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A study of the infrared spectra of a group of hydroxyalkylamine hydrochlorides

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A STUDY OF THE INFRARED SPECTRA
OF
A GROUP OF HYDROXYALKYLAMINE HYDROCHLORIDES

by
Lawrence Ingram Briel, II

THESIS

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of the
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for the Degree of
Master of Science - Chemistry

August 1964

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ABSTRACT

The infrared spectra of twenty amine hydrochlorides were obtained with the Perkin-Elmer Model 21 recording spectrophotometer. The positions of the absorption bands were compared with literature values for pertinent structural group frequencies. A system of coding the spectral data was devised so that an IBM 1620 digital computer could make the comparisons for a large number of group frequencies. Good agreement was observed between the positions of the absorption bands in the experimental spectra and those of pertinent group frequencies reported in the literature.

Of the ten symmetrical diamines which were studied, six contained the primary hydroxyl group. Two similar compounds without this group, 2,8-dimethyl-3,7-diaza-5-nonanol dihydrochloride and 2,2,8,8-Tetramethyl-3,7-diaza-5-nonanol dihydrochloride, were synthesized. These two were not found in the literature.

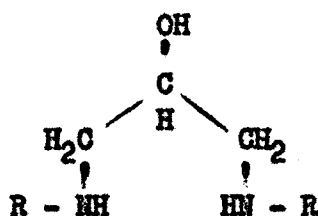
When the compounds were purified by recrystallization, many of them were highly hygroscopic and required special techniques to remove moisture before taking the spectra.

ACKNOWLEDGMENT

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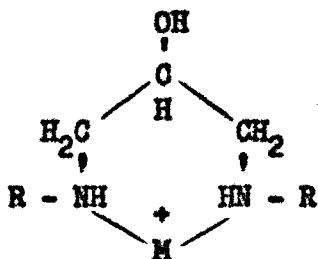
I. INTRODUCTION

The coordinating properties of a special series of polyhydroxyamines, viz., those possessing the symmetrical structure:



1,3-Bis(poly(hydroxymethyl)methylamino)-2-propanol

in which "R" represents one of six groups (Table I), have been studied previously by workers in this laboratory (Davis (9), Erdmanis (10), Gladding (12), Jackson (15), Moore (21), and O'Rear (23)) and elsewhere by means of stability constant data for the chelates of these compounds with various transition-metal cations in aqueous media. While the principal attachment of these organic bases (called "ligands") to the metal ions appears to occur at the sites of the two amino nitrogens, forming a six-membered chelate ring:



there is the possibility of the formation of additional chelate linkages to the cation by the hydroxyl groups of the ligand, especially under conditions of high pH, where the alcoholic protons may be removed. While evidence has not been found which establishes unequivocally the specific role of the hydroxyl groups in the chelating properties of the ligands of this

series, the stability constant data for the chelates of these compounds, with the copper (II) and nickel (II) ions, suggests that either these ligands are quadridentate--in which case two of the hydroxyl groups of the ligand would also participate in chelation--or the chelates which are formed under these conditions are polynuclear in nature and their apparently simple stoichiometry is deceptive.

It was thought that the infrared spectra of these chelates might yield valuable information about the nature of the various types of chemical bonds that are present, and clarify the role of the hydroxyl groups in the coordinating properties of the ligands. To interpret the significance of these spectra, reference spectra of the ligands were desired so that the effects of chelation on the bonds could be determined by observing the differences in the two sets of spectra. However, a search of the spectral literature revealed that no reference spectra on these ligands were available, and it became necessary to make a preliminary study of the spectra of these compounds before attempting to interpret those of the chelates.

This thesis is concerned with the preliminary study, i.e., the recording and study of the infrared spectra of this series of polyhydroxyamines, and also the parent series of monoamines from which the symmetrical diamines were prepared. Similarities, as well as differences, in the spectrum of a parent monoamine and the spectrum of its corresponding diamine will be noted; and comparisons will be drawn among the spectra of the two series.

Table I (the symmetrical diamines) and Table II (the parent monoamines) show the compounds studied, their official names, and our code numbers which were used to represent them. These numbers have been found to be a con-

venient means of discussing the relatively large number of similar compounds. The first two digits of the number refer respectively to the number of carbon atoms and the number of oxygen atoms in the parent monoamine group. The parent itself is indicated when the third digit is "1"; the symmetrical diamine (in which the 2-propanol group bridges two identical monoamines) is indicated when the third digit is "2".

TABLE I.

