

ADAS Subroutine d7alFs

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      SUBROUTINE D7ALFS( NDMET , NDCONF , NDTHET , ndlev , ndrtn ,
&                      IODIMD , IPMET  , IPMETR , IZ      , IZ0    ,
&                      NTHETA , THETA  , ITREF  , IGRPA  ,
&                      NORB   , VORB   , iz1    ,
&                      il     , ia     , isa    , xja    , wa     ,
&                      cstrga , icnte  , aval   , iela   , ie2a   ,
&                      NCUT   , N0A    , PARMR  ,
&                      ALFRA  , ALFRA0 , ALFRAR , ALRAPX ,
&                      NCONFIG ,
&                      WVMIN  , WVMAX  ,
&                      ECF    , FCF    , PCF    , WCF    , W      ,
&                      NCF    , LCF    , NDCF    , LDCF    , NDMIN  ,
&                      E      , DE0    , DE     , FM0    , FM     ,
&                      IINAA  , IIPNAA , NCTAA  , NCTAAC , ECTAA  ,
&                      NTRANS , ITYPE  , N1A    , NCUTT  , PARMD  ,
&                      ALFDA  , ALFPART, AGNGPX ,
&                      KGRPA  , NSYS
&                      )
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C
C ***** FORTRAN77 SUBROUTINE: D7ALFS *****
C
C
C PURPOSE:
C
C     (1) CALCULATES RADIATIVE AND DIELECTRONIC VALUES AND
C         PARAMETERS FROM SPECIFIC ION FILES WHICH HAVE EISSNER
C         CONFIGURATION NOTATION
C
C     (2) CONSIDERS METASTABLE LEVEL INDICES AND EVALUATES NCUT
C         IDENTIFIES DIPOLE TRANSITION OF TYPE DN=0 AND DN>0
C         EVALUATES OSCILLATOR STRENGTHS AND AVERAGE ENERGY
C         OF TRANSITION
C
C     (3) SEPARATES TRANSITION ARRAYS FOR EACH METASTABLE AND
C         EVALUATES WAVELENGTH RANGES OF TRANSITION ARRAYS
C
C     (4) EVALUATES POWER IN EACH TRANSITION ARRAY
C
C     (5) CALCULATES IONISATION, RADIATIVE & DIELECTRONIC
C         RECOMBINATION VALUES AND PARAMETERS.
C
C
C CALLING PROGRAM: ADAS407
C
C SUBROUTINE:
C
C INPUT : (I*4)  IUNIT    = UNIT NUMBER FOR SPECIFIC ION FILE FOR
C INPUT : (I*4)  NDMET    = MAXIMUM NUMBER OF METASTABLES ALLOWED
C INPUT : (I*4)  NDTHET   = MAXIMUM NUMBER OF TEMPS. FOR MAINCL FILE
C INPUT : (I*4)  NDCONF   = MAXIMUM NUMBER OF CONFIGURATIONS OR
C                          DIPOLE TRANSITIONS PER PARENT ALLOWED
C INPUT : (I*4)  IODIMD   = MAXIMUM NUMBER OF ORBITALS
C
C INPUT : (I*4)  NPMET    = NO. OF RECOMBINING ION (PARENT) METASTABLES
C INPUT : (I*4)  IPMETR() = INDICES OF RECOMBINING ION (PARENT)
C                          METASTABLES IN LEVEL LIST
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C
C INPUT : (I*4)  IZ      = RECOMBINING ION CHARGE
C INPUT : (I*4)  IZ0    = NUCLEAR CHARGE
C
C INPUT : (I*4)  NTHETA  = NUMBER OF TEMPERATURES FOR MAINCL FILE
C INPUT : (R*8)  THETA() = Z-SCALED TEMPERATURES FOR MAINCL FILE
C INPUT : (I*4)  ITREF   = MAINCL TEMPERATURE INDEX FOR MATCHING
C
C INPUT : (I*4)  IGRPA() = NUMBER OF ELECTRONS ALLOWED IN EACH SHELL
C                        1ST DIM: SHELL INDEX (1=1S, 2=2S ETC)
C
C INPUT : (R*8)  NORB    = NUMBER OF ELECTRON ORBITALS REQUIRED
C INPUT : (R*8)  VORB()  = EFFECT. PRINC. QUANT. NO. FOR ORBITAL
C                        1ST DIM: SHELL INDEX (1=1S, 2=2S ETC)
C OUTPUT: (I*4)  N0A(,)  = LOWEST ALLOWED N-SHELL
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: SPIN SYSTEM INDEX
C I/O   : (R*4)  PARMR(,,) = PARAMETERS OF RADIATIVE RECOMBINATION
C                        APPROXIMATE FORMS
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: SPIN SYSTEM INDEX
C                        3RD DIM: PARMS.  1: EFF. N FOR LOWEST LEVEL
C                                           2: PHASE SPACE FACTOR
C                                           3: ENERGY DISPLACEMENT
C                                           4: SCALING MULTIPLIER
C OUTPUT: (R*8)  ALFRA(,,) = TOTAL RADIATIVE RECOMB. COEFFTS. (CM3 S-1)
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: SPIN SYSTEM INDEX
C                        3RD DIM: TEMPERATURE INDEX
C OUTPUT: (R*8)  ALFRA0(,,) = GROUND RADIATIVE RECOMB. COEFFTS. (CM3 S-1)
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: SPIN SYSTEM INDEX
C                        3RD DIM: TEMPERATURE INDEX
C OUTPUT: (R*8)  ALFRAR(,,) = EXCIT. RADIATIVE RECOMB. COEFFTS. (CM3 S-1)
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: SPIN SYSTEM INDEX
C                        3RD DIM: TEMPERATURE INDEX
C OUTPUT: (R*8)  ALFRAPX() =
C OUTPUT: (I*4)  NCONFIG  = NUMBER OF CONFIGURATIONS
C
C OUTPUT: (R*8)  WVMIN(,) = MINIMUM WAVELENGTH FOR TRANSITION ARRAY (A)
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: CONFIGURATION INDEX
C OUTPUT: (R*8)  WVMAX(,) = MAXIMUM WAVELENGTH FOR TRANSITION ARRAY (A)
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: CONFIGURATION INDEX
C OUTPUT: (R*8)  ECF(,)   = AVERAGE ENERGY FOR TRANSITION ARRAY (RYD)
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: CONFIGURATION INDEX
C OUTPUT: (R*8)  FCF(,)   = SUMMED OSCIL. STRENGTH FOR TRANSITION ARRAY
C                        1ST DIM: PARENT INDEX
C                        2ND DIM: CONFIGURATION INDEX
C OUTPUT: (R*8)  PCF(,)   = RADIATED POWER FOR TRANSITION ARRAY AT

