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Technical Report PTR-81-10

N2 PRESSURE - BROADENED O3 LINE WIDTHS
AND STRENGTHS NEAR 1129.4 CM-1

By
G. E. Copeland, Principal Investigator
L. N. Majorana
C. N. Harward
and
R. J. Steinkamp

Progress Report
For the period October 25, 1980 - October 24, 1981

Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia 23665

Under
Research Grant NAG1-1
James M. Hoell, Technical Monitor
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\textbf{N}_2 \text{ PRESSURE-BROADENED O}_3 \text{ LINE WIDTHS AND STRENGTHS NEAR 1129.4 CM}^{-1}

By

G.E. Copeland\textsuperscript{1}, L.N. Majorana\textsuperscript{2}, C.N. Harward\textsuperscript{3},
and R.J. Steinkamp\textsuperscript{4}

\textbf{ABSTRACT}

A Beer's Law experiment was performed with a tunable diode laser to find the \textit{N}_2 \text{ pressure-broadening characteristics of a single O}_3 \text{ absorption line at 1129.426 cm}^{-1} (v1 Band, J, K_a, K_c = 31, 1, 31 + 32, 0, 32) for \textit{N}_2 \text{ pressures from 10 to 100 torr (O}_3 \text{ pressure = 3.16 torr). S}_2 \text{ line positions were used for wavelength calibration. Line shapes were iteratively fitted to a Lorentz function. Results were } \delta(\text{HWHM in MHz}) = 47.44(\pm 5.34) \text{ MHz} + 1.730 (\pm 0.088) \text{ MHz/torr } p(\text{torr}) \text{ with } p = 0.9897. \text{ This intercept compares well with the Doppler O}_3 - O}_3 \text{ broadened (at 3.16 torr) width of 44.52 Hz (ref. 1). Any difference is most likely in laser frequency uncertainty. This results in a HWHM line width of 0.044 cm}^{-1}\text{ atm}^{-1} \text{ at 760 torr and 285 K. The line strengths integrated over } \Delta\nu=0.055 \text{ cm}^{-1} \text{ were found to be N}_2 \text{ pressure dependent: } S(\text{cm}^{-2}\text{torr}^{-1}) = 1.334 \times 10^{-4} p(\text{torr})^{-1.314} \text{ with } p = -0.9957.

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INTRODUCTION

With the advent of semiconductor lasers and their recent application to spectroscopy (refs. 2-4), there has been a revolution in the study of infrared spectra. Use of the tunable diode laser (TDL) has permitted high-resolution (<0.0001 cm⁻¹) studies of several molecules of high current interest (ClO, HNO₃, SO₂, CF₂Cl₂, etc.). This study is concerned with the experimental determination of the pressure-broadened characteristics of a single O₃ line near 1129.4 cm⁻¹. This line has been suggested as a possible candidate for remote sensing experiments using either infrared heterodyne spectroscopy or differential lidar, since it is relatively well isolated from other atmospheric lines, has significant strength, and is relatively insensitive to temperature changes. A Beer's Law experiment is performed to determine the absorption coefficients and nitrogen (N₂) broadening parameters.

APPARATUS AND PROCEDURE

A simplified schematic of the apparatus is shown in figure 1. The radiation source is a PbSnTe TDL whose output is passed through collimating optics and a monochromator for mode selection. The output from the monochromator is divided by a beam splitter which directs 40 percent through a solid germanium etalon onto an LN₂-cooled HgCdTe detector. The remaining 60 percent is split into 2 beams. One beam is directed through a reference gas cell to a second detector and the other through the 50-cm O₃ absorption cell to a third detector. A more detailed description of the apparatus is to be found in the report by Majorana (ref. 5).