SYMMETRICAL DIAMINE LIGANDS

Code	Formula *	IUPAC Name
002	$\text{H}_3\text{N}^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_3^+$	1,3-Diamino-2-propanol
212	$\text{HO}-\text{CH}_2-\text{CH}_2-\text{NH}_2^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_2^+-\text{CH}_2-\text{CH}_2-\text{OH}$	3,7-Diaza-1,5,9-nonanetriol
302	$(\text{CH}_3)_2\text{CH}-\text{NH}_2^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_2^+-\text{CH}(\text{CH}_3)_2$	2,8-Dimethyl-3,7-diaza-5-nonanol
312	$(\text{HO}-\text{CH}_2)(\text{CH}_3)\text{CH}-\text{NH}_2^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_2^+-\text{CH}(\text{CH}_3)(\text{CH}_2-\text{OH})$	2,8-Dimethyl-3,7-diaza-1,5,9-nonanetriol
322	$(\text{HO}-\text{CH}_2)_2\text{CH}-\text{NH}_2^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_2^+-\text{CH}(\text{CH}_2-\text{OH})_2$	2,8-Bis(hydroxymethyl)-3,7-diaza-1,5,9-nonanetriol
402	$(\text{CH}_3)_3\text{C}-\text{NH}_2^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_2^+-\text{C}(\text{CH}_3)_3$	2,2,8,8-Tetramethyl-3,7-diaza-5-nonanol
412	$(\text{HO}-\text{CH}_2)(\text{CH}_3)_2\text{C}-\text{NH}_2^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_2^+-\text{C}(\text{CH}_3)_2(\text{CH}_2-\text{OH})$	2,2,8,8-Tetramethyl-3,7-diaza-1,5,9-nonanetriol
422	$(\text{HO}-\text{CH}_2)_2(\text{CH}_3)\text{C}-\text{NH}_2^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_2^+-\text{C}(\text{CH}_3)(\text{CH}_2-\text{OH})_2$	2,8-Bis(hydroxymethyl)-2,8-dimethyl-3,7-diaza-1,5,9-nonanetriol
432	$(\text{HO}-\text{CH}_2)_3\text{C}-\text{NH}_2^+-\text{CH}_2-\text{CH}(\text{OH})-\text{CH}_2-\text{NH}_2^+-\text{C}(\text{CH}_2-\text{OH})_3$	2,2,8,8-Tetrakis(hydroxymethyl)-3,7-diaza-1,5,9-nonanetriol
---	$\text{H}_3\text{N}^+-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{NH}_3^+$	1,3-Diaminopropane

* The formulas are those of the dipositive ions of the dihydrochlorides.

TABLE II.

PARENT MONOAMINE LIGANDS

Code No.	Formula	IUPAC Name
101	$\text{CH}_3\text{-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	Aminomethane hydrochloride
201	$\text{CH}_3\text{-CH}_2\text{-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	Aminoethane hydrochloride
211	$\text{HO-CH}_2\text{-CH}_2\text{-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	2-Aminoethanol hydrochloride
301	$(\text{CH}_3)_2\text{CH-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	2-Aminopropane hydrochloride
311	$(\text{HO-CH}_2)(\text{CH}_3)\text{CH-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	2-Amino-1-propanol hydrochloride
321	$(\text{HO-CH}_2)_2\text{CH-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	2-Amino-1,3-propanediol hydrochloride
401	$(\text{CH}_3)_3\text{C-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	2-Amino-2-methylpropane hydrochloride
411	$(\text{HO-CH}_2)(\text{CH}_3)_2\text{C-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	2-Amino-2-methyl-1-propanol hydrochloride
421	$(\text{HO-CH}_2)_2(\text{CH}_3)\text{C-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	2-Amino-2-methyl-1,3-propanediol hydrochloride
431	$(\text{HO-CH}_2)_3\text{C-}\overset{+}{\text{N}}\text{H}_3\text{.Cl}^-$	2-Amino-2-hydroxymethyl-1,3-propanediol hydrochloride

II. FUNDAMENTALS

A. THE ORIGIN OF INFRARED SPECTRA

Infrared spectra arise from changes in the different modes of motion of molecules that are possible on the absorption of a quantum of electromagnetic radiation at wavelengths between 1 and 50 microns. Molecules are composed^{of} atoms which are linked by means of interacting forces called chemical bonds. The atoms are never at rest, but are constantly vibrating about their equilibrium positions, which results in an alternate stretching and contracting of the bonds (Figure 1). As a first approximation, the molecule behaves like a set of masses connected by springs which follow Hooke's law. Thus, when the atoms are displaced from their equilibrium positions, they experience a restoring force which is proportional to the amount of displacement and opposite in direction:

$$f = -kx \quad (1)$$

The work done on the molecular system in distorting the bonds is stored as potential energy:

$$dU = kx dx \quad (2)$$

Integration gives the change in the potential energy as a function of the displacement:

$$U = \frac{1}{2}k x^2 \quad (3)$$

The constant "k" is called the "force constant" of the chemical bond.

For the simple case of a diatomic molecule, if the bond is assumed to be a classical harmonic oscillator, the positions of the two atoms as a function of time can be derived from Newton's second law of motion:

