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DF LASER FREQUENCIES

R. K. Long, et al

Ohio State University

Prepared for:

Advanced Research Projects Agency

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OF LASER FREQUENCIES

R. K. Long
F. S. Mills
G. L. Trusty

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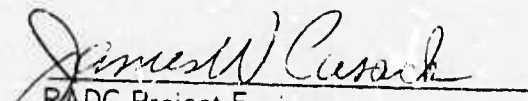
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FOREWORD

This report, Ohio State University Research Foundation Report Number 3271-7 (seventh Quarterly Report), was prepared by the Ohio State University ElectroScience Laboratory, Department of Electrical Engineering at Columbus, Ohio. Research was conducted under Contract F30602-72-C-0016. Mr. James W. Cusack, RADC (OCSE), of Rome Air Development Center, Griffiss Air Force Base, New York, is the Project Engineer.

PUBLICATION REVIEW

This technical report has been reviewed and is approved.


RADC Project Engineer

ABSTRACT

This report presents calculations of DF laser absorption coefficients for the Mid-Latitude Summer sea level atmospheric model. The individual gases which cause the absorption at each laser wavelength are identified. Results are compared with those previously published by R. A. McClatchey. The calculated results are being used to guide the experimental measurement program.

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I. INTRODUCTION

The best information, prior to experiments, as to the expected molecular absorption coefficients at DF laser wavelengths are obtainable from calculations based upon the Air Force Cambridge Research Laboratories line data tape[1]. Dr. R. A. McClatchey has published a report containing DF predictions based on the data tape[2]. The calculations presented here are extensions of that work in that:

- 1) The list of laser lines is different. Our line list includes all of the lines which have been observed in our pulsed probe laser, some of which were not included in the McClatchey report. Also we now have new wavenumbers for some of the lines.
- 2) A small correction for the H₂O continuum absorption which was omitted by McClatchey has been included. The data for this continuum absorption is given in the report on the AFCRL line data[1] which in turn is based on experimental work done by Burch[3].
- 3) Our calculations are presented only for one of McClatchey's atmospheric models (Mid-Latitude Summer) and only for sea level. We have, however, given the absorption coefficients for each component gas as well as the total coefficient so that one can see the relative importance of each absorber at each wavelength.
- 4) We have also made plots for each absorbing gas. These plots generally cover 5 or 10 wavenumbers to a page so that the laser line position relative to the absorption lines can be clearly seen. This is helpful in deciding whether small errors in either the absorption or laser line positions could result in a large change in the predicted coefficient.
- 5) Finally a calculation was made using a super-Lorentz line shape for the water vapor[4] in order to see what effect this would have on the coefficients.

II. DETAILS OF THE DF CALCULATIONS

All of the calculations were made for the AFCRL[5] mid-latitude sea level summer model. Table I lists some of the pertinent data. The derivation of the various conversion factors used is given in Appendix A.

TABLE I
Source of Absorption Line Data: AFCRL/GOAT TAPE
Atmospheric Model: AFCRL Mid-Latitude Summer

T	= 294 °K
P	= 760 torr
p(H ₂ O)	= 14.26 torr
p(N ₂ O)	= 2.13E-4 (.28 ppm)
p(CH ₄)	= 1.216E-3 torr (1.6 ppm)
p(CO ₂)	= .251 torr (330 ppm)
p(O ₃)	= 2.31E-5 torr (6E-5 g/m ³)
p(CO)	= 5.70E-5 torr (.075 ppm)

N₂ Continuum: AFCRL Report 434, Fig. 4.[1]

H₂O Continuum: AFCRL Report 434, Fig. 2.[1]

Bound = 25 cm⁻¹

The calculated absorption coefficients consist of three components: (1) molecular absorption, (2) water vapor continuum, and (3) pressure induced nitrogen absorption.

The data for the molecular absorption component was calculated using the AFCRL data tape[1]. This tape contains values for the frequency, strength, half-width, and lower energy state for H₂O, N₂O, CH₄, CO₂, CO, O₃, and O₂ lines in the wavelength band of interest. In our calculations a Lorentz line shape was used with all lines within 25 cm⁻¹ of the calculation frequency being included in the summation. Another program parameter (SLOW) allows the exclusion of lines having a line strength less than SLOW from the summation if desired in order to save computer time. For this report SLOW was set to 10⁻²⁷ to effectively include all lines in the data tabulation.

The program computes $\ln T = -k u$ where T is the fractional transmittance, k is the absorption coefficient in (mol-cm⁻²)⁻¹ and u is the absorber amount in mol-cm⁻².

The line strength is defined as $S = \int k dv$ and is in units of cm⁻¹(mol-cm⁻²)⁻¹. The halfwidth is in cm⁻¹. The Lorentz shape is given by

$$(1) \quad k = \sum_i \frac{S_i \alpha_i}{\pi[(\nu - \nu_i)^2 + \alpha_i^2]} \quad .$$

The line strengths and half-widths are given at STP and must be corrected to model conditions. We have used the following relationships.

1. Halfwidth

$$(2) \quad \alpha_i = \alpha_{i0} \left(\frac{P_e}{P_0} \right) \left(\frac{T_0}{T} \right)^{CX}$$

The effective pressure P_e [8] is given by

$$(3) \quad P_e = \frac{B P_a + F P_f}{760} \quad \text{atmospheres}$$

where

P_a = absorber pressure in torr

P_f = broadener pressure in torr

B = self-broadening coefficient

F = foreign-broadening coefficient.

For nitrogen F is equal to one and the empirical values for B , assuming nitrogen broadening, are given in Table II for each gas [8].

TABLE II

	B	BX	CX
N ₂ O	1.24	1.0	.5
CH ₄	1.3	1.5	.5
H ₂ O	5.	1.5	.62
CO ₂	1.3	1.0	.58
O ₃	1.0	1.5	.5
CO	1.02	1.0	.5

The exponent CX is also given in Table II. Although theoretically CX = 0.5 for all of the gases, we have used for H₂O and CO₂ the average empirical values originally suggested by Calfee and Benedict[9].

The line strengths were corrected to the model temperature by use of the relation

$$(4) \quad S_i = S_{i0} \left(\frac{T_0}{T} \right)^{BX} \exp \left(\frac{-E''}{k} \frac{T_0 - T}{T_0} \right)$$

where $k = 0.6951 \text{ cm}^{-1}/\text{deg K}$
 $E'' = \text{lower energy state in cm}^{-1} \text{ from data tape.}$

The coefficients BX for each of the molecules are listed in Table II.

The absorber amount, u, was computed from the formula

$$(5) \quad u = .733952 \times 10^{22} (p_a/760/T) \cdot \lambda \text{ mol-cm}^{-2}$$

where $p_a = \text{absorber partial pressure in torr} = \text{ppm by volume} \times 10^{-6} \times P$
 $T = \text{model temperature in deg K}$
 $\lambda = \text{path in cm.}$
 $P = \text{total pressure in torr.}$

Our program accepts the absorber partial pressure p_a in torr with the values given in Table I being used for the present work.

The AFCRL mid-latitude summer model gives the sea level H₂O density as 14.1 gm/m³ and using Eq. (3) of Appendix A the resulting p_a is 14.26 torr.

It is useful to note that there are 2438 water lines tabulated on the data tape between 2400 and 2850 cm⁻¹ of which 2150 or 88% are HDO. Also a composition factor of 0.03% for the HDO was assumed in compilation of the tape[1]. It is noted that this composition differs from the value of 0.027% which was given in the earlier water vapor data compilation by Gates, Calfee, Hansen and Benedict.

It is necessary in connection with the computation of absorber amount to have conversion factors between various systems of units. Although this information is available elsewhere[5,10] the derivations and resulting constants have been given in Appendix A of this report.

The water vapor continuum and pressure induced nitrogen absorption coefficients were derived from Figs. 2 and 4, respectively, of Reference [1].

Figure i which was derived from the experimental data of Burch[3] shows the wavelength dependence of the water vapor continuum absorption coefficient for 14.26 torr water vapor at sea level. The sea level absorption coefficient for 296°K and 14.26 torr H₂O is given by

$$k(\nu) = 1.813 \times 10^{25} p_a^2 C_s^0(\nu) \text{ km}^{-1}$$

where C_s^0 is from Burch's data and P_a is the H₂O pressure in atmospheres.

Note that Burch[3] measured a C_s/C_b of approximately 8 whereas a value of 5 was assumed in the line by line calculations, see Table II. Also note that the Burch results used here (296°K) are actually extrapolated from measurements made at higher temperatures[3].

Figure ii shows the nitrogen absorption coefficient at 296°K[1]. The calculations in this report are all for a pressure of one atmosphere, thus the values from Fig. ii are used directly.

III. COMPUTED MID-LATITUDE SUMMER ABSORPTION COEFFICIENTS

The calculated results for 30 DF laser lines are given in Table III. The six components which make up the total absorption coefficient are tabulated separately.

The AFCRL data tape lists no CO lines between 2400 and 2850 cm⁻¹ and the ozone absorption coefficient at the 30 DF lines was less than 10⁻⁵ km⁻¹ for a concentration of 6 x 10⁻⁵ g/m³. Therefore these two gases are not included.

Except for six DF lines between 2546.42 and 2594.25 cm⁻¹, nearly all of the absorption is caused by water vapor and nitrogen. For these six lines N₂O absorption is a significant factor. In the concentrations assumed, CH₄ absorption is a minor factor for all lines.

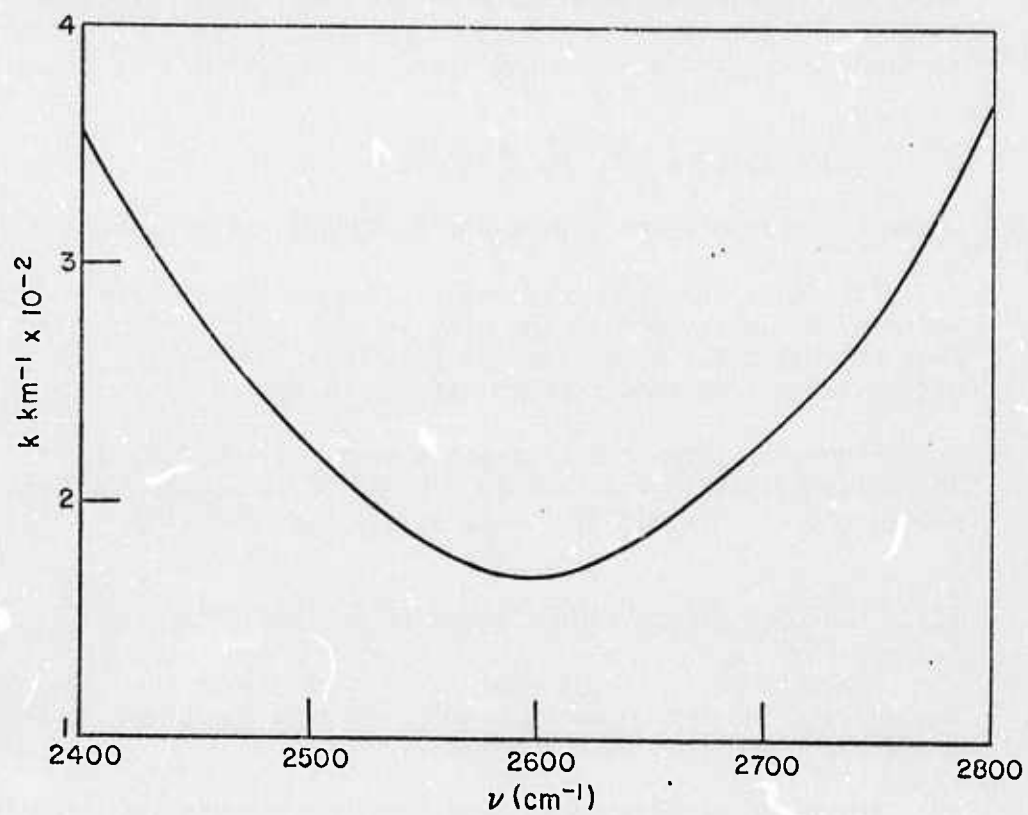


Fig. i. Water vapor continuum absorption coefficient adapted from Burch #4784[3] for $p_{\text{H}_2\text{O}} = 14.2$ torr and $T = 296^\circ\text{K}$ at 760 torr total pressure.

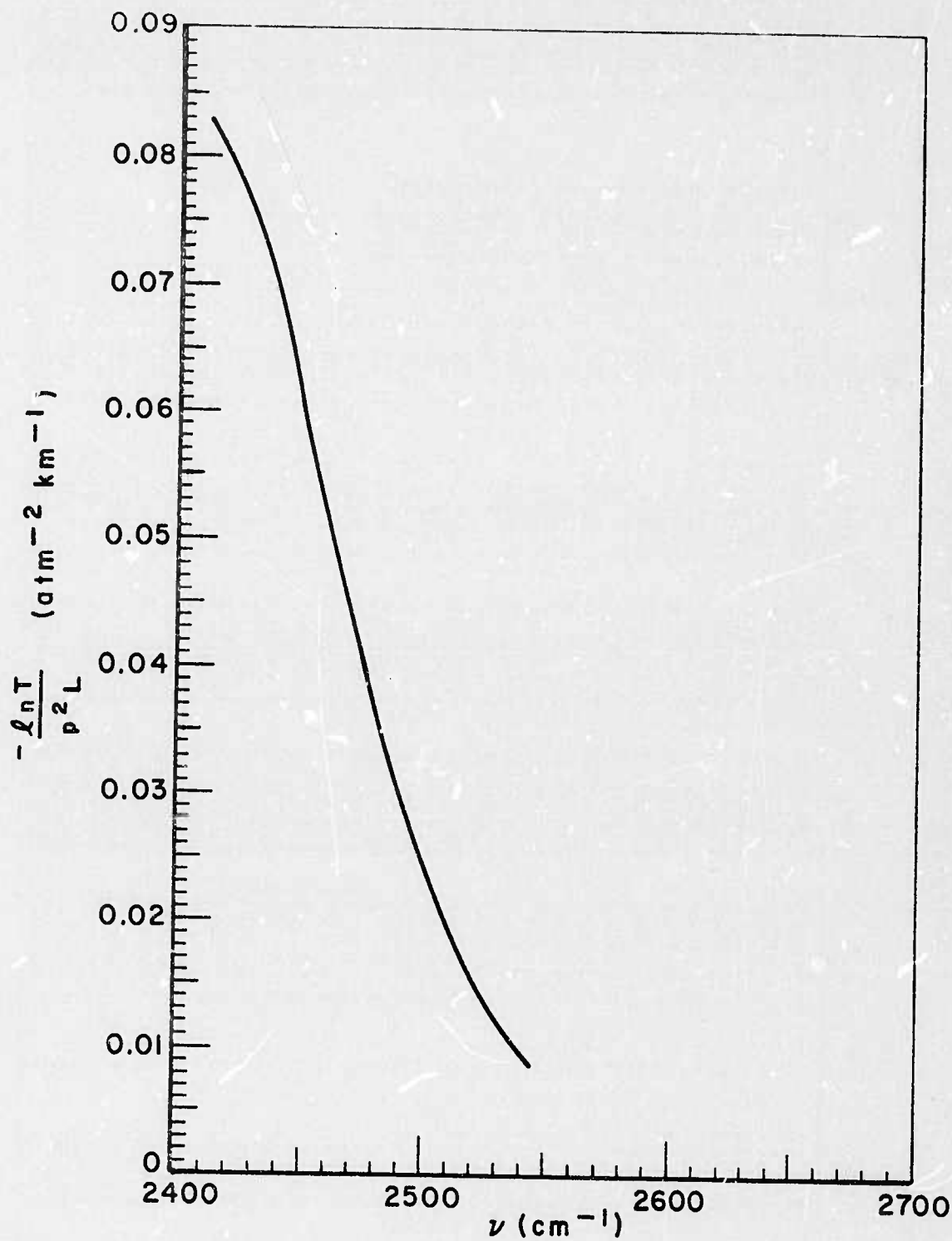


Fig. ii. Nitrogen absorption from Fig. 4 of AFCRL 73-0096, $T = 296^\circ \text{K}$.

TABLE III
Mid-Latitude Summer Sea Level Absorption Coefficients
Calculated from AFCRL Absorption Line-Data

Line	Iden	S*	N ₂ O	CH ₄	CO ₂	H ₂ O	H ₂ O Cont	N ₂	Total
2445.41	3-2,12	c	2.519E-3	4.268E-9	1.042E-2	3.095E-5	2.85E-2	6.6E-2	1.075E-1
2471.29	3-2,11	c	4.087E-3	7.683E-8	3.713E-5	4.997E-3	2.52E-2	4.6E-2	8.032E-2
2496.77	3-2,10	c	8.055E-4	1.109E-5	5.381E-8	6.540E-4	2.27E-2	2.5E-2	4.917E-2
2500.48	2-1,13	b	7.635E-3	2.881E-6	2.735E-8	1.267E-4	2.22E-2	2.5E-2	5.496E-2
2521.81	3-2,9	c	4.511E-4	2.748E-6	2.094E-7	2.321E-4	2.05E-2	1.5E-2	3.619E-2
2527.42	2-1,12	b	8.387E-4	1.841E-5	1.814E-7	2.539E-4	2.00E-2	1.4E-2	3.511E-2
2546.42	3-2,8	c	1.399E-2	1.833E-3	1.196E-7	1.347E-3	1.86E-2	8.0E-3	4.377E-2
2553.97	2-1,11	b	9.655E-3	7.757E-5	1.036E-7	5.113E-4	1.82E-2	7.1E-3	3.554E-2
2570.51	3-2,7	a	3.367E-2	3.174E-5	7.826E-8	4.783E-3	1.75E-2	5.0E-3	6.098E-2
2580.10	2-1,10	b	4.458E-2	2.618E-6	6.763E-8	2.684E-3	1.70E-2	3.6E-3	6.787E-2
2583.47	1-0,13	b	2.517E-2	5.008E-6	6.441E-8	3.580E-3	1.69E-2	3.45E-3	4.91 E-2
2594.25	3-2,6	c	1.954E-3	1.612E-5	5.553E-8	6.666E-3	1.68E-2	2.6E-3	2.804E-2
2605.80	2-1,9	b	5.362E-4	2.046E-4	4.792E-8	1.937E-2	1.68E-2	2.3E-3	3.921E-2
2611.14	1-0,12	b	9.147E-5	3.795E-6	4.492E-8	8.245E-3	1.70E-2	2.1E-3	2.744E-2
2617.44	3-2,5	c	1.170E-5	7.513E-5	4.174E-8	2.872E-3	1.72E-2	2.0E-3	2.216E-2
2631.06	2-1,8	b	1.229E-7	7.884E-4	3.591E-8	1.476E-2	1.78E-2	1.9E-3	3.525E-2
2638.39	1-0,11	b	1.271E-8	5.999E-4	3.327E-8	2.472E-1	1.82E-2	1.6E-3	2.676E-1
2655.85	2-1,7	b	1.103E-11	6.015E-4	2.805E-8	7.905E-2	1.93E-2		9.895E-2
2665.22	1-0,10	b	1.418E-11	1.975E-3	2.573E-8	1.512E-2	2.00E-2		3.709E-2
2680.17	2-1,6	b	2.291E-11	3.103E-4	2.260E-8	3.689E-2	2.12E-2		5.84 E-2
2691.61	1-0,9	b	3.647E-11	3.223E-3	2.057E-8	5.509E-2	2.20E-2		8.03 E-2
2703.99	2-1,5	b	7.099E-11	2.073E-6	1.867E-8	5.454E-3	2.30E-2		2.846E-2
2717.54	1-0,8	b	2.441E-9	2.335E-6	1.688E-8	8.986E-2	2.41E-2		1.14 E-1
2727.30	2-1,4	b	2.679E-8	1.475E-4	1.574E-8	4.248E-2	2.51E-2		6.773E-2
2743.00	1-0,7	b	4.321E-6	2.850E-4	1.414E-8	3.300E-2	2.69E-2		6.019E-2
2750.09	2-1,3	b	4.062E-5	8.969E-4	1.350E-8	1.255E-2	2.75E-2		4.099E-2
2767.97	1-0,6	b	1.029E-4	4.949E-3	1.206E-8	5.130E-2	3.08E-2		8.715E-2
2792.43	1-0,5	b	8.076E-4	6.103E-4	1.044E-8	3.732E-2	3.50E-2		7.374E-2
2816.38	1-0,4	b	1.158E-3	2.859E-3	9.144E-9	6.043E-2	4.00E-2		1.044E-1
2839.78	1-0,3	b	4.945E-7	7.241E-4	8.100E-9	5.749E-2	4.50E-2		1.032E-1

*Source of laser line data

a - Mills (OSU)

b - calculated from molecular constants (P.K.L. Yin, OSU Physics Dept.)

c - Deutsch (7)

There is also a remarkable uniformity in the calculated coefficients for 29 of the 30 laser lines, the exception being the 1-0₁₁ line at 2638.39 cm⁻¹. The laser lines miss all of the regions of intense absorption. This fortunate situation will also be clear from an examination of the plots to be given in a later section.

Table IV shows the output spectrum of a 200 watt DF laser which

TABLE IV
Distribution of Power for TRW 200 Watt DF Laser
Including Mid-Latitude Summer Absorption
Coefficient from Table III

Line	Iden	Percent	Coefficient
2496.77	3-2,10	.8	
2521.81	3-2,9	3.6	
2546.42	3-2,8	2.6	
2570.51	3-2,7	12.8	.061
2580.10	2-1,10	2.6	
2594.25	3-2,6	4.3	
2605.80	2-1,9	5.6	
2617.44	3-2,5	.8	
2631.06	2-1,8	12.3	.0353
2655.85	2-1,7	11.3	.099
2680.17	2-1,6	12.8	.0584
2691.61	1-0,9	.5	
2703.99	2-1,5	1.0	
2717.54	1-0,8	4.0	
2743.00	1-0,7	4.1	
2767.97	1-0,6	6.1	
2792.43	1-0,5	4.1	
		100.0	

was constructed at TRW, Inc. Fifty percent of the total power is obtained on four lines: 3-2₇ and 2-1₆, 2-1₇, and 2-1₈. For the 3-2₇ line 84 percent of the absorption is caused by N₂O and N₂ with N₂O being the most important. For the above 2-1 lines from 86 to 99% of the absorption is due to water vapor.

Table V shows the spectrum of the TRW propagation test laser and the predicted absorption coefficients from Table III.

TABLE V
DF Laser Calculated Absorption Coefficients for Mid-Latitude
Summer Sea Level Model with Normalized Relative
Intensities of DF Lines in TRW Propagation
Test Laser (3 cm Active Length).

Iden	Freq (cm^{-1})	Normalized Relative Intensity	Absorption Coefficient (km^{-1})
4-3,7		.08	
3-2,10	2496.77	.045	.0492
4-3,6		.163	
3-2,9	2521.81	.102	.0362
4-3,5		.08	
3-2,8	2546.42	.364	.0438
3-2,7	2570.51	.489	.061
2-1,10	2580.10	.07	.0679
3-2,6	2594.25	.688	.028
2-1,9	2605.80	.244	.0392
3-2,5	2617.44	.432	.022
2-1,8	2631.06	.648	.0353
2-1,7	2655.85	.693	.099
2-1,6	2680.17	1.00	.058
1-0,9	2691.61	.248	.080
2-1,5	2703.99	.307	.0285
1-0,8	2717.54	.494	.114
1-0,7	2743.00	.670	.0602
1-0,6	2767.97	.642	.087
1-0,5	2792.43	.21	.0737

IV. PLOTS

In order to provide additional insight into the molecular absorption problem, plots of N_2O , CH_4 , and water vapor absorption were also prepared.

The water vapor plots do not include the water continuum of Fig. i. The water plots are for 15 torr H_2O at 294°K , i.e., a relative humidity of 80 percent, a total pressure of 760 torr and a path length of 10 km. The laser wavelengths of Table III are clearly marked.

In all 54 plots were made. Figures 1-18 are the CH_4 plots. The path length was one km in all cases. The CH_4 pressure was varied from 0.1 to 30.0 torr to produce an onscale plot. Note from Table I that these partial pressures are all much greater than the 1.3×10^{-3} torr assumed in the sea level model atmosphere. The plots are mostly useful in examining the nature of the spectrum in the vicinity of the DF laser wavelengths in order to estimate which absorption coefficients from Table III may be in error due to incorrect data on either the absorption line or laser line positions. For example, see the 3-2 P(8) line, Fig. 3; 2-1 P(9), Fig. 5; 2-1 P(7), Fig. 8; 2-1 P(3), Fig. 14; etc. It is interesting also to examine the plots for the four high power laser lines given in Table IV.

Figures 19-35 give the plots for N_2O . Again the path length was one km and the partial pressure was from .002-30 torr as compared to the sea level model which contains 2.3×10^{-4} torr N_2O .

Figures 36-54 give the water vapor plots. In this case the path length was increased to 10 km and the partial pressure was maintained at 15 torr.

Experiments are being undertaken at Ohio State University where DF laser sources are being used together with a one km multitraversal absorption cell or an acoustic spectrophone in order to obtain direct information as to the accuracy of the predictions which have been given in this report.

V. COMPARISON TO AFCRL CALCULATIONS

We have attempted to compare our results with those reported earlier by McClatchey[2]. First, the calculations presumably use the same input line-data, namely the AFCRL GOAT tape[1]. Nevertheless differences in the results were noted which presumably must be due to differences in some of the other variables. There are some differences in approach where one cannot say that one is correct and the other not. Also we have not had a copy of Dr. McClatchey's computer program so that we are not entirely sure that the information given below is correct. Nevertheless from a study of some of the AFCRL reports[1,2] we have concluded that for the measurements reported in AFCRL-72-0312 the following data was used:

BOUND = 20 cm^{-1}
 BX as in Table II
 CX = 0.5 all gases
 Mid-Latitude Summer Model as in Table I
 Lorentz line shape
 B = 1.0 all gases.