This arrangement permits simultaneous recording of the O₃ absorption spectra, the etalon fringes for relative frequency calibration, and the SO₂ reference gas spectrum for conversion to absolute frequency (ref. 4). The detector output, the TDL current, and SO₂ and O₃ pressures were read by a 12-bit A/D and transferred to a 7-track tape by a PDP8/e minicomputer for later analysis. O₃ spectra were taken at 8 N₂ pressures (10-100 torr) at 285 K. SO₂ at 1 torr was used as the reference spectrum since a detailed atlas exists (ref. 6). The 1129.418 cm⁻¹ line of SO₂ (ν₁, ν₂, ν₃, j, Kₐ, Kₑ)
[1,0,0,33,3,31 +0,0,0,34,2,32] was selected as the standard reference line because of its proximity to the O₃ line under study and the recent heterodyne confirmation of its position at 1129.41835 cm⁻¹.

THE DATA AND ITS ANALYSIS

The data were collected and processed in the same manner as described by Majorana (ref. 5). Strip chart records were digitized and recorded on tape for later transfer to the ODU DEC System 10 computer. After input of data into the proper data format, each of the N₂-broadened O₃ profiles was processed using the program QUICK. One of the output products from program QUICK is a plot of the absorption coefficient as a function of wavenumber, as well as generation of data files containing the coefficient and the transmittance functions.

For the foreign gas broadening study done in this research, the proper broadening function is a Lorentz function. Therefore, the Voigt function-fitting routine developed by Majorana and Copeland (ref. 5) cannot be used efficiently. A new program, BROAD (listed in the Appendix) was developed to fit in a nonlinear least squares sense a Lorentzian to the absorption coefficient: that is, a fit of the data is made to the function

\[ y = A₄ + \frac{A₁}{(\omega - A₂)^2 + \left(\frac{A₃}{2}\right)^2} \]  

where \( A₁ \) is the numerator of the Lorentzian, \( A₂ \) is the center frequency (in cm⁻¹), \( A₃ \) is the half-width at half maximum (HWHM) of the profile, and \( A₄ \) is the background.

The program BROAD makes extensive use of the data-fitting routines developed by Bevington (ref. 8) and provides a file for plotting its fitted function together with the data for the user. The program begins by asking the user the name of the input data file. The program reports the number of
data points, the date the data was taken, the total (O\textsubscript{3} + N\textsubscript{2}) pressure in torr, and the minimum and maximum values of the absorption coefficient. The subroutine CHOP is called, and the user may reduce the size on high and low wavenumber ends of the spectrum to analyze. The total wavenumber interval across the data is reported, and the user may normalize the data if needed. The function AREA is called, and the integral of the absorption coefficient over wavenumber is calculated, i.e., the strength in units of \text{cm}^{-2}\text{torr}^{-1}. The user may select any of three different procedures in which to weight the data during the fitting procedure (MODE = +1, 0, -1) which correspond to the Bevington weight convention (ref. 8).

The program BROAD was designed to fit Lorentzians to either convex or concave data sets, i.e., A\textsubscript{4} near zero or A\textsubscript{4} maximum. The program automatically detects each case and, assuming only one spectral line, then makes initial guesses at the parameters A\textsubscript{1}, A\textsubscript{2}, A\textsubscript{3}, A\textsubscript{4} and at their initial movements DELTAA(1-4). These are reported to the user. The program uses the grid-search method, subroutine GRIDLS, and the DO loop 100 is entered. After each exit from GRIDLS, the reduced chi square statistic is compared with the previous value. If it has not changed by more than two percent, iteration is stopped and the program reports the final chi square, the number of iterations, the final values of the parameters A\textsubscript{1} to A\textsubscript{4}, and estimates of their errors. Finally, the total pressure in torr and the half-width at half maximum in both \text{cm}^{-1} and MHz are reported. The user may then select to see a recap of the data and the best fit and plot such as a graphics terminal. An example output of program BROAD is shown in the appendix.

RESULTS

These results are the first report to date of ozone line width broadening in the v1 band using N\textsubscript{2} as the foreign gas. Table 1 lists the N\textsubscript{2} pressure, the fitted half-widths, and the line strengths for the case where the initial ozone pressure was 3.16 torr. Figures 2 through 10 show the Lorentz fit to the absorption coefficient from the program BROAD.
The half-widths as a function of pressure are shown in figure 11. We find they can be represented by

\[ \delta \text{(HWHM in MHz)} = A + B \, p_{N_2} \]  

with

\[ A = 47.4 \pm 6.3 \text{ MHz} \]

and

\[ B = 1.730 \pm 0.01 \text{ MHz/torr} \]

with a linear correlation coefficient of 0.9897. The intercept value 47.4 ± 5.3 MHz corresponds to the O_3 - O_3 broadened width at 3.16 torr O_3. This self-broadening half-width compares well with the results of Majorana et al. (ref. 1), who found a width of 44.52 MHz. The two values agree well within error bounds. Any significant difference could be traced to frequency instability in the diode laser.

