

## ADAS Subroutine `xxdtes`

```
subroutine xxdtes( cstrg , leiss , lstan , nvfce )
c
c-----
c
c ***** fortran77 subroutine: xxdtes *****
c
c purpose: Detects if the configuration string from a specific ion
c           level list line is of eissner form , standard form or
c           neither.
c
c           If neither, the subroutine checks to see if it is a
c           bundle (* in the string) or based on a parent ([..] in
c           the string). If the string is of Eissner or standard
c           form, the n-shell and l-shell of the outermost
c           (valence) electron is returned.
c
c           A version of this routine with a more extended return of
c           parameters and bale to handle very long configuration
c           strings is available as 'g5dtes.for'.
c
c calling programs: general use
c
c subroutine:
c
c input : (c*(*)) cstrg      = configuration character string
c output: (l*4)  leiss      = .true. => eissner form
c                   .false. => not eissner form
c output: (l*4)  lstan      = .true. => standard form
c                   .false. => not standard form
c output: (i*4)  nvfce      = outer electron n-shell if recognisable
c
c           (l*4)  lbndl     = .true. => bundled form ('*' found)
c                   .false. => not bundled form
c           (l*4)  lprnt     = .true. => parent form ('[...] found)
c                   .false. => not parent form
c           (c*19) cstr_top = leading part of config. string in Eissner
c                   format (no leading blank, trailing blanks)
c           (c*(*)) cstr_tail= trailing part of config. string in Eissner
c                   format (no leading blank, trailing blanks)
c           (i*4)  lvfce     = outer electron l-shell if recognisable
c
c           (i*4)  i         = general use
c           (i*4)  iabt      = return code (see specific function)
c                   0 => ok
c                   1 => fault detected
c           (i*4)  icfsel    = 1 => standard form out, standard form in
c                   2 => eissner form out, standard form in
c                   3 => standard form out, eissner form in
c                   4 => eissner form out, eissner form in
c           (i*4)  ishel    = shell counter
c           (i*4)  ip       = parity of configuration
c           (i*4)  maxn     = n_shell sum for configuration
```

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c      (i*4)  nshel  = number of shells identified ffrom string
c      (i*4)  ndword = maximum number of words in string
c      (i*4)  nfirst = first word to be extracted from string
c      (i*4)  nwords = number of words in string
c      (i*4)  nela() = number of electrons in each shell
c      (i*4)  ifirst()= position of first char. of word in string
c      (i*4)  ilast() = position of last char. of word in string
c
c      (c*1)  cdelim = separators for words in string
c      (c*19) cstrgo  = general use string
c      (c*19) strg    = standard form configuration string
c      (c*19) strge   = eissner form configuration string
c      (c*1)  cheisa()= eissner character for orbitals
c      (c*2)  chstda()= standard orbital spec. for each shell
c      (c*2)  cnela() = chars. for no. of equiv. elec. in shell
c                      (eissner form case)
c      (c*1)  chqa()  = index to hexadecimal conversions
c      (c*1)  chra()  = char. for no. of. equiv. elec. in shell
c                      (standard form case)

```

c routines:

routine	source	brief description
i4fctn	adas	converts character string to integer
i4ngrp	adas	returns n quantum number in the eissner single hexadecimal character form
i4pgrp	adas	returns parity of orbital given the eissner single hexadecimal character form
i4schr	adas	returns numerical value for number of equivalent electrons given as hex> char.
cstgrp	adas	returns term of orbital given in the eissner single hexadecimal character form
ceigrp	adas	returns eissner code for orbital
xxword	adas	finds number of words in a string
xxcmps	adas	compare standard config. strings

```

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```

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c date:    19/02/03

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C VERSION: 1.1                      DATE: 19-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C          - PUT UNDER S.C.C.S. CONTROL

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C VERSION: 1.2                      DATE: 14-10-96
C MODIFIED: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C          - ADDED CHANGES DATED 01/10/96 ABOVE

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C VERSION: 1.3                      DATE: 28-08-97

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C MODIFIED: HUGH SUMMERS
C           - ADDED CHANGES TO CHECK 'G' STATES
C
C VERSION: 1.4                      DATE: 19/02/03
C MODIFIED: HUGH SUMMERS
C           - Rewrite based on g5dtes.for
C
C VERSION: 1.5                      DATE: 28/09/2004
C MODIFIED: Martin O'Mullane
C           - Incorrect redirection when checking the Eissner pattern.
C           The if statement block checking ir jumped out of the
C           current sub-block to the end of the previous sub-block
C           rather than to the end of its own sub-block.
C
C VERSION: 1.6                      DATE: 17/05/2007
C MODIFIED: Allan Whiteford
C           - Updated comments as part of subroutine documentation
C           procedure.

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C-----

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CHARACTER*(*)	CSTRG	
INTEGER	NVLCE	
LOGICAL	LEISS,	LSTAN