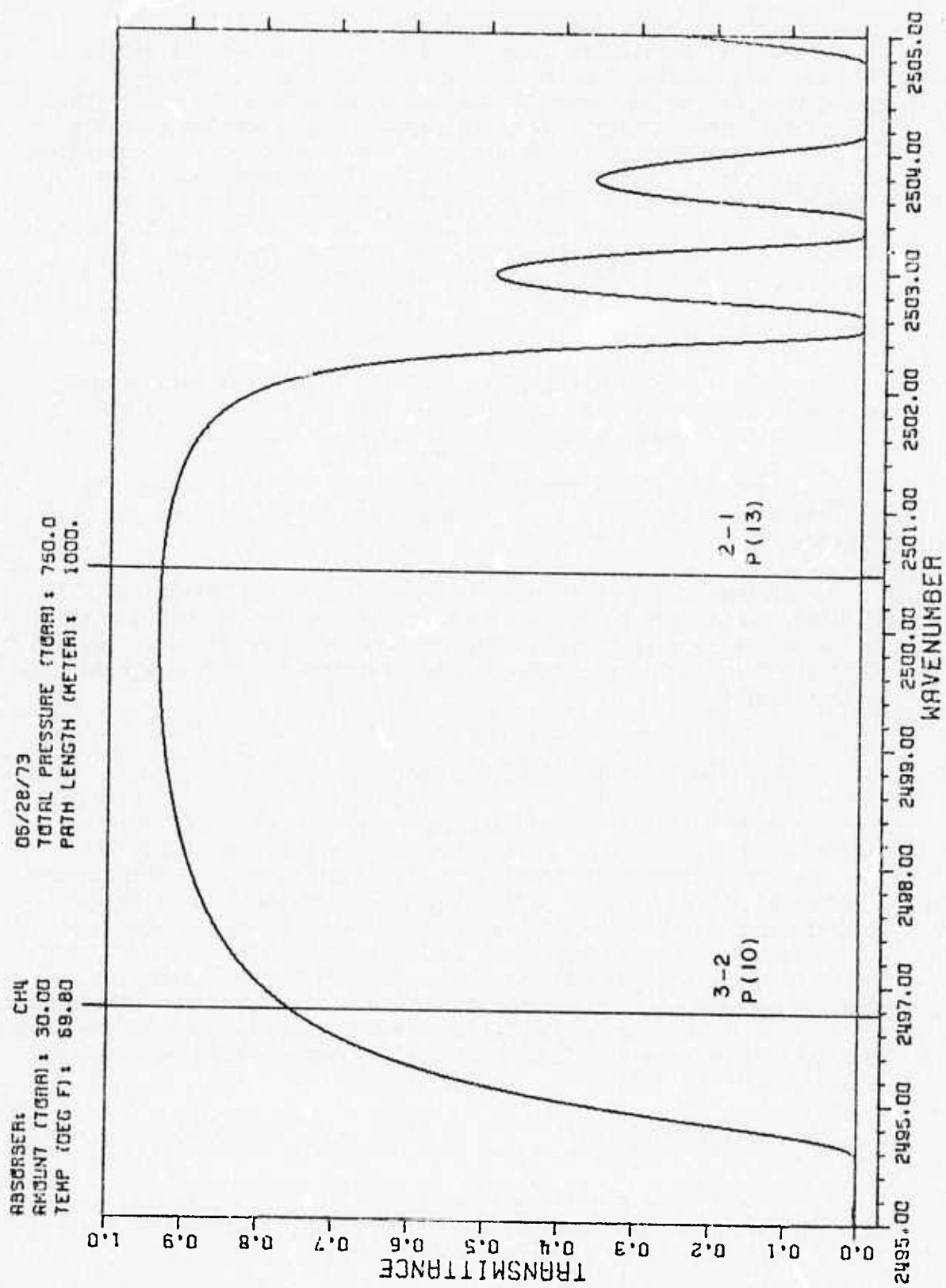


Fig. 1

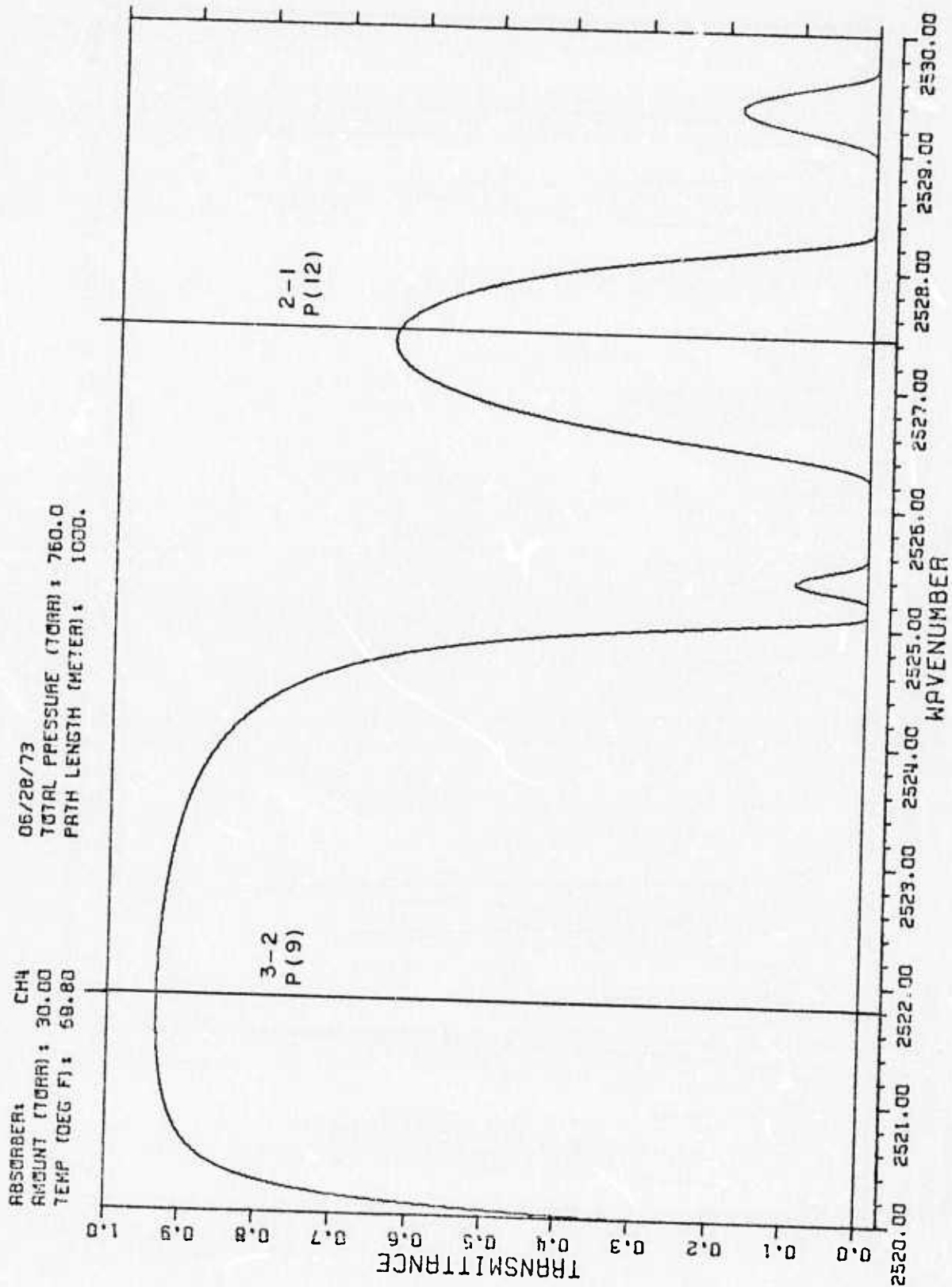


Fig. 2

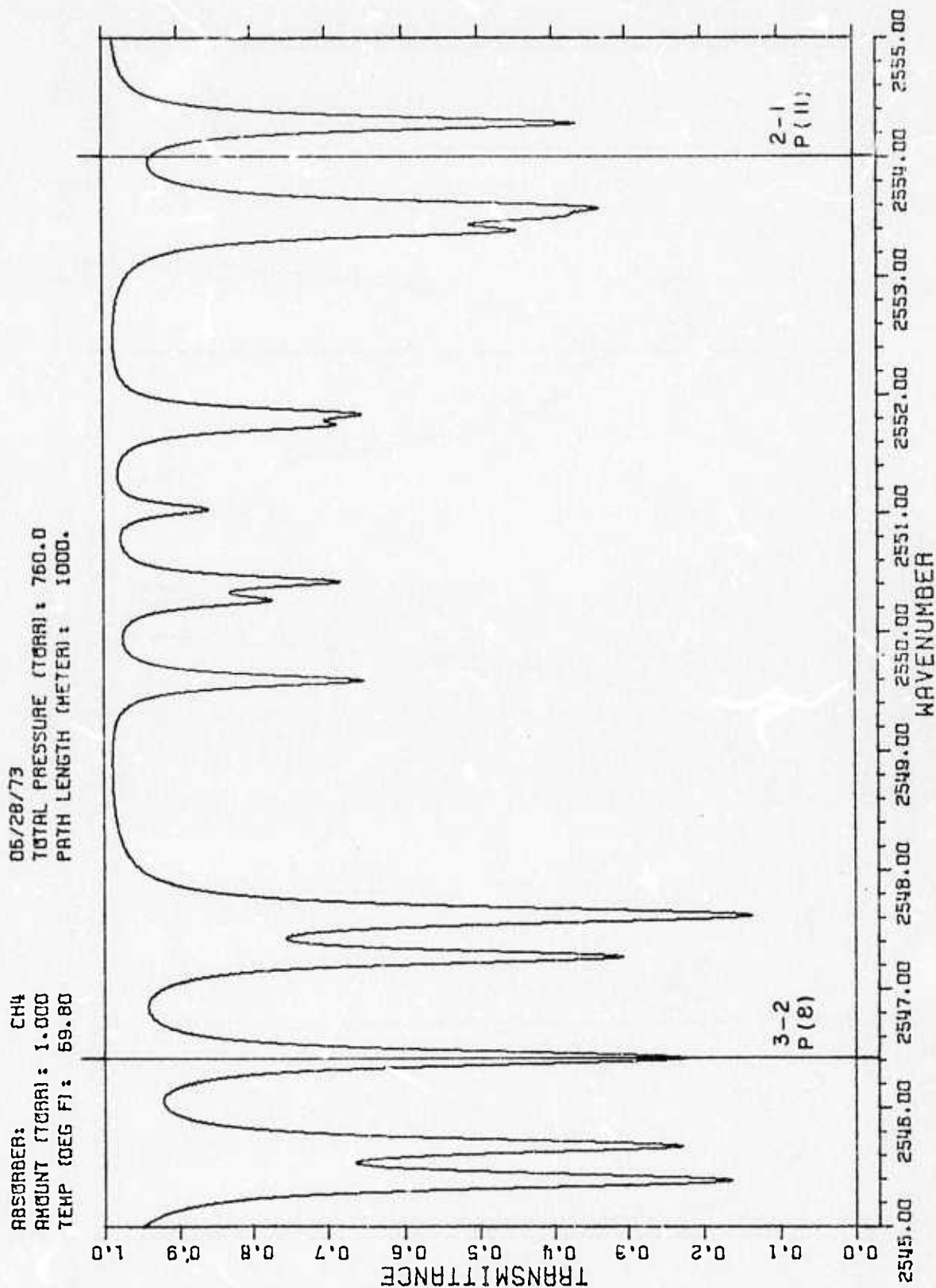


Fig. 3

ABSORBER: CH₄
AMOUNT (TORR): 10.00
TEMP (DEG F): 69.60

06/28/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

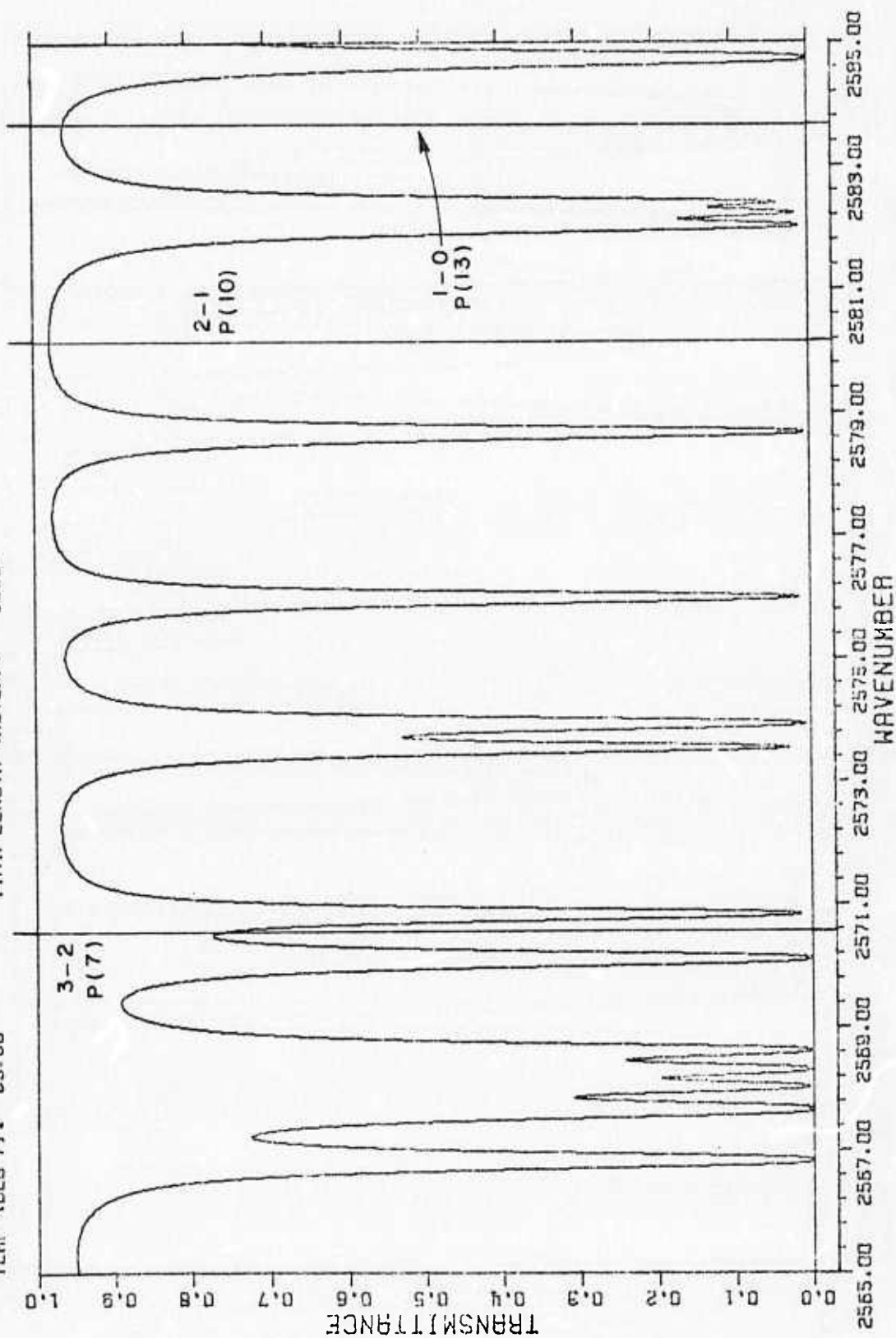


Fig. 4

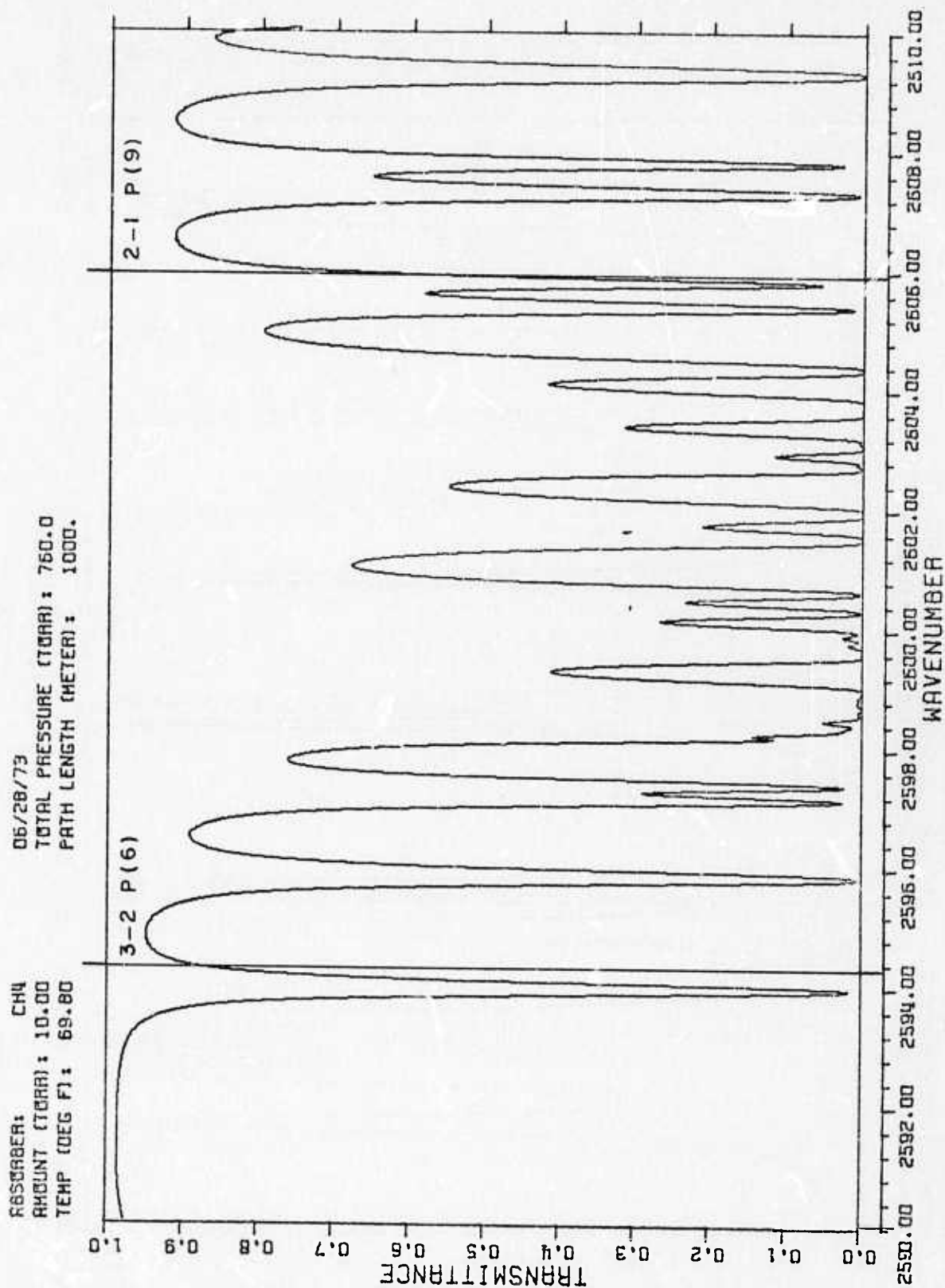


Fig. 5

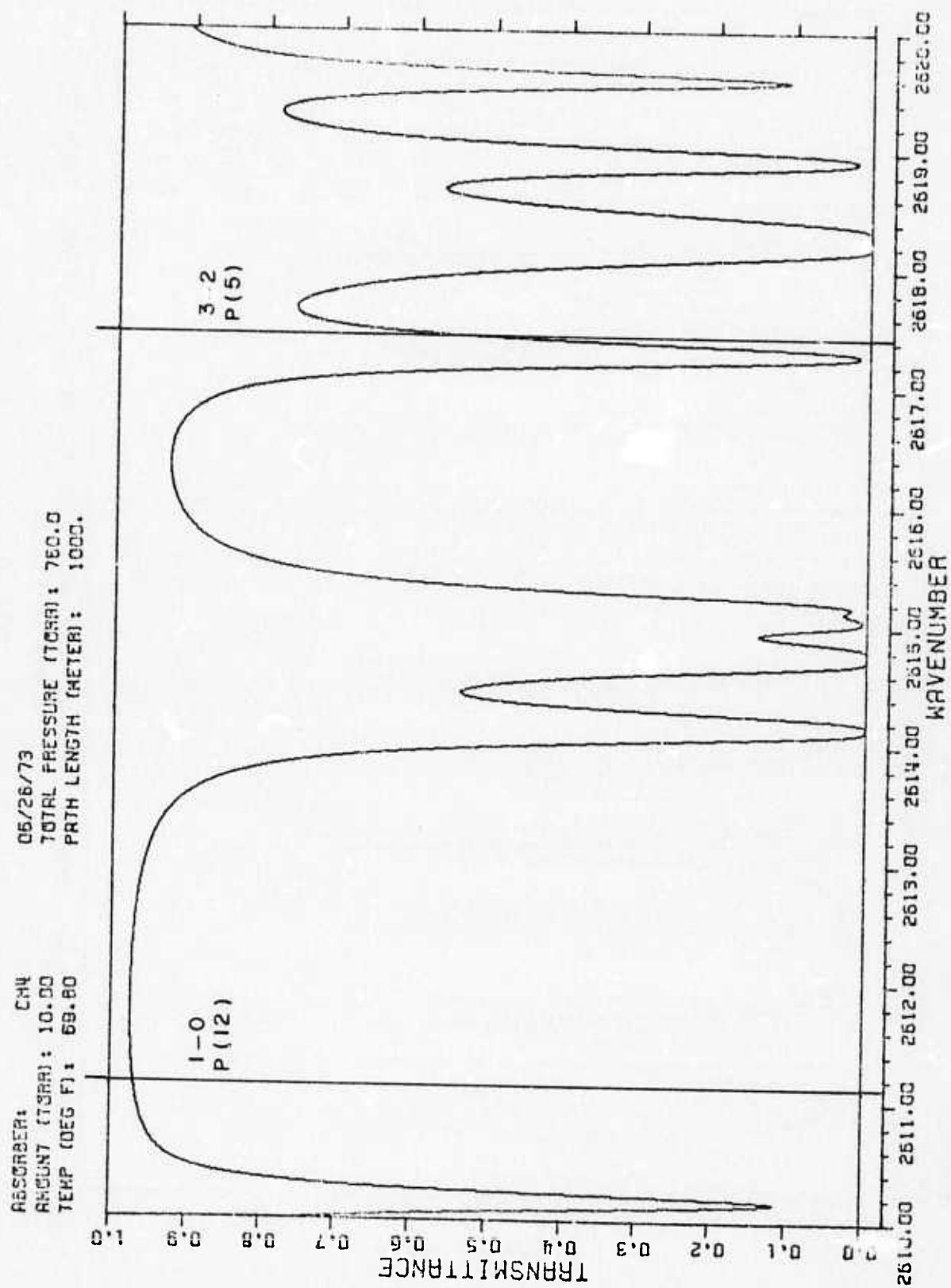


Fig. 6

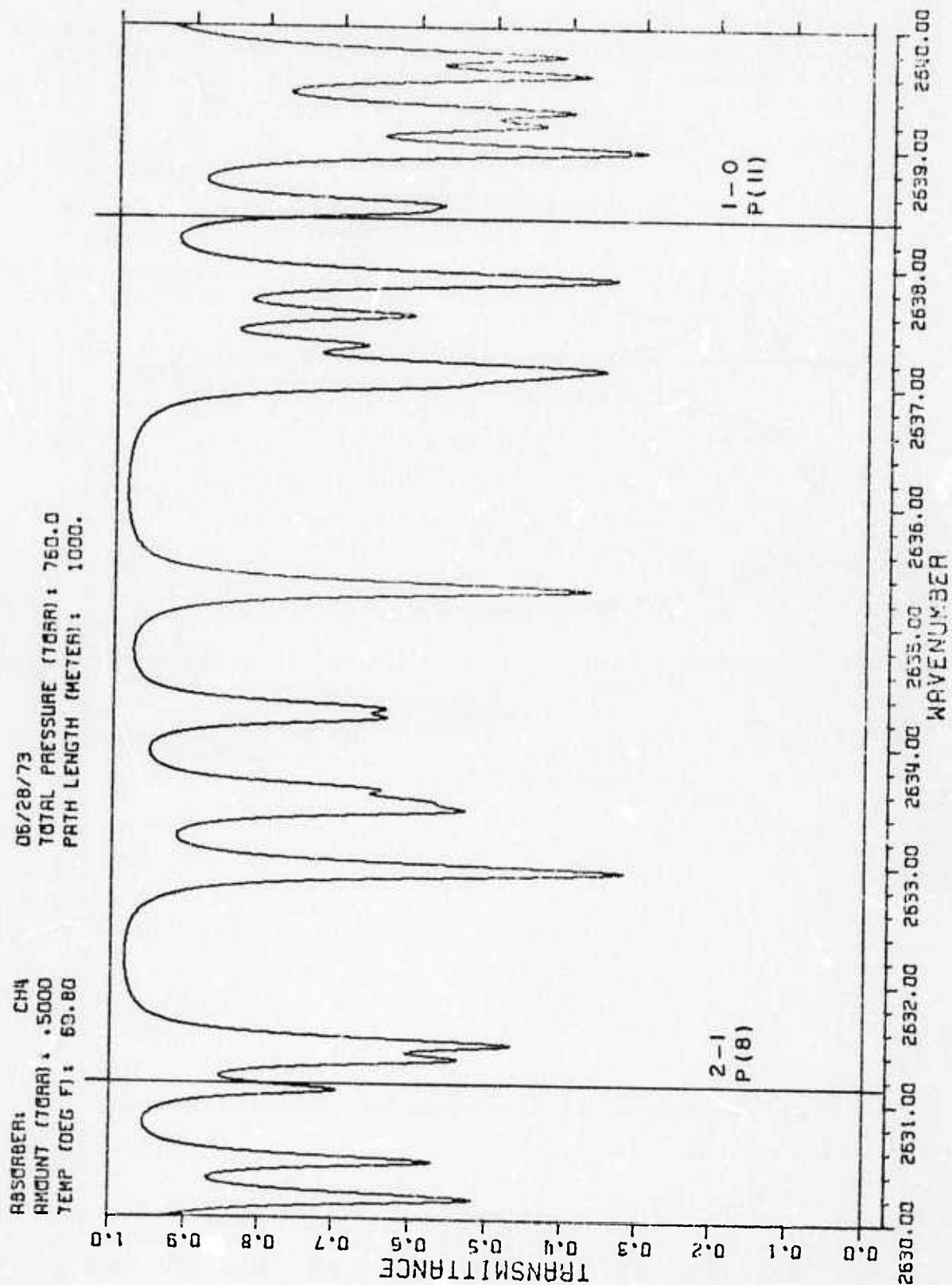


Fig. 7

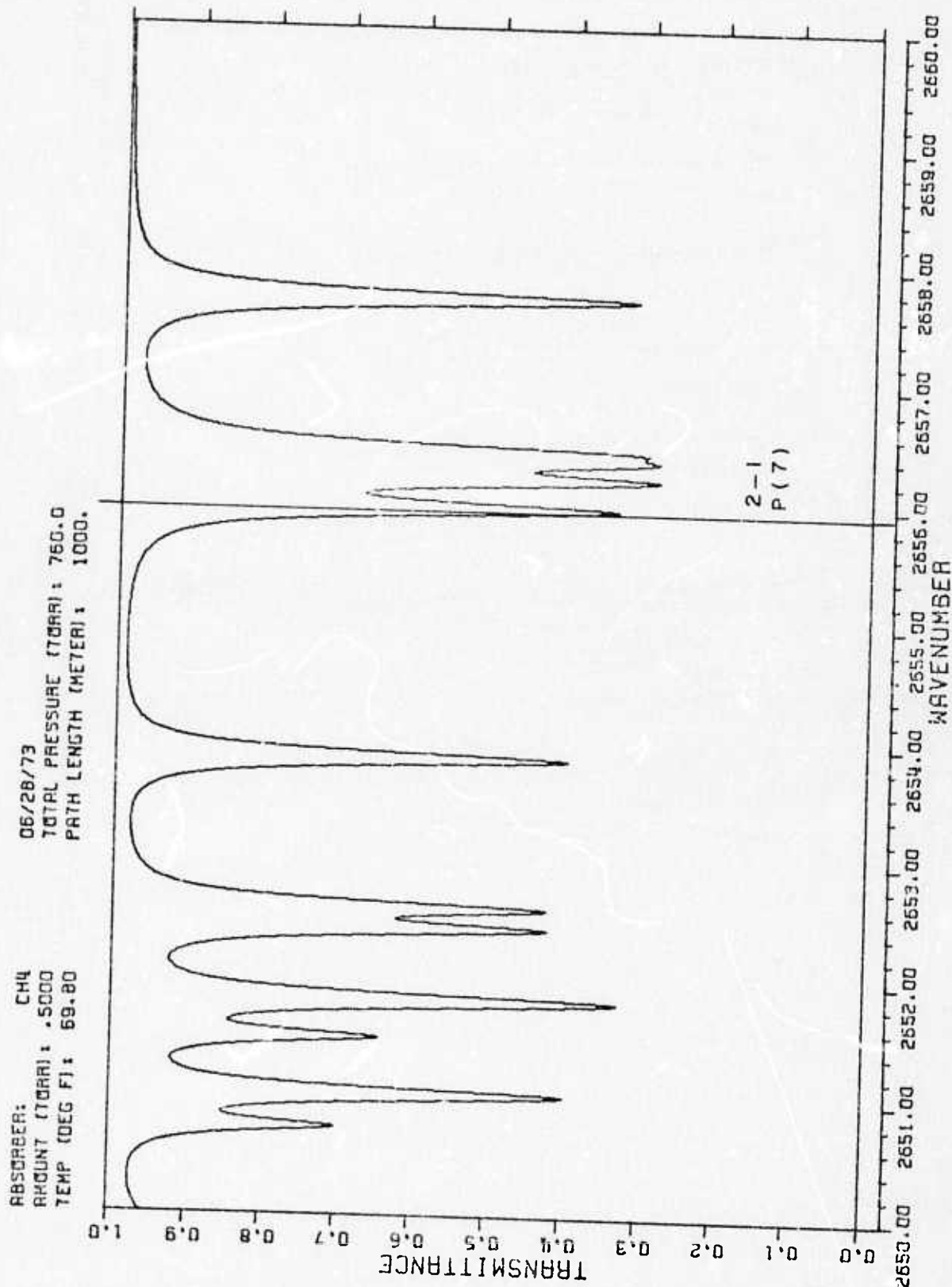


Fig. 8

ABSORBER: CH4
AMOUNT (TORR): .5000
TEMP (DEG F): 69.80

06/28/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

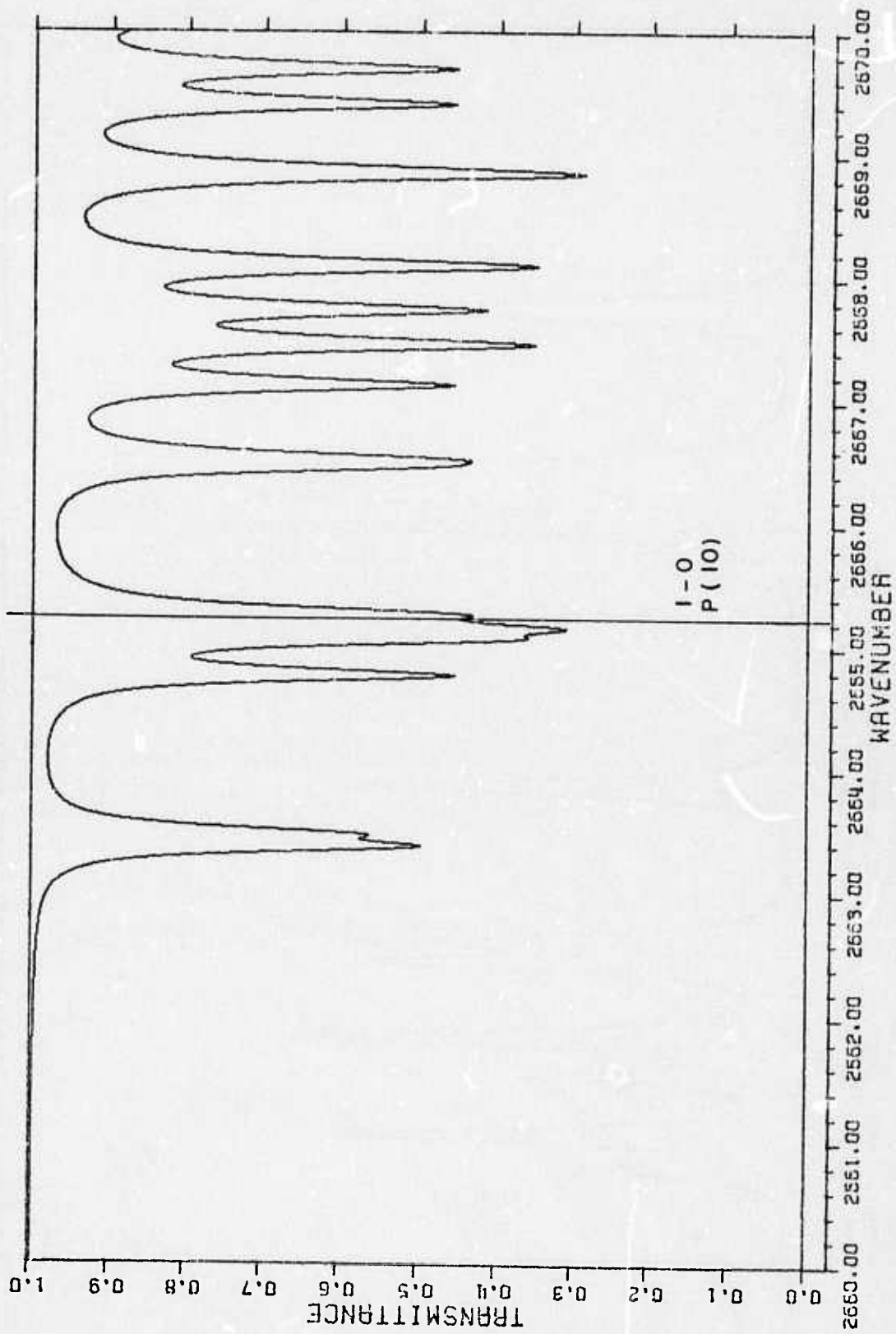


Fig. 9

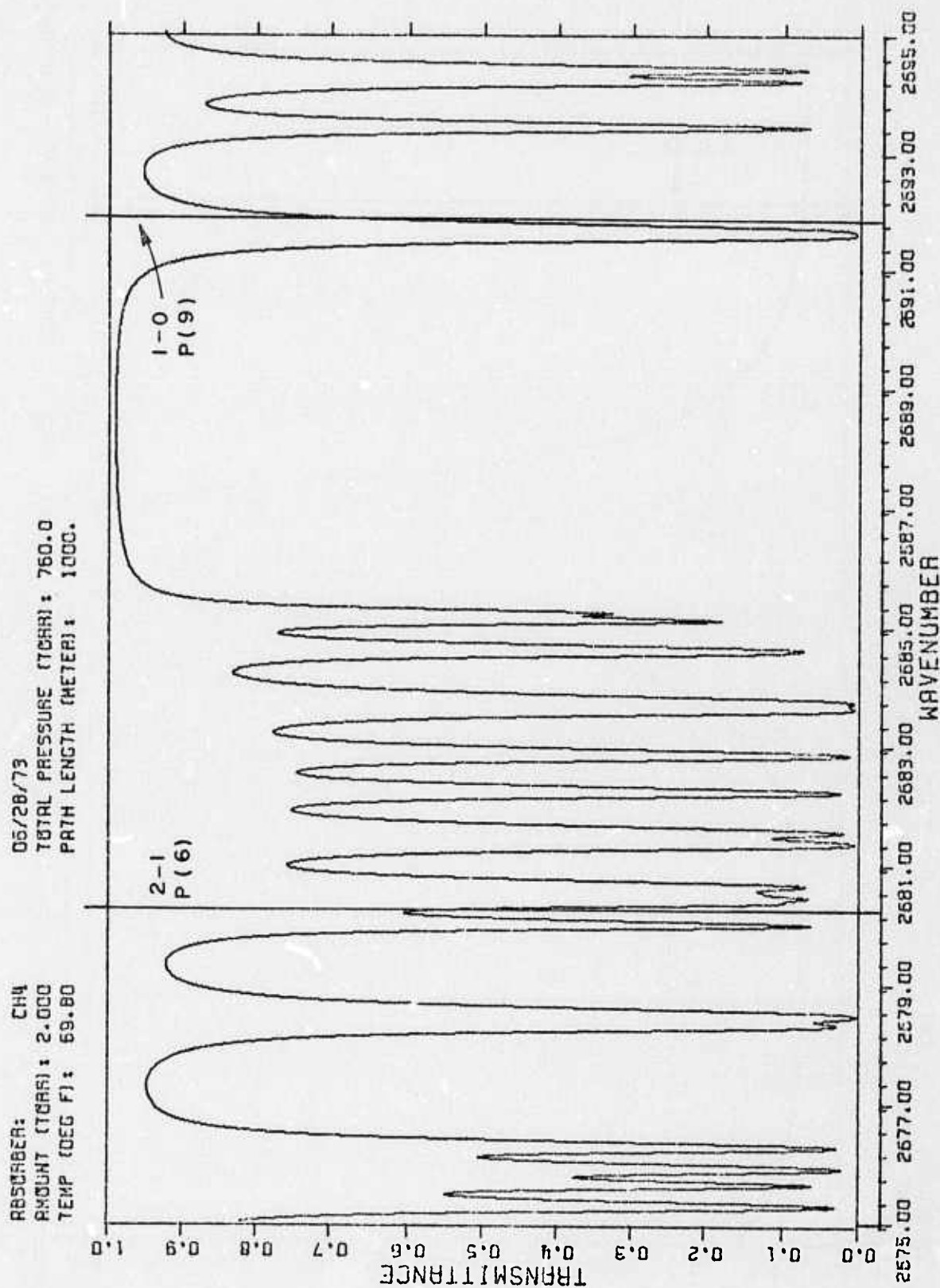