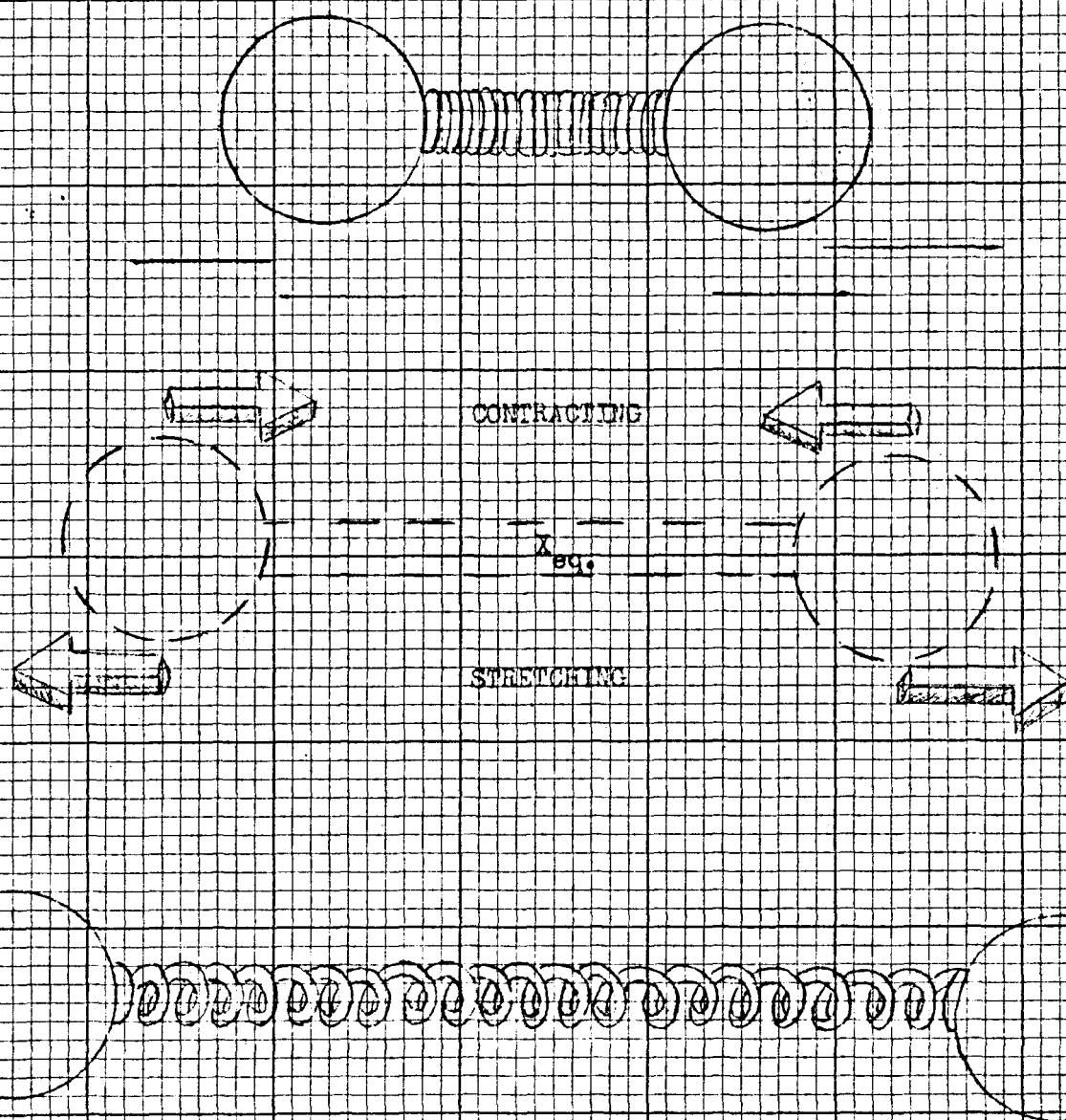
$$f = ma \quad (4)$$

which, for the system of two masses, becomes:

$$f = \mu a \quad (5)$$

Figure 1.

THE IDEALIZED VIBRATORY DISTORTIONS OF A CHEMICAL BOND



where the reduced mass " μ " is defined as:

$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \quad (6)$$

Since acceleration is the second derivative of displacement with respect to time:

$$a = \frac{d^2x}{dt^2} \quad (7)$$

Equations (5) and (7) can be substituted into Equation (1) to obtain:

$$-kx = \mu \cdot \frac{d^2x}{dt^2} \quad (8)$$

a solution of which is:

$$x = A \sin (k/\mu)^{\frac{1}{2}} \cdot t \quad (9)$$

where the constant "A" represents the maximum value of the displacement, i.e., the vibrational amplitude. Thus, the positions of the atoms change sinusoidally with time, and the interval which corresponds to one vibration is $2\pi(\mu/k)^{\frac{1}{2}}$. The reciprocal of this quantity is the frequency of vibration:

$$\nu_{\text{classical}} = \frac{1}{2\pi(k/\mu)^{\frac{1}{2}}} \quad (10)$$

However, chemical bonds are not classical harmonic oscillators, since they absorb energy only in discrete quanta. Erwin Schroedinger's solution to this problem differs from the classical approach by permitting only certain values of energy to be imparted to the vibrating system, the allowed energies forming a pattern of "levels" which are spaced by the amount:

$$\Delta \epsilon_{\text{vibrational}} = \frac{(k/\mu)^{\frac{1}{2}}}{2\pi c} \quad (11)$$

where "c" is the velocity of light (3×10^{10} cm/sec.) and $\Delta \epsilon_{\text{vib.}}$ is measured in units of reciprocal centimeters. Transitions among the levels are

induced by electromagnetic radiation when a dipole vector of the bond is oscillating with the same frequency as the electric vector of the radiation, and absorption occurs when the quantum of energy satisfies the equation:

$$\epsilon = (v \pm \frac{1}{2}) h\nu \text{ classical} \quad (12)$$

where "h" is Planck's constant (6.625×10^{-27} erg-sec.) and "v" is a non-negative integer. (2)

For polyatomic molecules each bond has its own pattern of vibrational energy levels which depends on the masses of the atoms and the force constant of the bond. Consequently, polyatomic molecules give rise to a large number of vibrational transitions and to a characteristic absorption maximum for each different type of chemical bond that is present. Infrared spectra are graphical representations of these absorption maxima as functions of the wavelength (or frequency) of the radiation being absorbed.

B. PRACTICAL APPLICATIONS OF INFRARED DATA

Since the vibrational frequencies are characteristic of the different chemical bonds which are present in a molecule, they are very useful in identifying the structural units which occur in unknown compounds. Not all of the possible vibrations are suitable for this type of analysis, since some vibrational "group frequencies" have been found to change for different molecular environments. However, the approximate constancy of the spectral position of many group frequencies has been established for a number of different chemical bonds, and the reliability of these positions has been verified in the literature (3, 4, 5, 7, 13, 17, 19, 22, 29, 31, 32, 33).

