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FORTRAN program for calculation of thermodynamic properties of minerals from vibrational spectra

by

Susan Werner Kiefferl

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1U.S. Geological Survey
2255 North Gemini Drive
Flagstaff, Arizona 86001

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CONTENTS Page

ABSTRACT

A VAX-VMS FORTRAN program is presented for calculation of the thermodynamic properties of minerals, including heat capacity at constant volume (C_V) and at constant pressure (C_P), harmonic and anharmonic entropy (S), enthalpy (H), free energy (G), and free energy function [(G-H)/T]. These properties can be calculated as a function of temperature (T) and pressure (P). They can also be calculated for the O^{16} and O^{18} isotopic species of minerals, yielding a fractionation factor. The program assumes that the actual lattice vibrational spectrum of the mineral can be approximated by discrete spectral parts (acoustic, optic, or Einstein) as described in Kieffer (1978a,b,c; 1980; 1982, 1985).

The VAX-VMS FORTRAN program described can be obtained by sending a 1200 foot magnetic tape, certified for 6250 BPI, to Susan W. Kieffer, U.S. Geological Survey, 2255 N. Gemini Drive, Flagstaff, Arizona 86001.

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INTRODUCTION

Interpretation of mineral thermodynamic properties is dependent on knowledge of mineral vibrational spectra. In some cases where thermodynamic properties of minerals cannot be measured because of lack of samples (e.g., high-pressure polymorphs) or instability of samples to calorimetric techniques (e.g., breakdown of structure or decomposition of hydrous minerals), the thermodynamic properties can be estimated from vibrational properties. The theory of this is discussed in Kieffer (1978a,b,c; 1980; 1982; and 1985) and is not repeated here. A VAX-VMS FORTRAN program (THERMO) for implementation of this theory is described in this report. Sample data sets and results are given for the following minerals: (a) fosterite and fayalite at 1 bar pressure vs. temperature; (b) quartz at several pressures and temperatures; and (c) O^{16} and O^{18} species of calcite, with calculation of the isotopic fractionation factors.

PROGRAM NOTES: STRUCTURE OF PROGRAM

The program calculates the thermodynamic properties from lattice vibrational spectra, approximated as shown in figure 1. The program can accomodate a spectrum consisting of three acoustic branches (two shear and one longitudinal), three optic continua, and four Einstein oscillators. Any of these optical parts of the spectrum can be eliminated by simply setting the relevant parameters to 0 in the input data; the acoustic branches must be retained.

The program is not interactive. Data are called from a file called DATARUN.DAT and results are placed in a file called RESULTS.PRT. The main program THERMO calls the FUNCTION JNDEX (a table-search function developed by H. Kieffer) and the SUBROUTINE QG92 (a 9-point Gaussian quadrature integration routine.)

The program consists of the following parts, labeled with comment statements:

- Part 1. A table of Debye functions is generated so that the calorimetric Debye temperature can be calculated from either measured or calculated values of specific heat.
- Part 2. Input data are read and printed out; if calculations at more than one pressure are requested, the program returns to this point so that the physical parameters for the mineral (this and next part) are recalculated.
- Part 3. The acoustic branch parameters, dispersion curves, mean acoustic velocity and acoustic Debye temperature are calculated.
- Part 4. Experimental heat capacity data vs. temperature are read and the calorimetric Debye temperatures corresponding to each data set are calculated.
- Part 5. Model values of the thermodynamic functions are calculated for the temperatures specified.
- Part 6. Isotopic fractionation factors can be calculated.
- Part 7. Model spectra are calculated.
- Part 8. The calculations can be repeated for different pressure conditions.

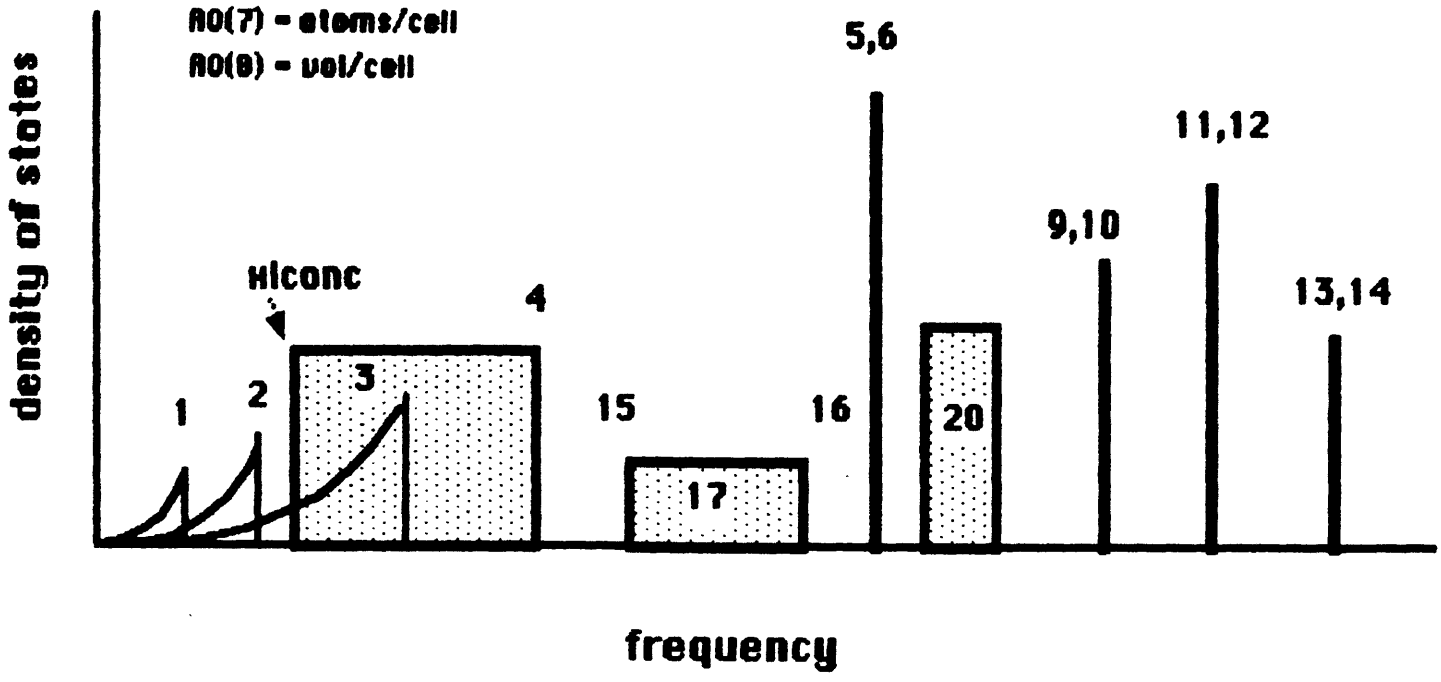

Figure 1. Schematic diagram of the spectrum allowed in THERMO. The numbers refer to the A0(i) parameters described in the report, e.g., A0(1), A0(2), and A0(3) are acoustic velocities; A0(4) is the cutoff frequency for the lower optic continuum, and A0(5) and A0(6) are the parameters for one of the Einstein oscillators.

PROGRAM NOTES: INPUT

There is no program limit on the number of minerals that can be placed in DATARUN.DAT and run by the program. However the print-out options and the temperature ranges described in the next two items cannot be varied from one mineral to the next within the file because the iteration through the minerals begins after reading these data; separate runs must be made to vary the print-out options or the temperature ranges.

Print-out options (specified on line 1 of DATARUN): In development of the program, it was convenient to print out various values at different places in the program. These are specified through the variables LP(I). Most print-out requests have been suppressed in this version by conversion to comment statements, but can be reinstated by specifying nonzero LP values on the first line of the data file and uncommenting the appropriate statements. Seven print-out options and one calculation option are available, depending on whether the LP values are zero or nonzero. The format is 8I5. The default is all zeros, with no print-out at these places in the program.

1. If LP1.NE.0, a table of the Debye function is printed.
2. If LP2.NE.0, acoustic, continuum, and Einstein contributions to the heat capacity are separately printed.
3. If LP3.NE.0, a formal table used for publication is printed.
4. If LP4.NE.0, the vibrational spectrum is calculated and printed.
5. If LP5.NE.0, FSTORE and FTTAL are printed, just before FRAC.FACTOR is calculated.
6. If LP6.NE.0, various indices are printed.
7. If LP7.NE.0, FSTORE can be printed in several places (used for debugging program).
8. (This is not a print-out option, but is a calculation option: If LP8.NE.0, the anharmonic correction is added to the Helmholtz energy).

Temperature (specified on lines 2,3,4 of DATARUN): Temperature is specified in Kelvins. The program automatically calculates the properties at 298.15 K as the first values. Temperature can be specified over three additional separate sub-ranges, so that the interval between temperatures can be varied, e.g., one sub-range could be from 0 to 100 K in 10 K increments, the next could be from 150 to 500 K in 50 K increments, and the third could be from 600 to 2000 K in 100 K increments.

I123(4), I123(5) and I123(6) are the lower and upper bounds of the first temperature range, and the temperature increment for the range, respectively.

I123(7), I123(8) and I123(9) specify the second range in the same order as above.

I123(10), I123(11), and I123(12) specify the third range in the same order as above.

Mineral neumonic and instruction for calculation of isotopic fractionation factors (line 5 of DATARUN): A neumonic is used for the mineral, XNAME, format 19A4. (In most of Kieffer's cases, the first four letters of the mineral name are used and the rest of the field can be used to comment.) The last four columns of this card (IFRAC, format I4) are used to declare whether

or not the oxygen isotopic fractionation factor is to be calculated. (The program could calculate isotopic fractionation of other species, e.g., sulfur and hydrogen, if a few statements particular to oxygen in the program were removed to data statements). If fractionation calculations are not desired, this field is blank (or zero). If fractionation factors are being calculated, the calculations must first be run for one composition (e.g., the O^{16} form), and then, sequentially, for the other composition (e.g., the O^{18} form). When this parameter, IFRAC, is nonzero for the second mineral, the appropriate energies of the second and first minerals are subtracted and the fractionation factors are determined.

Pressure increments (line 6 of DATARUN): The pressures at which the calculations are to be done are specified in bars. Up to eight pressures can be specified.

Grüneisen parameters (line 7 of DATARUN): There are two possible ways to calculate the thermodynamic properties at high pressure: (1) If high pressure spectral data are available, then these parameters can be entered directly in the AA(I) field. The program should be "fooled" into using these parameters by setting the pressure (line 6) equal to 1 bar, thus suppressing the pressure calculation that is normally applied to the spectra. (2) Up to six Grüneisen parameters can be specified on line 7 and they will be used to shift the 1-bar spectrum as described in Kieffer (1982). In the present program, the first three Grüneisen parameters are for the three acoustic branches respectively. the fourth Grüneisen parameter is used for all optic continua; the fifth is used for the first three Einstein oscillators, and the sixth is used for the last Einstein oscillator. Thus, care is required to order the Einstein oscillators and the Grüeisen parameters properly.

Values of mineral properties used by the model (lines 8,9,10 of DATARUN): The physical parameters of the model are specified here. They are read in as A0(I), in format 20F10.3.

1 - 3. A0(1), A0(2), A0(3), acoustic velocities, in km/sec. A0(1) and A0(2) are the shear velocities; A0(3) is the longitudinal velocity.

4. A0(4) is the upper cutoff of the first optic continuum, in cm^{-1}. If it is equal to 0.0, the program assumes that there are no other continua.

5. A0(5) is an Einstein frequency, in cm^{-1}.

6. A0(6) is the fraction of oscillators at the frequency A0(5).

7. A0(7) is the number of atoms per unit cell.

8. A0(8) is the volume of the unit cell, in cubic Angstroms.

9. A0(9) is a second Einstein frequency, in cm^{-1}.

10. A0(10) is the fraction of oscillators associated with A0(9).

11 and 13. A0(11) and A0(13) are two more Einstein oscillators, in cm^{-1}.

12 and 14. A0(12) and A0(14) are the fractions of the spectrum associated with A0(11) and A0(13) respectively.

15, 16, 18, and 19. A0(15,16) and A0(18,19) are the lower and upper bounds of additional optic continua if they are required, in cm^{-1}.

17 and 20. A0(17) is the fraction of oscillators in the continuum described by A0(15) and A0(16); A0(20) is the fraction of oscillators in the continuum described by A0(18) and A0(19).

More values of mineral properties (line 11 of DATARUN): The following four properties are specified in format 8F10.3:

1. RHO is crystal density in g/cm^3.
2. WTMOL is molecular weight.
3. P is the number of atoms in the formula unit.
4. RR is the number of oxygens per primitive cell.

Coefficients for calculation of C_p-C_v and their derivatives (line 12 of DATARUN, format 8F10.3):

1. VMOLAR is molar volume, in cm^3/mole.
2. ALPHA0, ALPHA1, and ALPHA2 are coefficients for thermal expansion as a function of temperature (expressed as a second-order polynomial):

$$\varepsilon = \varepsilon_0 + \varepsilon_1 T + \varepsilon_2 T^2.$$

3. BULK and DBULK are the bulk modulus (in Mbar) and its temperature derivative (in Mbar/K):

$$B = B_0 + (\partial B_0/\partial T)\Delta T.$$

4. CPTEST is a parameter which is set equal to zero if no correction from C_p to C_v is to be done on the experimental data that are read in below. If this parameter is not zero, the correction is made, but only above 300 K because thermal expansion data generally are not available (or important) at the lower temperatures.
5. PBULK is the pressure derivative of the bulk modulus, $\partial B/\partial P$.

Data for the lowest optical continuum (this is the only optic continuum to which a dispersion relation is applied for the lower cutoff frequency (line 13 of DATARUN,format 4F10.3):

1. XLCONC is the lowest cutoff frequency, in cm^{-1}, observed in either the far infrared, in Raman spectra, or estimated otherwise. This should be the value for K = 0, since dispersion is automatically computed by this program.
2. XM1 and XM2 are two factors used to calculate the dispersion of the lowest optic mode across the Brillouin zone, from the value XLCONC at K = 0 to a lower value at the zone center. Kieffer uses the masses of units (expressed in atomic mass units) believed to be involved in the low-frequency vibrations, e.g., XM1 and XM2 are atomic or cluster masses; XM1 should be the larger of the two. To use different dispersion relations, the statements for XLCONE and XLCON1 in the program can be changed. To suppress dispersion (i.e., to have a flat mode), set XM2 = 0.0, XM1 = any nonzero value.

Experimental C_p data to be used for comparison with calculated values (lines 14,15...of DATARUN, depending on number of data points): First, on line 14, read in the number of experimental data sets (T, C_p, DUMMY) to follow; format I10. Then, read in the data in format 2(3F10.3) (T in K; C_p in cal/mol-K); DUMMY is a dummy field and can be zeros.

After the experimental data or dummy data, another mineral can be added, beginning the data sequence with the mineral neumonic.

PROGRAM NOTES: OUTPUT

The program prints out all of the input data, appropriately labeled.

The temperature ranges are listed on the first page of output; this page is otherwise blank. Each mineral in a run begins on a new page. The output on these pages is as follows:

Line 1 is the label of the mineral, with a zero or nonzero indicating the choice about isotopic fractionation calculations.

Lines 2 and 3 give the molar volume (VMOLAR), the three thermal expansion parameters (labeled ALPHA0, ALPHA1 AND ALPHA2), the bulk modulus (BULK M), the temperature derivative of the bulk modulus (DBULK), the parameter CPTEST described above, and the pressure derivative of the bulk modulus (DK/DP). Units are the same as input.

Line 4 gives the six Grüeisen parameters.

Line 5 gives the pressure.

Line 6 gives the volume in cm^3, and the dilatation (0 if the pressure is 1 bar; calculated according to a Murnaghan equation of state for higher pressures; see Kieffer, 1982).

Line 7 gives the log of the ratio (18/16)**(3r/2), where r = RR is the number of oxygens in the unit cell.

Lines 8,9,10,11,12 and 13 reproduce the mineral input data in an obvious way.

Line 14 gives the input data for the lowest frequency of the first optic continuum, including the input value of frequency at K = 0 and the two dispersion constants.

Line 15 gives the calculated dispersion of frequency for this mode at $K = K_{max}$ (in cm^{-1} and in rad/sec).

Line 16 gives the radius of the Brillouin zone, in cm^{-1}.

