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Algorithm for the Calculation of Absorption Coefficient-Pressure Broadened Molecular Transitions

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22 July 1977



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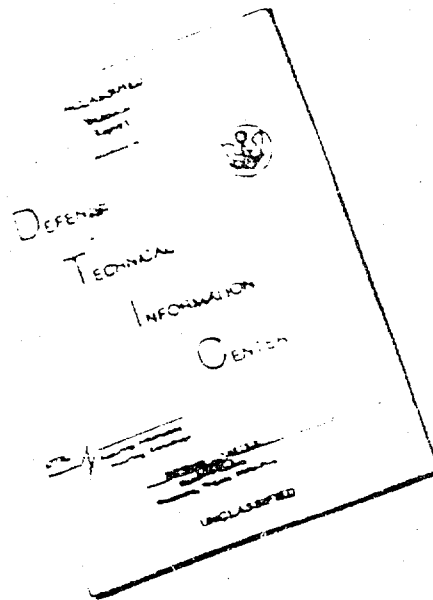
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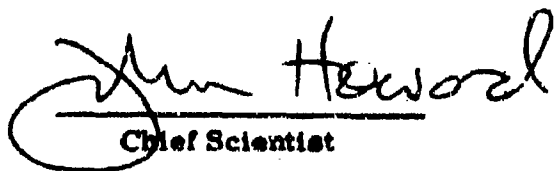
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This report describes an algorithm for the accelerated computation of the convolution of a Lorentz line shape (pressure broadened) with spectral line data. A computational savings of approximately 10 has been achieved over conventional methods. The Lorentz function has been decomposed into three functions, each of which is convolved independently at optional sampling intervals. Criteria for the determination of the sampling interval of the Lorentz function for a resultant error of 0.1 percent is described. The report contains		

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20. Abstract (Continued)

a listing of the computer program based on the algorithm and sample results in the spectral region 3550 to 3650 cm^{-1} due to water and carbon dioxide.

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Contents

1. INTRODUCTION	5
2. DECOMPOSITION OF THE LORENTZ LINE SHAPE	8
3. SAMPLING INTERVAL	15
4. APPLICATION OF THE ALGORITHM	22
5. EXTENSIONS OF THE METHOD	26
6. LINE SHAPES OTHER THAN LORENTZIAN	27
7. THE PROGRAM	27
REFERENCES	35
APPENDIX A	37
APPENDIX B	57

Illustrations

1. Decomposition of the Lorentz Function into Three Domains: -3 to 3 halfwidths, -12 to 12 halfwidths and -48 to 48 halfwidths	10
2. Functional Behavior of the Decomposed Functions Over Their Respective Limits	11

Illustrations

3. Reconstruction of the Shape of a Single Line of Strength π , halfwidth, $\alpha = 0.1$, Using a Sampling Interval of $\delta x = \alpha/4$ With a Sampling Point Positioned at the Spectral Line Center	20
4. Result of the Convolution of the Three Individual Functions With the Spectral Line Data From 3570 cm^{-1} to 3650 cm^{-1} and a Sampling Interval $DV = 0.01 \text{ cm}^{-1}$	23
5. Spectral Transmission Results From 3570 cm^{-1} to 3650 cm^{-1} at a Sampling Interval of $DV = 0.01 \text{ cm}^{-1}$ for Conditions as in Figure 4: $P = 500$ millibars, $T = 240 \text{ K}$, H_2O Column Density $= 2.9 \times 10^{18}$, and CO_2 Column Density $= 7.6 \times 10^{18} \text{ mol/cm}^2$	24
6. Flow Diagram for HIRACC Program	29
7. Flow Diagram for SUBROUTINE CONVEN	32
8. Flow Diagram for SUBROUTINE PANEL	33

Tables

1. Tabulation of the Decomposed Functions Used to Describe the Lorentz Function	12
2. Effect of Sampling Interval on the Reconstruction of the Lorentz Function Using $(\sin x/x)$ Interpolation and Four Point Lagrange Interpolation	18
A1. Listing of HIRACC Program	38
A2. Loader Map for HIRACC Program	46
A3. Sample Output From HIRACC Program	49
A4. Data Cards for HIRACC Program	55
B1. Listing of TPLLOT Program	58
B2. Loader Map for TPLLOT Program	60
B3. Sample Output From TPLLOT Program	63
B4. Data Cards for TPLLOT Program	64

Algorithm for the Calculation of Absorption Coefficient-Pressure Broadened Molecular Transitions

1. INTRODUCTION

This report describes an algorithm and associated program to perform the convolution of a line shape function with an array of absorption transitions for which the wavenumber values, the intensities, and the halfwidths are specified. The algorithm has been developed with the objectives of minimizing the number of operations to perform the convolution and of developing a program having reasonable computer storage requirements. The decrease in computational operations achieved by the present method may be utilized to decrease computer time requirements for current problems or, if necessary, to perform more extensive calculations that were not previously considered feasible.

The program described in this report uses a given line shape function (the Lorentz function) which is assumed to be independent of molecular species. The algorithm enables the calculation of the absorption coefficient at equally spaced output wavenumber increments over a specified wavenumber region. A uniform path is assumed for which the temperature, pressure, and absorber amounts are specified. The program has been written to be compatible with the AFGL line listing,¹ and performs the function of program LIN previously utilized in HITRAN (Received for publication 21 July 1977)

1. McClatchey, R. A., Benedict, W. S., Clough, S. A., Burch, D. E., Calfee, R. F., Fox, K., Rothman, L. S., and Garing, J. S. (1973) AFGL Atmospheric Absorption Line Parameters Compilation, Report No. AFGL-TR-73-0086, Environmental Research Papers, No. 434.

calculations. The algorithm has been developed with the goal of keeping the error in the absorption coefficient to within 0.1 percent.

The concept that has been developed involves the decomposition of the given line shape function into three functions which are independently convolved with the parameters for each spectral line. The first function is narrow and describes the central portion of the Lorentzian line shape, the second function is broader describing the intermediate region of the shape, and the third function is broad and may be considered to describe the "near" wing contribution of the line. The functions have been carefully chosen so that the required spectral information is retained as each function is sampled at the same number of points by the convolution process. The spectrum is reconstructed at the final stage by properly interpolating the three functions into the output array of absorption coefficients. Also included in this report is a program that performs a subsequent interpolation providing an essentially continuous resultant spectrum without requiring the convolution calculations to be performed at more output points than are required.

2. DECOMPOSITION OF THE LORENTZ LINE SHAPE

The Lorentz shape is generally applicable for pressure broadened lines for which the transition wavenumber value is large compared to the line halfwidth, and has been discussed by many authors.^{2, 3, 4} The absorption coefficient, $A_i(\nu)$, as a function of wavenumber, ν , resulting from the convolution of the Lorentz line shape with a molecular transition of wavenumber ν_i , intensity S_i , and width α_i (halfwidth at half maximum: HWHM) is given by

$$A_i(\nu) = \frac{S_i}{\pi} \frac{\alpha_i}{\alpha_i^2 + (\nu - \nu_i)^2} = \frac{S_i}{\pi \alpha_i} \frac{1}{1 + \left(\frac{\nu - \nu_i}{\alpha_i} \right)^2} \quad (1)$$

and the total absorption coefficient is given by

$$A(\nu) = \sum_i A_i(\nu) \quad (2)$$

2. Goody, R.M. (1964) Atmospheric Radiation I, Theoretical Basis, Oxford, Clarendon Press.
3. Breene, R.B., Jr. (1961) The Shift and Shape and Spectral Lines, Pergamon Press, New York.
4. Mitchell, A.C.G., and Zemansky, M.W. (1934) Resonance Radiation and Excited Atoms, The Macmillan Co., New York.

For computational purposes, it becomes advantageous to define a dimensionless variable z which for a single line is defined as

$$z = \frac{\nu - \nu_1}{\alpha_1} \quad (3)$$

where z is the wavenumber difference from the line center, ν_1 , in terms of the halfwidth of the transition. The absorption coefficient for a single line in terms of z is

$$A(z) = \frac{S}{\sigma} \frac{1/\pi}{1 + z^2} = \left(\frac{S}{\sigma}\right) L(z) \quad (4)$$

where the Lorentz function is

$$L(z) = \frac{1/\pi}{1 + z^2} \quad (5)$$

This definition has the computational advantage that $L(z)$ is explicitly independent of halfwidth and may be tabulated as a numerical function with argument z .

The function $L(z)$ has pathologically slow convergence to zero as has been discussed by Goody² and others. In order to avoid computation of the Lorentz function at values of the argument for which the function is slowly varying, the function has been decomposed into three bounded regions ($0 \leq |z| \leq Z_l$, $l = 1, 3$). We have chosen $Z_1 = 3$, $Z_2 = 12$, and $Z_3 = 48$ resulting in three functions with similar functional behavior over the bounds 0 to 3 halfwidths, 0 to 12 halfwidths and 0 to 48 halfwidths respectively.

The decomposition has been performed in a progressive manner by creating the first function (denoted as the "fast function," $XF(z)$) as the difference between the Lorentz function and an even quartic function $Q_1(z)$ chosen such that the value, the first derivative and the second derivative of $XF(z)$ are zero at the boundary Z_1 . $XF(z)$ is given by

$$XF(z) = 1/\pi (L(z) - Q_1(z)) \quad \text{for} \quad 0 \leq |z| \leq Z_1 \quad (6)$$

where

$$L'(z) = \pi L(z) = \frac{1}{1 + z^2} \quad (7)$$

$$Q_1(z) = a_1 + b_1 z^2 + c_1 z^4 \quad (8)$$

and

$$c_1 = 1/(1 + Z_b^2)^3, \quad b_1 = -c_1(1 + 3 Z_b^2) \quad \text{and} \quad a_1 = c_1(1 + 3 Z_b^2 + 3 Z_b^4). \quad (9)$$

For $Z_b = Z_1 = 3$ we obtain

$$c_1 = \frac{1}{10^3}, \quad b_1 = -\frac{28}{10^3}, \quad \text{and} \quad a_1 = \frac{271}{10^3}. \quad (10)$$

Consequently, we have for the "fast function"

$$XF(z) = 1/\pi (1/(1 + z^2) - (a_1 + b_1 z^2 + c_1 z^4)) \quad 0 \leq |z| \leq 3, \quad (11)$$

$$XF(z) = 0 \quad 3 \leq |z|. \quad (12)$$

The second function, the "slow function," $XS(z)$, is constructed in a similar manner by defining an even quartic function, $Q_2(z)$, in the domain $3 \leq |z| \leq 12$ which matches the Lorentzian at $z = Z_b = Z_2 = 12$. We obtain by performing operations similar to those above

$$XS(z) = 1/\pi (L'(z) - Q_2(z)) \quad \text{for} \quad 3 \leq |z| \leq 12 \quad (13)$$

with the coefficients for $Q_2(z)$ given by

$$c_2 = \frac{1}{145^3}, \quad b_2 = -433 \cdot c_2, \quad \text{and} \quad a_2 = 62641 \cdot c_2. \quad (14)$$

The "slow function" is then defined as

$$XS(z) = 1/\pi (Q_1(z) - Q_2(z)) \quad 0 \leq |z| \leq 3, \quad (15)$$

$$XS(z) = 1/\pi (1/(1 + z^2) - (a_2 + b_2 z^2 + c_2 z^4)) \quad 3 \leq |z| \leq 12, \quad (16)$$

$$XS(z) = 0 \quad 12 \leq |z|. \quad (17)$$

The third function, the "very slow function," $XVS(z)$, is defined as the Lorentzian for $12 \leq |z| \leq 48$ and as $Q_2(z)$ for $0 \leq |z| \leq 12$.

The following tabular form of the decomposition into the respective domains will make the process more clear:

FUNCTION	DOMAIN		
	$0 \leq z \leq 3$	$3 \leq z \leq 12$	$12 \leq z \leq 48$
XF(z)	$\frac{1}{\pi} (L'(z) - Q_1(z))$	0	0
XS(z)	$\frac{1}{\pi} (Q_1(z) - Q_2(z))$	$\frac{1}{\pi} (L'(z) - Q_2(z))$	0
XVS(z)	$\frac{1}{\pi} Q_2(z)$	$\frac{1}{\pi} Q_2(z)$	$\frac{1}{\pi} L'(z)$

(18)

Note that the three functions sum to the Lorentzian in each domain and that the functions are continuous in value, first and second derivative across the boundaries of the domains.

While the choices of the functions and the boundaries may appear to be somewhat arbitrary, an examination of the result demonstrates the advantage of the imposed conditions. Figure 1 is a plot of the three functions from -48 to +48 half-widths and indicates the dependence of XF(z), XS(z), and XVS(z) as a function of the variable z. It should be noted that 40.71 percent of the integral of the Lorentz function is contained in XF, 42.47 percent in XS, and 15.50 percent in XVS. The remaining 1.32 percent is outside the 48 halfwidth cutoff.

The three functions are represented in Figure 2 with the horizontal axis determined by the boundary of each function and the vertical axis chosen appropriately for each function. The three functions in this representation are seen to be functionally similar and as a consequence, it is possible to sample each function at the same sampling interval to perform the convolution. One hundred and fifty one (151) values of each symmetric function are stored in the computer program, and it is these values that are plotted in Figure 2 as indicated by the index on the top horizontal axis. The tabulation of this number of values for the functions precludes the necessity for interpolation in the convolution calculation. The values of the functions are tabulated in Table 1.

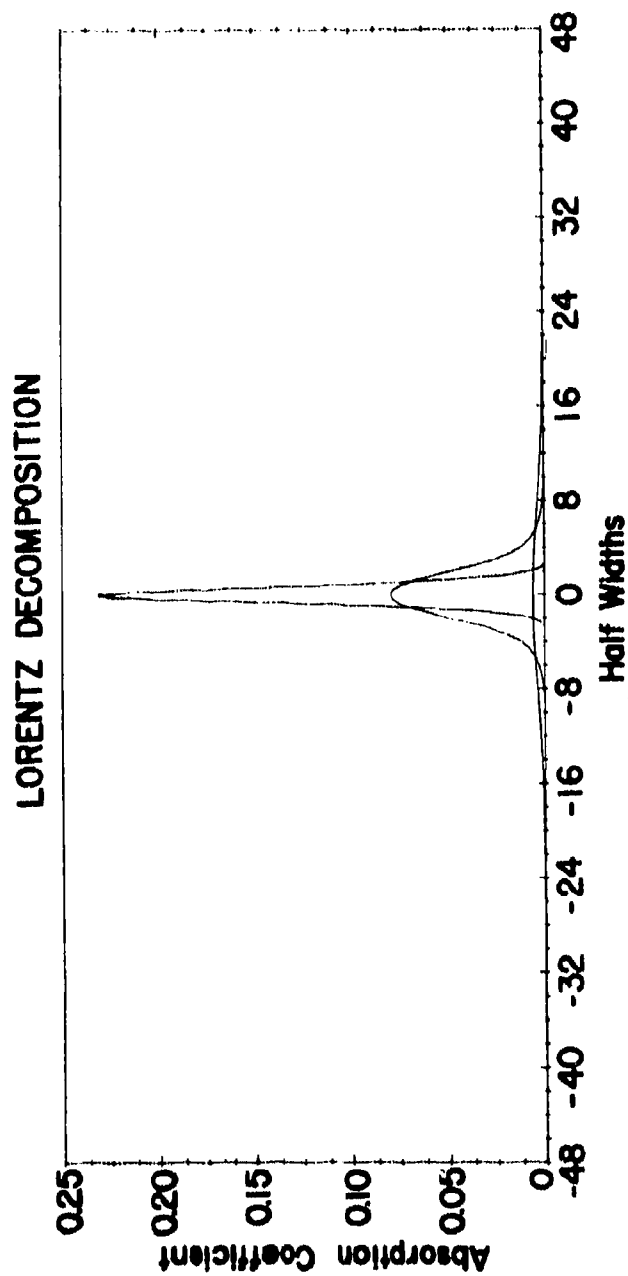


Figure 1. Decomposition of the Lorentz Function into Three Domains: -3 to 3 halfwidths, -12 to 12 halfwidths and -48 to 48 halfwidths. The sum of the three functions gives $L(z) = (1/\pi)(1/1 + z^2)$