Fig. 10

ABSORBER: CH₄
AMOUNT (TORR): 30.00
TEMP (DEG F): 69.80

06/28/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

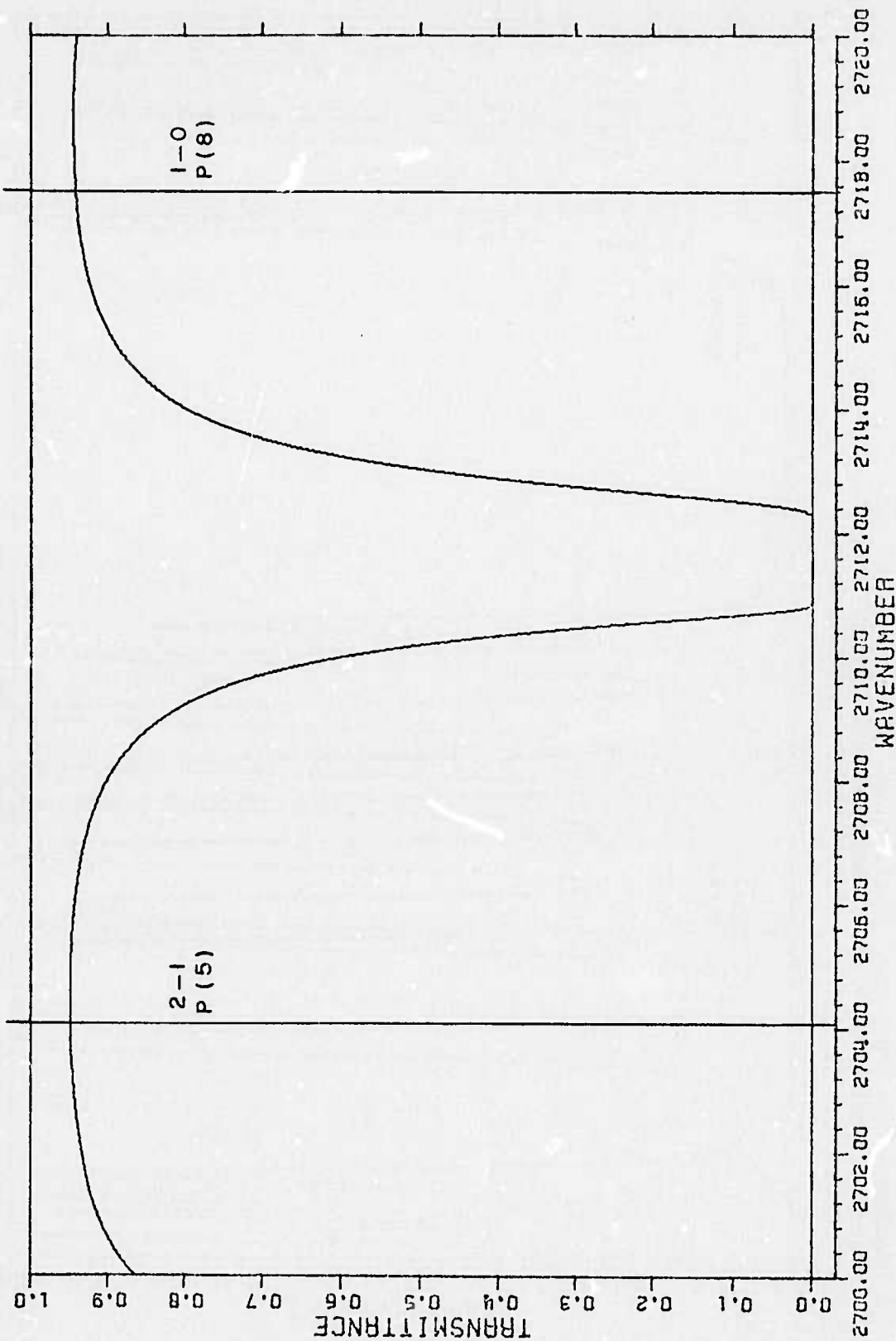


Fig. 1

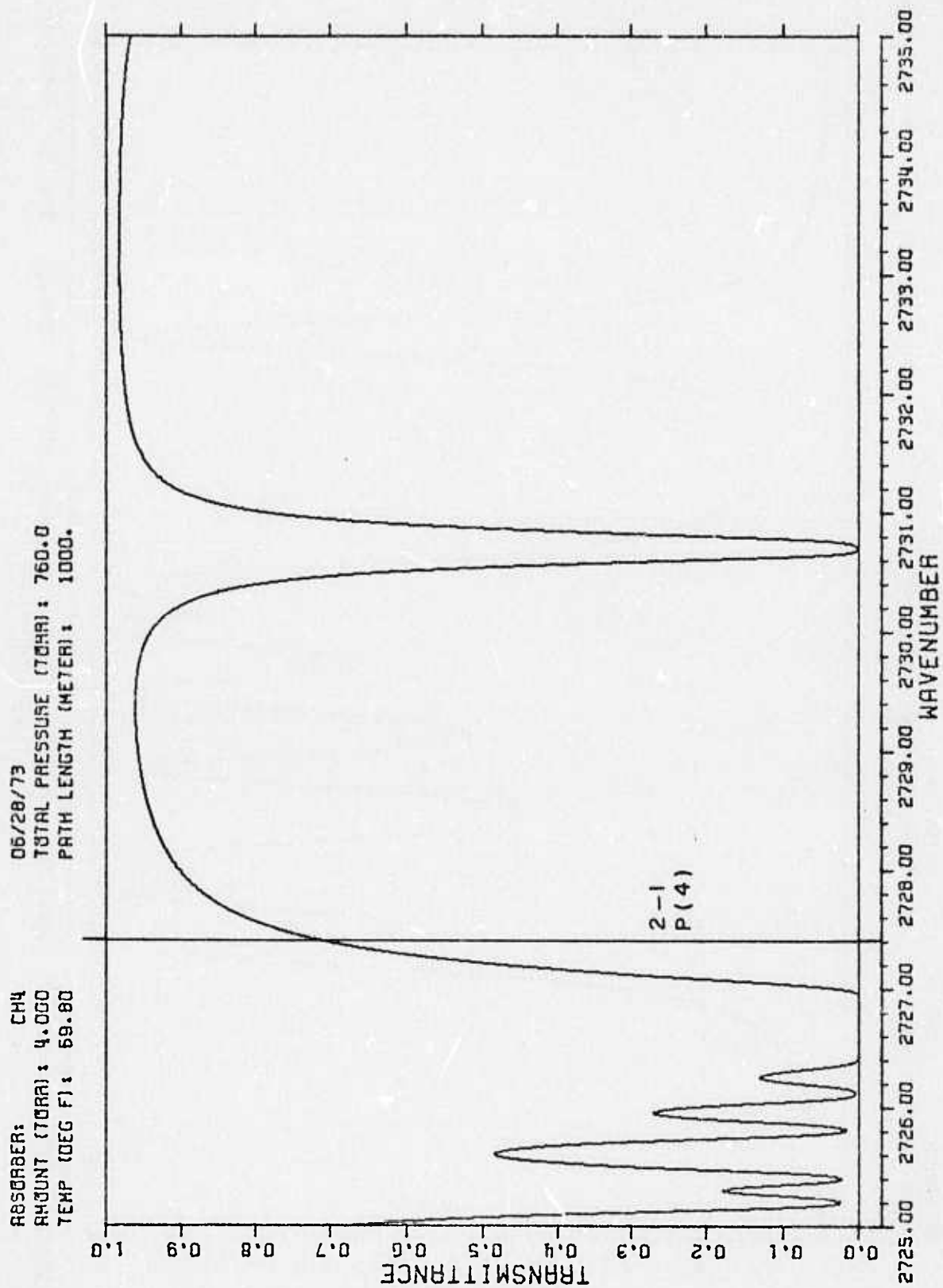


Fig. 12

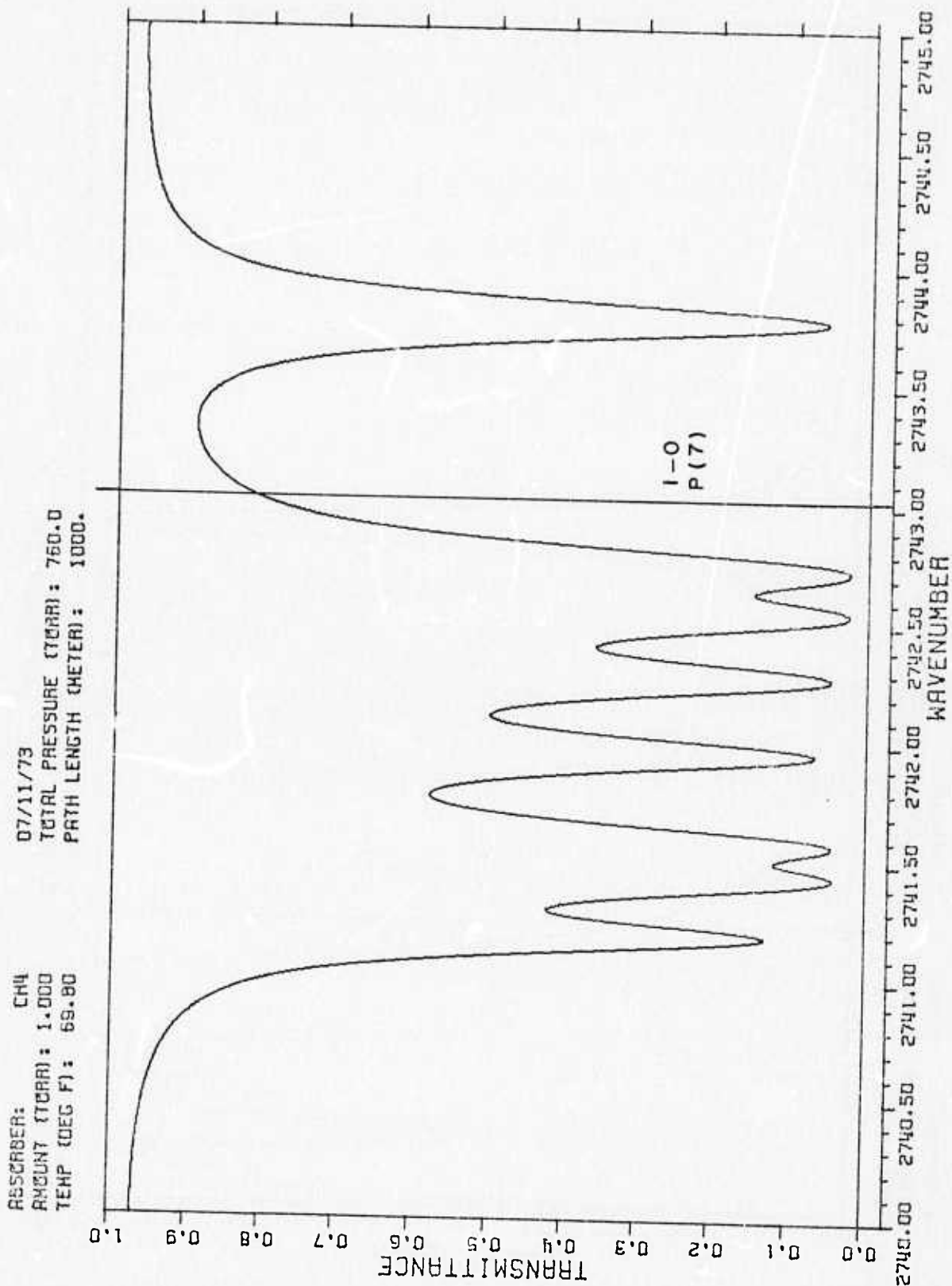


Fig. 13

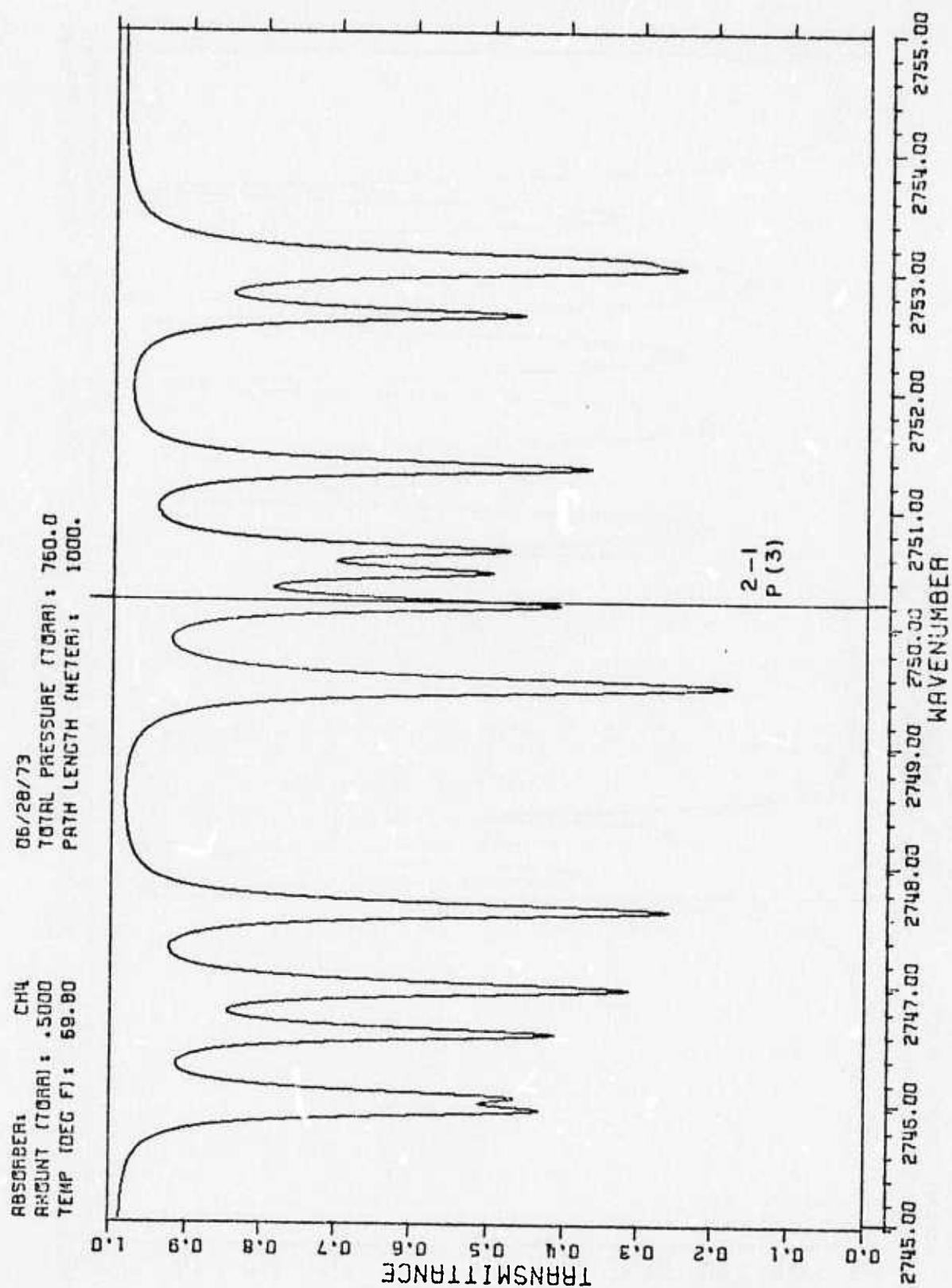


Fig. 14

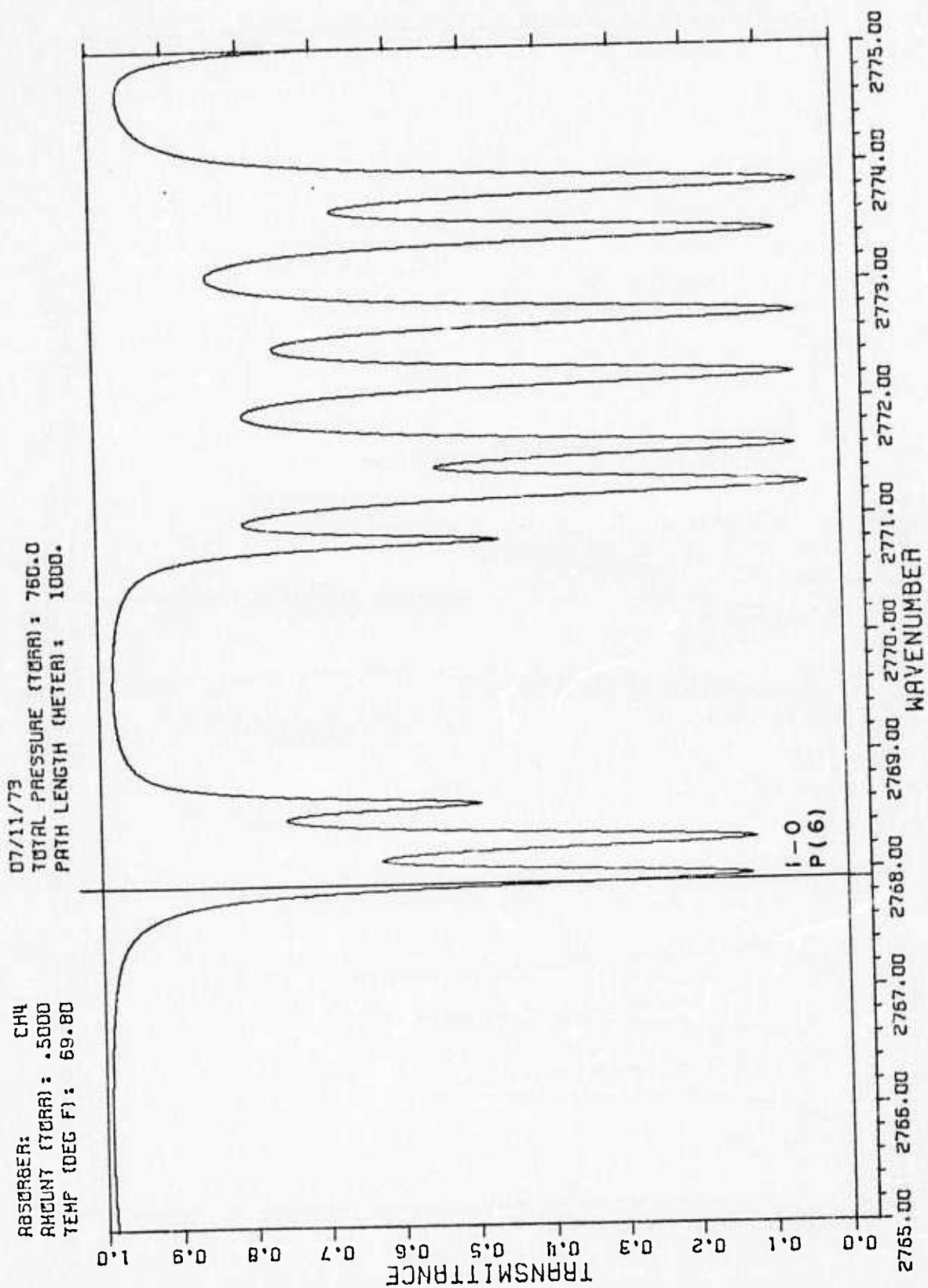


Fig. 15

ABSORBER: CH4
AMOUNT (TORR): 1.000
TEMP (DEG F): 69.80

07/13/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

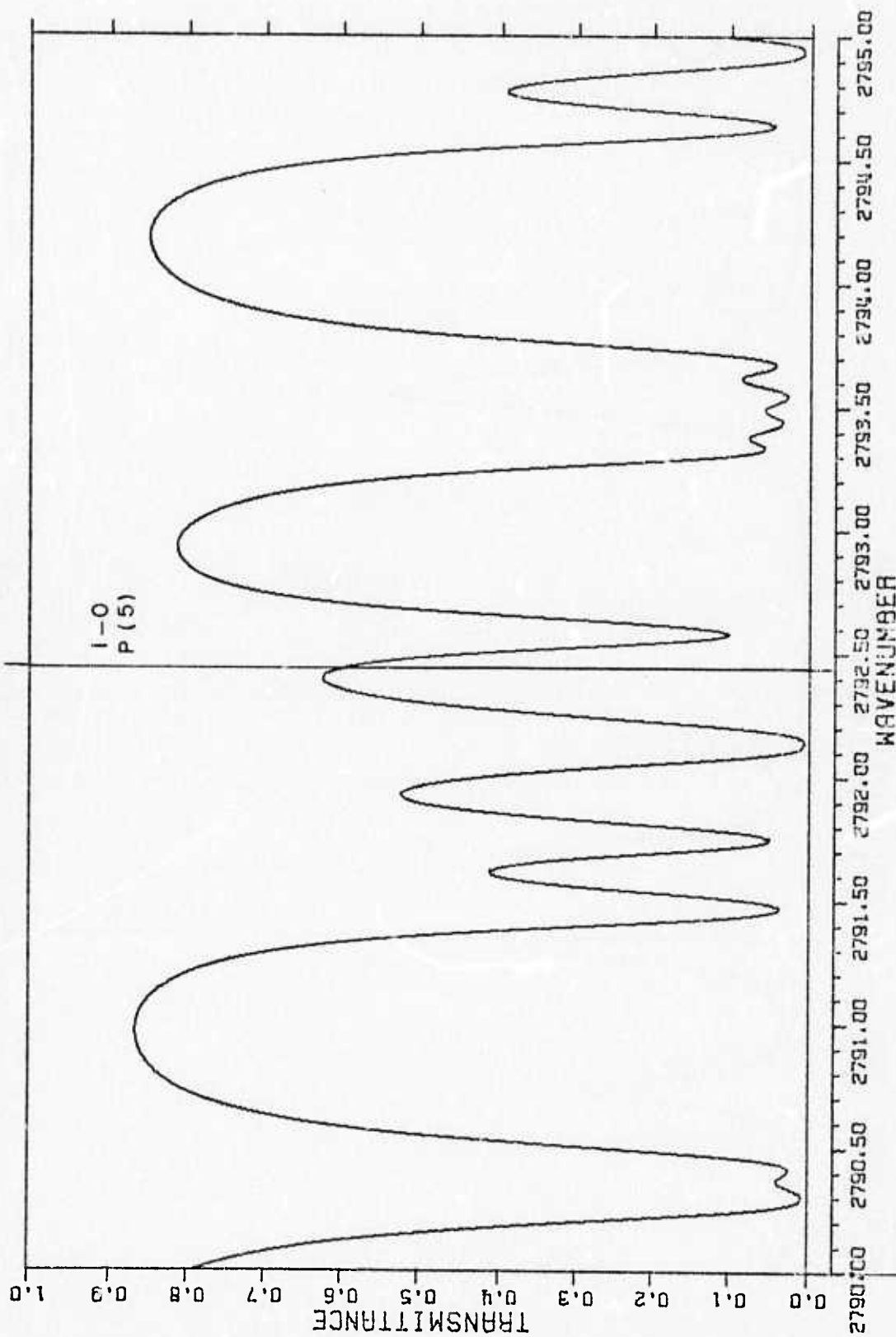


Fig. 16

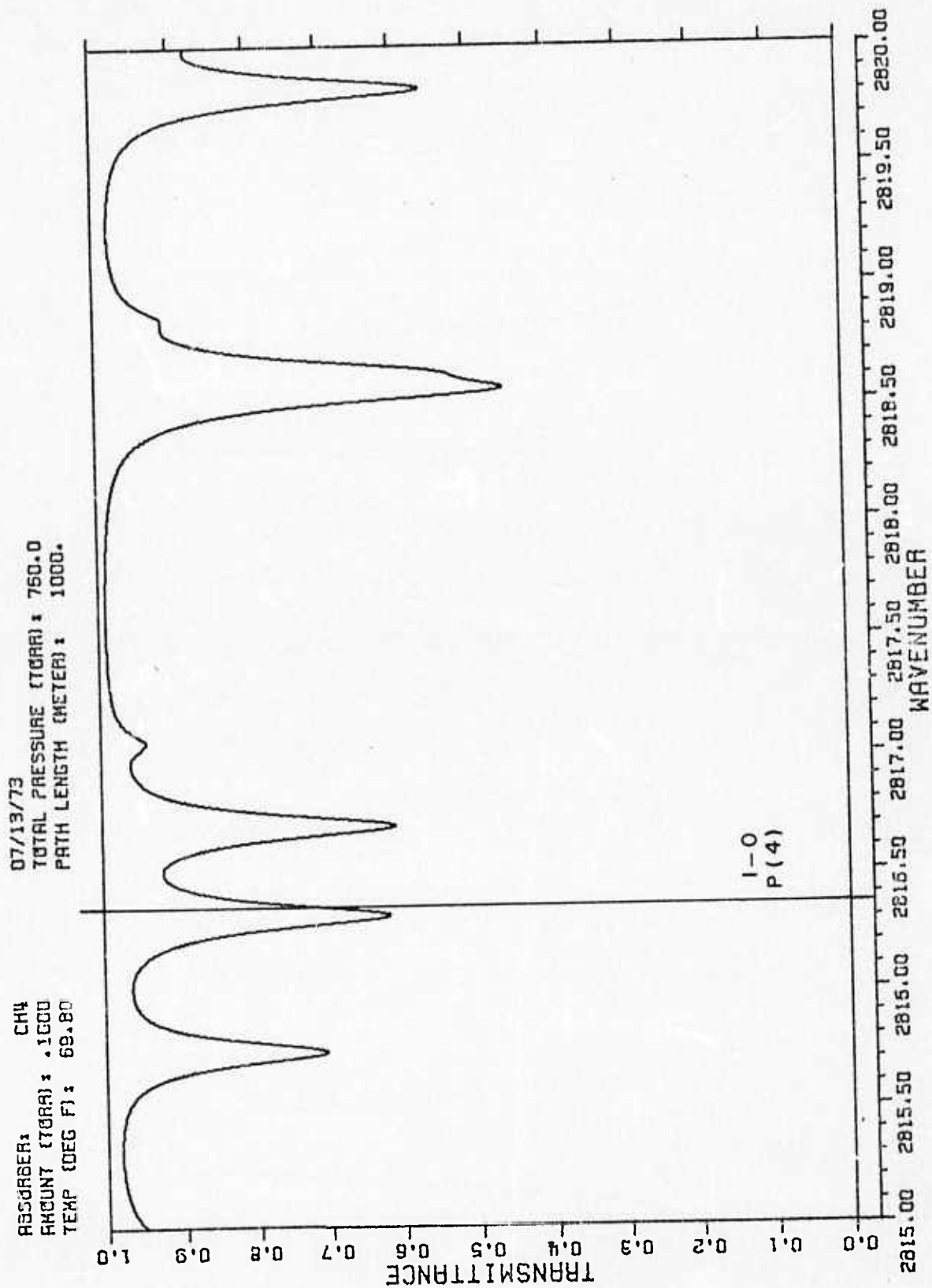


Fig. 17

RECORDER: CH4 07/13/73
PUNCT (TORR): 1.000 TOTAL PRESSURE (TORR): 760.0
TEMP (DEG F): 69.80 PATH LENGTH (CMETER): 1000.