The strength of the absorption line is defined as the integral over wavenumber of the absorption coefficient; that is, strength \( S \) is given by

\[ S(\text{cm}^{-2}\text{torr}^{-1}) = \int k(\nu) d\nu \]  

Generally, \( S \) is a constant for self-broadened data; however, we find \( S \) to be \( N_2 \) pressure dependent. Figure 12 shows the strength for this transition as a function of \( N_2 \) pressure. We find that the strength can be represented as a power function of the \( N_2 \) pressure, i.e., \( S = A p_{N_2}^B \), where \( A = 1.334 \times 10^{-4} \) and \( B = 1.314 \pm 0.049 \) with a correlation coefficient of -0.9957. Since \(-1.34\) is essentially \(-4/3\), then we find the strength varies as pressure of nitrogen raised to the \(-4/3\) power. This curious result may be due to several effects: chemical decomposition of \( O_3 \) due to collisions with \( N_2 \) or formation of weak Van de Waals molecules with \( N_2 \), i.e., \( O_3 + N_2 \rightarrow O_3N_2 \) and the resulting modification of residual ozone concentration.
APPENDIX

PROGRAM BROAD

This program is designed to perform the main data processing tasks as described in detail in the section "The Data and Its Analysis." This program is written in Fortran-10 and runs on a Dec System-10 time shared computer under the Topel0 operating system. Extensive use is made of the following data handling routines selected from those of Bevington (ref. 3) and are not listed here:

GRIDLS(X,Y,SIGMAY,NPTS,TERMS,MODE,A,DELTA,SIGMAA,YFIT,CHISQR)
INTEG(X,Y,NPTS,1,X1,X2,SUM)
MATINV(ARRAY,TERMS,DET)
FUNCTION FCHISQ(Y,SIGMAY,NPTS,NFREE,MODE,YFIT)
FUNCTION AREA(X,Y,NPTS,TERMS)

LISTING

PROGRAM BROAD

C Written by
C DR. G. E. COPELAND
C DEPARTMENT OF PHYSICS AND GEOPHYSICAL SCIENCES
C OLD DOMINION UNIVERSITY
C NASA HETERODYNE GRANT

DIMENSION YLABEL(16),XLABEL(10),TITLE(35),SIGMAX(400),
1SIGMAY(400)
DIMENSION X(400),Y(400),YFIT(400),A(4),SIGMAA(4)
DIMENSION DELTA(4)
DOUBLE PRECISION FILE

C SPEED OF LIGHT IN CM PER SECOND
C
C C = 2.9979250E10

C DATA FOR THE LABELS ON THE GRAPH
C
C DATA XLABEL/'W','A','V','E','N','U','M','B','E','R'/
DATA YLABEL/'A','B','S',
1'C','0', 'E', 'F', '1','B','A', 'S', 'L', 'E',
2,'T', 'Z', 'H', '4', '3', 'C', 'W', '1', 'L', 'O', 'R', 'E', '

DATA TITLE/0,'13', 'K', '1', 'E', 'E', 'E', 'A', 'T', '1', '1',
1'2', '9', '4', '9', '3', '9', 'A', 'S', 'L', 'T', 'F', 'I', 'F', 'E', 'A'

DATA YLB3/'R', 'E', 'S', 'I', 'D', 'U', 'A', 'L', 'S'/

TYPE 92 FORMAT(' L O R E N T Z I A N FITTING FUNCTION')
WRITE(5,10010)
ACCEPT 10020 ,FILE
OPEN(UNIT =21,DEVICE='DSK',ACCESS='SEQIN',FILE=FILE)
READ(21,*1NPTS,K2,K3,K4,P3
IF(NPTS.GT.400) TYPE 41
FORMAT(' TOO MANY DATA POINTS ENLARGE THE DIMENSIONS')
IF(NPTS.GT.400) STOP
TYPE 222,NPTS