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C             SELELECTED TEMPERATURE (CF. ITSEL)
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (R*8) WCF(,) = STATISTICAL WEIGHT FOR UPPER SHELL OF ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (R*8) W() = STATISTICAL WEIGHT FOR PARENT
C             1ST DIM: PARENT INDEX
C OUTPUT: (I*4) NCF(,) = N-SHELL OF ACTIVE ELEC. IN PARENT FOR ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (I*4) LCF(,) = L-SHELL OF ACTIVE ELEC. IN PARENT FOR ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (I*4) NDCF(,) = N-SHELL CHANGE OF ACTIVE ELECTRON FOR ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (I*4) LDCF(,) = L-SHELL CHANGE OF ACTIVE ELECTRON FOR ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (I*4) NDMIN() = ?
C             1ST DIM: PARENT INDEX
C OUTPUT: (R*8) E() = AVERAGE ENERGY FOR TRANSITION ARRAY (RYD)
C             1ST DIM: PARENT INDEX
C OUTPUT: (R*8) DE0() = MEAN DELTA N = 0 TRANSITION ENERGY (CM-1)
C             1ST DIM: PARENT INDEX
C OUTPUT: (R*8) DE() = MEAN DELTA N > 0 TRANSITION ENERGY (CM-1)
C             1ST DIM: PARENT INDEX
C OUTPUT: (R*8) FM0() = DELTA N = 0 OSCILLATOR STRENGTH
C             1ST DIM: PARENT INDEX
C OUTPUT: (R*8) FM() = DELTA N > 0 OSCILLATOR STRENGTH
C             1ST DIM: PARENT INDEX
C OUTPUT: (I*4) IINAA(,) = UPP. LEVEL INDEX OF DIPOLE TRANS FOR ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (I*4) IIPNAA(,) = PAR. LEVEL INDEX OF DIPOLE TRANS FOR ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (I*4) NCTAA(,) = ?
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (I*4) NCTAAC(,) = SECONDARY AUGER N-SHELL CUT-OFF FOR ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C OUTPUT: (R*8) ECTAA(,) = IONIS. ENERGY CUT-OFF (CM-1) FOR ARRAY
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX
C
C OUTPUT: (I*4) NTRANS() = NUMBER OF DIPOLE TRANSITIONS FOR PARENT
C             1ST DIM: PARENT INDEX
C OUTPUT: (I*4) ITYPE(,) = TYPE OF DIELECTRONIC CORE TRANSITION
C             1ST DIM: PARENT INDEX
C             2ND DIM: CONFIGURATION INDEX