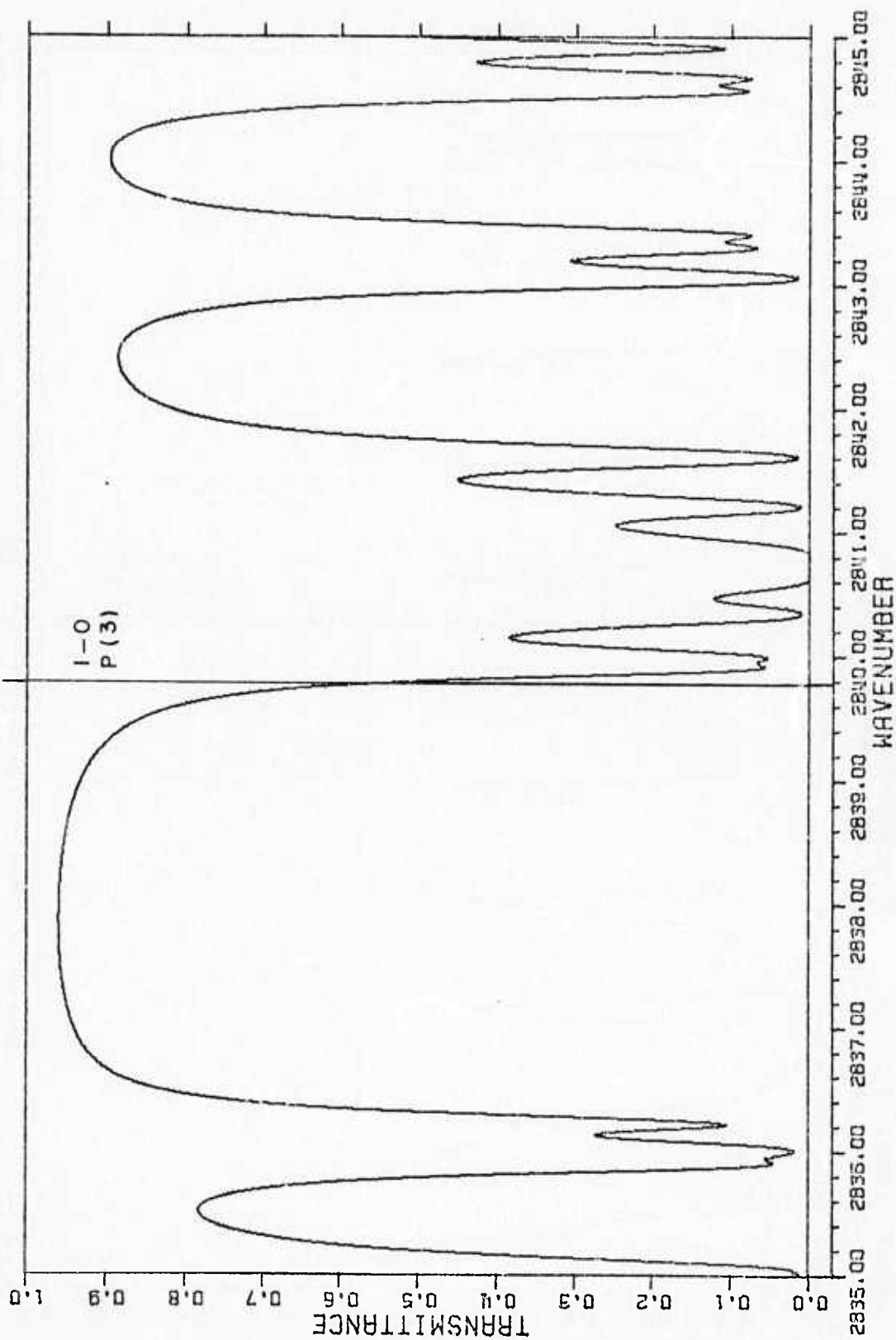


Fig. 18

ABSORBER: N2O
AMOUNT (TORR): .0100
TEMP (DEG F): 69.80

06/28/73
TOTAL PRESSURE (TORR): 750.0
PATH LENGTH (METER): 1000.