FORMAT(' NUMBER OF DATA PAIRS =',I4)

FORMAT(1X,0,MONTH=0,12,1DAY=0,13,1YEAR=0,14)

TYPE 4519,P3
FORMAT(' PRESSURE IS ',F7.2,' TORR')

READ THE DATA IN THE FILE INTO X AND Y ARRAYS

CALL READDT(X,Y,NPTS)

DO 31 I=1,NPTS

CALL ROUTINE TO CHOP OUT 1ST AND LAST OF DATA TO GET RID OF OUTER LINES

CALL CHOP(NPTS,X,Y)

ASK IF DATA IS TO NORMALIZED

TYPE 77
FORMAT( ' DO YOU WANT THE DATA NORMALIZED?<Y=1,N=0>'$)
ACCEPT *,ANNOR
IF ( ANNOR .EQ. 0) GOTO 79
YES NORMALIZE IT

ANSW = AREA(X, Y, NPTS, 3)

SCALE THE Y ARRAY NOW

DO 732 I = 1, NPTS
  732 Y(I) = Y(I) / ANSW

TYPE 765, ANSW

FORMAT(' INTEGRAL OVER THE DATA IS = ', 1PE)

OPEN(UNIT=22, DEVICE='DSK', ACCESS='SEQOUT', FILE='PLTTEK.DAT')

NSHET = 1
NGRP = 2
WRITE(22, 10190) NSHET

INPUT MODE +1, 0, -1.

MODE = +1 IS THE INSTRUMENTAL
MODE = -1 IS STATISTICAL
MODE = 0 NO WEIGHTING

WRITE(5, 10100) MODE = -1
ACCEPT *, MODE

CALCULATE MEAN IN X AND Y-
  YMEAN = 0.0
  XMEAN = 0.0
DO 50 I = 1, NPTS
  SIGMAX(I) = 0.0
  XMEAN = X(I) + XMEAN
  SIGMA(I) = 0.0
  YMEAN = YMEAN + Y(I)
  CONTINUE

XMEAN = XMEAN / FLOAT(NPTS)
YMEAN = YMEAN / FLOAT(NPTS)

CALCULATE 'SD' OF 'Y' AND 'SD' OF 'X' (SDY, SDX)
SDX = 0.0
SDY = 0.0
DO 70 I = 1, NPTS
  DX = (X(I) - XMEAN)**2 + SDX
  SDX = (X(I) - YMEAN)**2 + SDY
  SIGMAX(I) = SQRT((X(I) - XMEAN)**2)
  SIGMA(I) = SQRT((Y(I) - YMEAN)**2)
  CONTINUE
SDX = SQRT(SDX/FLOAT(NPTS-1))
SDY = SQRT(SDY/FLOAT(NPTS-1))
WE HAVE SDY, SDX TO PROVIDE START UP VALUES FOR
THE GRID SEARCH

YMAX=Y(1)
DO 80 I=2,NPTS
IF( YMAX .LT. Y(I) ) YMAX=Y(I)
80 CONTINUE

INTERMS=4
YMIN=Y(1)
DO 81 I=2,NPTS
IF( YMIN .GT. Y(I) ) YMIN=Y(I)
81 CONTINUE

GUESS ROUTINE

A(4)=( Y(1) +Y(NPTS) )*0.5
TYPE * , YMIN, YMEAN, YMAX, XMIN, XMEAN, XMAX
A(2)=XMEAN

IF(Y(1) .LT. YMEAN ) GOTO 811

CURVE IS CONCAVE

ICON=1
TYPE 877
FORMAT( ' CURVE IS CONCAVE' )
YMID=Y(1)-( Y(1)-YMIN)*0.5
DO 992 I=1,NPTS
IF( Y(I) .LT. YMID ) XL=X(I)
IF( Y(I) .LT. YMID ) ILEFT=I
IF( Y(I) .LT. YMID ) GOTO 993
992 CONTINUE
STOP '992'

