

ADAS Subroutine d7exps

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SUBROUTINE D7EXPS( NDMET , NDCONF , NDTHET , NDORB , NDLEV ,
&
& ndtrn , ndqdn , LTADJ ,
&
& IZ , IZ0 , IZ1 ,
&
& il , ia , isa , ila , xja ,
&
& cstrga , wa , bwno , iorb , qdorbb ,
&
& ipl , ipa , ipsa , ipla , xpja ,
&
& cstrgpa , wpa , bwnop ,
&
& icnte2 , iela2 , ie2a2 , aval2 ,
&
& NTHETA , THETA , ITSELA , NPMET , IPMETR ,
&
& ISPRT , ISPSYS , NSYS , INPAR , ILPAR ,
&
& ENPAR , TRMPRT , SPNFAC ,
&
& NORB , VORB , LEICHR ,
&
& CI4 , EIONA , IZETA4 , NZETA , SAO ,
&
& IONLEV , XITRUE , NCUT , N0A , PARMR ,
&
& ALFRA , ALFRA0 , ALFRAR , NCONFG ,
&
& WVMIN , WVMAX ,
&
& ECF , FCF , PCF , WCF , W ,
&
& NCF , LCF , NDCF , LDCE , NDMIN ,
&
& E , DE0 , DE , FM0 , FM ,
&
& IINAA , IIPNAA , NCTAA , NCTAAC , ECTAA ,
&
& NTRANS , ITYPEA , N1A , NCUTT , PARM ,
&
& EDISGP , SCALGP , ADIELO , ALFDA , ALFPART ,
&
& LLINK , ILINK , LEISS , NMET , IMETR
&
& )

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C-----
C
C ***** FORTRAN77 SUBROUTINE: D7EXPS *****
C
C
C PURPOSE:
C
C (1) GENERATES APPROXIMATE FORM PARAMETERS AND NUMERICAL
C VALUES FOR IONISATION AND RECOMBINATION RATES FROM
C SPECIFIC ION FILES
C
C (2) RETURNS DATA REQUIRED FOR A MAINCL INPUT FILE RESOLVED
C INTO PARENT/SPIN SYSTEM COMPONENTS.
C
C (3) RETURNS PARAMETERS REQUIRED FOR AN ATOMPARS FILE
C
C CALLING PROGRAM: ADAS407
C
C SUBROUTINE:
C
C INPUT : (I*4) IUNIT = UNIT NUMBER FOR SPECIFIC ION FILE FOR
C RECOMBINED ION
C
C INPUT : (I*4) IUNIT1 = UNIT NUMBER FOR SPECIFIC ION FILE FOR
C RECOMBINING ION
C
C INPUT : (I*4) NDMET = MAXIMUM NUMBER OF METASTABLES ALLOWED
C
C INPUT : (I*4) NDTHET = MAXIMUM NUMBER OF TEMPS. FOR MAINCL FILE
C
C INPUT : (I*4) NDCONF = MAXIMUM NUMBER OF CONFIGURATIONS ALLOWED
C
C INPUT : (I*4) NDORB = MAXIMUM NUMBER OF ELECTRON ORBITALS
C
C
C INPUT : (L*4) LTADJ = .TRUE. => ADJUST PARMS FROM SPECIAL TABLES