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C OUTPUT: (I*4) N1A(,) = LOWEST ALLOWED N-SHELL VIA DIELECTRONIC
C TRANSITION
C 1ST DIM: PARENT INDEX
C 2ND DIM: CONFIGURATION INDEX
C OUTPUT: (I*4) NCUTT() = N-SHELL ALT. AUG. CUT-OFF FOR DIELECTRONIC
C TRANSITION
C 1ST DIM: PARENT INDEX
C 2ND DIM: CONFIGURATION INDEX
C OUTPUT: (R*4) PARMD(,,) = PARAMETERS OF DIELECTRONIC RECOMBINATION
C APPROXIMATE FORMS
C 1ST DIM: PARENT INDEX
C 3RD DIM: PARMS. 1: EFF. N FOR LOWEST LEVEL
C 2: PHASE SPACE FACTOR
C 3: ENERGY DISPLACEMENT
C 4: SCALING MULTIPLIER
C 5: EFF. N FOR LOWEST LEVEL
C 6: PHASE SPACE FACTOR
C 7: ENERGY DISPLACEMENT
C 8: SCALING MULTIPLIER
C 9: ENERGY DISPLACEMENT
C 10: SCALING MULTIPLIER
C 3RD DIM: CONFIGURATION INDEX
C OUTPUT: (R*8) ALFDA(,) = TOTAL DIELECTRONIC RECOMB. COEFFTS. WITHOUT
C SPIN SYSTEM DIVISION (CM3 S-1)
C 1ST DIM: PARENT INDEX
C 3RD DIM: TEMPERATURE INDEX
C OUTPUT: (R*8) ALFPART(,)=PARTIAL DIELECT. RECOMB. COEFFTS. (CM3 S-1)
C 1ST DIM: PARENT INDEX
C 2ND DIM: CONFIGURATION INDEX
C 3RD DIM: TEMPERATURE INDEX
C OUTPUT: (R*8) AGNGPX() = ?
C
C OUTPUT: (I*4) NIA() = ?
C OUTPUT: (I*4) LIA() = ?
C OUTPUT: (R*8) WIA() = ?
C OUTPUT: (I*4) NIA() = ?
C OUTPUT: (I*4) LIA() = ?
C OUTPUT: (R*8) WIA() = ?
C OUTPUT: (R*8) WIA() = ?
C
C OUTPUT: (I*4) KGRPA() = INDEX POINTER TO ELECTRON ORBITALS.
C OUTPUT: (I*4) NSYS() = NUMBER OF SPIN SYSTEMS (1 OR 2)
C 1ST DIM: PARENT INDEX
C OUTPUT: (I*4) NCUT() = N-SHELL CUT-OFF
C 1ST DIM: PARENT INDEX
C
C
C NOTE:
C
C ROUTINES:
C ROUTINE SOURCE BRIEF DESCRIPTION
C -----
C NVGOEL ADAS CALC. RAD. RECOM. COEFFTS. TO N-SHELLS

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C GPCALL ADAS CALC. DIELECTRONIC COEFFTS. TO N-SHELLS
C
C AUTHOR: H. P. SUMMERS, JET
C K1/1/57
C JET EXT. 4941
C
C DATE: 29/06/94
C
C UPDATES: 09/08/94 - HPS - CORRECT PARAMETER LIST FOR GPCALL TO INCLUDE
C IFSEL. SET IFSEL =1, BUT IT IS NOT USED
C UPDATES: 07/03/96 - HPS - PUT DIMENSIONALITY OF A NUMBER OF VECTORS OF
C LENGTH 15 TO INTERNAL PARAMETER ITDIMD
C
C UPDATES: 15/03/96 - PEB - CORRECT ERROR: WIA(,) AND WJA(,) CHANGED TO
C REAL*8 FROM INTEGER.
C
C UNIX-IDL PORT:
C WILLIAM OSBORN, TESSELLA SUPPORT SERVICES PLC.
C
C DATE: 22ND APRIL 1996
C
C VERSION: 1.1 DATE: 22-04-96
C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION. NO CHANGES TO IBM VERSION
C
C VERSION: 1.2 DATE: 14-05-96
C MODIFIED: WILLIAM OSBORN
C REARRANGED ARGUMENTS TO STAY UNDER
C LIMIT OF 20 CONTINUATION CHARACTERS AT ARCETRI AND GARCHING
C
C VERSION: 1.3 DATE: 20-08-96
C MODIFIED: HUGH SUMMERS + WILLIAM OSBORN
C ADDED TRAP FOR ZERO POWER FOR A PARENT. THIS
C IS NOT A FULL SOLUTION (CF. D7AUTS COMMENTS)
C VERSION: 1.4 DATE: 24-06-97
C MODIFIED: HUGH SUMMERS
C CHANGED PARAMETER KTERM FROM 100 TO 300
C KTRAN FROM 1000 TO 3200
C
C
C VERSION : 1.5
C DATE : 23-05-2003
C MODIFIED: Martin O'Mullane
C - Pass in adf04 data rather than rewinding and
C reading it again.
C - Remove all unused variables and reduced length of
C parameter list.
C - Remove redundant code and format statements.
C
C
C VERSION : 1.6
C DATE : 04-11-2003
C MODIFIED: Hugh Summers