Group frequencies are usually described in terms of the motions that the atomic nuclei of a molecular structural unit undergo during the vibration. The simplest and most commonly encountered motion of the nuclei, viz., diatomic stretching, has already been described. If three atoms are bound linearly and a stretching vibration occurs, it may be a symmetric motion, in which the two end-nuclei move in-and-out in phase (Figure 2-a); or it may be an asymmetric motion, in which the two end-nuclei move alternately (Figure 2-b). All vibratory motions of nuclei other than stretching vibrations are classified as "deformation vibrations."

A linear unit of three atoms such as the one shown in Figure 2 can undergo a bending deformation, in which the end-nuclei move alternately off-and-back to the principal axis (Figure 3). A non-linear unit of three atoms can also undergo a bending deformation, in which the end-nuclei move alternately toward-and-away from each other (Figure 4); non-linear bending is called "scissoring."

In addition to the bending and scissoring deformations, there are three other types, called "wagging," "rocking," and "twisting." The wagging deformation occurs when the two end-nuclei move in phase alternately above-and-below the plane of the unit (Figure 5). The rocking deformation occurs when the two end-nuclei move in phase in the plane of the unit, in such a manner that the bond angle is alternately expanded and compressed (Figure 6). The twisting deformation is an oscillatory motion of the plane of the unit about the bond connecting it to the rest of the molecule (Figure 7).

For a simple non-linear molecule such as H_2O , the three absorption bands which appear in the infrared spectrum have been assigned to three fundamental vibrations: a symmetric stretching (Figure 8), which has a frequency ν_1 ; a scissors (Figure 9), which has a frequency ν_2 ; and an

Figure 2 (a). SYMMETRIC STRETCHING

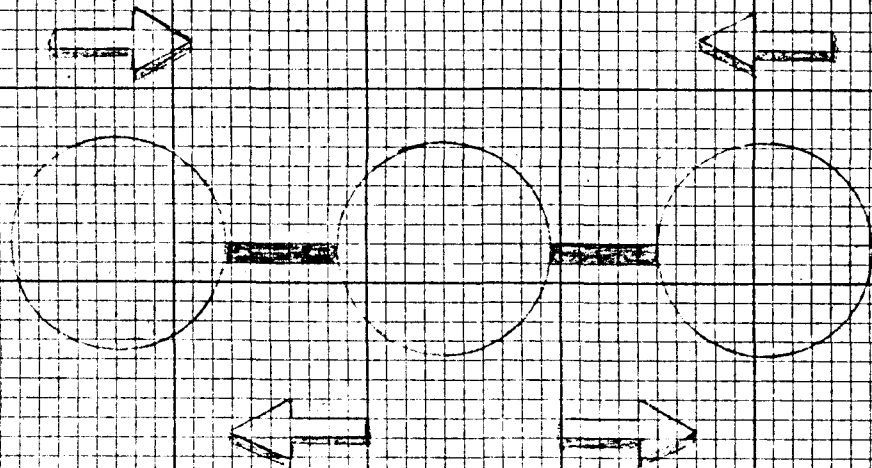


Figure 2 (b). ASYMMETRIC STRETCHING

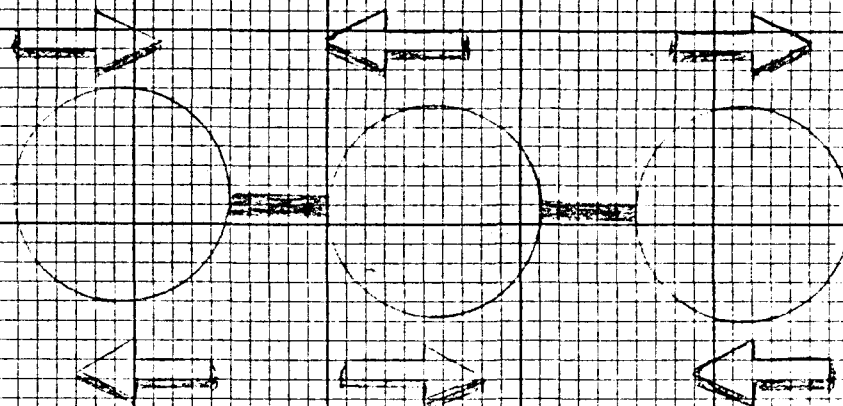
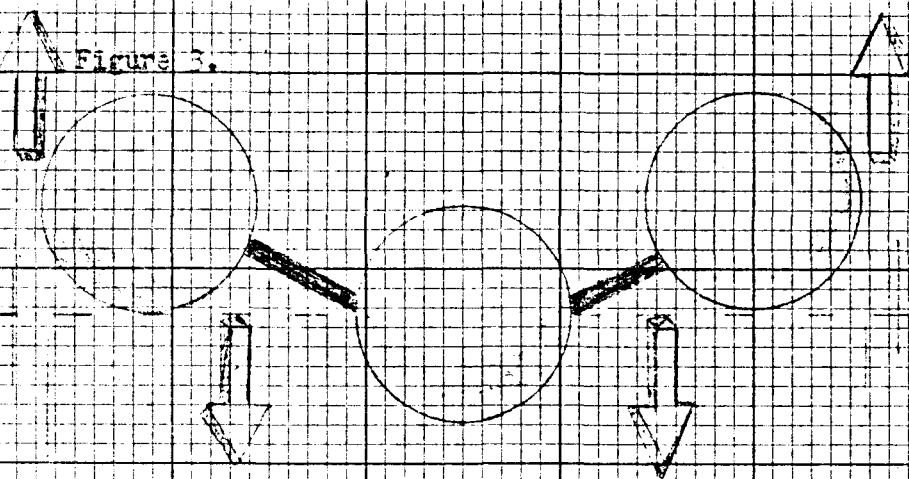
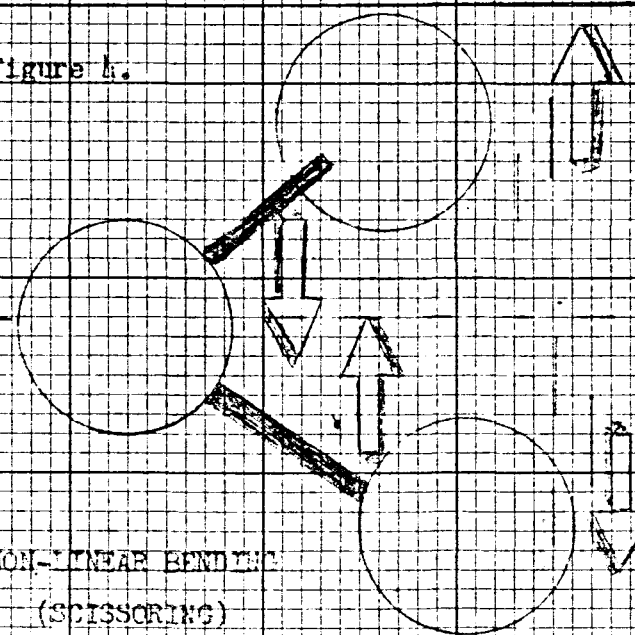