Line 17 gives the upper limits of the three acoustic modes, in cm^{-1}.

Lines 18, 19, 20 and 21 repeat the input data in units of rad/sec.

Lines 22--26 are a table of four lines, plus a heading, giving the shape of the acoustic modes. The first column specifies the distance across the Brillouin zone, K, normalized to K_{max} and has four values: 1.0, 0.5, 0.333, and 0.25. The other three tables give the frequency of the two shear (TA1, TA2) and longitudinal (LA) acoustic branches, in rad/sec.

Line 27 gives the mean acoustic velocity (km/s) and the elastic Debye temperature (K).

Line 28 is a statement of the number of experimental values read in, and a table of their values. The table begins on the second page of output for each mineral. It lists temperature (K), C_p*, the C_p*-C_v* correction (ANENTR), and C_v* (these three in cal/mole*-K), the calculated calorimetric Debye temperature (THETA-CAL), THETA-CAL divided by the elastic Debye temperature (THETA-CAL/EL), and the temperature divided by the elastic Debye temperature (TEMP/THETAEL).

The calculated values then follow in labeled rows. INDEX is simply a counting index. TEMP is temperature in Kelvin. C_v is the calculated monatomic equivalent heat capacity at constant volume, in cal/mole*-K. Theta is the calorimetric Debye temperature for the calculated values, in K. AC, CONT, and OPTIC are, respectively, the heat capacity contributions of the three acoustic branches, all of the optic continua, and all of the Einstein oscillators. These three columns should add up to C_v in column 4. INT.ENERG is the internal energy, in cal/mole*. HELMHLTZ is the Helmholtz Free energy, G

(cal/mol*). ENRGY FN is the Gibbs energy function (G-H)/T (cal/mol-K). S-AN is the calculated C_V to C_P correction based on the input data for thermal expansion and bulk modulus. Remember that the input data are often not known below 300 K, but the program ignores that in this section. FRAC.FAC is the isotopic fractionation factor. It will be 0.0000 if no fractionation calculation is requested, and will also be 0.0000 for the O^{16} species. The calculated value will appear for the O^{18} species. The last column, gives 1/T.

The third page of output contains the information about the spectrum used for the model. The information about the acoustic branches is contained in a table. The first three columns of this table give the frequency in three forms: NU = frequency in sec^{-1}; OMEGA = circular frequency in rad/sec; W = frequency in wave numbers, cm^{-1}. The last column is density of states and can be considered to be arbitrary units. If the acoustic modes overlap any of the optic continua, the continuum is added into the density of states to give a total density of states acoustic + optic. Information about the levels of the optic continua and Einstein oscillators is contained in individual statements below the acoustic mode table. The information on this page can be used to construct schematic spectra, e.g., as in Kieffer, 1978c, 1980.

If more than one mineral is run, this output sequence will repeat, beginning with the mineral neumonic.