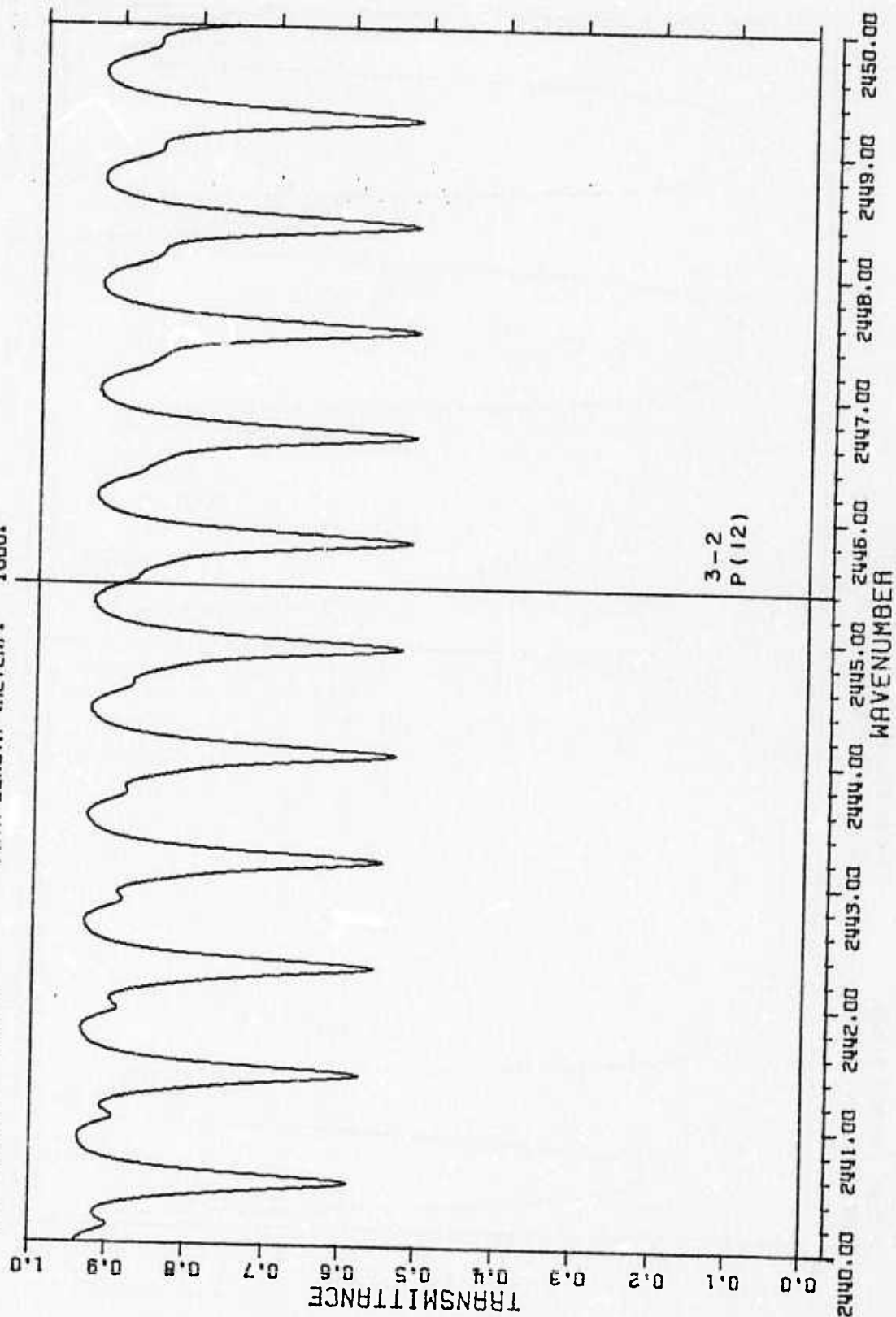


Fig. 19

ABSORBER: N2O
AMOUNT (TORR): .0100
TEMP (DEG F): 69.60

06/28/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

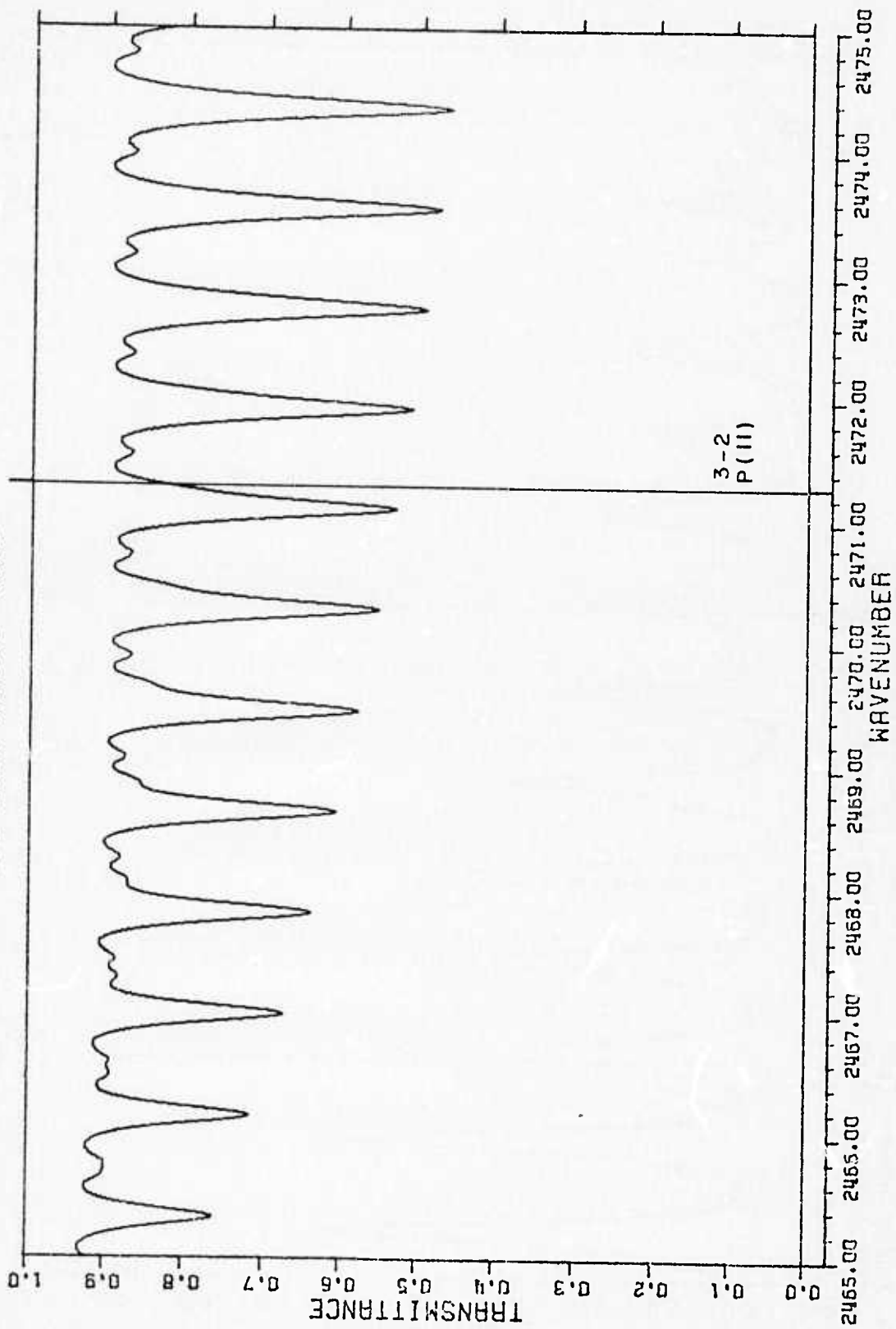


Fig. 20

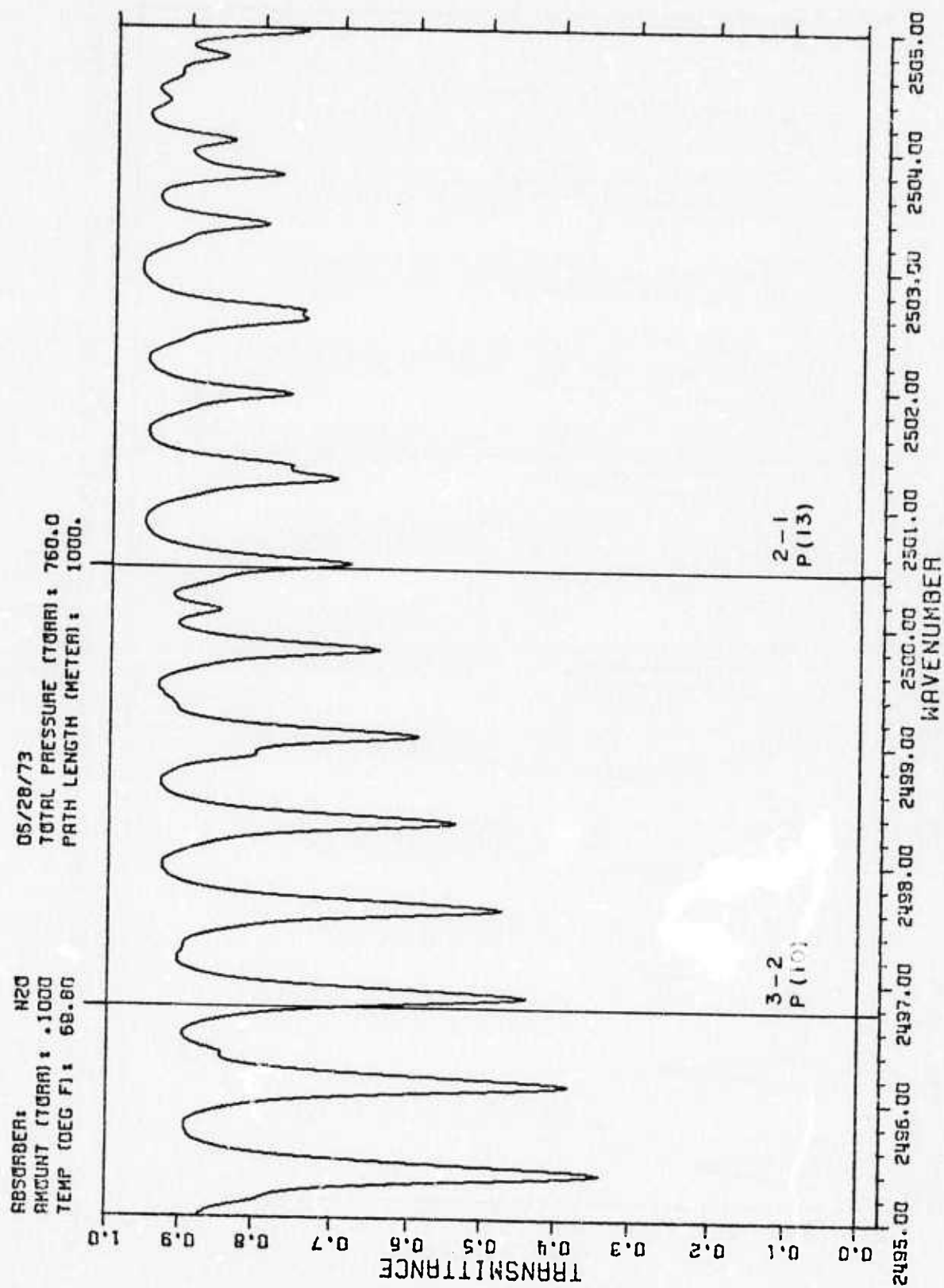


Fig. 21

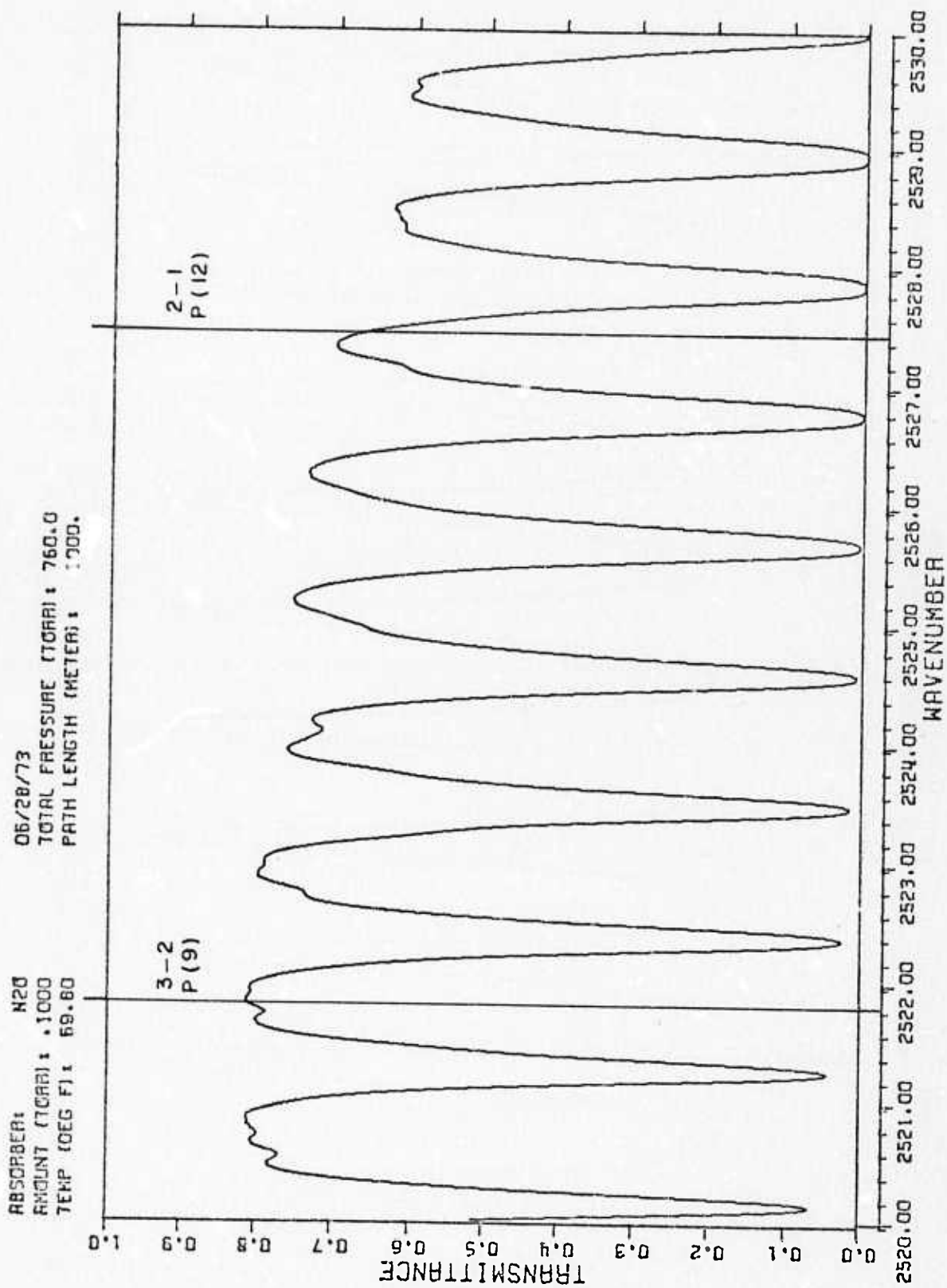


Fig. 22

ABSORBER: N₂O
AMOUNT (TORR): .0100
TEMP (DEG F): 59.80

06/28/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

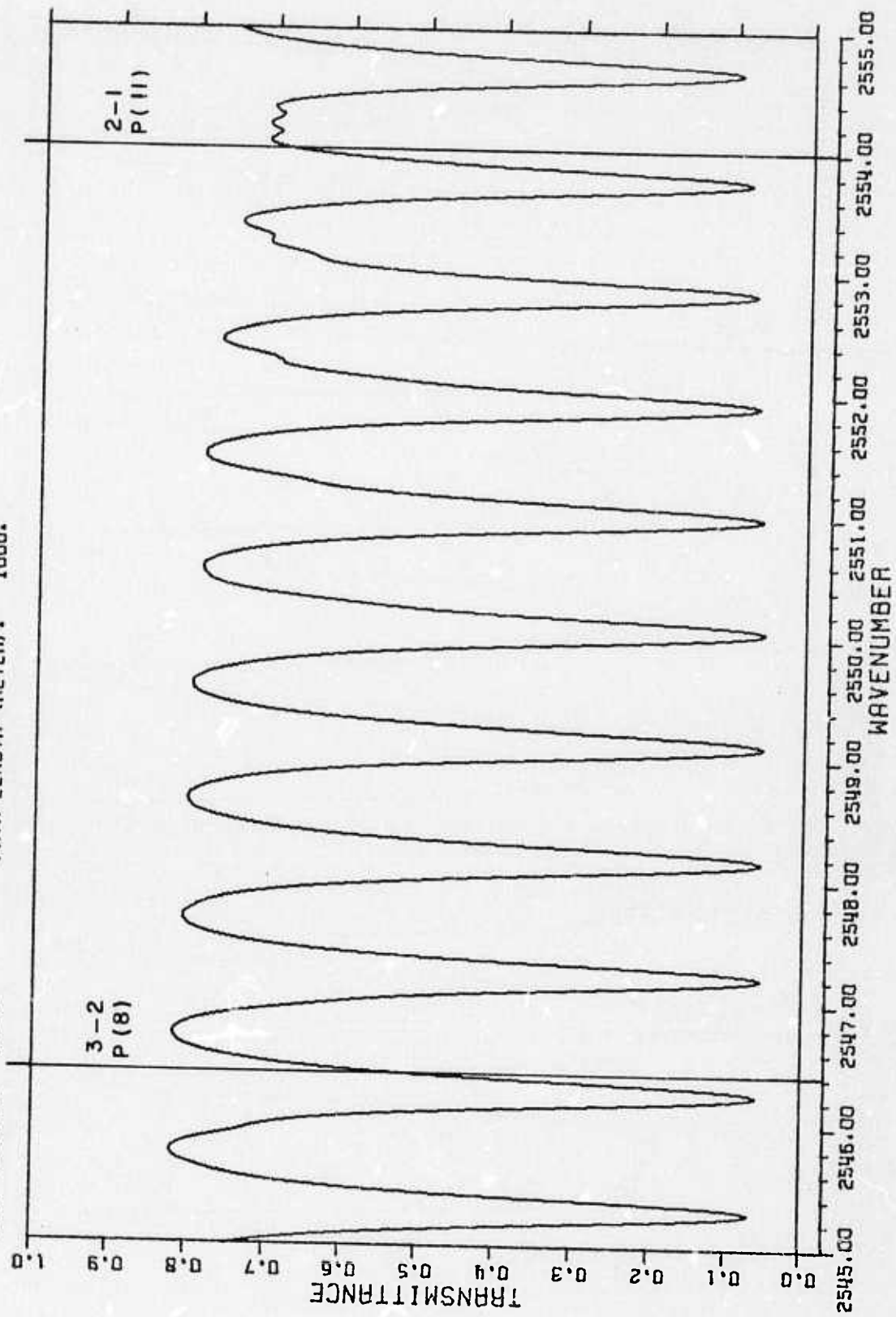


Fig. 23

ABSORBER: N2O
AMOUNT (TORR): .0020
TEMP (DEG F): 69.00

06/28/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

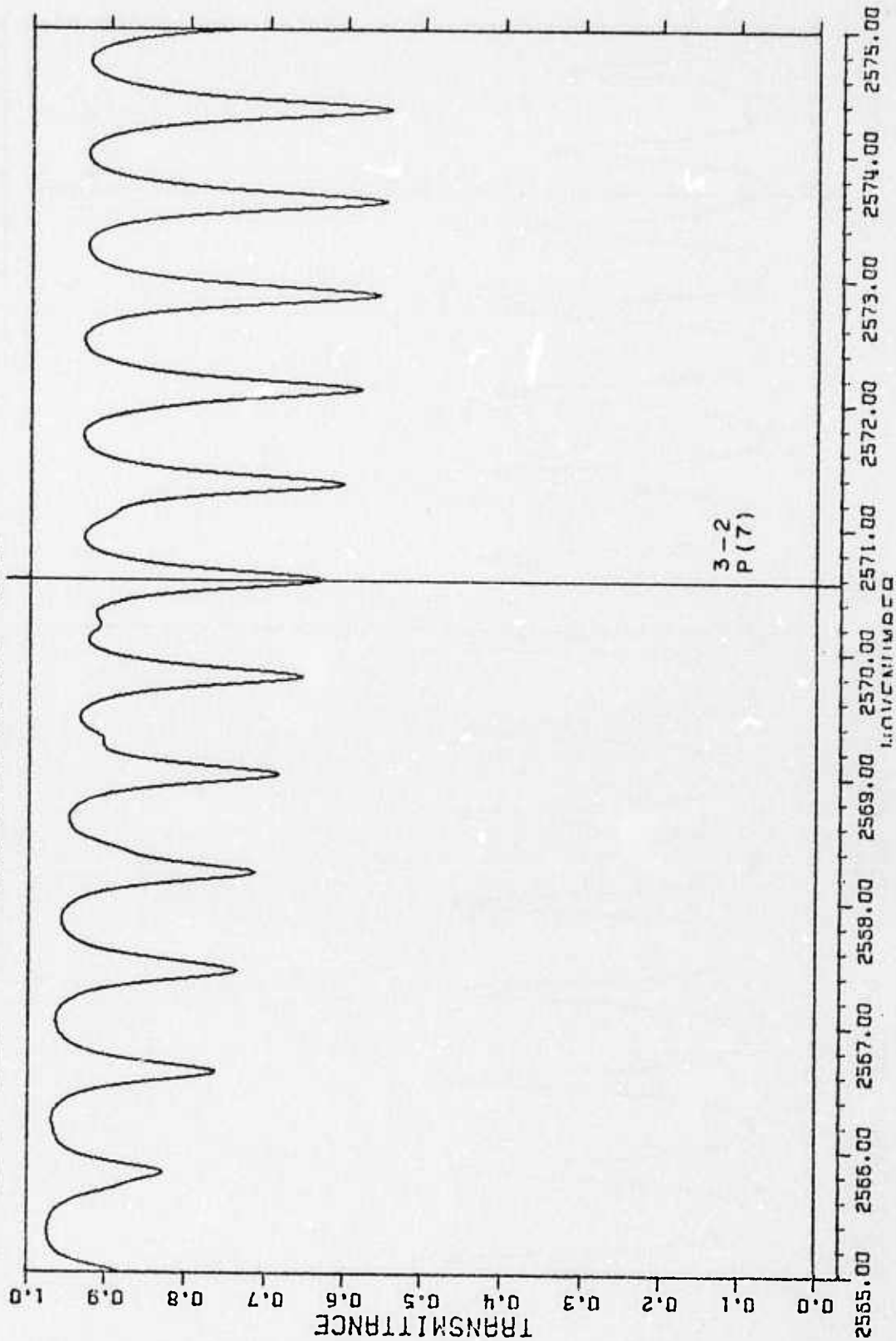


Fig. 24

ABSORBER: N2O
AMOUNT (TORR): .0020
TEMP (DEG F): 69.80

06/28/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

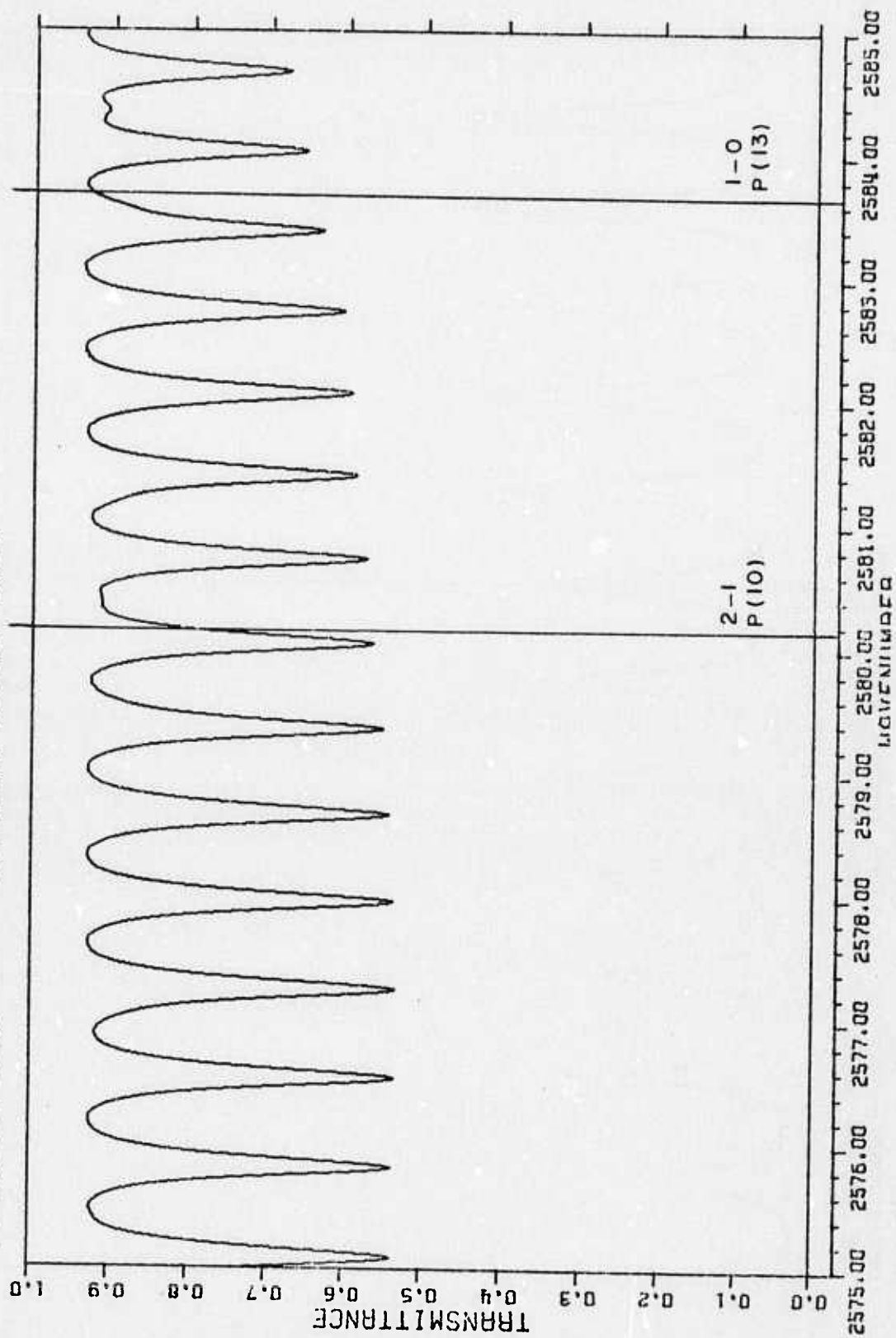


Fig. 25

ABSORBER: N2O
AMOUNT (TORR): .1000
TEMP (DEG F): 69.80

06/20/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

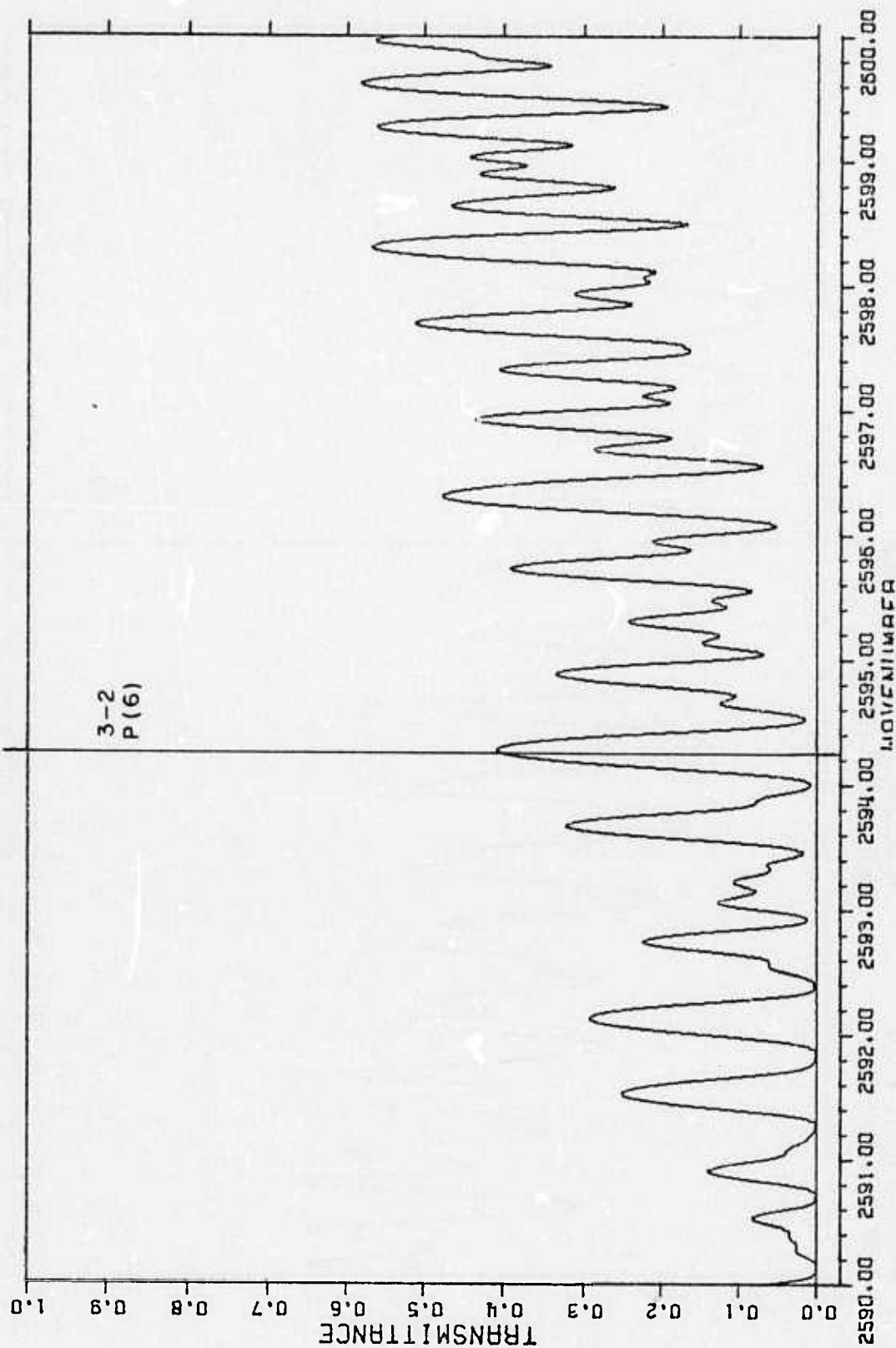


Fig. 26

ABSORBER: N2O
AMOUNT (TORR): .1000
TEMP (DEG F): 69.80

06/29/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

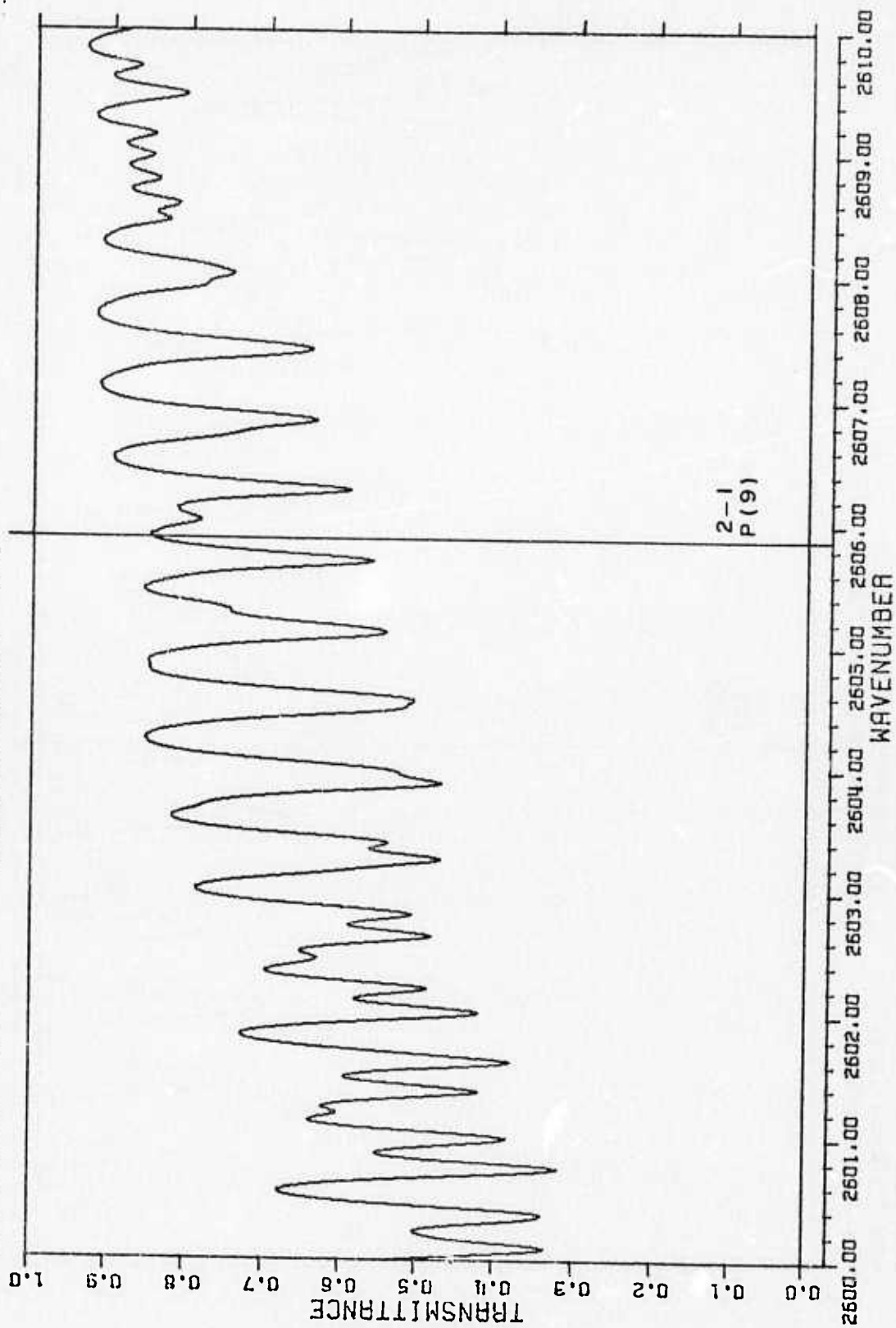


Fig. 27

ABSORBER: N2O
AMOUNT (TORR): 2.000
TEMP (DEG F): 69.80

06/29/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

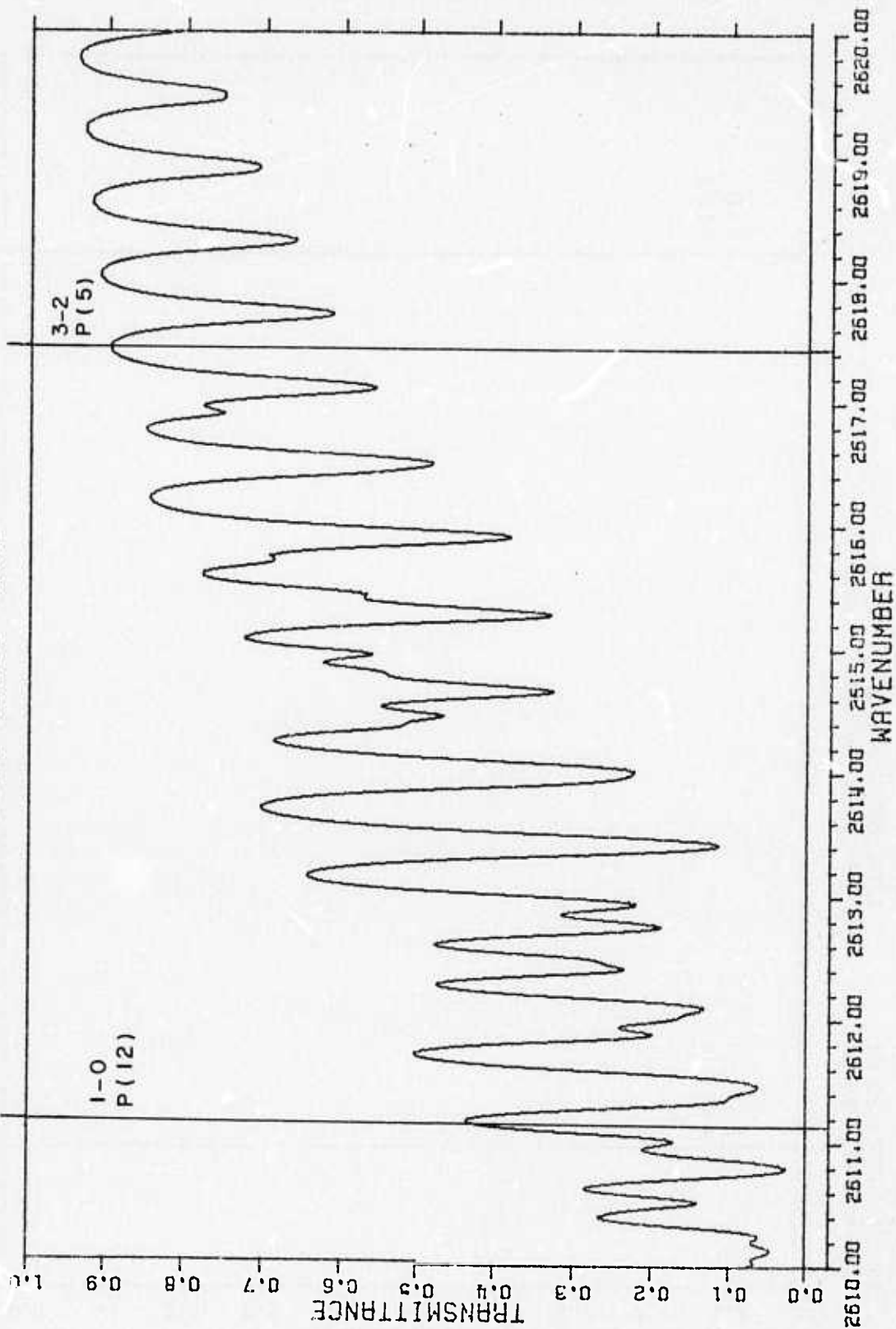


Fig. 28

ABSORBER: N2O
AMOUNT (TORR): 30.00
TEMP (DEG F): 69.80

06/29/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

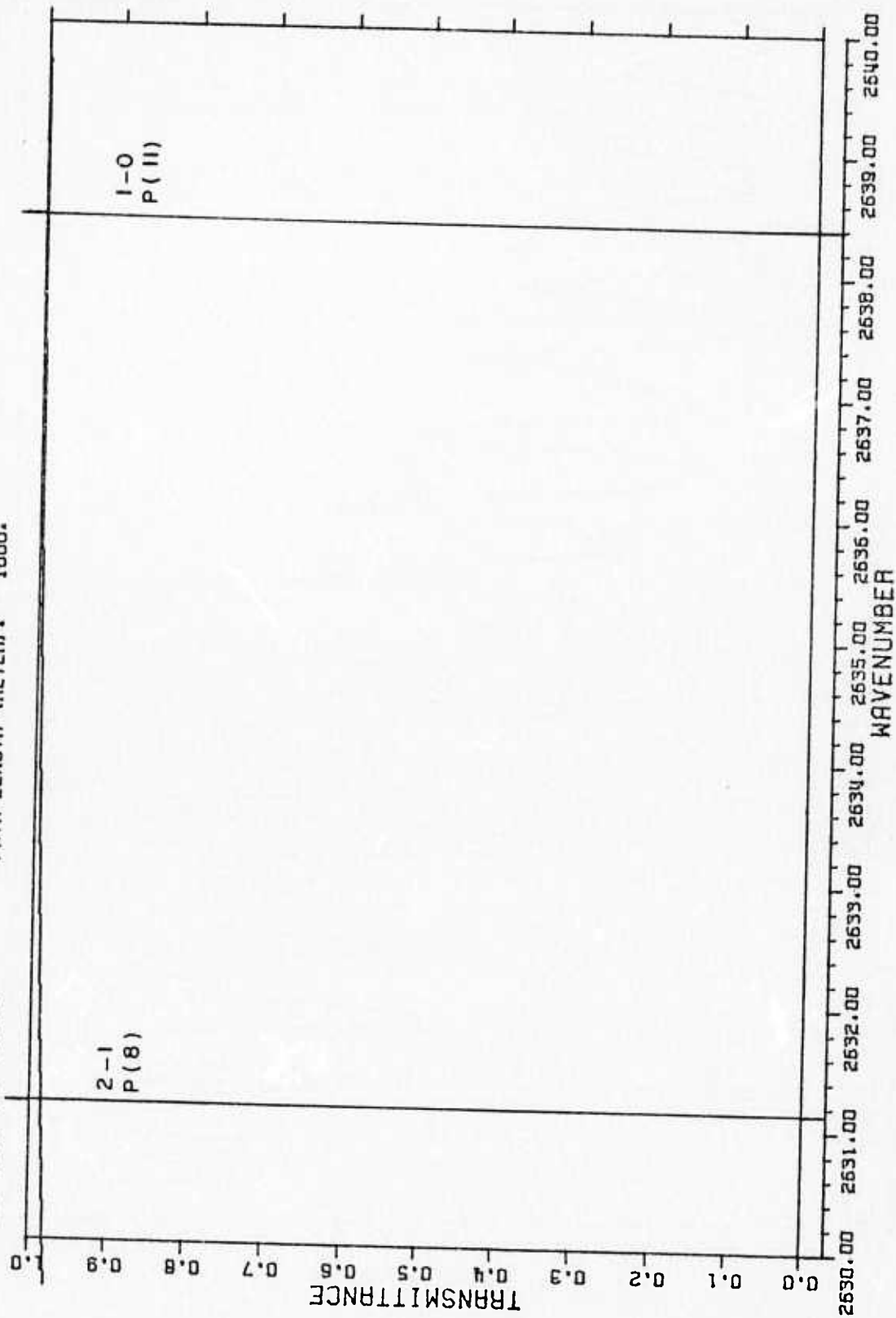


Fig. 29

ABSORBER: N2O
AMOUNT (TORR): 5.000
TEMP (DEG F): 59.80

07/11/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

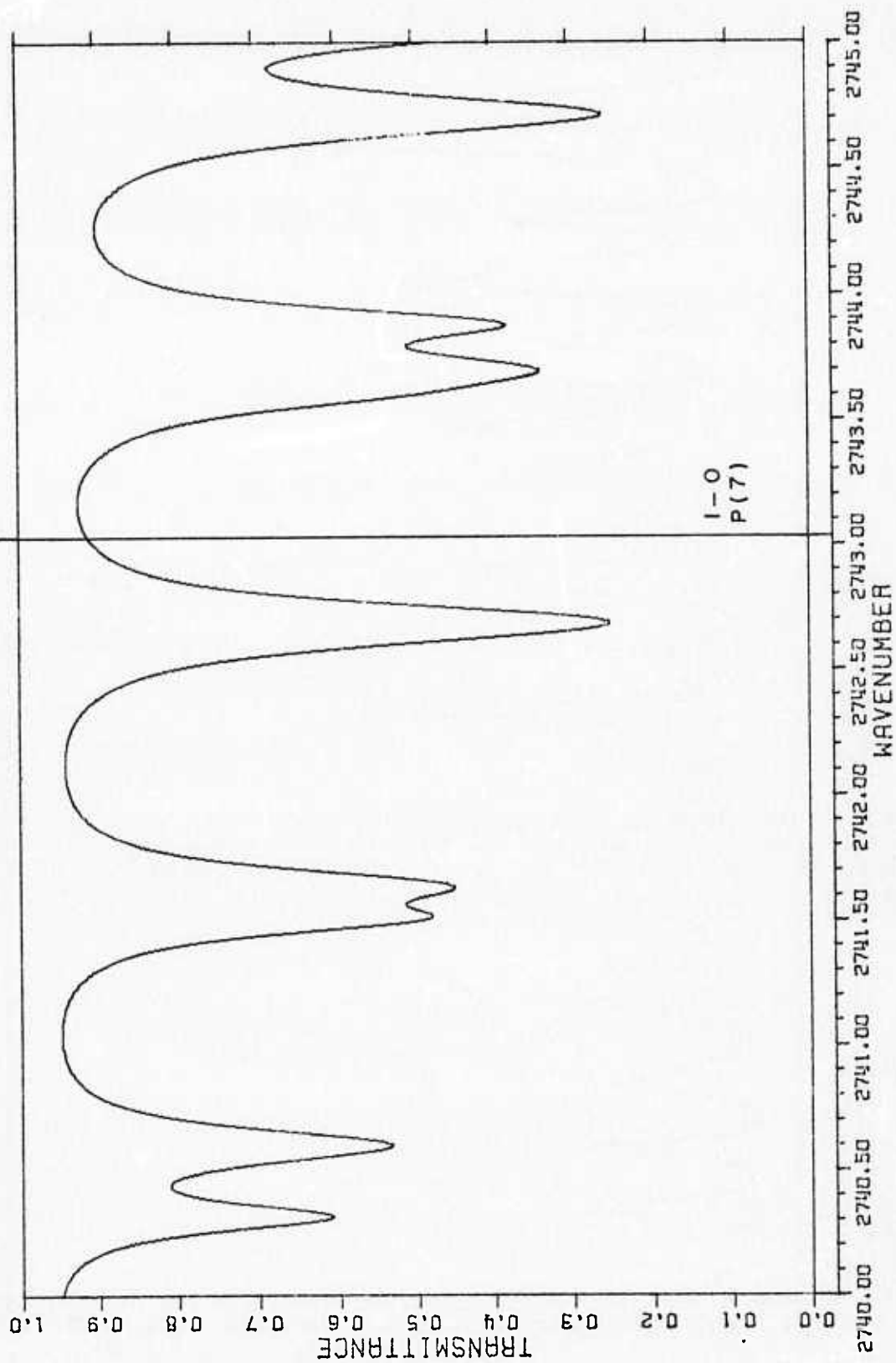


Fig. 30

ABSORBER: N2O
AMOUNT (TORR): 1.000
TEMP (DEG F): 69.80

06/28/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

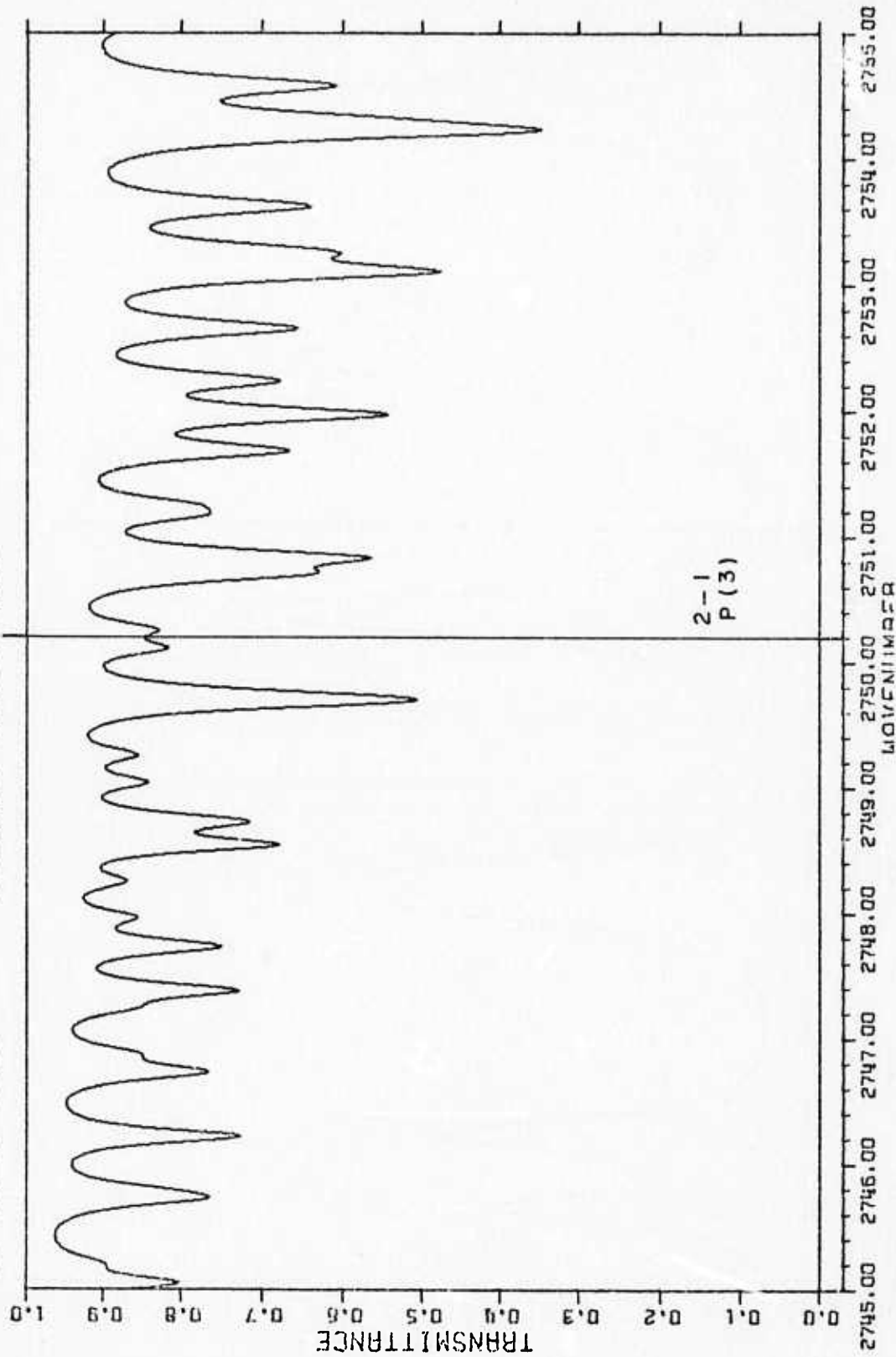


Fig. 31

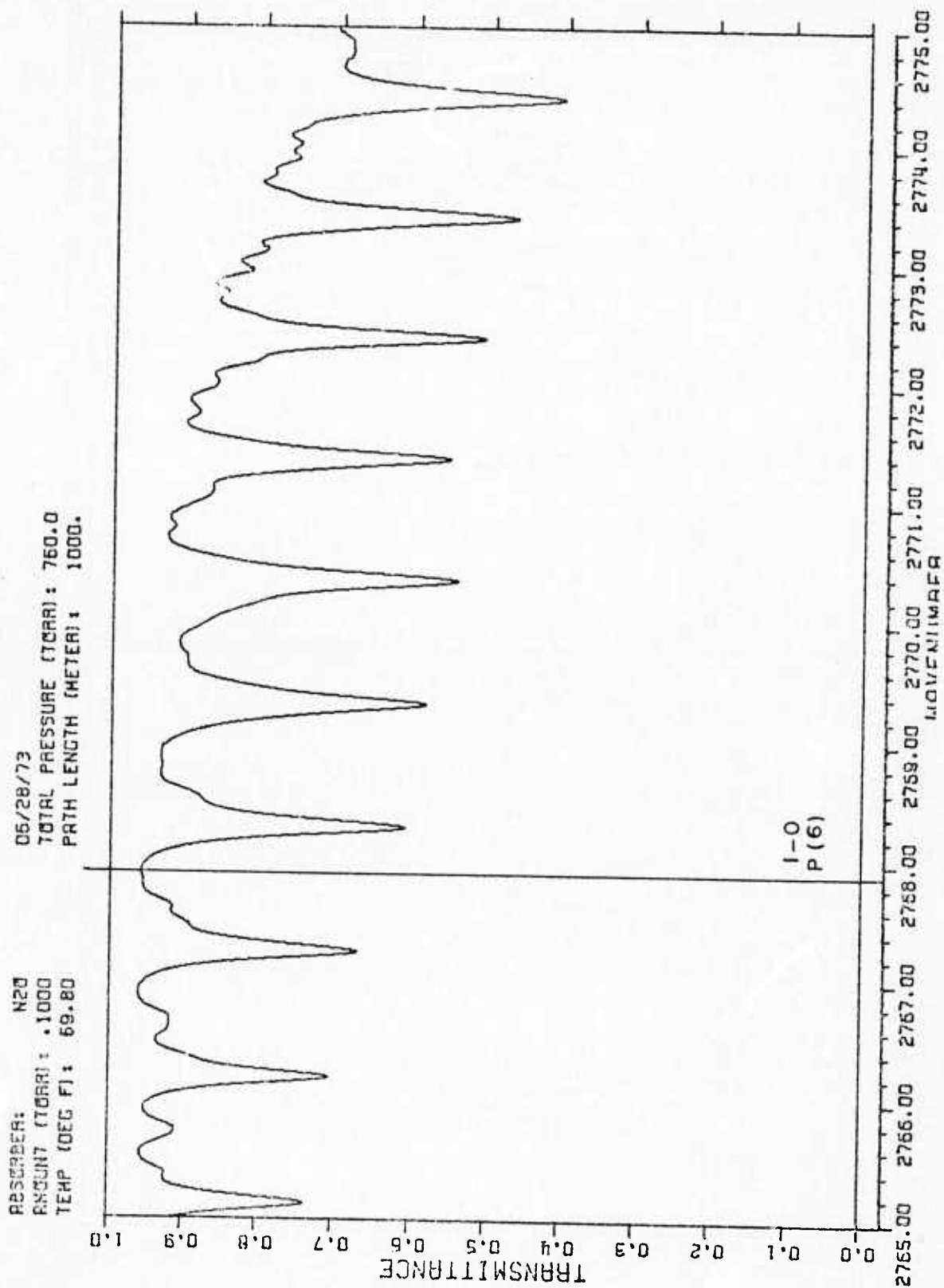


Fig. 32

ABSORBER: N2O
AMOUNT (TORR): .1000
TEMP (DEG F): 69.80

07/13/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

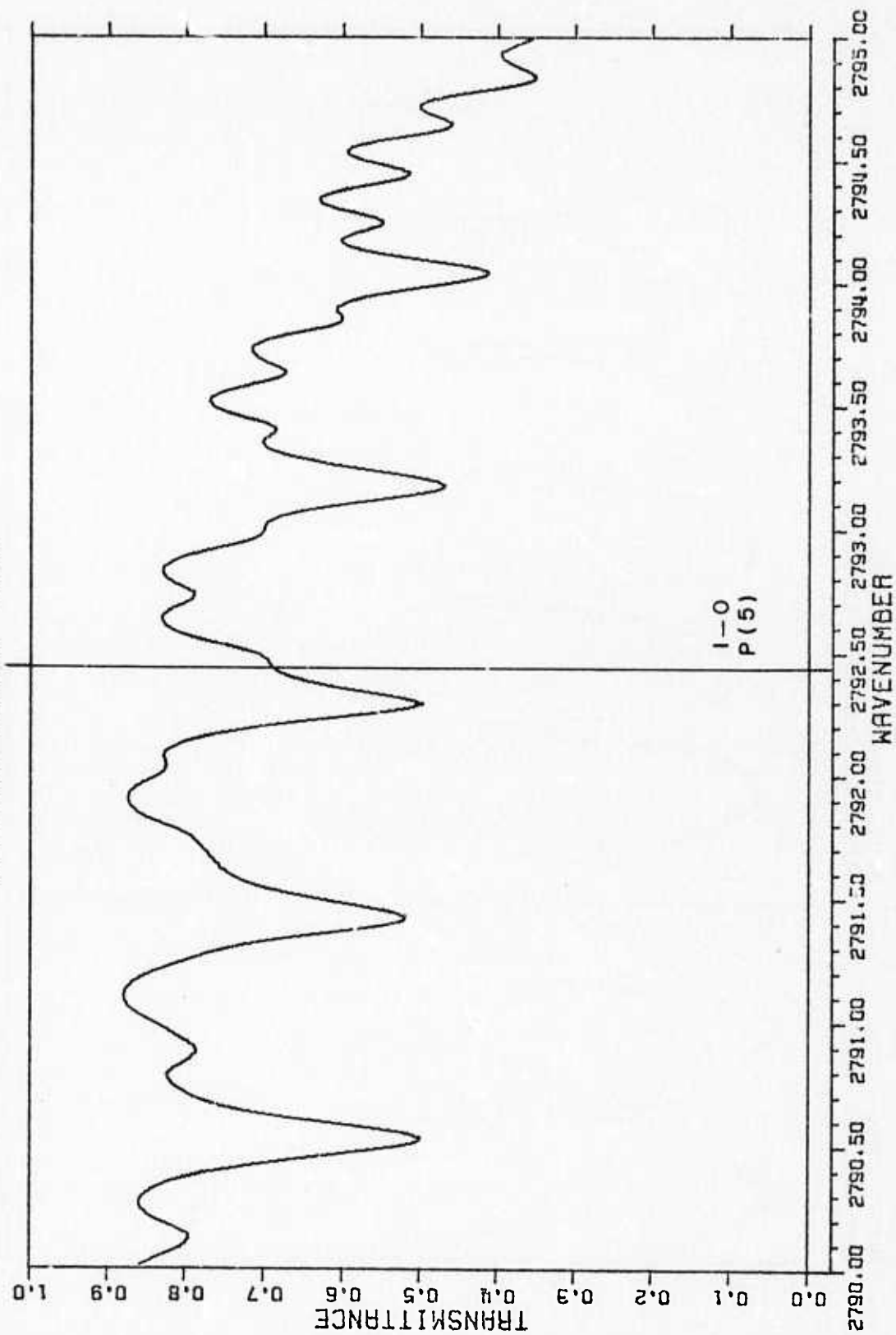


Fig. 33

ABSORBER: N2O
AMOUNT (GRAMS): .1000
TEMP (DEG F): 69.80

07/13/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 1000.

