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      PROGRAM TB
C  PROGRAM CALCULATES BRIGHTNESS TEMP. OF THE JOVIAN PLANETS
C  AS A FUNCTION OF WAVELENGTH.
C
C  PROGRAM ESPECIALLY FOR Neptune, based upon Sushil/romani's cloud models
C  L AMMONIA
C f77 -O -o sus susnep_v2003_orton.for
C
C ifort -132 susnep_2012_orton.for -o sus.exe
C ./sus.exe       to run it
C  man ifort to look for compiling options, like -132
C
C  This program has improved NH3 (joined Spilker and Joiner/Steffes
C  This program has H2S de Boer (H2S2, slightly better compared to lab data than
C  my older program, improved H2O, and PH3.
C Note: PH3 abundace is absent right now; need to add saturation curves, etc.
C
C  AS 1,VOL2:JTP.DAT    CONTAINS TEMP PRESS DATA IN UPPER ATM.
C  AS 2,VOL2:JPAR.DAT       PARTIAL PRESS DATA ARE CALCUL AND PUT IN THIS
C  AS 3,VOL2:JTPZ.DAT        TEMP PRESS ALT ARE CALC AND PUT HERE
C  AS 5,VOL2:JAMMON.DAT    INPUT
C  AS 6,SPR:
C  AS 7,VOL2:KAKAR.DAT    CONTAINS AMMONIA LINES AND CP FOR H2
C  RUN WITH JTP.JOB
C  M5 EQ 0  CALCULATE TABLES; NE 0 ASSUMES TABLES EXIST ALLREADY
      dimension Ttab(10),frequ(2428)
      dimension abeh2h2(2428,10),abnh2h2(2428,10)
      dimension abeh2he(2428,10),abnh2he(2428,10)
      dimension abeh2ch4(2428,10),abnh2ch4(2428,10)
      DIMENSION VKAK(16,16),DVKAK(16,16)
      DIMENSION TC(45),CPH2D(45)
      DIMENSION RR(18),CSZA(18),DCSZA(18),STR(19)
      DIMENSION ZT(7000),ZDELZ(7000),ZTPR(7000),ZPH2(7000),ZPH2S(7000),
     +          ZPHE(7000),ZPNH3(7000),ZPH2O(7000),ZPCH4(7000),ZSOLN(7000),
     +          ZPCO(7000),ZPCO13(7000),ZPHCN(7000),ZPPH3(7000)
      DIMENSION XWAVE(30000),XTEMP(30000), XNADIR(30000),VSET(30000)
      DIMENSION TAU(7000),FINT(7000),GTAU(5,7000)
      DIMENSION CLH2O(7000),CLNH4SH(7000),CLNH3(7000),CLH2S(7000)
      DIMENSION CLCH4(7000),CLAR(7000)
      real*4  F0(311),S0(311),EL(311),aph3,wgths(311)
      real*4  FP0(728),SP0(728),ELP(728)
      REAL*4 wgtS0(40),wgtFGB(40),wgtSB(40)
      real*4 t3,gm,vline,fjk,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,
     +       deltot,PCO,PCO13,PHCN
      COMMON/orton/Ttab,frequ,abeh2h2,abnh2h2,abeh2he,abnh2he,
     +             abeh2ch4,abnh2ch4,nfreq,ntemp
      COMMON/ph3/FP0,SP0,ELP,wgtS0,wgtFGB,wgtSB
      COMMON/h2s/F0,S0,EL,wgths
      COMMON/CL/CLH2O,CLNH4SH,CLNH3,CLH2S,CLCH4,CLAR
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
      COMMON/U2/C1,C2,C3,C4
      COMMON/U3/VKAK,DVKAK
      COMMON/U4/T1,T2,T3,T4,T5,T6,T7
      COMMON/U5/SP,SL,SLAM,SLH2O,KB,KS
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
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      COMMON/V3/QROT,QR1,QR2,S1,S2,S3,S4,P1,P2,P3,P4
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
      COMMON/V6/P5,P6,P7,P8
      COMMON/V7/PRO1(20),PRO2(20),STOR(20)
      COMMON/V9/TEMP,BETA,SQ,TAU1,TAU2
      COMMON/V10/TAU,FINT,GTAU
      COMMON/W1/FP,REB,RHO(20)
      COMMON/ABUN/AB1,AB2,AB3,AB4,AB5,AB6
      COMMON/ATM/TC,CPH2D
      COMMON/ZP/ZT,ZDELZ,ZTPR,ZPH2,ZPHE,ZPNH3,ZPH2O,ZPCH4,ZPH2S,
     +          ZPCO,ZPCO13,ZPHCN,ZPPH3
C     VSET ARE WAVENUMBERS (CM-1).
      DATA CSZA/.9978,.9911,.9798,.9638,.9428,.9165,
     1  .8844,.8459,.8000,.750,.700,.650,.600,.500,
     2  .400,.300,.200,.100/
      DATA DCSZA/.10,.0668,.0668,.0667,.0667,.0667,
     1  .0667,.0666,.0640,.0571,.0492,.0429,.0530,
     2  .0583,.0440,.0316,.0205,.0126/
      DATA STR/0.0,.10,.1666,.2333,.30,.3667,.4334,
     1  .50,.5667,.6307,.6878,.737,.7799,.8329,
     2  .8912,.9352,.9668,.9873,1.0/
C
      OPEN(1,NAME='neptune.paulCO_cloud21_fletcher_best_dry')
      OPEN(10,NAME='nepcloud_CO.cloud21_fletcher_best_dry')
      Open(2,NAME='npar.dat')
      OPEN(3,NAME='ntpz.dat')
      OPEN(5,NAME='nammon.dat')
C     OPEN(6,NAME='nepco_spectotal_allgases_dry.dat')
      OPEN(6,NAME='test.dat')
      Open(7,NAME='kakar.dat')
      open(11,NAME='orton_H2.tables',form='formatted')
C     TO SUPPRESS THE LENGHTLY PRINT OUT OF INTERMEDIATE VALUES,
C     SET NOPR AND NOPR2 TO 0 (NOT EQUAL TO 1).
C     NOPR3 CONTROLS PRINT OUT OF MIXING RATIOS
C     DEN=INTEGRATED CLOUD DENSITY; ALT=ALTITUDE RANGE OF CLOUD
C     for some reason I thought I calculated H2-CH4 I guess,
C               but this hasn't been done
      CZB=0.0
      DEN=7.2e6
      NOPR=0
      NOPR2=0
      NOPR3=0
      NOPR4=1
C
C     READ IN ORTON'S H2 TABLES
      read (11,*) ntemp,Tmax,Tmin
      dltemp=(alog(Tmax)-alog(Tmin))/float(ntemp-1)
      do n=1,ntemp
         Ttab(n)=alog(Tmin)+(n-1)*dltemp
      enddo
C
      read (11,*) nfreq
      read (11,*) (frequ(i),i=1,nfreq)
      do n=1,nfreq
         read (11,*) (abeh2h2(n,i),i=1,ntemp)
      enddo
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      do n=1,nfreq
         read (11,*) (abnh2h2(n,i),i=1,ntemp)
      enddo
      do n=1,nfreq
         read (11,*) (abeh2he(n,i),i=1,ntemp)
      enddo
      do n=1,nfreq
         read (11,*) (abnh2he(n,i),i=1,ntemp)
      enddo
      do n=1,nfreq
         read (11,*) (abeh2ch4(n,i),i=1,ntemp)
      enddo
      do n=1,nfreq
         read (11,*) (abnh2ch4(n,i),i=1,ntemp)
      enddo
C

      READ(5,779) MII
      READ(5,779) KQQ
  779 FORMAT(I2)
      READ(5,773) SIZE
C      WRITE(6,772) SIZE
      SIZE=SIZE/2.0
  772 FORMAT(2X,'WATER DROPLET SIZE',2X,E10.5,/)
  773 FORMAT(F10.4)
C     EQUIL: IQ=2, FP=S1, REB=1.0
C     NORMAL: IQ=0; FP=0.25; REB=0
C     INTERM: IQ=1; REB=1.0.; FP=S1
C     IQ=2: TEMP FOR EQUIL. CASE
      READ (5,778) IQ,REB,FP
      if(NOPR4.eq.1) WRITE(6,778) IQ,REB,FP
  778 FORMAT(I2,2F10.4)
C
      DO 1357 I=1,18
          RR(I)=ACOS(CSZA(I))
          RR(I)=SIN(RR(I))
          if(NOPR4.eq.1) WRITE(6,1345) CSZA(I),DCSZA(I),RR(I)
 1345     FORMAT(3E15.5)
 1357 CONTINUE
      DO 2345 J=1,16
          DO 2345 K=1,J
              READ(7,3333) VKAK(J,K)
 2345 CONTINUE
      DO 2346 J=1,16
          DO 2346 K=1,J
              READ(7,2222) DVKAK(J,K)
              IF(NOPR.EQ.1) WRITE(6,4444) J,K,VKAK(J,K),DVKAK(J,K)
              VKAK(J,K)=1.0E-3*VKAK(J,K)
 2346 CONTINUE
 3333 FORMAT(F12.3)
 2222 FORMAT(F8.1)
C
      READ(7,103) (TC(I),CPH2D(I),I=1,36)
      READ(7,108) (TC(I),CPH2D(I),I=37,38)
  108 FORMAT(2(F3.0,F4.3,1X))
      READ(7,104) (TC(I),CPH2D(I),I=39,44)
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  103 FORMAT(9(F3.0,F4.3,1X))
  104 FORMAT(6(F4.0,F4.3,1X))
  105 FORMAT(5(F5.0,1X,F7.3))
C     for equilibrium H2
      IF(IQ.EQ.2) READ(7,103) (TC(I),CPH2D(I),I=1,24)
C     WRITE(6,105) (TC(I),CPH2D(I),I=1,44)
      close(7)
C     read in H2S lines  THIS IS OLD
c     OPEN(7,NAME='h2s_file.list')
c     read(7,7465) (F0(i),S0(i),EL(i),i=1,311)
c7465 format(F13.4,9x,F7.4,3x,F9.4,32x)
      OPEN(7,NAME='H2S_deboer.LIN')
      read(7,*) (F0(i),S0(i),EL(i),wgths(i),i=1,311)
      close(7)
      OPEN(7,NAME='ph3_file.list')
      read(7,*) (FP0(i),SP0(i),ELP(i),i=1,728)
      close(7)
      OPEN(7,NAME='ph3wgt.dat')
      read(7,*) (k,wgtS0(i),wgtFGB(i),wgtSB(i),i=1,40)
      close(7)
C
 4444 FORMAT(I5,I5,2X,F15.4,2X,F15.4)
C
      READ(5,1041) M5,NL
 1041 FORMAT(I1,1X,I4)
      if(NOPR4.eq.1) WRITE(6,1046) M5,NL
 1046 FORMAT(2X,'PARAMETER M5 IS EQUAL TO',/,2I5)
 1049 FORMAT(F10.4)
C     G=1130.0
      G=1140.0
      GE=G
      if(NOPR4.eq.1) WRITE(6,1050) G
 1050 FORMAT(2X,'THE GRAVITY G IS ',/,F12.4)
C     READ(5,1045) AB1,AB2,AB3,AB4,AB5,AB6
 1045 FORMAT(6E10.3)
C     WRITE(6,1047) AB1,AB2,AB3,AB4,AB5,AB6
 1047 FORMAT(2X,'ABUNDANCES H2,HE,NH3,H2O,CH4,H2S ARE',/,6E12.5)
      IF(M5.EQ.0) CALL ATMOS(NL,SOL)
      if(NOPR4.eq.1) WRITE(6,1051) NL
 1051 FORMAT(2X,'THE PARAMETER NL AFTER ATMOS IS EQUAL TO',/,I6)
      NL2=NL-1
      REWIND 2
      REWIND 3
      do i=1,NL
          READ(3,23) ZT(I),ZDELZ(I),ZSOLN(I),CLH2O(I),CLNH4SH(I),
     +               CLNH3(I),CLH2S(I),CLCH4(I),CLAR(I)
      enddo
C  zpco etc are partial pressures
      do i=1,NL
          READ(2,13) ZTPR(I),ZPH2(I),ZPHE(I),ZPNH3(I),ZPH2O(I),
     +               ZPCH4(I),ZPH2S(I),ZPPH3(i),ZPCO(i),ZPCO13(i),ZPHCN(i)
      enddo
   23 FORMAT(10X,F10.4,8E13.8)
   13 FORMAT(11E13.8)
C
      READ(5,1060) NWN
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      if(NOPR4.eq.1) WRITE(6,1060) NWN
 1060 FORMAT(I5)
C     The following could be changed in the future to a read vset(1) and dvset
C     DO 31 I=1,NWN
C  31 READ(5,1061) VSET(I)
 1061 FORMAT(2F10.4)
C     WILL PERFORM THE CALCULATIONS FOR THE WAVENUMBERS
      read(5,1061) vset(1),vsetlast
      dvset=(vset(1)-vsetlast)/nwn
      do n=2,nwn
          vset(n)=vset(n-1)-dvset
      enddo
C
      DO 200 N=1,NWN
          VNU=VSET(N)
          FREQ=C*VNU*1.0E9
          VVNU=1.0/VNU
C      WRITE(6,9) VNU,FREQ,VVNU
   9      FORMAT(/,/,2X,'V(CM-1),FREQ(HZ) ',1P,3(2X,E10.3))
C     INITIALIZE THE OPTICAL DEPTH TO ZERO.
          DH2=0.0
          DHE=0.0
          DNH3=0.0
          DH2O=0.0
          DCH4=0.0
          DH2S=0.0
          dco=0.0
          dco13=0.0
          dhcn=0.0
          dpph3=0.0
          DOPTD=0.0
C         SUM OVER THE VARIOUS PRESSURE LEVELS.
          DO 100 M=1,NL2
C             SPECIFY THE PRESSSURES OF H2,HE,NH3,H2O,AND CH4.
              T=ZT(M)
              DELZ=ZDELZ(M)
              PH2=ZPH2(M)
              PHE=ZPHE(M)
              PNH3=ZPNH3(M)
              PH2O=ZPH2O(M)
              PCH4=ZPCH4(M)
              PH2S=ZPH2S(M)
              PPH3=ZPPH3(M)
              pco=zpco(M)
              pco13=zpco13(M)
              phcn=zphcn(M)
              TPR=ZTPR(M)
              T1=273./T
              T2=300./T
              T3=T2**C2
              T4=T1**C1
              T5=T1**C2
              T6=1.0/(T**3.5)
              T7=4.8/T
              ARGON=tpr*6.0E-14
              wtmol=PH2*2.0158 + PHE*4.0026 + PH2O*18.0153 + PCH4*16.04 + PNH3*
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                  17.03
     1            + PH2S*34.08 + ARGON*39.06 + PCO*28.01 + PHCN*27.018+ PPH3*
         33.9976
               wtmol=wtmol*1.67e-24/tpr
C              CALL THE VARIOUS SUBROUTINES WHICH CALCULATE THE ABSORPTION
    COEFFICIENTS.
               IF(IQ.GE.1) CALL PART(T)
               IF(IQ.GE.1) FP=S1
               IF(TPR.gt.1.0.and.PNH3.NE.0.0.and.vnu.lt.1.0) CALL NH3TOM(VNU,T,ANH
                   3)
               IF(TPR.le.1.0.and.PNH3.NE.0.0.and.vnu.lt.1.0) CALL NH3(VNU,T,ANH3)
               if(vnu.ge.1.0.and.PNH3.ne.0.0)  CALL NH3JOIN(VNU,T,ANH3)
               IF(PNH3.EQ.0.0) ANH3=0.0
               CALL H2O(VNU,T,AH2O)
C              AH2O=0.0
C              ANH3=0.0
C
C              H2H2 WITH MASSIE FORMALISM
C              H2H2JS WITH JOINER-STEFFES FORMALISM; not very good
C              H2H2OR  with Orton's tables;  this is best, but note the range
    inside which it works.
               if(vnu.le.frequ(1)) CALL H2H2(VNU,T,A,B)
               if(T.le.Tmin) CALL H2H2(VNU,T,A,B)
               if(T.ge.Tmax) CALL H2H2(VNU,T,A,B)
               if(T.gt.Tmin.and.T.lt.Tmax.and.vnu.gt.frequ(1))
     +             CALL H2H2OR(IQ,VNU,T,A,B,CZB)
               CALL absbr_H2S2(ah2s,t,tpr,vnu)
C              Ah2S=0.0
c              CALL absbr_ph3(aph3,t,tpr,vnu,ZPPH3)
C              CALCULATE THE OPTICAL DEPTH TAU
C              ACO = absco(lco,fr0,freq,tpr,T,wtmol)
C              the line shape to be used is determined in absco routine.
               call absx_co(aco,t,tpr,vnu)
C              statement above is including all CO lines,  VVW only; this is
    useful for continuum measurements
               ACO=ACO*pco/tpr
C              ****still an error in CO13. Also when simply running absx_co13 --
    assumed to be continuum
C              I need to test this. Note that fr0 is wrong for CO13 if the CO12
    parameters are used
C              ACO13=0.0
C              ACO13 = absco13(lco,fr0,freq,tpr,T,wtmol)
C              call absx_co13(aco13,t,tpr,vnu)
C              ACO13=ACO13*pco13/tpr
c              write(6,1345) aco,pco,tpr
               A8=0.0
c              goto 9191
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    UDSCLOUDSCLOUDSCLOUDSCLOUDS
               IF(MII.NE.1) GOTO 9191
c              H2O liquid and ice
               IF(T.LT.273.0) THEN
                   CALL DIEL(2,0,VVNU,T,E1,E2,D1,D2)
                   X1=SIZE
                   X2=X1*2.0*3.1415/VVNU
                   CALL MIE(X2, D1, D2, QABS)
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                    X=18*1.67E-24
                    Y=SIZE*SIZE*SIZE/8.0E-24
                    X=X*Y
                    XDEN=CLH2O(M)/X
                    A8=A8+XDEN*QABS*3.1415*DELZ*size*size
                ENDIF
                IF(T.GE.273.0) THEN
                    CALL DIEL(1,0,VVNU,T,E1,E2,D1,D2)
C                   X1 IS RADIUS PARTICLE
                    X1=SIZE
                    X2=X1*2.0*3.1415/VVNU
                    CALL MIE(X2, D1, D2, QABS)
C                   TAKE MOLEC.SIZE FEW ANGSTROMS; OR ITS RADIUS 2.00E-8
C                   TAKE H2O-NH3 SOLUTION CLOUD WITH H2O-ICE /WATER PROPERTIES
C                   X=MASS GR/CM3;
                    X=18*1.67E-24
                    Y=SIZE*SIZE*SIZE/8.0E-24
C                   WEIGHT OF ONE DROPLET IS X*Y
                    X=X*Y
C                   NUMBER OF DROPLETS PER CM**3:
                    XDEN=ZSOLN(M)/X
                    A8=A8+XDEN*QABS*3.1415*DELZ*size*size
                ENDIF
c               goto 9191
C               NH4SH CLOUD
                X1=SIZE
                X2=X1*2.0*3.1415/VVNU
                D1=1.7
                D2=.05
                CALL MIE(X2, D1, D2, QABS)
                X=51*1.67E-24
                Y=SIZE*SIZE*SIZE/8.0E-24
                X=X*Y
                XDEN=CLNH4SH(M)/X
                A8=A8+XDEN*QABS*3.1415*DELZ*size*size
                GOTO 9191
C               NH3-ICE
                D1=1.3
                D2=.05
                X1=SIZE
                X2=X1*2.0*3.1415/VVNU
                CALL MIE(X2, D1, D2, QABS)
                X=17*1.67E-24
                Y=SIZE*SIZE*SIZE/8.0E-24
                X=X*Y
                XDEN=CLNH3(M)/X
                A8=A8+XDEN*QABS*3.1415*DELZ*size*size
C               H2S-ICE
                D1=1.3
                D2=.01
                X1=SIZE
                X2=X1*2.0*3.1415/VVNU
                CALL MIE(X2, D1, D2, QABS)
                X=34*1.67E-24
                Y=SIZE*SIZE*SIZE/8.0E-24
                X=X*Y
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              XDEN=CLH2S(M)/X
              A8=A8+XDEN*QABS*3.1415*DELZ*size*size
              GOTO 9191
CLOUDSCLOUDSCLOUDSCLOUDSCLOUDSCLOUDSCLOUDSCLOUDSCLOUDSCLOUDSCLOUDSCLOUDSCLO
    UDSCLOUDSCLOUDSCLOUDSCLOUDS
C             CALCULATE THE OPTICAL DEPTH TAU
 9191         CONTINUE
C             FOR MASSIE FORMALISM USE FOLLOWING EXPRESSIONS
              DENH2=PH2/T
              DENHE=PHE/T
              DENCH4=PCH4/T
              A2=DENH2*DENH2*A*5.246E-3*DELZ/2.9979
              A3=DENH2*DENHE*B*5.246E-3*DELZ/2.9979
              A12=0.
C             For Orton tables (best to use): amagat is p(bar)*269.6/T with
    269.6=273.15/1.013
              if(T.gt.Tmin.and.T.lt.Tmax.and.vnu.gt.frequ(1))
     +             A2=DENH2*DENH2*273.*273.*delz*A/1.013/1.013
              if(T.gt.Tmin.and.T.lt.Tmax.and.vnu.gt.frequ(1))
     +             A3=DENH2*DENHE*273.*273.*delz*B/1.013/1.013
              if(T.gt.Tmin.and.T.lt.Tmax.and.vnu.gt.frequ(1))
     +             A12=DENH2*DENCH4*273.*273.*DELZ*CZB/1.013/1.013
C
              AH2HE=(A2+A3+A12)
C             WRITE(6,1003) T,PH2,A,B,CZB,A2,A3,A12
C             write(6,1004) nfreq,ntemp
c 1003        FORMAT(8(1X,E10.3))
c 1004        format(2I10)
c             Joiner\Steffes formalism:
c             AH2HE=AH2H2*DELZ
C             we absorb PH3 absorption into dh2s
              A4=ANH3*DELZ
              A5=AH2O*DELZ
              A6=AH2S*DELZ
              A9=APH3*DELZ
              DH2=DH2+A2
              DHE=DHE+A3
              DCH4=DCH4+A12
              DNH3=DNH3+A4
              DH2O=DH2O+A5
              DH2S=DH2S+A6+A9
              DCO=DCO+ACO*delz
              DHCN=DHCN+AHCN*delz
              DCO13=DCO13+ACO13*delz
              A7=A4+A5+AH2HE+A8+A6+A9+ACO*DELZ
C             NH3, H2O, HCN and 13CO do not make a difference.
              DOPTD=DOPTD+A7
C             TAU IS THE OPTICAL DEPTH.
              TAU(M)=DOPTD
              GTAU(1,M)=DH2
              GTAU(2,M)=DHE
              GTAU(3,M)=DNH3
              GTAU(4,M)=DH2O
              GTAU(5,M)=DH2S
c             wt=a7/delz*exp(-tau(m))
c             write weighting function
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c             WRITE(6,262) T,TPR,DELZ,wt
  262         FORMAT(4E15.5)
  100     CONTINUE
C         EVALUATE THE BRIGHTNESS TEMPERATURE OF THE CALCULATED INTENSITY.
          DBT=0.0
          DDR=0.0
          DO 2001 JJ=1,18
              CS=CSZA(JJ)
              DC=DCSZA(JJ)
              CALL BRIGHT(VNU,FREQ,NL,CS,BRI)
C             CALL BRIGHTor(VNU,FREQ,NL,CS,BRI)
              STR(JJ)=BRI
              DBT=DBT+BRI*RR(JJ)*DC
              DDR=DDR+RR(JJ)*DC
2001      CONTINUE
          DBT=DBT/DDR
          WAVEL=1./VNU
          GHZ=C*VNU
C         WRITE(6,225) VNU,WAVEL,GHZ
225       FORMAT(2X,'V(CM-1)',4X,'WAVELENGTH(CM)',3X,'FREQ(GHZ)',
     1           /,1P,E11.4,3X,E11.4,4X,E11.4)
C         WRITE(6,226)
226       FORMAT('       ')
C         WRITE(6,235) wavel,STR(1),DBT
235       FORMAT(' wavel, wave^-1, center disk, DISK-AVERAGED TB',/,1P,6X,3E11.4)
C
          XWAVE(N)=WAVEL
          XTEMP(N)=DBT
          XNADIR(N)=STR(1)
  200 CONTINUE
      DO 290 N=1, NWN
         x=1./xwave(N)
         GHZ=C*VSET(N)
         WRITE(6,5768) GHZ,XWAVE(N), x, XNADIR(N), XTEMP(N)
  290 CONTINUE
 5768 FORMAT(5F20.8)
      STOP
      END
CENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDEND
CENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDEND
CENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDEND