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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
C          (I*4)  ITDIMD  = PARAMETER = LIMIT NUMBER OF TEMPERATURES
C                               INTRINSIC TO ROUTINE
C          (I*4)  IMDIMD  = PARAMETER = LIMIT NUMBER OF METASTABLES
C                               INTRINSIC TO ROUTINE
C          (I*4)  IODIMD  = PARAMETER = LIMIT NUMBER OF ELEC. ORBITALS
C          (R*8)  SPNFAC(,) = SPIN WEIGHT FRACTION FOR PARENT/SPIN SYSTEM
C                               1ST DIM: PARENT INDEX
C                               2ND DIM: RECOMBINED ION SPIN SYSTEM INDEX
C          (R*8)  SPNSUM() = SPIN SYSTEM WEIGHT SUM BASED ON PARENT
C                               1ST DIM: PARENT INDEX
C          (I*4)  IGRPA()  = NUMBER OF ELECTRONS ALLOWED IN EACH SHELL
C                               1ST DIM: SHELL INDEX (1=1S, 2=2S ETC)
C          (C*1)  EICHR()  = EISSNER NOTATION CHARACTER FOR ORBITAL
C                               1ST DIM: ORBITAL INDEX
C          (L*4)  LEICHR() = .TRUE. => EISSNER ORBITAL USED
C                               .FALSE => EISSNER ORBITAL NOT USED
C          (I*4)  KGRPA()  = NUMBER OF ELECTRONS IN EACH SHELL
C                               1ST DIM: SHELL INDEX (1=1S, 2=2S ETC)
C          (R*8)  VORB()   = EFFECT. PRINC. QUANT. NO. FOR ORBITAL
C                               1ST DIM: SHELL INDEX (1=1S, 2=2S ETC)
C          (R*8)  EPSIL()  = ENERGY OF ORBITAL (RYDBERG)
C                               1ST DIM: SHELL INDEX (1=1S, 2=2S ETC)
C          (R*8)  SAO(,,)  = BEST ESTIMATE OF METASTABLE AVERAGED
C                               IONISATION RATE
C                               1ST DIM: PARENT INDEX
C                               2ND IND: SPIN SYSTEM INDEX
C                               3RD IND: TEMPERATURE INDEX
C          (C*1)  CHLA()   = CONVERTS NUMERICAL VALUE FOR L QUANTUM
C                               TO CHARACTER VALUE (CAPITAL).  NOTE
C                               THAT L+1 (<11) IS THE CALL PARAMETER.
C          (I*4)  ILPRT()  = RECOMBINING ION (PARENT) TOTAL ORBITAL
C                               ANGULAR MOMENTUM
C                               1ST DIM: PARENT INDEX

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C NOTE:

C ROUTINES:

ROUTINE	SOURCE	BRIEF DESCRIPTION
D7AUTS	ADAS	ANALYSES FOR IONISATION RATE PARAMETERS
D7ALFS	ADAS	ANALYSES FOR RECOMBINATION PARAMETERS

C AUTHOR: H. P. SUMMERS, JET
C K1/1/57
C JET EXT. 4941

C DATE: 27/06/94

C
C UPDATE: 04/07/95 - HPS CORRECTED ERROR BARE NUCLEUS CASE TO ENSURE
C NSHEL=1, NEL=1 CHEISA(1)='1' SET.
C NOTE: INSUM, ILSUM ARE NOT SATISFACTORY IN
C THE BARE NUCLEUS CASE. STILL TO RECONSIDER
C THE ALGORITM FOR DECIDING INNER CLOSED SHELLS
C BARE NUCLEUS MAKES A FALSE ASSUMPTION BUT
C WITHOUT SERIOUS CONSEQUENCE.
C UPDATE: 07/03/96 - HPS REMOVED VALUE ASSIGNMENT OF NTHETA
C REMOVED VALUE ASSIGNMENT OF MAXDTA
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.
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 VERSION: 1.3 DATE: 20-08-96
C MODIFIED: HUGH SUMMERS + WILLIAM OSBORN
C - CORRECTED ASSIGNMENT OF 'TRMPRT'
C - ADDED FOLLOWING TO CALL PARAMETERS
C LLINK,ILINK,LEISS,NMET AND IMETR
C VERSION: 1.4 DATE: 24-09-96
C MODIFIED: HUGH SUMMERS + WILLIAM OSBORN
C - INTRODUCED ILPRT AND CORRECT OUTPUT TRMPRT
C
C
C VERSION : 1.5
C DATE : 23-05-2003
C MODIFIED: Martin O'Mullane
C - Pass through adf04 data for d7alfs and d7auts.
C - Do not rewind files to get parent data; use
C the new arguments.
C - Make implicit none.
C - Remove all unused variables and reduced length of
C parameter list.
C - Remove redundant code and format statements.
C
C VERSION : 1.6
C DATE : 04-11-2003
C MODIFIED: Hugh Summers
C - checked iodimd consistency with passed ndorb.
C - Extended igrpa eichr,chla
C - corrected array indexing error in applying corrad
C to parmd(ipar,6,j)
C