PROGRAM LISTING

```
C PROGRAM THERMO TO COMPUTE THERMODYNAMIC FUNCTIONS AS A FUNCTION
C  OF P AND T; ALSO TO CALCULATE ISOTOPIC FRACTIONATION FACTORS.
C
C ALL OUTPUT GOES TO FILE RESULTS.PRT
C
C PROGRAM BY SUSAN W. KIEFFER, U.S. GEOLOGICAL SURVEY, EVOLVED FROM
C  1978 TO 1985.  THIS VERSION JULY 1986 FOR U.S.G.S. OPEN FILE REPT.
C
      DIMENSION XX(200),YY(200),TEMP(200),CP(200),CV(200),THETA(200)
     1,CSUB(6),AA(20),ESUB(6),SSUB(6),FSUB(6),A(20),A0(20)
      DIMENSION AAA(3),ARAD(20),CALOR(200)
      DIMENSION DRATIO(1490),CDEBYE(1490),LAB(11)
      DIMENSION EE(200),SS(200),FF(200),EN(200),I123(12),FSTORE(200)
      DIMENSION WE(13),E0(13),E1(13),AL(13),ALB(13),XMINER(19)
      DIMENSION IPR(8),GAMMA(6)
C
C
      DATA PLANCK,BOLTZ,SPEED/6.624E-27,1.380E-16,3.000E+10/
      DATA INC/1/
      DATA PI/3.14159/
      DATA AVOG/6.022E+23/
      DATA LAB/'C1  ','C2  ','C3  ','CONT','ERFQ','ENUM','ATMS','CELL',
     1'E2','Q2','XL'/
C
C
C
C.....
C.....
C.....
 1005 FORMAT (16I5)
 1006 FORMAT (3I10)
 1020 FORMAT (I10)
 1021 FORMAT (2(3F10.3))
 1022 FORMAT (7F15.3)
 1027 FORMAT (1H0,'THERE ARE ',I5,' EXPERIMENTAL VALUES.')
 1028 FORMAT (1H0,'TEMPERATURE RANGES:'4(3X,3I7))
 1029 FORMAT (3F10.3)
 2000 FORMAT (8F10.3)
 2001 FORMAT (1H,10F9.3)
 2002 FORMAT (19A4,I4)
 2003 FORMAT (1H0,9E10.3)
 2004 FORMAT (1H ,F7.3,3F9.3,F11.3,F6.3,F9.3,2F11.3,F6.3)
 2005 FORMAT (1H ,F9.3,F6.3,F9.3,F6.3,F12.3,F9.3,F7.3,2F11.3,F9.3)
 2006 FORMAT(I5,I6,F7.3,F8.4,I6,3F8.4,F12.3,F8.4,F12.3,F8.4,F7.3,
     1F7.4,E10.3)
 2007 FORMAT (1H1)
 2008 FORMAT (1H0,' VM IS ',F10.3,' KM/S.  THETA(ELASTIC) IS ',F10.3,
     1' K.')
 2009 FORMAT (2F10.3)
 2010 FORMAT(1H0,'INDEX TEMP T/THETA   CV    THETA     AC      CONT     OPT
     1IC     INT.ENER  ENTRPY    HELMHLTZ ENRGY FN S-AN FRAC FAC   1/
     1TEMP')
 2011 FORMAT (25H  CV TOO LARGE FOR TABLE )
 2012 FORMAT (8F10.3)
 2013 FORMAT (18H  NERNST COEFF IS ,E10.3)
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```
2014 FORMAT (1H ,8F9.3)
2015 FORMAT(1HO,'V1-KM/S  V2-KM/S  V3-KM/S  FREQ-UP   FREQ-EIN1   Q1
    1    NO.ATMS   VOL-CM3  FREQ-EIN2   Q2  ')
2016 FORMAT(1HO,'       RHO      WTMOL  ATMS/MOLWT  NO.OXYGENS/CELL')
2017 FORMAT(1HO,2X,' VMOLAR',3X,'ALPHA0',4X,'ALPHA1',3X,'ALPHA2',3X,
    1'BULK M',3X,'DBULK',2X,'CPTEST',4X,'DK/DP')
2018 FORMAT(1H1,'**********************EXPERIMENTAL DATA**************
    1**********************************************')
2019 FORMAT (1HO,'    TEMPERATURE            CP             ANENTR
    1            CV          THETA-CAL      THETA-CAL/EL     TEMP/THETAEL')
2020 FORMAT (1HO, 'CUTOFF WAVENUMBERS ARE  ',  3F9.3,   '   CM-1.   ')
2021 FORMAT (1HO,'  EIN3      Q3      EIN4      Q4         CONT2    CONT2,U
    1  CONT2,Q     CONT3,L     CONT3,U    CONT3,Q')
2022 FORMAT (F20.2,F20.6)
2023 FORMAT (10I10)
2030 FORMAT (1HO,19A4,I4)
2031 FORMAT (4F10.3)
2033 FORMAT(1HO,'              K/KMAX                    TA1
    1                  TA2                      LA  (*  E+13 RAD/SEC)')
2034 FORMAT (1HO,4E20.3)
2035 FORMAT (1HO,'RADIUS OF BRILLOUIN ZONE IS ',F10.5,  '*E+08 CM-1. ')
2036 FORMAT (1HO,'CONTINUUM EXTENDS FROM',2F10.3,'  CM-1.   ')
2037 FORMAT(1HO,'    FREQ1       FREQ2       FREQ3      FREQ-UP     FREQ-EIN
    1   Q1         ATOMS/CL     VOL/UCL      FREQ-E2        Q2')
2038 FORMAT (1H ,10E11.3)
2039 FORMAT (1HO,'GEEO(CONTINUUM LEVEL) IS',E10.3,'FROM',F10.1,'TO',
    1F10.1,'CM-1.')
2040 FORMAT (1HO,'LOWEST OPTICAL MODE AT K=0 IS',F10.1,' CM-1;DISPERSIO
    1N CONSTANTS ARE ',2F8.1)
2041 FORMAT(1HO,'LOWER CONTINUUM CUTOFF IN MODEL IS',F10.1,' CM-1 OR',
    1E10.3,'  RAD/SEC.   ')
2042 FORMAT(1HO,'ANHARMONIC ENTROPY IS',E20.3,'ENTROPY UNITS PER MOLE')
2043 FORMAT (1HO,'PRESSURE IS',F8.1,3X,' KB.')
2044 FORMAT (1HO,  'PRESSURE IS',F5.1,2X,' BAR.')
2045 FORMAT (1HO,'VOLUME IS',F8.2,'  CM3.',6X,'DILATATION IS',F8.3,'.')
2046 FORMAT (1HO,  'THE GAMMAS ARE:   ',6F8.2,'.')
2050 FORMAT (1HO,'GEE1(CONTINUUM LEVEL) IS',E10.3,'FROM',F10.1,'TO',
    1F10.1,'CM-1.')
2051 FORMAT (1HO,'GEE2(CONTINUUM LEVEL) IS',E10.3,'FROM',F10.1,'TO',
    1F10.1,'CM-1.')
2052 FORMAT (1HO,'EINSTEIN OSC. FREQ. ARE',4F10.1,' CM-1.')
2053 FORMAT (1HO,'THEIR ABUNDANCES ARE ',4F10.3,'(OF TOTAL = 1.0).')
2202 FORMAT (1HO,'****SPECTRUM CALCULATION IS FINISHED!!**')
2203 FORMAT (1H1)
2206 FORMAT (1H ,'                  NU                  OMEGA
    1                    W          DENSITY OF STATES')
2207 FORMAT (1H ,2E20.3,F20.1,E20.3)
2210 FORMAT (1HO)
2211 FORMAT (1H )
2212 FORMAT(1H ,'  TEMP.       CV*     E*-E298*       S*          F*     -(F*
    1-E298*)/T    ANHARM.  S*')
2213 FORMAT(1H ,'    (K) (CAL/MOL*K)(CAL/MOL*)(CAL/MOL*K)(CAL/MOL*) (CAL
    1/MOL*K)    (CAL/MOL*K)')
2214 FORMAT (1H ,I5,F12.2,2F10.2,F13.2,F10.2,F13.2)
2215 FORMAT (1HO,19X,'(E298=',F10.2,'  CAL/MOL*)')
2216 FORMAT (1HO,'MODEL PARAMETERS  (KEY AND UNITS GIVEN IN TABLE NOTES
    1):')
2217 FORMAT(1HO,5X,'A1         A2         A3         A4         A5         A
    16         A7         A8         A9         A10     ')
2218 FORMAT (1H ,10F10.3)
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```
 2219 FORMAT (1HO,'    A11        A12        A13        A14        A15
     1 A16        A17        A18        A19        A20    ')
 2220 FORMAT (1H ,'DENSITY IS',F6.3,'  G/C.C. ')
 2221 FORMAT (1H ,'ELASTIC DEBYE TEMPERATURE IS ',F10.3,'  KM/SEC. ')
 2222 FORMAT (1HO,'LOG MASS RATIO IS',F10.4)
 2223 FORMAT (10I10)
 2224 FORMAT(1H ,'LOWEST OPTIC MODE AT K=0 IS TAKEN AS',F6.1,'  CM-1. ')
 2225 FORMAT(1H ,'WITH DISPERSION CONSTANTS TAKEN AS ATOMIC MASSES',
     1F5.1,' AND',F5.1,', THIS WAVE NUMBER DROPS TO',F8.1,' CM-1 AT KMAX
     2. ')
C
C
      OPEN (UNIT=1,FILE='DATARUN',STATUS='OLD', FORM='FORMATTED')
      OPEN (UNIT=7,FILE='RESULTS.PRT', STATUS='NEW',
     1FORM='FORMATTED')
      W=PLANCK/BOLTZ*SPEED
      PLUNCK=PLANCK*SPEED
      C19=1.986467
      AVOG3=3.0*AVOG
      PI23 = (2.0/PI)**3
      C1816=18./16.
      AVOGB=AVOG*BOLTZ*2.389E-08
C
C
      READ (1,1005) LP1,LP2,LP3,LP4,LP5,LP6,LP7,LP8,LP9,LP10
      WRITE (7,2007)
C
C PART 1: GENERATE DEBYE TABLE SO THAT THETA(CALORIMETRIC) CAN BE CALC.
C
C     GENERATE DEBYE TABLE SO THAT THETA(CALORIMETRIC) CAN BE CALCULATED.
C     TABLE RUNS FROM 0.10 TO 14.99 FOR "X"
C     INTRODUCE FAKE STHETA AND S, SO THAT THE FUNCTION DD CAN BE USED
C
C
      DO 14 J=1,1490
      S=J+9
      DRATIO(J)=S/100.0
      XL=0.005
      XU=DRATIO(J)
      CALL GG92(0,XL,XU,DUM,S,CDEBYE(J),DUM,DUM,DUM)
C                                                          LP1
                IF (LP1.NE.0) WRITE (7,2022) XU, CDEBYE(J)
   14 CONTINUE
C
C PART 2: READ INPUT TEMPERATURE AND MINERAL DATA.
C
      I123(1)=29815
      I123(2)=29815
      I123(3)=100
      READ (1,1006) (I123(I),I=4,12)
      WRITE (7,1028) I123
C
   13 CONTINUE
      READ (1,2002,END=15) XMINER  ,IFRAC
      READ (1,2023) (IPR(I),I=1,8)
      READ (1,2000) (GAMMA(IG),IG=1,6)
      READ (1,2000) (AO(I),I=1,20)
      READ (1,2000) RHOO,WTMOL,P,RR
      READ (1,2012) VMOLAR, ALPHAO,ALPHA1,ALPHA2, BULK,DBULK,CPTEST,
     1PBULK
```

```
C
      VMOLO=VMOLAR
      BULKDR=PBULK
      XPOW=3.0*RR/2.
      FCST=ALOG(C1816**XPOW)
C     DISPERSION IS ALLOWED FOR THE LOWER BOUND OF ONLY THE FOLLOWING MODE
C     IF THERE IS ONLY ONE OPTIC CONTINUUM, IT MUST GO HERE.
      READ (1,2031) XLCONC,XM1,XM2
      XLCON2=XLCONC
      XLCONE=XLCONC/((1+XM2/XM1)**0.5)
      XLCON1=XLCONE*(0.0188E+13)
      WRITE (7,2007)
      WRITE (7,2030) XMINER,IFRAC
      WRITE (7,2017)
      WRITE (7,2014) VMOLAR,ALPHA0,ALPHA1,ALPHA2,BULK,DBULK,CPTEST,
     1PBULK
      WRITE (7,2046) (GAMMA(IG),IG=1,6)
C
C     ITERATE THROUGH PRESSURE LOOP; CHANGE ALL MINRAL PARAMETERS TO
C       ACCOUNT FOR COMPRESSION.
      DO 250 INDX=1,8
      XP=IPR(INDX)
      IF (XP.EQ.0) GO TO 250
      XPX=XP/1000.0
      XM=XP*1.0E-06
C     WRITE MINERAL DATA
C
      IF (XPX.GE.1.) GO TO 251
      WRITE (7,2044) XP
      GO TO 252
  251 WRITE (7,2043) XPX
  252 CONTINUE
C     CALCULATE NEW VOLUME AND DILATATION.
      VMOL1=VMOLO/(BULKDR*XM/BULK+1.0)**(1.0/BULKDR)
      DILAT=(VMOL1/VMOLO-1.0)
      WRITE (7,2045) VMOL1,DILAT
C
C     CALCULATE AA(I) FROM A0(I)
      IF (XP.GT.1.0) GO TO 254
      DO 253 ISET=1,20
      AA(ISET)=A0(ISET)
  253 CONTINUE
      GO TO 255
  254 CONTINUE
      AA(1)=A0(1)*(1.0-(GAMMA(1)+0.3333)*DILAT)
      AA(2)=A0(2)*(1.0-(GAMMA(2)+0.3333)*DILAT)
      AA(3)=A0(3)*(1.0-(GAMMA(3)+0.3333)*DILAT)
      AA(4)=A0(4)*(VMOLO/VMOL1)**GAMMA(4)
      AA(5)=A0(5)*(VMOLO/VMOL1)**GAMMA(5)
      AA(6)=A0(6)
      AA(7)=A0(7)
      AA(8)=A0(8)/(BULKDR*XM/BULK+1.0)**(1.0/BULKDR)
      AA(9)=A0(9)*(VMOLO/VMOL1)**GAMMA(5)
      AA(10)=A0(10)
      AA(11)=A0(11)*(VMOLO/VMOL1)**GAMMA(5)
      AA(12)=A0(12)
      AA(13)=A0(13)*(VMOLO/VMOL1)**GAMMA(6)
      AA(14)=A0(14)
      AA(15)=A0(15)*(VMOLO/VMOL1)**GAMMA(4)
      AA(16)=A0(16)*(VMOLO/VMOL1)**GAMMA(4)
```

```
      AA(17)=AO(17)
      AA(18)=AO(18)*(VMOLO/VMOL1)**GAMMA(4)
      AA(19)=AO(19)*(VMOLO/VMOL1)**GAMMA(4)
      AA(20)=AO(20)
  255 CONTINUE
      RHO=RHOO*(BULKDR* XM/BULK+1.0)** (1.0/BULKDR)
      XLCON=XLCONE*(VMOLO/VMOL1)**GAMMA(4)
      XLCON3=XLCONC*(VMOLO/VMOL1)**GAMMA(4)
      XLCON4=XLCON*(0.0188E+13)
C
      WRITE (7,2222) FCST
      WRITE (7,2015)
      WRITE (7,2004) (AA(I), I=1,10)
      WRITE (7,2021)
      WRITE (7,2005) (AA(I), I=11,20)
      WRITE (7,2016)
      WRITE (7,2001) RHO, WTMOL,P,RR
      WRITE (7,2040) XLCON3,XM1,XM2
      WRITE (7,2041) XLCON, XLCON4
      IF (LP6.NE.0) WRITE (7,2223) I
      IF (IFRAC.NE.0) GO TO 286
      DO 285 I=1,200
      FSTORE(I)=0.0
  285 CONTINUE
  286 CONTINUE
C                                                                    LP7
                IF (LP7.NE.0) WRITE (7,2001) (FSTORE(IM), IM=1,50)
C
C PART 3: CALCULATION OF ACOUSTIC BRANCHES.
C
C     CONVERT ACOUSTIC VELOCITIES TO CUTOFF FREQUENCIES, IN CM-1, ASSUMING
C        SINE-WAVE DISPERSION.  CALC RADIUS OF BRILLOUIN ZONE.
C
      AA33=(AA(8)**0.3333)
      A(1)=132.31*AA(1)/AA33
      A(2)=132.31*AA(2)/AA33
      A(3)=132.31*AA(3)/AA33
      DO 16 I=4,20
   16 A(I)=AA(I)
      PI7=PI23/A(7)
      A56=A(5)*A(6)
      A910=A(9)*A(10)
      A1112=A(11)*A(12)
      A1314=A(13)*A(14)
      A76=1.0-1.0/A(7)-A(6)-A(10)-A(12)-A(14)
      RBRIL=(2.0*3.14159)*((3.0/(4.0*PI*A(8)))**0.3333)
      WRITE (7,2035) RBRIL
      WRITE (7,2020) (A(I), I=1,3)
C
C     CONVERT FREQUENCIES IN CM-1 TO FREQUENCIES IN RAD SEC-1.
      AA18=0.0188E+13
      ARAD(1)=A(1)*AA18
      ARAD(2)=A(2)*AA18
      ARAD(3)=A(3)*AA18
      ARAD(4)=A(4)*AA18
      ARAD(5)=A(5)*AA18
      ARAD(6)=A(6)
      ARAD(7)=A(7)
      ARAD(8)=A(8)
      ARAD(9)=A(9)*AA18
```

```
      ARAD(10)=A(10)
      ARAD(11)=A(11)*AA18
      ARAD(12)=A(12)
      ARAD(13)=A(13)*AA18
      ARAD(14)=A(14)
      ARAD(15)=A(15)*AA18
      ARAD(16)=A(16)*AA18
      ARAD(17)=A(17)
      ARAD(18)=A(18)*AA18
      ARAD(19)=A(19)*AA18
      ARAD(20)=A(20)
      WRITE (7,2037)
      WRITE (7,2038) (ARAD(I),I=1,10)
      WRITE (7,2021)
      WRITE (7,2038) (ARAD(I),I=11,20)
C
C                                                              LP7
            IF (LP7.NE.0) WRITE (7,2001) (FSTORE(IM),IM=1,50)
C     CALCULATE ACOUSTIC DISPERSION CURVES
C
      WRITE (7,2033)
      DO 75 I=1,4
      DISP=I
      DISPN = 1.0/DISP
      DISP=PI/(2.0*DISP)
      DO 74 J=1,3
      AAA(J) =A(J)*SIN(DISP)*(0.0188E+13)/6.28318
   74 CONTINUE
      WRITE (7,2034) DISPN,AAA(1),AAA(2),AAA(3)
   75 CONTINUE
C
C
C     COMPUTE ELASTIC DEBYE TEMPERATURE FROM AA(1),AA(2), AA(3)
C
      ACALC1=AA(1)**(-3.0)
      ACALC2=AA(2)**(-3.0)
      ACALC3=AA(3)**(-3.0)
      VM=1.4422*((ACALC1+ACALC2+ACALC3)**(-0.3333))
      STHETA=(251.45*(RHO/(WTMOL/P))**0.3333)*VM
      ST3=STHETA**3
      WRITE (7,2008) VM,STHETA
C
C
C  PART 4: READ AND WRITE EXPERIMENTAL DATA POINTS.
C     SKIP THIS SECTION IF PRESSURE IS GREATER THAN 1 BAR SO DATA NOT
C        READ OR PRINTED AGAIN.
      IF (XP.GT.1.0) GO TO 40
C
      READ (1,1020) NUM
      NUM1=NUM+1
      WRITE (7,1027) NUM
C
C     INITIALIZE TEMPERATURE,CP, AND THETA ARRAYS TO 0.0,STHETA.
C     ASSUME DATA GIVEN ARE CP; TEST THIS HYPOTHESIS BELOW.
      TEMP(1)=0.0
      CP(1)=0.0
      THETA(1)=STHETA
C*****(IF THETA IS ENTERED IN COL. 3 OR 6 ON THE DATA CARDS, IT WILL
C       BE RECALCULATED HERE.)  THEREFORE, CONSIDER THETA(K) TO BE A
C       DUMMY COLUMN.
```

```
C
      READ (1,1021) (TEMP(K),CP(K),THETA(K),K=2,NUM1)
      WRITE (7,2018)
      WRITE (7,2019)
C
C     CHANGE CP TO CV
      DO 22 I=2,NUM1
C     CALCULATE V,ALPHA AND BULK MODULUS AT TEMP OF DATA POINTS
      DT=TEMP(I)-300.0
      ALPHAT=ALPHA0+ALPHA1*TEMP(I)+ALPHA2*TEMP(I)**2
      BULKT=BULK+DBULK*DT
      VT=VMOLAR+VMOLAR*ALPHAT*DT*1E-06
      ANENTR=VT*(ALPHAT**2)*TEMP(I)*2.389E-08*BULKT/P
      CV(I)=CP(I)
      IF (DT.LE.0.0) GO TO 23
C     TEST HERE IF CV DATA READ IN
      IF (CPTEST.EQ.2222.0) GO TO 23
      CV(I)=CP(I)-ANENTR
   23 CONTINUE
   24 CONTINUE
C     CALCULATE CALORIMETRIC DEBYE TEMPERATURE FROM CV(I)
C     IF (THETA/T).LE.15,CALORIMETRIC THETA IS LOOKED UP IN TABLE  OTHERWISE
C        IS CALCULATED FROM T-CUBED RULE
      IF (THETA(1)/TEMP(I).LE.15.0) GO TO 30
C
C     IF (CV.LT.0.002) THETA IS SET EQUAL TO ELASTIC VALUE
      IF (CV(I).GT.0.002) GO TO 34
      THETA(I)=THETA(1)
      GO TO 31
   34 CONTINUE
      THETA(I)=((464.39985*TEMP(I)**3)/CV(I))**0.3333
      GO TO 31
   30 CONTINUE
      ISERCH=JNDEX(CV(I),CDEBYE,1490)
      IF (ISERCH.GE.0) GO TO 32
      ISERCH=1
      WRITE (7,2011)
   32 CONTINUE
      THETA(I)=DRATIO(ISERCH)*TEMP(I)
   31 CONTINUE
      THETAN=THETA(I)/STHETA
      TEMPN=TEMP(I)/STHETA
      WRITE (7,1022) TEMP(I), CP(I),ANENTR,CV(I),THETA(I),THETAN,TEMPN
   22 CONTINUE
   40 CONTINUE
C
C
C PART 5: BEGIN LOOP THEROUGH TEMPERATURE INCREMENTS FOR CALCULATIONS.
C                                                                  LP3
                IF (LP3.EQ.0) GO TO 76
      WRITE (7,2007)
      WRITE (7,2030) XMINER
      WRITE (7,2210)
      WRITE (7,2211)
      WRITE (7,2212)
      WRITE (7,2211)
      WRITE (7,2213)
      WRITE (7,2211)
      GO TO 77
   76 CONTINUE
```

```
      WRITE (7,2010)
   77 CONTINUE
C     INITIALIZE INDEX PARAMETERS FOR ARRAYS
      INDEX=0
C     JJJ=1=CALC FOR T=298.15,, JJJ=2=CALC FOR FIRST TEMP RANGE, JJJ=3=ETC.
      DO 8 JJJ=1,4
C
      IMP=3*(JJJ-1)
      I1=I123(IMP+1)
      I2=I123(IMP+2)
      I3=I123(IMP+3)
C
C     BEGIN CALCULATIONS FOR EACH TEMPERATURE RANGE
C
C                                                                    LP7
                IF (LP7.NE.0) WRITE (7,2001) (FSTORE(IM),IM=1,50)
      DO 2 IS=I1,I2,I3
      INDEX=INDEX+1
      S=IS
      T2=1000000./(S*S)
      IF (JJJ.EQ.1) S=S/100.0
      SRATIO=STHETA/S
      XX(INDEX)=S
C
C*****COMPUTE ACOUSTIC CONTRIBUTION
C*****COMPUTE THREE ACOUSTIC BRANCHES WITH SINE WAVE DISPERSION.
C*****FORMULAS LOOK DIFFERENT FROM THOSE PUBLISHED IN KIEFFER PAPERS
C        BECAUSE VARIABLE CHANGED TO Z = ARC SIN FREQ/FREQMAX.
C
   71 CONTINUE
      XL=0.005
      XU=PI/2.0
      DO 1 I=1,3
      CALL QG92 (1,XL,XU,A(I),S,CSUB(I),ESUB(I),FSUB(I),SSUB(I))
    1 CONTINUE
      B= 3.0*C19*PI7*(CSUB(1)+CSUB(2)+CSUB(3))
      EAC=AVOG3*PI7*(ESUB(1)+ESUB(2)+ESUB(3))
      SAC=AVOG3*PI7*(SSUB(1)+SSUB(2)+SSUB(3))
      FAC=AVOG3*PI7*S*(FSUB(1)+FSUB(2)+FSUB(3))
C
C
C*****COMPUTE CONTRIBUTIONS OF OPTIC CONTINUA.
   72 CONTINUE
      F=0.0
      ECONT=0.0
      SCONT=0.0
      FCONT=0.0
      IF (A(4).EQ.0.0) GO TO 4
      XL=XLCON
      XLOWER=XLCON*0.0188E+13
      XU=A(4)
      C=(A76-A(17)-A(20))/(XU-XL)
      DO 73 I=4,6
      IF (I.EQ.4) GO TO 725
      IF (I.EQ.6) GO TO 726
      IF (A(15).EQ.0) GO TO 73
      XL=A(15)
      XU=A(16)
      C=A(17)/(XU-XL)
      GO TO 725
```

```
  726 IF (A(18).EQ.0) GO TO 73
      XL=A(18)
      XU=A(19)
      C=A(20)/(XU-XL)
  725 CALL GG92 (2,XL,XU,DUM,S,CSUB(I),ESUB(I),FSUB(I),SSUB(I))
      F=F+3.0*C19*C*CSUB(I)
      ECONT=ECONT+AVOG3*C*ESUB(I)
      FCONT=FCONT + AVOG3*C*S*FSUB(I)
      SCONT=SCONT+AVOG3*C*SSUB(I)
   73 CONTINUE
    4 CONTINUE
C
C*****COMPUTE CONTRIBUTIONS OF EINSTEIN OSCILLATORS.
      XO=0.0
      EEIN=0.0
      SEIN=0.0
      FEIN=0.0
      IF (A(5).EQ.0.0) GO TO 209
      DO 9 IEIN=5,13,2
      IF (IEIN.EQ.7) GO TO 9
      IF (A(IEIN).EQ.0) GO TO 9
      WE (IEIN)=W*A(IEIN)/S
      IF (WE(IEIN).LT.30.0) GO TO 80
      XO=XO
      SEIN=SEIN
      FEIN=FEIN+AVOG3*A(IEIN+1)*BOLTZ*S*WE(IEIN)/2.
      EEIN=EEIN+AVOG3*PLUNCK*A(IEIN+1)*A(IEIN)/2.
      GO TO 9
   80 EO(IEIN)=EXP(WE(IEIN))
      E1(IEIN)=EO(IEIN)-1.0
      AL(IEIN)=ALOG(1.-1.0/EO(IEIN))
      ALB(IEIN)=AL(IEIN)*BOLTZ
   81 XO=XO+(EO(IEIN)*(WE(IEIN)/E1(IEIN))**2)*A(IEIN+1)
      EEIN=EEIN+AVOG3*PLUNCK*A(IEIN+1)*((A (IEIN)/E1(IEIN))+A (IEIN)/2.)
      SEIN=SEIN+AVOG3*((PLUNCK*A(IEIN)*A(IEIN+1)/(S*E1(IEIN)))-A(IEIN+1
     1)*ALB(IEIN))
      FEIN=FEIN+AVOG3*A(IEIN+1)*BOLTZ*S*(AL(IEIN)+WE(IEIN)/2.)
    9 CONTINUE
  209 CONTINUE
      XO=3.0*C19*XO
C
C*****CHANGE ERGS TO CALORIES
C
      EAC=EAC*2.3889E-08
      ECONT=ECONT*2.3889E-08
      EEIN=EEIN*2.3889E-08
      ETTAL=EAC + ECONT + EEIN
      SAC=SAC*2.3889E-08
      SCONT=SCONT*2.3889E-08
      SEIN=SEIN*2.3889E-08
      STTAL = SAC + SCONT + SEIN
      FAC=FAC*2.3889E-08
      FCONT=FCONT*2.3889E-08
      FEIN=FEIN*2.3889E-08
      FTTAL=FAC+FCONT+FEIN
      CTOTAL=B+F+XO
      YY(INDEX)=CTOTAL
C                                                              LP2
                  IF (LP2.NE.0) WRITE (7,2003) EAC,ECONT,EEIN,SAC,SCONT,
     1SEIN,FAC,FCONT,FEIN
```

```
C
C  COMPUTE CALORIMETRIC DEBYE TEMPERATURES FOR THE CALCULATED VALUES.
C
      IF (THETA(1)/S.LE.15.0) GO TO 27
      CALOR(INDEX)=S*(464.39985/CTOTAL)**0.3333
       GO TO 28
   27 CONTINUE
      JSERCH=JNDEX(YY(INDEX),CDEBYE,1490)
      IF (JSERCH.GE.0) GO TO 20
      JSERCH=1
      WRITE (7,2011)
   20 CONTINUE
      CALOR(INDEX)=DRATIO(JSERCH)*S
   28 CONTINUE
      SRATI1=1.0/SRATIO
      IF (JJJ.GT.1) GO TO 282
      E298=ETTAL
      S298=STTAL
      F298=FTTAL
      IF (IFRAC.GT.0) GO TO 282
      F29816=FTTAL
  282 CONTINUE
      ENFN=-(FTTAL-E298)/S
  284 EE(INDEX)=ETTAL
      SS(INDEX)=STTAL
      FF(INDEX)=FTTAL
      EN(INDEX)=ENFN
      IKS=S
      ICAL=CALOR(INDEX)
C   CALCULATE ANHARMONIC TERMS
      DT=S-300.0
      ALPHAT=ALPHA0+ALPHA1*S+ALPHA2*S**2
      BULKT=BULK+DBULK*DT
      VT=VMOLAR+VMOLAR*ALPHAT*DT*1.0E-06
      ANENTR=VT*(ALPHAT**2)*S*2.389E-08*BULKT/P
      A2=0.5*ANENTR*S
C                                                                    LP8
      IF (LP8.EQ.0) GO TO 290
      FTTAL=FTTAL+A2
  290 CONTINUE

C PART 6:   CALCULATE ISOTOPIC FRACTIONATION FACTORS
C
      FS3S=0.0
C                                                                    LP5
                IF (LP5.NE.0) WRITE (7,2001) FSTORE(INDEX),FTTAL
      IF (IFRAC.EQ.0) GO TO 283
      FS1=FSTORE(INDEX)-FTTAL
      IF (JJJ.GT.1) GO TO 287
      FS1=F29816-FTTAL
  287 FS1S=FS1/S
      FS2S=FS1S*A(7)/AVOGB
      FS3S=(FS2S-FCST)/RR
  283 IF (JJJ.EQ.1) GO TO 288
      FSTORE(INDEX)=FTTAL
  288 CONTINUE
      ETTALT=ETTAL-E298
C                                                                    LP3
                IF (LP3.NE.0) WRITE (7,2214) IKS,CTOTAL,ETTALT,STTAL,
     1FTTAL,ENFN,ANENTR
```

```
C                                                                    LP3
                IF (LP3.NE.0) GO TO 7
      WRITE (7,2006) INDEX, IKS, SRATI1, CTOTAL, ICAL, B, F, XO, ETTAL,
     1STTAL, FTTAL, ENFN, ANENTR, FS3S, T2
    7 CONTINUE
      IF(JJJ.EQ.1) INDEX=0
    2 CONTINUE
C                                                                    LP6
                IF (LP6.NE.0) WRITE (7,2223) JJJ, I, IS, INDEX, IEIN
C
    8 CONTINUE
C                                                                    LP3
                IF (LP3.EQ.0) GO TO 10
      WRITE (7,2215) E298
      WRITE (7,2216)
      WRITE (7,2217)
      WRITE (7,2218) (A(I), I=1,10)
      WRITE (7,2219)
      WRITE (7,2218) (A(I), I=11,20)
      WRITE (7,2224) XLCON2
      WRITE (7,2225) XM1, XM2, XLCON
      WRITE (7,2220) RHO
      WRITE (7,2221) STHETA
C
   10 CONTINUE
C
C PART 7:  COMPUTE VIBRATIONAL SPECTRUM
C
C                                                                    LP4
                IF (LP4.EQ.0) GO TO 6
      WRITE (7,2203)
      WRITE (7,2206)
C
C     COMPUTE HEIGHT OF CONTINUUM SPECTRUM
      GEE0=0.0
      GEE1=0.0
      GEE2=0.0
      IF (A(4).EQ.0) GO TO 211
      GEE0=A(7)*A76/(ARAD(4)-XLOWER)
      IF (A(16).EQ.0) GO TO 211
      GEE1=A(7)*A(17)/(ARAD(16)-ARAD(15))
      IF (A(19).EQ.0) GO TO 211
      GEE2=A(7)*A(20)/(ARAD(19)-ARAD(18))
  211 CONTINUE
      GEE0=GEE0*AVOG3
      GEE1=GEE1*AVOG3
      GEE2=GEE2*AVOG3
      PI237=PI23*P/A(7)
      IIX=ARAD(3)/2.0E12
      DO 201 IX=1,IIX
      XNU=IX*2.0E12
C     INITIALIZE ACOUSTIC TERM TO 0.0
      ACOUS=0.0
      DO 206 II=1,3
      IF(XNU.GT.ARAD(2).AND.II.LT.3) GO TO 206
      IF (XNU.GT.ARAD(1).AND.II.LT.2) GO TO 206
      TERM1=(ASIN(XNU/ARAD(II)))**2/(ARAD(II
     1)**2-XNU**2)**0.5
      ACOUS=ACOUS+TERM1
  206 CONTINUE
```

```
      SPECTR=ACOUS*AVOG3*PI237
C  TEST IF ACOUSTIC BRANCHES OVERLAP ANY OF THE OPTIC CONTINUA.
      IF (XNU.GE.XLOWER) SPECTR=SPECTR+GEE0
      IF (XNU.GE.ARAD(15)) SPECTR=SPECTR+GEE1
      IF (XNU.GE.ARAD(18)) SPECTR=SPECTR+GEE2
      XXXNU=XNU/6.28318
      XNUCM=XXXNU/SPEED
      WRITE (7,2207) XXXNU,XNU,XNUCM, SPECTR
  201 CONTINUE
  202 CONTINUE
      WRITE (7,2039) GEE0,XLCON,A(4)
      WRITE (7,2050) GEE1,A0(15),A0(16)
      WRITE (7,2051) GEE2,A0(18),A0(19)
      WRITE (7,2052) A0(5), A0(9),A0(11), A0(13)
      WRITE (7,2053) A0(6),A0(10),A0(12), A0(14)
      WRITE (7,2202)
C*****END CALCULATION OF VIBRATIONAL SPECTRUM
C
    6 CONTINUE
C                                                                    LP7
                IF (LP7.NE.0) WRITE (7,2001) (FSTORE(IM),IM=1,50)
  250 CONTINUE
      GO TO 13
   15 CONTINUE
      CLOSE (UNIT=1)
      CLOSE (UNIT=7, DISPOSE='KEEP')
      STOP
      END
C
C
      FUNCTION JNDEX(X,T,N)
C (INPUT VALUE,ARRAY TO SEARCH,ARRAY SIZE)
C FINDS INTERVAL T(I) INCLUSIVE TO T(I+1) EXCLUSIVE THAT CONTAINS X
C T(N) IS INCLUDED IN T(N-1) INTERVAL
C METHOD IS REPEATED BINOMIAL DIVISION OF TABLE
C INDEX: 0= LESS THAN TWO POINTS IN TABLE
C        -1=X OFF T(1) END OF TABLE
C        -2=X OFF T(N) END OF TABLE
C IF T MULTIVALUED AT X, RETURNS REGION WITH SLOPE OF SAME SIGN AS AVERAGE
C TEST FOR POSSIBLE BAD RETURN IS:
C     IF(INDEX.LT.1) GO TO (I>N,I<1,N<2),INDEX+3
C
      DIMENSION T(N)
      IF(N.LT.2) GO TO 880
      IF((X-T(1))*(X-T(N))) 80,881,883
80    IF(T(N).GT.T(1)) GO TO 81
C K=LOWER(MOST NEGATIVE) BOUND, KK=UPPER BOUND, J=MIDPOINT(TEST -0&-T)
      K=N
      J=1
      GO TO 82
81    K=1
      J=N
82    KK=J
83    IF(IABS(KK-K).LE.1) GO TO 85
      J=(K+KK)/2
      IF(X-T(J))82,87,84
84    K=J
      GO TO 83
85    IF(KK.GT.K) GO TO 86
      INDEX=KK
```

```
      GO TO 9
86    INDEX=K
      GO TO 9
87    INDEX=J
      GO TO 9
880   INDEX=0
      GO TO 9
881   IF(X.EQ.T(1)) GO TO 882
      INDEX=N-1
      GO TO 9
882   INDEX=1
      GO TO 9
883   IF(ABS(X-T(1)).LE.ABS(X-T(N))) GO TO 884
      INDEX=-2
      GO TO 9
884   INDEX=-1
      GO TO 9
9     JNDEX=INDEX
      RETURN
      END
C
C
C
      SUBROUTINE QG92 (K,XL,XU,A,S,G,E,F,R)
      DIMENSION QX(9),QC(9)
      DATA C1,C2,PLUNCK,W/1.38E-16,1.987E-16,1.987E-16,1.44/
      DATA QX/0.0159199,0.0819844,0.1933143,0.3378733,0.50,0.6621267,
     10.8066857,0.9180156,0.9840801/,QC/0.04063719,0.09032408,0.1303053,
     20.1561735,0.1651197,0.1561735,0.1303053,0.09032408,0.04063719/
      G=0.
      E=0.
      F=0.
      R=0.
      B=XU-XL
C     9 POINT GAUSSIAN QUADRATURE
C     K=0=DEBYE FUNCTION, 1=ACOUSTIC CONTR., =2=CONTINUUM CONTRIBUTION
C      XL,XU = X RANGE
C      A=A(I)     S=TEMPERATURE KELVIN
C     RETURN INTEGRALS
C         G=HEAT CAPACITY
C         E=INTERNAL ENERGY
C         F=HELMHOLTZ FREE ENERGY
C         R=ENTROPY
      DO 8 I=1,9
      X=XL + QX(I)*B
      C=QC(I)
      IF (K-1) 3,4,5
    3 G=G+C*1.78782E7*EXP(X)*(X**2/(EXP(X)-1.0))**2/S**3
      GO TO 8
    4 AX=A*SIN(X)
      AXS=AX/S
      WXS=W*AXS
      IF (WXS.GT.30) GO TO 10
      EW=EXP(WXS)
      EW1=EW-1.
      AL=ALOG(1.-1./EW)
      C=C*X**2
      G=G+C*(WXS/EW1)**2*EW
      E=E+C*(AX/EW1+AX/2.)
      F=F+C*C1*(AL+WXS/2.0)
```

```
      R=R+C*(C2*AXS/EW1-C1*AL)
      GO TO 8
   10 G=G
      R=R
      E=E+(C*AX/2.)
      F=F+(C*C1*WXS/2.0)
      GO TO 8
    5 WXS=W*X/S
      IF (WXS.GT.35) GO TO 11
      IF (WXS.GT.150.) GO TO 8
      EW=EXP(WXS)
      EW1=EW-1.
      AL=ALOG(1.-1./EW)
      G=G+C*WXS**2/(EW-2.+1./EW)
      E=E+C*(X/EW1+X/2.)
      F=F+C*C1*(AL+WXS/2.)
      R=R+C*(C2*X/S)/(EW1)-(C1*AL)*C
      GO TO 8
   11 R=R
      G=G
      E=E+(C*X/2.)
      F=F+(C*C1*WXS/2.)
    8 CONTINUE
      E=E*PLUNCK*B
      G=G*B
      F=F*B
      R=R*B
      RETURN
      END
```