DO 994 I=ILEFT,NPTS
IF( Y(I) .GT. YMID ) XR=X(I)
IF( Y(I) .GT. YMID ) GOTO 995
994 CONTINUE
STOP '994'

993 CONTINUE

CURVE IS CONVEX

TYPE 878
FORMAT( ' CURVE IS CONVEX' )
YMID=Y(1)+(YMAX-Y(1))*0.5
DO 8121 I=1,NPTS
IF( Y(I) .GT. YMID ) XL=X(I)
IF( Y(I) .GT. YMID ) ILEFT=I
IF( Y(I) .GT. YMID ) GOTO 8131
8121 CONTINUE
STOP '8121'


DO 814 I=ILEFT,NPTS
   IF( Y(I) .LT. YMID) XR=X(I)
   IF( Y(I) .LT. YMID) GOTO 995
814  CONTINUE
   STOP '814'
995  A(3)=XR-XL
C A3 IS FWHM
C A(1)=(0.25* A(3)**2+(XMEAN-A(2))**2)*( YMAX-A(4) +0.5)
C IF( Y(I).GT. YMIN) A(1)=A(1)
C GOT A1,A2,A3,A4
C TYPE *,A
C NOW HAVE FINISHED THE
C GENERATION OF GUESSES ON A1,A2,A3,A4 FOR A LORENTZIAN FUNCTION
C Y=A4 + A1/( ( X-A2)**2+( A3/2)**2)
C
WRITE(5,10120)
WRITE(5,10110)(I,A(I),I=1,NTERMS)
C FINISHED STARTING VALUES
C NOW FIND THE INCREMENTS ON A(1),A(2),A(3)
C SET STEP SIZE IN MEAN = 6SDX/20
DELTAA(3)=A(3)/10.
C SET STEP SIZE ON COEFFICIENT A1
DELTAA(1)=A(1)/10.
C SET STEP SIZE ON COEFFICIENT A2
DELTAA(2)=(XMEAN+SDX)/10.0
C GIVE GUESS ON DELTAA(4)----BACKGOUND
DELTAA(4)=A(4)/10.0
C
ENTER LOOP
C ITERATE 20 TIMES AT MOST
KNT=0
DO 100 K=1,15
   CALL GRIDLS(X,Y,SIGMAY,NPTS,NTERMS,MODE,A,DELTAA,1
   SIGMAA,YFIT,CHISQR)
   TYPE 887,K,CHISQR
   IF(K .GT. 1) GOTO 90
   SAVE=CHISQR
   SAVIT-SAVE
   KNT=1
   GOTO 100
90   XCHI=100.0*(CHISQR-SAVE)/CHISQR
   IF( XCHI .GT. 0.0 ) GOTO 110
C CRITERION OF CONVERGENCE IS CHISQR DOES NOT CHANGE BY 1 PER CENT
OR IF CHISQR IS LESS THAN 0.02 OF THE 1ST CHISQR FOUND

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IF( ABS(XCHI) .LT. 0.5 ) GOTO 110
IF( CHISQR .LT. 0.020*SAVIT) GOTO 110
SAVE = CHISQR
KNT=KNT+1
100  CONTINUE
110  CONTINUE

WRITE(5,10130) KNT
RETURNED VALUES ARE A,SIGMAA,YFIT,CHISQR
WRITE(5,10140)
DO 120 I = 1, NTERMS
WRITE(5,10150),I,A(I),SIGMAA(I)
CONTINUE
WRITE(5,10160),CHISQR
WRITE(5,10161),P3

TOTAL PRESSURE IS =F6.2,' TORR'
A3K=A(3)*.5
A3MHZ=A3K*C/1.E+6
TYPE 345 ,A3K,A3MHZ
FORMAT(1X,'HWHM =',F9.6,' CM-1 OR ',F12.4' MHZ')
WRITE(5,10170)
ANS1=0
ACCEPT *,ANS1
IF(ANS1.EQ.1)GO TO 150
140  WRITE(5,10180)
ACCEPT *,ANS2
IF(ANS2.EQ.0) STOP
WRITE(22,10190) NGRP
WRITE(22,10190),NPTS
WRITE(22,10080)(YLABEL(I),I=1,16)
WRITE(22,10080)(XLABEL(I),I=1,10)
WRITE(22,10200)(TITLE(I),I=1,35)
WRITE(22,3451),A3K,A3MHZ,P3
OUTPUT TO TEKTRONIX PLOTTING FILE