Figure 3.



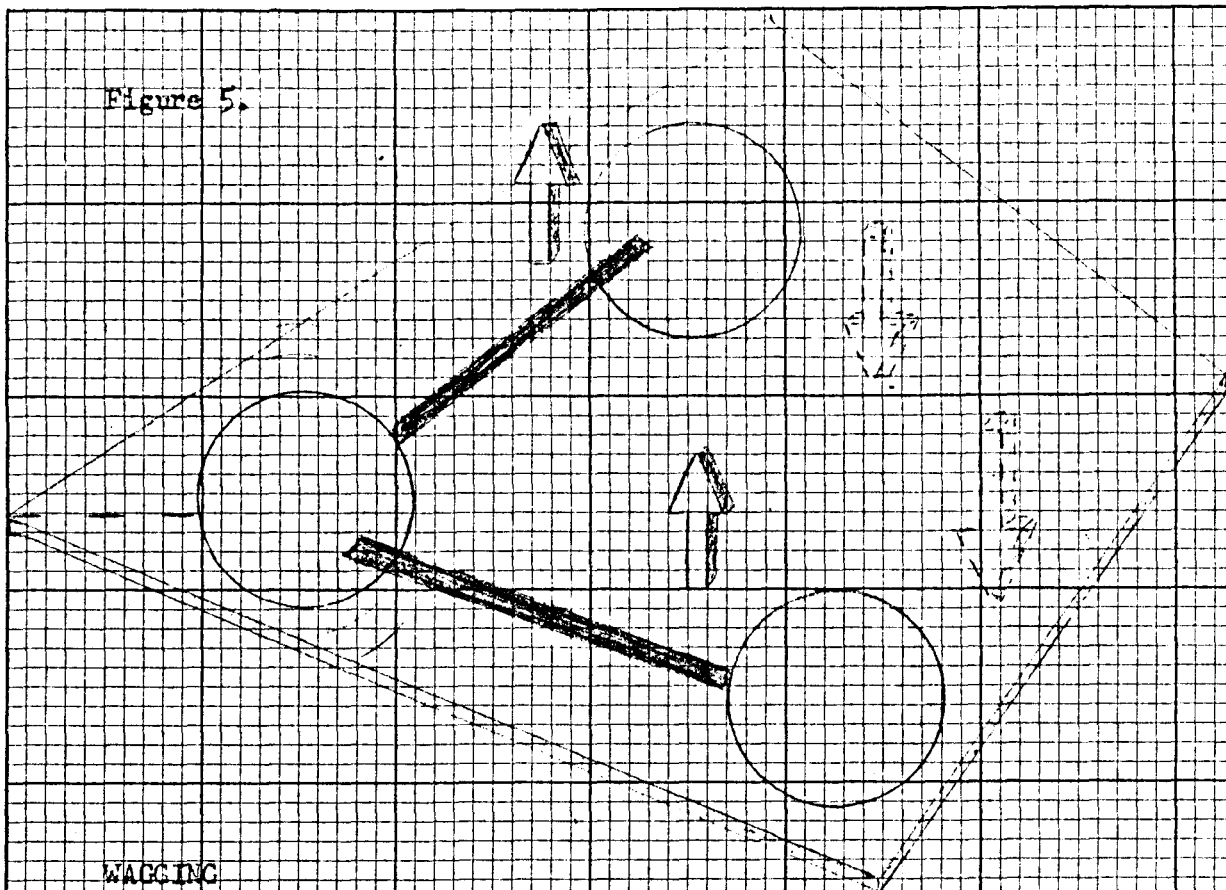
LINEAR BENDING

Figure 4.