SAMPLE DATA FILE (DATARUN.DAT)*

```
    0    0    0    1    0    0    0    0    0    0    0    0    0    0
        10         100          10
       150         500          50
       600        1200         200
FAYALITE
         1
     1.000      1.000      1.000      1.000      1.000      1.000
     3.814      3.814      5.433    196.000    900.000      0.142     28.000    308.100
   825.000      0.048                                               196.000    540.000
     0.533
     4.393    203.790      7.000     16.000
    46.390     25.860      0.005      0.000      1.098      0.000                4.000
    94.000     56.000     16.000
         2
   298.150      4.538      5.064    600.000      5.757      8.733
FORSTERITE
         1
     1.300      1.300      1.300      1.300      1.300      1.300
     4.900      4.965      8.560    620.000    930.000      0.142     28.000    290.000
   837.000      0.048

     3.210    140.6        7.000     16.000
    43.798     17.969      0.026      0.000     1.3447-0.000210      300.000      4.900
   144.000     92.000     24.000
         9
   .53.200      0.260    646.000    104.300      1.192    717.600
   155.800      2.221    776.000    196.300      2.888    815.000
   256.100      3.638    855.000    300.000      4.069    873.000
   400.000      4.696    908.000    500.000      5.077    930.000
   600.000      5.341    924.000
CALCITE (0-16)
         1
     1.           1.           1.           1.           1.           1.
     2.930        3.700        6.530      200.000    712.000        0.133     10.000    122.60
   881.000        0.067     1070.000        0.067   1460.000        0.133    200.000    325.000
     0.200      300.000      387.000        0.100
     2.712      100.091        5.000        6.000
    36.940        4.285        0.030        0.000        0.747        0.000    300.000      4.
    99.000       60.000       40.000
        22
    20.000        0.078      363.200       25.000        0.154      361.500
    30.000        0.250      368.400       35.000        0.360      380.100
    40.000        0.468      390.400       50.000        0.746      416.500
    60.000        1.006      444.000       70.000        1.262      469.000
    80.000        1.498      495.200       95.700        1.788      540.700
   118.600        2.220      591.800      141.500        2.546      645.200
   159.700        2.768      685.100      180.000        2.984      727.200
   196.500        3.170      752.600      209.200        3.266      780.300
   227.400        3.336      830.000      241.900        3.406      866.000
   261.000        3.666      863.900      272.500        3.774      872.000
   279.800        3.808      887.000      294.300        3.886      909.400
CALCITE (0-18)                                                                  1
         1
     1.           1.           1.           1.           1.           1.
2.845941     3.593850     6.342660      188.600    674.690        0.133     10.000    122.600
   871.130        0.067     1008.670        0.067   1436.150        0.133    196.452    319.2345
     0.200      291.000      375.390        0.100
2.874572     106.091          5.000        6.000
    36.940        3.766        0.028        0.000        0.797        0.000    300.000      4.
    93.357       60.000       40.000
         2
   279.800        3.808      887.000      294.300        3.886      909.400
QUARTZ (SEE TABLE NOTES RE DIFFERENCES FROM MODEL IN PAPER 3)  0-16
         1           10         1000      1000000
     0.023        0.023        1.180        0.703        0.850        0.850
     3.761        4.463        6.024      550.000    1200.000        0.074      9.000    113.000
  1162.000        0.037     1117.000        0.074   1080.000        0.037    697.000    809.000
     0.1852
     2.650       60.000        3.000        6.000
    22.700      -32.176        0.173        0.000        0.377-0.0001000     2222.000      6.400
   128.000       16.000       16.000
         2
   300.000        3.544     1032.000      400.000        4.197     1120.000
```

*DATARUN.DAT is called by the program. Results go into RESULT.PRT.

OUTPUT FROM RUN WITH SAMPLE DATA FILE

```
TEMPERATURE RANGES:
  29815  29815    100
     10    100     10
    100     10    150
    500     50    600
   1200    200
```

FAYALITE 0

VMOLAR	ALPHA0	ALPHA1	ALPHA2	BULK M	DBULK	CPTEST	DK/DP
46.390	25.860	0.005	0.000	1.098	0.000	0.000	4.000

THE GAMMAS ARE: 1.00 1.00 1.00 1.00 1.00 1.00.

PRESSURE IS 1.0 BAR.

VOLUME IS 46.39 CM3. DILATATION IS 0.000.

LOG MASS RATIO IS 2.8268

V1-KM/S	V2-KM/S	V3-KM/S	FREQ-UP	FREQ-EIN1	Q1	NO.ATMS	VOL-CM3	FREQ-EIN2	Q2
3.814	3.814	5.433	196.000	900.000	0.142	28.000	308.100	825.000	0.048

EIN3	Q3	EIN4	Q4	CONT2	CONT2,U	CONT2,Q	CONT3,L	CONT3,U	CONT3,Q
0.000	0.000	0.000	0.000	196.000	540.000	0.533	0.000	0.000	0.000

RHO	WTMOL	ATMS/MOLWT	NO.OXYGENS/CELL
4.393	203.790	7.000	16.000

LOWEST OPTICAL MODE AT K=0 IS 94.0 CM-1; DISPERSION CONSTANTS ARE 56.0 16.0

LOWER CONTINUUM CUTOFF IN MODEL IS 82.9 CM-1 OR 0.156E+14 RAD/SEC.

RADIUS OF BRILLOUIN ZONE IS 0.57724*E+08 CM-1.

CUTOFF WAVENUMBERS ARE 74.730 74.730 106.451 CM-1.

