

ADAS Subroutine rd2bs

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FUNCTION RD2BS(N,L,N2,L2)
IMPLICIT REAL*8(A-H,O-Z)
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C
C  PURPOSE: GENERATION OF HYDROGENIC BOUND-BOUND RADIAL INTEGRALS USING
C           RECURRENCE RELATIONS.
C
C-----
C  VERSION   : 1.1
C  DATE      : 18-03-1999
C  MODIFIED  : ???
C
C  VERSION   : 1.2
C  DATE      : 05-10-2000
C  MODIFIED  : ???
C             - Removed junk from columns > 72
C
C  VERSION   : 1.3
C  DATE      : 16-05-2007
C  MODIFIED  : Allan Whiteford
C             - Updated comments as part of subroutine documentation
C             procedure.
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SC=64.0
SCL=0.015625
EN=N
EN2=EN*EN
EK=N2
EK=1.0/EK
EK2=-EK*EK
V=1.0+EN2*EK2
W=1.0+EN*EK
W=W*W
U=8.0*EN2/(W*W)
P=1.0
JS=0
SC2=SC*SC
SCL2=SCL*SCL
DO 5 I=1,N
EI=I
P=P*U*(1.0+EI*EI*EK2)/(EI*(2.0*EI-1.0))
AP=DABS(P)
IF(SCL2.LE.AP)GO TO 5
JS=JS-1
P=SC2*P
5 CONTINUE
P=2.0*EN*EK*P
P=4.0*EK*DSQRT(P)/(V*V)
NL=N+1
DO 10 I=NL,N2
P=P*V/W
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AP=DABS (P)
IF (SCL.LE.AP) GO TO 10
JS=JS-1
P=SC*P
10 CONTINUE
IF (L2.EQ.L+1) GO TO 11
IF (L2.EQ.L-1) GO TO 20
RD2BS=0.0
GO TO 7
11 T2=P
U=(2.0*EN-1.0)*V
U=DSQRT (U)
T3=0.5*U*T2
NU=N-2
IF (L-NU) 14, 13, 12
12 T3=T2
13 GO TO 40
14 DO 16 I=L2, NU
LI=NU-I+L
EL1=LI+1
EL2=LI+2
ES=EL2*EL2
T1=T2
T2=T3
T3=(4.0*(EN2-ES)+EL2*(2.0*EL2-1.0)*V)*T2-2.0*EN*U*T1
U=(EN2-EL1*EL1)*(1.0+ES*EK2)
U=DSQRT (U)
T3=T3/(2.0*EN*U)
AT3=DABS (T3)
IF (AT3.LE.SC) GO TO 16
JS=JS+1
T3=SCL*T3
T2=SCL*T2
16 CONTINUE
GO TO 40
20 T2=P
EN1=N-1
U=V/(1.0+EN1*EN1*EK2)
T2=DSQRT (U)*T2/(2.0*EN)
U=(2.0*EN-1.0)*(1.0+(EN-2.0)*(EN-2.0)*EK2)
U=DSQRT (U)
T3=(4.0+EN1*V)*(2.0*EN-1.0)*T2/(2.0*EN*U)
NU=N-3
IF (L-NU-1) 24, 23, 22
22 T3=T2
23 GO TO 40
24 DO 26 I=L, NU
LI=NU-I+L
EL=LI
EL1=LI+1
ES=EL1*EL1
T1=T2
T2=T3

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T3=(4.0*(EN2-ES)+EL1*(2.0*EL1+1.0)*V)*T2-2.0*EN*U*T1
U=(EN2-ES)*(1.0+EL*EL*EK2)
U=DSQRT(U)
T3=T3/(2.0*EN*U)
AT3=DABS(T3)
IF(AT3.LE.SC)GO TO 26
JS=JS+1
T3=SCL*T3
T2=SCL*T2
26 CONTINUE
40 RD2BS=EN2*EN2*T3*T3*4096.0**JS
7 RETURN
END
INTEGER L, L2, N, N2
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