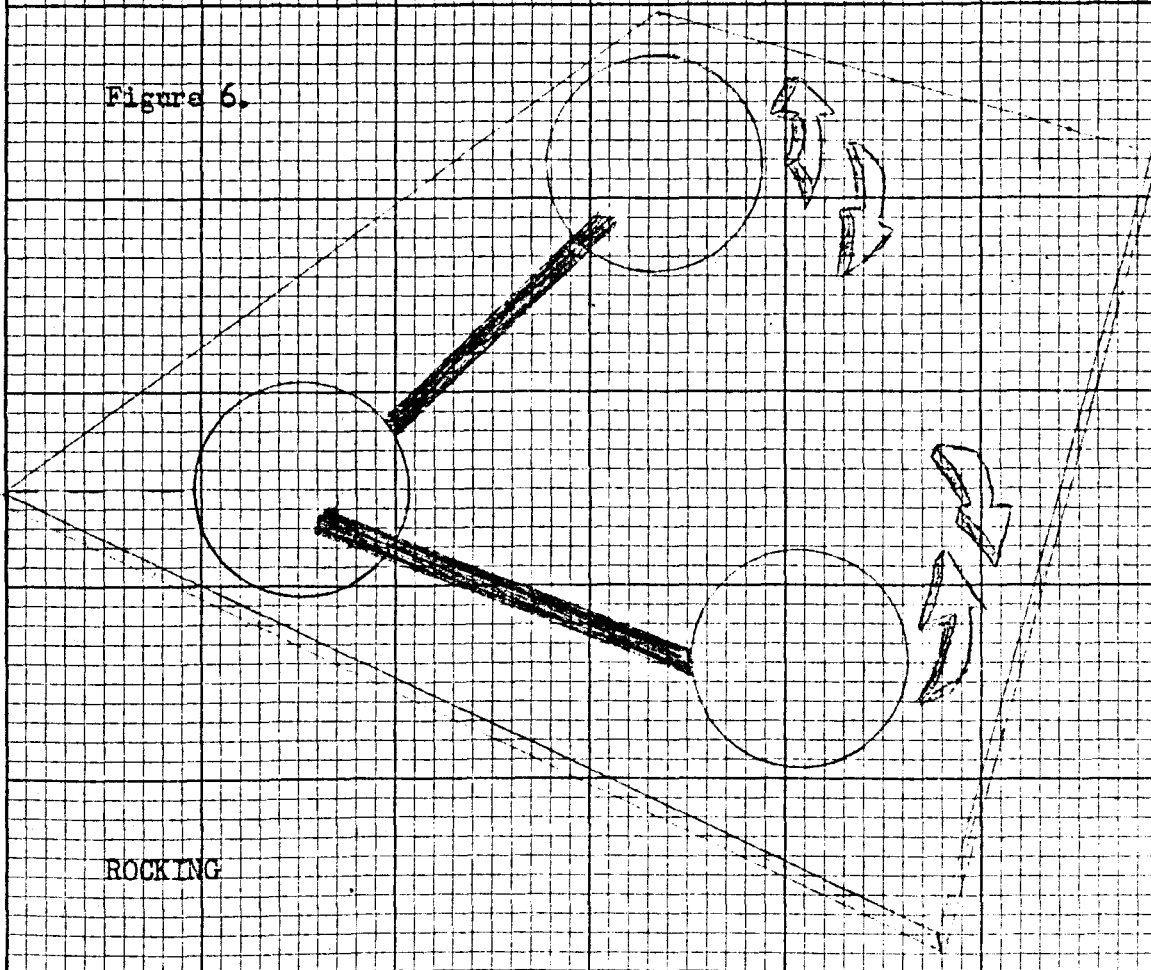
NON-LINEAR BENDING
(SCISSORING)

Figure 5.



WAGGING

Figure 6.



ROCKING

TOISEING

Figure 7.