FREQ1	FREQ2	FREQ3	FREQ-UP	FREQ-E	Q1	ATOMS/CL	VOL/UCL	FREQ-E2	Q2
0.140E+14	0.140E+14	0.200E+14	0.368E+14	0.169E+15	0.142E+00	0.280E+02	0.308E+03	0.155E+15	0.480E-01

EIN3	Q3	EIN4	Q4	CONT2	CONT2,U	CONT2,Q	CONT3,L	CONT3,U	CONT3,Q
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.368E+14	0.102E+15	0.533E+00	0.000E+00	0.000E+00	0.000E+00

K/KMAX	TA1	TA2	LA (* E+13 RAD/SEC)
0.100E+01	0.224E+13	0.224E+13	0.319E+13
0.500E+00	0.158E+13	0.158E+13	0.225E+13
0.333E+00	0.112E+13	0.112E+13	0.159E+13
0.250E+00	0.856E+12	0.856E+12	0.122E+13

VM IS 4.139 KM/S. THETA(ELASTIC) IS 554.147 K.

THERE ARE 2 EXPERIMENTAL VALUES.

**********EXPERIMENTAL DATA**********

TEMPERATURE	CP	ANENTR	CV	THETA-CAL	THETA-CAL/EL	TEMP/THETAEL
298.150	4.538	0.039	4.538	715.560	1.291	0.538
600.000	5.757	0.088	5.669	600.000	1.083	1.083

INDEX	TEMP	T/THETA	CV	THETA	AC	CONT	OPTIC	INT. ENER	ENTRPY	HELMHLTZ	ENRGY FN	S-AN FRAC FAC	1/TEMP
1	298	0.538	4.3319	778	0.2104	3.8213	0.3002	2444.753	4.4760	1110.346	4.4756	0.039 0.0000	0.112E-02
1	10	0.018	0.0037	501	0.0036	0.0001	0.0000	1714.674	0.0011	1714.764	72.9989	0.001 0.0000	0.100E+05
2	20	0.036	0.0585	398	0.0361	0.0224	0.0000	1714.905	0.0151	1714.704	36.5024	0.002 0.0000	0.250E+04
3	30	0.054	0.2122	389	0.0832	0.1290	0.0000	1716.185	0.0649	1714.340	24.3471	0.004 0.0000	0.111E+04
4	40	0.072	0.4277	407	0.1201	0.3076	0.0000	1719.350	0.1544	1713.273	18.2870	0.005 0.0000	0.625E+03
5	50	0.090	0.6666	433	0.1453	0.5213	0.0000	1724.809	0.2752	1711.147	14.6721	0.006 0.0000	0.400E+03
6	60	0.108	0.9099	460	0.1622	0.7478	0.0000	1732.686	0.4182	1707.695	12.2843	0.007 0.0000	0.278E+03
7	70	0.126	1.1502	487	0.1737	0.9764	0.0000	1742.983	0.5765	1702.731	10.6003	0.008 0.0000	0.204E+03
8	80	0.144	1.3843	512	0.1819	1.2023	0.0000	1755.653	0.7453	1696.129	9.3578	0.010 0.0000	0.156E+03
9	90	0.162	1.6106	534	0.1878	1.4226	0.0002	1770.624	0.9214	1687.801	8.4106	0.011 0.0000	0.123E+03
10	100	0.180	1.8280	556	0.1922	1.6351	0.0006	1787.813	1.1023	1677.685	7.6707	0.012 0.0000	0.100E+03
11	150	0.271	2.7585	640	0.2033	2.5375	0.0177	1903.503	2.0277	1599.443	5.6354	0.018 0.0000	0.444E+02
12	200	0.361	3.4460	702	0.2074	3.1572	0.0814	2059.381	2.9199	1475.499	4.8463	0.025 0.0000	0.250E+02
13	250	0.451	3.9573	747	0.2093	3.5623	0.1857	2244.939	3.7460	1308.551	4.5448	0.032 0.0000	0.160E+02
14	300	0.541	4.3444	780	0.2104	3.8294	0.3046	2452.772	4.5028	1102.041	4.4757	0.039 0.0000	0.111E+02
15	350	0.632	4.6408	801	0.2110	4.0107	0.4191	2677.570	5.1953	859.322	4.5298	0.046 0.0000	0.816E+01
16	400	0.722	4.8699	820	0.2115	4.1377	0.5207	2915.414	5.8302	583.446	4.6533	0.054 0.0000	0.625E+01
17	450	0.812	5.0485	832	0.2117	4.2295	0.6072	3163.382	6.4141	277.125	4.8170	0.062 0.0000	0.494E+01
18	500	0.902	5.1894	840	0.2120	4.2977	0.6797	3419.288	6.9533	-57.251	5.0040	0.070 0.0000	0.400E+01
19	600	1.083	5.3922	852	0.2122	4.3898	0.7902	3948.729	7.9181	-802.008	5.4113	0.088 0.0000	0.278E+01
20	800	1.444	5.6198	872	0.2125	4.4853	0.9219	5051.952	9.5035	-2550.743	6.2444	0.126 0.0000	0.156E+01
21	1000	1.805	5.7353	870	0.2126	4.5309	0.9918	6187.844	10.7704	-4582.493	7.0272	0.169 0.0000	0.100E+01
22	1200	2.165	5.8011	876	0.2127	4.5561	1.0324	7341.254	11.8218	-6844.791	7.7413	0.218 0.0000	0.694E+00

NU	OMEGA	W	DENSITY OF STATES
0.318E+12	0.200E+13	10.6	0.401E+09
0.637E+12	0.400E+13	21.2	0.168E+10
0.955E+12	0.600E+13	31.8	0.414E+10
0.127E+13	0.800E+13	42.4	0.848E+10
0.159E+13	0.100E+14	53.1	0.167E+11
0.191E+13	0.120E+14	63.7	0.365E+11
0.223E+13	0.140E+14	74.3	0.444E+12
0.255E+13	0.160E+14	84.9	0.185E+13
0.286E+13	0.180E+14	95.5	0.186E+13
0.318E+13	0.200E+14	106.1	0.222E+13

GEE0(CONTINUUM LEVEL) IS 0.184E+13FROM 82.9TO 196.0CM-1.

GEE1(CONTINUUM LEVEL) IS 0.417E+12FROM 196.0TO 540.0CM-1.

GEE2(CONTINUUM LEVEL) IS 0.000E+00FROM 0.0TO 0.0CM-1.

EINSTEIN OSC. FREQ. ARE 900.0 825.0 0.0 0.0 CM-1.

THEIR ABUNDANCES ARE 0.142 0.048 0.000 0.000(OF TOTAL = 1.0).

****SPECTRUM CALCULATION IS FINISHED!!**

FORSTERITE 0

VMOLAR	ALPHA0	ALPHA1	ALPHA2	BULK M	DBULK	CPTEST	DK/DP
43.798	17.969	0.026	0.000	1.345	0.000	300.000	4.900

THE GAMMAS ARE: 1.30 1.30 1.30 1.30 1.30 1.30.

PRESSURE IS 1.0 BAR.

VOLUME IS 43.80 CM3. DILATATION IS 0.000.

LOG MASS RATIO IS 2.8268

V1-KM/S	V2-KM/S	V3-KM/S	FREQ-UP	FREQ-EIN1	G1	NO. ATMS	VOL-CM3	FREQ-EIN2	G2
4.900	4.965	8.560	620.000	930.000	0.142	28.000	290.000	837.000	0.048

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

RHO	WTMOL	ATMS/MOLWT	NO. OXYGENS/CELL
3.210	140.600	7.000	16.000

LOWEST OPTICAL MODE AT K=0 IS 144.0 CM-1; DISPERSION CONSTANTS ARE 92.0 24.0

LOWER CONTINUUM CUTOFF IN MODEL IS 128.2 CM-1 OR 0.241E+14 RAD/SEC.

RADIUS OF BRILLOUIN ZONE IS 0.98901*E+08 CM-1.

CUTOFF WAVENUMBERS ARE 97.965 99.265 171.139 CM-1.

FREQ1	FREQ2	FREQ3	FREQ-UP	FREQ-E	G1	ATOMS/CL	VOL/UCL	FREQ-E2	G2
0.184E+14	0.187E+14	0.322E+14	0.117E+15	0.175E+15	0.142E+00	0.280E+02	0.290E+03	0.157E+15	0.480E-01

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00

K/KMAX	TA1	TA2	LA (* E+13 RAD/SEC)
0.100E+01	0.293E+13	0.297E+13	0.512E+13
0.500E+00	0.207E+13	0.210E+13	0.362E+13
0.333E+00	0.147E+13	0.149E+13	0.256E+13
0.250E+00	0.112E+13	0.114E+13	0.196E+13

VM IS 5.476 KM/S. THETA(ELASTIC) IS 747.220 K.

THERE ARE 9 EXPERIMENTAL VALUES.

**********EXPERIMENTAL DATA**********

TEMPERATURE	CP	ANENTR	CV	THETA-CAL	THETA-CAL/EL	TEMP/THETAEL
53.200	0.260	0.004	0.260	643.720	0.861	0.071
104.300	1.192	0.009	1.192	714.455	0.956	0.140
155.800	2.221	0.015	2.221	772.768	1.034	0.209
196.300	2.888	0.021	2.888	808.756	1.082	0.263
256.100	3.638	0.031	3.638	847.691	1.134	0.343
300.000	4.069	0.040	4.069	861.000	1.152	0.401
400.000	4.696	0.064	4.632	920.000	1.231	0.535
500.000	5.077	0.094	4.983	960.000	1.285	0.669
600.000	5.341	0.131	5.210	996.000	1.333	0.803

INDEX	TEMP	T/THETA	CV	THETA	AC	CONT	OPTIC	INT. ENER	ENTRPY	HELMHLTZ	ENRGY FN	S-AN FRAC FAC	1/TEMP
1	298	0.399	3.9763	885	0.2075	3.4882	0.2806	2591.589	3.3475	1593.663	3.3471	0.040 0.0000	0.112E-02
1	10	0.013	0.0013	716	0.0013	0.0000	0.0000	1997.249	0.0004	1997.372	59.4217	0.001 0.0000	0.100E+05
2	20	0.027	0.0162	611	0.0149	0.0013	0.0000	1997.315	0.0044	1997.354	29.7118	0.001 0.0000	0.250E+04
3	30	0.040	0.0669	572	0.0452	0.0217	0.0000	1997.694	0.0191	1997.249	19.8114	0.002 0.0000	0.111E+04
4	40	0.054	0.1620	568	0.0775	0.0845	0.0000	1998.802	0.0503	1996.917	14.8668	0.003 0.0000	0.625E+03
5	50	0.067	0.2951	579	0.1047	0.1904	0.0000	2001.059	0.1001	1996.180	11.9082	0.004 0.0000	0.400E+03
6	60	0.080	0.4549	598	0.1261	0.3287	0.0000	2004.789	0.1677	1994.855	9.9456	0.005 0.0000	0.278E+03
7	70	0.094	0.6318	619	0.1426	0.4891	0.0000	2010.207	0.2509	1992.774	8.5545	0.006 0.0000	0.204E+03
8	80	0.107	0.8192	640	0.1552	0.6639	0.0000	2017.450	0.3473	1989.793	7.5225	0.007 0.0000	0.156E+03
9	90	0.120	1.0125	661	0.1650	0.8474	0.0001	2026.599	0.4548	1985.790	6.7311	0.008 0.0000	0.123E+03
10	100	0.134	1.2082	681	0.1726	1.0352	0.0005	2037.695	0.5716	1980.665	6.1092	0.009 0.0000	0.100E+03
11	150	0.201	2.1432	760	0.1932	1.9350	0.0149	2121.917	1.2418	1935.781	4.3721	0.015 0.0000	0.444E+02
12	200	0.268	2.9181	818	0.2014	2.6445	0.0722	2249.104	1.9682	1855.586	3.6800	0.022 0.0000	0.250E+02
13	250	0.335	3.5240	857	0.2054	3.1486	0.1701	2410.689	2.6869	1739.096	3.4100	0.030 0.0000	0.160E+02
14	300	0.401	3.9915	885	0.2076	3.4990	0.2849	2598.955	3.3721	1587.447	3.3471	0.040 0.0000	0.111E+02
15	350	0.468	4.3519	906	0.2090	3.7451	0.3978	2807.781	4.0152	1402.571	3.3972	0.051 0.0000	0.816E+01
16	400	0.535	4.6309	920	0.2099	3.9217	0.4993	3032.486	4.6150	1186.625	3.5124	0.064 0.0000	0.625E+01
17	450	0.602	4.8487	931	0.2105	4.0513	0.5869	3269.530	5.1731	941.743	3.6663	0.078 0.0000	0.494E+01
18	500	0.669	5.0204	940	0.2109	4.1488	0.6607	3516.251	5.6929	669.925	3.8433	0.094 0.0000	0.400E+01
19	600	0.803	5.2678	954	0.2115	4.2820	0.7743	4031.189	6.6311	52.644	4.2316	0.131 0.0000	0.278E+01
20	800	1.071	5.5452	960	0.2121	4.4221	0.9111	5115.136	8.1885	-1435.516	5.0339	0.227 0.0000	0.156E+01
21	1000	1.338	5.6861	970	0.2124	4.4896	0.9841	6238.918	9.4418	-3202.751	5.7943	0.357 0.0000	0.100E+01
22	1200	1.606	5.7664	972	0.2125	4.5271	1.0268	7384.062	10.4856	-5198.490	6.4917	0.523 0.0000	0.694E+00

NU	OMEGA	W	DENSITY OF STATES
0.318E+12	0.200E+13	10.6	0.162E+09
0.637E+12	0.400E+13	21.2	0.666E+09
0.955E+12	0.600E+13	31.8	0.157E+10
0.127E+13	0.800E+13	42.4	0.301E+10
0.159E+13	0.100E+14	53.1	0.523E+10
0.191E+13	0.120E+14	63.7	0.875E+10
0.223E+13	0.140E+14	74.3	0.149E+11
0.255E+13	0.160E+14	84.9	0.282E+11
0.286E+13	0.180E+14	95.5	0.968E+11
0.318E+13	0.200E+14	106.1	0.208E+10
0.350E+13	0.220E+14	116.7	0.281E+10
0.382E+13	0.240E+14	127.3	0.385E+10
0.414E+13	0.260E+14	137.9	0.429E+12
0.446E+13	0.280E+14	148.5	0.432E+12
0.477E+13	0.300E+14	159.2	0.438E+12
0.509E+13	0.320E+14	169.8	0.499E+12

GEE0(CONTINUUM LEVEL) IS 0.424E+12FROM 128.2TO 620.0CM-1.

GEE1(CONTINUUM LEVEL) IS 0.000E+00FROM 0.0TO 0.0CM-1.

GEE2(CONTINUUM LEVEL) IS 0.000E+00FROM 0.0TO 0.0CM-1.

EINSTEIN OSC. FREQ. ARE 930.0 837.0 0.0 0.0 CM-1.

THEIR ABUNDANCES ARE 0.142 0.048 0.000 0.000(OF TOTAL = 1.0).

****SPECTRUM CALCULATION IS FINISHED!!**

CALCITE (O-16) 0

VMOLAR	ALPHA0	ALPHA1	ALPHA2	BULK M	DBULK	CPTEST	DK/DP
36.940	4.285	0.030	0.000	0.747	0.000	300.000	4.000

THE GAMMAS ARE: 1.00 1.00 1.00 1.00 1.00 1.00.

PRESSURE IS 1.0 BAR.

VOLUME IS 36.94 CM3. DILATATION IS 0.000.

LOG MASS RATIO IS 1.0600

V1-KM/S	V2-KM/S	V3-KM/S	FREQ-UP	FREQ-EIN1	Q1	NO. ATMS	VOL-CM3	FREQ-EIN2	Q2
2.930	3.700	6.530	200.000	712.000	0.133	10.000	122.600	881.000	0.067

EIN3	Q3	EIN4	Q4	CONT2	CONT2,U	CONT2,Q	CONT3,L	CONT3,U	CONT3,Q
1070.000	0.067	1460.000	0.133	200.000	325.000	0.200	300.000	387.000	0.100

RHO	WTMOL	ATMS/MOLWT	NO. OXYGENS/CELL
2.712	100.091	5.000	6.000

LOWEST OPTICAL MODE AT K=0 IS 99.0 CM-1; DISPERSION CONSTANTS ARE 60.0 40.0

LOWER CONTINUUM CUTOFF IN MODEL IS 76.7 CM-1 OR 0.144E+14 RAD/SEC.