      SUBROUTINE BRIGHT(VNU,FREQ,NL,CMU,BRI)
      DIMENSION ZT(7000),ZDELZ(7000)
      DIMENSION TEM(7000),TOPR(7000)
      DIMENSION TAU(7000),FINT(7000),GTAU(5,7000)
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
      COMMON/V10/TAU,FINT,GTAU
      COMMON/ZP/ZT,ZDELZ
C     BR IS THE INTENSITY AT THE TOP OF THE ATMOSPHERE.
C     CMU IS THE COSINE OF THE SOLAR ZENITH ANGLE.
C     FINT(I) IS THE FRACTION OF THE INTENSITY CONTRIBUTED BY LEVEL I.
C     BR IS GIVEN BY EQUATION 90,PAGE 16 OF CHANDRASEKHAR'S
C     RADIATIVE TRANSFER BOOK.  BR IS DERIVED FROM THE INTENSITY
C     CALCULATED FROM EQUATION 90. EQUATION 90 ASSUMES THAT
```

```
C     THE SOURCE FUNCTION IS SIMPLY GIVEN BY THE PLANCK FUNCTION.
      BR=0.0
      YY=FREQ
      A1=2.0*6.626E-9*YY*YY*YY/(C*C)
      A2=6.626*1.0E-11*YY/1.3806
C     WRITE(6,190)
C190  FORMAT(2X,'LEVEL,H*FREQ/KT,EXP(-TAU),DTAU,B(T),',/,
C    1  2X,'TAU,DINT,PARTIAL SUM OF I')
      L1=NL
      L2=L1-1
      BR=0.0
      DO 200 L=2,L2
          K=L1+1-L
          K2=K-1
          S1=ZT(K)
          S2=ZT(K2)
          TAVE=0.5*(S1+S2)
          A4=A2/TAVE
          A5=(TAU(K)+TAU(K2))/(2.0*CMU)
          A6=(TAU(K)-TAU(K2))/CMU
          PL=A1/(EXP(A4)-1.00)
          CALL EX(A5,A7)
          DINT=PL*A7*A6
          BR=BR+DINT
          FINT(K)=DINT
C         if(cmu.gt.0.99) WRITE(6,205) K,Tave,A7,A6,PL,TAU(K),DINT,BR
 205      FORMAT(2X,I4,7(2X,E10.3))
 200  CONTINUE
C     A8 IS THE BRIGHTNESS TEMPERATURE CORRESPONDING TO BR.
      A7=A1/BR
      A8=A2/(ALOG(1.00+A7))
C     WRITE(6,888) FREQ,CMU,BR,A8
 888  FORMAT(2X,'FREQ,CMU,BR,T ARE ',/,4E15.5)
      BRI=A8
      RETURN
      END
CENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDEND
      SUBROUTINE BRIGHTor(VNU,FREQ,NL,CMU,BRI)
      real*8 BR,DINT,PL,A44,A55,A66,A77,A88,A99,A11,A22,YY
      DIMENSION ZT(7000),ZDELZ(7000)
      DIMENSION TEM(7000),TOPR(7000)
      DIMENSION TAU(7000),FINT(7000),GTAU(5,7000)
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
      COMMON/V10/TAU,FINT,GTAU
      COMMON/ZP/ZT,ZDELZ
C     BR IS THE INTENSITY AT THE TOP OF THE ATMOSPHERE.
C     CMU IS THE COSINE OF THE SOLAR ZENITH ANGLE.
C     FINT(I) IS THE FRACTION OF THE INTENSITY CONTRIBUTED BY LEVEL I.
C     BR IS GIVEN BY EQUATION 90,PAGE 16 OF CHANDRASEKHAR'S
C     RADIATIVE TRANSFER BOOK.  BR IS DERIVED FROM THE INTENSITY
C     CALCULATED FROM EQUATION 90. EQUATION 90 ASSUMES THAT
C     THE SOURCE FUNCTION IS SIMPLY GIVEN BY THE PLANCK FUNCTION.
      BR=0.0
      YY=FREQ
      A11=2.0*6.626E-9*YY*YY*YY/(C*C)
```

```
      A22=6.626*1.0E-11*YY/1.3806
C     WRITE(6,190)
C190  FORMAT(2X,'LEVEL,H*FREQ/KT,EXP(-TAU),DTAU,B(T),',/,
C    1  2X,'TAU,DINT,PARTIAL SUM OF I')
      L1=NL
      L2=L1-1
      BR=0.0
      K=NL
      S1=ZT(K)
      TAVE=S1
      A44=A22/TAVE
      PL=A11/(EXP(A44)-1.00)
C     determine BR at bottom atm
      BR=PL
C     if(cmu.gt.0.99) WRITE(6,204) K,Tave,PL,BR,tau(K)
 204  format(I5,4E15.5)
      DO 200 L=2,L2
          K=L1+1-L
          K2=K-1
          S1=ZT(K)
          S2=ZT(K2)
          TAVE=0.5*(S1+S2)
          A44=A22/TAVE
C         A5=TAU(K2)/CMU
          A55=(TAU(K)+TAU(K2))/(2.0*CMU)
          A66=(TAU(K)-TAU(K2))/CMU
          PL=A11/(EXP(A44)-1.00)
          CALL EX(A66,A77)
C         DINT=PL*A7*A6
          BR=BR*A77+PL*(1.-A77)
C         if(cmu.gt.0.99) WRITE(6,205) K,Tave,BR,A77,A66,PL,TAU(K),TAU(K2)
 205      FORMAT(2X,I4,7(2X,E10.3))
 200  CONTINUE
C     A8 IS THE BRIGHTNESS TEMPERATURE CORRESPONDING TO BR.
      A99=A11/BR
      A88=A22/(DLOG(A99+1.000))
C     WRITE(6,888) FREQ,CMU,BR,A8
 888  FORMAT(2X,'FREQ,CMU,BR,T ARE ',/,4E15.5)
      BRI=A88
      RETURN
      END
CENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDENDEND
      SUBROUTINE ATMOS(NN,SOL)
      DIMENSION XP(7000),XT(7000), XG(7000), H2S(7000), CH4(7000),
     +          co(7000),co13(7000),hcn(7000)
      DIMENSION TEMPA(7000),TEMPW(7000),TEMPP(7000),TEMPHY(7000)
      DIMENSION TEMPHE(7000),TEMPXG(7000),HELIUM(7000),XH(7000)
      DIMENSION TEMPT(7000),TMPCH4(7000),TMPH2S(7000),TSOLN(7000),
     +          tmpph3(7000),tmpco(7000),tmphcn(7000)
      DIMENSION ZDELZ(7000),TDELZ(7000),SOLN(7000),fosf(7000)
      DIMENSION AMMON(7000),WATER(7000),DRUK(7000),HYDR(7000),fosfien(7000)
      DIMENSION TC(45),CPH2D(45)
      DIMENSION TCLH2O(7000),TCLNH4SH(7000),TCLNH3(7000),TCLH2S(7000)
      DIMENSION TCLCH4(7000),TCLAR(7000)
      DIMENSION CLH2O(7000),CLNH4SH(7000),CLNH3(7000),CLH2S(7000)
      DIMENSION CLCH4(7000),CLAR(7000)
```

```
      COMMON/CL/CLH2O,CLNH4SH,CLNH3,CLH2S,CLCH4,CLAR
      COMMON/U2/C1,C2,C3,C4
      COMMON/U5/SP,SL,SLAM,SLH2O,KB,KS
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/ABUN/AB1,AB2,AB3,AB4,AB5,AB6
      COMMON/ATM/TC,CPH2D
C
C     AMMON,WATER MIXING RATIOS NH3,H2O
C     THEY ARE READ IN AT PRESSURE LEVELS OF
C     .01,.02,.03,.05,.07,.1,.2,.3,.5,.7,1,2,3,5,7,10  BARS.
      TFLAT=1.0E10
      KOUNT=0
      ZZZ=0.0
      READ(1,19) JMAX
  19  FORMAT(1x,I5)
      write(6,19) JMAX
      SOL=0.0
      ZD=0.0
      zdelz(1)=0.0
      DO 8079 II=1, JMAX
          READ(1,*) XH(II),XT(II),XP(II),HYDR(II),HELIUM(II),CH4(II),
     +              AMMON(II),WATER(II),H2S(II),SOLN(II)
C         read(1,*) s,XH(II),XP(II),XT(II)
C         Hydr(ii)=0.831
C         helium(ii)=0.149
C         h2s(ii)=0.0
C         water(ii)=2.0E-4
C         ammon(ii)=1.0E-4
C         ch4(ii)=2.0E-2
          co(ii)=1.0E-6
          if(xp(ii).ge.0.1585) co(ii)=0.0
C         ***NOTE: check on pco in lats loop; do 50 M=1,----
          co13(ii)=co(ii)*1.0E-2
          hcn(ii)=0.0
          soln(ii)=0.0
 222      FORMAT(F5.1,2X,F6.2,E13.3,2F7.3,5(E10.3))
 223      FORMAT(I5,F7.2,E11.3,2F7.3,4(E10.3))
c         IF(II.GT.1) ZDELZ(II)=(XH(II-1)-XH(II))*1.0E5*900./1130.
          IF(II.GT.1) ZDELZ(II)=abs(XH(II-1)-XH(II))*1.0E5
c         SOLN(II)=SOLN(II)/10.0
          IF(II.NE.1) SOL=SOL+SOLN(II)*ZDELZ(II)
          IF(SOLN(II).GT.0.0) ZD=ZD+ZDELZ(II)
C         IF(XT(II).GT.400.0) ammon(ii)=1.94E-4
          fosfie=0.0
          fosfien(ii)=fosfie
C         CALCULATE VAPOR PRESSURE FOR NH3
C         Skip steps if Paul's files are used
      goto 8079
      if(ammon(ii).gt.3.0E-6) ammon(ii)=3.0E-6
      IF(XT(II).GT.195.0) GOTO 608
      PNH3=1.342E7*EXP(-3753.6/XT(II))
      PRNH3=PNH3/XP(II)
      IF(PRNH3.GE.AMMON(II)) PNH3=AMMON(II)*XP(II)
      AMMON(II)=PNH3/XP(II)
  608 CONTINUE
C     calculate vapor pressure for water
```

```
C     skip step if Paul's profiles are used
      goto 8079
      IF(XT(II).le.273.) goto 9910
      IF(XT(II).gt.273.) goto 9920
 9910 PH2O=1.013*4.327E7*EXP(-6194./XT(II))
      PRH2O=PH2O/XP(II)
      GOTO 9921
 9920 PH2O=1.013*1.5350E6*EXP(-5273./XT(II))
      PRH2O=PH2O/XP(II)
 9921 IF(PRH2O.GE.water(ii)) PH2O=water(ii)*xp(ii)
      water(ii)=PH2O/xp(ii)
c     TT=XT(ii)*XT(ii)
c     VPCH4S = 4.425070D0 - 453.92414D0/XT(ii) - 4055.6016D0/TT
c    1   + 115352.19D0/XT(ii)**3 - 1165560.7D0/XT(ii)**4
c      PCH4 = (10.0D0**VPCH4S) * 1.013
c      PRCH4=PCH4/XP(II)
c      if(PRCH4.ge.CH4(ii)) PCH4=ch4(II)*XP(II)
C      if(xt(ii).lt.80.) CH4(ii)=0.0
 8079  continue
C  skip step if Paul's profiles are used
       goto 8069
C
       xtabun=ammon(jmax)+water(jmax)+H2S(jmax)+ch4(jmax)+co(jmax)
       fhe=helium(jmax)/hydr(jmax)
       fxtab=xtabun/hydr(jmax)
       DO 8089 II=1, JMAX
       xabun=ch4(ii)+ammon(II)+water(ii)+H2S(ii)+co(ii)
       fac=(xabun/xtabun)*fxtab
       hydr(ii)=1.0/(1.0+fhe+fac)
       helium(ii)=hydr(ii)*fhe
 8089  continue
 8069  continue
C
        DO i=1,jmax
            j=jmax+1-i
c           read(10,*) x,y,z,soln(j),clh2o(j),clnh4sh(j),
c    +                 clnh3(j),clh2s(j),clch4(j),clar(j)
            soln(j)=0.
            clh2o(j)=0.
            clnh4sh(j)=0.
            clnh3(j)=0.
            clh2s(j)=0.
            clch4(j)=0.
            clar(j)=0.
        enddo
        ZDELZ(1)=ZDELZ(2)
c       SOL=SOL/ZD
C       WRITE(6,994) SOL,ZD
  994   FORMAT('DENSITY AND ALTITUDE RANGE ARE',2E12.4)
        TT=XT(1)
        PR=XP(1)
        JM=JMAX-1
C       skip all te rest?
C       goto 6904
        DO 601 II=1,JM
            X=ALOG(XT(II+1)/XT(II))
```

```
          Y=ALOG(XP(II+1)/XP(II))
          XG(II)=X/Y
  601   CONTINUE
        write(6,*) xg(jm)
        TEMPT(1)=XT(1)
        TEMPP(1)=XP(1)
        TEMPHY(1)=HYDR(1)
        TEMPHE(1)=HELIUM(1)
        TMPCH4(1)=CH4(1)
        TEMPA(1)=AMMON(1)
        TEMPW(1)=WATER(1)
        TMPph3(1)=fosfien(1)
        TMPco(1)=co(1)
        tmphcn(1)=hcn(1)
        TMPH2S(1)=H2S(1)
        TEMPXG(1)=XG(1)
        TDELZ(1)=ZDELZ(1)
        TSOLN(1)=SOLN(1)
        TCLH2O(1)=CLH2O(1)
        TCLNH4SH(1)=CLNH4SH(1)
        TCLNH3(1)=CLNH3(1)
        TCLH2S(1)=CLH2S(1)
        TCLCH4(1)=CLCH4(1)
        TCLAR(1)=CLAR(1)
        DO 387 IJ=1,2
            KMAX=JMAX
            JJ=1
            write(6,*) jmax,jm
            DO 102 II=2,JMAX
                DO 101 KK=1,3
                    JJ=JJ+1
                    TEMPXG(JJ)=XG(II)
                    TEMPT(JJ)=KK*(XT(II)-XT(II-1))/3.0 + XT(II-1)
                    TEMPP(JJ)=KK*(XP(II)-XP(II-1))/3.0 + XP(II-1)
                    TEMPHY(JJ)=KK*(HYDR(II)-HYDR(II-1))/3.0 + HYDR(II-1)
                    TEMPHE(JJ)=KK*(HELIUM(II)-HELIUM(II-1))/3.0 + HELIUM(II-1)
                    TMPCH4(JJ)=KK*(CH4(II)-CH4(II-1))/3.0 + CH4(II-1)
                    TEMPA(JJ)=KK*(AMMON(II)-AMMON(II-1))/3.0 + AMMON(II-1)
                    TEMPW(JJ)=KK*(WATER(II)-WATER(II-1))/3.0 + WATER(II-1)
                    TMPH2S(JJ)=KK*(H2S(II)-H2S(II-1))/3.0 + H2S(II-1)
                    TMPco(JJ)=KK*(co(II)-co(II-1))/3.0 + co(II-1)
                    TMPHcn(JJ)=KK*(Hcn(II)-hcn(II-1))/3.0 + hcn(II-1)
                    TMPph3(JJ)=KK*(fosfien(II)-fosfien(II-1))/3.0 + fosfien(II-1)
                    TDELZ(JJ)=ZDELZ(II)/3.0
                    TSOLN(JJ)=kk*(SOLN(II)-soln(ii-1))/3.0 + soln(ii-1)
                    if(soln(ii).eq.0..and.soln(ii-1).gt.0.)
     +                  tsoln(jj)=(4-kk)*soln(ii-1)/3.0
                    TCLH2O(JJ)=kk*(CLH2O(II)-clh2o(ii-1))/3.0 + clh2o(ii-1)
                    if(clh2o(ii).eq.0..and.clh2o(ii-1).gt.0.)
     +                  tclh2o(jj)=(4-kk)*clh2o(ii-1)/3.0
                    TCLNH4SH(JJ)=kk*(CLNH4SH(II)-clnh4sh(ii-1))/3.0 + clnh4sh(ii-
                        1)
                    if(clnh4sh(ii).eq.0..and.clnh4sh(ii-1).gt.0.)
     +                  tclnh4sh(jj)=(4-kk)*clnh4sh(ii-1)/3.0
                    TCLNH3(JJ)=CLNH3(II)
                    TCLH2S(JJ)=CLH2S(II)
```