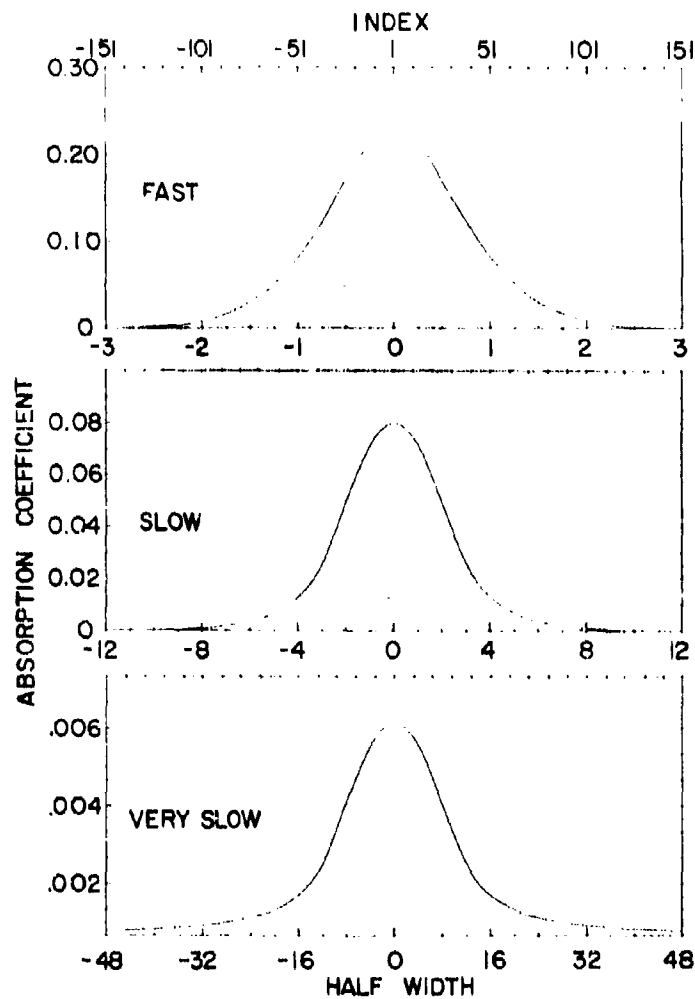


Figure 2. Functional Behavior of the Decomposed Functions Over Their Respective Limits. Plots are direct plots of the functions in terms of the storage index of the program. The fast function (XF) is on the top, the slow function (XS) is in the middle, and the very slow functions (XVS) are on the bottom

Table 1. Tabulation of the Decomposed Functions Used to Describe the Lorentz Function. The variable z is defined as the wavenumber difference from the line center in terms of the halfwidth, α , that is, $z = |(\nu - \nu_0)/\alpha|$. Plots of the three tabulated functions appear in Figure 2 and Figure 3

INDEX		"FAST" FUNCTION FN		"SLOW" FUNCTION FN		"VERY SLOW" FUNCTION FN
	z		z		z	
1	0.000	2.320E-01	0.000	7.972E-02	0.000	6.540E-03
2	.020	2.319E-01	.010	7.966E-02	.320	6.516E-03
3	.040	2.316E-01	.140	7.949E-02	.640	6.522E-03
4	.060	2.309E-01	.240	7.921E-02	.960	6.499E-03
5	.080	2.301E-01	.320	7.882E-02	1.280	6.467E-03
6	.100	2.290E-01	.400	7.811E-02	1.600	6.425E-03
7	.120	2.277E-01	.480	7.770E-02	1.920	6.375E-03
8	.140	2.261E-01	.560	7.697E-02	2.240	6.316E-03
9	.160	2.243E-01	.640	7.614E-02	2.560	6.249E-03
10	.180	2.223E-01	.720	7.521E-02	2.880	6.173E-03
11	.200	2.202E-01	.800	7.418E-02	3.200	6.088E-03
12	.220	2.178E-01	.880	7.305E-02	3.520	5.996E-03
13	.240	2.152E-01	.960	7.182E-02	3.840	5.896E-03
14	.260	2.125E-01	1.040	7.050E-02	4.160	5.789E-03
15	.280	2.096E-01	1.120	6.910E-02	4.480	5.675E-03
16	.300	2.066E-01	1.200	6.761E-02	4.800	5.554E-03
17	.320	2.034E-01	1.280	6.605E-02	5.120	5.427E-03
18	.340	2.001E-01	1.360	6.441E-02	5.440	5.294E-03
19	.360	1.967E-01	1.440	6.270E-02	5.760	5.155E-03
20	.380	1.932E-01	1.520	6.093E-02	6.080	5.012E-03
21	.400	1.896E-01	1.600	5.911E-02	6.400	4.864E-03
22	.420	1.859E-01	1.680	5.723E-02	6.720	4.712E-03
23	.440	1.821E-01	1.760	5.531E-02	7.040	4.556E-03
24	.460	1.783E-01	1.840	5.335E-02	7.360	4.398E-03
25	.480	1.745E-01	1.920	5.136E-02	7.680	4.237E-03
26	.500	1.706E-01	2.000	4.934E-02	8.000	4.075E-03
27	.520	1.667E-01	2.080	4.731E-02	8.320	3.911E-03
28	.540	1.628E-01	2.160	4.528E-02	8.640	3.747E-03
29	.560	1.588E-01	2.240	4.324E-02	8.960	3.584E-03
30	.580	1.549E-01	2.320	4.121E-02	9.280	3.421E-03
31	.600	1.510E-01	2.400	3.920E-02	9.600	3.261E-03
32	.620	1.470E-01	2.480	3.722E-02	9.920	3.103E-03
33	.640	1.432E-01	2.560	3.527E-02	10.240	2.948E-03
34	.660	1.393E-01	2.640	3.338E-02	10.560	2.797E-03
35	.680	1.355E-01	2.720	3.153E-02	10.880	2.652E-03
36	.700	1.317E-01	2.800	2.976E-02	11.200	2.512E-03
37	.720	1.279E-01	2.880	2.806E-02	11.520	2.379E-03
38	.740	1.242E-01	2.960	2.646E-02	11.840	2.255E-03
39	.760	1.205E-01	3.040	2.495E-02	12.160	2.138E-03
40	.780	1.169E-01	3.120	2.354E-02	12.480	2.031E-03
41	.800	1.134E-01	3.200	2.223E-02	12.800	1.931E-03
42	.820	1.099E-01	3.280	2.100E-02	13.120	1.839E-03
43	.840	1.065E-01	3.360	1.986E-02	13.440	1.752E-03
44	.860	1.031E-01	3.440	1.878E-02	13.760	1.672E-03
45	.880	9.984E-02	3.520	1.776E-02	14.080	1.598E-03
46	.900	9.661E-02	3.600	1.683E-02	14.400	1.528E-03
47	.920	9.345E-02	3.680	1.594E-02	14.720	1.462E-03
48	.940	9.035E-02	3.760	1.511E-02	15.040	1.401E-03
49	.960	8.733E-02	3.840	1.432E-02	15.360	1.343E-03
50	.980	8.437E-02	3.920	1.358E-02	15.680	1.289E-03
51	1.000	8.149E-02	4.000	1.288E-02	16.000	1.239E-03
52	1.020	7.867E-02	4.080	1.222E-02	16.320	1.191E-03
53	1.040	7.592E-02	4.160	1.160E-02	16.640	1.145E-03
54	1.060	7.324E-02	4.240	1.101E-02	16.960	1.103E-03
55	1.080	7.063E-02	4.320	1.046E-02	17.280	1.062E-03
56	1.100	6.809E-02	4.400	9.930E-03	17.600	1.024E-03
57	1.120	6.561E-02	4.480	9.432E-03	17.920	9.882E-04
58	1.140	6.320E-02	4.560	8.960E-03	18.240	9.539E-04
59	1.160	6.086E-02	4.640	8.513E-03	18.560	9.214E-04
60	1.180	5.858E-02	4.720	8.089E-03	18.880	8.909E-04

Table 1. Tabulation of the Decomposed Functions Used to Describe the Lorentz Function. The variable z is defined as the wavenumber difference from the line center in terms of the halfwidth, α , that is, $z = (\nu - \nu_0)/\alpha$. Plots of the three tabulated functions appear in Figure 2 and Figure 3 (Cont.)

INDEX	"FAST"		"SLOW"		"VERY SLOW"	
	Z	FUNCTION FN	Z	FUNCTION FN	Z	FUNCTION FN
61	1.200	5.637E-02	4.800	7.687E-03	19.200	8.611E-04
62	1.220	5.422E-02	4.840	7.305E-03	19.520	8.332E-04
63	1.240	5.213E-02	4.960	6.942E-03	19.840	8.066E-04
64	1.260	5.010E-02	5.040	6.597E-03	20.160	7.813E-04
65	1.280	4.813E-02	5.120	6.269E-03	20.480	7.571E-04
66	1.300	4.622E-02	5.200	5.958E-03	20.800	7.340E-04
67	1.320	4.437E-02	5.280	5.661E-03	21.120	7.120E-04
68	1.340	4.258E-02	5.360	5.379E-03	21.440	6.910E-04
69	1.360	4.084E-02	5.440	5.111E-03	21.760	6.708E-04
70	1.380	3.915E-02	5.520	4.855E-03	22.080	6.516E-04
71	1.400	3.752E-02	5.600	4.611E-03	22.400	6.331E-04
72	1.420	3.594E-02	5.680	4.379E-03	22.720	6.155E-04
73	1.440	3.441E-02	5.760	4.158E-03	23.040	5.985E-04
74	1.460	3.293E-02	5.840	3.947E-03	23.360	5.822E-04
75	1.480	3.150E-02	5.920	3.746E-03	23.680	5.666E-04
76	1.500	3.012E-02	6.000	3.555E-03	24.000	5.517E-04
77	1.520	2.879E-02	6.080	3.372E-03	24.320	5.373E-04
78	1.540	2.749E-02	6.160	3.198E-03	24.640	5.234E-04
79	1.560	2.625E-02	6.240	3.032E-03	24.960	5.101E-04
80	1.580	2.504E-02	6.320	2.873E-03	25.280	4.973E-04
81	1.600	2.388E-02	6.400	2.722E-03	25.600	4.850E-04
82	1.620	2.276E-02	6.480	2.578E-03	25.920	4.731E-04
83	1.640	2.168E-02	6.560	2.441E-03	26.240	4.616E-04
84	1.660	2.064E-02	6.640	2.309E-03	26.560	4.506E-04
85	1.680	1.963E-02	6.720	2.184E-03	26.880	4.399E-04
86	1.700	1.866E-02	6.800	2.065E-03	27.200	4.297E-04
87	1.720	1.773E-02	6.880	1.951E-03	27.520	4.197E-04
88	1.740	1.684E-02	6.960	1.843E-03	27.840	4.102E-04
89	1.760	1.597E-02	7.040	1.739E-03	28.160	4.009E-04
90	1.780	1.514E-02	7.120	1.641E-03	28.480	3.920E-04
91	1.800	1.435E-02	7.200	1.547E-03	28.800	3.833E-04
92	1.820	1.358E-02	7.280	1.457E-03	29.120	3.749E-04
93	1.840	1.284E-02	7.360	1.372E-03	29.440	3.668E-04
94	1.860	1.214E-02	7.440	1.291E-03	29.760	3.590E-04
95	1.880	1.146E-02	7.520	1.213E-03	30.080	3.514E-04
96	1.900	1.081E-02	7.600	1.140E-03	30.400	3.441E-04
97	1.920	1.019E-02	7.680	1.070E-03	30.720	3.369E-04
98	1.940	9.594E-03	7.760	1.003E-03	31.040	3.300E-04
99	1.960	9.024E-03	7.840	9.397E-04	31.360	3.233E-04
100	1.980	8.479E-03	7.920	8.796E-04	31.680	3.169E-04
101	2.000	7.958E-03	8.000	8.224E-04	32.000	3.105E-04
102	2.020	7.460E-03	8.080	7.682E-04	32.320	3.044E-04
103	2.040	6.985E-03	8.160	7.167E-04	32.640	2.985E-04
104	2.060	6.532E-03	8.240	6.679E-04	32.960	2.927E-04
105	2.080	6.101E-03	8.320	6.217E-04	33.280	2.871E-04
106	2.100	5.690E-03	8.400	5.779E-04	33.600	2.817E-04
107	2.120	5.299E-03	8.480	5.365E-04	33.920	2.764E-04
108	2.140	4.928E-03	8.560	4.973E-04	34.240	2.713E-04
109	2.160	4.575E-03	8.640	4.603E-04	34.560	2.663E-04
110	2.180	4.241E-03	8.720	4.254E-04	34.880	2.614E-04
111	2.200	3.924E-03	8.800	3.925E-04	35.200	2.567E-04
112	2.220	3.624E-03	8.880	3.619E-04	35.520	2.521E-04
113	2.240	3.341E-03	8.960	3.323E-04	35.840	2.476E-04
114	2.260	3.073E-03	9.040	3.049E-04	36.160	2.433E-04
115	2.280	2.821E-03	9.120	2.791E-04	36.480	2.390E-04
116	2.300	2.584E-03	9.200	2.550E-04	36.800	2.349E-04
117	2.320	2.361E-03	9.280	2.324E-04	37.120	2.308E-04
118	2.340	2.152E-03	9.360	2.113E-04	37.440	2.269E-04
119	2.360	1.956E-03	9.440	1.916E-04	37.760	2.231E-04
120	2.380	1.773E-03	9.520	1.732E-04	38.080	2.194E-04

Table 1. Tabulation of the Decomposed Functions Used to Describe the Lorentz Function. The variable z is defined as the wavenumber difference from the line center in terms of the halfwidth, α , that is, $z = [(\nu - \nu_0)/\alpha]$. Plots of the three tabulated functions appear in Figure 2 and Figure 3 (Cont.)