RADIUS OF BRILLOUIN ZONE IS 0.78477*E+08 CM-1.

CUTOFF WAVENUMBERS ARE 78.049 98.560 173.945 CM-1.

FREQ1	FREQ2	FREQ3	FREQ-UP	FREQ-E	Q1	ATOMS/CL	VOL/UCL	FREQ-E2	Q2
0.147E+14	0.185E+14	0.327E+14	0.376E+14	0.134E+15	0.133E+00	0.100E+02	0.123E+03	0.166E+15	0.670E-01

EIN3	Q3	EIN4	Q4	CONT2	CONT2,U	CONT2,Q	CONT3,L	CONT3,U	CONT3,Q
0.201E+15	0.670E-01	0.274E+15	0.133E+00	0.376E+14	0.611E+14	0.200E+00	0.564E+14	0.728E+14	0.100E+00

K/KMAX	TA1	TA2	LA (* E+13 RAD/SEC)
0.100E+01	0.234E+13	0.295E+13	0.520E+13
0.500E+00	0.165E+13	0.209E+13	0.368E+13
0.333E+00	0.117E+13	0.147E+13	0.260E+13
0.250E+00	0.894E+12	0.113E+13	0.199E+13

VM IS 3.622 KM/S. THETA(ELASTIC) IS 467.846 K.

THERE ARE 22 EXPERIMENTAL VALUES.

**********EXPERIMENTAL DATA**********

TEMPERATURE	CP	ANENTR	CV	THETA-CAL	THETA-CAL/EL	TEMP/THETAEL
20.000	0.078	0.000	0.078	362.276	0.774	0.043
25.000	0.154	0.000	0.154	360.973	0.772	0.053
30.000	0.250	0.000	0.250	368.566	0.788	0.064
35.000	0.360	0.000	0.360	378.700	0.809	0.075
40.000	0.468	0.000	0.468	394.800	0.844	0.085
50.000	0.746	0.000	0.746	415.500	0.888	0.107
60.000	1.006	0.000	1.006	442.200	0.945	0.128
70.000	1.262	0.000	1.262	467.600	0.999	0.150
80.000	1.498	0.000	1.498	492.800	1.053	0.171
95.700	1.788	0.001	1.788	538.791	1.152	0.205
118.600	2.220	0.001	2.220	588.256	1.257	0.254
141.500	2.546	0.001	2.546	640.995	1.370	0.302
159.700	2.768	0.002	2.768	680.322	1.454	0.341
180.000	2.984	0.002	2.984	721.800	1.543	0.385
196.500	3.170	0.003	3.170	746.700	1.596	0.420
209.200	3.266	0.003	3.266	774.040	1.654	0.447
227.400	3.336	0.004	3.336	825.462	1.764	0.486
241.900	3.406	0.004	3.406	858.745	1.836	0.517
261.000	3.666	0.005	3.666	856.080	1.830	0.558
272.500	3.774	0.006	3.774	863.825	1.846	0.582
279.800	3.808	0.006	3.808	878.572	1.878	0.598
294.300	3.886	0.007	3.886	900.558	1.925	0.629

INDEX	TEMP	T/THETA	CV	THETA	AC	CONT	OPTIC	INT.ENER	ENTRPY	HELMHLTZ	ENRGY FN	S-AN FRAC	FAC	1/TEMP
1	298	0.637	3.7688	948	0.5820	2.6644	0.5224	3008.220	4.3249	1718.813	4.3247	0.007	0.0000	0.112E-02
1	10	0.021	0.0058	431	0.0056	0.0002	0.0000	2334.595	0.0017	2334.632	67.3588	0.000	0.0000	0.100E+05
2	20	0.043	0.0840	353	0.0605	0.0235	0.0000	2334.938	0.0225	2334.542	33.6839	0.000	0.0000	0.250E+04
3	30	0.064	0.2738	357	0.1552	0.1186	0.0000	2336.659	0.0897	2334.021	22.4733	0.000	0.0000	0.111E+04
4	40	0.085	0.5132	382	0.2437	0.2695	0.0000	2340.570	0.2006	2332.601	16.8905	0.000	0.0000	0.625E+03
5	50	0.107	0.7651	411	0.3150	0.4501	0.0000	2346.955	0.3420	2329.908	13.5662	0.000	0.0000	0.400E+03
6	60	0.128	1.0147	440	0.3703	0.6444	0.0000	2355.853	0.5036	2325.693	11.3754	0.000	0.0000	0.278E+03
7	70	0.150	1.2544	469	0.4127	0.8416	0.0001	2367.201	0.6780	2319.793	9.8347	0.000	0.0000	0.204E+03
8	80	0.171	1.4796	496	0.4454	1.0339	0.0004	2380.876	0.8603	2312.106	8.7014	0.000	0.0000	0.156E+03
9	90	0.192	1.6876	522	0.4706	1.2158	0.0012	2396.716	1.0466	2302.573	7.8405	0.001	0.0000	0.123E+03
10	100	0.214	1.8776	548	0.4904	1.3840	0.0032	2414.544	1.2343	2291.168	7.1705	0.001	0.0000	0.100E+03
11	150	0.321	2.5967	670	0.5442	2.0050	0.0476	2527.709	2.1422	2206.432	5.3453	0.002	0.0000	0.444E+02
12	200	0.427	3.0831	780	0.5657	2.3508	0.1666	2670.225	2.9589	2078.500	4.6486	0.003	0.0000	0.250E+02
13	250	0.534	3.4623	872	0.5762	2.5482	0.3378	2834.063	3.6886	1911.979	4.3850	0.005	0.0000	0.160E+02
14	300	0.641	3.7796	951	0.5821	2.6679	0.5296	3015.198	4.3482	1710.790	4.3248	0.007	0.0000	0.111E+02
15	350	0.748	4.0518	1011	0.5857	2.7449	0.7211	3211.016	4.9514	1478.075	4.3718	0.010	0.0000	0.816E+01
16	400	0.855	4.2864	1064	0.5881	2.7970	0.9013	3419.472	5.5078	1216.404	4.4795	0.014	0.0000	0.625E+01
17	450	0.962	4.4886	1102	0.5897	2.8337	1.0652	3638.824	6.0243	927.934	4.6229	0.019	0.0000	0.494E+01
18	500	1.069	4.6625	1135	0.5909	2.8605	1.2111	3867.555	6.5062	614.524	4.7874	0.025	0.0000	0.400E+01
19	600	1.282	4.9401	1182	0.5924	2.8960	1.4516	4348.059	7.3815	-80.796	5.1484	0.040	0.0000	0.278E+01
20	800	1.710	5.2988	1240	0.5940	2.9321	1.7727	5374.717	8.8559	-1709.937	5.8977	0.086	0.0000	0.156E+01
21	1000	2.137	5.5045	1270	0.5947	2.9491	1.9607	6456.101	10.0616	-3605.467	6.6137	0.159	0.0000	0.100E+01
22	1200	2.565	5.6298	1284	0.5951	2.9584	2.0764	7569.748	11.0765	-5722.048	7.2752	0.266	0.0000	0.694E+00

NU	OMEGA	W	DENSITY OF STATES
0.318E+12	0.200E+13	10.6	0.474E+09
0.637E+12	0.400E+13	21.2	0.198E+10
0.955E+12	0.600E+13	31.8	0.478E+10
0.127E+13	0.800E+13	42.4	0.953E+10
0.159E+13	0.100E+14	53.1	0.178E+11
0.191E+13	0.120E+14	63.7	0.346E+11
0.223E+13	0.140E+14	74.3	0.101E+12
0.255E+13	0.160E+14	84.9	0.419E+12
0.286E+13	0.180E+14	95.5	0.486E+12
0.318E+13	0.200E+14	106.1	0.394E+12
0.350E+13	0.220E+14	116.7	0.395E+12
0.382E+13	0.240E+14	127.3	0.397E+12
0.414E+13	0.260E+14	137.9	0.400E+12
0.446E+13	0.280E+14	148.5	0.404E+12
0.477E+13	0.300E+14	159.2	0.414E+12
0.509E+13	0.320E+14	169.8	0.454E+12

GEE0(CONTINUUM LEVEL) IS 0.390E+12FROM 76.7TO 200.0CM-1.

GEE1(CONTINUUM LEVEL) IS 0.154E+12FROM 200.0TO 325.0CM-1.

GEE2(CONTINUUM LEVEL) IS 0.110E+12FROM 300.0TO 387.0CM-1.

EINSTEIN OSC. FREQ. ARE 712.0 881.0 1070.0 1460.0 CM-1.

THEIR ABUNDANCES ARE 0.133 0.067 0.067 0.133(OF TOTAL = 1.0).

****SPECTRUM CALCULATION IS FINISHED!!**

CALCITE (O-18) 1

VMOLAR	ALPHA0	ALPHA1	ALPHA2	BULK M	DBULK	CPTEST	DK/DP
36.940	3.766	0.028	0.000	0.797	0.000	300.000	4.000

THE GAMMAS ARE: 1.00 1.00 1.00 1.00 1.00 1.00.

PRESSURE IS 1.0 BAR.

VOLUME IS 36.94 CM3. DILATATION IS 0.000.

LOG MASS RATIO IS 1.0600

V1-KM/S	V2-KM/S	V3-KM/S	FREQ-UP	FREQ-EIN1	G1	NO.ATMS	VOL-CM3	FREQ-EIN2	G2
2.846	3.594	6.343	188.600	674.690	0.133	10.000	122.600	871.130	0.067

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
1008.670	0.067	1436.150	0.133	196.452	319.234	0.200	291.000	375.390	0.100

RHO	WTMOL	ATMS/MOLWT	NO.OXYGENS/CELL
2.875	106.091	5.000	6.000

LOWEST OPTICAL MODE AT K=0 IS 93.4 CM-1; DISPERSION CONSTANTS ARE 60.0 40.0

LOWER CONTINUUM CUTOFF IN MODEL IS 72.3 CM-1 OR 0.136E+14 RAD/SEC.

RADIUS OF BRILLOUIN ZONE IS 0.78477*E+08 CM-1.

CUTOFF WAVENUMBERS ARE 75.810 95.732 168.959 CM-1.

FREQ1	FREQ2	FREQ3	FREQ-UP	FREQ-E	G1	ATOMS/CL	VOL/UCL	FREQ-E2	G2
0.143E+14	0.180E+14	0.318E+14	0.359E+14	0.127E+15	0.133E+00	0.100E+02	0.123E+03	0.164E+15	0.670E-01

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
0.190E+15	0.670E-01	0.270E+15	0.133E+00	0.369E+14	0.600E+14	0.200E+00	0.547E+14	0.706E+14	0.100E+00

K/KMAX	TA1	TA2	LA (* E+13 RAD/SEC)
0.100E+01	0.227E+13	0.286E+13	0.506E+13
0.500E+00	0.160E+13	0.203E+13	0.357E+13
0.333E+00	0.113E+13	0.143E+13	0.253E+13
0.250E+00	0.868E+12	0.110E+13	0.193E+13

VM IS 3.519 KM/S. THETA(ELASTIC) IS 454.425 K.

THERE ARE 2 EXPERIMENTAL VALUES.

**********EXPERIMENTAL DATA**********

TEMPERATURE	CP	ANENTR	CV	THETA-CAL	THETA-CAL/EL	TEMP/THETAEL
279.800	3.808	0.005	3.808	878.572	1.933	0.616
294.300	3.886	0.006	3.886	900.558	1.982	0.648

INDEX	TEMP	T/THETA	CV	THETA	AC	CONT	OPTIC	INT. ENER	ENTRPY	HELMHLTZ	ENRGY FN	S-AN FRAC FAC	1/TEMP
1	298	0.656	3.8323	927	0.5827	2.6804	0.5692	2952.490	4.4663	1620.923	4.4661	0.006 0.0989	0.112E-02
1	10	0.022	0.0065	414	0.0063	0.0003	0.0000	2262.815	0.0019	2262.848	68.9642	0.000 5.8495	0.100E+05
2	20	0.044	0.0966	337	0.0657	0.0310	0.0000	2263.211	0.0259	2262.745	34.4873	0.000 2.8369	0.250E+04
3	30	0.066	0.3056	344	0.1637	0.1420	0.0000	2265.155	0.1019	2262.150	23.0113	0.000 1.8345	0.111E+04
4	40	0.088	0.5599	370	0.2530	0.3068	0.0000	2269.464	0.2241	2260.552	17.2985	0.000 1.3354	0.625E+03
5	50	0.110	0.8207	400	0.3241	0.4966	0.0000	2276.364	0.3770	2257.566	13.8985	0.000 1.0379	0.400E+03
6	60	0.132	1.0748	430	0.3787	0.6961	0.0000	2285.843	0.5491	2252.947	11.6590	0.000 0.8411	0.278E+03
7	70	0.154	1.3163	458	0.4202	0.8959	0.0001	2297.802	0.7330	2246.544	10.0849	0.000 0.7018	0.204E+03
8	80	0.176	1.5416	485	0.4519	1.0890	0.0006	2312.095	0.9235	2238.264	8.9278	0.000 0.5982	0.156E+03
9	90	0.198	1.7487	512	0.4763	1.2704	0.0020	2328.550	1.1171	2228.061	8.0492	0.000 0.5183	0.123E+03
10	100	0.220	1.9374	538	0.4954	1.4372	0.0048	2346.983	1.3112	2215.919	7.3657	0.001 0.4550	0.100E+03
11	150	0.330	2.6530	660	0.5468	2.0459	0.0603	2463.016	2.2424	2126.711	5.5052	0.001 0.2695	0.444E+02
12	200	0.440	3.1423	766	0.5673	2.3801	0.1949	2608.406	3.0756	1993.342	4.7957	0.002 0.1808	0.250E+02
13	250	0.550	3.5248	857	0.5773	2.5694	0.3780	2775.291	3.8188	1820.637	4.5274	0.004 0.1300	0.160E+02
14	300	0.660	3.8432	930	0.5829	2.6838	0.5765	2959.585	4.4900	1612.638	4.4662	0.006 0.0980	0.111E+02
15	350	0.770	4.1142	990	0.5863	2.7571	0.7708	3158.559	5.1029	1372.583	4.5140	0.009 0.0764	0.816E+01
16	400	0.880	4.3462	1040	0.5885	2.8066	0.9510	3370.073	5.6675	1103.125	4.6234	0.013 0.0611	0.625E+01
17	450	0.990	4.5448	1075	0.5901	2.8414	1.1133	3592.324	6.1908	806.495	4.7689	0.017 0.0499	0.494E+01
18	500	1.100	4.7147	1110	0.5912	2.8668	1.2567	3823.765	6.6784	484.611	4.9358	0.022 0.0414	0.400E+01
19	600	1.320	4.9843	1152	0.5926	2.9005	1.4912	4309.086	7.5626	-228.399	5.3015	0.036 0.0298	0.278E+01
20	800	1.760	5.3300	1208	0.5941	2.9347	1.8012	5343.213	9.0478	-1894.949	6.0593	0.078 0.0175	0.156E+01
21	1000	2.201	5.5269	1230	0.5947	2.9508	1.9814	6429.904	10.2595	-3829.505	6.7820	0.145 0.0114	0.100E+01
22	1200	2.641	5.6465	1248	0.5951	2.9596	2.0919	7547.425	11.2779	-5986.039	7.4488	0.244 0.0080	0.694E+00

NU	OMEGA	W	DENSITY OF STATES
0.318E+12	0.200E+13	10.6	0.518E+09
0.637E+12	0.400E+13	21.2	0.216E+10
0.955E+12	0.600E+13	31.8	0.526E+10
0.127E+13	0.800E+13	42.4	0.106E+11
0.159E+13	0.100E+14	53.1	0.201E+11
0.191E+13	0.120E+14	63.7	0.408E+11
0.223E+13	0.140E+14	74.3	0.598E+12
0.255E+13	0.160E+14	84.9	0.449E+12
0.286E+13	0.180E+14	95.5	0.416E+12
0.318E+13	0.200E+14	106.1	0.418E+12
0.350E+13	0.220E+14	116.7	0.419E+12
0.382E+13	0.240E+14	127.3	0.421E+12
0.414E+13	0.260E+14	137.9	0.425E+12
0.446E+13	0.280E+14	148.5	0.431E+12
0.477E+13	0.300E+14	159.2	0.447E+12

GEE0(CONTINUUM LEVEL) IS 0.413E+12FROM 72.3TO 188.6CM-1.