C - Increased extended electron list strings to 93
 C - Changed minimum A-value, aminsc to 1.0D3
 C - match iodimd to ndorb for internal dimensions
 C
 C VERSION : 1.6
 C DATE : 06-01-2004
 C MODIFIED: Martin O'Mullane
 C - Remove redundant nia, lia, wia, nja, lja and wja
 C arguments.
 C - Pre-process configuration string with a new
 C routine (ceprep) to account for leading d10 and
 C f10-f14 terms.
 C - Add error trapping code to check for overruns
 C and index=0 errors.
 C
 C VERSION : 1.7
 C DATE : 15-11-2004
 C MODIFIED: Martin O'Mullane
 C - Increase to 3500 levels and 500000 transitions.

CHARACTER*18	CSTRGA (NDLEV)	
INTEGER	IA (NDLEV) ,	ICNTE, IE1A (NDTRN)
INTEGER	IE2A (NDTRN) ,	IGRPA (IODIMD)
INTEGER	I INAA (NDMET, NDCONF) ,	I IPNAA (NDMET, NDCONF)
INTEGER	IL, IODIMD,	IPMET
INTEGER	IPMETR (NDMET) ,	ISA (NDLEV) , ITREF
INTEGER	ITYPE (NDMET, NDCONF) ,	IZ, IZ0
INTEGER	IZ1, KGRPA (IODIMD)	
INTEGER	LCF (NDMET, NDCONF) ,	LDCF (NDMET, NDCONF)
INTEGER	N0A (NDMET, 2) ,	N1A (NDMET, NDCONF)
INTEGER	NCF (NDMET, NDCONF) ,	NCONFG
INTEGER	NCTAA (NDMET, NDCONF) ,	NCTAAC (NDMET, NDCONF)
INTEGER	NCUT (NDMET) ,	NCUTT (NDMET, NDCONF)
INTEGER	NDCF (NDMET, NDCONF) ,	NDCONF, NDLEV
INTEGER	NDMET, NDMIN (NDMET) ,	NDTHET
INTEGER	NDTRN, NORB,	NSYS (NDMET) , NTHETA
INTEGER	NTRANS (NDMET)	
REAL*8	AGNGPX (ITDIMD) ,	ALFDA (NDMET, NDTHET)
REAL*8	ALFPART (NDMET, NDCONF, NDTHET)	
REAL*8	ALFRA (NDMET, 2, NDTHET)	
REAL*8	ALFRA0 (NDMET, 2, NDTHET)	
REAL*8	ALFRAR (NDMET, 2, NDTHET) ,	ALRAPX (ITDIMD)
REAL*8	AVAL (NDTRN) ,	DE (NDMET) , DE0 (NDMET)
REAL*8	E (NDMET) ,	ECF (NDMET, NDCONF)
REAL*8	ECTAA (NDMET, NDCONF) ,	FCF (NDMET, NDCONF)
REAL*8	FM (NDMET) ,	FM0 (NDMET)
REAL*8	PARMD (NDMET, 10, NDCONF) ,	PARMR (NDMET, 2, 4)
REAL*8	PCF (NDMET, NDCONF) ,	THETA (NDTHET)
REAL*8	VORB (IODIMD) ,	W (NDMET)
REAL*8	WA (NDLEV) ,	WCF (NDMET, NDCONF)
REAL*8	WVMAX (NDMET, NDCONF) ,	WVMIN (NDMET, NDCONF)
REAL*8	XJA (NDLEV)	