INDEX	"FAST" FUNCTION FN		"SLOW" FUNCTION FN		"VERY SLOW" FUNCTION FN	
	z		z		z	
121	2.400	1.602E-03	9.600	1.561E-04	38.400	2.157E-04
122	2.420	1.442E-03	9.680	1.403E-04	38.720	2.122E-04
123	2.440	1.294E-03	9.760	1.256E-04	39.040	2.087E-04
124	2.460	1.157E-03	9.840	1.121E-04	39.360	2.053E-04
125	2.480	1.030E-03	9.920	9.995E-05	39.680	2.020E-04
126	2.500	9.131E-04	10.000	8.806E-05	40.000	1.988E-04
127	2.520	8.055E-04	10.080	7.753E-05	40.320	1.957E-04
128	2.540	7.070E-04	10.160	6.791E-05	40.640	1.926E-04
129	2.560	6.170E-04	10.240	5.915E-05	40.960	1.896E-04
130	2.580	5.352E-04	10.320	5.121E-05	41.280	1.867E-04
131	2.600	4.610E-04	10.400	4.403E-05	41.600	1.838E-04
132	2.620	3.942E-04	10.480	3.758E-05	41.920	1.810E-04
133	2.640	3.343E-04	10.560	3.182E-05	42.240	1.783E-04
134	2.660	2.809E-04	10.640	2.669E-05	42.560	1.756E-04
135	2.680	2.336E-04	10.720	2.215E-05	42.880	1.730E-04
136	2.700	1.920E-04	10.800	1.818E-05	43.200	1.705E-04
137	2.720	1.557E-04	10.880	1.472E-05	43.520	1.680E-04
138	2.740	1.244E-04	10.960	1.174E-05	43.840	1.655E-04
139	2.760	9.758E-05	11.040	9.194E-06	44.160	1.631E-04
140	2.780	7.498E-05	11.120	7.054E-06	44.480	1.608E-04
141	2.800	5.620E-05	11.200	5.280E-06	44.800	1.585E-04
142	2.820	4.088E-05	11.280	3.834E-06	45.120	1.563E-04
143	2.840	2.865E-05	11.360	2.653E-06	45.440	1.541E-04
144	2.860	1.915E-05	11.440	1.791E-06	45.760	1.519E-04
145	2.880	1.203E-05	11.520	1.124E-06	46.080	1.498E-04
146	2.900	6.947E-06	11.600	6.479E-07	46.400	1.478E-04
147	2.920	3.549E-06	11.680	3.306E-07	46.720	1.458E-04
148	2.940	1.494E-06	11.760	1.790E-07	47.040	1.438E-04
149	2.960	4.418E-07	11.840	4.104E-08	47.360	1.419E-04
150	2.980	5.511E-08	11.920	5.113E-09	47.680	1.400E-04
151	3.000	0.	12.000	0.	48.000	1.381E-04

The rationalization for terminating the convolution at 48 halfwidths is based on three considerations: (1) evidence that the line shape deviates from Lorentz behavior for $(\nu - \nu_0)$ of the order of 5 cm^{-1} , corresponding to $z \approx 48$ for a typical atmospheric line at atmospheric pressure (Winters et al;⁵ Holstein;⁶ Breene;³ Burch;⁷) (2) the value of the Lorentzian at 48 halfwidths is 1.38×10^{-4} which is

5. Winters, B.H., Silverman, S., and Benedict, W.S. (1964) Line shape in the wing beyond the band head of the 4.3μ band of CO_2 , J. Quant. Spect. Rad. Trans., 4:527.
6. Holstein, T. (1950) Pressure broadening of spectral lines, Phys. Rev. 79:744; see also L. Spitzer Phys. Rev. 58:348 (1940).
7. Burch, D.E., Grynak, D.A., Patty, R.R. and Bartky, C.E. (1968) The Shapes of Collision Broadened CO_2 Lines, Philco Ford Corp., Aeronutronic Report U-3203.

sufficiently small for most calculations, and (3) calculation beyond 48 halfwidths requires an unwarranted increase in computational effort. Although the value of the Lorentz function may justify termination of the calculation at 48 halfwidths, it must not be forgotten that 1.32 percent of the integrated absorption is beyond this region. This is a result of the previously mentioned slow convergence of $1/x^2$ (Goody,² and Townes and Schawlow⁸). It is suggested that calculations of the far wings of the lines can more appropriately be done in a parametrized tabulation of what is currently referred to as the continuum for each of the molecular species of interest. The contribution of this continuum function to the absorption coefficient may be calculated at large sampling intervals in the wavenumber domain with negligible effect on computational time.

3. SAMPLING INTERVAL

General discussions of the proper choice of the sampling interval appear in the literature for the type of "line by line" calculations described in this report.^{9, 10, 11, 12} These references are primarily concerned with the effect of the sampling interval on the integral of the absorption coefficient or absorptance over a specified wavenumber interval. That approach is particularly appropriate to the case in which an instrumental scanning function that is broad compared to the spectral line widths, is being convolved with the true line spectrum. The present discussion is concerned with the development of a quantitative evaluation of the error introduced in the reconstruction of the spectrum in the interval between sampled points.

An approach that provides direct insight into the problem of determining the sampling interval is that obtained from information theory and the Nyquist sampling theorem. Simple and readily comprehensible discussions of this are provided by

8. Townes, C. H., and Schawlow, A. L. (1955) Microwave Spectroscopy, McGraw Hill-Book Co., New York.
9. Drayson, D. R. (1967) The Calculation of Long Wave Radiative Transfer in Planetary Atmospheres, Report No. 07584-1-T, University of Michigan, Ann Arbor.
10. Kyle, T. G. (1968) Net interval for calculating absorption spectra, J. Opt. Soc. Am. 58:192.
11. Scott, N. A. (1974) A direct method of computation of the transmission function of an inhomogeneous gaseous medium, I: Description of the method, J. Quant. Spect. Rad. Trans. 14:891.
12. Kunde, V. G., and McQuire, W. C. (1974) Direct integration transmittance model, J. Quant. Spect. Rad. Trans. 14:803.

Brigham¹³ and Bracewell.¹⁴ The sampling theorem states that if the Fourier transform of a function is zero for all frequencies greater than frequency f_0 , then the continuous function $g(x)$ can be uniquely determined from its sampled values, $g_n(n\delta x)$, if the sampling interval is chosen as

$$\delta x = \frac{1}{2f_0} \quad (19)$$

In particular, the continuous function $g(x)$ can be reconstructed for all x by convolving the continuous interpolating function

$$s(x) = \frac{1}{\delta x} \frac{\sin\left(\pi \frac{x}{\delta x}\right)}{\left(\pi \frac{x}{\delta x}\right)} \quad (20)$$

with the sampled function $g_n(n\delta x)$ where n is integer. That is,

$$g(x) = g_n(n\delta x) * s(x) \quad (21)$$

or explicitly for the discrete convolution we have

$$g(x) = \sum_{n=-\infty}^{\infty} g_n(n\delta x) \frac{\sin \pi \left(\frac{x}{\delta x} - n\right)}{\pi \left(\frac{x}{\delta x} - n\right)} \quad (22)$$

In the present case, the Fourier transform of the Lorentz function does not have a frequency, f_0 , beyond which the transform is zero. Consequently by sampling at discrete intervals, it is not possible to exactly reconstruct the continuous function. However, by properly choosing the interval, the difference between the exact and reconstructed functions can be held within a predetermined limit. The Lorentz function is given as

$$g(x) = \frac{1}{\pi} \frac{a}{a^2 + x^2} \quad (23)$$

13. Brigham, E.O. (1974) The Fast Fourier Transform, Englewood Cliffs, New Jersey.

14. Bracewell, R.M. (1965) The Fourier Transform and Its Applications, McGraw-Hill, New York.

where $x = \nu - \nu_0$, α is the halfwidth, and ν_0 is the wavenumber value of the transition. The Fourier transform of $g(x)$ is

$$\mathcal{F}(g(x)) = \mathcal{F}(f) = e^{-2\pi\alpha f} \quad (24)$$

where $\mathcal{F}$ is the Fourier transform operator. If the value of the transform is assumed to be zero beyond a frequency, f_0 , this is equivalent to multiplying the complete transform by a rectangular box, $\mathcal{L}(f)$, where

$$\mathcal{L}(f) = \begin{cases} 1 & |f| < f_0 \\ \frac{1}{2} & |f| = f_0 \\ 0 & |f| > f_0 \end{cases} \quad (25)$$

We may define the sampling interval as before such that

$$\delta x = \frac{1}{2f_0} \quad (26)$$

The Fourier transform of $\mathcal{L}(f)$ in the x domain is given by

$$s(x) = \frac{1}{\delta x} \frac{\sin\left(\pi \frac{x}{\delta x}\right)}{\left(\pi \frac{x}{\delta x}\right)} \quad (27)$$

which is identical to the scanning function prescribed by the Nyquist sampling theorem (Eq. (20)).

In order to evaluate the error caused by the discrete sampling interval and the associated truncation of the function in the Fourier domain, calculations have been made using the interpolating function, Eq. (27), convolved with the sampled Lorentz function

$$g_s(n\delta x) = \frac{1}{\pi} \frac{\alpha}{\alpha^2 + (n\delta x)^2} \quad (28)$$

as indicated in Eq. (23). For these convolution calculations, a more relevant definition of the sampling interval, δx , is given in terms of the halfwidth, α ,

$$\delta x = \frac{\alpha}{N} \quad (29)$$

The results are evaluated for sampling intervals expressed in fractions, $1/N$, of the halfwidth. For this definition, we have for the sampled Lorentz function

$$g_N \left(\frac{n}{N} \right) = \frac{1}{\pi n} \frac{1}{1 + \left(\frac{n}{N} \right)^2} \quad (30)$$

A quantitative evaluation of the effect of the sampling interval, is the RMS deviation of the function interpolated at three intermediate points per interval from the function calculated exactly at the same intermediate points. The results of these calculations are given in Table 2. These results are a measure of the amount of information lost due to the choice of sampling interval. As the sampling interval becomes infinitesimally small, the RMS deviation approaches zero. It is seen that for an interval of $a/4$, that is, $N = 4$, the RMS deviation is negligibly small and essentially all of the information is retained.

Table 2. Effect of Sampling Interval on the Reconstruction of the Lorentz Function Using $(\sin x/x)$ Interpolation and Four Point Lagrange Interpolation. Interpolations are calculated at three equally spaced points between the sampled values. In all cases the maximum percent deviation using the four point Lagrange occurs in the first sampled interval. Deviations are calculated as the difference between the interpolated value and the exact value of the function

Sampling Interval		Interpolation Method		
		$\frac{\sin x}{x}$	Four Point Lagrange	
N	$\delta x = \frac{a}{N}$	rms deviation	rms deviation	max percent deviation
1	a	1.1×10^{-3}	3.5×10^{-3}	-1.9
2	$\frac{a}{2}$	0.067	0.20	-0.99
3	$\frac{a}{3}$	0.0035	0.087	-0.37
4	$\frac{a}{4}$	0.00063	0.028	-0.15

There is another consideration that must be taken into account in this situation. Although the information is retained for a sampling interval of $a/4$, the computational effort to retrieve this information using the $(\sin x/x)$ interpolation is large and in some cases may be of the same magnitude as that required to evaluate the function directly at the intermediate intervals.

In order to retrieve sufficient information with reasonable computational effort and stay within a specified error criterion for the absorption coefficient calculation, a four point interpolation function has been used instead of the prohibitively long "sin x/x" interpolation. The output points are assumed to be equally spaced. Values for the weighting factors necessary to perform the interpolation at three equally spaced intermediate points are given by the following three equations:

$$g\left(x + \frac{\delta x}{4}\right) = -\frac{7}{128} g(x - \delta x) + \frac{105}{128} g(x) + \frac{35}{128} g(x + \delta x) - \frac{5}{128} g(x + 2\delta x) \quad (31)$$

$$g\left(x + \frac{\delta x}{2}\right) = -\frac{1}{16} g(x - \delta x) + \frac{9}{16} g(x) + \frac{1}{16} g(x + \delta x) - \frac{1}{16} g(x + 2\delta x) \quad (32)$$

$$g\left(x + \frac{3\delta x}{4}\right) = -\frac{5}{128} g(x - \delta x) + \frac{35}{128} g(x) + \frac{105}{128} g(x + \delta x) - \frac{7}{128} g(x + 2\delta x) \quad (33)$$

The interpolation scheme that has been employed in this development is due to Lagrange and is well described by Acton.¹⁵ In Table 2, the maximum percent deviation in the interpolated values is indicated. This error always occurs within one or two intervals from the line center. For a sampling interval of $\alpha/4$, the error is 0.15 percent. Although this error at the line center is slightly larger than desirable, the added complication of using a more refined interpolation does not presently seem warranted. Furthermore, the percent error decreases rapidly away from the line center.

The four point interpolation scheme is used for interpolating the "very slow array," and the "slow array" into the "fast array." This is required since the sampling criterion of $\alpha/4$ has been used for the calculation of the three arrays where the effective α is appropriate to each array.

Similarly, for the presentation of the final results, the fast array is interpolated into a plotting array in a separate program which represents the final result. Figure 3 depicts the effect of this interpolation scheme as compared to the result obtained with linear interpolation. It should be noted that the error for a complete spectrum can only be the same or less than that for a single line. This is readily concluded from the superposition theorem.

One final consideration that provides information on the sampling interval, is the Rayleigh criterion.¹⁶ For two spectral lines of unit strength and equal half-widths, separated by two halfwidths, let us determine the sampling interval required to exactly reproduce the minimum between the two spectral lines.

15. Acton, F. S. (1970) Numerical Methods That Work, New York.

16. Born, M., and Wolf, E. (1965) Principles of Optics, Oxford, Pergamon Press.

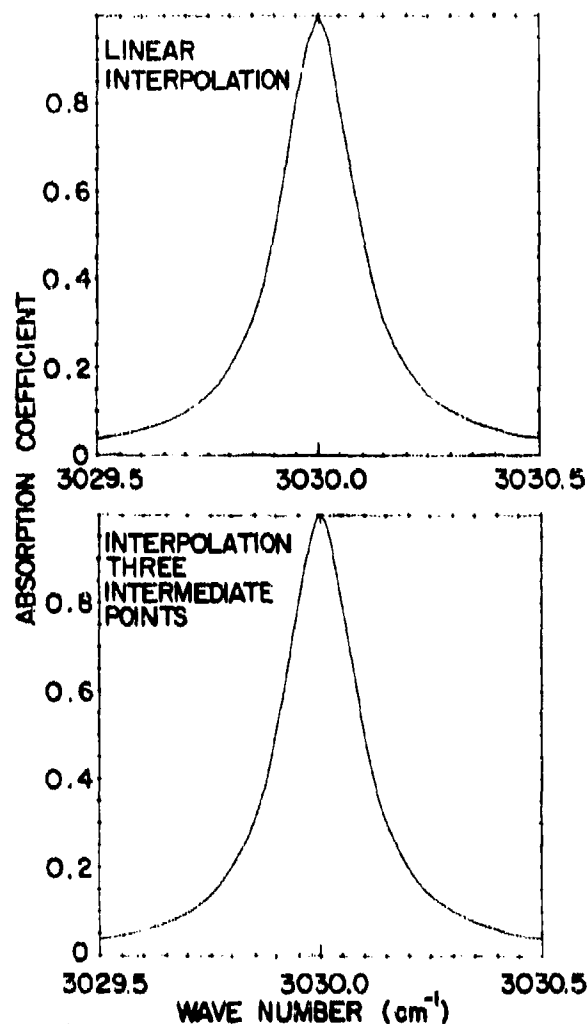


Figure 3. Reconstruction of the Shape of a Single Line of Strength τ , halfwidth, $\alpha = 0.1$, Using a Sampling Interval of $\delta x = \alpha/4$ With a Sampling Point Positioned at the Spectral Line Center. The upper curve uses linear interpolation of the convolution output and the lower curve uses the 4 point Lagrange interpolation. To emphasize the line center, the region from -5 to $+5$ halfwidths is depicted

Consider one line centered at $x = 0$ and the other line centered at $x = x_0$. We have for the two Lorentz functions

$$g_1(x) = \frac{1}{\pi} \frac{\alpha}{\alpha^2 + x^2} \quad (34)$$

and

$$g_2(x) = \frac{1}{\pi} \frac{\alpha}{\alpha^2 + (x - x_0)^2} \quad (35)$$

The Fourier transform for this pair is given by

$$g(f) = e^{-2\pi\alpha f} + e^{-2\pi\alpha f} \cos(2\pi x_0 f) \quad (36)$$

The Rayleigh criterion postulates $x_0 = 2\alpha$ giving for the transform

$$g(f) = e^{-2\pi\alpha f} (1 + \cos 4\pi\alpha f) \quad (37)$$

To exactly reproduce the minimum between the doublet, one period of the oscillatory function is required, giving

$$4\pi\alpha f_0 = 2\pi \quad (38)$$

so that the cut off frequency is

$$f_0 = \frac{1}{2\alpha} \quad (39)$$

and the sampling interval from the Nyquist theorem, is

$$\delta x = \frac{1}{2f_0} = \alpha \quad (40)$$

This result indicates that the sampling interval of $\alpha/4$, previously determined, is well within the Rayleigh criterion for resolving a Lorentzian doublet separated by two halfwidths.

