX
C 2ND.DIM: PARENT PAIR INDEX
C OUTPUT: (L*4) LAUGA(,) = .TRUE. => AUGER RATE PRESENT FOR N-SHELL
C .FALSE.=> AUGER RATE NOT PRESENT
C 1ST.DIM: REPRESENTATIVE N-SHELL INDEX
C 2ND.DIM: PARENT PAIR INDEX
C OUTPUT: (I*4) IPRTI() = INITIAL PARENT BLOCK INDEX
C OUTPUT: (C*5) TPRTI() = INITIAL PARENT BLOCK TERM
C OUTPUT: (I*4) ISPRTI() = INITIAL PARENT BLOCK SPIN MULTIPLICITY
C OUTPUT: (R*8) TEA() = ELECTRON TEMPERATURES (K)
C OUTPUT: (R*8) DIELR(,,) = TERM SELECTIVE DIELEC. COEFFTS.(CM3 S-1)
C 1ST.DIM: LEVEL INDEX
C 2ND.DIM: INITIAL PARENT INDEX
C 3RD.DIM: TEMPERATURE INDEX
C OUTPUT: (L*4) LDIELR(,) = .TRUE. => DIEL. PRESENT FOR LEVEL INDEX
C .FALSE.=> DIEL. NOT PRESENT FOR LEVEL INDEX
C 1ST.DIM: LEVEL INDEX
C 2ND.DIM: INITIAL PARENT INDEX
C OUTPUT: (I*4) IPRTF(,) = FINAL PARENT BLOCK INDEX
C OUTPUT: (C*5) TPRTF(,) = FINAL PARENT BLOCK TERM
C OUTPUT: (I*4) ISPRTF(,) = FINAL PARENT BLOCK SPIN MULTIPLICITY
C OUTPUT: (I*4) NSYSF(,) = NO, . OF SPIN SYSTEMS BUILT ON FINAL PARENT

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C OUTPUT: (I*4) ISYS(,,) = N-SHELL SPIN SYSTEM INDEX FOR FINAL PARENT
C OUTPUT: (I*4) ISPSYS(,,)=N-SHELL SPIN SYSTEM FOR FINAL PARENT
C OUTPUT: (R*8) DIELN(,,,,) =N-SHELL DIELEC. COEFFTS.(CM3 S-1)
C           1ST.DIM: REPR. N-SHELL INDEX
C           2ND.DIM: INITIAL PARENT INDEX
C           3RD.DIM: FINAL PARENT INDEX
C           4TH.DIM: SPIN SYSTEM INDEX
C           5TH.DIM: TEMPERATURE INDEX
C OUTPUT: (R*8) LDIELN(,) = .TRUE. => DIEL. PRESENT FOR REPR. N-SHELL
C           .FALSE.=> DIEL. NOT PRESENT FOR N-SHELL
C           1ST.DIM: REPR. N-SHELL INDEX
C           2ND.DIM: INITIAL PARENT INDEX
C           3RD.DIM: FINAL PARENT INDEX
C           4TH.DIM: SPIN SYSTEM INDEX
C OUTPUT: (R*8) DIELT(,,,,) =N-SHELL DIELEC. COEFFTS.(CM3 S-1)
C           1ST.DIM: INITIAL PARENT INDEX
C           2ND.DIM: FINAL PARENT INDEX
C           3RD.DIM: SPIN SYSTEM INDEX
C           4TH.DIM: TEMPERATURE INDEX
C OUTPUT: (R*8) AATP() =SPECIFIC METASTABLE TO METASTABLE SEC.