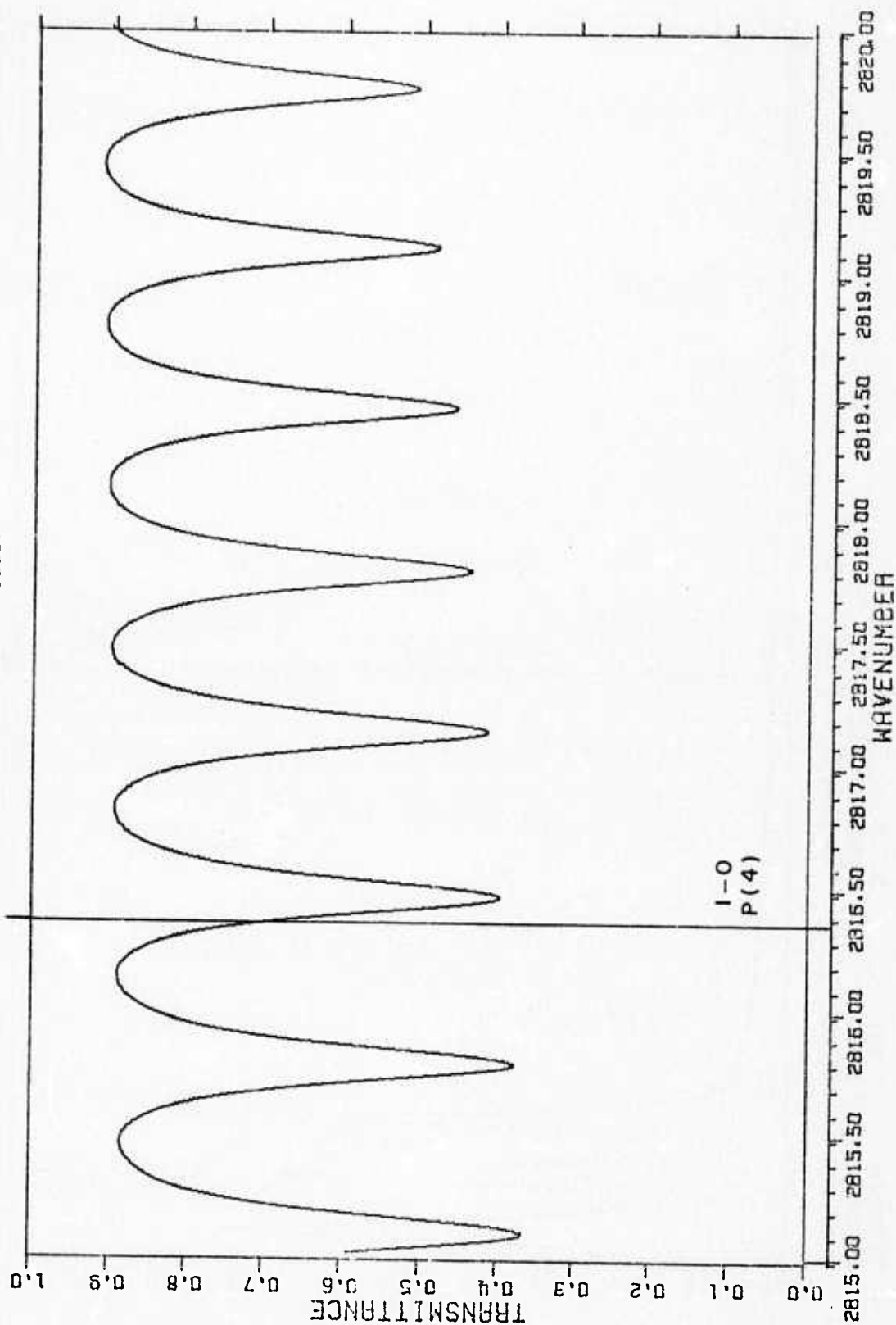


Fig. 34

ABSORBER: N2D
AMOUNT (TERR): 10.00
TEMP (DEG F): 69.80

07/18/73
TOTAL PRESSURE (TERR): 760.0
PATH LENGTH (METER): 1000.