4. APPLICATION OF THE ALGORITHM

In the previous sections, two basic steps for an improved computational procedure to perform the convolution of the Lorentz line shape with a set of absorption line data have been described: (1) the decomposition of the line shape into bounded domains, and (2) the criterion for determining the sampling interval. In this section we describe the application of the algorithm to obtain the absorption coefficient as a function of wavenumber for a set of spectral line data parameters that are appropriate for the specified values of temperature, pressure, and column density. Three separate convolutions utilizing the fast (XF), the slow (XS), and the very slow (XVS) functions are performed on the data set. The results of the three convolutions for a specific set of data are displayed in transmittance in Figure 4. For this case the average halfwidth is of the order of 0.04 cm^{-1} so that the sampling interval used is $\delta x = \alpha/4 = 0.01 \text{ cm}^{-1}$. Each convolution function is sampled at approximately 24 values corresponding to intervals of 0.01 cm^{-1} for the fast function, 0.04 cm^{-1} for the slow function, and 0.16 cm^{-1} for the very slow function. Seventy-two (72) points have been sampled to reproduce the Lorentzian from -48 to $+48$ halfwidths instead of 384 (4×96) which would be required if the function were sampled at equal intervals of $\alpha/4$ (0.01 cm^{-1}). Consequently, the algorithm as applied in this case provides a computational savings of a factor $5 \frac{1}{3}$. The actual saving using an optimized version of the conventional method compared to the present method is a factor of 10. The additional factor of two is due to the use of tabulated rather than calculated functions and to reduced overhead time in setting up the inner convolution loop. The results of the two computational methods are given in Figure 5 and no differences are discernable. It should be noted that the lower spectrum of Figure 5 is equivalent to the product of the three functions presented in Figure 4, since the functions are all on a transmittance scale.

Some further consideration needs to be given to the method described here with respect to the theoretical computational gain. If the assumption is made that the line shape function can be decomposed into M functions, and that the sampling interval is the same for the first decomposed function as for the total Lorentz function, $\alpha/4$, then the gain, G , is

$$G = \frac{N_{\text{tot}}}{\sum_m^M N_m \left(\frac{\delta x_1}{\delta x_m} \right)} \quad (41)$$

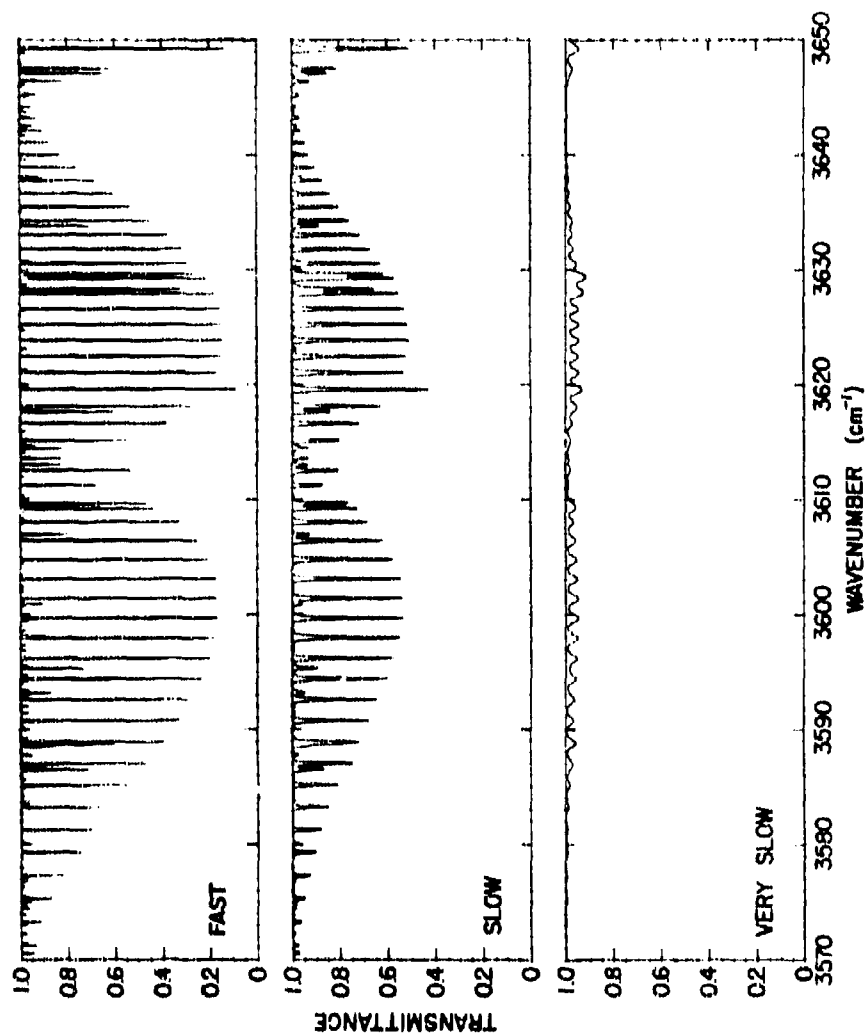


Figure 4. Results of the Convolution of the Three Individual Functions With the Spectral Line Data From 3570 cm^{-1} to 3650 cm^{-1} and a Sampling Interval $\Delta\nu = 0.01\text{ cm}^{-1}$. From top to bottom the plots are the result of the fast function, slow function and very slow function convolutions respectively. The conditions are $P = 500$ millibars, $T = 240\text{ K}$, H_2O column density $= 2.9 \times 10^{18}$, and CO_2 column density $= 7.6 \times 10^{18}\text{ mol/cm}^2$. The results are expressed in transmittance to increase the dynamic range of the presentation. The product of the three spectra give the total result shown in the upper spectrum of Figure 5

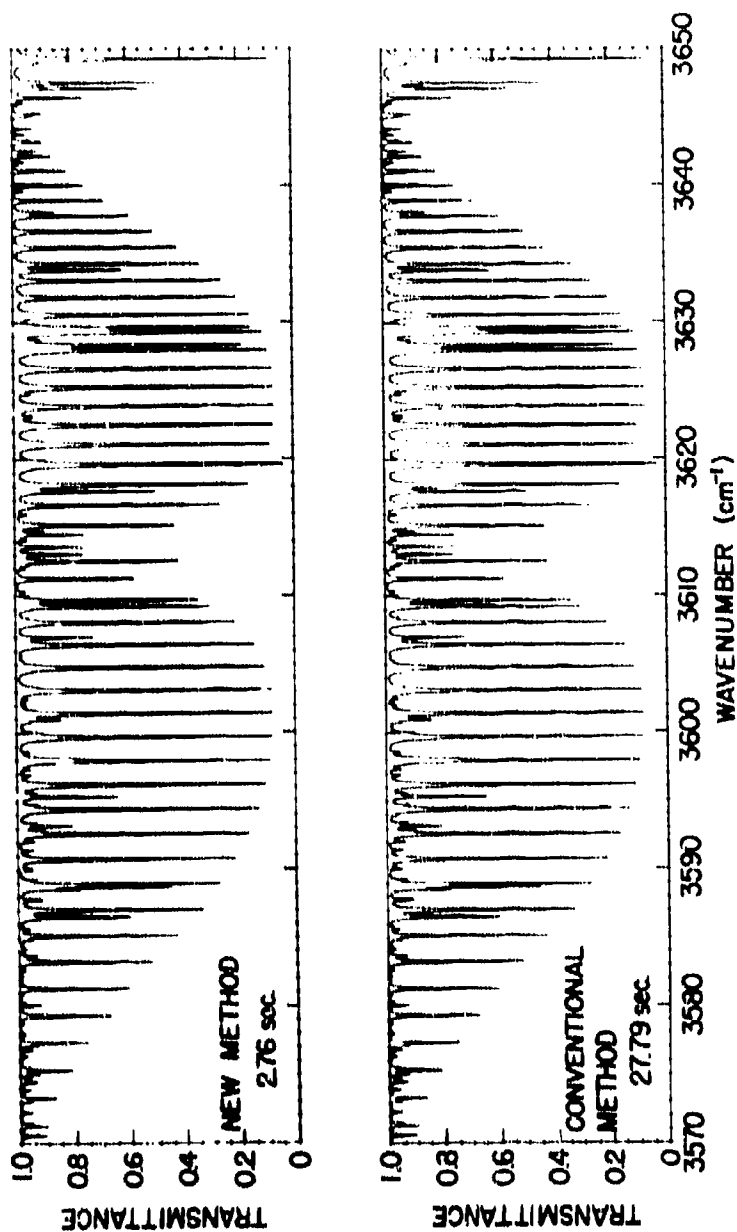


Figure 5. Spectral Transmission Results From 3570 cm^{-1} to 3650 cm^{-1} at a Sampling Interval of $\text{DV} = 0.01 \text{ cm}^{-1}$ for Conditions as in Figure 4: $P = 500 \text{ millibars}$, $T = 240 \text{ K}$, H_2O Column Density = 2.9×10^{18} , and CO_2 Column Density = $7.6 \times 10^{18} \text{ mol/cm}^2$. The upper trace is the result of the new algorithm and required 2.76 sec of computer time; the lower trace utilizing the conventional procedure required 27.79 sec. The times are for a CDC 6600 computer; read time has not been included. The AFGL line file was used for the spectral data from which 4401 lines were required

In this expression, N_{tot} is the total number of halfwidths over which the function is to be computed, N_m is the number of halfwidths spanned by the m 'th decomposed function, and $\delta x_1 / \delta x_m$ is the ratio of the sampling interval of the first function to that required for the m 'th function. In the present case for $N_{\text{tot}} = 48$, we have:

$$G = \frac{48}{(3 \cdot 1 + 12 \cdot \frac{1}{4} + 48 \cdot \frac{1}{16})} = \frac{48}{9} = 5 \frac{1}{3} \quad (42)$$

There are some constraints that are not explicit in the above expression; in particular, there are limitations on how small N_m can be and still have the function be reconstructable at the sampling interval. The algorithm provides greater improvement as the extent of the convolution is increased. For instance, if it were desired to reproduce the function over 192 halfwidths using four decomposed functions, a given choice would give a gain of

$$G = \frac{192}{(3 \cdot 1 + 12 \cdot \frac{1}{4} + 48 \cdot \frac{1}{16} + 192 \cdot \frac{1}{64})} = \frac{192}{12} = 16 \quad (43)$$

It must be emphasized that this choice, though workable, is not unique and other choices might provide greater improvement.

The algorithm, as it has been developed, must include protection against lines having halfwidths deviating significantly from the average. For anomalously wide lines, the convolution process can overflow the output arrays at the beginning and ending of the panels. In this case the line width is reset to the maximum width that can be treated: twice the average value. A series of + signs and the line identification are outputted when such a situation is encountered. In general, wide lines are not a problem since the widest lines do not vary significantly from the mean. This case also provides protection when a sampling interval, D , is chosen which is not consistent with the mean halfwidth of the lines being considered or when the line width is incorrect on the input data file.

There are a number of anomalously narrow lines that are encountered such as the high J , low K_a water lines of type measured by Eng et al.¹⁷ For such lines, that is, $\alpha_1 \ll \bar{\alpha}$, where α_1 is the width of the i 'th line and $\bar{\alpha}$ is the mean width, not only does the algorithm fail, but depending on the phasing of the sampling interval, the contribution of the transition can be missed entirely. Such lines have been

17. Eng, R. S., Kelley, P. L., Mooradian, A., Calawa, A. R., and Harmon, T. C. (1973) Tunable laser measurements of water vapor transitions in the vicinity of $5 \mu\text{m}$, Chem. Phys. Letters 19:524.

treated by setting the halfwidth to the sampling interval, that is, $\alpha_1 = DV$. In this case, a series of - signs and the line identification are printed out. Although the convolution will be undersampled for such lines, information pertaining to the line is retained. The only strictly correct way to handle these narrow lines, is to choose a DV equal to $\alpha_1/4$ where α_1 is characteristic of the narrowest line encountered. Such a choice of DV may necessitate the use of the conventional convolution method, since the sampling interval is so small. Computational requirements may dictate the calculation of the absorption coefficient over a small wavenumber region around the lines in question. In general, these lines are relatively weak, and except in cases such as laser transmission problems the method used here proves to be satisfactory.

5. EXTENSIONS OF THE METHOD

As has been indicated in the previous section, the calculation of the far line wings may be readily incorporated into the program. However, for the reasons stated it is recommended that this far wing contribution be handled as a continuum contribution in the wavenumber domain. Similarly, the variation of line shape with molecular species may be incorporated into the algorithm. It is well known that the wings of air broadened CO_2 lines are "subLorentzian" and a very slow function specific to the CO_2 molecular species could be utilized in place of the Lorentz very slow function. However, there is no compelling evidence that the subLorentzian behavior occurs within 5 cm^{-1} of the line center at atmospheric pressure so again, it is considered more appropriate to include the absorption due to the far wings of the CO_2 lines as a properly chosen continuum function. The best available theories indicate that the subLorentzian behavior is wavenumber dependent. Incorporation of this effect is not amenable to a direct extension of the algorithm since the argument of the Lorentz function is in terms of halfwidths. The wing modification may be readily added to the calculation by including the contribution into the very slow array before the three arrays are combined into the final output array. Continuum contributions of this type are important for CO_2 in spectral regions such as the 01001 band center where the wing contribution from the Q branch is not negligible as at 667.2 cm^{-1} and beyond the band head from 780 cm^{-1} to 890 cm^{-1} .

The convolution method described here offers even more significant computational savings for the multilayer case as it is generally applied to atmospheric modeling. The sampling interval is determined for each layer based on the average halfwidth which is a function of temperature and pressure for the layer. The remaining problem is to merge the results of each layer using appropriate

interpolation techniques to obtain the transmission or emission for the case being considered. In the conventional approach to the problem, the calculations are performed at the finest sampling interval required and is the same for all layers; that is, the sampling interval required to perform the absorption coefficient calculation at 60 km is the same as that used at 0 km. This approach requires the calculation of many more output points than is necessary at altitudes below the original altitude with a proportional increase in computational effort. With the scheme proposed here, the computational time is the same for each layer.

6. LINE SHAPES OTHER THAN LORENTZIAN

The present method is clearly not restricted to any particular function such as the Lorentz function. The Doppler line shape may readily be tabulated either directly or as decomposed functions depending on the definition of halfwidth. For many atmospheric modeling cases, the line shape of greatest interest is the Voigt¹⁸ shape. Current efforts are being directed toward incorporating the Voigt line shape into the new algorithm. Preliminary indications are that the Voigt profile, computed to an accuracy similar to that attained for the Lorentz, will require only slightly more computer time than that required for the Lorentz function. Details of the procedure for calculating the Voigt shape will appear in a subsequent publication. Although the program assumes a symmetric line shape and only half the scanning function is stored, an asymmetric shape can be utilized by storing the entire function and making minor changes to the program.

7. THE PROGRAM

The program has been written to use line parameter input data consistent with that contained on the AFGL line parameter tape.¹ The line data is reformatted onto a binary file which contains the line data pertinent to the molecules and wavenumber range of interest. This step has been taken to keep read time consistent with the time required to perform the calculational part of the program. The control parameters are read from the input file and written to the output file; "tape 3" is the binary file containing the line parameter data; and KKFILE is the binary output file. KKFILE contains a header record which includes the identification information, SECANT, temperature, pressure, molecular identification, and molecular column densities of the homogeneous layer. The first record for each output panel is a header record for the panel which contains the wavenumber values

18. Voigt, S. Münch, Ber. (1912) p. 403.

of the first and last absorption coefficient values of the panel, the wavenumber increment between output points and the number of output points. The second record of the panel contains the array of absorption coefficient values resulting from the convolution calculation. The current version of the program outputs a maximum of 2400 values; in general, the first and last panel are shorter.