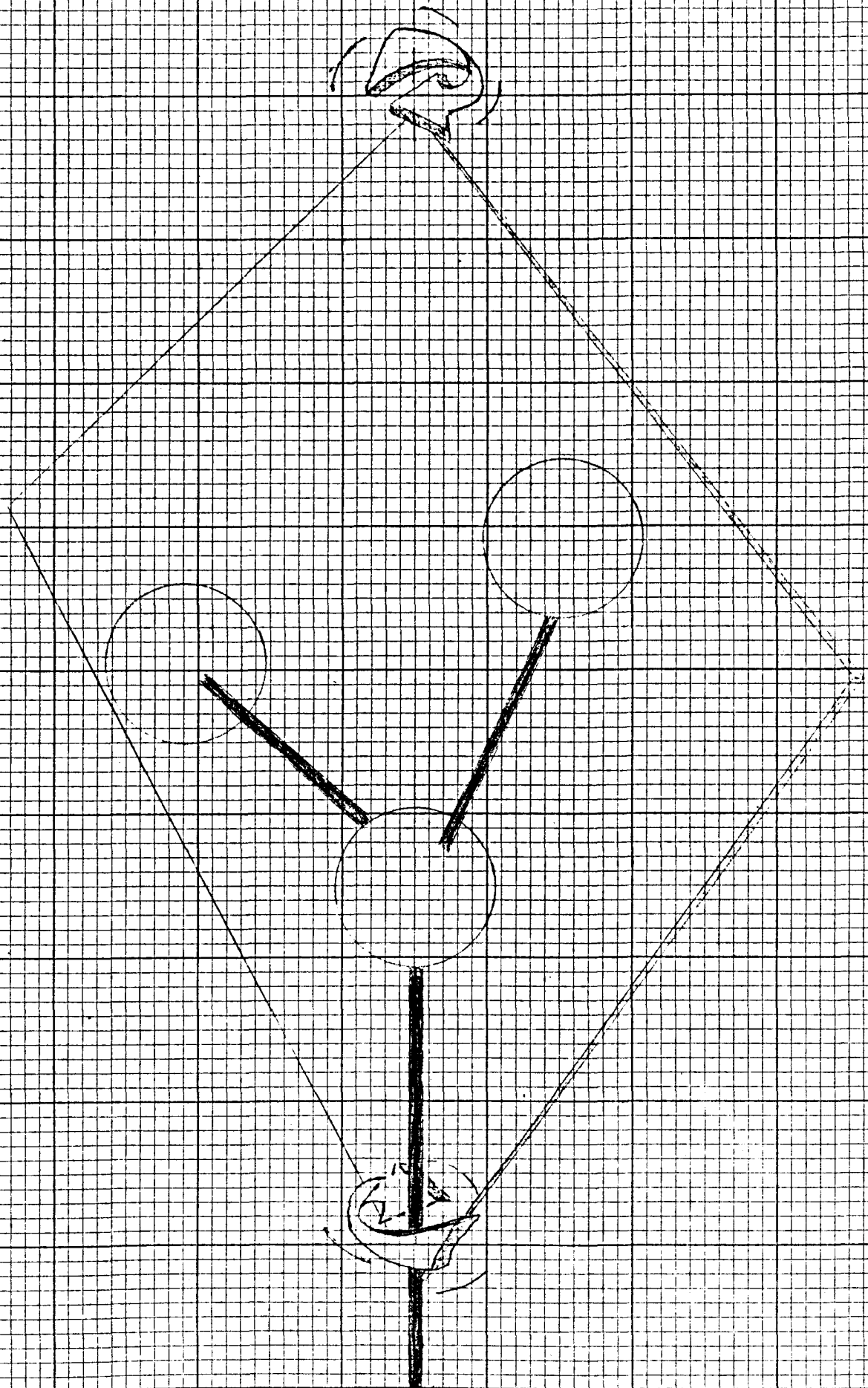
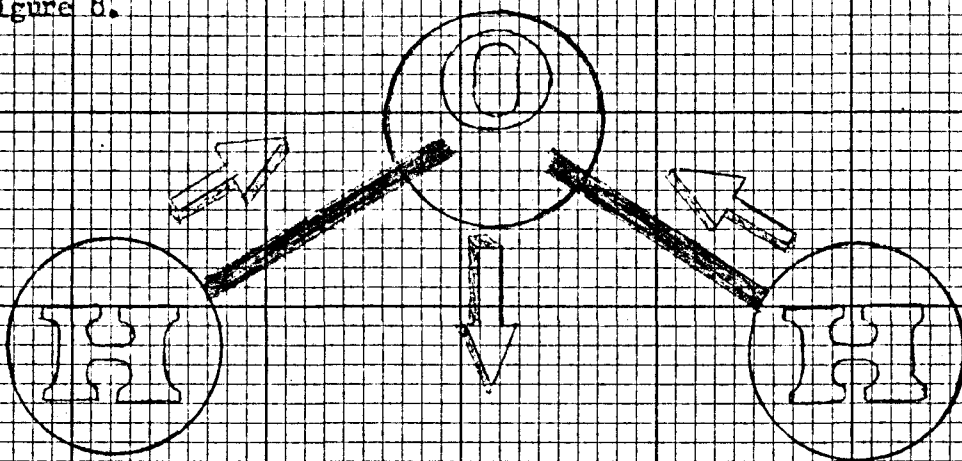
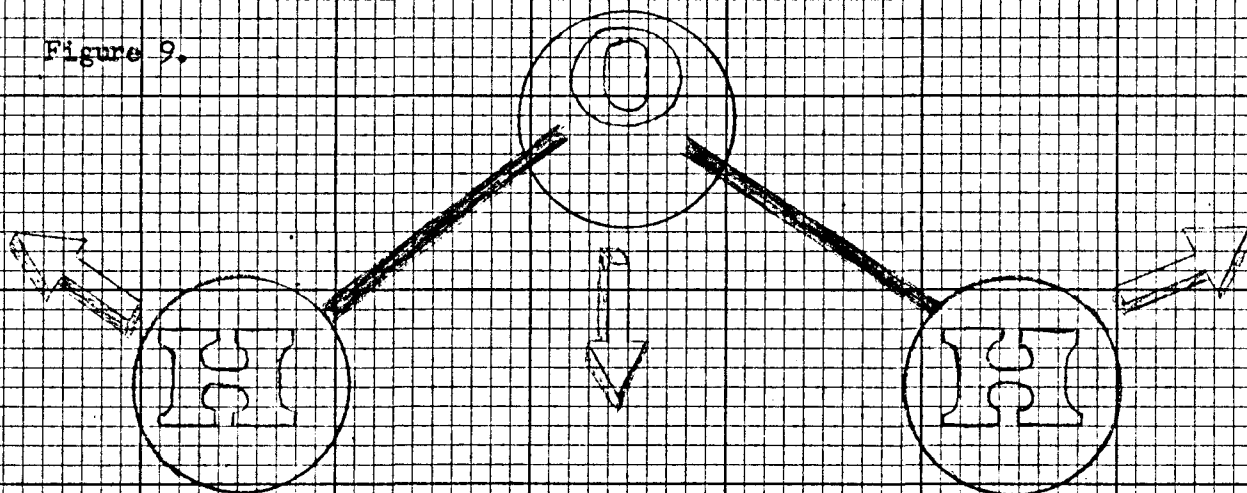


Figure 8.