GEE1(CONTINUUM LEVEL) IS 0.157E+12FROM 196.5TO 319.2CM-1.

GEE2(CONTINUUM LEVEL) IS 0.114E+12FROM 291.0TO 375.4CM-1.

EINSTEIN OSC. FREQ. ARE 674.7 871.1 1008.7 1436.2 CM-1.

THEIR ABUNDANCES ARE 0.133 0.067 0.067 0.133(OF TOTAL = 1.0).

****SPECTRUM CALCULATION IS FINISHED!!**

QUARTZ (SEE TABLE NOTES RE DIFFERENCES FROM MODEL IN PAPER 3) O-16 0

VMOLAR	ALPHA0	ALPHA1	ALPHA2	BULK M	DBULK	CPTEST	DK/DP
22.700	-32.176	0.173	0.000	0.377	0.000	2222.000	6.400

THE GAMMAS ARE: 0.02 0.02 1.18 0.70 0.85 0.85.

PRESSURE IS 1.0 BAR.

VOLUME IS 22.70 CM3. DILATATION IS 0.000.

LOG MASS RATIO IS 1.0600

V1-KM/S	V2-KM/S	V3-KM/S	FREQ-UP	FREQ-EIN1	G1	NO. ATMS	VOL-CM3	FREQ-EIN2	G2
3.761	4.463	6.024	550.000	1200.000	0.074	9.000	113.000	1162.000	0.037

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
1117.000	0.074	1080.000	0.037	697.000	809.000	0.185	0.000	0.000	0.000

RHO	WTMOL	ATMS/MOLWT	NO. OXYGENS/CELL
2.650	60.000	3.000	6.000

LOWEST OPTICAL MODE AT K=0 IS 128.0 CM-1; DISPERSION CONSTANTS ARE 16.0 16.0

LOWER CONTINUUM CUTOFF IN MODEL IS 90.5 CM-1 OR 0.170E+14 RAD/SEC.

RADIUS OF BRILLOUIN ZONE IS 0.80639*E+08 CM-1.

CUTOFF WAVENUMBERS ARE 102.945 122.160 164.887 CM-1.

FREQ1	FREQ2	FREQ3	FREQ-UP	FREQ-E	G1	ATOMS/CL	VOL/UCL	FREQ-E2	G2
0.194E+14	0.230E+14	0.310E+14	0.103E+15	0.226E+15	0.740E-01	0.900E+01	0.113E+03	0.218E+15	0.370E-01

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
0.210E+15	0.740E-01	0.203E+15	0.370E-01	0.131E+15	0.152E+15	0.185E+00	0.000E+00	0.000E+00	0.000E+00

K/KMAX	TA1	TA2	LA (* E+13 RAD/SEC)
0.100E+01	0.308E+13	0.366E+13	0.493E+13
0.500E+00	0.218E+13	0.258E+13	0.349E+13
0.333E+00	0.154E+13	0.183E+13	0.247E+13
0.250E+00	0.118E+13	0.140E+13	0.189E+13

VM IS 4.425 KM/S. THETA(ELASTIC) IS 567.220 K.

THERE ARE 2 EXPERIMENTAL VALUES.

**********EXPERIMENTAL DATA**********

TEMPERATURE	CP	ANENTR	CV	THETA-CAL	THETA-CAL/EL	TEMP/THETAEL
300.000	3.544	0.008	3.544	1023.000	1.804	0.529
400.000	4.197	0.037	4.197	1100.000	1.939	0.705

INDEX	TEMP	T/THETA	CV	THETA	AC	CONT	OPTIC	INT. ENER	ENTRPY	HELMHLTZ	ENRGY FN	S-AN	FRAC FAC	1/TEMP
1	298	0.526	3.5320	1019	0.6443	2.7250	0.1626	2975.262	3.4799	1937.861	3.4795	0.008	0.0000	0.112E-02
1	10	0.018	0.0028	547	0.0028	0.0000	0.0000	2405.082	0.0009	2405.205	57.0057	0.001	0.0000	0.100E+05
2	20	0.035	0.0399	453	0.0325	0.0074	0.0000	2405.237	0.0103	2405.163	28.5049	0.001	0.0000	0.250E+04
3	30	0.053	0.1619	426	0.1114	0.0505	0.0000	2406.177	0.0467	2404.907	19.0118	0.002	0.0000	0.111E+04
4	40	0.071	0.3400	441	0.2085	0.1315	0.0000	2408.658	0.1169	2404.115	14.2787	0.002	0.0000	0.625E+03
5	50	0.088	0.5333	471	0.2967	0.2367	0.0000	2413.019	0.2134	2402.481	11.4556	0.002	0.0000	0.400E+03
6	60	0.106	0.7239	504	0.3682	0.3557	0.0000	2419.306	0.3275	2399.788	9.5912	0.002	0.0000	0.278E+03
7	70	0.123	0.9063	538	0.4238	0.4824	0.0000	2427.458	0.4528	2395.894	8.2767	0.002	0.0000	0.204E+03
8	80	0.141	1.0800	572	0.4668	0.6132	0.0000	2437.390	0.5852	2390.708	7.3069	0.002	0.0000	0.156E+03
9	90	0.159	1.2454	604	0.5000	0.7454	0.0000	2449.015	0.7219	2384.175	6.5676	0.002	0.0000	0.123E+03
10	100	0.176	1.4031	636	0.5259	0.8772	0.0000	2462.254	0.8613	2376.260	5.9900	0.002	0.0000	0.100E+03
11	150	0.264	2.0940	771	0.5958	1.4954	0.0028	2550.246	1.5654	2315.567	4.3980	0.000	0.0000	0.444E+02
12	200	0.353	2.6595	878	0.6235	2.0118	0.0242	2669.426	2.2473	2220.106	3.7758	0.000	0.0000	0.250E+02
13	250	0.441	3.1375	960	0.6370	2.4208	0.0797	2814.566	2.8931	2091.435	3.5353	0.002	0.0000	0.160E+02
14	300	0.529	3.5460	1023	0.6446	2.7352	0.1662	2981.804	3.5018	1931.403	3.4795	0.008	0.0000	0.111E+02
15	350	0.617	3.8931	1067	0.6492	2.9744	0.2696	3167.893	4.0748	1741.832	3.5241	0.019	0.0000	0.816E+01
16	400	0.705	4.1856	1104	0.6522	3.1566	0.3769	3369.933	4.6140	1524.463	3.6270	0.037	0.0000	0.625E+01
17	450	0.793	4.4303	1129	0.6542	3.2966	0.4795	3585.365	5.1212	1280.941	3.7652	0.062	0.0000	0.494E+01
18	500	0.881	4.6345	1150	0.6557	3.4055	0.5733	3811.984	5.5986	1012.811	3.9249	0.096	0.0000	0.400E+01
19	600	1.058	4.9475	1176	0.6577	3.5598	0.7300	4291.681	6.4724	408.382	4.2781	0.197	0.0000	0.278E+01
20	800	1.410	5.3277	1208	0.6596	3.7291	0.9389	5322.615	7.9528	-1039.469	5.0184	0.562	0.0000	0.156E+01
21	1000	1.763	5.5335	1220	0.6605	3.8136	1.0594	6409.920	9.1651	-2755.069	5.7303	1.209	0.0000	0.100E+01
22	1200	2.116	5.6549	1236	0.6610	3.8612	1.1326	7528.973	10.1850	-4692.881	6.3901	2.218	0.0000	0.694E+00

NU	OMEGA	W	DENSITY OF STATES
0.318E+12	0.200E+13	10.6	0.159E+09
0.637E+12	0.400E+13	21.2	0.651E+09
0.955E+12	0.600E+13	31.8	0.152E+10
0.127E+13	0.800E+13	42.4	0.287E+10
0.159E+13	0.100E+14	53.1	0.486E+10
0.191E+13	0.120E+14	63.7	0.783E+10
0.223E+13	0.140E+14	74.3	0.125E+11
0.255E+13	0.160E+14	84.9	0.208E+11
0.286E+13	0.180E+14	95.5	0.168E+12
0.318E+13	0.200E+14	106.1	0.144E+12
0.350E+13	0.220E+14	116.7	0.169E+12
0.382E+13	0.240E+14	127.3	0.132E+12
0.414E+13	0.260E+14	137.9	0.135E+12
0.446E+13	0.280E+14	148.5	0.140E+12
0.477E+13	0.300E+14	159.2	0.160E+12

GEE0(CONTINUUM LEVEL) IS 0.126E+12FROM 90.5TO 550.0CM-1.

GEE1(CONTINUUM LEVEL) IS 0.143E+12FROM 697.0TO 809.0CM-1.

GEE2(CONTINUUM LEVEL) IS 0.000E+00FROM 0.0TO 0.0CM-1.

EINSTEIN OSC. FREQ. ARE 1200.0 1162.0 1117.0 1080.0 CM-1.

THEIR ABUNDANCES ARE 0.074 0.037 0.074 0.037(OF TOTAL = 1.0).

****SPECTRUM CALCULATION IS FINISHED!!**

PRESSURE IS 10.0 BAR.

VOLUME IS 22.70 CM3. DILATATION IS 0.000.

LOG MASS RATIO IS 1.0600

V1-KM/S	V2-KM/S	V3-KM/S	FREQ-UP	FREQ-EIN1	G1	NO.ATMS	VOL-CM3	FREQ-EIN2	G2
3.761	4.463	6.024	550.010	1200.027	0.074	9.000	112.997	1162.026	0.037

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
1117.025	0.074	1080.024	0.037	697.013	809.015	0.185	0.000	0.000	0.000

RHO	WTMOL	ATMS/MOLWT	NO.OXYGENS/CELL
2.650	60.000	3.000	6.000

LOWEST OPTICAL MODE AT K=0 IS 128.0 CM-1; DISPERSION CONSTANTS ARE 16.0 16.0

LOWER CONTINUUM CUTOFF IN MODEL IS 90.5 CM-1 OR 0.170E+14 RAD/SEC.

RADIUS OF BRILLOUIN ZONE IS 0.80640*E+08 CM-1.

CUTOFF WAVENUMBERS ARE 102.947 122.162 164.895 CM-1.

FREQ1	FREQ2	FREQ3	FREQ-UP	FREQ-E	G1	ATOMS/CL	VOL/UCL	FREQ-E2	G2
0.194E+14	0.230E+14	0.310E+14	0.103E+15	0.226E+15	0.740E-01	0.900E+01	0.113E+03	0.218E+15	0.370E-01

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
0.210E+15	0.740E-01	0.203E+15	0.370E-01	0.131E+15	0.152E+15	0.185E+00	0.000E+00	0.000E+00	0.000E+00

K/KMAX	TA1	TA2	LA (* E+13 RAD/SEC)

0.100E+01	0.308E+13	0.366E+13	0.493E+13
0.500E+00	0.218E+13	0.258E+13	0.349E+13
0.333E+00	0.154E+13	0.183E+13	0.247E+13
0.250E+00	0.118E+13	0.140E+13	0.189E+13

VM IS 4.425 KM/S. THETA(ELASTIC) IS 567.232 K.

INDEX	TEMP	T/THETA	CV	THETA	AC	CONT	OPTIC	INT. ENER	ENTRPY	HELMHLTZ	ENRGY FN	S-AN	FRAC FAC	1/TEMP
1	298	0.526	3.5319	1019	0.6443	2.7250	0.1626	2975.302	3.4798	1937.922	3.4794	0.008	0.0000	0.112E-02
1	10	0.018	0.0028	547	0.0028	0.0000	0.0000	2405.131	0.0009	2405.255	57.0047	0.001	0.0000	0.100E+05
2	20	0.035	0.0399	453	0.0325	0.0074	0.0000	2405.286	0.0103	2405.213	28.5045	0.001	0.0000	0.250E+04
3	30	0.053	0.1619	426	0.1114	0.0505	0.0000	2406.226	0.0467	2404.956	19.0115	0.002	0.0000	0.111E+04
4	40	0.071	0.3399	441	0.2085	0.1315	0.0000	2408.707	0.1169	2404.164	14.2784	0.002	0.0000	0.625E+03
5	50	0.088	0.5333	471	0.2966	0.2367	0.0000	2413.068	0.2134	2402.531	11.4554	0.002	0.0000	0.400E+03
6	60	0.106	0.7238	504	0.3682	0.3557	0.0000	2419.355	0.3275	2399.838	9.5911	0.002	0.0000	0.278E+03
7	70	0.123	0.9063	538	0.4238	0.4824	0.0000	2427.507	0.4528	2395.943	8.2766	0.002	0.0000	0.204E+03
8	80	0.141	1.0799	572	0.4668	0.6132	0.0000	2437.438	0.5852	2390.758	7.3068	0.002	0.0000	0.156E+03
9	90	0.159	1.2453	604	0.4999	0.7454	0.0000	2449.063	0.7219	2384.225	6.5675	0.002	0.0000	0.123E+03
10	100	0.176	1.4031	636	0.5259	0.8772	0.0000	2462.302	0.8612	2376.310	5.9899	0.002	0.0000	0.100E+03
11	150	0.264	2.0939	771	0.5958	1.4953	0.0028	2550.292	1.5654	2315.620	4.3979	0.000	0.0000	0.444E+02
12	200	0.353	2.6595	878	0.6235	2.0118	0.0242	2669.470	2.2472	2220.161	3.7757	0.000	0.0000	0.250E+02
13	250	0.441	3.1375	960	0.6370	2.4207	0.0797	2814.608	2.8930	2091.492	3.5352	0.002	0.0000	0.160E+02
14	300	0.529	3.5459	1023	0.6446	2.7352	0.1662	2981.844	3.5017	1931.464	3.4795	0.008	0.0000	0.111E+02
15	350	0.617	3.8931	1067	0.6492	2.9743	0.2696	3167.930	4.0748	1741.897	3.5240	0.019	0.0000	0.816E+01
16	400	0.705	4.1856	1104	0.6522	3.1565	0.3768	3369.969	4.6139	1524.532	3.6269	0.037	0.0000	0.625E+01
17	450	0.793	4.4303	1129	0.6542	3.2966	0.4795	3585.399	5.1211	1281.014	3.7651	0.062	0.0000	0.494E+01
18	500	0.881	4.6345	1150	0.6557	3.4055	0.5733	3812.015	5.5985	1012.889	3.9248	0.096	0.0000	0.400E+01
19	600	1.058	4.9475	1176	0.6577	3.5598	0.7300	4291.708	6.4723	408.470	4.2781	0.197	0.0000	0.278E+01
20	800	1.410	5.3277	1208	0.6596	3.7291	0.9389	5322.637	7.9527	-1039.361	5.0183	0.562	0.0000	0.156E+01
21	1000	1.763	5.5335	1220	0.6605	3.8136	1.0594	6409.939	9.1650	-2754.938	5.7302	1.209	0.0000	0.100E+01
22	1200	2.116	5.6548	1236	0.6610	3.8612	1.1326	7528.989	10.1849	-4692.728	6.3900	2.218	0.0000	0.694E+00

NU	OMEGA	W	DENSITY OF STATES
0.318E+12	0.200E+13	10.6	0.159E+09
0.637E+12	0.400E+13	21.2	0.651E+09
0.955E+12	0.600E+13	31.8	0.152E+10
0.127E+13	0.800E+13	42.4	0.287E+10
0.159E+13	0.100E+14	53.1	0.486E+10
0.191E+13	0.120E+14	63.7	0.783E+10
0.223E+13	0.140E+14	74.3	0.125E+11
0.255E+13	0.160E+14	84.9	0.208E+11
0.286E+13	0.180E+14	95.5	0.168E+12
0.318E+13	0.200E+14	106.1	0.144E+12
0.350E+13	0.220E+14	116.7	0.169E+12
0.382E+13	0.240E+14	127.3	0.132E+12
0.414E+13	0.260E+14	137.9	0.135E+12
0.446E+13	0.280E+14	148.5	0.140E+12
0.477E+13	0.300E+14	159.2	0.160E+12

GEE0(CONTINUUM LEVEL) IS 0.126E+12FROM 90.5TO 550.0CM-1.

GEE1(CONTINUUM LEVEL) IS 0.143E+12FROM 697.0TO 809.0CM-1.

GEE2(CONTINUUM LEVEL) IS 0.000E+00FROM 0.0TO 0.0CM-1.