The program consists of the main program HIRACC; subroutines SHAPE, MOLEC, RDFILE, CONVFN, and PANEL; and the function QVRFAC. The overall strategy of the program is indicated in Figure 6. All the subroutines are called from the main program and the flow of the program is easily traced. Subroutine SHAPE sets up the three convolution functions XF, XS, XVS used to define the Lorentz function from 0 to 48 halfwidths.

Subroutine MOLEC in conjunction with function QVRFAC, makes the molecular identifications with the line parameter file, and determines the correction factors for the line intensities (SCOR) and the halfwidths (ALFCOR). The quantity, SCOR, is the correction factor due to the temperature dependence of the vibrational and rotational partition sums. The vibrational partition sum is calculated for a given molecular type as

$$Q_v(T) = \prod_{i=1}^N \frac{1}{\left(1 - e^{-h\nu_i/kT}\right) d_i} \quad (44)$$

where ν_i is a fundamental vibrational frequency and d_i is the degeneracy of the vibration. The temperature dependence of the rotational partition sum is given by

$$\frac{Q_R(T_0)}{Q_R(T)} = \left(\frac{T_0}{T}\right)^F \quad (45)$$

where $F = 1$ for linear molecules and 1.5 for nonlinear molecules. The reference temperature, T_0 , is taken as 298 K, consistent with the AFGL Line Listing. For further discussion of these topics, see Herzberg¹⁹ pp 503 ff. The partition sum calculations are performed by QVRFAC and the necessary molecular parameters are contained in data statements in subroutine MOLEC. The quantity, ALFCOR, is the correction factor due to the pressure and temperature dependence of the collision broadened halfwidth. The temperature dependence of the halfwidth has

19. Herzberg, G. (1945) Molecular Spectra and Molecular Structure II. Infrared and Raman Spectra. D. Van Nostrand and Co., Princeton.

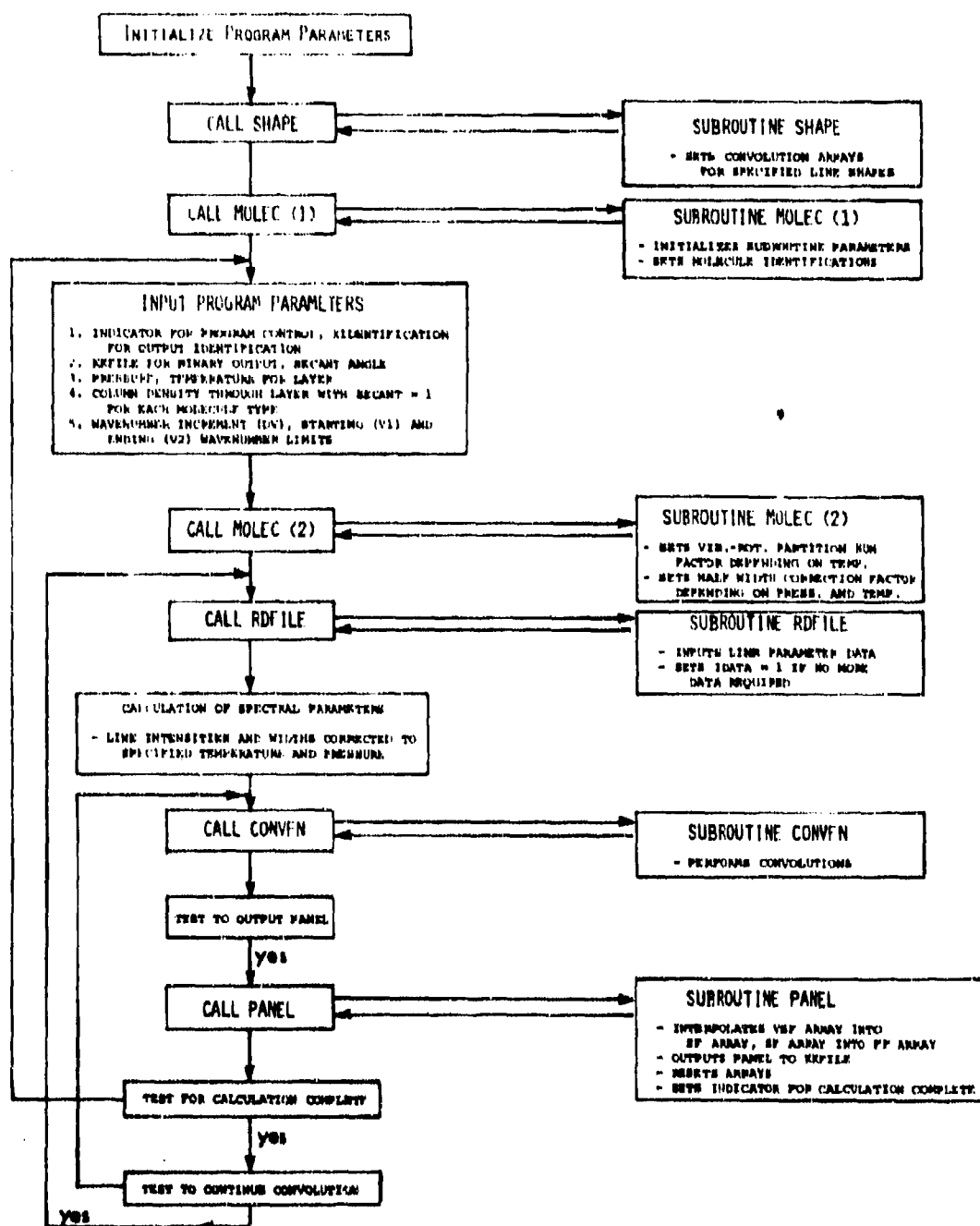


Figure 6. Flow Diagram for HIRACC Program

been taken as $(T_0/T)^{0.5}$ although calculations based on the Anderson - Tsao - Curnutte theory are reported to give a temperature dependence $\propto (T_0/T)^{0.75}$ (Varanasi²⁰).

Subroutine RDFILE reads the blocked binary line parameters over the wavenumber range for which line data is required. The line parameters include the wavenumber value of the transition (GNU, cm^{-1}), the intensity of the transition at 296⁰K (S , $\text{cm}^{-1}/(\text{mol}/\text{cm}^2)$), the collision broadened halfwidth at half maximum for 296⁰K and atm pressure (ALFAO, cm^{-1}), the lower state energy of the transition (EPP, cm^{-1}), and the molecule identification number (MOL). If the line parameter data is insufficient to complete the specified calculation, the message "end of file on disk" is printed on the output file. If no further line data is required IDATA is set to 1, and control is returned to the main program.

At this stage of the main program, an effective optical depth is calculated for each line which is dependent on the column density of the layer, the secant of the angle through the layer, the temperature of the layer, and the halfwidth of the line, $\alpha(\text{ALFI})$.

The effective depth, u' ,

$$u' = \left(\frac{1}{\alpha}\right) \cdot w \cdot \sec \cdot \left(\frac{Q_{VR}(T_0)}{Q_{VR}(T)}\right) \cdot \left[\exp\left(\frac{E''}{kT_0} - \frac{E''}{kT}\right)\right] \cdot \left[\frac{1 - \exp\left(-\frac{h\nu}{kT}\right)}{1 - \exp\left(-\frac{h\nu}{kT_0}\right)}\right] \quad (46)$$

where w is the absorber column density, E'' is the lower state energy, $Q_{VR} = Q_V Q_R$, and the other quantities have been previously defined. In terms of the program coding the effective depth appears as:

```
EFDPHTH=RECALF*W*SEC*SCOR*EXP(EPP/XKTFAC)*(1.-EXP(-GNU/TEMPO))/
(1.-EXP(-GNU/TAVE)).
```

As previously discussed, the proper sampling interval, DV, should be 0.25 times the average line halfwidth. If the halfwidth, ALFI, is less than the sampling interval, the halfwidth is set to the sampling interval and a series of minus signs is written to the output file. If the halfwidth exceeds a maximum value (ALFMAX) where $\text{ALFMAX} = \text{BOUND}/46$ and BOUND is the maximum value in wavenumbers over which a line can be calculated, the halfwidth is reset to ALFMAX, and a series of + signs is written to the output file. Included in the records indicating the

20. Varanasi, P., and Ko, F.K. (1977) Intensity and transmission measurements in the ν_3 fundamental of N_2O at low temperatures, Thirty Second Symposium on Molecular Spectroscopy, Paper RF'5, Columbus, Ohio

resetting of the halfwidth is the wavenumber value of the transition (GNU), the intensity (S) and the halfwidth (ALFAO) values of the transition from the line parameter tape, the calculated value of the halfwidth (ALFI), the value to which the halfwidth (DV or ALFMAX), and molecular identification number (M). If the number of halfwidth changes (NCHNG) exceeds 100, the computation is terminated.

Subroutine CONVFN is a tightly written subprogram in which considerable effort has been taken to minimize operations in the DO 30 loop. This subroutine performs the triple convolution of XP, XS, and XVS with the line data putting the results in the proper elements of FF, SF, and VSF respectively. A simplified flow diagram appears in Figure 7. Control indicator IPANEL is set to IDATA if the DO loop over the lines (40) is satisfied indicating whether a panel is complete or more lines are required. If the line DO loop (40) is not completed, IPANEL is set to 1 indicating that a complete panel has been calculated. Control is returned to the main program.

If IPANEL has been set to 1, subroutine PANEL is called. Subroutine PANEL performs a four point Lagrange interpolation of the VSF array into the SF array and the SF array into the FF array, thus combining the results of three independent convolutions into a final result. A general flow diagram of panel is given in Figure 8. Care is taken to store array values required for the interpolation of subsequent panels. VFT is the wavenumber value of the first element of the FF array, which is common to the first element of the SF and VSF arrays. A binary header record is written to the binary file (KKFILE) for each panel which includes the wavenumber value (V1P) of the first element of the panel (FF(NLO)), the wavenumber value (V2P) of the last element of the panel (FF(NHI)), the wavenumber increment (DV), and the number of absorption coefficient values outputted (NLIM). The second binary record contains the NLIM values of the absorption coefficient from the FF array. The arrays are appropriately shifted and reset in preparation for the computation of subsequent panels. Control is again returned to the main program, HIRACC.

After a panel is written to KKFILE, a record is written to the output file indicating the current value of the time, the time spent in RDFILE, in CONVFN, and in PANEL (the units are seconds). Also included in this record are the first and last wavenumber values of the panel, the wavenumber increment, and the number of values in the panel. A second record is written to the output file indicating the average value of the halfwidth, the number of lines read since the last panel was completed, and the total number of lines read since the initiation of the convolution calculation. Control is returned to statement 10 if the calculation is complete, or to statement 140 to continue the convolution process.

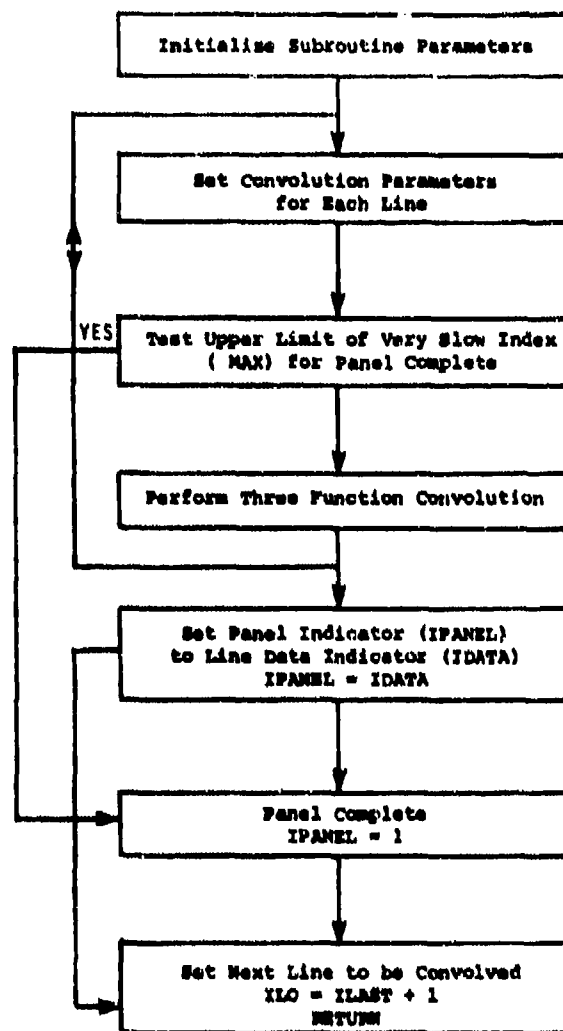


Figure 7. Flow Diagram for SUBROUTINE CONVFN

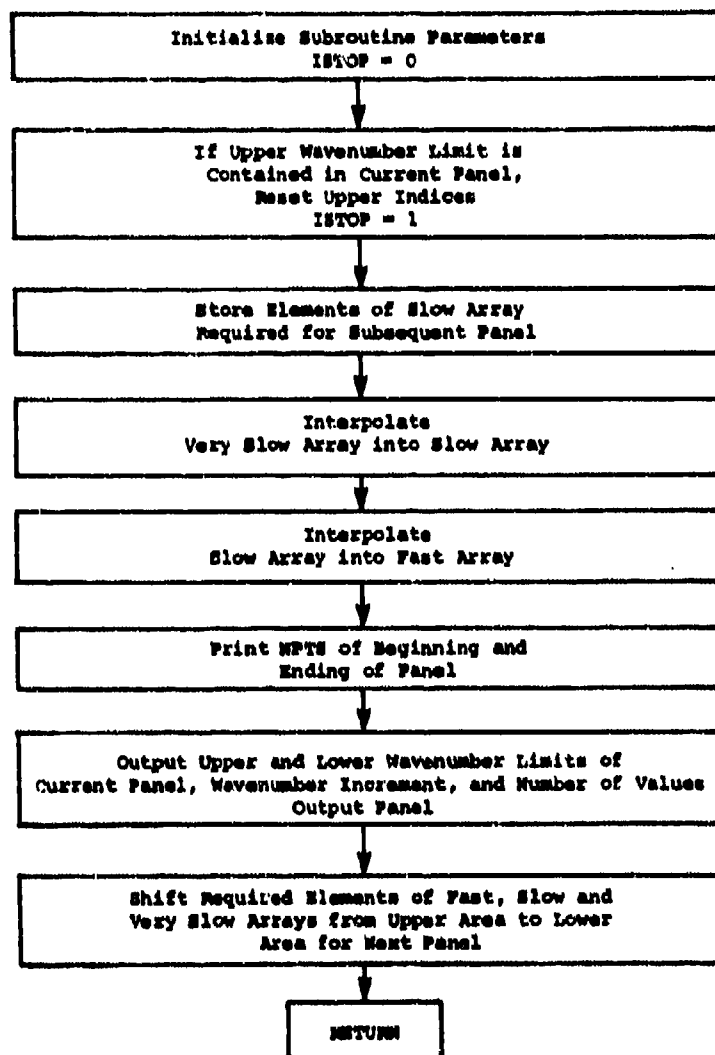


Figure 8. Flow Diagram for SUBROUTINE PANEL

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Appendix A

A listing of the Fortran program HIRACC is given in Table A1, together with the loader map, the input data, and the program output for the results which appear in Figure 5. In the output, it should be noted that one line is encountered that has a halfwidth which is larger than that allowed by the program. This line at $3558.4830 \text{ cm}^{-1}$ is an HDO line, molecular type 1, which has an erroneous halfwidth on the AFGL line tape used. The width for this line is reset to $\text{ALFMAX} = 0.08 \text{ cm}^{-1}$. Two H_2O lines occur at $3579.0810 \text{ cm}^{-1}$ which have anomalously narrow halfwidths. The values of these halfwidths are correct and are the high J, low K_A water lines of the type measured by Eng et al.¹ The widths for these lines are reset to $\text{DV} = 0.01 \text{ cm}^{-1}$. The beginning and ending sections of the output panels are printed out including the location in the FF array, the dimensionless absorption coefficient, and the wavenumber value associated with the respective elements of the FF array.