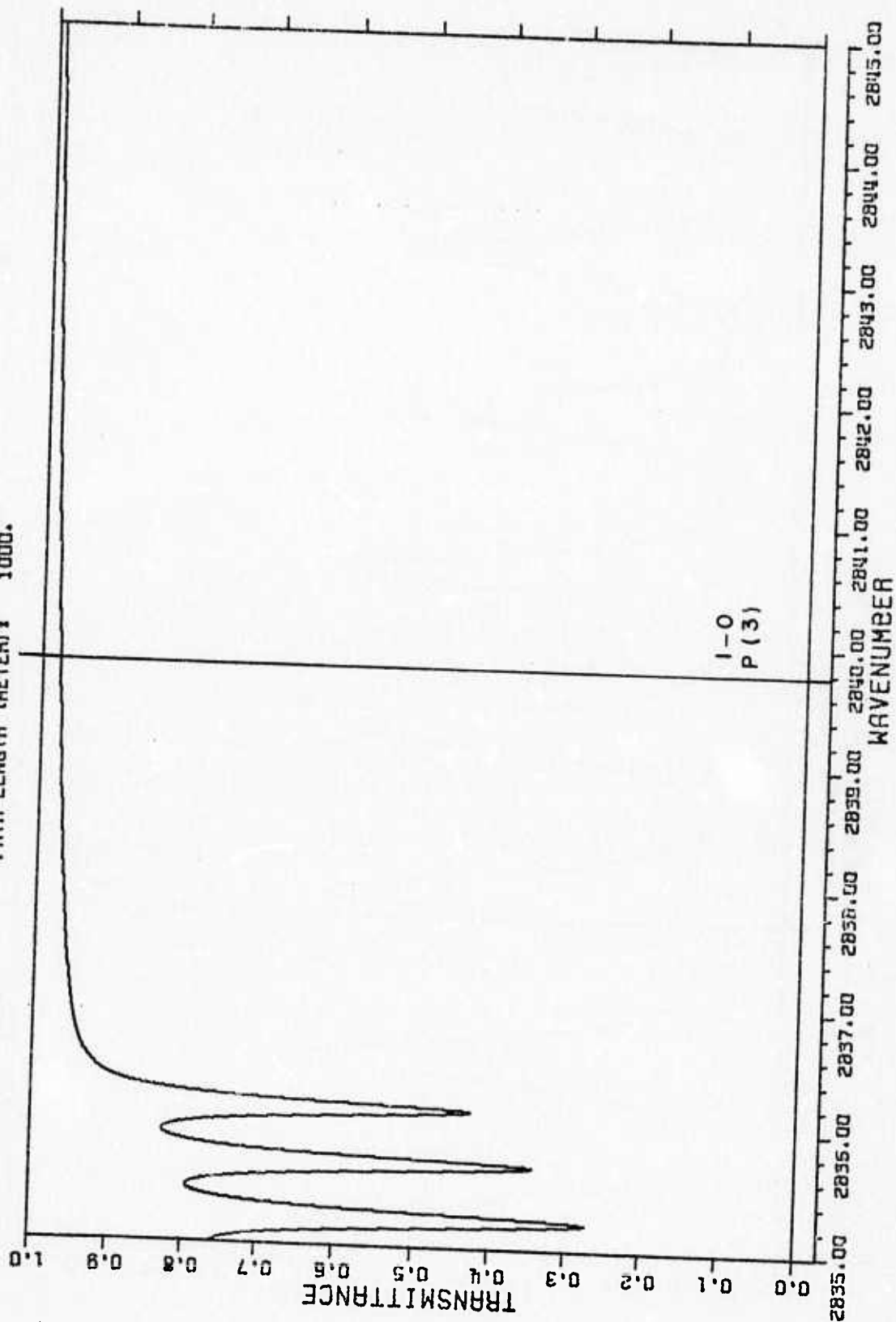


Fig. 35

ABSORBER: M20
AMOUNT (TORR): 15.00
TEMP (DEG F): 69.80

07/17/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 10000

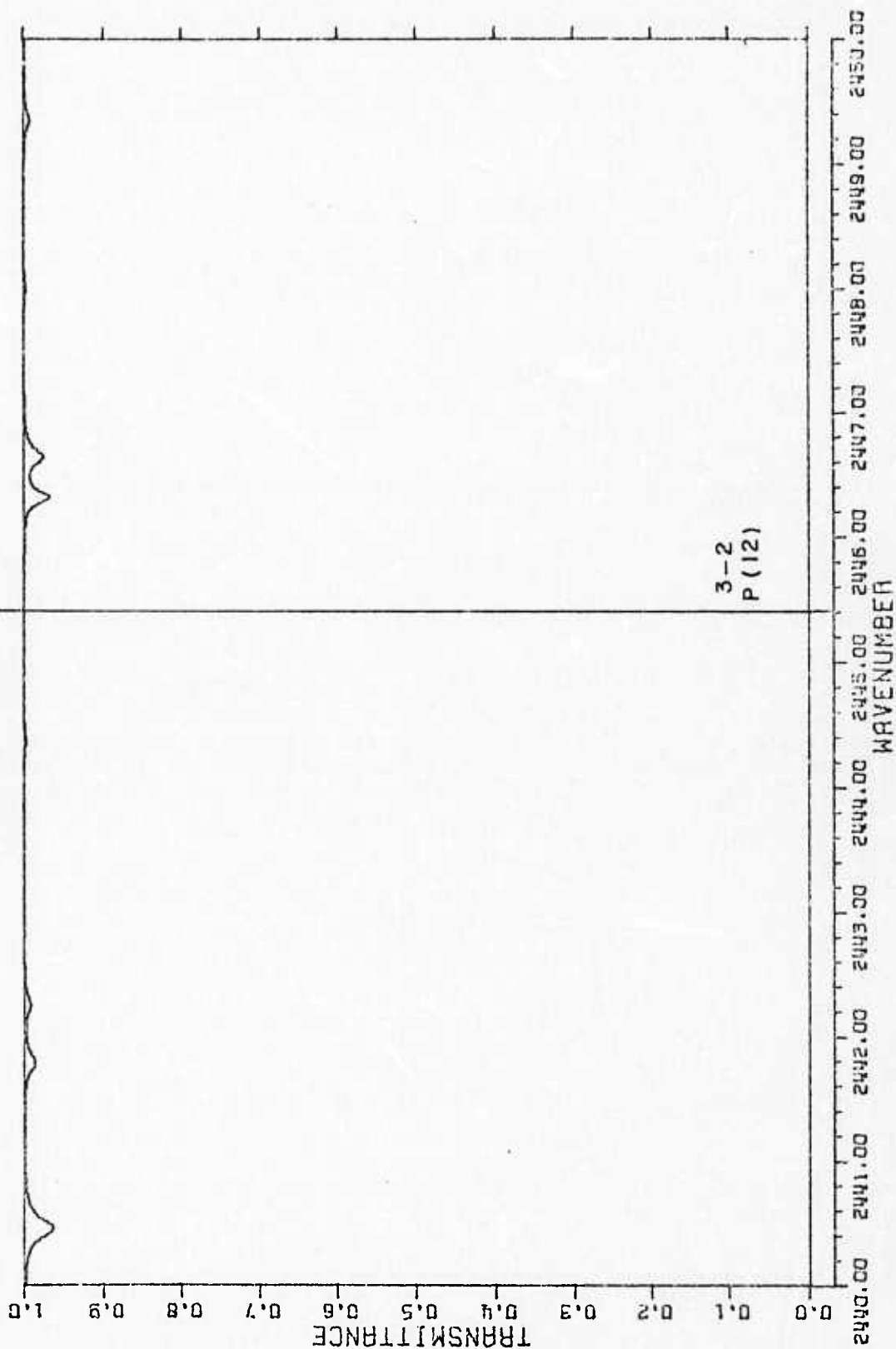


Fig. 36

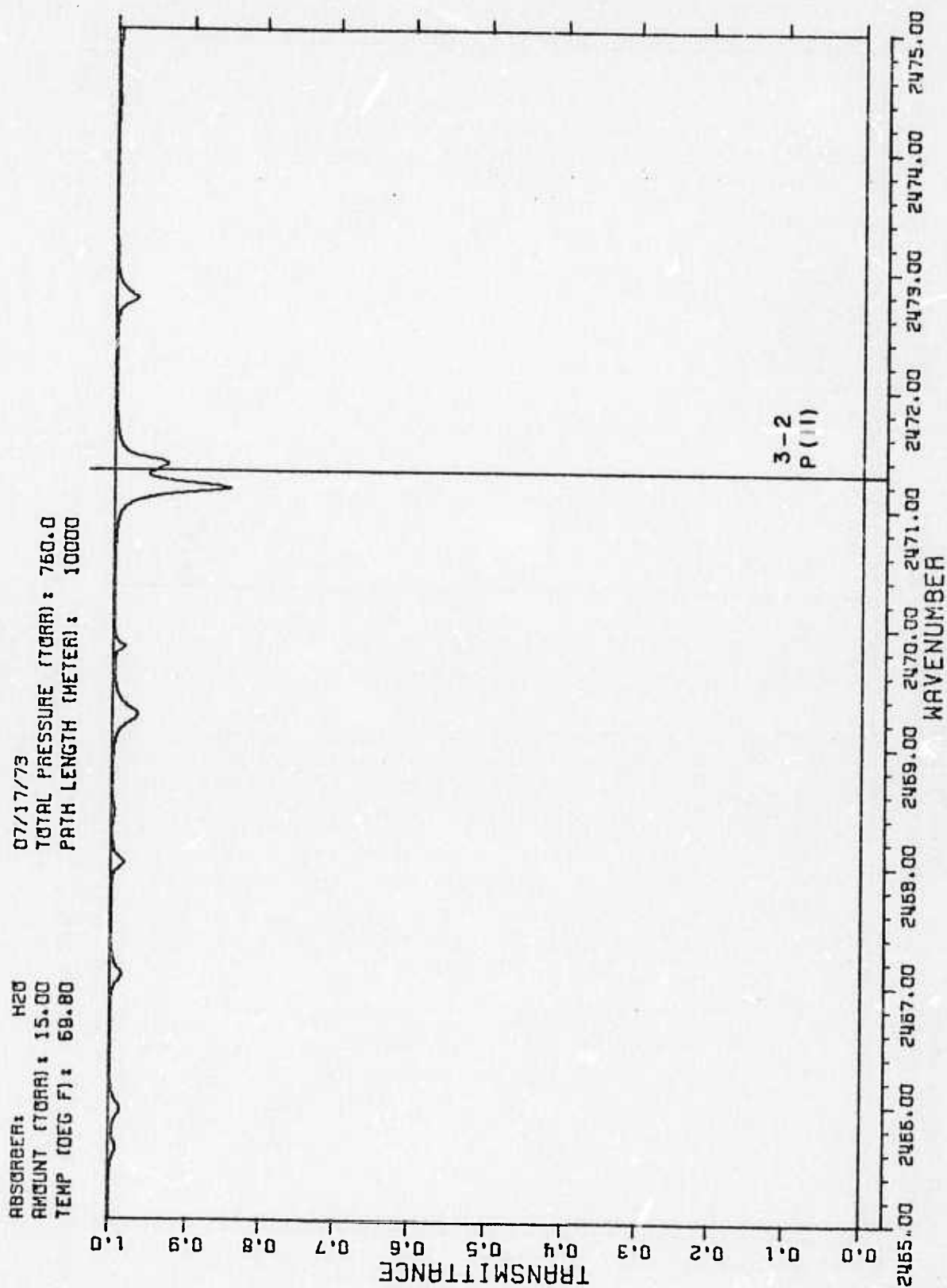


Fig. 37

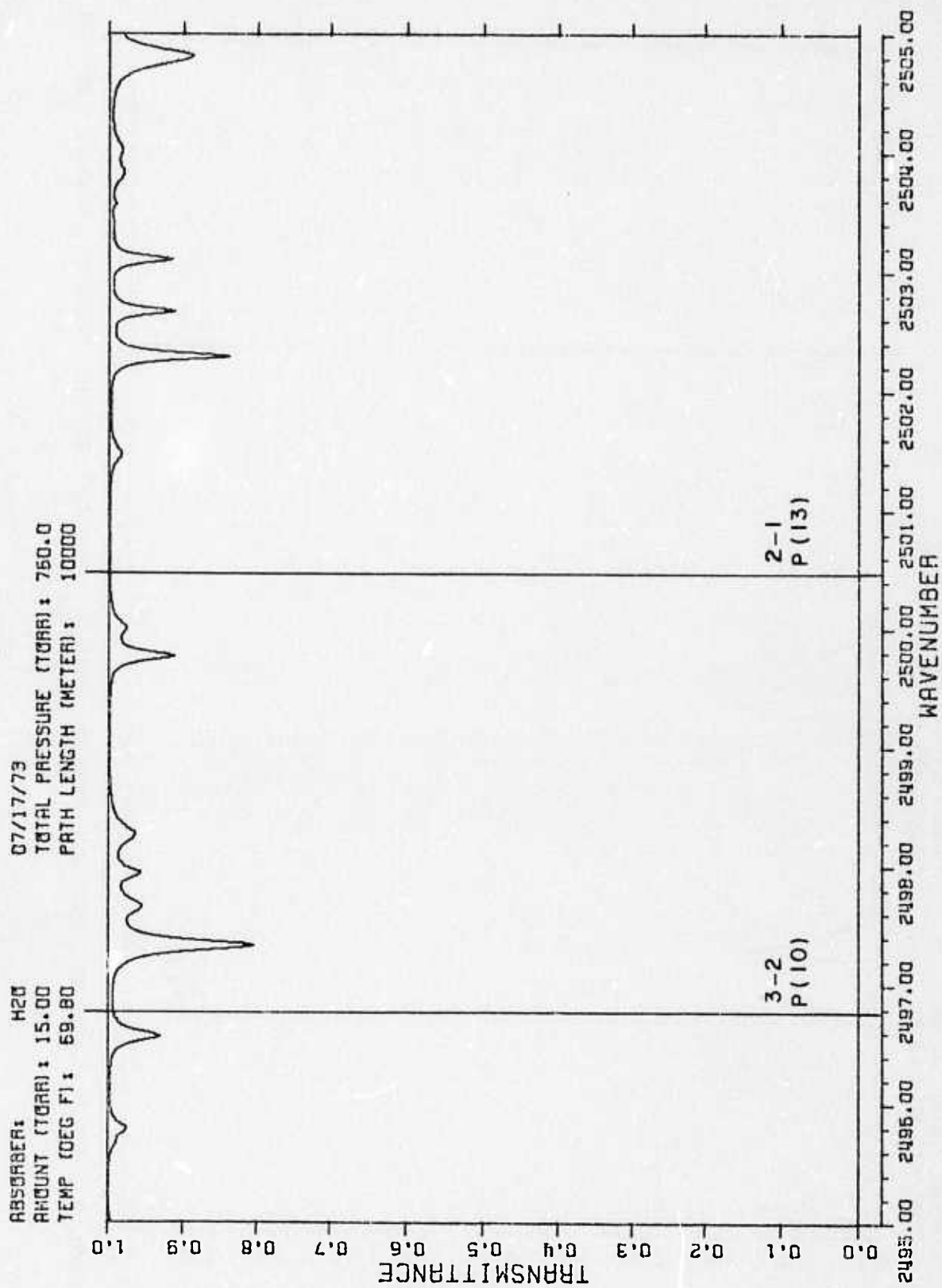


Fig. 38

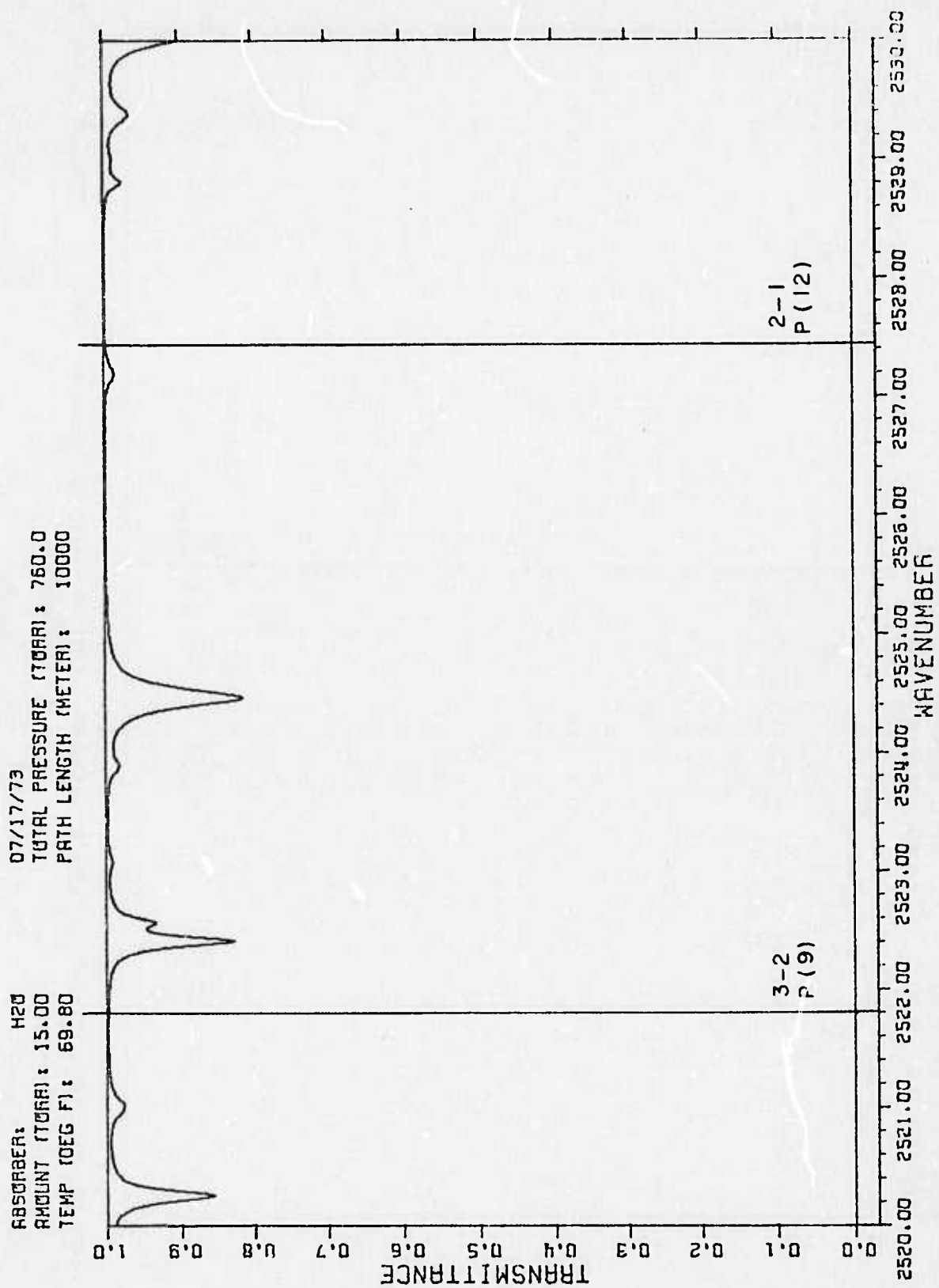


Fig. 39

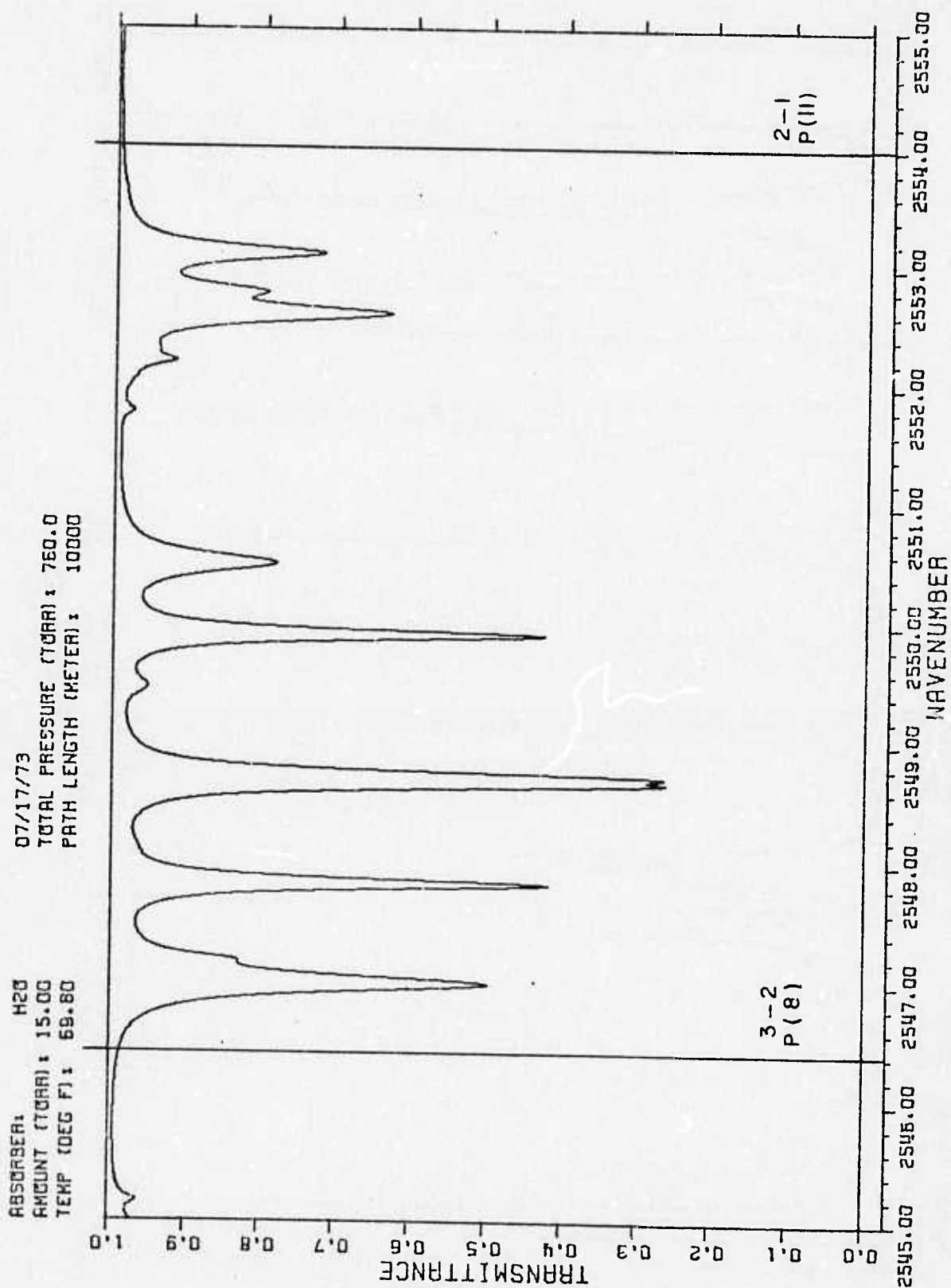


Fig. 40

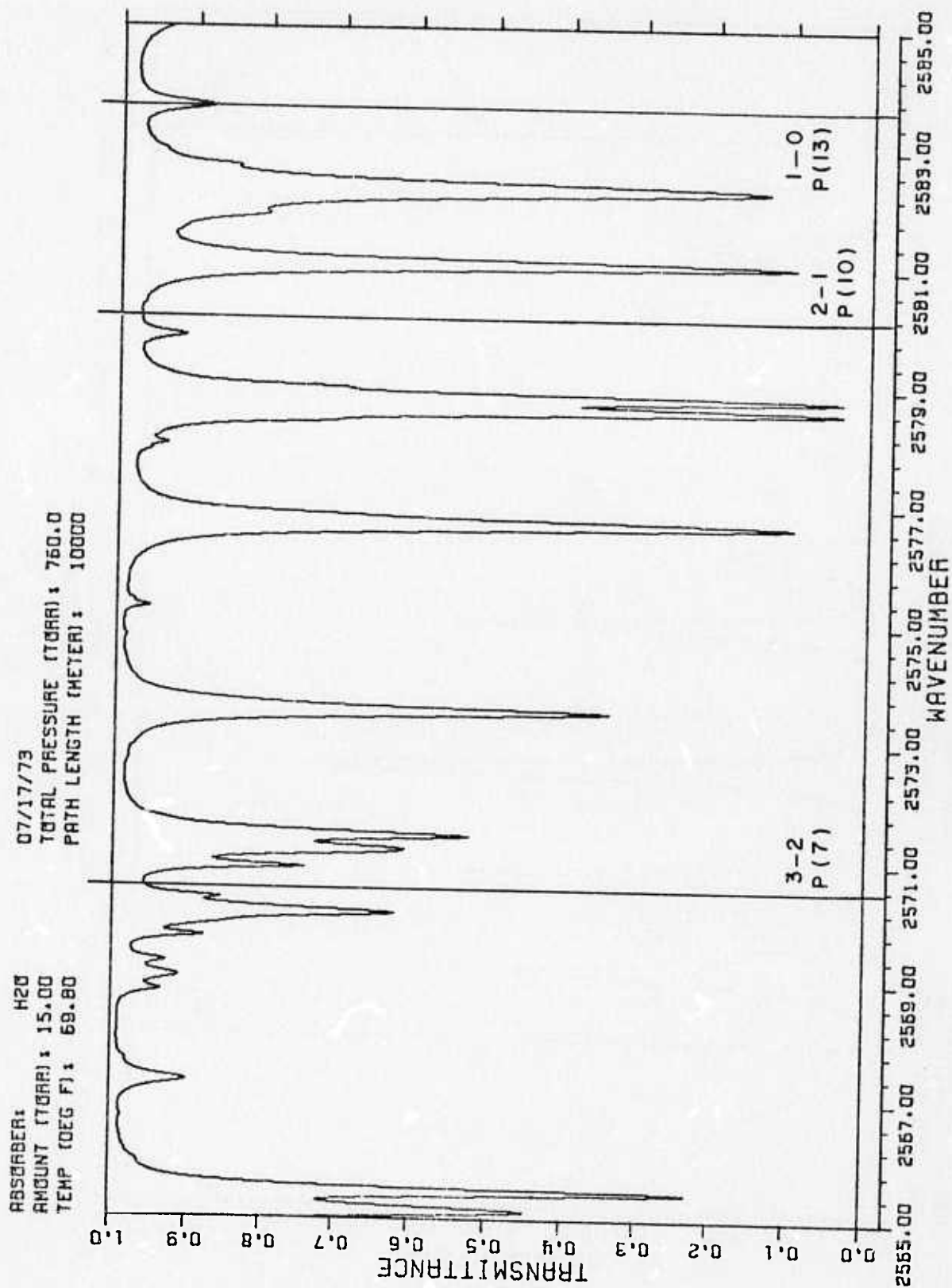


Fig. 41

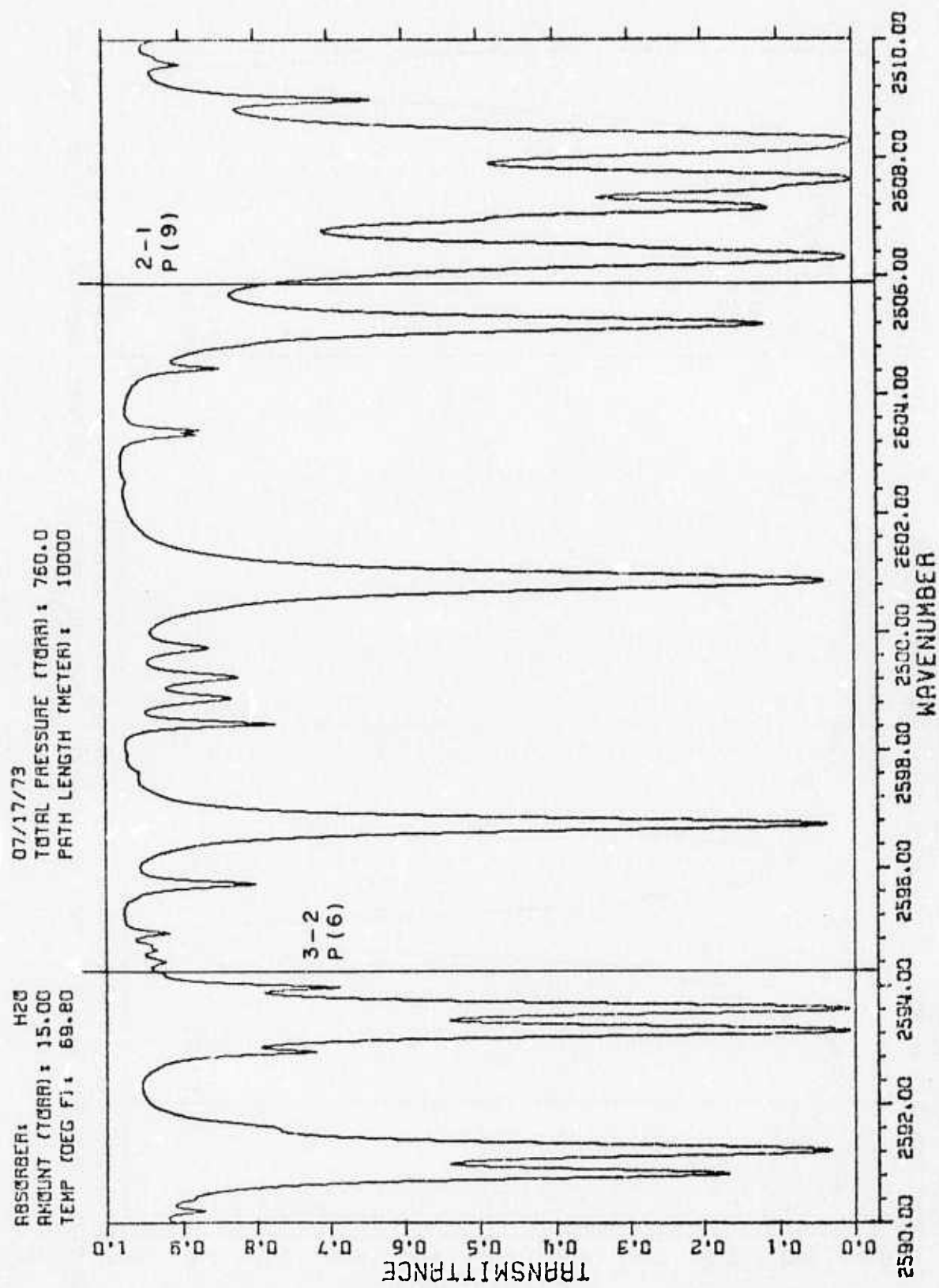


Fig. 42

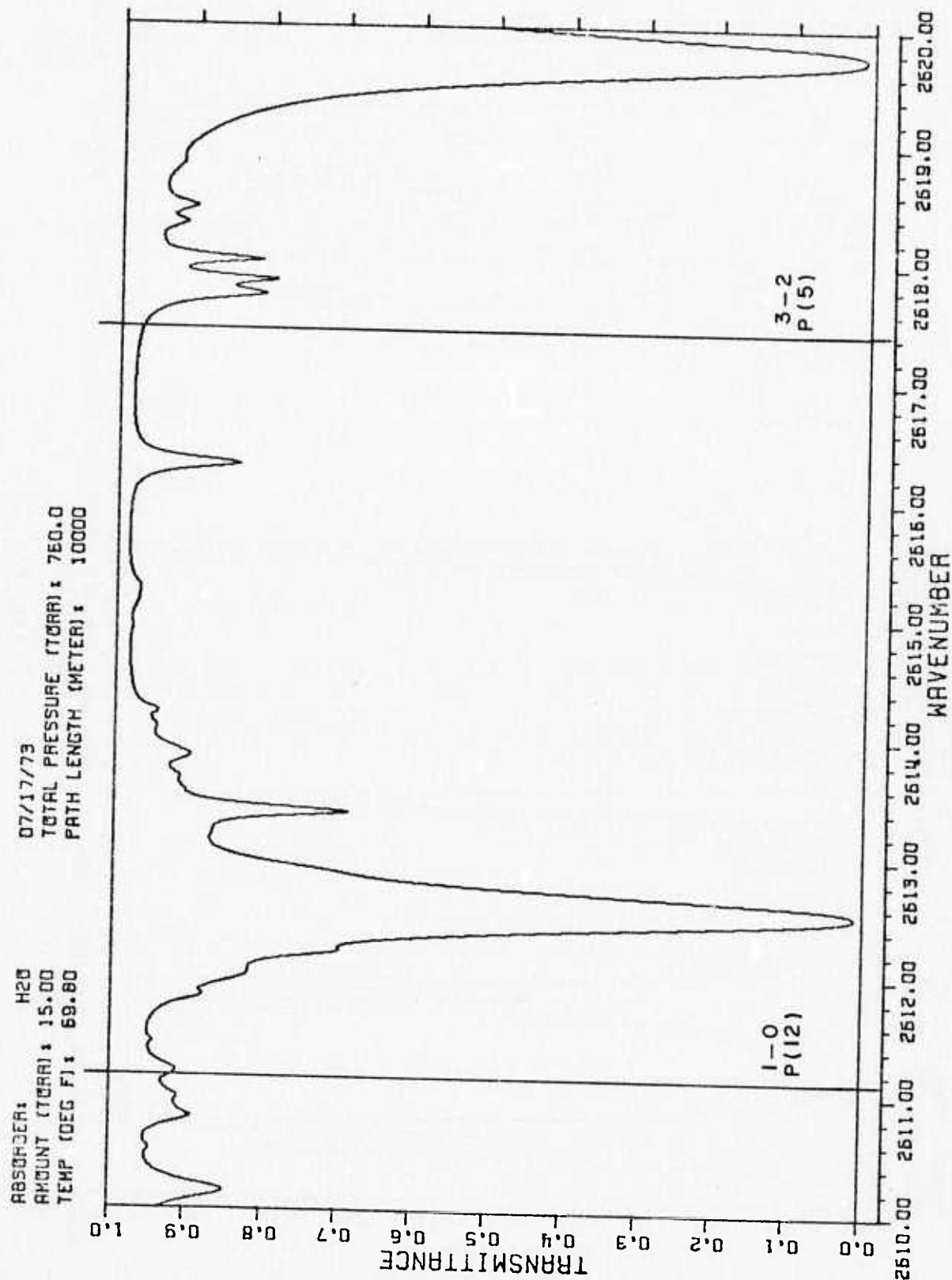


Fig. 43

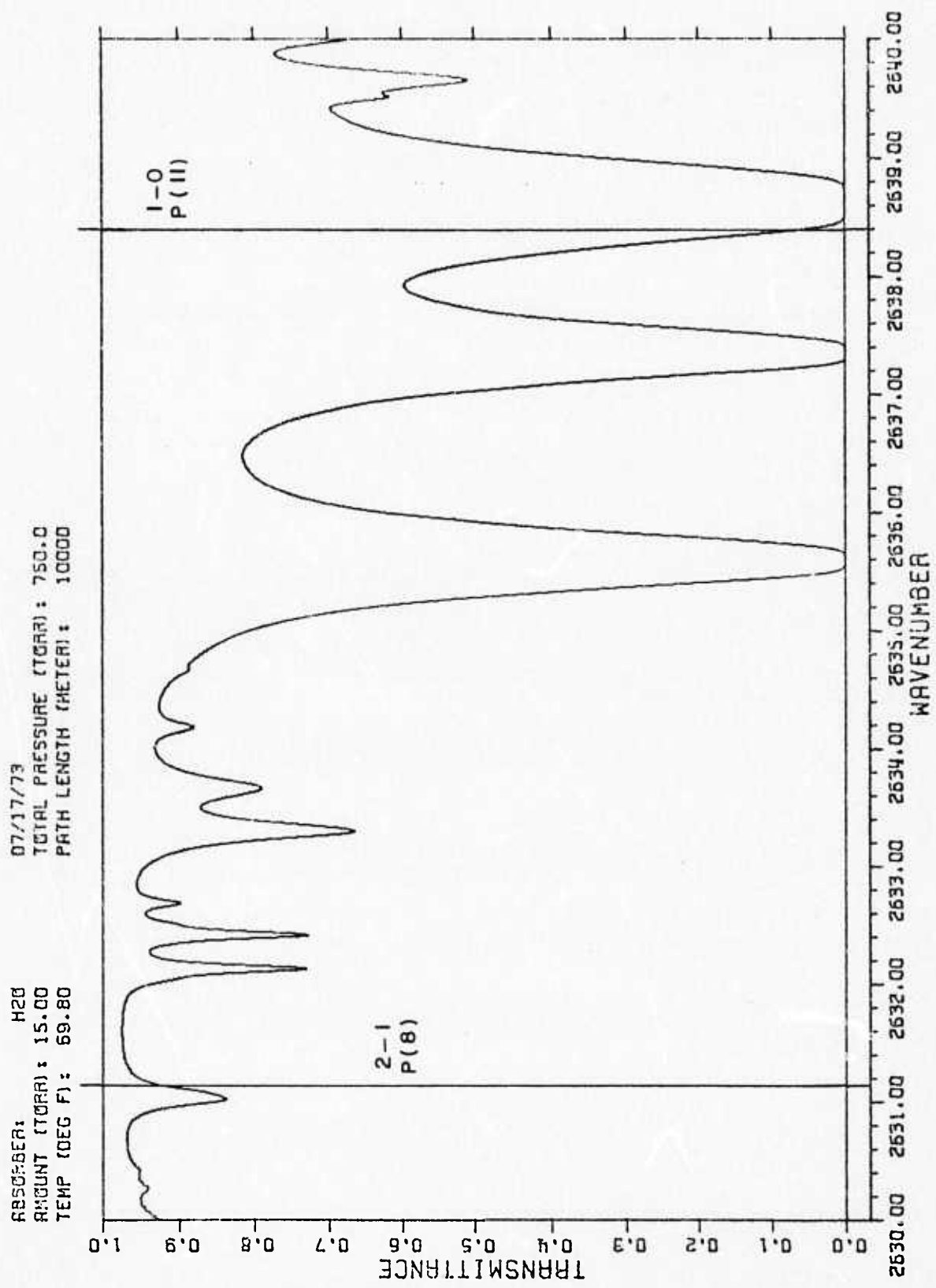


Fig. 44

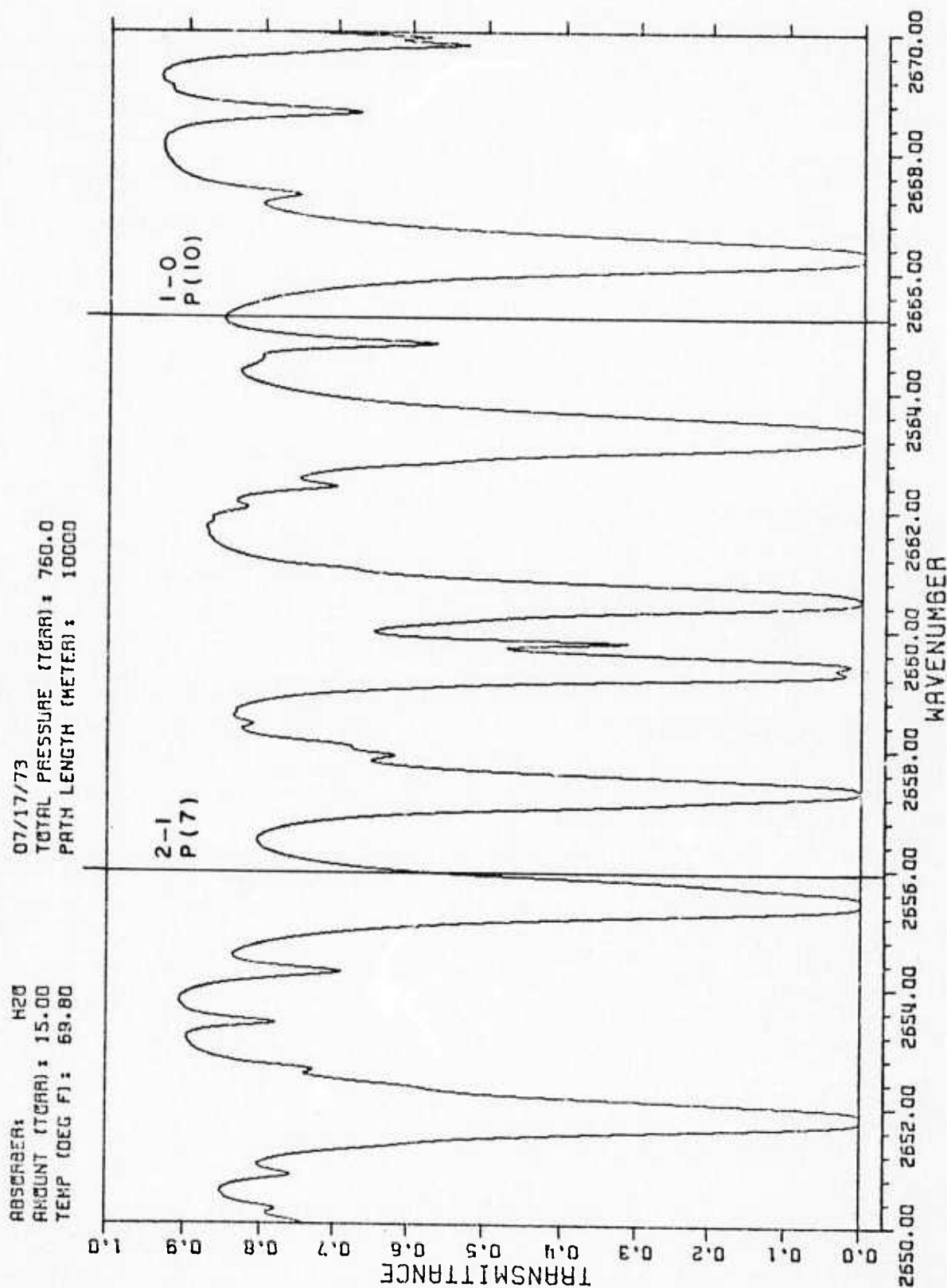


Fig. 45

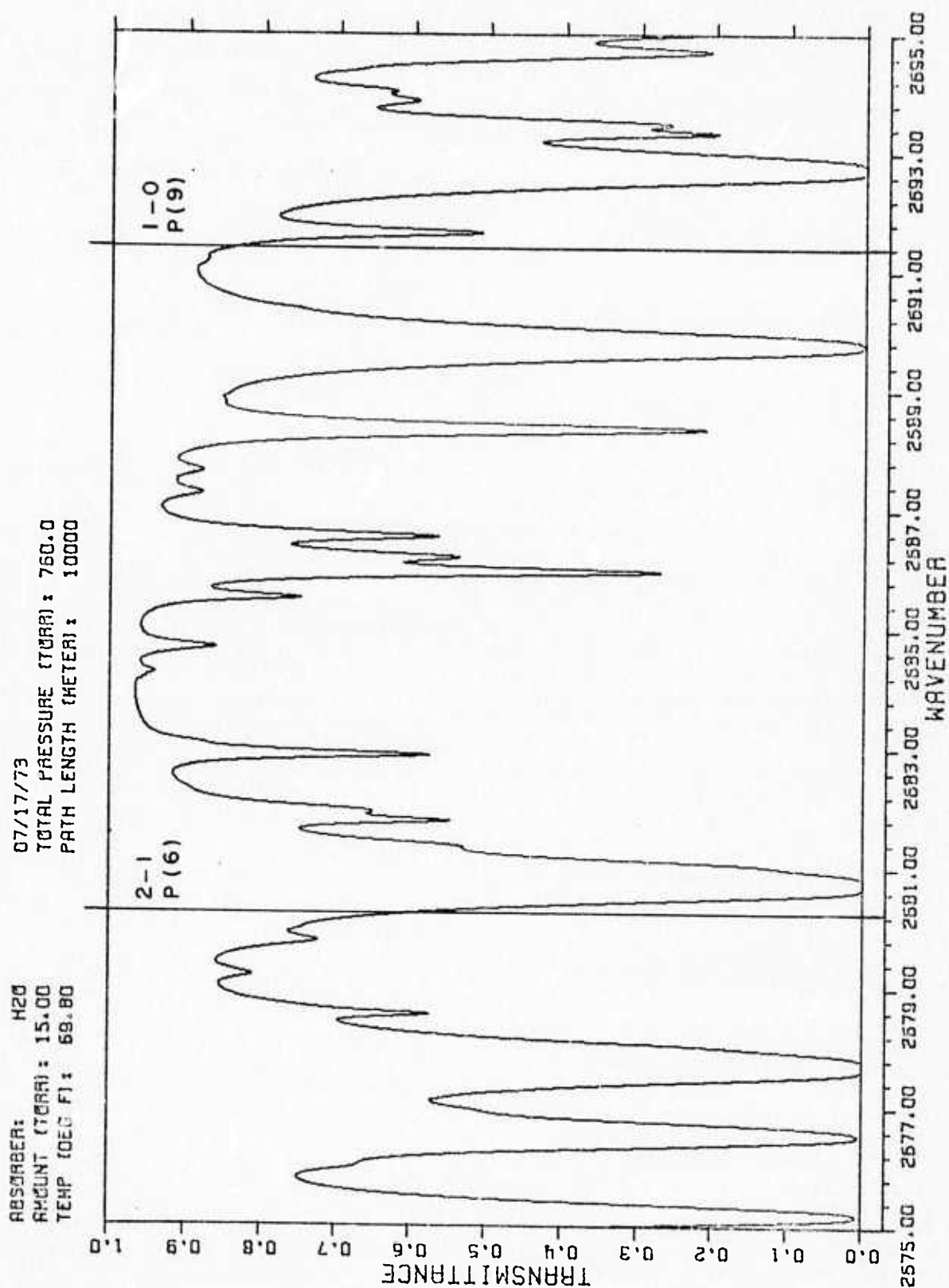


Fig. 46

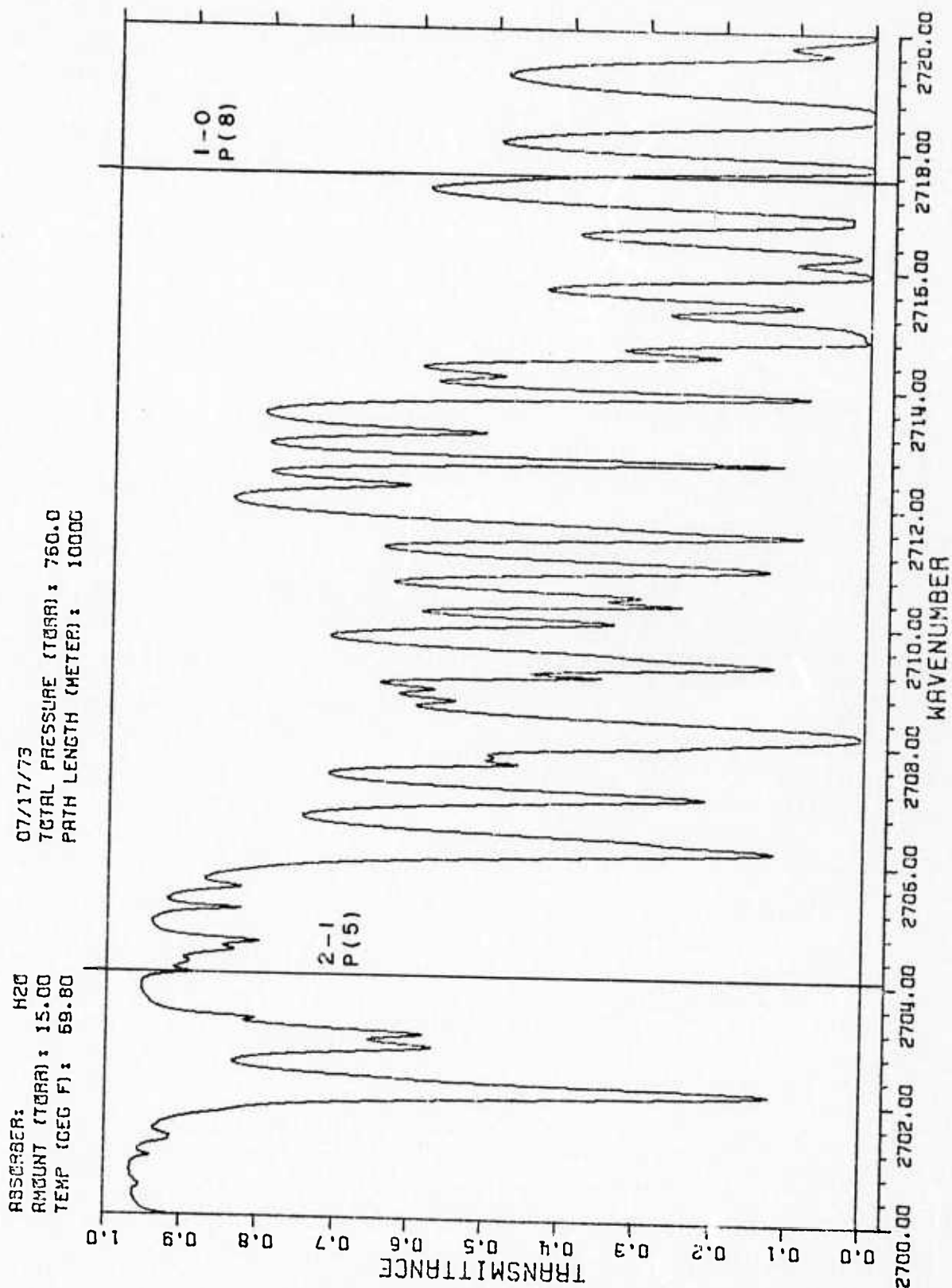


Fig. 47

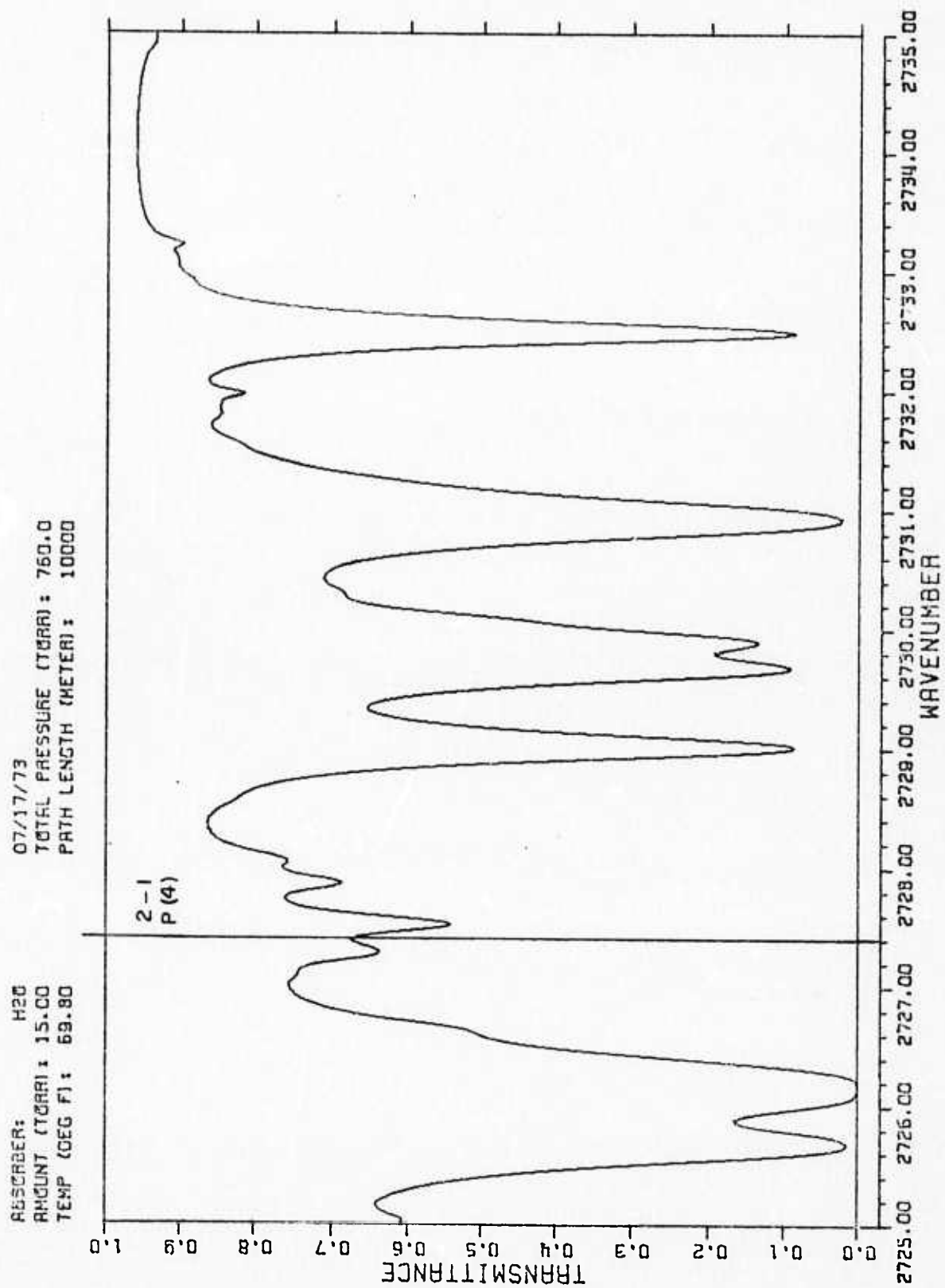


Fig. 48

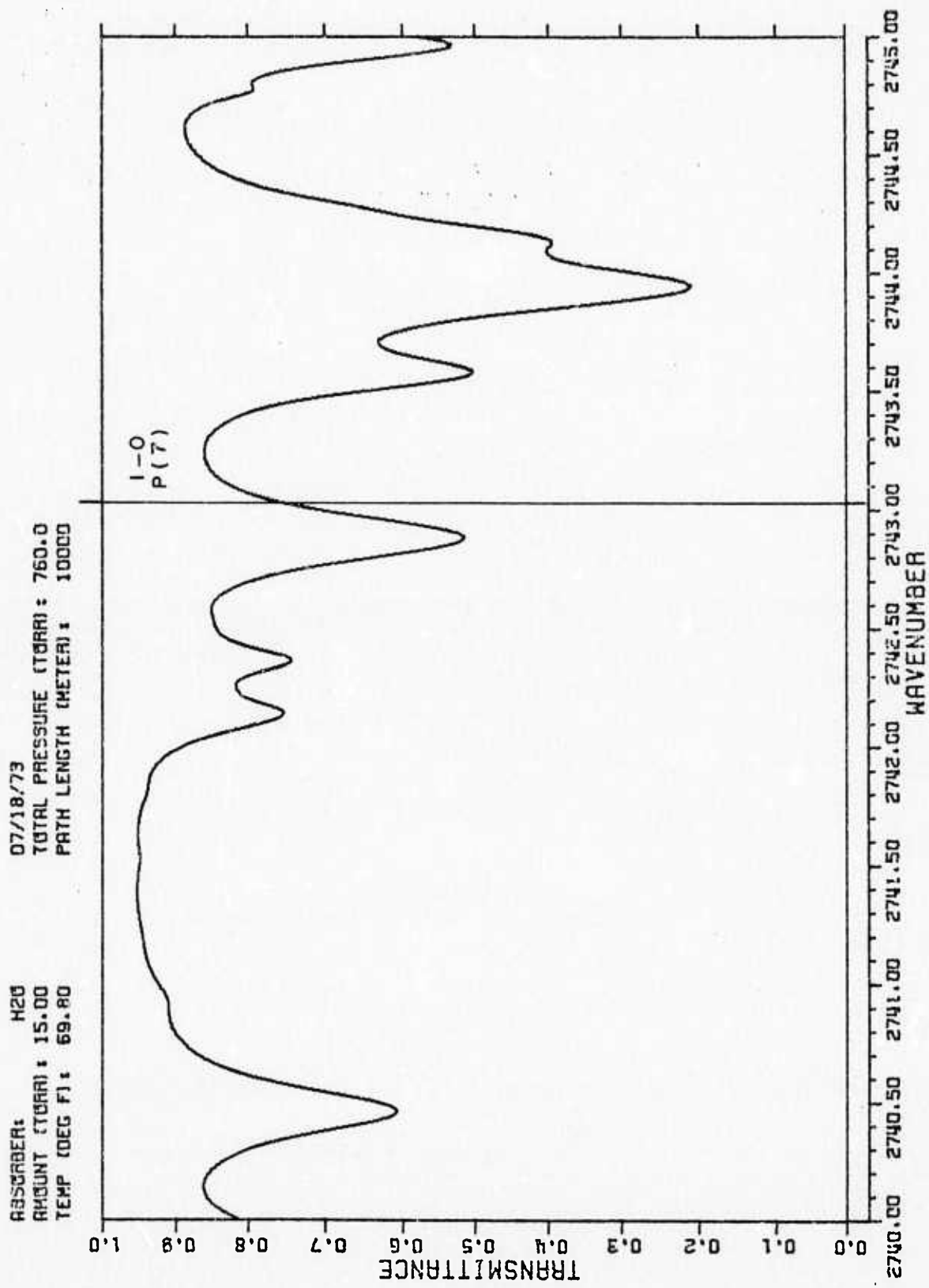


Fig. 49

ABSORBER: H₂O
AMOUNT (TORR): 15.00
TEMP (DEG F): 69.80

07/17/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 10000

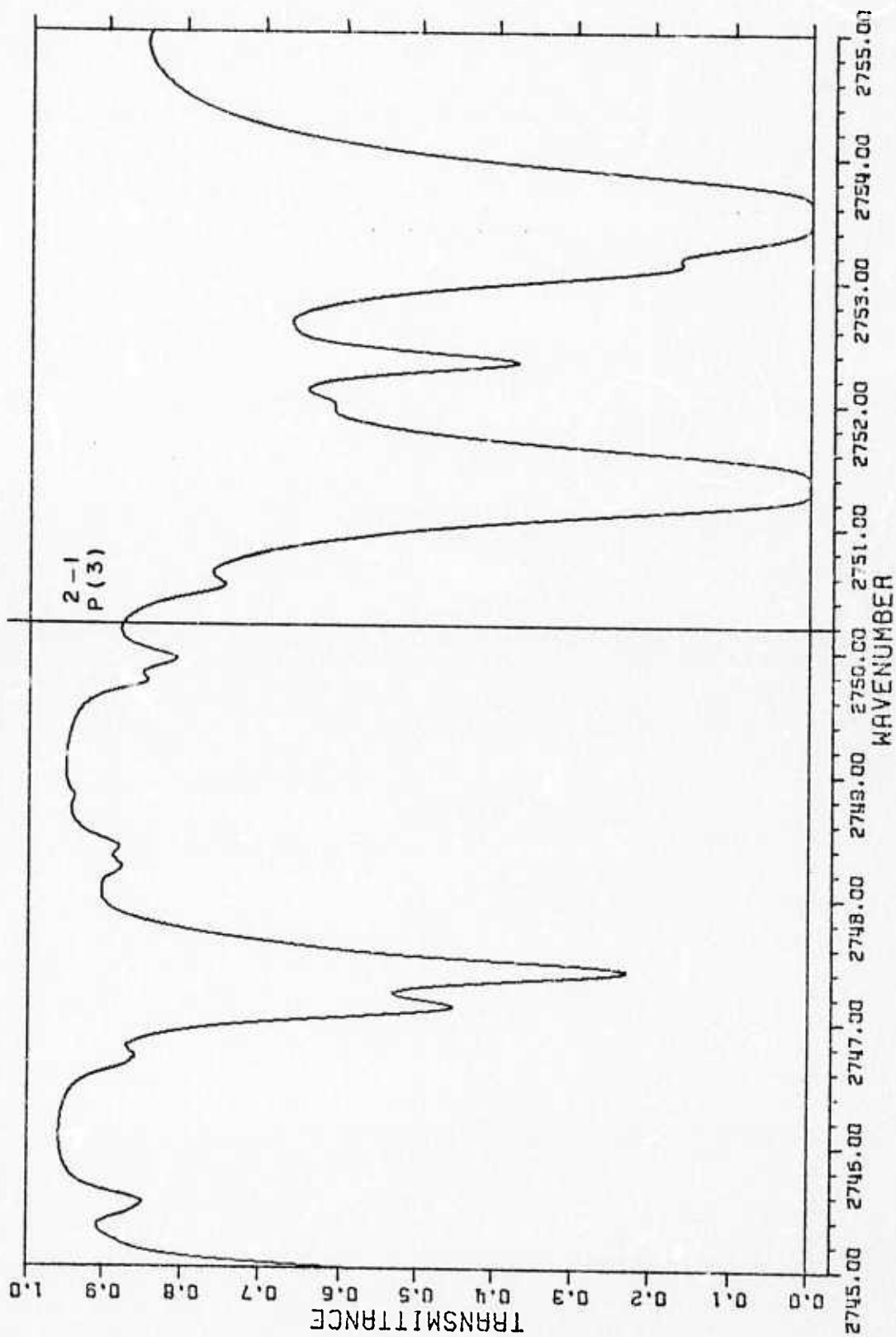


Fig. 50

ABSORBER: H2O
AMOUNT (TCRR): 15.00
TEMP (DEG F): 69.80

07/17/73
TOTAL PRESSURE (TCRR): 760.0
PATH LENGTH (METER): 10000

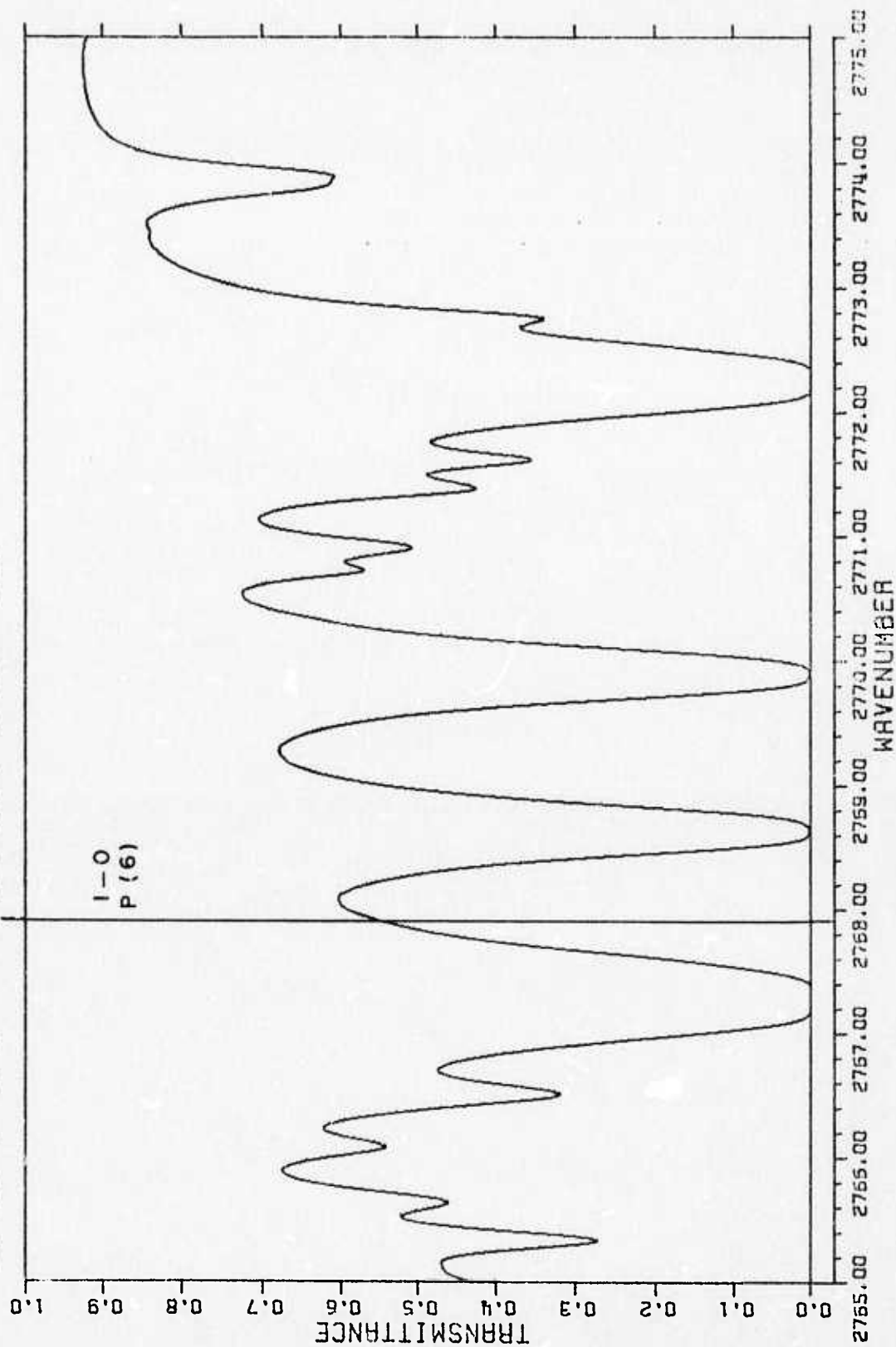


Fig. 51

07/17/73
TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 10000

ABSORBER: H₂O
AMOUNT (TORR): 15.00
TEMP (DEC F): 69.80

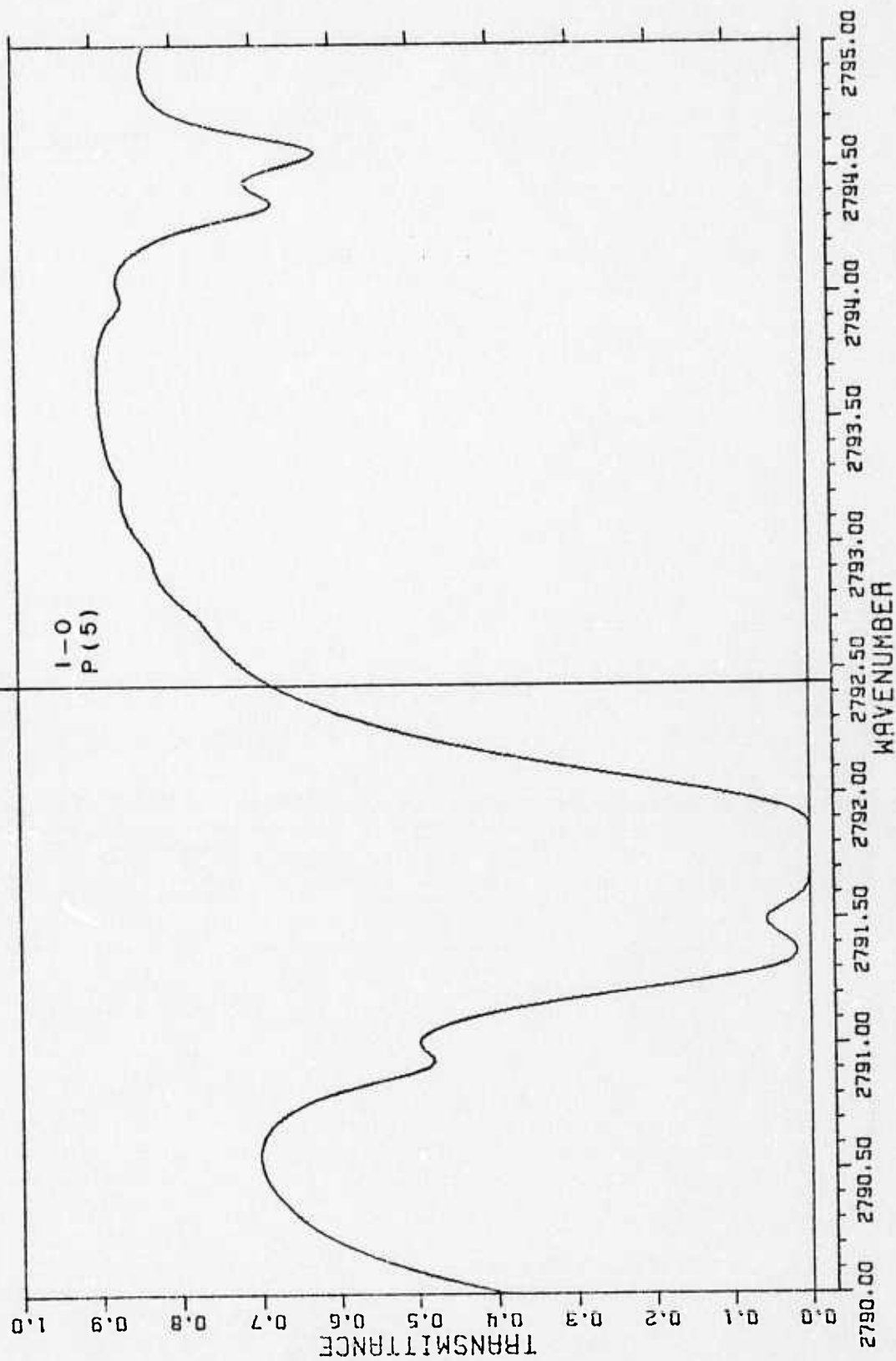


Fig. 52

ABSORBER: H₂O
AMOUNT (TORR): 15.00
TEMP (DEG F): 69.80

07/17/73

TOTAL PRESSURE (TORR): 760.0
PATH LENGTH (METER): 10000

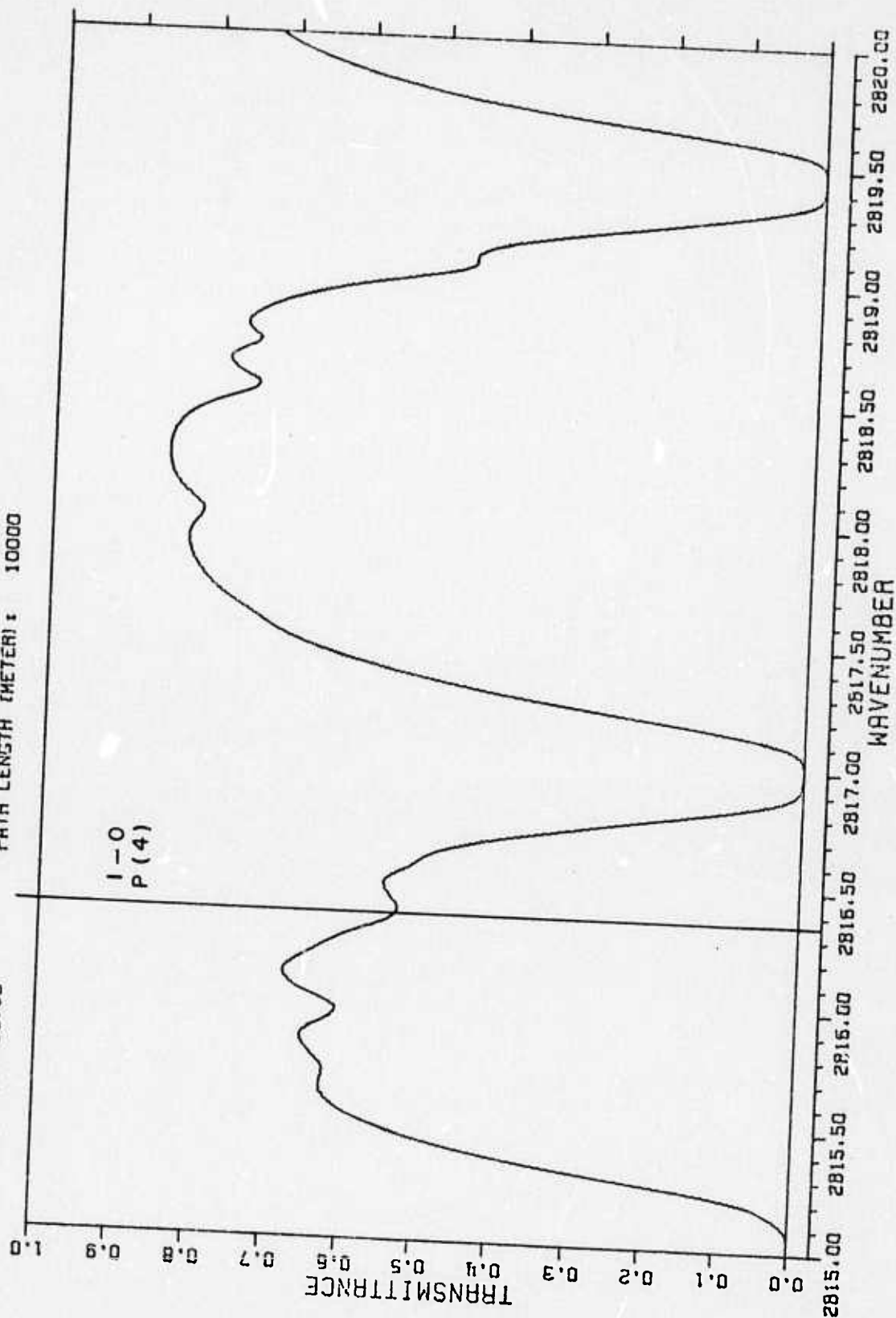


Fig. 53

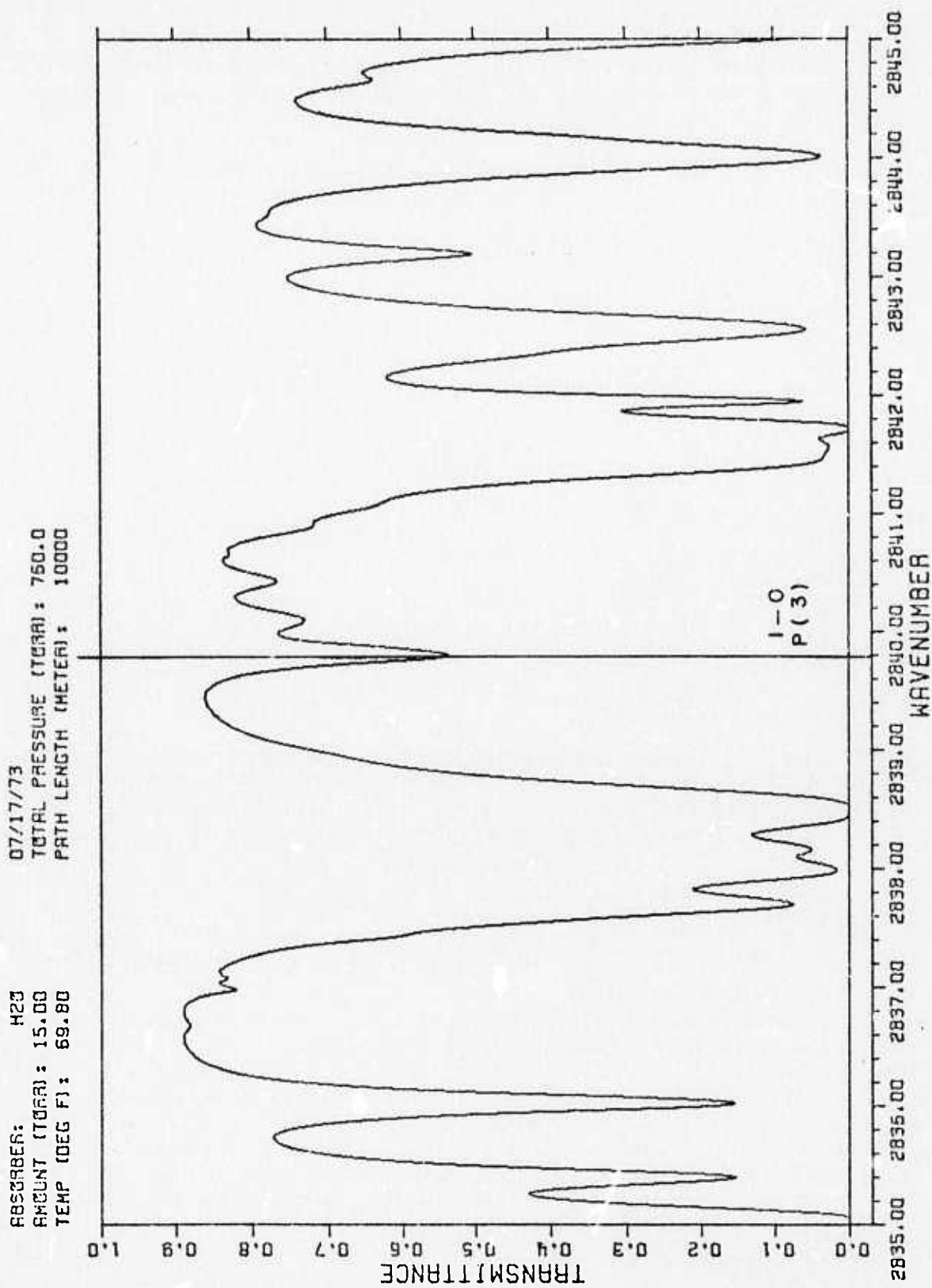


Fig. 54

SLOW was set to include all lines on the tape. DF line frequencies were for the purposes of the comparison set to the values in AFCRL-72-0312.

The results of the comparison are given in Table VI. The water

TABLE VI

LINE FREQUENCY (AFCRL)	LINE IDEN	k_{AFCRL} (REPT. 72-0312)	k_{OSU}	$\frac{\Delta k}{\text{AFCRL}} \times 100$
2445.29	3-2,12	6.706E-2	7.007E-2	+ 4.5
2471.34	3-2,11	4.925E-2	5.598E-2	+13.7
2496.61	3-2,10	3.057E-2	2.966E-2	- 3.0
2500.32	2-1,13	2.445E-2	2.547E-2	+ 4.2
2521.81	3-2,9	1.521E-2	1.566E-2	+ 3.0
2527.47	2-1,12	1.419E-2	1.516E-2	+ 6.9
2546.37	3-2,8	3.262E-2	3.286E-2	+ 0.7
2553.97	2-1,11	1.462E-2	1.730E-2	+18.3
2570.51	3-2,7	5.098E-2	4.316E-2	-15.3
2580.16	2-1,10	2.808E-2	2.929E-2	+ 4.3
2594.23	3-2,6	9.654E-3	1.154E-2	+19.5
2605.87	2-1,9	2.337E-2	2.425E-2	+ 3.8
2611.10	1-0,12	8.700E-3	9.085E-3	+ 4.4
2617.41	3-2,5	4.165E-3	4.571E-3	+ 9.7
2631.09	2-1,8	7.276E-3	1.500E-2	+106.1
2655.97	2-1,7	4.094E-2	4.480E-2	+ 9.4
2665.20	1-0,10	1.861E-2	1.621E-2	-12.9
2680.28	2-1,6	4.569E-2	4.930E-2	+ 7.9
2703.98	2-1,5	4.132E-3	4.875E-2	+18.0
2727.38	2-1,4	2.663E-2	3.623E-2	+36.0
2750.05	2-1,3	3.023E-2	1.324E-2	-56.2

vapor continuum was not included in our computation since it was not included in AFCRL-72-0312[11].

Predictions made on the basis of the data tape and using a Lorentz line shape are not expected to be accurate to any better than 10 or 20 percent and in some cases at CO laser wavelengths we have experimental data[4] indicating that a much larger discrepancy exists. With respect to calculations made at two locations it is not clear why large discrepancies occur for some lines when the calculation and data input are supposedly identical.

In a calculation involving so much input data, it would probably take a significant joint effort to discover the reasons, and then it might simply be a legitimate difference in approach. At the present we do not have the funds to pursue the matter, if indeed it is worth pursuing, but we did feel that completeness required us to make the comparison, especially since we were using Dr. McClatchey's data and did not wish to make an obvious error in doing so.

The over one hundred percent difference for the 2-1 P(8) line bothers us since it is one of the high power DF lines, see Table IV.

Finally we should comment that the calculations were repeated using a super-Lorentz line shape[4] for water vapor but the results were nearly the same as for the Lorentz line shape. This is in opposition to the situation at 5μ where the water vapor coefficient was found to be very sensitive to line shape. Perhaps the reason is that here we do not have intense absorption lines so that the calculated coefficient is due to the lines near the calculation frequency. This could be tested by sharply lowering the value of BOUND to see if the effect on the absorption coefficient is small. This was not done, however.