WRITE FITTED DATA AND GENERATE NEW X VALUES

WRITE OUT THESE X AND YFIT
DO 813 I=1,NPTS
813  WRITE(22,10220) X(I),YFIT(I)
99   CONTINUE
CLOSE(UNIT=22,DEVICE='DSK',ACCESS='SEQOUT',FILE='PLTTEK.DAT')
STOP
C
OUTPUT A DATA MATRIX IN TERMINAL
150 CONTINUE
Q=0.0
C
FIND AVG OF ABS(% ERROR)
C
WRITE(5,10240)
DO 88 I=1,NPTS,10
Z=((Y(I)-YFIT(I))/YFIT(I))*100.0
Q=Q+ABS(Z)
88 WRITE(5,10250) X(I),Y(I),YFIT(I),Z
Q=10.0*Q/FLOAT(NPTS)
WRITE(5,10230)Q
WRITE(5,10240)
GO TO 140
887 FORMAT(' FINISHED ITERATION ',I2,' CHI SQ =',1PE)
10010 FORMAT(1X,'WHAT IS INPUT FILE NAME<CONTAINS OUTPUT FROM
QUICK>?)
10020 FORMAT(A10)
10060 FORMAT(10A1)
10080 FORMAT(40A1)
10090 FORMAT(40Al)
10100 FORMAT(1X,'WHICH MODE DO YOU WISH TO FIT DATA',/,
1 1X, '1=INSTRUMENTAL FITS= 1/VARIANCE',/, 2
1X,'0= NO WGH'T',/,
3 1X, ' -1= STATISTICAL=1/Y',/,
1X,'?'$)
10110 FORMAT(5X,'A(',I1,') =',1PE)
10120 FORMAT(5X,'START VALUES')
10130 FORMAT(1X,'THERE WERE ',I3,' ITERATIONS')
10140 FORMAT(1X,'USING Y=A4+Al/( (X-A2)**2 + 0.25*A3 **2)
11',1X, 'YOU OBTAIN:')
10150 FORMAT(5X,'A0,Il,') =l,1PE,t+/- '11PE)
10160 FORMAT(5X,'CHI SQUARED -',1PE)
10170 FORMAT(1X,/,1X,'D0 YOU WANT A DATA RECAP? YES-1,N0-0?'$)
10180 FORMAT(2X,I)
10190 FORMAT(40A1)
10200 FORMAT(5X,'A1-',4(1X,lPE9.2)
10210 FORMAT(2X,lPE,2X)
10220 FORMAT(1X,'MEAN OF THE ABSOLUTE VALUE OF THE % ERROR =',1F)
10230 FORMAT(1X,'PER CENT DIFF')
10240 FORMAT(2X,/,8X,'X-DATA',8X,'Y-DATA',8X,'YFIT',8X,'PER CENT DIFF')
10250 FORMAT(1X,3(1PE,3X),OPF10.2)
END
C
FUNCTION FUNCTN(X,I,A)
PURE LORENTZIAN FUNCTION

\[ Y = A_4 + \frac{(A_1)}{(x-A_2)^2 + (A_3/2)^2} \]

PLUS A BACKGROUND

C

DIMENSION X(1), A(1)
10 XI = X(I)
30 Z = XI - A(2)
30 Z2 = Z * Z
Functn = A(1) / (Z2 + (A(3) * A(3) * 0.25))
Functn = Functn + A(4)
50 RETURN
END