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74/74 QP7=1 FTH 4,5+414 07/11/77

38

Table A 1. Listing of HIRACC Program (Cont.)

PROGRAM HIRACC		
75		000840
	NBOUND=48.*(DXVS/DXF)	000850
	MAXF=MLIMF/NBOUND	000860
	MAXVS=(MAXF/4)+1	000870
	MAXVS=(MAXVS/4)+1	000880
	CALL SHAPE (XF,YF,XVS)	000890
80	CALL MOLECD(1,MHOLID,7,TEMPO,TAVE,P0,PAVE,SCOR,ALFCOR)	000900
	LIMIN=250	000910
10	PRINT 900	000920
	TIMROF=TIMCONV-TIMPL=0.	000930
	READ 902, IND,(XIO(I),I=1,7)	000940
85	IF (IND.NE.1) GO TO 160	000950
	PRINT 904. (XIO(I),I=1,7)	000960
	REWIND 3	000970
	TEOP=0	000980
90	READ 905, KKFILE,SECANT	000990
	PRINT 910, KKFILE	001000
	PRINT 910, SECANT	001010
	READ 920, PAVE,TAVE	001020
	PRINT 920, PAVE,TAVE	001030
	READ 920, (M(M),M=1,7)	001040
95	PRINT 930, (MHOLID(M),M(M),M=1,7)	001050
	READ 935, DV,V1,V2	001060
	PRINT 940, DV,V1,V2	001070
	IF (DV.LE.0.01) GO TO 160	001080
100	DVS=(DXVS/DXF)*DV	001090
	DVS=(DXVS/DXF)*DV	001100
	BOUND=FLOAT(NBOUND)*DV/2.	001110
	PRINT 942, BOUND	001120
	ALFMAX=BOUND/48.	001130
	NLO=NBOUND+1	001140
105	NHI=NLIMF+NSHIFT-1	001150
	DO 60 I=1,MAXF	001160
90	FF(I)=0.	001170
	DO 60 J=1,MAXV	001180
60	SP(I)=0.	001190
110	DO 70 I=1,MAXVS	001200
70	VSF(I)=0.	001210
	PRINT 900	001220
C	WRITE (KKFILE) (XIO(I),I=1,7),SECANT,PAVE,TAVE,(MHOLID(M),M=1,7),	001230
115	(M(M),M=1,7), DV,V1,V2	001240
C		001250
	VFT=V1-2.*BOUND	001260
	VROT=V1-BOUND	001270
	VTOP=V2+BOUND	001280
120	C	001290
	P0=1013.0	001300
	TEMPO=296.0	001310
	XKTD=0.8951*TEMPO	001320
	XKT=0.8951*TAVE	001330
125	XKTFAC=(1./XKTD)-(1./XKT)	001340
	CALL MOLECD(2,MHOLID,7,TEMPO,TAVE,P0,PAVE,SCOR,ALFCOR)	001350
	DO 80 M=1,7	001360
80	U(M)=M(M)*SCOR(M)*SECANT	001370
	LIMCON=0	001380
130	NCHMG=0	001390
C		001400
90	CONTINUE	001410
	ICNT=0	001420
	SUMALP=0.	001430
135	C	001440
100	CONTINUE	001450
C		001460
	CALL SECOND (TIME0)	001470
	IF (TEOP.NE.0) GO TO 140	001480
140	CALL MOFILE (GNU,3,ALFAS,APP,HOLI)	001490
	CALL SECOND (TIME)	001500
	TIMROF=TIMROF+TIME-TIME0	001510
C		001520
	IF (TEOP.NE.0) GO TO 140	001530
145	C	001540
O	MODIFY LINE DATA FOR TEMPERATURE,PRESSURE, AND COLUMN DENSITY	001550
C		001560
	DO 130 I=ILO,IHI	001570
	M=MOL(I)	001580
150	(FDPH(I)=B(I)*U(M)	001590

Table A1. Listing of HIRACC Program (Cont.)

```

PROGRAM HIRACC
      IF (EFDPTH(I).LE.0.) GO TO 130
      ICNT=ICNT+1
      ALFI=ALFAS(I)*ALFDOOR(M)
      IF (ALFI.GE.DV) GO TO 110
155  PRINT 945, GNU(I),S(I),ALFAS(I),ALFI,DV,M
      ALFI=DV
      NCHNG=NCHNG+1
      110  IF (ALFI.LE.ALPHAX) GO TO 120
      PRINT 950, GNU(I),S(I),ALFAS(I),ALFI,ALPHAX,M
160  ALFI=ALPHAX
      NCHNG=NCHNG+1
      120  CONTINUE
      SUMALF=SUMALF+ALFI
      RECALF(I)=1./ALFI
165  EFDPTH(I)=EFDPTH(I)*EXP((PP(I)*KKTFAC)*RECALF(I)*
      $ (1.-EXP(-GNU(I)/TAVE)))/(1.-EXP(-GNU(I)/TEMPO))
      130  CONTINUE
      IF (NCHNG.GT.100) GO TO 140
      140  CONTINUE
170  C
      CALL CONVPN (GNU,EFDPTH,RECALF,MOL,FF,SF,VSF,XP,XS,XVS)
      C
      IF (IPANEL.EQ.0) GO TO 100
      C
175  150  CONTINUE
      C
      CALL PANEL (FF,SF,VSF,KKFILE)
      C
      CALL SECOND (TIME)
180  PRINT 955, TIME,TIMRDF,TIMCNV,TIMPNL,V1P,V2P,DV,NLIN
      AVALF=SUMALF/FLOAT(ICNT)
      LINCNT=LINCNT+ICNT
      PRINT 960, AVALF,ICNT,LINCNT
      SUMALF=0.
185  ICNT=0
      IF (ISTOP.NE.1) GO TO 140
      END FILE KKFILE
      GO TO 10

C
190  160  CONTINUE
      STOP
      C
      C
195  980  FORMAT (1H1)
      992  FORMAT(11,F10.3)
      994  FORMAT(1X,F10.3)
      996  FORMAT(1X,F10.6)
      998  FORMAT(1X,F10.3)
      1000  FORMAT(1X,OUTPUT FILE NO. = 19)
      1002  FORMAT(1X,SECANT = F10.5)
      1004  FORMAT(1X,PE10.3)
      1006  FORMAT(1X,PRES(MB) = F12.9/ 10 TEMP(K) = F11.2)
      1008  FORMAT(1XMO COLUMN DENSITY(MOLECULES/CM^2) ,
      1010  / (1X,A6, * = F10.3) )
      1012  FORMAT (1X,F10.4)
      1014  FORMAT(1X DV(CM-1) = F12.4/10 V1(CM-1) = F12.4/10 V2(CM-1) =
      1016  F12.4)
      1018  FORMAT(1XMO 2*BOUND(CM-1) = ,F8.4)
      1020  FORMAT (1X -----F10.4,E14.3,3F10.6,15)
      1022  FORMAT (1X *****F10.4,E14.3,3F10.6,15)
      1024  FORMAT (1X,10X,TIME,11X,READ,4X,CONVOLUTION,10X,PAVEL,8X,
      1026  1*V1,13X,V2,11X,DV*8X,NVALUES,14F10.3,3F10.4,F10.4,110)
      1028  FORMAT (1X AVERAGE WIDTH = F10.9, NO. LINES = I10,
      1030  TOTAL NO. OF LINES=F10.7)
      1032  END
210  END

```

Table A1. Listing of HIRACC Program (Cont.)

SUBROUTINE SHAPE

74/74 OPT=1

FTN 4,5+414

07/11/77

```

1      SUBROUTINE SHAPE (XF,XS,XVS)
COMMON /XSUM/ RFOPI
COMMON /MXK/ NMF,DXF,NF,NMS,DXS,NS,NMVS,DXVS,NXVS,NFMX,NSHX,NVSH
18K
5      DIMENSION XF(1), XS(1), XVS(1)
      XLCRNZ(2)=1./ (1.+X2)
      SFN(X2)=A1+X1*XP+X1*X2*X2
      VSFN(X2)=A2+X2*X2+CP*X2*X2
      AQ(Z0)=(1.+3.*Z0**2+3.*Z0**4)/(1.+20**2)**3
10     RQ(Z0)=-(1.+3.*Z0**2)/(1.+20**2)**3
      CQ(Z0)=1./ (1.+20**2)**3
C      MATCH AT Z1 HALFWIDTHS
      Z1=4.
      A1=AQ(Z1)
15     R1=RQ(Z1)
      C1=CQ(Z1)
C      MATCH AT Z2 HALFWIDTHS
      Z2=12.
      A2=AQ(Z2)
20     R2=RQ(Z2)
      C2=CQ(Z2)
      TOTAL=0.
      DO 10 I=1,NFMX
25     10     XF(I)=0.
      XF(I)=RECPI*(XLCRNZ(I)-SFN(I))
      SUM=XF(I)
      DO 20 JJ=2,NF
      X=FLOAT(JJ-1)*DXF
      XZ=X*X
30     XF(JJ)=RECPI*(XLCRNZ(X2)-SFN(X2))
      SUM=SUM+XF(JJ)*2.
20     CONTINUE
      XFINF)=0.
      SUM=SUM+DXF
35     TOTAL=TOTAL+SUM
      DO 30 I=1,NSHX
30     XS(I)=0.
      XS(I)=RECPI*(SFN(0.1)-VSFN(0.1))
      SUM=XS(I)
40     NS1=FLOAT(NMF)/DXS+1.001
      DO 40 JJ=2,NS1
      X=FLOAT(JJ-1)*DXS
      XZ=X*X
45     XS(JJ)=RECPI*(SFN(X2)-VSFN(X2))
      SUM=SUM+XS(JJ)*2.
40     CONTINUE
      NS1=NS1+1
      DO 50 JJ=NS1P,NS
      X=FLOAT(JJ-1)*DXS
      XZ=X*X
50     XS(JJ)=RECPI*(XLCRNZ(X2)-VSFN(X2))
      SUM=SUM+XS(JJ)*2.
50     CONTINUE
      XS(NS)=0.
      SUM=SUM+DXS
55     TOTAL=TOTAL+SUM
      DO 60 I=1,NVSHX
60     XVS(I)=0.
      XVS(I)=RECPI*VSFN(0.1)
      SUM=XVS(I)
60     NVS1=FLOAT(NMS)/DXVS+1.001
      DO 70 JJ=2,NVS1
      X=FLOAT(JJ-1)*DXVS
      XZ=X*X
65     XVS(JJ)=RECPI*VSFN(X2)
      SUM=SUM+XVS(JJ)*2.
70     CONTINUE
      NVS1=NVS1+1
      DO 80 JJ=NS1P,NVVS
      X=FLOAT(JJ-1)*DXVS
      XZ=X*X
75     XVS(JJ)=RECPI*(XLCRNZ(X2))
      SUM=SUM+XVS(JJ)*2.
80     CONTINUE
      SUM=SUM+DXVS
      TOTAL=TOTAL+SUM
      RETURN
C
C
60     C
      END

```

Table A1. Listing of HIRACC Program (Cont.)

SUBROUTINE MOLEC	74/74	OPT=1	PTN 4.8+414	07/11/77
1	SUBROUTINE MOLEC (IND, MMOLID, NMOLEC, TEMPO, TEMP, P0, P, SCOR, ALFCOR)			003060
	DIMENSION MMOLID(1), SCOR(1), ALFCOR(1)			003070
	DIMENSION M(7,4), ND(7,4)			003080
	COMMON /XMOLEC/ MM(7), MV(7), M1(7), M2(7), M3(7), M4(7), QV(7), ROTFAC(7)			003090
9	1 M2(7), M3(7), M4(7), QV(7), ROTFAC(7)			003100
	DATA MM(1), MV(1), M1(1), M2(1), M3(1), M4(1), QV(1), ROTFAC(1)			003110
	1 QV(1), ROTFAC(1)			003120
	1 6M M20 .3, 3691.7, 1, 1995.8, 1, 3755.8, 1, 0, .0, 1.0004, 1.5 /			003130
	DATA MM(2), MV(2), M1(2), M2(2), M3(2), M4(2), QV(2), ROTFAC(2)			003140
10	2 QV(2), ROTFAC(2)			003150
	2 6M CO2 .3, 1364.0, 1, 647.3, 2, 2349.3, 1, 0, .0, 1.0040, 1.0 /			003160
	DATA MM(3), MV(3), M1(3), M2(3), M3(3), M4(3), QV(3), ROTFAC(3)			003170
	3 QV(3), ROTFAC(3)			003180
	3 6M O3 .3, 1103.2, 1, 700.9, 1, 1042.1, 1, 0, .0, 1.0056, 1.5 /			003190
15	DATA MM(4), MV(4), M1(4), M2(4), M3(4), M4(4), QV(4), ROTFAC(4)			003200
	4 QV(4), ROTFAC(4)			003210
	4 6M N2O .3, 1264.9, 1, 588.8, 2, 2223.0, 1, 0, .0, 1.1267, 1.0 /			003220
	DATA MM(5), MV(5), M1(5), M2(5), M3(5), M4(5), QV(5), ROTFAC(5)			003230
	5 QV(5), ROTFAC(5)			003240
20	5 6M CO .1, 2143.3, 1, 0, .0, 0, .0, 1.0000, 1.0 /			003250
	DATA MM(6), MV(6), M1(6), M2(6), M3(6), M4(6), QV(6), ROTFAC(6)			003260
	6 QV(6), ROTFAC(6)			003270
	6 6M CH4 .4, 2914. .1, 1533.3, 2, 3018.0, 3, 1247.9, 3, 1.0066, 1.5 /			003280
	DATA MM(7), MV(7), M1(7), M2(7), M3(7), M4(7), QV(7), ROTFAC(7)			003290
25	7 QV(7), ROTFAC(7)			003300
	7 6M O2 .1, 1483.5, 1, 0, .0, 0, .0, 1.0007, 1.0 /			003310
	MOLEC MAKES THE MOLECULAR IDENTIFICATIONS			003320
				003330
30				003340
	ALFCOR IS THE FACTOR BY WHICH THE COLLISION WIDTH MUST BE CHANGED			003350
	DUE TO THE DEPENDENCE ON PRESSURE AND TEMPERATURE			003360
	THE TEMPERATURE DEPENDENCE IS TAKEN AS (T0/T)**0.5			003370
35				003380
	SCOR IS THE FACTOR BY WHICH THE LINE INTENSITY IS CHANGED DUE TO			003390
	TEMPERATURE DEPENDENCE OF THE VIB AND ROT PARTITION SUMS			003400
				003410
	IF (IND.EQ.2) GO TO 28			003420
	NDIM=7			003430
40	NVDIM=4			003440
	DO 30 M=1, NMOLEC			003450
	M(1)=M1(M)			003460
	M(2)=M2(M)			003470
	M(3)=M3(M)			003480
45	M(4)=M4(M)			003490
	ND(M,1)=M1(M)			003500
	ND(M,2)=M2(M)			003510
	ND(M,3)=M3(M)			003520
	ND(M,4)=M4(M)			003530
50	MMOLID(M)=MM(M)			003540
	RETURN			003550
55	28 CONTINUE			003560
	PRATIO=P/P0			003570
	TRATIO=TEMPO/TEMP			003580
	DO 30 M=1, NMOLEC			003590
	SCOR(M)=QVRFAC(M,TEMP,TRATIO,QV,ROTFAC,M,ND,NDIM,NVDIM)			003600
	ALFCOR(M)=PRATIO*(TRATIO**0.5)			003610
60	30 CONTINUE			003620
	RETURN			003630
	END			003640

Table A 1. Listing of HIRACC Program (Cont.)

