

ADAS Subroutine bbprs3

SUBROUTINE BBPRS3(STRING, IA, LCLSHL)

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C
C ***** FORTRAN77 SUBROUTINE: BBPRS3 *****
C
C PURPOSE:  TO ANALYSE A CONFIGURATION CHARACTER STRING INTO A  INTEGER
C           ARRAY OF OCCUPATION NUMBERS IN A STANDARD ORDER
C
C CALLING PROGRAM: ADAS211
C
C NOTES: THE STANDARD ORDER IS 1S,2S,2P,3S,3P,3D . . . . ., 4F (15 VALUES)
C        CLOSED SHELLS WITHIN THE ACTIVE N-SHELLS ARE ASSUMED FULLY
C        OCCUPIED
C
C SUBROUTINE:
C
C INPUT : (C*(*))STRING   = STRING TO BE PARSED
C         (L*4)  LCLSHL   = SWITCH ON CLOSED SHELL ASSUMPTION
C
C OUTPUT: (I*4)  IA()     = SET OF OCCUPATION NUMBERS IN STANDARD
C                           ORDER
C
C ROUTINES: NONE
C
C AUTHOR:  HP SUMMERS
C         K1/1/57
C         JET EXT. 4941
C
C DATE:    29/06/92
C
C UPDATE:  W.J. DICKSON  7/10/92
C         ADDED PARAMETER LCLSHL TO SWITCH OFF CLOSED SHELL
C         APPROXIMATION
C
C UPDATE:  H. P. SUMMERS  1/10/96
C         PERMITTED LOWER AND UPPER CASE ORBITAL L-VALUES
C         IN CONFIGURATION STRINGS. DETECT RETURNED L<0
C
C UNIX-IDL PORT:
C
C AUTHOR:  WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C
C DATE:    4TH JULY 1996
C
C VERSION: 1.1                               DATE: 04-07-96
C MODIFIED: WILLIAM OSBORN
C           - FIRST VERSION.
C
C VERSION: 1.2                               DATE: 14-10-96
C MODIFIED: WILLIAM OSBORN
C           - ADDED CHANGES DATED 1/10/96 ABOVE
C
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C VERSION: 1.3

DATE: 17-05-07

C MODIFIED: Allan Whiteford

C - Removed non-standard control character from
C comments.

C

C-----

CHARACTER* (*)	STRING
INTEGER	IA(15)
LOGICAL	LCLSHL