---- ---- ---------- -------------------------

SUBROUTINE READDT(X, Y, N)
DIMENSION X(1), Y(1)
C10 READ(21, 211) KK, N, K1, K2, K3, K4, K10, TAPENO, P3
C211 FORMAT(1X, I2, 1X, 3(I2, 1X), I1, 1X, A5, 1X, F)
READ(21, END = 22, *) (X(I), Y(I), I = J, J+4), J = 1, N, 5)
334 FORMAT(10(I1, 1PE8.2))
C WRITE(5, 334) (X(I), Y(I), I = J, J+4), J = 1, N, 5)
RETURN
22 CONTINUE
TYPE 33
33 FORMAT(' RAN OUT OF DATA IN READDT --- RECAP FOLLOWS')
TYPE 34, N
34 FORMAT(' NUMBER OF DATA POINTS = ', I)
WRITE(5, *) (X(I), Y(I), I = J, J+4), J = 1, N, 5)
RETURN
SUBROUTINE CHOP(N,X,Y)
DIMENSION X(1),Y(1)
DIMENSION XSAV(400),YSAV(400)

CHOP OUT PARTS OF THE ARRAY AND REPLACE IT IN THE ORIGINAL ARRAYS

NSAV=N
DO 10 I=1,NSAV
XSAV(I)=X(I)
10 YSAV(I)=Y(I)
YMIN=Y(1)
DO 20 I=2,NSAV
IF(YMIN .GT.Y(I)) IMIN=I
20 CONTINUE
TYPE 100,YMIN,IMIN
100 FORMAT('MINIMUM VALUE OF Y = ',F,F,' AT POINT ',I3)
YMAX=Y(1)
DO 201 I=2,NSAV
IF(Y(I) .GT. YMAX) IMAX=I
201 CONTINUE
TYPE 2011,YMAX,IMAX
2011 FORMAT('MAXIMUM VALUE OF Y = ',F,' AT POINT ',I3)
109 TYPE 110
110 FORMAT('DO YOU WANT TO CHOP PARTS OF THE ARRAY OFF? <Y=1,NO=0> ')
ACCEPT *,ANS
IF(ANS.EQ.0) RETURN
IF(ANS.EQ.1) GOTO 150
GOTO 109
150 CONTINUE
TYPE 160
160 FORMAT('INPUT OF LEFT DATA POINT TO START NEW ARRAY? ')
ACCEPT *,IST
161 FORMAT('INPUT OF DATA POINT ON RIGHT TO STOP THE ARRAY? ')
ACCEPT *,ISP
IF(ISP.LT.IST) GOTO 109
C
REPORT THE DIFFERENCE IN FREQUENCY BETWEEN THE 2 LIMITS

DIFF=X(ISP)-X(IST)
TYPE 1601,DIFF
1601 FORMAT('WAVENUMBER CHANGE ACROSS THIS SAMPLE = ',F8.7,' CM-1')
DO 30 I=IST,ISP
X(I-IST+1)=XSAV(I)
30 CONTINUE
Y(I-IST+1)=YSAV(I)
N=ISP-IST
RETURN
END

RUN BROAD

L O R E N T Z I A N FITTING FUNCTION
WHAT IS INPUT FILE NAME<CONTAINS OUTPUT FROM EARL>? FIL5
NUMBER OF DATA PAIRS = 200
MONTH =12 DAY = 19 YEAR = 79
PRESSURE IS 53.59 TORR
MINIMUM VALUE OF Y = -0.0000024 AT POINT 180
MAXIMUM VALUE OF Y = 0.0000723 AT POINT 93
DO YOU WANT TO CHOP PARTS OF THE ARRAY OFF?<Y=1,ND=0> 1
INPUT # OF LEFT DATA POINT TO START NEW ARRAY? 20
INPUT # OF DATA POINT ON RIGHT TO STOP THE ARRAY? 180
WAVENUMBER CHANGE ACROSS THIS SAMPLE = .0484009 CM-1
DO YOU WANT THE DATA NORMALIZED?<Y=1,N=0> 1
INTEGRAL OVER THE DATA IS = 8.1862793E-07
WHICH MODE DO YOU WISH TO FIT DATA
+1=INSTRUMENTAL FITS= 1/VARIANCE
0= NO WGT
-1= STATISTICAL=1/Y = ? 0
CURVE IS CONVEX