EINSTEIN OSC. FREQ. ARE 1200.0 1162.0 1117.0 1080.0 CM-1.

THEIR ABUNDANCES ARE 0.074 0.037 0.074 0.037(OF TOTAL = 1.0).

****SPECTRUM CALCULATION IS FINISHED!!**

PRESSURE IS 1.0 KB.

VOLUME IS 22.64 CM3. DILATATION IS -0.003.

LOG MASS RATIO IS 1.0600

V1-KM/S	V2-KM/S	V3-KM/S	FREQ-UP	FREQ-EIN1	G1	NO. ATMS	VOL-CM3	FREQ-EIN2	G2
3.765	4.467	6.048	551.018	1202.686	0.074	9.000	112.703	1164.601	0.037

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
1119.500	0.074	1082.417	0.037	698.290	810.497	0.185	0.000	0.000	0.000

RHO	WTMOL	ATMS/MOLWT	NO.OXYGENS/CELL
2.657	60.000	3.000	6.000

LOWEST OPTICAL MODE AT K=0 IS 128.2 CM-1; DISPERSION CONSTANTS ARE 16.0 16.0

LOWER CONTINUUM CUTOFF IN MODEL IS 90.7 CM-1 OR 0.170E+14 RAD/SEC.

RADIUS OF BRILLOUIN ZONE IS 0.80710*E+08 CM-1.

CUTOFF WAVENUMBERS ARE 103.132 122.381 165.688 CM-1.

FREQ1	FREQ2	FREQ3	FREQ-UP	FREQ-E	G1	ATOMS/CL	VOL/UCL	FREQ-E2	G2
0.194E+14	0.230E+14	0.311E+14	0.104E+15	0.226E+15	0.740E-01	0.900E+01	0.113E+03	0.219E+15	0.370E-01

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
0.210E+15	0.740E-01	0.203E+15	0.370E-01	0.131E+15	0.152E+15	0.185E+00	0.000E+00	0.000E+00	0.000E+00

K/KMAX	TA1	TA2	LA (* E+13 RAD/SEC)

0.100E+01	0.309E+13	0.366E+13	0.496E+13
0.500E+00	0.218E+13	0.259E+13	0.351E+13
0.333E+00	0.154E+13	0.183E+13	0.248E+13
0.250E+00	0.118E+13	0.140E+13	0.190E+13

VM IS 4.430 KM/S. THETA(ELASTIC) IS 569.475 K.

INDEX	TEMP	T/THETA	CV	THETA	AC	CONT	OPTIC	INT. ENER	ENTRPY	HELMHLTZ	ENRGY FN	S-AN FRAC	FAC	1/TEMP
1	298	0.524	3.5275	1022	0.6442	2.7220	0.1613	2979.245	3.4727	1943.992	3.4723	0.008	0.0000	0.112E-02
1	10	0.018	0.0028	549	0.0028	0.0000	0.0000	2410.024	0.0009	2410.147	56.9098	0.001	0.0000	0.100E+05
2	20	0.035	0.0395	454	0.0322	0.0073	0.0000	2410.177	0.0102	2410.106	28.4570	0.001	0.0000	0.250E+04
3	30	0.053	0.1608	427	0.1107	0.0501	0.0000	2411.111	0.0464	2409.852	18.9798	0.002	0.0000	0.111E+04
4	40	0.070	0.3383	442	0.2075	0.1308	0.0000	2413.578	0.1162	2409.064	14.2545	0.002	0.0000	0.625E+03
5	50	0.088	0.5312	471	0.2955	0.2356	0.0000	2417.920	0.2122	2407.440	11.4361	0.002	0.0000	0.400E+03
6	60	0.106	0.7214	505	0.3671	0.3543	0.0000	2424.184	0.3259	2404.761	9.5747	0.002	0.0000	0.278E+03
7	70	0.123	0.9036	539	0.4228	0.4808	0.0000	2432.310	0.4508	2400.884	8.2623	0.002	0.0000	0.204E+03
8	80	0.141	1.0771	572	0.4658	0.6112	0.0000	2442.214	0.5828	2395.720	7.2941	0.002	0.0000	0.156E+03
9	90	0.158	1.2423	605	0.4991	0.7432	0.0000	2453.809	0.7192	2389.212	6.5559	0.002	0.0000	0.123E+03
10	100	0.176	1.4000	637	0.5251	0.8748	0.0000	2467.017	0.8582	2381.326	5.9792	0.002	0.0000	0.100E+03
11	150	0.264	2.0904	772	0.5954	1.4922	0.0028	2554.839	1.5610	2320.822	4.3895	0.000	0.0000	0.444E+02
12	200	0.352	2.6555	880	0.6233	2.0084	0.0239	2673.828	2.2418	2225.609	3.7682	0.000	0.0000	0.250E+02
13	250	0.440	3.1332	960	0.6369	2.4174	0.0789	2818.760	2.8866	2097.237	3.5280	0.002	0.0000	0.160E+02
14	300	0.528	3.5415	1023	0.6444	2.7322	0.1649	2985.780	3.4946	1937.547	3.4723	0.008	0.0000	0.111E+02
15	350	0.616	3.8887	1071	0.6491	2.9717	0.2679	3171.645	4.0669	1748.355	3.5168	0.019	0.0000	0.816E+01
16	400	0.704	4.1813	1104	0.6521	3.1542	0.3750	3373.466	4.6055	1531.397	3.6196	0.037	0.0000	0.625E+01
17	450	0.792	4.4263	1129	0.6542	3.2945	0.4775	3588.688	5.1122	1288.313	3.7576	0.062	0.0000	0.494E+01
18	500	0.880	4.6307	1150	0.6557	3.4037	0.5713	3815.109	5.5892	1020.644	3.9172	0.096	0.0000	0.400E+01
19	600	1.055	4.9443	1182	0.6577	3.5584	0.7282	4294.455	6.4623	417.190	4.2701	0.197	0.0000	0.278E+01
20	800	1.407	5.3254	1208	0.6596	3.7283	0.9375	5324.846	7.9419	-1028.562	5.0098	0.562	0.0000	0.156E+01
21	1000	1.759	5.5319	1220	0.6605	3.8130	1.0584	6411.770	9.1538	-2741.946	5.7212	1.209	0.0000	0.100E+01
22	1200	2.111	5.6537	1236	0.6610	3.8608	1.1319	7530.545	10.1735	-4677.477	6.3806	2.218	0.0000	0.694E+00

NU	OMEGA	W	DENSITY OF STATES
0.318E+12	0.200E+13	10.6	0.158E+09
0.637E+12	0.400E+13	21.2	0.646E+09
0.955E+12	0.600E+13	31.8	0.151E+10
0.127E+13	0.800E+13	42.4	0.285E+10
0.159E+13	0.100E+14	53.1	0.483E+10
0.191E+13	0.120E+14	63.7	0.777E+10
0.223E+13	0.140E+14	74.3	0.124E+11
0.255E+13	0.160E+14	84.9	0.206E+11
0.286E+13	0.180E+14	95.5	0.167E+12
0.318E+13	0.200E+14	106.1	0.144E+12
0.350E+13	0.220E+14	116.7	0.167E+12
0.382E+13	0.240E+14	127.3	0.131E+12
0.414E+13	0.260E+14	137.9	0.134E+12
0.446E+13	0.280E+14	148.5	0.140E+12
0.477E+13	0.300E+14	159.2	0.157E+12

GEE0(CONTINUUM LEVEL) IS 0.125E+12FROM 90.7TO 551.0CM-1.

GEE1(CONTINUUM LEVEL) IS 0.143E+12FROM 697.0TO 809.0CM-1.

GEE2(CONTINUUM LEVEL) IS 0.000E+00FROM 0.0TO 0.0CM-1.

EINSTEIN OSC. FREQ. ARE 1200.0 1162.0 1117.0 1080.0 CM-1.

THEIR ABUNDANCES ARE 0.074 0.037 0.074 0.037(OF TOTAL = 1.0).

****SPECTRUM CALCULATION IS FINISHED!!**

PRESSURE IS 1000.0 KB.

VOLUME IS 14.45 CM3. DILATATION IS -0.363.

LOG MASS RATIO IS 1.0600

V1-KM/S	V2-KM/S	V3-KM/S	FREQ-UP	FREQ-EIN1	G1	NO. ATMS	VOL-CM3	FREQ-EIN2	G2
4.248	5.041	9.336	755.411	1761.248	0.074	9.000	71.950	1705.475	0.037

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
1639.429	0.074	1585.123	0.037	957.312	1111.141	0.185	0.000	0.000	0.000

RHO	WTMOL	ATMS/MOLWT	NO. OXYGENS/CELL
4.162	60.000	3.000	6.000

LOWEST OPTICAL MODE AT K=0 IS 175.8 CM-1; DISPERSION CONSTANTS ARE 16.0 16.0

LOWER CONTINUUM CUTOFF IN MODEL IS 124.3 CM-1 OR 0.234E+14 RAD/SEC.

RADIUS OF BRILLOUIN ZONE IS 0.93732*E+08 CM-1.

CUTOFF WAVENUMBERS ARE 135.147 160.373 297.021 CM-1.

FREQ1	FREQ2	FREQ3	FREQ-UP	FREQ-E	G1	ATOMS/CL	VOL/UCL	FREQ-E2	G2
0.254E+14	0.302E+14	0.558E+14	0.142E+15	0.331E+15	0.740E-01	0.900E+01	0.720E+02	0.321E+15	0.370E-01

EIN3	G3	EIN4	G4	CONT2	CONT2,U	CONT2,G	CONT3,L	CONT3,U	CONT3,G
0.308E+15	0.740E-01	0.298E+15	0.370E-01	0.180E+15	0.209E+15	0.185E+00	0.000E+00	0.000E+00	0.000E+00

K/KMAX	TA1	TA2	LA (* E+13 RAD/SEC)

0.100E+01	0.404E+13	0.480E+13	0.889E+13
0.500E+00	0.286E+13	0.339E+13	0.628E+13
0.333E+00	0.202E+13	0.240E+13	0.444E+13
0.250E+00	0.155E+13	0.184E+13	0.340E+13

VM IS 5.140 KM/S. THETA(ELASTIC) IS 765.902 K.

INDEX	TEMP	T/THETA	CV	THETA	AC	CONT	OPTIC	INT. ENER	ENTRPY	HELMHLTZ	ENRGY FN	S-AN	FRAC FAC	1/TEMP
1	298	0.389	2.8092	1255	0.6194	2.1632	0.0266	3836.206	2.4352	3110.324	2.4346	0.008	0.0000	0.112E-02
1	10	0.013	0.0011	754	0.0011	0.0000	0.0000	3402.895	0.0004	3403.073	43.3133	0.001	0.0000	0.100E+05
2	20	0.026	0.0122	673	0.0113	0.0008	0.0000	3414.149	0.0034	3414.264	21.0971	0.001	0.0000	0.250E+04
3	30	0.039	0.0590	596	0.0470	0.0121	0.0000	3414.465	0.0156	3414.180	14.0675	0.002	0.0000	0.111E+04
4	40	0.052	0.1500	582	0.1050	0.0450	0.0000	3415.479	0.0441	3413.898	10.5577	0.002	0.0000	0.625E+03
5	50	0.065	0.2681	599	0.1692	0.0989	0.0000	3417.552	0.0899	3413.241	8.4593	0.002	0.0000	0.400E+03
6	60	0.078	0.3982	627	0.2301	0.1681	0.0000	3420.876	0.1501	3412.052	7.0692	0.002	0.0000	0.278E+03
7	70	0.091	0.5322	660	0.2845	0.2477	0.0000	3425.523	0.2215	3410.202	6.0858	0.002	0.0000	0.204E+03
8	80	0.104	0.6660	694	0.3318	0.3341	0.0000	3431.511	0.3012	3407.594	5.3577	0.002	0.0000	0.156E+03
9	90	0.118	0.7977	729	0.3726	0.4251	0.0000	3438.826	0.3873	3404.155	4.8006	0.002	0.0000	0.123E+03
10	100	0.131	0.9264	763	0.4075	0.5189	0.0000	3447.443	0.4779	3399.832	4.3637	0.002	0.0000	0.100E+03
11	150	0.196	1.5169	918	0.5197	0.9972	0.0000	3508.860	0.9679	3363.855	3.1490	0.000	0.0000	0.444E+02
12	200	0.261	2.0200	1050	0.5740	1.4449	0.0012	3597.562	1.4748	3302.778	2.6671	0.000	0.0000	0.250E+02
13	250	0.326	2.4498	1162	0.6030	1.8388	0.0080	3709.498	1.9726	3216.523	2.4787	0.002	0.0000	0.160E+02
14	300	0.392	2.8221	1260	0.6199	2.1746	0.0276	3841.411	2.4526	3105.803	2.4347	0.008	0.0000	0.111E+02
15	350	0.457	3.1493	1340	0.6306	2.4550	0.0638	3990.760	2.9125	2971.583	2.4704	0.019	0.0000	0.816E+01
16	400	0.522	3.4394	1408	0.6377	2.6861	0.1156	4155.506	3.3520	2814.879	2.5533	0.037	0.0000	0.625E+01
17	450	0.588	3.6974	1462	0.6427	2.8755	0.1792	4333.927	3.7720	2636.688	2.6656	0.062	0.0000	0.494E+01
18	500	0.653	3.9266	1510	0.6463	3.0306	0.2497	4524.505	4.1734	2437.964	2.7965	0.096	0.0000	0.400E+01
19	600	0.783	4.3097	1578	0.6511	3.2632	0.3954	4936.808	4.9241	1982.503	3.0895	0.197	0.0000	0.278E+01
20	800	1.045	4.8424	1664	0.6559	3.5375	0.6490	5855.761	6.2424	862.036	3.7177	0.562	0.0000	0.156E+01
21	1000	1.306	5.1698	1710	0.6581	3.6823	0.8294	6858.849	7.3603	-501.228	4.3374	1.209	0.0000	0.100E+01
22	1200	1.567	5.3782	1728	0.6594	3.7665	0.9523	7914.411	8.3220	-2071.808	4.9233	2.218	0.0000	0.694E+00

NU	OMEGA	W	DENSITY OF STATES
0.318E+12	0.200E+13	10.6	0.644E+08
0.637E+12	0.400E+13	21.2	0.261E+09
0.955E+12	0.600E+13	31.8	0.601E+09
0.127E+13	0.800E+13	42.4	0.110E+10
0.159E+13	0.100E+14	53.1	0.180E+10
0.191E+13	0.120E+14	63.7	0.275E+10
0.223E+13	0.140E+14	74.3	0.404E+10
0.255E+13	0.160E+14	84.9	0.580E+10
0.286E+13	0.180E+14	95.5	0.832E+10
0.318E+13	0.200E+14	106.1	0.122E+11
0.350E+13	0.220E+14	116.7	0.189E+11
0.382E+13	0.240E+14	127.3	0.128E+12
0.414E+13	0.260E+14	137.9	0.103E+12
0.446E+13	0.280E+14	148.5	0.112E+12
0.477E+13	0.300E+14	159.2	0.204E+12
0.509E+13	0.320E+14	169.8	0.927E+11
0.541E+13	0.340E+14	180.4	0.929E+11
0.573E+13	0.360E+14	191.0	0.932E+11
0.605E+13	0.380E+14	201.6	0.935E+11
0.637E+13	0.400E+14	212.2	0.939E+11
0.668E+13	0.420E+14	222.8	0.945E+11
0.700E+13	0.440E+14	233.4	0.951E+11
0.732E+13	0.460E+14	244.0	0.960E+11
0.764E+13	0.480E+14	254.6	0.972E+11
0.796E+13	0.500E+14	265.3	0.991E+11
0.828E+13	0.520E+14	275.9	0.102E+12
0.859E+13	0.540E+14	286.5	0.110E+12

GEE0(CONTINUUM LEVEL) IS 0.914E+11FROM 124.3TO 755.4CM-1.

GEE1(CONTINUUM LEVEL) IS 0.104E+12FROM 697.0TO 809.0CM-1.

GEE2(CONTINUUM LEVEL) IS 0.000E+00FROM 0.0TO 0.0CM-1.

EINSTEIN OSC. FREQ. ARE 1200.0 1162.0 1117.0 1080.0 CM-1.

THEIR ABUNDANCES ARE 0.074 0.037 0.074 0.037(OF TOTAL = 1.0).

****SPECTRUM CALCULATION IS FINISHED!!**