C           AUGER PATHS FOR TERMS
C OUTPUT: (R*8) DTOT(,,,,) =TOTAL DR COEFFICINETS (CM3 S-1) TABULATED
C           AT BOTTOM OF FILE
C           1ST.DIM: INITIAL PARENT INDEX
C           2ND.DIM: ELECTRON TEMPERATURE INDEX
C
C           (I*4)  INDX      = GENERAL INDEX
C           (I*4)  INDX1    = GENERAL INDEX
C           (I*4)  II       = GENERAL INDEX
C           (I*4)  I        = GENERAL INDEX
C           (I*4)  IPI      = GENERAL INDEX
C           (I*4)  IPF      = GENERAL INDEX
C           (I*4)  IPFS     = GENERAL INDEX
C           (I*4)  J        = GENERAL INDEX
C           (I*4)  K        = GENERAL INDEX
C           (I*4)  IFORM    = FORMAT OF FILE:
C                           1: LS 93 DATA
C                           2: LS 00 DATA
C                           3: IC 00 DATA
C
C           (L)    LDATA    = GENERAL READ/DO NOT READ FLAG
C           (L)    LNOPI    = FLAG TO DETERMINE WHETHER HAVE PASSED
C           INTO A NEW INITIAL PARENT BLOCK
C
C           (C*20) C20      = GENERAL CHARACTER STRING
C
C ROUTINES:
C           ROUTINE      SOURCE      BRIEF DESCRIPTION
C           -----
C           I4UNIT       ADAS        FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C           I4EIZ0       ADAS        RETURNS NUCL. CHARGE FROM ELEMENT SYMBOL
C           R8FCTN       ADAS        CONVERTS FROM CHARACTER TO REAL VARIABLE
C           XXWORD       ADAS        EXTRACT POSITION OF NUMBER IN BUFFER

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C DASUMD ADAS SUM DR OVER REPRESANTITIVE N-SHELLS
 C
 C
 C BASED ON DADATA V1.2
 C
 C AUTHOR: A D WHITEFORD, UNIVERSITY OF STRATHCLYDE
 C
 C DATE: 02/05/05
 C
 C-----
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CHARACTER*10	CAPRS (NDAUG)	
CHARACTER* (*)	CSTRGA (NDLEV) ,	CSTRPA (NDPRT)
CHARACTER*2	SEQSYM	
CHARACTER*5	TPRTF (NDPRT, NDPRT) ,	TPRTI (NDPRT)
INTEGER	IA (NDLEV) , IAPRS,	IL
INTEGER	ILA (NDLEV) , ILPA (NDPRT) ,	IPA (NDPRT)
INTEGER	IPAUG (NDAUG, 2) ,	IPRTF (NDPRT, NDPRT)
INTEGER	IPRTI (NDPRT) ,	IREPA (NDREP)
INTEGER	ISA (NDLEV) , ISPA (NDPRT) ,	ISPRTF (NDPRT, NDPRT)
INTEGER	ISPRTI (NDPRT)	
INTEGER	ISPSYS (NDPRT, NDPRT, 2) ,	ISYS (NDPRT, NDPRT, 2)
INTEGER	IUNIT, IZ,	IZ0, IZ1
INTEGER	NDAUG, NDLEV,	NDPRT, NDREP
INTEGER	NDT, NPRNT,	NPRNTF, NPRNTI
INTEGER	NREP, NREPA (NDREP)	
INTEGER	NSYSF (NDPRT, NDPRT) ,	NTE
LOGICAL	LAUGA (NDREP, NDAUG)	
LOGICAL	LDIELN (NDREP, NDPRT, NDPRT, 2)	
LOGICAL	LDIELR (NDLEV, NDPRT)	
REAL*8	AATP (NDLEV, NDPRT) ,	AUGA (NDREP, NDAUG)
REAL*8	BWNP, BWRN	
REAL*8	DIELN (NDREP, NDPRT, NDPRT, 2, NDT)	
REAL*8	DIELR (NDLEV, NDPRT, NDT)	
REAL*8	DIELT (NDPRT, NDPRT, 2, NDT) ,	DTOT (NDPRT, NDT)
REAL*8	TEA (NDT) , WA (NDLEV) ,	WPA (NDPRT)
REAL*8	XJA (NDLEV) , XJPA (NDPRT)	