

ADAS Subroutine adwlpol

SUBROUTINE ADWLPOL (Z0, NLQS, NSHELL, NA, LA, EA, QDA, ALFAA, JSN, JEALFA,
&ACC, XMAX, H, LAM, IREPT, IEXT, ANS, OPEN17)
IMPLICIT REAL*8 (A-H, O-Z)

C VERSION OF DWLPOL FOR USE BY ADASRRC. IT AVOIDS ALFA SEARCH FOR FREE
C WAVE FUNCTIONS BY USING SAME SCREENING PARAMETERS AS BOUND STATE
C ***** H.P. SUMMERS, JET 30 JUNE 1992 *****
C
C PURPOSE: EVALUATES LAM-POLE RADIAL MATRIX ELEMENTS USING DISTORTED
C WAVES
C
C BOUND-BOUND, BOUND-FREE AND FREE-FREE CASES ARE HANDLED. THE
C DISTORTED WAVES ARE IN A JUCYS OR SLATER TYPE POTENTIAL.
C ***** H.P. SUMMERS, JET 24 APRIL 1985 *****
C INPUT
C Z0=NUCLEAR CHARGE (+VE)
C NLQS(I)=N, L, IQ FOR EACH SCREENING SHELL I=1 TO NSHELL
C NSHELL=NUMBER OF SCREENING SHELLS
C NA(1),NA(2)=INITIAL AND FINAL STATE PRINCIPAL QUANTUM NUMBERS.
C SET TO ZERO FOR FREE STATES
C LA(1),LA(2)=INITIAL AND FINAL STATE ORBITAL QUANTUM NUMBERS.
C EA(1),EA(2)=ENERGIES (RYD) OF INITIAL AND FINAL STATES
C SET <0 FOR BOUND STATES, SET >0 FOR FREE STATES.
C QDA(1),QDA(2)=QUANTUM DEFECTS FOR INITIAL AND FINAL STATES.
C EXTRAPOLATED QUANTUM DEFECT USED FOR FREE STATE
C ALFAA(1,I),ALFAA(2,I)=SCREENING PARAMETERS FOR INITIAL AND FINAL
C STATES FOR EACH SHELL I=1 TO NSHELL.
C JSN=-1 JUCYS POTENTIAL
C =0 SLATER POTENTIAL
C JEALFA=0 SEARCH FOR ENERGIES GIVEN POTENTIAL (NO EFFECT FOR
C FREE STATES)
C =1 SEARCH FOR ALFAA PARAMETERS FOR POTENTIAL GIVEN ENERGIES
C AND QUANTUM DEFECTS.
C ACC=SEARCH ACCURACY SETTING
C XMAX=RANGE FOR NUMERICAL WAVE FUNCTION GENERATION AND STORAGE
C H=STEP INTERVAL FOR NUMERICAL WAVE FUNCTION STORAGE
C LAM=MULTIPOLE (FOR RADIAL INTEGRAL <X**LAM>)
C IREPT=0 FULL WAVE FUNCTION DETERMINATION
C =1 REPETITION WITH SAME WAVE FUNCTIONS AS IN PREVIOUS CASE
C =2 USE SAME BOUND WAVE FUNCTIONS AS IN PREVIOUS CASE,
C USE FREE WAVE FUNCTIONS IN SAME POTENTIAL AS IN PREVIOUS
C BUT WITH POSSIBLY DIFFERENT ENERGIES.
C IEXT=0 NORMAL OPERATION WITH INTERNALLY GENERATED WAVE FUNCTIONS
C =1 USE EXTERNAL WAVE FUNCTIONS SUPPLIED IN FUNCTION
C GEXT(X,N,L) WITH N AND L SPECIFYING ORBITAL.
C OPEN17 = FLAG WHETHER UNIT 17 IS OPENED OR NOT
C OUTPUT
C ANS=RADIAL INTEGRAL (AT. UNITS)
C
C
C UPDATE: HP SUMMERS 16/06/95 ALTER DEFINIAITON OF NLQS AS
C 1000*N+100*L+iQ TO AVOID PROBLEM WHEN\

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C                                     NUMBER OF EQUIVALENT ELECTRONS IS 10.
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: 19-08-96
C MODIFIED: WILLIAM OSBORN
C          - COMMENTED-OUT DIAGNOSTIC OUTPUT.
C          - ADDED OPEN17 PARAMETER.
C
C VERSION: 1.3                        DATE: 23-08-96
C MODIFIED: WILLIAM OSBORN
C          - CORRECTED OUTPUT TO STREAM 17
C
C VERSION: 1.4                        DATE: 19-12-01
C MODIFIED: Martin O'Mullane
C          - Removed junk from > column 72.
C
C VERSION: 1.5                        DATE: 16-05-07
C MODIFIED: Allan Whiteford
C          - Modified comments as part of subroutine documentation
C          procedure.

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      INTEGER          IEXT,          IREPT,          JEALFA,          JSN
      INTEGER          LA(2),          LAM,          NA(2)
      INTEGER          NLQS(10),       NSHELL
      LOGICAL          OPEN17
      REAL*8           ACC,          ALFAA(2,10), ANS,          EA(2)
      REAL*8           H,            QDA(2),          XMAX,          Z0

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