

ADAS Subroutine xxcftr

SUBROUTINE XXCFTR(ICFSEL , CSTRGI , CSTRGO)

```
C
C-----
C
C ***** FORTRAN77 SUBROUTINE: XXCFTR *****
C
C PURPOSE: CONVERTS A CONFIGURATION CHARACTER STRING, SUCH AS OCCURS
C           IN A SPECIFIC ION FILE LEVEL LIST, BETWEEN EISSNER AND
C           STANDARD FORMS
C
C CALLING PROGRAMS: GENERAL USE
C
C SUBROUTINE:
C
C INPUT : (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 INPUT : (C*(*)) CSTRGI = CONFIGURATION STRING IN INPUT FORM
C OUTPUT: (C*(*)) CSTRGO = CONFIGURATION STRING IN OUTPUT FORM
C
C           (I*4)   I       = GENERAL USE
C           (I*4)   ISHEL  = SHELL COUNTER
C           (I*4)   IP     = PARITY OF CONFIGURATION
C           (I*4)   MAXN   = N_SHELL SUM FOR CONFIGURATION
C           (I*4)   NSHEL  = NUMBER OF SHELLS IDENTIFIED fFROM STRING
C           (I*4)   NELA() = NUMBER OF ELECTRONS IN EACH SHELL
C
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                   (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
C           (L*4)   LEISS  = .TRUE.  => EISSNER FORM
C                   .FALSE. => NOT EISSNER FORM
C
C ROUTINES:
C
C ROUTINE      SOURCE      BRIEF DESCRIPTION
C-----
C I4UNIT       ADAS        FETCH UNIT NUMBER FOR OUTPUT OF MESSAGES
C I4NGRP       ADAS        RETURNS N QUANTUM NUMBER IN THE
C                   EISSNER SINGLE HEXADECIMAL CHARACTER FORM
C I4PGRP       ADAS        RETURNS PARITY OF ORBITAL GIVEN THE
C                   EISSNER SINGLE HEXADECIMAL CHARACTER FORM
C I4SCHR       ADAS        RETURNS NUMERICAL VALUE FOR NUMBER OF
C                   EQUIVALENT ELECTRONS GIVEN AS HEX> CHAR.
C CSTGRP       ADAS        RETURNS TERM OF ORBITAL GIVEN IN THE
```

C EISSNER SINGLE HEXADECIMAL CHARACTER FORM
C CEIGRP ADAS RETURNS EISSNER CODE FOR ORBITAL
C
C
C NOTE: THE ROUTINE IS USED TO CONVERT THE CONFIGURATION CHARACTER
C STRING OCCURRING IN ADF04 FILE LEVEL LISTS. THE STRING
C LENGTH ALLOCATED TO THIS IS *18 FOLLOWING 1 BLANK SPACE
C AFTER THE LEVEL INDEX. A PROBLEM ARISES WHEN THE FIRST
C SHELL CONTAINS MORE THAN 9 EQUIVALENT ELECTRONS. IN THIS
C CASE, OVERSPILL IS ALLOWED INTO THE BLANK CHARACTER SPACE.
C THE ROUTINE WILL ANALYSE A *19 STRING INCLUDING THE USUALLY
C BLANK LOCATION OR A *18 STRING EXCLUDING IT. IN THE LATTER
C CASE AN INTELLIGENT GUESS IS MADE AS TO WHETHER THE OMITTED
C BLANK SHOULD IN FACT BE A '1'. THIS SITUATION OCCURS FOR A
C LEADING CLOSED D-SHELL.
C
C AUTHOR: H. P. SUMMERS, UNIVERSITY OF STRATHCLYDE
C JA8.08
C TEL. 0141-553-4196
C
C DATE: 25/10/95
C
C
C UPDATE: 19/02/03 H. P. SUMMERS - EXTENDED RANGE AND STRINGS
C
C
C UNIX-IDL PORT:
C
C VERSION: 1.1 DATE: 19-1-96
C MODIFIED: TIM HAMMOND (TESSELLA SUPPORT SERVICES PLC)
C - PUT UNDER SCCS CONTROL
C
C VERSION: 1.2 DATE: 19-02-03
C MODIFIED: H. P. SUMMERS
C - EXTENDED RANGE AND STRINGS
C
C-----
C-----
C CHARACTER*(*) CSTRGI, CSTRGO
C INTEGER ICFSEL