APPENDIX A

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      PROGRAM ONE (INPUT,OUTPUT,PLOT,TAPE5=INPUT,TAPE6=OUTPUT)
C  NUMERICAL APPROXIMATION OF THE ENERGY PERTURBATION
C  IN THE HYDROGEN MOLECULE
      COMMON X,A0,DELTA,E
      DIMENSION DISTAN(30),EPLUS(30),EMINUS(30)
      CALL PLOTS
      EMIN=0.0
      EMAX=60.
      DMAX=6.0
      DMIN=0.0
      AE=EMAX/6.
      CALL PLOT(0.0,3.0,-3)
      CALL AXIS(0.0,0.0,15HDISTANCE = R/A0,-15,6.0,0.,0.0,1.0,0)
      CALL AXIS(0.0,-3.,24HENERGY(IN ELECTRON-VOLT),+24,10.0,90.,
     1 -EMAX/2.0,AE,-1)
      WRITE(6,6)
    6 FORMAT(12X, *ENERGY PERTURBATION IN THE HYDROGEN MOLECULE,
     1 (E+,E-,J,K,J(PRIME),K(PRIME),AND E**2/R  IN ELECTRON-VOLT)*,///
     2 10X,*E+*,6X,*E-*,4X,*DISTAN=R/A0*,4X,*R  (CM.)*,8X,*J*,
     2 13X,*K*,8X,*DELTA*,3X,*DELTA**2*,3X,*J(PRIME)*,
     2 5X,*K(PRIME)*,7X,*E**2/R*/)
      A0=.5282E-08
C  THE ENERGY E+ (OR E-) IN ELECTRON-VOLT
      DO 8 I=1,28
      DI=I+2
      DISTAN(I)=2.0*DI/10.
C  R IN CENTIMETER
      R=DISTAN(I)*A0
      X=DISTAN(I)
      E=4.770/(10.**10)
C  ELECTRONIC CHARGE IN ARSOLUTE E.S.U.
      A=(E**2/A0)*(-1./X+EXP(-2*X)*(1.+1./X))
      B=(-E**2/A0)*EXP(-X)*(1.+X)
      DELTA=EXP(-X)*(1.+X+X**2/3.)
      PJ=(E**2/A0)*(1./X-EXP(-2*X)*(1./X+11./8.+3*X/4.+X**2/6.))
      CALL INTLOG(PK)
      EPLUS(I)=(E**2/R)+(2*A+PJ+2*DELTA*B+PK)/(1.0+DELTA**2)
      EMINUS(I)=(E**2/R)+(2*A+PJ-2*DELTA*B-PK)/(1.0-DELTA**2)
      Q=E**2/R
      TANT=.6285E+12
      EPLUS(I)=EPLUS(I)*TANT
      EMINUS(I)=EMINUS(I)*TANT
      A=A*TANT
      B=B*TANT
      PJ=PJ*TANT
      PK=PK*TANT
      Q=Q*TANT
      TEMP=DELTA**2
      WRITE(6,7)EPLUS(I),EMINUS(I),DISTAN(I),R,A,B,DELTA,TEMP,PJ,PK,Q
    7 FORMAT(6X,3F8.3,E14.3,2F14.5,2F8.3,2F14.5,E14.3)
    8 CONTINUE
      DISTAN(29)=0.0
      DISTAN(30)=1.0
      EPLUS(29)=0.0
      EPLUS(30)=AE
      CALL LINE(DISTAN,EPLUS,28,1,0,0)
      DISTAN(29)=0.0
      DISTAN(30)=1.0
      EMINUS(29)=0.0
      EMINUS(30)=AE
      CALL LINE(DISTAN,EMINUS,28,1,0,0)
      CALL PLOT(0.0,0.999)
      STOP
      END
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```
      SUBROUTINE INTLOG(PK)
      COMMON X,A0,DELTA,E
      GAMMA=.577215665
      PDELTA=EXP(X)*(1.-X+X**2/3.)
C FOR THE CASE *X GREATER THAN 2 WE HAVE THE FOLLOWING EXPRESSION
      FI1=(EXP(-4*X)/(-4*X))*(.9999965-.9989710/(4*X)+
     1 1.9487646/((4*X)**2)-4.9482092/((4*X)**3)+
     1 11.7850792/((4*X)**4)-20.4523840/((4*X)**5)
     1 +21.1491469/((4*X)**6)-9.5240410/((4*X)**7))
      FI2=(EXP(-2*X)/(-2*X))*(.9999965-.9989710/(2*X)+
     1 1.9487646/((2*X)**2)-4.9482092/((2*X)**3)+
     1 11.7850792/((2*X)**4)-20.4523840/((2*X)**5)
     1 +21.1491469/((2*X)**6)-9.5240410/((2*X)**7))
      PK=(E**2/(5*A0))*(-EXP(-2*X)*(-25./8.+23*X/4.+
     1 3*X**2+X**3/3.)+(6./X)*(DELTA**2*(GAMMA+ALOG(X))+
     1 PDELTA**2*EI1-2*DELTA*PDELTA*EI2))
      RETURN
      END
```