S T A R T U P V A L U E S
A(1 ) = -1.5973438E-03
A(2 ) = 1.1294275E+03
A(3 ) = 8.4991455E-03
A(4 ) = 3.6646686E-01
FINISHED ITERATION # 1 CHI SQ = 1.2879837E+02
FINISHED ITERATION # 2 CHI SQ = 1.2755936E+02
FINISHED ITERATION # 3 CHI SQ = 1.2667750E+02
FINISHED ITERATION # 4 CHI SQ = 1.2597696E+02
FINISHED ITERATION # 5 CHI SQ = 1.2537410E+02
THERE WERE 5 ITERATIONS USING Y=A4+A1/( (X-A2)**2 + 0.25*A3 **2)
YOU OBTAIN:
A(1) = 1.6568207E-03+/- 4.1651741E-06
A(2) = 1.1294275E+03+/- 3.5054553E-03
A(3) = 9.0509854E-03+/- 1.4426374E-05
A(4) = -3.5671993E-01+/- 7.9056752E-02
CHI SQUARED = 1.2537410E+02
TOTAL PRESSURE IS = 53.59 TORR
HWHM = 0.004525 CM-1 OR 135.6709 MHZ
DO YOU WANT A DATA RECAP? YES=1, NO=0

DO YOU WANT TO PLOT DATA ON GRAPHICS? (YES=1, NO=0)

STOP

END OF EXECUTION

CPU TIMES: 1.46  ELAPSED TIME: 1:3.32

EXIT
REFERENCES


5. Majorana, L.N.; Copeland, G.E.; and Harward, C.N.: Ozone Line Widths and Strengths near 1129.4 cm\(^{-1}\). Final Report (before grant continuation) for NASA Grant NAG1-1, March 1981 (GDU technical report No. PTR-81-6).


Table 1. Half-widths (HWHM) and strengths vs. N$_2$ pressure, for O$_3$ broadened with O$_3$ pressure = 3.16 torr at 285 K.

<table>
<thead>
<tr>
<th>SN$_2$ Pressure (torr)</th>
<th>Half-widths (mKaysers)</th>
<th>Strengths$^{a,b}$ cm$^{-2}$torr$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>1.615</td>
<td>48.43</td>
</tr>
<tr>
<td>10.15</td>
<td>1.929</td>
<td>57.83</td>
</tr>
<tr>
<td>15.10</td>
<td>2.290</td>
<td>68.66</td>
</tr>
<tr>
<td>19.95</td>
<td>2.784</td>
<td>83.47</td>
</tr>
<tr>
<td>30.30</td>
<td>3.819</td>
<td>114.5</td>
</tr>
<tr>
<td>50.43</td>
<td>4.491</td>
<td>134.6</td>
</tr>
<tr>
<td>60.48</td>
<td>4.945</td>
<td>148.3</td>
</tr>
<tr>
<td>90.80</td>
<td>7.600</td>
<td>227.8</td>
</tr>
<tr>
<td>100.6</td>
<td>6.834</td>
<td>205.0</td>
</tr>
</tbody>
</table>

$^a$Integration over 55 mKaysers

$^b$Numbers in ( ) are powers of 10
Figure 1. Optical setup for simultaneous measurement of reference gas spectrum, test gas spectrum and etalon tuning curve.
Figure 2. Absorption coefficient vs. wavenumber at pressure = 3.16 torr.

Figure 3. Absorption coefficient vs. wavenumber at pressure = 13.31 torr.
Figure 4. Absorption coefficient vs. wavenumber at pressure = 18.26 torr.

Figure 5. Absorption coefficient vs. wavenumber at pressure = 23.11 torr.
Figure 6. Absorption coefficient vs. wavenumber at pressure = 33.46 torr.

Figure 7. Absorption coefficient vs. wavenumber at pressure = 53.59 torr.
Figure 8. Absorption coefficient vs. wavenumber at pressure = 63.64 torr.

Figure 9. Absorption coefficient vs. wavenumber at pressure = 93.80 torr.
Figure 10. Absorption coefficient vs. wavenumber at pressure = 103.80 torr.
Figure 11. Half-width vs. pressure of $N_2$ with 3.16 torr of $O_3$. 