

ADAS Subroutine xxdata_00

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      subroutine xxdata_00( iunit  , dsname  ,
&                          izdimd  , iodimd  , imdimd  ,
&                          esym    , iz0    , bwnoa   , eeve   ,
&                          iorba   , na     , la      , iqa    ,
&                          cstr_std ,
&                          imeta   , eeve    ,
&                          iorbma  , nma    , lma     , iqma   ,
&                          cstrm_std ,
&                          lexist   , lresol
&                          )
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C ***** fortran77 subroutine: xxdata_00 *****

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C purpose: to fetch data from an adf00 data set and detect its main
C characteristics.

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- C 1. element symbol and nuclear charge
- C 2. ionisation potentials (cm-1 and eV)
- C 3. shell occupancies in the normal collating order

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C calling program: various

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C ionisation potential: eV
C configuration: standard form nlq (incl. integers
C for n>9 and q>9 , lower case
C letter for l and space separators)

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C subroutine:

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C input : (i*4) iunit = unit to which input file is allocated
C input : (c*(*)) dsname = name of opened data set on iunit
C input : (i*4) izdimd = maximum nuclear charge
C input : (i*4) iodimd = max. number of orbitals
C input : (i*4) imdimd = max. number of metastables

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C output: (c*2) esym = element symbol.
C output: (i*4) iz0 = nuclear charge read
C output: (r*8) bwnoa() = ionisation potential (cm-1) of each stage
C 1st dim: index = nuclear charge +1
C output: (r*8) eeve() = ionisation potential (eV) of each stage
C 1st dim: index = nuclear charge +1
C output: (i*4) iorba() = number of orbital shells in configuration
C 1st dim: index = nuclear charge +1
C output: (i*4) na(,) = principal quantum number of shell
C 1st dim: index = nuclear charge +1
C 2nd dim: shell index
C output: (i*4) la(,) = orbital ang. momentum qu. no. of shell
C 1st dim: index = nuclear charge +1
C 2nd dim: shell index
C output: (i*4) iqa(,) = occupancy. of shell

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c          1st dim: index = nuclear charge +1
c          2nd dim: shell index
c
c output: (c*(*)) cstr_std()= configuration string in standard form
c          1st dim: index = nuclear charge +1
c
c output: (r*8)   eevma(,) = excitation energy (eV) of each metastable
c          1st dim: index = nuclear charge +1
c          2nd dim: index = metastable index
c output: (i*4)   iorbma(,) = number of orbital shells in metas. config.
c          1st dim: index = nuclear charge +1
c          2nd dim: index = metastable index
c output: (i*4)   nma(,,) = principal quantum number of metas.shell
c          1st dim: index = nuclear charge +1
c          2nd dim: shell index
c          3rd dim: index = metastable index
c output: (i*4)   lma(,,) = orbital ang. mom. qu. no. of metas. shell
c          1st dim: index = nuclear charge +1
c          2nd dim: shell index
c          3rd dim: index = metastable index
c output: (i*4)   iqma(,,) = occupancy. of metas. shell
c          1st dim: index = nuclear charge +1
c          2nd dim: shell index
c          3rd dim: index = metastable index
c
c output: (c*(*)) cstrm_std(,)=meta. config. string in standard form
c          1st dim: index = nuclear charge +1
c          2nd dim: index = metastable index
c
c output: (l*4)   lexist = .true. => ionisation potential present
c                = .false. => not present
c output: (l*4)   lresol = .true. => metastable resolved adf00 file
c                = .false. => not metastable resolved adf00
c
c
c routines:
c routine      source      brief description
c -----
c i4unit       adas        fetch unit number for output of messages
c i4fctn       adas        converts from char. to integer variable
c xxslen       adas        finds string length excluding leading and
c                trailing blanks
c xxword       adas        parses a string into separate words
c                for ' (<>{}' delimiters
c xxcase       adas        changes a string to upper or lower case
c xfesym       adas        obtain element symbol from nuclear charge
c xfelem       adas        obtain element name from nuclear charge
c xxterm       adas        terminate program with a message
c
c
c author:      Hugh Summers, University of Strathclyde
c              JA7.08
c              tel. 0141-548-4196

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c
c date:    27/04/04
c
c update:  15/12/06  H. P. Summers - extended to handle metastable resolved
c                                adf00 files
c
c
c version: 1.1                                date: 27-04-04
c modified: H.P. Summers
c          - first version
c
c version: 1.2                                date: 05-01-07
c modified: H. P. Summers
c          - extended to handle metastable resolved
c                                adf00 files
c
c
c-----
c-----

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CHARACTER*(*)      CSTRM_STD (IZDIMD,IMDIMD) , CSTR_STD (IZDIMD)
CHARACTER*(*)      DSNAME
CHARACTER*2        ESYM
INTEGER            IMDIMD,          IMETA (IODIMD) ,          IODIMD
INTEGER            IORBA (IZDIMD)
INTEGER            IORBMA (IZDIMD,IMDIMD) ,          IQA (IZDIMD,IODIMD)
INTEGER            IQMA (IZDIMD,IODIMD,IMDIMD) ,          IUNIT
INTEGER            IZ0,          IZDIMD,          LA (IZDIMD,IODIMD)
INTEGER            LMA (IZDIMD,IODIMD,IMDIMD)
INTEGER            NA (IZDIMD,IODIMD)
INTEGER            NMA (IZDIMD,IODIMD,IMDIMD)
LOGICAL            LEXIST,          LRESOL
REAL*8             BWNOA (IZDIMD) ,          EEVA (IZDIMD)
REAL*8             EEVMA (IZDIMD,IODIMD)

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