```
                    TCLCH4(JJ)=CLCH4(II)
                    TCLAR(JJ)=CLAR(II)
  101           CONTINUE
                KMAX=KMAX+2
  376           CONTINUE
  102       CONTINUE
            JMAX=KMAX
            WRITE(6,19) JMAX
            DO 103 II=1,JMAX
                ZDELZ(II)=TDELZ(II)
                SOLN(II)=TSOLN(II)
                CLH2O(II)=TCLH2O(II)
                CLNH4SH(II)=TCLNH4SH(II)
                CLNH3(II)=TCLNH3(II)
                CLH2S(II)=TCLH2S(II)
                CLCH4(II)=TCLCH4(II)
                CLAR(II)=TCLAR(II)
                XT(II)=TEMPT(II)
                XP(II)=TEMPP(II)
                HYDR(II)=TEMPHY(II)
                HELIUM(II)=TEMPHE(II)
                CH4(II)=TMPCH4(II)
                AMMON(II)=TEMPA(II)
                WATER(II)=TEMPW(II)
                H2S(II)=TMPH2S(II)
                Hcn(II)=TMPHcn(II)
                co(II)=TMPco(II)
                fosfien(ii)=tmpph3(ii)
                XG(II)=TEMPXG(II)
  388           CONTINUE
  103       CONTINUE
  387   CONTINUE
C  if skipping extension of the adiabat, then (there is an error in the below,
    and it is better to use Paul's code)
 6904  continue
       KOUNT=0
CHEREIAMHEREIAM
       DO 50 M=1,JMAX
C   DELP IS THE DIFFERENCE IN THE PRESSURE LEVELS OF THE
C   MODEL ATMOSPHERE, IN LOG10 COORDINATES.
      PO=PR
      TO=TT
      IF(M.EQ.1) GOTO 50
      PR=XP(M)
      TT=XT(M)
      PCH4=CH4(M)*PR
      H2OMR=WATER(M)
      AMR=AMMON(M)
      PHE=HELIUM(M)*PR
      PH2S=H2S(M)*PR
      PNH3=AMR*PR
      PH2O=H2OMR*PR
      PH2=HYDR(M)*PR
    PPh3=fosfien(m)*pr
        if(pr.ge.0.1585) co(m)=0.0
        pco=co(m)*pr
```

```
        pco13=co13(m)*pr
        phcn=hcn(m)*pr
C
C  COMPUTE DELZ, DIFFERENCE IN HEIGHT BETWEEN THE TWO
C  PRESSURE LEVELS PO AND PR
C
      DELZ=ZDELZ(M)
      ZZZ=ZZZ+DELZ*1.0E-5
      TPR=PR
      WRITE(2,7) TPR,PH2,PHE,PNH3,PH2O,PCH4,PH2S,PCO,PCO13,PHCN
      IF(TT.GT.TFLAT)
     +WRITE(3,8) TPR,TFLAT,DELZ,SOLN(M),CLH2O(M),CLNH4SH(M),
     + CLNH3(M),CLH2S(M),CLCH4(M),CLAR(M)
      IF(TT.LE.TFLAT)
     +WRITE(3,8) TPR,TT,DELZ,SOLN(M),CLH2O(M),CLNH4SH(M),
     + CLNH3(M),CLH2S(M),CLCH4(M),CLAR(M)
    7 FORMAT(10E13.8)
    8 FORMAT(E10.5,F10.4,8E13.8)
       KOUNT=KOUNT+1
 50   CONTINUE
 9999 NN=KOUNT
      M5=0
 1049 FORMAT(F10.4)
  110 FORMAT(I1,1X,I4,I4)
      RETURN
      END
      SUBROUTINE MIE(X,A,B,QABS)
      COMPLEX ZM
      ZM=CMPLX(A,-B)
      ZM=4.0*X*((ZM*ZM-1.0)/(ZM*ZM+2.0))
      QABS=-AIMAG(ZM)
C      A2=2.0*A*B
C      A3=A2*A2
C      A4=(A*A)-(B*B)+2.0
C      A5=A4*A4
C      QABS=4.0*X*((3.0*B)/(A3+A5))
      RETURN
      END
C
C
      SUBROUTINE EX(TX,S)
C     SINCE THE COMPUTER DOES NOT LIKE TOO LARGE OR SMALL ARGUMENTS
C     FOR THE EXPONENTIAL FUNCTION, WE SET THE VALUE TO ZERO IF
C     NEED BE.
      IF (TX .GT. 75.0) S=0.0
      IF (TX .LT. 75.0) S=EXP(-TX)
      RETURN
      END
      BLOCK DATA
C     CONSTANTS USED IN THE PROGRAM ARE SPECIFIED HERE.
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/U2/C1,C2,C3,C4
C     PI,SPEED OF LIGHT,PLANCK'S CONST/TWO PI,TWO PI C,
C     BOLTZMANN'S CONST,AW,1 AMAGAT=2.69E19 CM-3.
C     AW IS 2*PI*PI/3*HB*C
      DATA PI,C,HB,TPC,BOLC,AW,DEN/3.14159,2.99792458E1,1.054,
```

```
     1  1.884,1.380622,2.082,2.687E19/
C     BAR IS 1.0E6 DYNES/CM2.
      DATA BAR/1.0E6/
C     THESE MOLECULAR CONSTANTS FOR NH3 ARE IN MHZ.
C     C1,C2,C3,C4 ARE 13/3,2/3,1/3,30*760*SQRT(293)
      DATA C1,C2,C3,C4/4.333,0.666,0.333,3.902E+05/
      END
C
      SUBROUTINE H2O(VNU,T,AH2O)
C     SEE BERGE AND GULKIS PAPER IN GEHRELS JUPITER BOOK,PG 676,1969.
C     SEE PAGE 118 OF GOODMAN'S THESIS.
C  Updated July 2003 with de Boer's thesis (p. 66), and refs therein
      REAL*4 AON,T,P,F,V
     real*4 gm,vline,fjk,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,PCO,PCO13,PHCN
     REAL*4 QLOG2,SHAPE2
     REAL*4 C,ZH2O,DV,VNU,gamma
      EXTERNAL QLOG2
      REAL*4 DF,DFC,DFD,EL(10),Q0(5),F0(10),FS,FV
      REAL*4 S0(10),S1(10),TCOR,X,X1,Y
     real*4 gh2(10),ghe(10),gh2o(10),xh2(10),xhe(10),xh2o(10)
C  S0 stands for A in de Boer's table 3.5
C       DATA Q0 /2.711, 2.5237, 2.2605, 1.8164,1.3778/ !LOG PF AT
     300,225,150,75,37.5K  Values aren't right, I think
      DATA Q0 /2.2507, 2.0645, 1.804, 1.3649,0.9335/ !LOG PF AT
          300,225,150,75,37.5K  These are right, I think
      DATA F0(1),S0(1),EL(1),gh2(1),ghe(1),gh2o(1),xh2(1),xhe(1),xh2o(1)
     &  /22235.15, 1.0, 644.0,  2.395, 0.67, 10.67, 0.90, 0.515, 0.626/
      DATA F0(2),S0(2),EL(2),gh2(2),ghe(2),gh2o(2),xh2(2),xhe(2),xh2o(2)
     &  /183310.12, 41.9, 196.0, 2.400, 0.71, 11.64, 0.95, 0.490, 0.649/
      DATA F0(3),S0(3),EL(3),gh2(3),ghe(3),gh2o(3),xh2(3),xhe(3),xh2o(3)
     &  /323000.0, 334.4, 1850.0, 2.395, 0.67, 9.59, 0.90, 0.515, 0.420 /
      DATA F0(4),S0(4),EL(4),gh2(4),ghe(4),gh2o(4),xh2(4),xhe(4),xh2o(4)
     &  /325153.8, 115.7, 454.0,  2.395, 0.67, 11.99, 0.90, 0.490, 0.619/
      DATA F0(5),S0(5),EL(5),gh2(5),ghe(5),gh2o(5),xh2(5),xhe(5),xh2o(5)
     &  /380196.8, 651.8, 306.0,  2.390, 0.63, 12.42, 0.85, 0.540, 0.630/
      DATA F0(6),S0(6),EL(6),gh2(6),ghe(6),gh2o(6),xh2(6),xhe(6),xh2o(6)
     &  /390000.0, 127.0, 2199.0,  2.395, 0.67, 9.16, 0.90, 0.515, 0.330/
      DATA F0(7),S0(7),EL(7),gh2(7),ghe(7),gh2o(7),xh2(7),xhe(7),xh2o(7)
     &  /436000.0, 191.4, 1507.0, 2.395, 0.67, 6.32, 0.90, 0.515, 0.290/
      DATA F0(8),S0(8),EL(8),gh2(8),ghe(8),gh2o(8),xh2(8),xhe(8),xh2o(8)
     &  /438000.0, 697.6, 1070.0, 2.395, 0.67, 8.34, 0.90, 0.515, 0.360 /
      DATA F0(9),S0(9),EL(9),gh2(9),ghe(9),gh2o(9),xh2(9),xhe(9),xh2o(9)
     &  /442000.0, 590.2, 1507.0, 2.395, 0.67, 6.52, 0.90, 0.515, 0.332 /
      DATA F0(10),S0(10),EL(10),gh2(10),ghe(10),gh2o(10),xh2(10),xhe(10),xh2o
          (10)
     &  /448000.8, 973.1, 412.0,  2.395, 0.67, 11.57, 0.90, 0.515, 0.510/
       COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
       COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C
C     CONVERT VNU(CM-1) TO GHZ. C = 29.97
     NLINES=10
     C=2.99791E1
     F=VNU*C*1.0E3                  !FREQU IN MHZ
```

```
      V=VNU*C             !FREQ IN GHZ
      rho=1.0E12*18.0*PH2O/(8.34143E7*T)  !rho in g/m^3
      PA=0.81*PH2 + 0.35*PHe
      AON=0.0
          DO N = 1,NLINES
      flc=f0(n)                        !line center in MHz
      VLINE=F0(N)/1.0E3       !LINE CENTER IN GHZ
          TCOR = S0(N) * exp(-EL(N)/T)
C  THE GROSS LINE SHAPE
          X2=(-v*v+vline*vline)
          X2=X2*X2
      g1=gh2(N)*PH2*(300.0/T)**xh2(N)
      g2=ghe(N)*PHe*(300.0/T)**xhe(N)
      g3=gh2o(N)*PH2O*(300.0/T)**xh2o(N)
      gamma=g1+g2+g3
          X3=gamma*gamma*4.*v*v
          FJK=TCOR*gamma/(X2+X3)
C  Divide FJK by 10 to test Steffes student's idea that DeBoer is off by 10.
      FJK=FJK/10.0
      AON=AON+FJK
C  perhaps multiply by 4/pi
      enddo
C     AON=AON*4.0/3.14159 !we think that it is all included in deBoer's stuff; It
      is
      X1=(300.0/T)**2.1
      X1=1.08E-11*X1*PA*v*v*rho
      X2=(300.0/T)**2.5
      X2=2.0*v*v*rho*X2*2.3E-5*AON
C     write(6,*) AON,X1,X2
      AON=X1+X2
C
C       H2O ABSORPTION COEFFICIENT IN CM-1 ;
         AH2O=AON
C
        RETURN
        END
        SUBROUTINE H2Oold(VNU,T,AH2O)
C This is the old H2O routine
C       SEE BERGE AND GULKIS PAPER IN GEHRELS JUPITER BOOK,PG 676,1969.
C       SEE PAGE 118 OF GOODMAN'S THESIS.
         COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
         COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
        COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
        COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
        COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C
C       CONVERT VNU(CM-1) TO GHZ. C = 29.97
        V=VNU*C
C
C       EVALUATE EQUATION 29.
        A2=V/29.97
        A3=(A2-0.74)*(A2-0.74)
        A4=(A2+0.74)*(A2+0.74)
        A5=9.88E-2*T5*((0.81*PH2)+(0.35*PHE))
        A5=A5/1.013
        A6=A5*A5
```

```
      A7=(A5/(A3+A6))+(A5/(A4+A6))
C     H2O ABSORPTION COEFFICIENT IN CM-1
      AH2O=PH2O*T4*V*V*((9.07E-9*A7)+(1.45E-7*A5))
C  CORRECTION TERM B(T)/B(293)   SEE GOODMAN,P.117
      AH2O=AH2O*1.179
      AH2O=AH2O/1.013
C
      IF (NOPR .EQ. 1) WRITE(6,10) V,A2,A3,A4,A5,A6,A7,AH2O
  10  FORMAT(2X,'H2O V(GHZ),A2,A3,A4,A5,A6,A7,AH2O',/,
     1  2X,1P,8(2X,E10.3),/)
      RETURN
      END
C
C
C
      SUBROUTINE NH3TOM(VNU,T,ANH3)
C     CALCULATE THE AMMONIA ABSORPTION COEFFICIENT (CM-1)
C     USED BY GULKIS AND POYNTER (1972),AND GIVEN IN BERGE
C     AND GULKIS, GEHRELS JUPITER BOOK,PAGE 675.
      DIMENSION VKAK(16,16),DVKAK(16,16)
       COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
      COMMON/U2/C1,C2,C3,C4
      COMMON/U3/VKAK,DVKAK
      COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C
C   VKAK(J,K)=CENTER FREQU FOR THE (J,K) TRANSITION ACCORDING TO THE
C  TABULATED VALUES OF POYNTER AND GULKIS (1975).
C  DVKAK(J,K) ARE THE CORRESPONDING SELF BROADENED LINE WIDTHS
C  AS TABULATED BY THEM (RESP. GHZ, MHZ/TORR)
C     CHANGE VNU(CM-1) TO GHZ.
      V=(C*VNU)
C  CHANGE PRESSURES FROM BARS TO ATM, AND BACK AT END OF SUBROUTINE; MARCH89
     PH2=PH2/1.013
     PHE=PHE/1.013
     PH2O=PH2O/1.013
     PNH3=PNH3/1.013
     PCH4=PCH4/1.013
     TPPR=PH2+PHE+PNH3+PH2O+PCH4
C     CORRECTION FRACTOR IS GIVEN ON PAGE 676 OF THE BERGE AND GULKIS
C     PAPER, GEHRELS JUPITER BOOK.
      CORBG=1.0075+((0.0308+(0.0552*(PH2/T)))*(PH2/T))
     CORR=-0.33664+T/110.4-T*T/70600.
     IF(T.GT.320.) CORR=1.1115
     IF(T.LT.180.) then
     x=(180.*180./70600.) - 0.337
     y=(1./110.4) - (180./35300.)
     corr=x + y*T
     endif
C
     CORR=CORR*CORBG
     IF(TPPR.LE.1.0) CORR=1.0
C
      SUM=0.0
C     CALCULATE THE INVERSION LINE WAVENUMBERS
```

```
C     FOR NH3, FROM THE DATA IN POYNTER AND KAKAR
C     AP J SUPPL SERIES,VOL 29,P87,1975.
C     J AND K ARE QUANTUM NUMBERS.
C
C     NLINE ARE THE NUMBER OF LINES TO BE CALCULATED.
      NLINE=16
C
      DO 10 J=1,NLINE
      L1=J*(J+1)
      L3=0
      DO 20 K=1,J
      L2=K*K
      L3=L3+1
C     SB IS THE SELF BRODENED LINE WIDTH OF NH3 IN MHZ/TORR.
C     C4 IS GIVEN IN THE BLOCK DATA STATEMENT.
C     SK IS 1.5 OR 3, DEPENDING UPON THE K VALUE.
      SK=1.5
      IF (L3 .NE. 3) GO TO 21
      SK=3.0
      L3=0
  21  VLINE=VKAK(J,K)
       SB=DVKAK(J,K)
      IF (NOPR .EQ. 1) WRITE(6,22) J,K,SK,VLINE,SB
  22  FORMAT(2X,'J,K,SK,VLINE(GHZ),SB(MHZ/TORR)',/,
     1 2X,I3,2X,I3,2X,F4.1,2X,1P,2(2X,E10.3))
C     CALCULATE A(J,K).
      CALL SAJTOM(T,VLINE,J,L1,L2,SK,SB,GM,GH2,AJK)
      IF(J.EQ.1.AND.K.EQ.1) ZZV=2.0*AJK*EXP(23.3/T)/3.0
C     FJK IS THE FREQUENCY DEPENDENT LINE SHAPE OF BEN REUVEN.
      CALL SFJTOM(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
      SB=AJK*FJK
      SUM=SUM+(CORR*AJK*FJK)
c  no correction term in Joiner/Steffes;
c     SUM=SUM+(AJK*FJK)
  20  CONTINUE
  10  CONTINUE
C
C  CALCULATE ROTATION LINE J=0;K=0
C  VLINE=5.73E5 MHZ; CHOSE DVLINE=14. MHZ
C
      L1=2
      L2=1
      VLINE=5.73E2
      SB=14.0
      GM=(2.318*T3*PH2)+(0.79*T3*PHE)+(0.75*T2*SB*PNH3)
      GM=GM
      CALL SFJK(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
      ZZV1=ZZV*7.0E-2*T*(1.0-EXP(-28.6/T))
      ZZV2=ZZV*5.25E-2*T*EXP(-23.3/T)*(1.0-EXP(-57.2/T))
      ZZV3=ZZV*7.50E-2*T*EXP(-28.6/T)*(1.0-EXP(-57.2/T))
      SUM=SUM+(ZZV1*FJK)
      L1=2
      L2=1
      VLINE=1169.0
      SB=23.8
      CALL SFJK(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
```

```
      SUM=SUM+(ZZV2*FJK)+(ZZV3*FJK)
C
C
C     THE AMMONIA ABSORPTION COEFFICIENT IS IN CM-1.
        ANH3=sum
      IF (NOPR .EQ. 1) WRITE(6,30) CORR,SUM,ANH3
   30 FORMAT(2X,'CORR,SUM,ANH3',2X,1P,3(2X,E10.3),/)
C
     PH2=PH2*1.013
     PHE=PHE*1.013
     PH2O=PH2O*1.013
     PNH3=PNH3*1.013
     PCH4=PCH4*1.013
      RETURN
      END
C
      SUBROUTINE NH3(VNU,T,ANH3)
C     CALCULATE THE AMMONIA ABSORPTION COEFFICIENT (CM-1)
C     USED BY GULKIS AND POYNTER (1972),AND GIVEN IN BERGE
C     AND GULKIS, GEHRELS JUPITER BOOK,PAGE 675.
      DIMENSION VKAK(16,16),DVKAK(16,16)
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
      COMMON/U2/C1,C2,C3,C4
      COMMON/U3/VKAK,DVKAK
      COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C
C   VKAK(J,K)=CENTER FREQU FOR THE (J,K) TRANSITION ACCORDING TO THE
C  TABULATED VALUES OF POYNTER AND GULKIS (1975).
C  DVKAK(J,K) ARE THE CORRESPONDING SELF BROADENED LINE WIDTHS
C  AS TABULATED BY THEM (RESP. GHZ, MHZ/TORR)
C     CHANGE VNU(CM-1) TO GHZ.
      V=(C*VNU)
C  CHANGE PRESSURES FROM BARS TO ATM, AND BACK AT END OF SUBROUTINE; MARCH89
     PH2=PH2/1.013
     PHE=PHE/1.013
     PH2O=PH2O/1.013
     PNH3=PNH3/1.013
     PCH4=PCH4/1.013
C     CORRECTION FRACTOR IS GIVEN ON PAGE 676 OF THE BERGE AND GULKIS
C     PAPER, GEHRELS JUPITER BOOK.
C
      CORR=1.0075+((0.0308+(0.0552*(PH2/T)))*(PH2/T))
C      CORR=SQRT(PH2/T)
C      CORR=1.0+(0.155*CORR+0.52*SQRT(CORR))*SQRT(CORR)
      IF (NOPR .EQ. 1) WRITE(6,5) V,CORR
    5 FORMAT(2X,'NH3 V(GHZ),CORR',2X,1P,2(2X,E10.3))
      IF (NOPR .EQ. 1) WRITE(6,6) C1,C2,C3,C4
    6 FORMAT(2X,'CONSTANTS C1,C2,C3,C4',2X,1P,4(2X,E10.3))
C
      SUM=0.0
C     CALCULATE THE INVERSION LINE WAVENUMBERS
C     FOR NH3, FROM THE DATA IN POYNTER AND KAKAR
C     AP J SUPPL SERIES,VOL 29,P87,1975.
C     J AND K ARE QUANTUM NUMBERS.
```

