

ADAS Subroutine xxprs3

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      subroutine xxprs3( string , ia_dim      , iz0      , iz      ,  
&                      ia      , ia_vlnce  
&                      )
```

***** fortran77 subroutine: xxprs3 *****

purpose: To analyse a configuration character string in Standard form into a integer array of occupation numbers in the normal collating order.

unified version of bbprs3 & g5prs3 and a replacement for these subroutines

calling program: various

notes: 1. the normal collating order is 1s,2s,2p,3s,3p,3d etc.
2. a strategy for deciding the occupancy of unspecified inner shells is implemented using the nuclear and ion charge. The strategy may be switched off.
3. opens a central ADAS adf00 file for an element on unit 10.

subroutine:

input : (c*(*))string = string to be parsed
input : (i*4) ia_dim = dimensionality of occupancy vector ia
input : (i*4) iz0 = nuclear charge
input : (i*4) iz = ion charge

output: (i*4) ia() = set of occupation numbers in standard collating list order
output: (i*4) ia_vlnce = outer occupied shell index in collating list

routines:

routine	source	brief description
i4unit	adas	fetch unit number for output of messages
xxopen	adas	inquire & open a data file on a unit
xxword	adas	parses a string into separate words
xxrmve	adas	removes occurrences of a char. in string
xxcase	adas	changes a string to upper or lower case
xxslen	adas	finds the length of a string excluding leading and trailing blanks
xfesym	adas	fetch the chemical symbol of an element

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CHARACTER* (*)	STRING			
INTEGER	IA (IA_DIM),	IA_DIM,	IA_VLNCE,	IZ
INTEGER	IZ0			