

ADAS Subroutine rdwbes

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C
    subroutine rdwbes( ndinfo,
&                      z0      , nlqs   , nshell , na      , la      ,
&                      ea      , qda    , alfaa  , jsn     , jealfa , acc    , xmax   , h      ,
&                      lam     , einc   , irept  , iext   , iochk  ,
&                      res    ,
&                      ninfo  , cinfoa )
C-----
C
C **** fortran77 program: rdwbes.for ****
C
C Purpose: Evaluates Born multipole integrals using distorted bound
C           waves. The distorted waves are in a Jucys or Slater type
C           potential.
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C Subroutine:
C
C Input : (i*4)  ndinfo   = maximum number of information strings
C Input : (r*8)  z0        = nuclear charge (+ve)
C Input : (i*4)  nlqs()   = 1000*n+100*l+iqfor each screening shell
C                           1st dim: screening shell index
C Input : (i*4)  nshell   = number of screening shells
C Input : (i*4)  na()     = initial (1) and final (2) state principal
C                           quantum numbers.
C Input : (i*4)  la()     = initial (1) and final (2) orbital quantum
C                           numbers.
C Input : (r*8)  ea()     = energies(ryd) of initial (1) and final (2)
C                           states - set <0 for bound states.
C Input : (r*8)  qda()   = quantum defects for initial (1) and
C                           final (2) states.
C Input : (r*8)  alfaa(,) = screening parameters
C                           1st dim: initial (1) and final (2) states
C                           2nd dim: screening shell index.
C Input : (i*4)  jsn      = -1 => Jucys potential
C                           = 0 => Slater potential
C Input : (i*4)  jealfa  = 0 => search for energies given potential
C                           = 1 => search for alfaa parameters for
C                           potential given energies and quantum
C                           defects.
C Input : (r*8)  acc      = search accuracy setting
C Input : (r*8)  xmax    = range for numerical wave function generation
C                           and storage
C Input : (r*8)  h       = step interval for numerical wave function
C                           storage
C Input : (i*4)  lam     = Born multipole
C Input : (r*8)  einc   = incident electron energy(ryd)
C Input : (i*4)  irept  = 0 =>full wave function determination
C                           = 1 => repeat with same wave functions as in
C                           previous case with irept=0
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C Input : (i*4) iext      = 0 normal operation with internally generated
C                               wave functions
C                               = 1 use external wave functions supplied in
C                               function gext(x,n,l) with n and l
C                               specifying orbital.
C Input : (i*4) iochk     = 1 => Born multipole integral evaluated
C                               = 2 => Ochkur multipole integral evaluated
C
C Output: (r*8) res       = multipole integral (at.unit)
C Output: (i*4) ninfo     = number of information strings
C Output (c*90) cinfoa() = information strings
C                               1st dim: index number of strings
C
C
C Routines:
C
C      routine      source      brief description
C      -----
C      zeff        adas        effective charge (+ve)
C      effz3       adas        evaluates effective potential
C      gext        adas        access external radial wave functions
C      zser        adas        power series expansion of z(r)
C      bdcf7       adas        generate bound radial distorted wave fn.
C      fcf6        adas        generate free radial distorted wave fn.
C      rbesf       adas        evaluate bessel function
C      ass2        adas        asymptotic integral contribution
C      dnamp       adas        asymp. wave fn. amplitude Taylor coeffs
C      phase       adas        asymp. wave fn. phase Taylor coeffs
C      ass         adas        asymptotic integral contribution
C
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C
C Date:   22/04/85
C
C Update: HP Summers 16/06/95 alter definition of nlqs as
C                               1000*n+100*l+iq to avoid problem when
C                               number of equivalent electrons is 10
C Update: HP Summers 21/05/04 restructure and add calculation
C                               information strings to parameter output
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CHARACTER*90	CINFOA(NDINFO)
INTEGER	IEXT, IOCHK,
INTEGER	JSN, LA(2), LAM,
INTEGER	NDINFO, NINFO, NLQS(10), NSHELL
REAL*8	ACC, ALFAA(2,10), EA(2), EINC
REAL*8	H, QDA(2), RES, XMAX
REAL*8	Z0