```
C
C     NLINE ARE THE NUMBER OF LINES TO BE CALCULATED.
      NLINE=16
C
      DO 10 J=1,NLINE
      L1=J*(J+1)
      L3=0
      DO 20 K=1,J
      L2=K*K
      L3=L3+1
C     SB IS THE SELF BRODENED LINE WIDTH OF NH3 IN MHZ/TORR.
C     C4 IS GIVEN IN THE BLOCK DATA STATEMENT.
C     SK IS 1.5 OR 3, DEPENDING UPON THE K VALUE.
      SK=1.5
      IF (L3 .NE. 3) GO TO 21
      SK=3.0
      L3=0
  21  VLINE=VKAK(J,K)
       SB=DVKAK(J,K)
      IF (NOPR .EQ. 1) WRITE(6,22) J,K,SK,VLINE,SB
  22  FORMAT(2X,'J,K,SK,VLINE(GHZ),SB(MHZ/TORR)',/,
     1 2X,I3,2X,I3,2X,F4.1,2X,1P,2(2X,E10.3))
C     CALCULATE A(J,K).
      CALL SAJK(T,VLINE,J,L1,L2,SK,SB,GM,GH2,AJK)
      IF(J.EQ.1.AND.K.EQ.1) ZZV=2.0*AJK*EXP(23.3/T)/3.0
C     FJK IS THE FREQUENCY DEPENDENT LINE SHAPE OF BEN REUVEN.
      CALL SFJK(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
      SB=AJK*FJK
      SUM=SUM+(CORR*AJK*FJK)
      IF (NOPR .EQ. 1) WRITE(6,23) AJK,FJK,SB
  23  FORMAT(2X,'AJK,FJK,(AJK*FJK)',2X,1P,3(2X,E10.3))
  20  CONTINUE
  10  CONTINUE
C
C  CALCULATE ROTATION LINE J=0;K=0
C  VLINE=5.73E5 MHZ; CHOSE DVLINE=14. MHZ
C
      L1=2
      L2=1
      VLINE=5.73E2
      SB=14.0
      GM=(2.318*T3*PH2)+(0.79*T3*PHE)+(0.75*T2*SB*PNH3)
      GM=GM
      CALL SFJK(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
      ZZV1=ZZV*7.0E-2*T*(1.0-EXP(-28.6/T))
      ZZV2=ZZV*5.25E-2*T*EXP(-23.3/T)*(1.0-EXP(-57.2/T))
      ZZV3=ZZV*7.50E-2*T*EXP(-28.6/T)*(1.0-EXP(-57.2/T))
      SUM=SUM+(ZZV1*FJK)
      L1=2
      L2=1
      VLINE=1169.0
      SB=23.8
      CALL SFJK(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
      SUM=SUM+(ZZV2*FJK)+(ZZV3*FJK)
C
C
```

```
C     THE AMMONIA ABSORPTION COEFFICIENT IS IN CM-1.
      ANH3=SUM
      IF (NOPR .EQ. 1) WRITE(6,30) CORR,SUM,ANH3
  30  FORMAT(2X,'CORR,SUM,ANH3',2X,1P,3(2X,E10.3),/)
C
    PH2=PH2*1.013
    PHE=PHE*1.013
    PH2O=PH2O*1.013
    PNH3=PNH3*1.013
    PCH4=PCH4*1.013
      RETURN
      END
C
C
C
      SUBROUTINE SAJK(T,VLINE,J,L1,L2,SK,SB,GM,GH2,AJK)
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
      COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C     GM IS GAMMA(J,K) IN GHZ.
C   2.318 IPV 3.318
      GM=(2.318*T3*PH2)+(0.79*T3*PHE)+(0.75*T2*SB*PNH3)
C      GM=(4.8*PH2*(T2**0.50))+(0.79*T3*PHE)+(0.75*T2*SB*PNH3)
C      GM=17.4*T2*PNH3+1.73*T8*PH2+0.40*T8*PHE
      A1=(2.*J+1.)*FLOAT(L2)/FLOAT(L1)
      A5=((2.98*L1)-(1.09*L2))*T7
C     AJK IS A(J,K),SEE EQN 24 OF BERGE AND GULKIS PAPER,GEHRELS
C     JUPITER BOOK,PAGE 675.
      CALL EX(A5,A10)
      AJK=1.23E3*A1*SK*PNH3*T6*A10
      IF (NOPR .EQ. 1) WRITE(6,10) GM,A1,A5,AJK
  10  FORMAT(2X,'GM,A1,A5,AJK',2X,1P,4(2X,E10.3))
      RETURN
      END
      SUBROUTINE SAJTOM(T,VLINE,J,L1,L2,SK,SB,GM,GH2,AJK)
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
      COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C     GM IS GAMMA(J,K) IN GHZ.
    PTOT=PH2+PHE+PNH3+PH2O+PCH4
c  spilker uses equations below
    GNH3=0.74
    GHE=0.46+T/3000.
    R=8.79*EXP(-T/83.)
    X=2.122*EXP(-T/116.8)
    Y=EXP(9.024-T/20.3)
    Y=(Y-0.9918+PH2)**R
    GH2=2.34*(1.0-X/Y)
c  Joanna Joiner uses:
c        gh2=1.69
c        ghe=0.75
c        gnh3=0.60
      GM=(GH2*T3*PH2)+(GHE*T3*PHE)+(GNH3*T2*SB*PNH3)
      A1=(2.*J+1.)*FLOAT(L2)/FLOAT(L1)
```

```
      A5=((2.98*L1)-(1.09*L2))*T7
C     AJK IS A(J,K),SEE EQN 24 OF BERGE AND GULKIS PAPER,GEHRELS
C     JUPITER BOOK,PAGE 675.
      CALL EX(A5,A10)
      AJK=1.23E3*A1*SK*PNH3*T6*A10
      IF (NOPR .EQ. 1) WRITE(6,10) GM,A1,A5,AJK
  10  FORMAT(2X,'GM,A1,A5,AJK',2X,1P,4(2X,E10.3))
      RETURN
      END
C
C
      SUBROUTINE SFJK(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
    real*4 t3,gm,vline,fjk,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,
     + deltot,PCO,PCO13,PHCN
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
       COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C     FJK IS THE BEN REUVEN LINE SHAPE,SEE EQN 25 OF BERGE AND
C     GULKIS ARTICLE,PAGE 675 OF GEHRELS JUPITER BOOK.
C
      X=PH2+PHE+PH2O+PNH3+PCH4
C  IF X.LT.1 ATM VAN VLECK-WEISKOPF LINE SHAPE CAN BE
C  USED; HOWEVER, BEN REUVEN IS STILL BETTER OUT IN THE
C  WINGS OF THE AMMONIA LINES.
c     A2 IS THE COUPLING FACTOR ZETA(J,K) IN GHZ.
C   GOTO 500
C  for Gross lineshape, goto 500 (first VVW, then gross
      IF(VLINE.GT.100.0) GOTO 500
      A2=(1.92*PH2*T3)+(0.49*T2*PNH3*SB)+
     1  (0.3*T3*PHE)
C      A2=(0.49*T2*PNH3*SB)+(0.3*T3*PHE)+
C     +(4.80*(T2**0.5)-0.6*(T2**2.0))*PH2
C      A2=(1.73*T8-0.87*T10)*PH2+
C     +  (0.40*T8-0.21*T9)*PHE+
C     +  (17.4*T2-6.0*T11)*PNH3
C      A2=0.655*GM
C     A4 IS THE PRESSURE SHIFT DEL (GHZ)
    A4=-0.45*PNH3
C     SQUARES OF VARIOUS TERMS.
      A5=(VLINE+A4)*(VLINE+A4)
C      A5=VLINE*VLINE
      A6=GM*GM
      A7=A2*A2
      A8=V*V
C     NUMERATOR
      A9=((GM-A2)*A8)+((GM+A2)*(A5+A6-A7))
      A10=A8-A5-A6+A7
C     DENOMINATOR
      A10=(A10*A10)+(4.0*A8*A6)
C     THE BEN REUVEN LINE SHAPE.
      FJK=2.0*A8*(A9/A10)
      IF (NOPR .EQ. 1) WRITE(6,10) A2,A4,A5,A6,A7,A8,A9,
     1  A10,FJK
      FFF=FJK
      GOTO 501
```

```
  500 CONTINUE
C  THE VAN VLECK-WEISKOPF LINE SHAPE
C
      Z1=0.755*PH2+0.231*PHE
      Z2=FLOAT(L2)/FLOAT(L1)
      Z1=Z1*(Z2**0.3333)
      Z2=SQRT(Z2)*PNH3*6.23
      Z=(Z1+Z2)*1.0E3/T
      X1=V*V*Z
      X2=(V-VLINE)*(V-VLINE)
      X3=(V+VLINE)*(V+VLINE)
      FJK=X1/(X2+Z*Z)+X1/(X3+Z*Z)
C      GOTO 501
  502 CONTINUE
C  THE GROSS LINE SHAPE
       X2=(-V*V+VLINE*VLINE)
       X2=X2*X2
      if(vline.lt.1000.) Z1=123.3551*PH2+60.7441*PHE
    if(vline.ge.1000.) z1=2.885*PH2+1.00*PHE
C      Z2=FLOAT(L2)/FLOAT(L1)
    Z2=300./T
      Z1=Z1*(Z2**0.3)
    if(vline.lt.1000.) Z=154.1939*PNH3*Z2
    if(vline.ge.1000.) Z=22.989*PNH3*Z2
       Z=Z1+Z
       X3=Z*Z*4.*V*V
       X1=v*VLINE*Z*4.
       X1=X1*V*VLINE
       FJK=X1/(X2+X3)
      FFF=FJK
  501 CONTINUE
  10  FORMAT(2X,'A2,A4,A5,A6,A7,A8,A9,A10,FJK',/,
     1  2X,1P,9(2X,E10.3))
      RETURN
      END
C
      SUBROUTINE SFJTOM(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
    real*4 t3,gm,vline,fjk,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,
     + deltot,PCO,PCO13,PHCN
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
       COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C
C     FJK IS THE BEN REUVEN LINE SHAPE,SEE EQN 25 OF BERGE AND
C     GULKIS ARTICLE,PAGE 675 OF GEHRELS JUPITER BOOK.
C
      X=PH2+PHE+PH2O+PNH3+PCH4
C  IF X.LT.1 ATM VAN VLECK-WEISKOPF LINE SHAPE SHOUL BE
C  USED; HOWEVER, BEN REUVEN IS STILL BETTER OUT IN THE
C  WINGS OF THE AMMONIA LINES. SO OPTION VAN VLECK-WEISKOPF
C  IS NEGLECTED BY SETTING IN NEXT LINE:
C  IF(X.LT.0.0) INSTEAD OF IF(X.LT.1.0)
C
C       IF(X.LT.1.) GOTO 500
C
```

```
C     A2 IS THE COUPLING FACTOR ZETA(J,K) IN GHZ.
c  spliker's formalism uses equations below
     ZNH3=0.5
     ZHE=0.28-T/1750.
     ZH2=5.7465+GH2*(-7.7644+GH2*(9.1931+GH2*(-5.6816+1.2307*GH2)))
     if(v.le.30.0) goto 600
c  Joanna Joiner's paper gives parameters below
C  These parameters are better at freq. (v in GHz) above 40 GHz
C  see de Boer's thesis, p. 61-64
         znh3=0.20
        zh2=1.35
         zhe=0.30
C
      IF(VLINE.GT.100.0) GOTO 500
 600   A2=(ZH2*PH2*T3)+(ZNH3*T2*PNH3*SB)+(ZHE*T3*PHE)
C     A4 IS THE PRESSURE SHIFT DEL (GHZ)
    A4=-0.45*PNH3
C     SQUARES OF VARIOUS TERMS.
      A5=(VLINE+A4)*(VLINE+A4)
      A6=GM*GM
      A7=A2*A2
      A8=V*V
C     NUMERATOR
      A9=((GM-A2)*A8)+((GM+A2)*(A5+A6-A7))
      A10=A8-A5-A6+A7
C     DENOMINATOR
      A10=(A10*A10)+(4.0*A8*A6)
C     THE BEN REUVEN LINE SHAPE.
      FJK=2.0*A8*(A9/A10)
      FFF=FJK
C      IF(V.LT.29.0) GOTO 501
c  April 2003: we skip VVW because Spilker's formalism does already
c  do the right thing, I believe
    GOTO 501
  500 CONTINUE
C  THE VAN VLECK-WEISKOPF LINE SHAPE
      Z1=0.755*PH2+0.231*PHE
      Z2=FLOAT(L2)/FLOAT(L1)
      Z1=Z1*(Z2**0.3333)
      Z2=SQRT(Z2)*PNH3*6.23
      Z=(Z1+Z2)*1.0E3/T
      X1=V*V*Z
      X2=(V-VLINE)*(V-VLINE)
      X3=(V+VLINE)*(V+VLINE)
      FJK=X1/(X2+Z*Z)+X1/(X3+Z*Z)
C      GOTO 501
  502 CONTINUE
C  THE GROSS LINE SHAPE
        X2=(-V*V+VLINE*VLINE)
        X2=X2*X2
       if(vline.lt.1000.) Z1=123.3551*PH2+60.7441*PHE
    if(vline.ge.1000.) z1=2.885*PH2+1.00*PHE
C      Z2=FLOAT(L2)/FLOAT(L1)
    Z2=300./T
      Z1=Z1*(Z2**0.3)
    if(vline.lt.1000.) Z=154.1939*PNH3*Z2
```

```
      if(vline.ge.1000.) Z=22.989*PNH3*Z2
         Z=Z1+Z
          X3=Z*Z*4.*V*V
          X1=v*VLINE*Z*4.
          X1=X1*V*VLINE
          FJK=X1/(X2+X3)
         FFF=FJK
  501 CONTINUE
  10  FORMAT(2X,'A2,A4,A5,A6,A7,A8,A9,A10,FJK',/,
     1  2X,1P,9(2X,E10.3))
      RETURN
      END
C
C
      SUBROUTINE H2H2(VNU,T,A,B)
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V3/QROT,QR1,QR2,S1,S2,S3,S4,P1,P2,P3,P4
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
      COMMON/V6/P5,P6,P7,P8
      COMMON/V7/PRO1(20),PRO2(20),STOR(20)
      COMMON/W1/FP,REB,RHO(20)
      COMMON/V9/TEMP,BETA,SQ,TAU1,TAU2
C     H2 OPACITIES ARE CALCULATED FOLLOWING THE PAPER "ANALYSIS OF
C     THE SHAPE OF THE FAR-INFRARED SPECTRA OF H2-H2 AND H2-HE
C     COLLISIONS,BY COHEN AND BIRNBAUM,APRIL 1981.
C     A RELATED PAPER IS GIVEN BY BIRNBAUM AND COHEN, CANADIAN
C     JOURNAL OF PHYSICS,VOL 54,PAGE 593,1976.
C     THIS WORK IS NBSIR 80-2175(R).
C     A AND B COEFFICIENTS IN THE TRAFTON TRADITION ARE CALCULATED.
C     SEE TRAFTON, ASTROPHYSICAL JOURNAL,V 147,PAGE 765,1967.
C
C     THE H2-H2 COLLISIONS ARE CONSIDERED HERE FOR THE A VALUES.
C
      TEMP=T
C     BOLTZMANN STATISTICS ARE CALCULATED.
      CALL JROT(TEMP)
C     EVALUATE SQ,TAU1,TAU2 PARAMETERS.
      CALL PARAM(1)
      IF (NOPR .EQ. 1) WRITE(6,330) SQ,TAU1,TAU2
 330  FORMAT(/,2X,'FOR H2-H2 COLLISIONS',/,2X,'SQ,TAU1,TAU2',
     1  2X,1P,3(2X,E10.3))
C     EVALUATE THE A FACTOR.
      CALL FAC(10,AFAC)
      IF (NOPR .EQ. 1) WRITE(6,355) AFAC
 355  FORMAT(2X,'AFAC=',2X,1P,E10.3)
C
      V=VNU
      IF (NOPR .EQ. 1) WRITE(6,310) V
 310  FORMAT(2X,'V(CM-1)= ',1P,E10.3)
C     OM IS TWO PI TIMES C TIMES THE WAVENUMBER.
C     FREQ IS SEC-1.
      OM=TPC*V
      FREQ=C*V*1.0E9
      BETA=1.0/(BOLC*TEMP)
      IF (NOPR .EQ. 1) WRITE(6,315) OM,FREQ,BETA
```

```
 315  FORMAT(2X,'OM(SEC-1),FREQ(SEC-1),BETA(ERG-1)',/,
     1  2X,1P,3(2X,E10.3))
C     EVALUATE THE 1-EXP TERM.
      TX=BETA*HB*OM
      CALL EX(TX,S)
C  AW2 SHOULD BE MULTIPLIED BY 1.0E-36
      AW2=AW*OM*(1.0-S)*SQ
      IF (NOPR .EQ. 1) WRITE(6,340) AW2
 340  FORMAT(2X,'AW2= ',1P,E10.3)
C
C     THE SIX TERMS OF EQUATION 7 OF NBS 80 ARE CALCULATED.
C     THE FIRST TERM IS EVALUATED.
      OM2=OM
      CALL GAMMA(OM2,GAM)
      IF (NOPR .EQ. 1) WRITE(6,356) TEMP,TAU1,TAU2,OM,BETA,GAM
 356  FORMAT(2X,1P,6(2X,E10.3))
      TERM1=AFAC*GAM
C         ZERO AND TWO ARE EVALUATED.
      CALL EVAL(0,2,OM,B1,B2)
      TERM2=(RHO(1)*B1)+(RHO(3)*B2)
C         ONE AND THREE ARE EVALUATED.
      CALL EVAL(1,3,OM,B1,B2)
      TERM3=(RHO(2)*B1)+(RHO(4)*B2)
      TERM3=(9.0/5.0)*TERM3
C         TWO AND FOUR ARE EVALUATED.
      CALL EVAL(2,4,OM,B1,B2)
      TERM4=(RHO(3)*B1)+(RHO(5)*B2)
      TERM4=(18.0/7.0)*TERM4
C         THREE AND FIVE ARE EVALUATED.
      CALL EVAL(3,5,OM,B1,B2)
      TERM5=(RHO(4)*B1)+(RHO(6)*B2)
      TERM5=(10.0/3.0)*TERM5
C
C  SUM3 SHOULD BE MULTIPLIED BY 1.0E-14
      SUM3=TERM1+TERM2+TERM3+TERM4+TERM5
      IF (NOPR .EQ. 1) WRITE(6,360) TERM1,TERM2,TERM3,TERM4,
     1  TERM5,SUM3
 360  FORMAT(2X,'TERM1,TERM2,TERM3,TERM4,TERM5,SUM',/,
     1  2X,1P,6(2X,E10.3))
C     NOTE:THE RESULT IS MULTIPLIED BY 1.0E36
      SUM=AW2*SUM3*2.9979E-4
C
C       NOTICE FACTOR OF 2.  NEED TO RESOLVE THIS DISCREPANCY
C       WITH BIRNBAUM. (FACTOR OF 2 GIVES D(V) VALUES WHICH
C       AGREE WITH BIRNBAUM'S GRAPHED VALUES.)
C
C     A(T) IN THE TRAFTON STYLE IS PUT INTO A
      A=SUM
      IF (NOPR .EQ. 1) WRITE(6,104) V,T,A
 104  FORMAT(2X,'V,T,A = ',2X,1P,3(2X,E10.3))
C
C     THE H2-HE COLLISIONS ARE CONSIDERED HERE FOR THE B VALUES.
C
      TEMP=T
C     BOLTZMANN STATISTICS ARE CALCULATED.
      CALL JROT(TEMP)
```