C VERSION : 1.7
 C DATE : 06-01-2004
 C MODIFIED: Martin O'Mullane
 C - Remove redundant nia, lia, wia, nja, lja and wja
 C variables.
 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

CHARACTER*18	CSTRGA (NDLEV) ,	CSTRGPA (NDLEV)
CHARACTER*2	TRMPRT (NDMET)	
INTEGER	IA (NDLEV) , ICNTE2,	IE1A2 (NDTRN)
INTEGER	IE2A2 (NDTRN) ,	IINAA (NDMET, NDCONF)
INTEGER	IIPNAA (NDMET, NDCONF) ,	IL
INTEGER	ILA (NDLEV) , ILINK (NDMET, NDMET, 2)	
INTEGER	ILPAR (NDMET) ,	IMETR (NDMET)
INTEGER	INPAR (NDMET) ,	IONLEV (NDMET, 2)
INTEGER	IORB, IPA (NDLEV) ,	IPL
INTEGER	IPLA (NDLEV) , IPMETR (NDMET)	
INTEGER	IPSA (NDLEV) , ISA (NDLEV) ,	ISPRT (NDMET)
INTEGER	ISPSYS (NDMET, 2) ,	ITSELA (NDMET)
INTEGER	ITYPEA (NDMET, NDCONF) ,	IZ, IZ0
INTEGER	IZ1, IZETA4 (NDMET, 2, NDORB)	
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) ,	NDORB
INTEGER	NDQDN, NDTHET, NDTRN,	NMET
INTEGER	NORB, NPMET,	NSYS (NDMET) , NTHETA
INTEGER	NTRANS (NDMET) ,	NZETA (NDMET, 2)
LOGICAL	LEICHR (NDORB) ,	LEISS
LOGICAL	LLINK (NDMET, NDMET, 2) ,	LTADJ
REAL*8	ADIELO (NDMET, 2, NDTHET) ,	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) ,	AVAL2 (NDTRN)
REAL*8	BWNO, BWNOP,	CI4
REAL*8	DE (NDMET) , DE0 (NDMET) ,	E (NDMET)
REAL*8	ECF (NDMET, NDCONF) ,	ECTAA (NDMET, NDCONF)
REAL*8	EDISGP, EIONA (NDMET, 2, NDORB)	
REAL*8	ENPAR (NDMET) ,	FCF (NDMET, NDCONF)
REAL*8	FM (NDMET) , FM0 (NDMET)	
REAL*8	PARMD (NDMET, 10, NDCONF) ,	PARMR (NDMET, 2, 4)
REAL*8	PCF (NDMET, NDCONF)	
REAL*8	QDORB ((NDQDN* (NDQDN+1)) /2)	
REAL*8	SAO (NDMET, 2, NDTHET) ,	SCALGP

REAL*8	SPNFAC (NDMET, 2),	THETA (NDTHET)
REAL*8	VORB (NDORB), W (NDMET),	WA (NDLEV)
REAL*8	WCF (NDMET, NDCONF),	WPA (NDLEV)
REAL*8	WVMAX (NDMET, NDCONF),	WVMIN (NDMET, NDCONF)
REAL*8	XITRUE (NDMET, 2),	XJA (NDLEV)
REAL*8	XPJA (NDLEV)	