	FUNCTION QVRFAC	7/4/74	OPT=1	FTN 4.5+414	87/11/77
1	FUNCTION QVRFAC(M,TEMP,TRATIO,QV8,ROTFAC,M,ND,NVDIM,NVDIM)				003666
	DIMENSION QV8(1),ROTFAC(1)				003670
	DIMENSION N(MDIM,NVDIM),ND(MDIM,NVDIM)				003680
	QV=1.				003690
5	DO 10 I=1,NVDIM				003700
	IF (ND(M,I).EQ.0) GO TO 20				003710
	SV=1.-EXP(-M(M,I)/TEMP)				003720
	IF (ND(I).GT.1) SV=SV**ND(M,I)				003730
10	QV=QV*SV				003740
20	QVRFAC=(QV8(M)/QV)**(TRATIO)**ROTFAC(M)				003750
	RETURN				003760
	C				003770
	END				003780

	SUBROUTINE RQFILE	7/4/74	OPT=1	FTN 4.5+414	87/11/77
1	SUBROUTINE RQFILE (GNU,R,ALPHA,EPP,MOL)				003790
	COMMON /XSUB/ NEDPI,LIMIN,ILO,IMI,VBOT,VTOP,V1,V2,QV,VFF,IEOP,IPAN				003800
	IEL,SEAT,ISTOP				003810
	DIMENSION GNU(1),S(1),ALPHA(1),EPP(1),MOL(1)				003820
	IDATA=0				003830
5	READ (3) VHIN,VHAX,NREC				003840
10	IF (IEOP(3)) 90,20				003850
	IF (VHAX.GE.VBOT) GO TO 30				003860
	READ (3) VHIN				003870
	GO TO 10				003880
20	READ (3) (GNU(I),S(I),ALPHA(I),EPP(I),MOL(I),I=1,NREC)				003890
	ILO=1				003900
	IMI=NREC				003910
	IF (VHIN.GE.VBOT) GO TO 90				003920
15	DO 40 I=1,NREC				003930
	ILO=I				003940
	IF (GNU(I).GE.VBOT) GO TO 90				003950
	CONTINUE				003960
	IF (VHAX.LE.VTOP) RETURN				003970
20	DO 60 I=1,NREC				003980
	IMI=I				003990
	IF (GNU(I).GT.VTOP) GO TO 70				004000
	CONTINUE				004010
	IF (IMI.LT.NREC) IDATA=1				004020
25	RETURN				004030
	PRINT *,IDATA				004040
	IEOP=1				004050
	RETURN				004060
30	C				004070
	C				004080
	FORMAT (' END OF FILE ON DISK')				004090
	END				004100

Table A1. Listing of HIRACC Program (Cont.)

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SUBROUTINE CONVPN 74/74 OPT=1 FTH 4.5+414 07/11/77

1 SUBROUTINE CONVPN (GNU,FFDPYH,RECALF,MOL,PF,SP,VSP,XF,NS,XVS) 004110
COMMON /XSIM/ RECP1,LIMIN,ILO,IMI,VBDT,VTOP,V1,V2,DV,VFT,TEOF,IPAN 004120
IEL,IData,IStop 004130
COMMON /XXX/ NHF,DXF,NF,NWS,DXS,NS,NHVS,DXVS,NXVS,NFMAX,NSMAX,NVSM 004140
IAX 004150
COMMON /SUM1/ MAXP,MAXS,MAXVS,NLIMP,NLIMS,NLIMVS,NLO,NHI,OVS,OVVS 004160
COMMON /XTIME/ TIME,TIMROF,TIMCNV,TIMPNL 004170
DIMENSION GNU(1), EVDPTH(1), RECALF(1), PF(1), SP(1) 004180
DIMENSION MOL(1) 004190
10 DIMENSION XF(1), XS(1), XVS(1), VSP(1) 004200
004210
004220
004230
004240
15 THE VERY SLOW CONVOLUTION IS PERFORMED FROM -NHVS TO +NHVS IN 004250
HALFWIDTHS 004260
004270
004280
004290
20 DXVS IS THE INTERVAL AT WHICH THE VERY SLOW FUNCTION IS STORED IN 004300
HALFWIDTHS 004310
004320
004330
004340
004350
25 JJ IS THE LOCATION IN THE VSP ARRAY FOR WHICH THE CONTRIBUTION 004360
TO THE ABSORPTION COEFFICIENT FROM THE I'YM LINE IS CALCULATED 004370
004380
004390
004400
004410
004420
004430
004440
004450
004460
004470
004480
004490
004500
004510
004520
004530
004540
004550
004560
004570
004580
004590
004600
004610
004620
004630
004640
004650
004660
004670
004680
004690
004700
004710
004720
004730
004740
004750
004760
004770
004780
004790
004800
004810
004820
004830
004840
004850
004860
004870
004880
004890
004900
004910
004920
004930
004940
004950
004960
004970
004980
004990
005000

30 CALL SECOND (TIME) 005010
RATVX=DVVS/DXVS 005020
FVS=FLOAT (NHVS)/DXVS 005030
CONF=DVVS/DV-1. 005040
CONS=DVVS/DVS-1. 005050
IF (ILO.GT.IMI) GO TO 50 005060
ON 40 I=ILO,IMI 005070
DEPTHI=EVDPTH(I) 005080
IF (DEPTHI.LE.0.) GO TO 40 005090
ISLOPE=RECALF(I)*RATVX 005100
ZINT=(GNU(I)-VF1)/DVVS 005110
SFVS=FVS/ZSLOPE 005120
JMAX=(ZINT*SFVS)+2. 005130
IF (JMAX.LE.MAXVS) GO TO 20 005140
ILAST=I-1 005150
GO TO 50 005160
20 JMIN=(ZINT-SFVS)+2. 005170
JMINF=(ZINT*CONF) 005180
JMINS=(ZINT*CONS) 005190
ZVS=(FLOAT (JMIN-2)-ZINT)*ZSLOPE 005200
ZS=ZVS*(FLOAT (JMINS)-ZINT*CONS)*ZSLOPE 005210
ZF=ZVS*(FLOAT (JMINF)-ZINT*CONF)*ZSLOPE 005220
OU 30 JJ=JMIN,JMAX 005230
JS=JMINS+JJ 005240
JF=JMINF+JJ 005250
ZVS=ZVS+ZSLOPE 005260
ZS=ZS+ZSLOPE 005270
ZF=ZF+ZSLOPE 005280
IZV=ABS(ZVS)+1.4 005290
IZS=ABS(ZS)+1.3 005300
IZF=ABS(ZF)+1.3 005310
VSP(JJ)=VBF(JJ)*DEPTHI*XVS(IZV) 005320
SF(JS)=SF(JS)+DEPTHI*NS(IZS) 005330
PF(JF)=PF(JF)+DEPTHI*NF(IZF) 005340
30 CONTINUE 005350
40 CONTINUE 005360
ILAST=IMI 005370
C IDATA=0 IF MORE DATA REQUIRED ** IDATA=1 IF NO MORE DATA REQUIRE 005380
IPANEL=IDATA 005390
70 GO TO 60 005400
50 CONTINUE 005410
IPANEL=1 005420
ILO=ILAST+1 005430
CALL SECOND (TIME) 005440
TIMCNV=TIMCNV+TIME-TIME0 005450
75 RETURN 005460
005470
005480
005490
005500
005510
005520
005530
005540
005550
005560
005570
005580
005590
005600
005610
005620
005630
005640
005650
005660
005670
005680
005690
005700
005710
005720
005730
005740
005750
005760
005770
005780
005790
005800
005810
005820
005830
005840
005850
005860
005870
005880
005890
005900
005910
005920
005930
005940
005950
005960
005970
005980
005990
006000
END

```

Table A1. Listing of HIRACC Program (Cont.)

SUBROUTINE PANEL

74/74

OPT61

FTN 4,5+64

07/11/77

```

1      SUBROUTINE PANEL (FF,VF,VSP,KKFILE)
COMMON /XSUS/ REOPT,LINIM,ILO,IMI,VBOT,VTOP,VI,V2,DV,VFT,IFUF,IPAN
1FL,IDATA,ISTOP
COMMON /SUB1/ MAXF,MAXS,MAXVS,NLINF,NLIMS,NLTHVS,NLO,NMI,DVS,DVVS
5      COMMON /XPANEL/ VIP,V2P,NLTH,NSHIFT,NPTS
COMMON /XTIME/ TIME,TINROF,TINCHV,TINPML
      DIMENSION FF(1),VF(1),VSP(1)
      DIMENSION IFSTOP(8)
      CALL SECOND (TIME0)
10     X00=-7./120.
      X01=109./120.
      X02=39./120.
      X03=-9./120.
      X10=-1./10.
15     X11=9./10.
      ISTOP=0
      NMHI=(V2-VFT)/DV+1.5
      IF (NMHI.GE.NNMI) ISTOP=1
      IF (ISTOP.EQ.1) NMH=NMHI
20     JMXPR=NLO+NPTS
      JJPR=NMH+NPTS
      LIMLO=(NLO-1)/4-1
      LIMHI=(NMH/4)+1
      C      SLOW FUNCTION VALUES NEEDED FOR SUBSEQUENT PANELS ARE SAVED
      DO 10 J=1,8
25     SPSTOR(J)=SP(LIMHI+J-5)
30     DO 20 J=NLO,NMI,4
      JVS=(J-1)/4+1
      SP(J)=VF(J)+VSP(JVS)
      SP(J+1)=SP(J+1)+X00*VSP(JVS-1)+X01*VSP(JVS)+X02*VSP(JVS+1)+X03*VSP
      1(JVS+2)
      SP(J+2)=SP(J+2)+X10*(VSP(JVS-1)+VSP(JVS+2))+X11*(VSP(JVS)+VSP(JVS+
      1))
      SP(J+3)=SP(J+3)+X03*VSP(JVS-1)+X02*VSP(JVS)+X01*VSP(JVS+1)+X00*VSP
35     1(JVS+2)
      CONTINUE
40     DO 30 J=NLO,NMI,4
      JS=(J-1)/4+1
      FF(J)=FF(J)+SP(JS)
      FF(J+1)=FF(J+1)+X00*SP(JS-1)+X01*SP(JS)+X02*SP(JS+1)+X03*SP(JS+2)
      FF(J+2)=FF(J+2)+X10*(SP(JS-1)+SP(JS+2))+X11*(SP(JS)+SP(JS+1))
      FF(J+3)=FF(J+3)+X03*SP(JS-1)+X02*SP(JS)+X01*SP(JS+1)+X00*SP(JS+2)
45     CONTINUE
      IF (NPTS.EQ.0) GO TO 60
      DO 40 J=NLO,JMXPR
      VP=VFT+FLOAT(J-1)*DV
      PRINT 900, J,FF(J),VP
50     DO 50 J=JJPR,NMI
      VP=VFT+FLOAT(J-1)*DV
      PRINT 900, J,FF(J),VP
60     CONTINUE
      DO 70 J=1,8
75     SP(LIMHI+J-5)=SPSTOR(J)
      NLIM=NMH+NLO+1
      V1P=VFT+FLOAT(NLO-1)*DV
      V2P=VFT+FLOAT(NMI-1)*DV
      C      V1P IS FIRST FREQ OF PANEL
      V2P IS LAST FREQ OF PANEL
      WRITE (KKFILE) V1P,V2P,DV,NLIM
80     WRITE (KKFILE) (FF(J),J=NLO,NMI)
      VFT=VFT+FLOAT(NLIM-1)*DV
      IF (ISTOP.EQ.1) GO TO 140
      JF=1
      DO 80 J=NLINF,MAXF
85     FF(J)=FF(J)
      JF=JF+1
      DO 90 J=JF,MAXF
90     FF(J)=0.
      JS=1
      DO 100 J=NLIMS,MAXS
100    SP(JS)=SP(J)
      JS=JS+1
      DO 110 J=JS,MAXS
110    VF(J)=0.
      JVS=1
75     DO 120 J=NLTHVS,MAXVS
      VSP(JVS)=VSP(J)
120    JVS=JVS+1
      DO 130 J=JVS,MAXVS
130    VSP(J)=0.
      NLO=NNSHIFT+1
140    CALL SECOND (TIME1)
      TINPML=TINPML+TIME-TIME0
      RETURN
      C
      C
      C
900    FORMAT (I10,2F8,2I2,5,F12,5)
      END

```

Table A2. Loader Map for HIRACC Program

CYBER LOADER 1.1-24								07/11/77 21.37.29.	PAGE 1
PROGRAM AND BLOCK ASSIGNMENTS.									
BLOCK	ADDRESS	LENGTH	FILE	DATE	PROCESSOR VER LEVEL	HARDWARE	COMMENTS		
/KSUB/	111	16							
/KX/	127	14							
/KXU/	143	12							
/KXU/	155	5							
/KXU/	162	4							
/KXU/	166	12486	LGO	07/11/77	FTN	666X I	OPT=1		
/KXU/	12572	262	LGO	07/11/77	FTN	666X I	OPT=1		
/KXU/	13659	124							
/KXU/	13659	228	LGO	07/11/77	FTN	666X I	OPT=1		
/KXU/	13621	111	LGO	07/11/77	FTN	666X I	OPT=1		
/KXU/	13621	164	LGO	07/11/77	FTN	666X I	OPT=1		
/KXU/	13716	238	LGO	07/11/77	FTN	666X I	OPT=1		
/KXU/	14346	467	LGO	07/11/77	FTN	666X I	OPT=1		
/KXU/	14635	23							
/KXU/	14668	131							
/KXU/	15011	64	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	COMMON CODED I/O ROUTINES AND COMMENTS.		
/KXU/	15011	8	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	FCL INITIALIZATION ROUTINE.		
/KXU/	15075	61	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	WRITE END OF LOGICAL FILE MARK.		
/KXU/	15156	41	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	INITIALIZE CONSTANTS.		
/KXU/	15217	318	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	COMMON FLOATING OUTPUT CODE.		
/KXU/	15527	651	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	FORTRAN OBJECT LIBRARY UTILITIES.		
/KXU/	16318	777	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	COMMON INPUT FORMATTING CODE.		
/KXU/	16427	168	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	FORTRAN RECORD FORTRAN RECORD.		
/KXU/	17407	456	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	OUTPUT FORMAT INTERPRETER.		
/KXU/	17665	172	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	FORTRAN WRITE FORTRAN RECORD.		
/KXU/	17857	75	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	COMMON COMMON AND NATURAL LOGARITHMS.		
/KXU/	23447	75	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	EXPONENTIAL FUNCTION. E TO POWER. OPTIMAL.		
/KXU/	23452	1	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	LINK BETWEEN SYSTEMS AND INITIALIZE-INITIAL CODE.		
/KXU/	23558	16	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	TEST FOR END OF FILE STATUS.		
/KXU/	23666	154	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	COMMON FLOATING INPUT CONVERTER.		
/KXU/	26242	352	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	COMMON APLIST AND FORMAT FOR KXU/COMPASS.		
/KXU/	28014	16	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	FCL MISC. UTILITIES.		
/KXU/	28032	42	SL-FORTRAN	08/11/76	COMPASS	3. 2-416	LOCATE AN FIT GIVEN A FILE NAME.		

Table A2. Loader Map for HIRACC Program (Cont.)

LOAD MAP - WTORC2					
PGMT.001	27435	11	SL-SYSIO	05/28/76 COMPASS	3. 75125
PGMT.002	27446	1335	SL-SYSIO	05/28/76 COMPASS	3. 75125
Z.58	39543	181	SL-SYSIO	05/28/76 COMPASS	3. 75125
L.50	38164	98	SL-SYSIO	05/28/76 COMPASS	3. 75125
P.300.00	38654	186	SL-SYSIO	05/28/76 COMPASS	3. 75125
SYS.00	38762	37	SL-SYSIO	05/15/77 COMPASS	3. 2-614
//	31021	12525			

PROCESS SYSTEM REQUEST,

.721 CP SECONDS

44100 CH STORAGE USED

78 TABLE MOVES

Table A3. Sample Output From HIRACC Program

OCO AND NOW , 3550 TO 3650 FOR REPORT

OUTPUT FILE NO. = 10

SECANT = 1.00000

PRESS(Pa) = 500.00000

TEMP(K) = 240.00

COLUMN DENSITY(MOLECULES/CM**2)

N2 = $2.900E+10$

CO2 = $7.600E+10$

O3 = -8.

N2O = -8.

CO = -8.

CH4 = -8.

O2 = -8.

DV(CM-1) = .0100

V1(CM-1) = 3550.0000

V2(CM-1) = 3650.0000

2*BOUND(CM-1) = 3.5400

Table A3. Sample Output From HIRACC Program (Cont.)

	TIME	READ	CONVOLUTION	PANEL	W1	W2	DV	NVALUES
	5.754	.340	.719	.867	3558.000	3566.630	.0130	1664
AVERAGE WIDTH =	.83868	NO. LINES =	1283	TOTAL NO. OF LINES =	1263			
*****	3558.738				.086688	.880888		1
769					.149E-07	.158888		
770					.19788E-02	3553.8300		
771					.18811E-02	3559.8188		
772					.17869E-02	3558.0288		
773					.16573E-02	3553.8388		
774					.16692E-02	3558.8488		
775					.17411E-02	3553.0588		
776					.18789E-02	3558.6688		
777					.28963E-02	3558.0788		
778					.24889E-02	3558.8488		
779					.28353E-02	3558.8988		
780					.14628E-02	3558.1888		
781					.41288E-02	3558.1188		
782					.86754E-02	3558.1288		
783					.48183E-02	3558.1388		
784					.44647E-02	3558.1688		
785					.38362E-02	3553.1588		
2416					.32832E-02	3553.1688		
2417					.56486E-01	3566.4788		
2418					.66591E-01	3566.4888		
2419					.78283E-01	3566.4988		
2420					.94324E-01	3566.5088		
2421					.11388E+00	3566.5188		
2422					.13222E+00	3566.5288		
2423					.15281E+00	3566.5388		
2424					.16691E+00	3566.5488		
2425					.17259E+00	3566.5588		
2426					.16592E+00	3566.5688		
2427					.15183E+00	3566.5788		
2428					.13229E+00	3566.5888		
2429					.11516E+00	3566.5988		
2430					.98761E-01	3566.6088		
2431					.87471E-01	3566.6188		
2432					.77873E-01	3566.6288		
					.78856E-01	3566.6388		

Table A3. Sample Output From HIRACC Program (Cont.)

TIME	READ	CONVOLUTION	PANEL	V1	V2	DV	NVALUES
6.638	.519	1.253	.142	3566.6480	3593.6300	.0100	2035
AVERAGE WIDTH =	.03554	NO. LINES =	1000	TOTAL NO. OF LINES =	2283		
33	3579.8818	.131E-07	.011750	.006441	.910800	1	
34	3579.8878	.396E-07	.012000	.006578	.310300	1	
35		.06222E-01	3566.64800				
36		.62001E-01	3566.65000				
37		.62345E-01	3566.66000				
38		.62964E-01	3566.67000				
39		.66502E-01	3566.68000				
40		.73269E-01	3566.69000				
41		.84911E-01	3566.70000				
42		.10070E+00	3566.71000				
43		.12546E+00	3566.72000				
44		.16105E+00	3566.73000				
45		.19919E+00	3566.74000				
46		.22946E+00	3566.75000				
47		.26841E+00	3566.76000				
48		.31559E+00	3566.77000				
49		.36333E+00	3566.78000				
50		.41763E-01	3566.79000				
51		.48074E-01	3593.47000				
52		.55933E-01	3598.49000				
53		.64602E-01	3598.49000				
54		.74266E-01	3593.51000				
55		.84465E-01	3598.52000				
56		.94345E-01	3598.53000				
57		.1.06314E-01	3598.54000				
58		.1.19843E-01	3598.55000				
59		.1.33757E-01	3598.56000				
60		.1.48293E-01	3598.57000				
61		.1.64084E-01	3598.58000				
62		.1.80955E-01	3598.59000				
63		.1.99524E-01	3598.60000				
64		.2.18559E-01	3598.61000				
65		.2.38363E+00	3599.62000				
66		.1.19196E+00	3598.63000				

Table A3. Sample Output From HIRACC Program (Cont.)

	TIME	READ	CONVOLUTION	PANEL	V1	V2	CV	NVALUES
33	7.354	.652	1.579	.227	3598.6400	3614.6300	.8100	24..
34								
35								
36								
37								
38								
39								
40								
41								
42								
43								
44								
45								
46								
47								
48								
49								
2416								
2417								
2418								
2419								
2420								
2421								
2422								
2423								
2424								
2425								
2426								
2427								
2428								
2429								
2430								
2431								
2432								
AVERAGE WIDTH =				NO. LINES =	759	TOTAL NO. OF LINES=	3033	

Table A3. Sample Output From HIRACC Program (Cont.)

	TIME	READ	CONVOLUTION	PANEL	V1	V2	OV	NVALUES
33	8.244	.827	2.222	.333	3614.640C	3630.6300	.6100	2432
34								
35								
36								
37								
38								
39								
40								
41								
42								
43								
44								
45								
46								
47								
48								
49								
2416								
2417								
2418								
2419								
2420								
2421								
2422								
2423								
2424								
2425								
2426								
2427								
2428								
2429								
2430								
2431								
2432								
AVERAGE WIDTH =		.83852	MC. LINES =	1000	TOTAL NO. OF LINES =	4633		

Table A3. Sample Output From HIRACC Program (Cont.)

	TIME 8.672	READ .912	CONVOLUTION 2.484	PANEL .356	V1 3638.6400	V2 3650.0000	DV .0100	NVALUES 1137
33								
34								
35								
36								
37								
38								
39								
40								
41								
42								
43								
44								
45								
46								
47								
48								
49								
1153								
1154								
1155								
1156								
1157								
1158								
1159								
1160								
1161								
1162								
1163								
1164								
1165								
1166								
1167								
1168								
1169								
AVERAGE WIDTH =		.03745	NO. LINES =	368	TOTAL NO. OF LINES =	4401		

Table A4. Data Cards for HIRACC Program