```
      IF (NOPR .EQ. 1) WRITE(6,200)
 200  FORMAT(/,2X,'FOR H2-HE COLLISIONS')
C     EVALUATE SQ,TAU1,TAU2 PARAMETERS.
C     FOR THE ISOTROPIC S AND TAU FACTORS.
      CALL PARAM(2)
      SQA=SQ
      TAU1A=TAU1
      TAU2A=TAU2
      IF (NOPR .EQ. 1) WRITE(6,210) SQA,TAU1A,TAU2A
 210  FORMAT(2X,'ISOTROPIC SQA,TAU1,TAU2A',2X,1P,3(2X,E10.3))
C     EVALUATE SQ,TAU1,TAU2 PARAMETERS.
C     FOR THE ANISOTROPIC S AND TAU FACTORS.
      CALL PARAM(3)
      SQB=SQ
      TAU1B=TAU1
      TAU2B=TAU2
      IF (NOPR .EQ. 1) WRITE(6,220) SQB,TAU1B,TAU2B
 220  FORMAT(2X,'ATISOTROPIC SQB,TAU1B,TAU2B',2X,1P,3(2X,E10.3))
C     EVALUATE THE A FACTOR.
      CALL FAC(10,AFAC)
      IF (NOPR .EQ. 1) WRITE(6,355) AFAC
C
      V=VNU
      IF (NOPR .EQ. 1) WRITE(6,310) V
C     OM IS TWO PI TIMES C TIMES THE WAVENUMBER.
C     FREQ IS SEC-1.
      OM=TPC*V
      FREQ=C*V*1.0E9
      BETA=1.0/(BOLC*TEMP)
      IF (NOPR .EQ. 1) WRITE(6,315) OM,FREQ,BETA
C     EVALUATE THE 1-EXP TERM.
      TX=BETA*HB*OM
      CALL EX(TX,S)
C     NOTE THAT THE SQ FACTOR IS NOT IN THE AW2 EXPRESSION.
C     FOR H2-HE, THERE IS AN ADDITIONAL FACTOR OF 2.
C     THE SQA AND SQB FACTORS WILL BE INTRODUCED LATER.
      AW2=2.0*AW*OM*(1.0-S)
      IF (NOPR .EQ. 1) WRITE(6,340) AW2
C
C     THE ISOTROPIC TERM IS CALCULATED HERE.
      SQ=SQA
      TAU1=TAU1A
      TAU2=TAU2A
      IF (NOPR .EQ. 1) WRITE(6,430) SQ,TAU1,TAU2
 430  FORMAT(2X,'ISOTROPIC SQ,TAU1,TAU2',2X,1P,3(2X,E10.3))
      OM2=OM
      CALL GAMMA(OM2,GAM)
      IF (NOPR .EQ. 1) WRITE(6,356) TEMP,TAU1,TAU2,OM,BETA,GAM
C     NOTE:THE RESULT IS MULTIPLIED BY 1.0E36
      TERM6=SQ*GAM
      IF (NOPR .EQ. 1) WRITE(6,357) SQ,GAM,TERM6
 357  FORMAT(2X,'ISOTROPIC SQ,GAM,TERM6 ',1P,6(2X,E10.3))
C
C     THE ANISOTROPIC TERMS ARE CALCULATED HERE.
C     THE SIX TERMS OF EQUATION 7 OF NBS 80 ARE CALCULATED.
      SQ=SQB
```

```
      TAU1=TAU1B
      TAU2=TAU2B
      IF (NOPR .EQ. 1) WRITE(6,431) SQ,TAU1,TAU2
 431  FORMAT(2X,'ANISOTROPIC SQ,TAU1,TAU2',2X,1P,3(2X,E10.3))
C     THE FIRST TERM IS EVALUATED.
      OM2=OM
      CALL GAMMA(OM2,GAM)
      IF (NOPR .EQ. 1) WRITE(6,356) TEMP,TAU1,TAU2,OM,BETA,GAM
      TERM1=AFAC*GAM
C         ZERO AND TWO ARE EVALUATED.
      CALL EVAL(0,2,OM,B1,B2)
      TERM2=(RHO(1)*B1)+(RHO(3)*B2)
C         ONE AND THREE ARE EVALUATED.
      CALL EVAL(1,3,OM,B1,B2)
      TERM3=(RHO(2)*B1)+(RHO(4)*B2)
      TERM3=(9.0/5.0)*TERM3
C         TWO AND FOUR ARE EVALUATED.
      CALL EVAL(2,4,OM,B1,B2)
      TERM4=(RHO(3)*B1)+(RHO(5)*B2)
      TERM4=(18.0/7.0)*TERM4
C         THREE AND FIVE ARE EVALUATED.
      CALL EVAL(3,5,OM,B1,B2)
      TERM5=(RHO(4)*B1)+(RHO(6)*B2)
      TERM5=(10.0/3.0)*TERM5
C
      SUM3=TERM1+TERM2+TERM3+TERM4+TERM5
C     THE ANISOTROPIC TERMS ARE MULTIPLED BY SQB
C     NOTE:THE RESULT IS MULTIPLIED BY 1.0E36
      SUM3=SQ*SUM3
C     ADD UP THE ISOTROPIC AND ANISOTROPIC TERMS.
      SUM3=SUM3+TERM6
      IF (NOPR .EQ. 1) WRITE(6,460) TERM1,TERM2,TERM3,TERM4,TERM5,
     1  SUM3
 460  FORMAT(2X,'TERM1,TERM2,TERM3,TERM4,TERM5,TOTAL SUM*SQ',/,
     1  2X,1P,7(2X,E10.3))
C     NOTE:THE RESULT IS MULTIPLIED BY 1.0E36
      SUM=AW2*SUM3*2.9979E-4
C
C       NOTICE FACTOR OF 2.  NEED TO RESOLVE THIS DISCREPANCY
C       WITH BIRNBAUM. (FACTOR OF 2 GIVES D(V) VALUES WHICH
C       AGREE WITH BIRNBAUM'S GRAPHED VALUES.)
C
C     B(T) IN THE TRAFTON STYLE IS PUT INTO B
      B=SUM
      IF (NOPR .EQ. 1) WRITE(6,404) V,T,B
 404  FORMAT(2X,'V,T,B = ',2X,1P,3(2X,E10.3),/)
C
C
      RETURN
      END
C Subroutine for H2H2 absorption from Joiner and Steffes
    SUBROUTINE H2H2JS(VNU,T,AH2H2)
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V3/QROT,QR1,QR2,S1,S2,S3,S4,P1,P2,P3,P4
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
```

```
      COMMON/V6/P5,P6,P7,P8
      COMMON/V7/PRO1(20),PRO2(20),STOR(20)
      COMMON/W1/FP,REB,RHO(20)
      COMMON/V9/TEMP,BETA,SQ,TAU1,TAU2
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
C
    X1=(273.0/T)**3.12
    X2=(273.0/T)**2.24
    X3=(273.0/T)**3.34
    X=PH2*X1 + 1.382*PHE*X2 + 9.322*PCH4*X3
      FREQ=C*VNU*1.0E9
      ZL=1.0/VNU
    Y=3.557E-11*PH2/(ZL*ZL)
    AH2H2=Y*X
    RETURN
    END
C Following subroutine is based on Orton's tables
C Following subroutine is based on Orton's tables
    SUBROUTINE H2H2OR(IQ,VNU,T,A,B,CZB)
      dimension Ttab(10),frequ(2428)
      dimension ah2h2e(10),ah2h2n(10),ah2hee(10),ah2hen(10)
      dimension ah2che(10),ah2chn(10)
      dimension abeh2h2(2428,10),abnh2h2(2428,10)
      dimension abeh2he(2428,10),abnh2he(2428,10)
      dimension abeh2ch4(2428,10),abnh2ch4(2428,10)
C      real*8 A,B,CZB,ah2e,ah2n,ahee,ahen,ache,achn
c      integer ntemp,nfreq
      COMMON/orton/Ttab,frequ,abeh2h2,abnh2h2,abeh2he,abnh2he,
     + abeh2ch4,abnh2ch4,nfreq,ntemp
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V9/TEMP,BETA,SQ,TAU1,TAU2
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
      COMMON/W1/FP,REB,RHO(20)
C
      algT=alog(T)
C  CHANGE PRESSURES FROM BARS TO ATM, AND BACK AT END OF SUBROUTINE;
C
        kp=0
        do 10 ip=1,nfreq
           if(vnu.ge.frequ(ip)) kp=kp+1
           if(vnu.lt.frequ(ip)) goto 11
 10        continue
C  so vnu is in between kp-1 and kp (after next line)
 11         kp=kp+1
            x=vnu-frequ(kp-1)
           do i=1,ntemp
            ah2h2e(i)=abeh2h2(kp-1,i)
     +      +x/(frequ(kp)-frequ(kp-1))*(abeh2h2(kp,i)-abeh2h2(kp-1,i))
            ah2h2n(i)=abnh2h2(kp-1,i)
     +      +x/(frequ(kp)-frequ(kp-1))*(abnh2h2(kp,i)-abnh2h2(kp-1,i))
            ah2hee(i)=abeh2he(kp-1,i)
     +      +x/(frequ(kp)-frequ(kp-1))*(abeh2he(kp,i)-abeh2he(kp-1,i))
            ah2hen(i)=abnh2he(kp-1,i)
     +      +x/(frequ(kp)-frequ(kp-1))*(abnh2he(kp,i)-abnh2he(kp-1,i))
            ah2che(i)=abeh2ch4(kp-1,i)
     +      +x/(frequ(kp)-frequ(kp-1))*(abeh2ch4(kp,i)-abeh2ch4(kp-1,i))
```

```
             ah2chn(i)=abnh2ch4(kp-1,i)
     +      +x/(frequ(kp)-frequ(kp-1))*(abnh2ch4(kp,i)-abnh2ch4(kp-1,i))
           enddo
C
           kp=0
        do 12 ip=1,ntemp
           if(algT.ge.Ttab(ip)) kp=kp+1
           if(algT.lt.Ttab(ip)) goto 13
 12     continue
C  so algT is in between kp-1 and kp
 13            kp=kp+1
               x=algT-Ttab(kp-1)
C
              ah2e=ah2h2e(kp-1)
     +         +x/(Ttab(kp)-Ttab(kp-1))*(ah2h2e(kp)-ah2h2e(kp-1))
              ah2n=ah2h2n(kp-1)
     +         +x/(Ttab(kp)-Ttab(kp-1))*(ah2h2n(kp)-ah2h2n(kp-1))
              ahee=ah2hee(kp-1)
     +         +x/(Ttab(kp)-Ttab(kp-1))*(ah2hee(kp)-ah2hee(kp-1))
              ahen=ah2hen(kp-1)
     +         +x/(Ttab(kp)-Ttab(kp-1))*(ah2hen(kp)-ah2hen(kp-1))
              ache=ah2che(kp-1)
     +         +x/(Ttab(kp)-Ttab(kp-1))*(ah2che(kp)-ah2che(kp-1))
              achn=ah2chn(kp-1)
     +         +x/(Ttab(kp)-Ttab(kp-1))*(ah2chn(kp)-ah2chn(kp-1))
C
        if(IQ.ge.1) A=exp(ah2e)
        if(IQ.ge.1) B=exp(ahee)
        if(IQ.ge.1) CZB=exp(ache)
        if(IQ.eq.0) A=exp(ah2n)
        if(IQ.eq.0) B=exp(ahen)
        if(IQ.eq.0) CZB=exp(achn)
C
C        write(6,667) (Ttab(i),i=1,10)
C        write(6,668) vnu,algt,nfreq,ntemp
C        write(6,669) abeh2h2(128,3),frequ(128)
C        write(6,666) T,A,B,CZB,ah2e,ahee,ache
 666    format(7E15.6)
 667    format(10f8.3)
 668    format(2f8.3,2I10)
 669    format(2E15.5)
    RETURN
    END
C
C
      SUBROUTINE EVAL(L,K,OM,B1,B2)
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
      COMMON/V9/TEMP,BETA,SQ,TAU1,TAU2
C     CALCULATE THE GAMMA VALUES.
C     SEE NBS 80.
      CALL EH2(L,E)
      B1=E
      CALL EH2(K,E)
      B2=E
C     B3 IS W(L,K) IN 2 PI RAD PER SEC.
```

```
      B3=TPC*(B2-B1)
      OM2=OM-B3
      IF (NOPR .EQ. 1) WRITE(6,10) L,K,OM,B3
   10 FORMAT(2X,I3,2X,1P,I3,2X,1P,2(2X,E10.3))
      CALL GAMMA(OM2,GAM)
      IF (NOPR .EQ. 1) WRITE(6,15) TEMP,TAU1,TAU2,OM2,BETA,GAM
   15 FORMAT(2X,1P,6(2X,E10.3))
      B1=GAM
      OM2=OM+B3
      CALL GAMMA(OM2,GAM)
      IF (NOPR .EQ. 1) WRITE(6,15) TEMP,TAU1,TAU2,OM2,BETA,GAM
      B2=GAM
      RETURN
      END
C
C
C
      SUBROUTINE PARAM(M)
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/V9/TEMP,BETA,SQ,TAU1,TAU2
C     SEE NBS 80 FOR THE SQ,TAU1,TAU2 PARAMETER VALUES.
      IF (M .EQ. 1) GO TO 10
      IF (M .EQ. 2) GO TO 20
      IF (M .EQ. 3) GO TO 30
C     FOR H2-H2 COLLISIONS.
   10 A1=TEMP/273.15
C      A2=142.0*EXP(0.26*ALOG(A1))
C      A3=4.85*EXP(-0.593*ALOG(A1))
C      A4=2.17*EXP(-0.523*ALOG(A1))
      A2=281.0*(A1**0.235)
      A3=4.68*(A1**(-0.605))
      A4=2.23*(A1**(-0.607))
      SQ=1.38*A2
      TAU1=A3
      TAU2=A4
      GO TO 40
C     FOR H2-HE COLLISIONS,THE ISOTROPIC PARAMETERS.
   20 CONTINUE
C     A1=TEMP/273.15
C      A2=112.0*EXP(0.93*ALOG(A1))
C      A3=1.74*EXP(-0.54*ALOG(A1))
C      A4=3.4*EXP(-0.30*ALOG(A1))
      A1=77.4/TEMP
      A2=33.53/A1
      A3=3.43*SQRT(A1)
      A4=6.56*SQRT(A1)
      SQ=1.38*A2
      TAU1=A3
      TAU2=A4
      GO TO 40
C     FOR H2-HE COLLISIONS,ANISOTROPIC PARAMETERS.
C     VALUES ARE FOR 195 DEGREES KELVIN.
   30 CONTINUE
C     A1=TEMP/273.15
C      A2=1.914E1
C      A3=4.13
```

```
C      A4=2.38
       A1=TEMP/77.4
       A2=12.06*(A1**0.57)
       A3=3.02*(A1**(-0.30))
       A4=8.94*(A1**(-0.60))
       SQ=1.38*A2
       TAU1=A4
       TAU2=A3
       GO TO 40
  40   RETURN
       END
C
C
C
       SUBROUTINE FAC(L,AFAC)
       COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
       COMMON/V7/PRO1(20),PRO2(20),STOR(20)
       COMMON/W1/FP,REB,RHO(20)
C      SEE NBS 80 FOR THE AFAC FACTOR,EQUATION 8.
       A8=0.0
       DO 10 I=1,L
       J=I-1
       A1=J
       A2=A1+1.00
       A3=2.0*A1
       A4=A3+1.00
       A5=A3-1.00
       A6=A3+3.00
       A7=(A1*A2*A4*RHO(I))/(A5*A6)
       A8=A8+A7
  10   CONTINUE
       AFAC=A8
       RETURN
       END
C
C
C
       SUBROUTINE BESSEL(Z,BES)
       COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
C      BES IS Z*K1(Z)
C      SEE PAGES 378-379 OF ABRAMOWITZ AND STEGUN,HANDBOOK OF
C      MATHEMATICAL FUNCTIONS.
C      EQNS. 9.8.3,9.8.4,9.8.7,9.8.8 ARE USED TO CALCULATE Z*K1(Z)
       IF (Z .LE. 2.00) GO TO 10
       IF (Z .GT. 2.00) GO TO 20
C      A1,A2,..ARE Z/2 TO THE 2,4,..POWER. SEE EQN 9.8.7.
C      BESI IS I1(Z).
  10   CALL BESS2(Z,BESI)
       A1=(Z*Z)/(2.0*2.0)
       A2=A1*A1
       A3=A2*A1
       A4=A3*A1
       A5=A4*A1
       A6=A5*A1
       BES=(Z*ALOG(Z/2.0)*BESI)+(1.000)+(.15443144*A1)
       BES=BES-(.67278579*A2)-(.18156897*A3)-(.01919402*A4)
```

```
      BES=BES-(.00110404*A5)-(.00004686*A6)
      GO TO 30
C     A1,A2,.. ARE Z/2 TO THE 1,2,.. POWER. SEE EQN 9.8.8.
   20 A1=2.0/Z
      A2=A1*A1
      A3=A2*A1
      A4=A3*A1
      A5=A4*A1
      A6=A5*A1
      BES=1.25331414+(.23498619*A1)-(.03655620*A2)
      BES=BES+(.01504268*A3)-(.00780353*A4)
      BES=BES+(.00325614*A5)-(.00068245*A6)
      CALL EX(Z,A1)
      BES=BES*SQRT(Z)*A1
   30 RETURN
      END
C
C
C
      SUBROUTINE BESS2(Z,BESSI)
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C     BESSI IS I1(Z).
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      IF (Z .LE. 3.75) GO TO 10
      IF (Z .GT. 3.75) GO TO 20
C     A1,A2,.. IS Z/3.75 TO THE 2,4,.. POWER. SEE EQN. 9.8.3.
   10 A1=(Z*Z)/(3.75*3.75)
      A2=A1*A1
      A3=A2*A1
      A4=A3*A1
      A5=A4*A1
      A6=A5*A1
      BESSI=0.5000+(.87890594*A1)+(.51498869*A2)
      BESSI=BESSI+(.15084934*A3)+(.02658733*A4)
      BESSI=BESSI+(.00301532*A5)+(.00032411*A6)
      BESSI=BESSI*Z
      GO TO 30
C     A1,A2,.. ARE 3.75/Z TO THE 1,2,.. POWER. SEE EQN. 9.8.4.
   20 A1=3.75/Z
      A2=A1*A1
      A3=A2*A1
      A4=A3*A1
      A5=A4*A1
      A6=A5*A1
      A7=A6*A1
      A8=A7*A1
      BESSI=.39894228-(.03988024*A1)-(.00362018*A2)
      BESSI=BESSI+(.00163801*A3)-(.01031555*A4)
      BESSI=BESSI+(.02282967*A5)-(.02895312*A6)
      BESSI=BESSI+(.01787654*A7)-(.00420059*A8)
      BESSI=BESSI*(EXP(Z)/SQRT(Z))
      IF ((Z .GT. 150.) .AND. (NOPR .EQ. 1)) WRITE(6,29)
   29 FORMAT(2X,'Z .GT. 150.,EXP PROBLEMS')
   30 RETURN
      END
C
```