Finally one notes that Table III includes predictions for nine 1-0 band DF frequencies which were not included in AFCRL-72-0312.

APPENDIX A

We are indebted to Calfee[9] and McClatchey[5] for much of the material below.

I. Conversion Factors

A. Conversion of (atm-cm)_{STP} to molecules cm⁻²[5]

The molecular weight, M , of any gas in grams occupies 22.4136 liters at STP[12] so one cm³ of any gas at STP weighs

$$\frac{M}{2.24136 \times 10^4} \text{ grams.}$$

Since 1 atm-cm_{STP} is equivalent to one cm of gas at STP per cm²

$$1 \text{ atm-cm}_{\text{STP}} = \frac{M}{2.24136 \times 10^4} \text{ gm cm}^{-2}.$$

Avogadro's number[12] can be used to compute the number, n , of molecules per cm³ of any gas

$$n = \frac{6.02252 \times 10^{23}}{2.24136 \times 10^4} = 2.687016 \times 10^{19} \text{ molecules cm}^{-3}.$$

Hence the desired result is

$$(1) \quad \boxed{1 \text{ atm-cm}_{\text{STP}} = 2.6870 \times 10^{19} \text{ molecules cm}^{-2}}.$$

B. Conversion of precipitable centimeters of water to mol cm⁻²[5]

$$1 \text{ atm-cm}_{\text{STP}, \text{H}_2\text{O}} = \frac{M}{2.24136 \times 10^4} = \frac{18.016}{2.24136 \times 10^4}$$

$$1 \text{ atm-cm}_{\text{STP}, \text{H}_2\text{O}} = 8.03798 \times 10^{-4} \text{ gm cm}^{-2}.$$

Using the constant developed in paragraph A, above we have the desired result

$$(2) \quad 1 \text{ pr-cm} = 3.3429 \times 10^{22} \text{ mol cm}^{-2} .$$

C. Partial pressure of water vapor from density and temperature[13].

From the referenced tables we have the relation

$$\rho = \frac{10^3 a \delta p_a / 760}{1 + \alpha T} \text{ gm m}^{-3}$$

where a = weight of one cubic meter of dry air at 0°C and 760 torr = 1.29278 kg.

δ = density of aqueous vapor relative to dry air = .62168

p_a = partial pressure H_2O in torr

α = coefficient of expansion of air for 1°C = .00366.

Rearranging we have the desired result

$$(3) \quad p_a = .9456 (1 + .00366 T) \rho \text{ torr}$$

where T = temperature in deg C

ρ = water vapor density in gm/m^3

D. Precipitable centimeters H_2O from partial pressure, temperature, and path length

$$w = \rho \ell .$$

Using the relation from paragraph C,

$$w = \frac{1.05821 p_a \cdot 10^{-6}}{1 + .00367 (T_{\text{OK}} - 273.13)} \cdot \ell \cdot 10^2$$

where ℓ is the path length in meters

p_a is water vapor pressure in torr.

Since the third term in the denominator is nearly unity, we can write

$$(4) \quad w = \frac{2.8834 \times 10^{-2} p_a \ell}{T} \text{ pr-cm} .$$

E. Conversion to atm-cm_{STP} from pressure, path length, and temperature of sample [5]

$$\text{atm-cm}_{\text{STP}} = \frac{\ell p_a}{760} \frac{273.13}{T}$$

$$(5) \quad \text{atm-cm}_{\text{STP}} = 3.5938 \times 10^{-1} \frac{p_a \ell}{T}$$

where p_a = absorber pressure in torr
 ℓ = path length in cm
 T = temperature in deg K.

F. Density computed from partial pressure, molecular weight, and temperature

This is of course the Gas Law

$$(6) \quad \rho = 1.6035 \times 10^{-5} \frac{p_a M}{T} \text{ gm cm}^{-3}$$

where p_a = pressure in torr
 M = molecular weight
 T = deg K.

G. Partial pressure of water vapor from mixing ratio [14]

$$(7) \quad p_a = \frac{r P}{.62168 + r} \text{ torr}$$

where r is the mixing ratio and P is the total pressure in torr.

From the data in the AFCRL models (5), one should compute mixing ratio as follows:

$$(8) \quad r = \frac{p_{H_2O}}{p_{air} - p_{H_2O} \frac{28.9785}{18.0153}}$$

Note that the constant .62168 in Eq. (7) is the ratio of the molecular weight of water vapor to that of dry air at STP, i.e., $18.0153/28.9785$, see reference 12. In the Smithsonian tables (14) the value used is 0.62197 apparently based on older molecular weight data.

H. Ozone partial pressure from density for AFCRL mid-latitude summer model (5)

$$(9) \quad p_a = \frac{d}{q} \times 760 \times \frac{6.0 \times 10^{-5}}{1.191 \times 10^3} \text{ torr}$$

where d = air density at STP = 28.9785 (12),
 q = molecular weight of ozone = 47.9982 (12),

and $6.0 \times 10^{-5} \text{ g/m}^3$ is the density of ozone and $1.191 \times 10^3 \text{ g/m}^3$ is the air density, both at sea level, of the AFCRL mid-latitude summer model. The result is $2.31 \times 10^{-5} \text{ torr}$.

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