```

1  020 AND MDH , 3558 TO 3656 FOR REPORT
    18 1.
    588.8E 86 246. E 88
    2.988E 18 7.688E 18 0.888E 88 0.888E 88 0.888E 88 0.888E 88
    .81      3558.      3658.
    99999
    *EOR
  
```

Appendix B

A listing of a Fortran program to plot the results from HIRACC in transmission is given in Appendix B. This program, entitled TPLLOT, was written for the CDC 6600 and the plotting functions are specific to that computer. This plot program is consistent with the sampling criterion and the interpolation methods described in this report. The four point Lagrange interpolation is used to generate three intermediate points for each output interval of HIRACC. The listing of the program, the output, and the input data, are given in Table B1. Two data cards are required: the first contains 30 characters of identification, and the second contains the upper and lower limits (cm^{-1}) of the wave number range and the distance in inches (DX) over which this wavenumber range is to be plotted.

REPRODUCED FROM HIRACC-6600 FILED

PROGRAM TPLOT

FIN 4,50414

07012177

80

Table B1. Listing of TPLOT Program (Cont.)

```

PROGRAM TPLOT
CONTINUE
IF (VIP,VT,V1) GO TO 80
ILO=(V1-VIP)/DV+5.001
IMI=ILO+600
75 IF (IMI,GE,LIMHI) IMI=LIMHI-1
80 IF (VZF,LT,VZ) GO TO 90
LIMHI=(VZ-VIP)/DV+5.001
90 IF (LIMHI,LT,600) IMI=LIMHI-1
CALL LPP (ILO,IMI,VIP,V1,DX,DV)
ILO=IMI
IMI=ILO+600
IF (IMI,LT,LIMHI) GO TO 90
IMI=LIMHI-1
95 IF (ILO,LT,(LIMHI-1)) GO TO 90
V(1)=V(LIMHI-3)
V(2)=V(LIMHI-2)
V(3)=V(LIMHI-1)
V(4)=V(LIMHI)
98 IF (LIMHI,LT,NLIM) GO TO 100
GO TO 90
100 CALL PLOT (Nsize+3.0,0.0,-3)
CALL KNOPLY
STOP
99 C
C
900 FORMAT (5I12,F10.6)
910 FORMAT (3A10)
920 FORMAT (3F12.3,E10)
100 930 FORMAT (4F10.3,4I5)
END

```

SUBROUTINE LPP

```

SUBROUTINE LPP (ILO,IMI,VIP,V1,DX,DV)
COMMON V(2000),NP(2000),VP(2000)
PRINT 910, ILO, IMI, VIP
DV1=DV/4.
DV2=DV1+DV1
DV3=DV2+DV1
K00=-7./128.
K01=109./128.
K02=39./128.
K03=-9./128.
K10=-1./16.
K11=9./16.
IP=1
IMAX=IMI-1
15 DO 10 I=ILO,IMAX
NP(IP)=VIP+DV*FLOAT(I-5)
NP(IP+1)=NP(IP)+DV1
NP(IP+2)=NP(IP)+DV2
NP(IP+3)=NP(IP)+DV3
20 VP(IP)=VIP
VP(IP+1)=K00*V(I-1)+K01*V(I)+K02*V(I+1)+K03*V(I+2)
VP(IP+2)=K10*V(I-1)+K11*V(I+1)+K12*V(I+2)
VP(IP+3)=K03*V(I-1)+K02*V(I)+K01*V(I+1)+K00*V(I+2)
IP=IP+4
25 10 CONTINUE
NP(IP)=VIP+DV*FLOAT(IMI-5)
VP(IP)=V(IMI)
CALL LINE (NP,VP,IP,1,0,1,V1,DX,0.0,0.0,1,0.00)
RETURN
30 C
C
900 FORMAT (5F12.3,F10.6)
910 FORMAT (2I10,F12.3," ILO,IMI,VIP")
35 END

```

Table B2. Loader Map for TPLOT Program

1

PAGE

18.31.45.

CYBER LOADER 1.1-28

87/12/77

TPLOT

FM OF THE LOAD 111
LUN#1 OF THE LOAD 50161

TRANSFER ADDRESS --- TPLOT 6262

PROGRAM AND BLOCK ASSIGNMENTS.

BLK#	ADDRESS	LENGTH	FILE	DATE	PROCESSOR	VER	LEVEL	MACHWARE	COMMENTS
TPLOT	111	7177	LGO	87/12/77	FTM	4.5	414	66X I	OPT=1
LGO	7318	282	LGO	87/12/77	FTM	4.5	414	66X I	OPT=1
NAME/	7512	6	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	7528	1	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	7521	1	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	7522	1	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	7523	5	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	7528	171	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	7721	54	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	7775	325	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18322	235	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18327	16	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18375	387	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18144	432	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18136	425	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18163	168	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18343	41	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18484	23	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18427	52	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18581	11	UL-PEN	18/06/76	COMPASS	3.0	2-414	66X I	OPT=2
NAME/	18512	318	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18222	233	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18255	66	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18363	75	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18448	467	UL-PEN	18/06/76	COMPASS	3.0	2-414	66X I	OPT=2
NAME/	18127	4	UL-PEN	18/06/76	COMPASS	3.0	2-414	66X I	OPT=2
NAME/	18133	576	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18731	23	UL-PEN	18/06/76	FTM	4.5	414	66X I	OPT=2
NAME/	18754	131	UL-PEN	18/06/76	COMPASS	3.0	2-414	66X I	OPT=2
NAME/	18185	64	UL-PEN	18/06/76	COMPASS	3.0	2-414	66X I	OPT=2
NAME/	18125	8	UL-PEN	18/06/76	COMPASS	3.0	2-414	66X I	OPT=2
NAME/	18171	16	UL-PEN	18/06/76	COMPASS	3.0	2-414	66X I	OPT=2

COMMON CODED I/O ROUTINES AND CONSTANTS.
PUL INITIALIZATION ROUTINE.
TEST FOR END OF FILE STATUS.

Table B2. Loader Map for TPLOT Program (Cont.)

LONG MAP - TPLOT					
ATERN, R4/	24426	1			
GET, F0/	24427	7			
GET, R1/	24436	5			
GET, R7/	24442	11			
GET, S0	24454	1835	SL-SYSIO	35/28/76 COMPASS	3. 75125
Z, SC	25911	181	SL-SYSIO	05/28/76 COMPASS	3. 75125
W, S0	25912	48	SL-SYSIO	35/28/76 COMPASS	3. 75125
F0U, S0	25942	186	SL-SYSIO	05/28/76 COMPASS	3. 75125
F0R, R0	25978	606	SL-SYSIO	05/28/76 COMPASS	3. 75125
C0R0, S0	26034	7	SL-SYSIO	35/28/76 COMPASS	3. 75125
C0R0, R0	26035	65	SL-SYSIO	05/28/76 COMPASS	3. 75125
C0R0, S0	26078	262	SL-SYSIO	35/28/76 COMPASS	3. 75125
C0R0, R0	26079	16	SL-SYSIO	05/28/76 COMPASS	3. 75125
C0R0, S0	26080	7	SL-SYSIO	35/28/76 COMPASS	3. 75125
C0R0, R0	26081	2	SL-SYSIO	05/28/76 COMPASS	3. 75125
C0R0, S0	26082	1362	SL-SYSIO	35/28/76 COMPASS	3. 75125
C0R0, R0	26083	260	SL-SYSIO	05/28/76 COMPASS	3. 75125
C0R0, S0	26084	23	SL-SYSIO	35/28/76 COMPASS	3. 75125
C0R0, R0	26085	114	SL-SYSIO	05/28/76 COMPASS	3. 75125
C0R0, S0	26086	142	SL-SYSIO	35/28/76 COMPASS	3. 75125
C0R0, R0	26087	7	SL-SYSIO	05/28/76 COMPASS	3. 75125
C0R0, S0	26088	67	SL-SYSIO	35/28/76 COMPASS	3. 75125
C0R0, R0	26089	166	SL-NUCLEUS	05/15/77 COMPASS	3. 2-614
C0R0, S0	26090	37	SL-NUCLEUS	30/15/77 COMPASS	3. 2-614
C0R0, R0	26091	16514			

REPLINE INTERFACE
PROCESS SYSTEM REQUEST.

.070 CP SECONDS

445688 CM STORAGE USED

67 TABLE MOVES

Table B3. Sample Output From TPLLOT Program

CLOUGH LOWENTZ(40) JULY 11,77			
3558.808	3658.818	48.888	
3558.908	3658.938	.818	1668
5	685	3558.808	ILO,IMI,VIP
1285	1285	3558.808	ILO,IMI,VIP
1285	1667	3558.808	ILO,IMI,VIP
3566.648	3638.638	.818	2484
3	683	3556.648	ILO,IMI,VIP
683	1283	3566.648	ILO,IMI,VIP
1283	1883	3566.648	ILO,IMI,VIP
1883	2483	3566.648	ILO,IMI,VIP
3598.648	3614.638	.818	2484
3	683	3598.648	ILO,IMI,VIP
683	1283	3598.648	ILO,IMI,VIP
1283	1883	3598.648	ILO,IMI,VIP
1883	2483	3598.648	ILO,IMI,VIP
3614.648	3638.638	.818	2484
3	683	3614.648	ILO,IMI,VIP
683	1283	3614.648	ILO,IMI,VIP
1283	1883	3614.648	ILO,IMI,VIP
1883	2483	3614.648	ILO,IMI,VIP
3638.648	3658.808	.818	1141
3	683	3638.648	ILO,IMI,VIP
683	1148	3638.648	ILO,IMI,VIP

END OF PLG'S.

Table B4. Data Cards for TPLOT Program

CLOWEN LORENTZ(40) JULY 11,77

3950. 3650. 40.