```
C
C
      SUBROUTINE GAMMA(OM2,GAM)
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
      COMMON/V9/TEMP,BETA,SQ,TAU1,TAU2
C     SEE EQNS 17 OF BIRNBAUM AND COHEN (CAN J PHYS,54,PG 593,1976)
C     ALSO EQUATION 5 OF NBS 80.
      A1=TAU1
      A2=TAU2
      A3=0.5*BETA*HB*OM2
      A4=1.00+(OM2*OM2*A1*A1*1.0E-6)
      A5=(A2*A2*1.0E-6)+((BETA*BETA*HB*HB)/4.0)
      GAM=(A1/(PI*A4))*EXP((A2/A1)+A3)
        A6=GAM
      Z=SQRT(A4*A5)*1.0E3/A1
      CALL BESSEL(Z,BES)
C  GAM SHOULD BE MULTIPLIED BY 1.0E-14
      GAM=GAM*BES
      IF (NOPR .EQ. 1) WRITE(6,10) A1,A2,A3,A4,A5,A6,Z,GAM
  10  FORMAT(2X,'TAU1,TAU2,A3,A4,A5,A6,Z,GAM',/,
     1  2X,1P,8(2X,E10.3))
      RETURN
      END
      SUBROUTINE EH2(J,E)
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
C     ENERGY VALUE IN WAVENUMBERS(CM-1) FOR THE
C     JTH ROTATIONAL LEVEL OF H2,SEE NBS 80,EQUATION 2.
      A1=J
      A2=A1+1.00
      A3=A1*A1
      A4=A2*A2
      A5=A3*A1
      A6=A4*A2
      E=(59.3392*A1*A2)-(0.04599*A3*A4)+(5.2E-5*A5*A6)
      RETURN
      END
C
C
C
      SUBROUTINE JROT(TEMP)
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
      COMMON/V7/PRO1(20),PRO2(20),STOR(20)
      COMMON/W1/FP,REB,RHO(20)
C     THE BOLTZMANN STATISTICS FOR H2 ARE CALCULATED
      CALL PART(TEMP)
C      RHO(L) GIVES THE FRACTION OF H2 IN THE
C     K=L-1 ROTATIONAL LEVEL,DIVIDED BY 2J+1.
C     AND MULTIPLIED BY FP FOR THE NORMAL CASE,AND
C     BY 1.00 IN THE EQUIL CASE (SEE SUBROUTINE
C     PART FOR DEFINITION OF STOR).
C     FRACT IS THE FRACTION OF H2 IN THE K=L-1 LEVEL.
C     NOTICE SEPARATE EQUIL AND NORMAL DEFINITIONS OF FRACT.
C     EQUIL CASE,KL=0 AND A2=1.00
```

```
C     NORMAL CASE,KL=10 AND A2=FP.
 345  FORMAT(/,2X,'BOLTZMANN STATISTICS FOR H2',/,
     1  2X,'KL IS EQUAL TO  ',I3)
C     FOR NORMAL CASE,FRACTION OF PARA IS 0.25
C       PARA LEVELS J=0,2,4..ARE SPECIFIED.
      DO 20 L=1,5
C  K=1,3,5,7,9
      K=((L-1)*2)+1
      J=K-1
      A1=(2*(K-1))+1
C
      POP=(REB*STOR(K))+((1.0-REB)*FP*STOR(K+10))
      RHO(K)=POP/A1
 350  FORMAT(2X,'J,FRACT,PRO1 ',2X,I3,2X,1P,2(2X,E10.3))
  20  CONTINUE
C       ORTHO LEVELS J=1,3,5.. ARE SPECIFIED.
      DO 21 L=1,5
      K=((L-1)*2)+2
      J=K-1
      A1=(2*(K-1))+1
      POP=(REB*STOR(K))+((1.0-REB)*(1.0-FP)*STOR(K+10))
      RHO(K)=POP/A1
  21  CONTINUE
      RETURN
      END
      SUBROUTINE PART(TEMP)
      COMMON/V3/QROT,QR1,QR2,S1,S2,S3,S4,P1,P2,P3,P4
      COMMON/V6/P5,P6,P7,P8
      COMMON/V7/PRO1(20),PRO2(20),STOR(20)
      DIMENSION CC(20),CC2(20)
C     SEE TATUM,AP J SUPPL SER,VOL 14,PAGE 21,1967
C     FOR THE EXPRESSIONS FOR THE BOLTZMANN STATISTICS
C     THAT APPLY TO THE GROUND STATE OF H2.
C     HERZBERG,MOLECULAR SPECT AND MOL STRUCT,VOL 4,CONSTS
C     OF DIATOMIC MOLECULES IS USED FOR THE BV,DE VALUES.
      HCK=1.4388
      BV=60.853-(3.062*0.5)
      DE=4.71E-2
      SNUC=0.5
      CI1=SNUC/((2.0*SNUC)+1)
      CI2=(SNUC+1)/((2.0*SNUC)+1)
      CONST=((2.0*0)+1)*((2.0*SNUC)+1)*((2.0*SNUC)+1)
      SUM=0.0
      SUM2=0.0
      L=0
      L1=1
      LR=5
      DO 31 J=1,LR
      DG1=(2.0*L)+1.0
      DG2=(2.0*L1)+1.0
      J1=L*(L+1)
      J2=L1*(L1+1)
      F=(BV*J1)-(DE*J1*J1)
      F2=(BV*J2)-(DE*J2*J2)
      CALL EH2(L,E)
      F=E
```

```
      CALL EH2(L1,E)
      F2=E
      TX=HCK*(F/TEMP)
      CALL EX(TX,S)
      CC(J)=S*CONST*CI1*DG1
      SUM=SUM+CC(J)
      TX2=HCK*(F2/TEMP)
      CALL EX(TX2,S2)
      CC2(J)=S2*CONST*CI2*DG2
      SUM2=SUM2+CC2(J)
      L=L+2
      L1=L1+2
   31 CONTINUE
      QROT=SUM+SUM2
      QR1=SUM
      QR2=SUM2
      S1=0.0
      S2=0.0
      S3=0.0
      S4=0.0
C     S1=PROB,TOTAL PARA,EQUILIBRIUM
C     S2=PROB,TOTAL ORTHO,EQUILIBRIUM
C     S3=PROB,TOTAL PARA,NORMAL
C     S4=PROB,TOTAL ORTHO,NORMAL
C     P1=PROB,TOTAL ORTHO/PARA,EQUILIBRIUM
C     P2=PROB,ORTHO J=1/PARA J=0,EQUILIBRIUM
C     P3=PROB,TOTAL ORTHO/PARA,NORMAL
C     P4=PROB,ORTHO J=1/PARA J=0,NORMAL
C     P5=PROB,ORTHO J=1,EQUILIBRIUM
C     P6=PROB,PARA J=0,EQUILIBRIUM
C     P7=PROB,ORTHO J=1,NORMAL
C     P8=PROB,PARA J=0,NORMAL
      DO 32 J=1,LR
      S1=S1+(CC(J)/QROT)
      S2=S2+(CC2(J)/QROT)
      S3=S3+(CC(J)/QR1)
      S4=S4+(CC2(J)/QR2)
   32 CONTINUE
      P1=S2/S1
      P2=CC2(1)/CC(1)
      P3=S4/S3
      P4=(CC2(1)/CC(1))*(QR1/QR2)
      P5=CC2(1)/QROT
      P6=CC(1)/QROT
      P7=CC2(1)/QR2
      P8=CC(1)/QR1
      DO 40 J=1,LR
      PRO1(J)=CC(J)/QROT
      PRO2(J)=CC2(J)/QROT
      PRO1(J+10)=CC(J)/QR1
      PRO2(J+10)=CC2(J)/QR2
   40 CONTINUE
C     STOR(I) I=1,2,3,4.. FOR JROT=0,1,2,3,..
C     EQUIL DISTRIBUTION FOR I=1 TO 10
C     NORMAL DISTRIBUTION FOR I=11 TO 20
      DO 50 J=1,LR
```

```
      L=((J-1)*2)+1
      L1=L+1
C     AA1=1.00,AA2=1.00 FOR STANDARD BOLTZMANN STATISTICS
C     WHERE THE DEGENERACY IS UPPSTAIRS AND DOWNSTAIRS.
C     AA1=.25*L,AA2=.75*L1 FOLLOWS EQUATION 9B OF
C     BIRNBAUM AND COHEN(WRONG?)
      AA1=1.00
      AA2=1.00
      STOR(L)=PRO1(J)/AA1
      STOR(L1)=PRO2(J)/AA2
      STOR(L+10)=PRO1(J+10)/AA1
      STOR(L1+10)=PRO2(J+10)/AA2
   50 CONTINUE
      RETURN
      END
      SUBROUTINE DIEL(I,NPR,W,TK,E1,E2,D1,D2)
    COMPLEX ZM,ZZ
    REAL*4 LF,LF0,LF1
    DIMENSION EIMAG(9),FR(9)
C  SUBROUTINE TO CALCULATE DIELECTRIC CONST/REFRACTIVE INDICES FOR
C  WATER, BASED UPON ULABY ET AL, 1981.
    F=30.0E9/W
      IF(I.EQ.1) GOTO 100
      IF(I.EQ.2) GOTO 200
  100 TEMP=TK-273.0
      A1=TEMP
      A2=A1*A1
      A3=A2*A1
    RELT=(1.1109E-10)-A1*(3.824E-12)+A2*(6.938E-14)-
     + A3*(5.096E-16)
      E0=88.045-0.4147*A1+A2*(6.295E-4)+A3*(1.075E-5)
    if(E0.LT.0.0) E0=0.0
      EINF=4.9
      E1=(E0-EINF)/(1+(F*RELT)*(F*RELT))
    E1=EINF+E1
    E2=F*RELT*(E0-EINF)
    E2=E2/(1+(F*RELT)*(F*RELT))
    IF(E2.LT.0.0) E2=0.0
      GOTO 900
  200  CONTINUE
    TEMP=TK-273.0
    FR(1)=1.0E8
    FR(2)=3.0E8
    FR(3)=1.0E9
    FR(4)=2.0E9
    FR(5)=3.0E9
    FR(6)=5.0E9
    FR(7)=1.0E10
    FR(8)=3.0E10
    FR(9)=1.0E11
    EIMAG(1)=8.0E-3
    EIMAG(2)=1.5E-3
    EIMAG(3)=8.0E-4
    EIMAG(4)=1.0E-3
    EIMAG(5)=1.2E-3
    EIMAG(6)=1.5E-3
```

```
      EIMAG(7)=3.0E-3
      EIMAG(8)=8.0E-3
      EIMAG(9)=2.0E-2
      E1=3.15
      LF=LOG10(F)
      IF(F.LE.FR(1)) THEN
      E2=8.0E-3
      GOTO 900
      ENDIF
      IF(F.GE.FR(9)) THEN
      E2=2.0E-2
          GOTO 900
      ENDIF
      IF(F.GT.FR(1).AND.F.LE.FR(2)) J=1
      IF(F.GT.FR(2).AND.F.LE.FR(3)) J=2
      IF(F.GT.FR(3).AND.F.LE.FR(4)) J=3
      IF(F.GT.FR(4).AND.F.LE.FR(5)) J=4
      IF(F.GT.FR(5).AND.F.LE.FR(6)) J=5
      IF(F.GT.FR(6).AND.F.LE.FR(7)) J=6
      IF(F.GT.FR(7).AND.F.LE.FR(8)) J=7
      IF(F.GT.FR(8).AND.F.LE.FR(9)) J=8
      LF0=ALOG10(FR(J))
      LF1=ALOG10(FR(J+1))
      DLF=(LF-LF0)/(LF1-LF0)
      X0=ALOG10(EIMAG(J))
      X1=ALOG10(EIMAG(J+1))
      DX=X0+DLF*(X1-X0)
      E2=10**DX
  900   CONTINUE
c     ZM=CMPLX(E1,-E2)
c     ZZ=SQRT(ZM)
c     D1=REAL(ZZ)
c     D2=-AIMAG(ZZ)
        D1=(E1+SQRT((E1*E1)+(E2*E2)))/2.0
        D1=SQRT(D1)
        IF(D1.EQ.0.0) GOTO 910
        D2=E2/(2.0*D1)
        GOTO 9999
  910 D2=0
 9999 RETURN
        END
C
C
C
         FUNCTION SHAPE2(P,T,F,FLC)
          implicit none
          REAL*4 SHAPE2
          real*4 DL,P,T,F,FLC,DFC,DL2
          DL=F-FLC
      DL2=F+FLC
c   line width is taken as water line width
      DFC = 0.08*P*((273/T)**0.666)
      DFC = DFC * 30.0        !LINEWIDTH IN MHZ
         SHAPE2=((F*F)/(FLC*FLC))*(DFC/(DL*DL+DFC*DFC)
       + +DFC/(DL2*DL2+DFC*DFC))
      SHAPE2=SHAPE2/3.1415926536      !DIVIDE BY PI
```

```
      RETURN
      END
C
      REAL*4 FUNCTION QLOG2(Q0,T)
      IMPLICIT NONE
      REAL*4 Q0(5),T
      REAL*4 SLOPE, TLOG
C LOG(T) FOR T=300,225,150,75, 37.5K
      REAL*4 TLOG0(5) /2.47712,2.35218,2.17609,1.8751, 1.5740/
      TLOG=ALOG10(T)
      IF(TLOG.GT.TLOG0(1)                          )GO TO 4
      IF(TLOG.LE.TLOG0(1) .AND. TLOG.GT. TLOG0(2))GO TO 5
      IF(TLOG.LE.TLOG0(2) .AND. TLOG.GT. TLOG0(3))GO TO 6
      IF(TLOG.LE.TLOG0(3) .AND. TLOG.GT. TLOG0(4))GO TO 7
      IF(TLOG.LE.TLOG0(4) .AND. TLOG.GT. TLOG0(5))GO TO 8
      IF(TLOG.LE.TLOG0(5)                         )GO TO 9
4     QLOG2=Q0(1)    !USE 300 K VALUE NEEDS TO BE FIXED
      GO TO 10
5     SLOPE=(Q0(2)-Q0(1))/(TLOG0(2)-TLOG0(1))
      QLOG2=Q0(1)+SLOPE*(TLOG-TLOG0(1))
      GO TO 10
6     SLOPE=(Q0(3)-Q0(2))/(TLOG0(3)-TLOG0(2))
      QLOG2=Q0(2)+SLOPE*(TLOG-TLOG0(2))
      GO TO 10
7     SLOPE=(Q0(4)-Q0(3))/(TLOG0(4)-TLOG0(3))
      QLOG2=Q0(3)+SLOPE*(TLOG-TLOG0(3))
      GO TO 10
 8    SLOPE=(Q0(5)-Q0(4))/(TLOG0(5)-TLOG0(4))
      QLOG2=Q0(4)+SLOPE*(TLOG-TLOG0(4))
      GO TO 10
 9    QLOG2=Q0(5)              !USE 37.5 K VALUE -NEEDS TO BE FIXED
10    CONTINUE
      RETURN
      END
C
C
      SUBROUTINE SAJph3(N,T,T3,GM)
        REAL*4 T,P,F,V
    real*8 x,ajk,fjk,tcor
    real*4 T3,gm,vline,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,deltot,PCO,PCO13,PHCN
    real*4  FP0(728),SP0(728),ELP(728)
    REAL*4 wgtS0(40),wgtFGB(40),wgtSB(40)
    integer*2 N
        COMMON/ph3/FP0,SP0,ELP,wgtS0,wgtFGB,wgtSB
        COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
C     GM IS GAMMA(N) IN GHZ.
    GH2=3.293
    GHE=1.6803
    Gph3=4.2157
    if(N.gt.40) goto 40
        GM=(GH2*T3*PH2)+(GHE*T3*PHE)
    GM=GM*wgtfgb(N)
    GM=GM+(GPH3*(300.0/T)*PPh3*wgtSB(N))
    goto 50
  40   GM=(GH2*T3*PH2)+(GHE*T3*PHE)
    GM=GM+(GPH3*(300.0/T)*PPh3)
```

```
  50  continue
      RETURN
      END
C
      SUBROUTINE SFJPH3(N,T,V,VLINE,GM,FJK)
        REAL*4 T,P,F,V
    real*8 x,ajk,fjk,tcor,y,z
        real*4 t3,gm,vline,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,deltot,PCO,PCO13,PHCN
    real*4  FP0(728),SP0(728),ELP(728)
    REAL*4 wgtS0(40),wgtFGB(40),wgtSB(40)
    integer*2 N
        COMMON/ph3/FP0,SP0,ELP,wgtS0,wgtFGB,wgtSB
        COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
C
    zeta=0.
    delta=0.0
C     FJK IS THE BEN REUVEN LINE SHAPE, FROM DEBOER AND STEFFES
C
    x = (gm+zeta)*((vline+delta)*(vline+delta) + GM*GM - zeta*zeta)
    x=x+(gm-zeta)*v*v
        y = (v*v - (vline+delta)*(vline+delta) - gm*gm + zeta*zeta)
    z=y*y  + 4.0*v*v*GM*GM
        FJK  = 29.97925*2.0*v*v*x/3.14159/z/vline/vline
      RETURN
      END
C
       SUBROUTINE ABSBR_h2s2(AON,T,P,VNU)
C
C THIS SUBROUTINE RETURNS QUANTITY AON, WHICH WHEN MULTIPLIED
C BY THE VOLUME MIXING RATIO, GIVES THE ABSORPTION COEFFICIENT
C OF H2S, IN UNITS OF 1/cm
C
C DEFINITIONS
C   AON ABSORPTION COEFFICIENT/VOLUME MIXING RATIO   1/cm
C   T   TEMPERATURE                   K
C       P   PRESSUME                BARS
C   F   FREQUENCY               MHZ
C
C ADDITIONAL FUNCTIONS REQUIRED
C   QLOG    BASE TEN LOGARITHM OF THE RATIO OF PARTITION
C       FUNCTION AT TEMPERATURE T TO PARTITION FUNCTION
C       AT T=300K
C   SHAPE(F,P)  LINE SHAPE FACTOR
C
C**********************************************************************
        IMPLICIT NONE
        REAL*4 AON,T,P,F,V
    real*4 t3,gm,vline,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,deltot,PCO,PCO13,PHCN
        real*4 DL,FLC,DL2
    REAL*4 C,DV,VNU,coef,hck
    real*8 x,ajk,fjk,tcor
        INTEGER*2 N,NLINES
        PARAMETER (NLINES=311)   !NUMBER OF SPECTRAL LINES
    real*4  F0(311),S0(311),EL(311),Q0(5),wgths(311)
    REAL*4 QLOG2,SHAPE2
        EXTERNAL QLOG2
```

```
      DATA Q0 /2.711, 2.5244, 2.2619, 1.8164, 1.3778/ !LOG PF AT
          300,225,150,75,37.5K
      COMMON/h2s/F0,S0,EL,wgths
       COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
C
    C=2.997925E1
    coef=7.244E21
    hck=1.438396    !hc/k
    V=VNU*C             !FREQ IN GHZ
    T3=(296./T)**0.6667
    AON=0.0
      DO N = 1,NLINES
    VLINE=F0(N)     !LINE CENTER IN GHZ
      TCOR = EXP(-(hck*EL(N)*(1./T - 3.3784E-03)))
    call sajh2s2(N,T,T3,GM)
      ajk=S0(N)*TCOR
      CALL SFJh2s2(N,T,V,VLINE,GM,FJK)
     AON=AON + ajk*FJK
     ENDDO
    x=(296.0/T)**3.5
    AON=7.244E21*x*AON*Ph2s/296.0       !2.4163E3 is from deboer
C
      RETURN
      END
C
      SUBROUTINE SAJh2s2(N,T,T3,GM)
       REAL*4 T,P,F,V
    real*8 x,ajk,fjk,tcor
    real*4 T3,gm,vline,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,deltot,PCO,PCO13,PHCN
    real*4  F0(311),S0(311),EL(311),wgths(311)
    integer*2 N
      COMMON/h2s/F0,S0,EL,wgths
       COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
C     GM IS GAMMA(N) IN GHZ.
    GH2=1.96
    GHE=1.20
    GH2S=wgths(N)
      GM=(GH2*T3*PH2)+(GHE*T3*PHE)+(GH2S*T3*PH2S)
      RETURN
      END
C
      SUBROUTINE SFJh2s2(N,T,V,VLINE,GM,FJK)
       REAL*4 T,P,F,V
    real*8 x,ajk,fjk,tcor,y,z
      real*4 t3,gm,vline,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,deltot,PCO,PCO13,PHCN
    real*4  F0(311),S0(311),EL(311),wgths(311)
    integer*2 N
      COMMON/h2s/F0,S0,EL,wgths
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
C
    zeta=gm
    delta=1.28*ph2s
C     FJK IS THE BEN REUVEN LINE SHAPE, FROM DEBOER AND STEFFES
C
    x = (gm+zeta)*((vline+delta)*(vline+delta) + GM*GM - zeta*zeta)
    x=x+(gm-zeta)*v*v
```

