

ADAS Subroutine rd2fs

FUNCTION RD2FS(N,L,L2,E2)

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C PURPOSE: GENERATION OF HYDROGENIC BOUND-FREE RADIAL INTEGRALS USING
C RECURRENCE RELATIONS.
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C UNIX-IDL PORT:
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C AUTHOR: WILLIAM OSBORN (TESSELLA SUPPORT SERVICES PLC)
C

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C

C VERSION: 1.1 DATE: 04-07-96

C MODIFIED: WILLIAM OSBORN
C - FIRST VERSION.
C

C VERSION: 1.2 DATE: 19-12-01

C MODIFIED: Martin O'Mullane
C - Removed junk from > column 72.
C

C VERSION: 1.3 DATE: 16-05-07

C MODIFIED: Allan Whiteford
C - Modified comments as part of subroutine documentation
C procedure.
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      IMPLICIT REAL*8 (A-H,O-Z)
      SC=64.0
      SCL=0.015625
      EN=N
      EN2=EN*EN
      EK2=-E2
      V=1.0+EN2*EK2
      EK=DSQRT(EK2)
      V=V*V
      U=8.0*EN2/V
      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
      IF(EK.GT.0.04D0)GO TO 6
      P=EN*P
      GO TO 7
6     P=EN*P/(1.0-DEXP(-6.283185/EK))
7     IF(EK.GT.1.0D-5)GO TO 8
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U=-2.0*EN
GO TO 9
8 U=-2.0*DATAN(EN*EK)/EK
9 T2=7.089815*DSQRT(P)*DEXP(U)/V
V=1.0+EN2*EK2
IF(L2.EQ.L+1)GO TO 11
IF(L2.EQ.L-1)GO TO 20
RD2FS=0.0
GO TO 50
11 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 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
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)

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```
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 RJS=JS
RD2FS=EN2*EN2*T3*T3*4096.0**RJS
50 RETURN
END
INTEGER          L,          L2,          N
REAL*8           E2
```