```
          y = (v*v - (vline+delta)*(vline+delta) - gm*gm + zeta*zeta)
        z=y*y  + 4.0*v*v*GM*GM
          FJK  = 29.97925*2.0*v*v*x/3.14159/z/vline/vline
        RETURN
        END
C
        SUBROUTINE NH3JOIN(VNU,T,ANH3)
C     CALCULATE THE AMMONIA ABSORPTION COEFFICIENT (CM-1)
C     USED BY GULKIS AND POYNTER (1972),AND GIVEN IN BERGE
C     AND GULKIS, GEHRELS JUPITER BOOK,PAGE 675.
        DIMENSION VKAK(16,16),DVKAK(16,16)
        COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
        COMMON/U2/C1,C2,C3,C4
        COMMON/U3/VKAK,DVKAK
        COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
        COMMON/V2/PI,HB,C,TPC,BOLC,AW,DEN,BAR,G
        COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C
C   VKAK(J,K)=CENTER FREQU FOR THE (J,K) TRANSITION ACCORDING TO THE
C  TABULATED VALUES OF POYNTER AND GULKIS (1975).
C  DVKAK(J,K) ARE THE CORRESPONDING SELF BROADENED LINE WIDTHS
C  AS TABULATED BY THEM (RESP. GHZ, MHZ/TORR)
C     CHANGE VNU(CM-1) TO GHZ.
        V=(C*VNU)
C  CHANGE PRESSURES FROM BARS TO ATM, AND BACK AT END OF SUBROUTINE; MARCH89
      PH2=PH2/1.013
      PHE=PHE/1.013
      PH2O=PH2O/1.013
      PNH3=PNH3/1.013
      PCH4=PCH4/1.013
C     CORRECTION FRACTOR IS GIVEN ON PAGE 676 OF THE BERGE AND GULKIS
C     PAPER, GEHRELS JUPITER BOOK.
C
      CORR=1.0
        IF (NOPR .EQ. 1) WRITE(6,5) V,CORR
    5   FORMAT(2X,'NH3 V(GHZ),CORR',2X,1P,2(2X,E10.3))
        IF (NOPR .EQ. 1) WRITE(6,6) C1,C2,C3,C4
    6   FORMAT(2X,'CONSTANTS C1,C2,C3,C4',2X,1P,4(2X,E10.3))
C
        SUM=0.0
C     CALCULATE THE INVERSION LINE WAVENUMBERS
C     FOR NH3, FROM THE DATA IN POYNTER AND KAKAR
C     AP J SUPPL SERIES,VOL 29,P87,1975.
C     J AND K ARE QUANTUM NUMBERS.
C
C     NLINE ARE THE NUMBER OF LINES TO BE CALCULATED.
        NLINE=16
C
        DO 10 J=1,NLINE
        L1=J*(J+1)
        L3=0
        DO 20 K=1,J
        L2=K*K
        L3=L3+1
C     SB IS THE SELF BRODENED LINE WIDTH OF NH3 IN MHZ/TORR.
C     C4 IS GIVEN IN THE BLOCK DATA STATEMENT.
```

```
C     SK IS 1.5 OR 3, DEPENDING UPON THE K VALUE.
      SK=1.5
      IF (L3 .NE. 3) GO TO 21
      SK=3.0
      L3=0
  21  VLINE=VKAK(J,K)
       SB=DVKAK(J,K)
      IF (NOPR .EQ. 1) WRITE(6,22) J,K,SK,VLINE,SB
  22  FORMAT(2X,'J,K,SK,VLINE(GHZ),SB(MHZ/TORR)',/,
     1 2X,I3,2X,I3,2X,F4.1,2X,1P,2(2X,E10.3))
C     CALCULATE A(J,K).
      CALL SAJKJOIN(T,VLINE,J,L1,L2,SK,SB,GM,GH2,AJK)
      IF(J.EQ.1.AND.K.EQ.1) ZZV=2.0*AJK*EXP(23.3/T)/3.0
C     FJK IS THE FREQUENCY DEPENDENT LINE SHAPE OF BEN REUVEN.
      CALL SFJKJOIN(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
      SB=AJK*FJK
      SUM=SUM+(CORR*AJK*FJK)
      IF (NOPR .EQ. 1) WRITE(6,23) AJK,FJK,SB
  23  FORMAT(2X,'AJK,FJK,(AJK*FJK)',2X,1P,3(2X,E10.3))
  20  CONTINUE
  10  CONTINUE
C
C  CALCULATE ROTATION LINE J=0;K=0
C  VLINE=5.73E5 MHZ; CHOSE DVLINE=14. MHZ
C
      L1=2
      L2=1
      VLINE=5.73E2
      SB=14.0
      GM=(1.89*T3*PH2)+(0.75*T3*PHE)+(0.60*T2*SB*PNH3)
      CALL SFJKJOIN(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
      ZZV1=ZZV*7.0E-2*T*(1.0-EXP(-28.6/T))
      ZZV2=ZZV*5.25E-2*T*EXP(-23.3/T)*(1.0-EXP(-57.2/T))
      ZZV3=ZZV*7.50E-2*T*EXP(-28.6/T)*(1.0-EXP(-57.2/T))
      SUM=SUM+(ZZV1*FJK)
      L1=2
      L2=1
      VLINE=1169.0
      SB=23.8
      CALL SFJKJOIN(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
C   multiply fjk by 4.0 to test sensitivity
C   FJK=4.0*FJK
      SUM=SUM+(ZZV2*FJK)+(ZZV3*FJK)
C
C
C     THE AMMONIA ABSORPTION COEFFICIENT IS IN CM-1.
      ANH3=SUM
c      IF (NOPR .EQ. 1) WRITE(6,30) CORR,SUM,ANH3
  30  FORMAT(2X,'CORR,SUM,ANH3',2X,1P,3(2X,E10.3),/)
C
    PH2=PH2*1.013
    PHE=PHE*1.013
    PH2O=PH2O*1.013
    PNH3=PNH3*1.013
    PCH4=PCH4*1.013
      RETURN
```

```
      END
C
      SUBROUTINE SAJKJOIN(T,VLINE,J,L1,L2,SK,SB,GM,GH2,AJK)
     real*4 t3,gm,vline,fjk,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,deltot,PCO,PCO13,PHCN
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
      COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C     GM IS GAMMA(J,K) IN GHZ.
      GM=(1.89*T3*PH2)+(0.75*T3*PHE)+(0.60*T2*SB*PNH3)
      A1=(2.*J+1.)*FLOAT(L2)/FLOAT(L1)
      A5=((2.98*L1)-(1.09*L2))*T7
C     AJK IS A(J,K),SEE EQN 24 OF BERGE AND GULKIS PAPER,GEHRELS
C     JUPITER BOOK,PAGE 675.
      CALL EX(A5,A10)
      AJK=1.23E3*A1*SK*PNH3*T6*A10
c      IF (NOPR .EQ. 1) WRITE(6,10) GM,A1,A5,AJK
  10  FORMAT(2X,'GM,A1,A5,AJK',2X,1P,4(2X,E10.3))
      RETURN
      END
C
      SUBROUTINE SFJKJOIN(T,L1,L2,V,VLINE,GM,GH2,SB,FJK)
     real*4 t3,gm,vline,fjk,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,deltot,PCO,PCO13,PHCN
      COMMON/V1/A1,A2,A3,A4,A5,A6,A7,A8,A9,A10
      COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
       COMMON/U4/T1,T2,T3,T4,T5,T6,T7,T8,T9,T10,T11
      COMMON/V4/NOPR,NOPR2,NOPR3,NOPR4
C
C     FJK IS THE BEN REUVEN LINE SHAPE,SEE EQN 25 OF BERGE AND
C     GULKIS ARTICLE,PAGE 675 OF GEHRELS JUPITER BOOK.
C
      X=PH2+PHE+PH2O+PNH3+PCH4
C  IF X.LT.1 ATM VAN VLECK-WEISKOPF LINE SHAPE CAN BE
C  USED; HOWEVER, BEN REUVEN IS STILL BETTER OUT IN THE
C  WINGS OF THE AMMONIA LINES.
c     A2 IS THE COUPLING FACTOR ZETA(J,K) IN GHZ.
c   GOTO 500
C  for Gross lineshape, goto 500 (first VVW, then gross
      IF(VLINE.GT.100.0) GOTO 500
      A2=(1.35*PH2*T3)+(0.30*T2*PNH3*SB)+
     1  (0.2*T3*PHE)
C     A4 IS THE PRESSURE SHIFT DEL (GHZ)
     A4=-0.45*PNH3
C     SQUARES OF VARIOUS TERMS.
      A5=(VLINE+A4)*(VLINE+A4)
C      A5=VLINE*VLINE
      A6=GM*GM
      A7=A2*A2
      A8=V*V
C     NUMERATOR
      A9=((GM-A2)*A8)+((GM+A2)*(A5+A6-A7))
      A10=A8-A5-A6+A7
C     DENOMINATOR
      A10=(A10*A10)+(4.0*A8*A6)
C     THE BEN REUVEN LINE SHAPE.
      FJK=2.0*A8*(A9/A10)
```

```
      IF (NOPR .EQ. 1) WRITE(6,10) A2,A4,A5,A6,A7,A8,A9,
     1  A10,FJK
    goto 501
  500 CONTINUE
C  THE VAN VLECK-WEISKOPF LINE SHAPE
c
      Z1=0.755*PH2+0.231*PHE
      Z2=FLOAT(L2)/FLOAT(L1)
      Z1=Z1*(Z2**0.3333)
      Z2=SQRT(Z2)*PNH3*6.23
      Z=(Z1+Z2)*1.0E3/T
      X1=V*V*Z
      X2=(V-VLINE)*(V-VLINE)
      X3=(V+VLINE)*(V+VLINE)
      FJK=X1/(X2+Z*Z)+X1/(X3+Z*Z)
C      GOTO 501
C  THE GROSS LINE SHAPE
       X2=(-V*V+VLINE*VLINE)
       X2=X2*X2
      if(vline.lt.1000.) Z1=123.3551*PH2+60.7441*PHE
    if(vline.ge.1000.) z1=2.885*PH2+1.00*PHE
C      Z2=FLOAT(L2)/FLOAT(L1)
    Z2=300./T
      Z1=Z1*(Z2**0.3)
    if(vline.lt.1000.) Z=154.1939*PNH3*Z2
    if(vline.ge.1000.) Z=22.989*PNH3*Z2
       Z=Z1+Z
       X3=Z*Z*4.*V*V
       X1=v*VLINE*Z*4.
       X1=X1*V*VLINE
       FJK=X1/(X2+X3)
 501    FFF=FJK
  10  FORMAT(2X,'A2,A4,A5,A6,A7,A8,A9,A10,FJK',/,
     1  2X,1P,9(2X,E10.3))
      RETURN
      END
c**********************************************************************
      function absco(j,fr0,f,p,t,wtmol)
c
c     this function calculates the absorption coeff of CO
C  f, fr0 in Hz; p in bar, but the routine expects:
C f, fr0 in Hz, and p in microbar
c     normalized by the CO mixing ratio (xco)
c     the formulae were taken from Clancy's PhD thesis
C
      if(j.eq.0) then
          absco = 0.0
          return
      endif
      p=p*1.0E6
c
      pi = 3.14159265308
c
c     offset frequency from line center
      fpm = f - fr0
      fpp = f + fr0
```

```
c
c     pressure broadened line width  in Hz
C  this is the same as in the SHAPE function (IdP)
C  note that microbar = dynes/cm^2
C + this number should be the half-width of CO in H2-broadened gas
C  which is about 0.071 cm-1/atm
C  or 2100 instead of old 3300
C for HCN that would be 2 times larger
C  the following line is pretty consistent with the Menger et al 2000
C  results for 2-1 transition
       wp = 2100.0 * p * (300.0/t)**0.7

c     doppler width (e-folding ... not FWHM)  in Hz
      wd = fr0 / 3.00e10 * sqrt(2.0*1.38e-16*t/wtmol)
C in his thesis wd is smaller by f. 1.20
c
c     number density of atmosphere (ideal gas p = dkt)
      d = p / 1.38e-16 / t
c
      a = wp/wd
      x = fpm/wd
c
c     use the Voigt function line shape
      shape = voigt(x,a) / wd
c
c     VanVleck-Weisskopf shape (for future use at large offsets)
      vvwshape =
     & 1.0 / pi * f*f/fr0/fr0 * (wp/(fpm*fpm+wp*wp)+wp/(fpp*fpp+wp*wp))
c
c     Lorentz Shape
      vl = wp / pi / (fpm*fpm + wp*wp)
c
c
        shape=shape*1.0E6
        v1=v1*1.0E6
        vvwshape=vvwshape*1.0E6
        fshape=shape
        if(v1.gt.fshape) fshape=v1
C  The following is correct, I think -- 15 April 2011
        if(vvwshape.gt.fshape) fshape=vvwshape
c  I think pin = p/1.013E6 so P in is in atm; it was written as *1.013E6
        pin = p / 1.01325E6
         xshape=fshape
C         xshape=vvwshape
        call absx_coline(j,aon,t,pin,f,xshape)
C  xshape: p in millibar, f in MHz (p/f); I don't think we need to use this
C vvwshape: p in microbar; f in Hz
C We multiply shape by 1E6 to correct answer to come out in bars and MHz
C
         absco = aon
c       write(6,1003) j,aon,absco,shape,f,x,a,wp,wd
c       write(6,1004) p,xshape,vvwshape,v1,shape
c 1003  format(I5,8E12.4)
c 1004  format(5E12.4)
      p=p/1.0E6
C  if other gases are considered, add them here as well I guess; e.g.
```

```
C  SO2, H2SO4 vapor. VVW line shape is probably OK for lower layers
c
      return
      end
c**********************************************************************
c**********************************************************************
      function absco13(j,fr0,f,p,t,wtmol)
c
c     this function calculates the absorption coeff of CO
C  f, fr0 in Hz; p in bar, but the routine expects:
C f, fr0 in Hz, and p in microbar
c     normalized by the CO mixing ratio (xco)
c     the formulae were taken from Clancy's PhD thesis
C
      if(j.eq.0) then
          absco13 = 0.0
          return
      endif
      p=p*1.0E6
c
      pi = 3.14159265308
c
c     offset frequency from line center
      fpm = f - fr0
      fpp = f + fr0
c
c     pressure broadened line width; take same parameters as for CO12
      wp = 2100.0 * p * (300.0/t)**0.7

c     doppler width (e-folding ... not FWHM)  in Hz
      wd = fr0 / 3.00e10 * sqrt(2.0*1.38e-16*t/wtmol)
c
c     number density of atmosphere (ideal gas p = dkt)
      d = p / 1.38e-16 / t
c
      a = wp/wd
      x = fpm/wd
c
c     use the Voigt function line shape
      shape = voigt(x,a) / wd
c
c     VanVleck-Weisskopf shape (for future use at large offsets)
      vvwshape =
     & 1.0 / pi * f*f/fr0/fr0 * (wp/(fpm*fpm+wp*wp)+wp/(fpp*fpp+wp*wp))
c
c     Lorentz Shape
      vl = wp / pi / (fpm*fpm + wp*wp)
c
        shape=shape*1.0E6
        v1=v1*1.0E6
        vvwshape=vvwshape*1.0E6
        fshape=shape
        if(v1.gt.fshape) fshape=v1
C  The following is correct, I think -- 15 April 2011
        if(vvwshape.gt.fshape) fshape=vvwshape
c  I think pin = p/1.013E6 so P in is in atm; it was written as *1.013E6
```

```
        pin = p / 1.01325E6
        xshape=fshape
C         xshape=shape
         call absx_co13line(j,aon,t,pin,f,xshape)
C  xshape: p in millibar, f in MHz (p/f)
C vvwshape: p in microbar; f in Hz
C We multiply shape by 1E6 to correct answer to come out in bars and MHz
       absco13 = aon
c       write(6,1003) j,aon,absco13,shape,f,x,a,wp,wd
c       write(6,1004) p,xshape,vvwshape,v1,shape
c 1003  format(I5,8E12.4)
c 1004  format(5E12.4)
      p=p/1.0E6
C  if other gases are considered, add them here as well I guess; e.g.
C  SO2, H2SO4 vapor. VVW line shape is probably OK for lower layers
c
      return
      end
c*******************************************************************
c*******************************************************************
      function voigt(xx,a)
C  Need to know: T, P, But it is all passed along in xx, a
c
c     voigt function subroutine obtained from D. van Blerkom
c
c     This is not the ONE TRUE Voigt funtion ...
c     The normal definition of voigt function is:
c            H(a,b) = a/pi * INTEGRAL ( exp(-y*y) / ((b-y)**2 + a**2) dy )
c            where a = wp / wd
c                  b = (f - fr0) / wd
c     We compute:
c            voigt = 1/sqrt(pi) * H(a,b)
c
c     Function requires further normalization by doppler width.
c
      dimension c(31)
      data ic/0/,epsiln/2.5e-12/
c
c
C       write(6,1003) xx,a
C 1003  format(2E12.4)
      if(ic.ne.0) goto 20
   10 k=-16
      pie  = 3.1415926535898
      sqp  = sqrt(pie)
      sqpp = 1./sqp
      pie3 = 3.0*pie
      pie32= pie3*pie
      piec = 0.5/(pie*sqp)
      do 15 n=1,31
         k=k+1
   15    c(n)=piec*exp(-float(k*k)/9.)
      ic=1
c
   20 x=abs(xx)
c
```

```
      if(a.gt.1000.0)  go to 40
      if(a.lt.0.001)  go to 45
c
      a1=3.0*a
      a2=a*a
      if(a.lt.0.1) go to 25
      x1=-pie3*a
      voigt=0.0
      rz=0.0
      b2=0.0
      if(x1.lt.-675.0) go to 30
      y1=pie3*x
      e1=exp(x1)
      rz=e1*cos(y1)
      b2=-e1*sin(y1)
      go to 30
   25 x1=pie3*x
      y1=pie3*a
      e1=exp(y1)
      e2=1.0/e1
      rz=0.5*(e1+e2)*cos(x1)
      b2=-0.5*(e2-e1)*sin(x1)
      qin=a2-x*x
      voigt=0.0
      if(qin.gt.-675.0) voigt=sqpp*exp(qin)*cos(2.0*a*x)
   30 b1=(1.0-rz)*a*1.5
      s=-8.0-1.5*x
      t=s*s+2.25*a2
      c2=-a*pie32
      do 35 n=1,31
         t=t+s+0.25
         s=s+0.5
         b1=a1-b1
         b2=-b2
         con=c2
         if(t.gt.epsiln) con=(b1+b2*s)/t
   35    voigt=voigt+con*c(n)
      return
c
c     large a limit
c
   40 qin=x*x/a+a
      voigt=1.0/(pie*qin)
      return
c
c     small a limit
c
   45 voigt=0.0
      x2=x*x
      if(x2.lt.675.0) voigt=sqpp*exp(-x2)
      return
      end
c*****************************************************************
            SUBROUTINE ABSX_CO13(AON,T,P,vnu)
C
c  Note: This subroutine is for 13CO.
```

```
C
C THIS SUBROUTINE RETURNS QUANTITY AON, WHICH WHEN MULTIPLIED
C BY THE VOLUME MIXING RATIO, GIVES THE ABSORPTION COEFFICIENT
C OF CO13, IN UNITS OF 1/KM
C
C DEFINITIONS
C   AON ABSORPTION COEFFICIENT/VOLUME MIXING RATIO   1/KM
C   T   TEMPERATURE                  K
C       P   PRESSUME                MILLIBARS
C   F   FREQUENCY               MHZ
C
C ADDITIONAL FUNCTIONS REQUIRED
C   QLOG    BASE TEN LOGARITHM OF THE RATIO OF PARTITION
C       FUNCTION AT TEMPERATURE T TO PARTITION FUNCTION
C       AT T=300K
C   SHAPE(F,P)  LINE SHAPE FACTOR
C
C  the Q0, F0, S0, EL data are from Poynter and Picket, JPL catalogue
C
C*****************************************************************
        IMPLICIT NONE
        REAL*4 AON,T,P,F,V,wtmol
    REAL*4 QLOG2,SHAPE2,SHAPE
    REAL*4 C,ZCO,DV,VNU
        EXTERNAL QLOG2,SHAPE2,SHAPE
        INTEGER*2 N,NLINES
        PARAMETER (NLINES=9)   !NUMBER OF SPECTRAL LINES
        REAL*4 DF,DFC,DFD,EL(NLINES),Q0(5),F0(NLINES),FS,FV
        REAL*4 S0(NLINES),S1(NLINES),TCOR,X,X1,Y
        DATA Q0 /2.0564, 1.9317, 1.7565, 1.4579, 1.1620/ !LOG PF AT
            300,225,150,75,37.5K
         DATA F0(1),S0(1),EL(1)
     &  /110201.3672, -5.0614, 0.0000/
        DATA F0(2),S0(2),EL(2)
     &  /220398.7031, -4.1698, 3.6759/
        DATA F0(3),S0(3),EL(3)
     &  /330588.0937, -3.6607, 11.0276/
        DATA F0(4),S0(4),EL(4)
     &  /440765.4375, -3.3127, 22.0549/
        DATA F0(5),S0(5),EL(5)
     &  /550926.7500, -3.0564, 36.7572/
        DATA F0(6),S0(6),EL(6)
     &  /661068.0625, -2.8609, 55.1341/
        DATA F0(7),S0(7),EL(7)
     &  /771185.3125, -2.7098, 77.1850/
        DATA F0(8),S0(8),EL(8)
     &  /881274.5625, -2.5933, 102.9090/
        DATA F0(9),S0(9),EL(9)
     &  /991331.8125, -2.5049, 132.3051/
    P=P*1000.0/1.013        !MILLIBAR
    C=2.99791E1
    F=vnu*C*1.0E3                   !FREQU IN MHZ
    AON=0.0
       DO N = 1,NLINES
       TCOR = EXP(1.4388*EL(N)*(3.33356E-03-1./T))
     & *(1.-EXP(-4.7993E-05*F0(N)/T))
```

```
     & /(1.-EXP(-1.5998E-07*F0(N)))
       AON=AON+TCOR*SHAPE(P,T,F,F0(N))*(10.**S0(N))
       enddo
       AON=AON*10**(Q0(1)-QLOG2(Q0,T)) !T DEPENDENCE OF PARTITION FUNCTION
       AON=0.72435E5*AON*P/T       !YIELD ABSORPTION COEFFICIENT IN 1/cm
C                                    WHEN MULTIPLIED BY MIXING RATIO
C
    P=P*1.013/1000.0
       RETURN
       END
C
c**********************************************************************
             SUBROUTINE ABSX_CO13line(n,AON,T,P,f,xshape)
C
c  Note: This subroutine is for 13CO.
C
C THIS SUBROUTINE RETURNS QUANTITY AON, WHICH WHEN MULTIPLIED
C BY THE VOLUME MIXING RATIO, GIVES THE ABSORPTION COEFFICIENT
C OF CO13, IN UNITS OF 1/KM
C
C DEFINITIONS
C   AON ABSORPTION COEFFICIENT/VOLUME MIXING RATIO   1/KM
C   T   TEMPERATURE                   K
C       P   PRESSUME                MILLIBARS
C   F   FREQUENCY               MHZ
C
C ADDITIONAL FUNCTIONS REQUIRED
C   QLOG    BASE TEN LOGARITHM OF THE RATIO OF PARTITION
C       FUNCTION AT TEMPERATURE T TO PARTITION FUNCTION
C       AT T=300K
C   SHAPE(F,P)  LINE SHAPE FACTOR
C
C  the Q0, F0, S0, EL data are from Poynter and Picket, JPL catalogue
C
C**********************************************************************
       IMPLICIT NONE
       REAL*4 AON,T,P,F,V,wtmol
    REAL*4 QLOG2,SHAPE2,xshape
    REAL*4 C,ZCO,DV,VNU
       EXTERNAL QLOG2,SHAPE2
       INTEGER*2 N,NLINES
       PARAMETER (NLINES=9)   !NUMBER OF SPECTRAL LINES
       REAL*4 DF,DFC,DFD,EL(NLINES),Q0(5),F0(NLINES),FS,FV
       REAL*4 S0(NLINES),S1(NLINES),TCOR,X,X1,Y
       DATA Q0 /2.0564, 1.9318, 1.7565, 1.4579, 1.1620/ !LOG PF AT
           300,225,150,75, 37.5K
        DATA F0(1),S0(1),EL(1)
     &  /110201.3672, -5.0614, 0.0000/
       DATA F0(2),S0(2),EL(2)
     &  /220398.7031, -4.1698, 3.6759/
       DATA F0(3),S0(3),EL(3)
     &  /330588.0937, -3.6607, 11.0276/
       DATA F0(4),S0(4),EL(4)
     &  /440765.4375, -3.3127, 22.0549/
       DATA F0(5),S0(5),EL(5)
     &  /550926.7500, -3.0564, 36.7572/
```

```
      DATA F0(6),S0(6),EL(6)
     &  /661068.0625, -2.8609, 55.1341/
      DATA F0(7),S0(7),EL(7)
     &  /771185.3125, -2.7098, 77.1850/
      DATA F0(8),S0(8),EL(8)
     &  /881274.5625, -2.5933, 102.9090/
      DATA F0(9),S0(9),EL(9)
     &  /991331.8125, -2.5049, 132.3051/
    P=P*1000.0/1.013        !MILLIBAR
    C=2.99791E1
      F=F/1.0E6
C   F=vnu*C*1.0E3                 !FREQU IN MHZ
    AON=0.0
C      xshape=SHAPE2(P,T,F,F0(N))
      TCOR = EXP(1.4388*EL(N)*(3.33356E-03-1./T))
     & *(1.-EXP(-4.7993E-05*F0(N)/T))
     & /(1.-EXP(-1.5998E-07*F0(N)))
      AON=AON+TCOR*xshape*(10.**S0(N))
      AON=AON*10**(Q0(1)-QLOG2(Q0,T)) !T DEPENDENCE OF PARTITION FUNCTION
      AON=0.72435E5*AON*P/T       !YIELD ABSORPTION COEFFICIENT IN 1/cm
C                                   WHEN MULTIPLIED BY MIXING RATIO
C
    P=P*1.013/1000.0
      F=F*1.0E6
      RETURN
      END
C
C*********************
C
      SUBROUTINE ABSX_CO(AON,T,P,vnu)
C
C THIS SUBROUTINE RETURNS QUANTITY AON, WHICH WHEN MULTIPLIED
C BY THE VOLUME MIXING RATIO, GIVES THE ABSORPTION COEFFICIENT
C OF CO, IN UNITS OF 1/cm
C
C DEFINITIONS
C   AON ABSORPTION COEFFICIENT/VOLUME MIXING RATIO   1/cm
C   T   TEMPERATURE                   K
C       P   PRESSUME                atm
C   F   FREQUENCY               MHZ
C
C ADDITIONAL FUNCTIONS REQUIRED
C   QLOG    BASE TEN LOGARITHM OF THE RATIO OF PARTITION
C       FUNCTION AT TEMPERATURE T TO PARTITION FUNCTION
C       AT T=300K
C   SHAPE(F,P)  LINE SHAPE FACTOR
C
C  the Q0, F0, S0, EL data are from Poynter and Picket, JPL catalogue
C
C*****************************************************************
      IMPLICIT NONE
      REAL*4 AON,T,P,F,V,wtmol
    REAL*4 QLOG2,SHAPE2,SHAPE
    REAL*4 C,ZCO,DV,VNU
      EXTERNAL QLOG2,SHAPE2,SHAPE
      INTEGER*2 N,NLINES
```

```
      PARAMETER (NLINES=8)   !NUMBER OF SPECTRAL LINES
      REAL*4 DF,DFC,DFD,EL(NLINES),Q0(5),F0(NLINES),FS,FV
      REAL*4 S0(NLINES),S1(NLINES),TCOR,X,X1,Y
      DATA Q0 /2.0369, 1.9123, 1.7370, 1.4386, 1.1429/ !LOG PF AT
          300,225,150,75,37.5K
      DATA F0(1),S0(1),EL(1)
     &  /115271.2018, -5.0105, 0.0000/
      DATA F0(2),S0(2),EL(2)
     &  /230538.0000, -4.1197, 3.8450/
      DATA F0(3),S0(3),EL(3)
     &  /345795.9899, -3.6118, 11.5350/
      DATA F0(4),S0(4),EL(4)
     &  /461040.7682, -3.2657, 23.0695/
      DATA F0(5),S0(5),EL(5)
     &  /576267.9305, -3.0118, 38.4481/
      DATA F0(6),S0(6),EL(6)
     &  /691473.0763, -2.8193, 57.6704/
      DATA F0(7),S0(7),EL(7)
     &  /806651.8060, -2.6715, 80.7354/
      DATA F0(8),S0(8),EL(8)
     &  /921799.7000, -2.5590, 107.6424/
    P=P*1000.0/1.013        !MILLIBAR
    C=2.99791E1
    F=VNU*C*1.0E3                  !FREQU IN MHZ
       AON=0.0
      DO N = 1,NLINES
      TCOR = EXP(1.4384*EL(N)*(3.3784E-03-1./T))
     & *(1.-EXP(-4.7993E-05*F0(N)/T))
     & /(1.-EXP(-1.5998E-07*F0(N)))
      AON=AON+TCOR*SHAPE(P,T,F,F0(N))*(10.**S0(N))
      enddo
      AON=AON*10**(Q0(1)-QLOG2(Q0,T)) !T DEPENDENCE OF PARTITION FUNCTION
      AON=0.72435E5*AON*P/T       !YIELD ABSORPTION COEFFICIENT IN 1/cm
C                                  WHEN MULTIPLIED BY MIXING RATIO
      P=P*1.013/1000.0
C      write(6,1003) n,aon,xz,xz2
 1003  format(I5,3E12.4)
C
      RETURN
      END
C
C*********************
C
      SUBROUTINE ABSX_COline(n,AON,T,P,f,xshape)
C
C THIS SUBROUTINE RETURNS QUANTITY AON, WHICH WHEN MULTIPLIED
C BY THE VOLUME MIXING RATIO, GIVES THE ABSORPTION COEFFICIENT
C OF CO, IN UNITS OF 1/cm
C
C DEFINITIONS
C   AON ABSORPTION COEFFICIENT/VOLUME MIXING RATIO   1/cm
C   T   TEMPERATURE                   K
C       P   PRESSUME                atm
C   F   FREQUENCY               MHZ
C
C ADDITIONAL FUNCTIONS REQUIRED
```

```
C   QLOG    BASE TEN LOGARITHM OF THE RATIO OF PARTITION
C       FUNCTION AT TEMPERATURE T TO PARTITION FUNCTION
C       AT T=300K
C   SHAPE(F,P)  LINE SHAPE FACTOR
C
C  the Q0, F0, S0, EL data are from Poynter and Picket, JPL catalogue
C
C*****************************************************************
        IMPLICIT NONE
        REAL*4 AON,T,P,F,V,wtmol
    REAL*4 QLOG2,SHAPE2,SHAPE,xshape
    REAL*4 C,ZCO,DV,VNU
        EXTERNAL QLOG2,SHAPE2,SHAPE
        INTEGER*2 N,NLINES
        PARAMETER (NLINES=8)   !NUMBER OF SPECTRAL LINES
        REAL*4 DF,DFC,DFD,EL(NLINES),Q0(5),F0(NLINES),FS,FV
        REAL*4 S0(NLINES),S1(NLINES),TCOR,X,X1,Y
        DATA Q0 /2.0369, 1.9123, 1.7370, 1.4386, 1.1429/ !LOG PF AT
            300,225,150,75, 37.5K
        DATA F0(1),S0(1),EL(1)
     &  /115271.2018, -5.0105, 0.0000/
        DATA F0(2),S0(2),EL(2)
     &  /230538.0000, -4.1197, 3.8450/
        DATA F0(3),S0(3),EL(3)
     &  /345795.9899, -3.6118, 11.5350/
        DATA F0(4),S0(4),EL(4)
     &  /461040.7682, -3.2657, 23.0695/
        DATA F0(5),S0(5),EL(5)
     &  /576267.9305, -3.0118, 38.4481/
        DATA F0(6),S0(6),EL(6)
     &  /691473.0763, -2.8193, 57.6704/
        DATA F0(7),S0(7),EL(7)
     &  /806651.8060, -2.6715, 80.7354/
        DATA F0(8),S0(8),EL(8)
     &  /921799.7000, -2.5590, 107.6424/
    P=P*1000.0/1.013        !MILLIBAR
    C=2.99791E1
    F=f/1.0E6               !FREQ IN MHz
C   F=VNU*C*1.0E3                  !FREQU IN MHZ
        AON=0.0
C        xshape=SHAPE(P,T,F,F0(N))
       TCOR = EXP(1.4384*EL(N)*(3.3784E-03-1./T))
     & *(1.-EXP(-4.7993E-05*F0(N)/T))
     & /(1.-EXP(-1.5998E-07*F0(N)))
       AON=AON+TCOR*xshape*(10.**S0(N))
       AON=AON*10**(Q0(1)-QLOG2(Q0,T)) !T DEPENDENCE OF PARTITION FUNCTION
       AON=0.72435E5*AON*P/T       !YIELD ABSORPTION COEFFICIENT IN 1/cm
C                                   WHEN MULTIPLIED BY MIXING RATIO
       P=P*1.013/1000.0
C       write(6,1003) n,aon,xz,xz2
C 1003  format(I5,3E12.4)
       f=f*1.0E6
C
       RETURN
       END
C
```

```
      SUBROUTINE ABSX_HCN(AON,T,P,vnu)
C
C THIS SUBROUTINE RETURNS QUANTITY AON, WHICH WHEN MULTIPLIED
C BY THE VOLUME MIXING RATIO, GIVES THE ABSORPTION COEFFICIENT
C OF Hcn, THIOFORMALDEHYDE, IN UNITS OF 1/KM
C
C DEFINITIONS
C   AON ABSORPTION COEFFICIENT/VOLUME MIXING RATIO   1/CM
C   T   TEMPERATURE                   K
C       P   PRESSUME                MILLIBARS
C   F   FREQUENCY               MHZ
C
C ADDITIONAL FUNCTIONS REQUIRED
C   QLOG    BASE TEN LOGARITHM OF THE RATIO OF PARTITION
C       FUNCTION AT TEMPERATURE T TO PARTITION FUNCTION
C       AT T=300K
C   SHAPE(P,T,F,FLC)    LINE SHAPE FACTOR
C
C  the Q0, F0, S0, EL data are from Poynter and Picket, JPL catalogue
C
C*****************************************************************
      IMPLICIT NONE
      REAL*4 AON,T,P,F,V
    REAL*4 QLOG2,SHAPE
    REAL*4 C,ZHCN,DV,VNU
      EXTERNAL QLOG2,SHAPE
      INTEGER*2 N,NLINES
      PARAMETER (NLINES=11)   !NUMBER OF SPECTRAL LINES
      REAL*4 DF,DFC,DFD,EL(NLINES),Q0(5),F0(NLINES),FS,FV
      REAL*4 S0(NLINES),S1(NLINES),TCOR,X,X1,Y
      DATA Q0 /2.6277,2.5031,2.3276,2.0286,1.7317/ !LOG PF AT
          300,225,150,75,37.5K
      DATA F0(1),S0(1),EL(1)
     & /177262.0156,  -3.8432,   2.9564/
      DATA F0(2),S0(2),EL(2)
     & /88630.4141,  -2.9588,     0.000/
      DATA F0(3),S0(3),EL(3)
     & /88631.8437,  -2.7370,     0.000/
      DATA F0(4),S0(4),EL(4)
     & /88633.9375,  -3.4359,     0.000/
      DATA F0(5),S0(5),EL(5)
     & /177259.6719,  -2.6671,     2.9564/
      DATA F0(6),S0(6),EL(6)
     & /177259.9219,  -2.5422,     2.9564/
      DATA F0(7),S0(7),EL(7)
     & /177261.1094,  -2.1900,     2.9564/
      DATA F0(8),S0(8),EL(8)
     & /177261.2188,  -1.9189,     2.9564/
      DATA F0(9),S0(9),EL(9)
     & /177263.4375,  -2.6671,     2.9564/
      DATA F0(10),S0(10),EL(10)
     & /265886.1875,  -1.0751,     8.8692/
      DATA F0(11),S0(11),EL(11)
     & /354505.4687,  -0.7220,  17.7382/
    P=P*1000.0/1.013        !MILLIBAR
    C=2.99791E1
```

```
      F=VNU*C*1.0E3                  !FREQU IN MHZ
      AON=0.0
         DO N = 1,NLINES
         TCOR = EXP(1.4388*EL(N)*(3.33356E-03-1./T))
       & *(1.-EXP(-4.7993E-05*F0(N)/T))
       & /(1.-EXP(-1.5998E-07*F0(N)))
         AON=AON + TCOR*SHAPE(P,T,F,F0(N))*(10.**S0(N))
         ENDDO
         AON=AON*10**(Q0(1)-QLOG2(Q0,T)) !T DEPENDENCE OF PARTITION FUNCTION
         AON=0.72435E5*AON*P/T        !YIELD ABSORPTION COEFFICIENT IN 1/cm
C                                       WHEN MULTIPLIED BY MIXING RATIO
C
      P=P*1.013/1000.0
         RETURN
         END
C*************
C
         FUNCTION SHAPE(P,T,F,FLC)
      implicit none
      REAL*4 SHAPE
      real*4 DL,P,T,F,FLC,DFC,DL2
C  HPFW for collisional broadening from Clancy's thesis, for CO
C P in mbar, F and DFC in MHz when called from absx_co routines
C CO 2-1: 2.1*P*((300.0/T)**0.7)
C       DFC=188.57*P/(T**0.75)
         DFC=2.1*P*((300.0/T)**0.7)
         DL=F-FLC
         DL2=F+FLC
         SHAPE=((F*F)/(FLC*FLC))*(DFC/(DL*DL+DFC*DFC)
       + +DFC/(DL2*DL2+DFC*DFC))
      SHAPE=SHAPE/3.1415926536        !DIVIDE BY PI
         RETURN
         END
C
         SUBROUTINE ABSBR_PH3(AON,T,P,VNU,zpph3)
C
C THIS SUBROUTINE RETURNS QUANTITY AON, WHICH WHEN MULTIPLIED
C BY THE VOLUME MIXING RATIO, GIVES THE ABSORPTION COEFFICIENT
C OF PH3, IN UNITS OF 1/cm
C
C DEFINITIONS
C   AON ABSORPTION COEFFICIENT/VOLUME MIXING RATIO   1/cm
C   T   TEMPERATURE                   K
C       P   PRESSUME                BARS
C   F   FREQUENCY               MHZ
C
C ADDITIONAL FUNCTIONS REQUIRED
C   QLOG    BASE TEN LOGARITHM OF THE RATIO OF PARTITION
C       FUNCTION AT TEMPERATURE T TO PARTITION FUNCTION
C       AT T=300K
C   SHAPE(F,P)  LINE SHAPE FACTOR
C
C*****************************************************************
         IMPLICIT NONE
         REAL*4 AON,T,P,F,V
      real*4 t3,gm,vline,ph2,phe,ph2s,pnh3,pch4,ph2o,pph3,
```

```
     + deltot,PCO,PCO13,PHCN
        real*4 DL,FLC,DL2,zpph3
      REAL*4 C,DV,VNU,coef,hck
      real*8 x,ajk,fjk,tcor
        INTEGER*2 N,NLINES
        PARAMETER (NLINES=320)   !NUMBER OF SPECTRAL LINES
      real*4  FP0(728),SP0(728),ELP(728),Q0(5)
      REAL*4 wgtS0(40),wgtFGB(40),wgtSB(40)
      REAL*4 QLOG2,SHAPE2
        EXTERNAL QLOG2
       DATA Q0 /2.905, 2.722, 2.4606, 2.0132, 1.5705/ !LOG PF AT 300,225,150,75,
           37.5K
        COMMON/ph3/FP0,SP0,ELP,wgtS0,wgtFGB,wgtSB
        COMMON/U1/PH2,PHE,PNH3,PH2O,PCH4,PH2S,PPH3,PCO,PCO13,PHCN
      C=2.997925E1
      coef=7.244E21
      hck=1.438396    !hc/k
      V=VNU*C             !FREQ IN GHZ
      T3=(300/T)**0.6667
      AON=0.0
        DO N = 1,NLINES
      VLINE=FP0(N)        !LINE CENTER IN GHZ
        TCOR = EXP(-(hck*ELP(N)*(1./T - 3.3333E-03)))
      call sajph3(N,T,T3,GM)
      if (N.gt.40) goto 40
      ajk=SP0(N)*wgtS0(N)*TCOR
      goto 50
   40    ajk=SP0(N)*TCOR
   50   continue
        CALL SFJph3(N,T,V,VLINE,GM,FJK)
       AON=AON + ajk*FJK
       ENDDO
      x=(300.0/T)**3.5
      AON=2.4163E3*x*AON*PPh3/300.0       !2.4163E3 is from deboer
C
       RETURN
       END

C
C
```