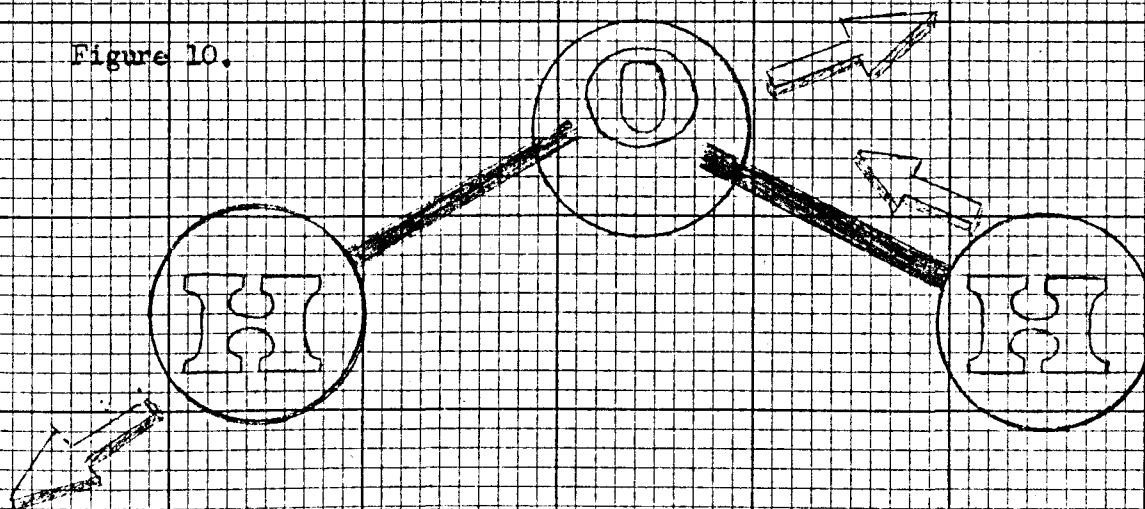
THE SYMMETRIC STRETCHING OF THE WATER MOLECULE

Figure 9.



THE SCISSORING DEFORMATION OF THE WATER MOLECULE

Figure 10.



THE ASYMMETRIC STRETCHING OF THE WATER MOLECULE

asymmetric stretching (Figure 10), which has a frequency ν_3 . Diagramming the vibrations in this way implies that the frequency ν_1 depends entirely on a stretching force constant, k_1 , while the scissoring fundamental, ν_2 , depends entirely on a scissoring force constant, k_2 ; and that there is no contribution of k_2 to the force constant that determines ν_1 , and vice versa. (32) This idealized concept of completely isolated stretching and deformation vibrational modes cannot be applied successfully to all the structural units of large (polyatomic) molecules, since it has been found that some structural units have vibrational modes which are rather easily perturbed by interactions from those of adjacent units in the molecule.(4) There are structural groups, however, which retain some of their characteristic vibrational modes throughout a large number of compounds, and these modes are the true "characteristic frequencies" for the structural group. When a particular mode can be associated with a definite group, it can be used for identification. Examples of characteristic frequencies for a large number of structural groups have been tabulated in the literature (4, 7, 13, 22, 26, 32), and are available for analyzing the infrared spectra of specific compounds for the presence of these groups.

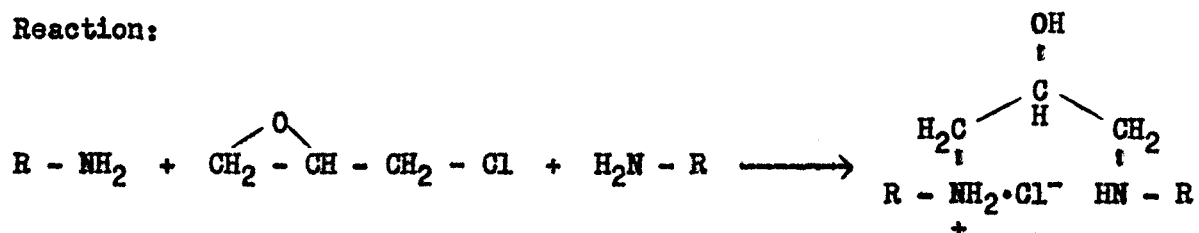
III. EXPERIMENTAL PROCEDURE

A. SYNTHESIS AND PURIFICATION

The procedure for the synthesis of the compounds of Table I was suggested originally by Pierce and Wotiz (25) and later modified slightly by O'Rear (23) and Jackson (15). For the compounds of Table I which were prepared by Davis (9) and Briel, the procedure used is outlined below.

Preparation of the Diamine Ligands

Reaction:



A solution of two moles of the amine in 300 ml. of absolute ethanol was placed in a one liter 3-neck flask. One of the small side necks was fitted with a thermometer which was immersed in the solution, the other with a separatory funnel containing a solution of one mole of epichlorohydrin in 150 ml. of absolute ethanol. The large center neck was adapted to a reflux condenser, above which was a cold trap for any of the reaction mixture which might be expelled from the flask during an especially vigorous moment in the reaction. To keep the temperature of the reaction mixture below 30°C, the flask was partially immersed in a water bath. Magnetic stirring of the reaction mixture was maintained throughout the entire course of the reaction.

The solution of epichlorohydrin was added by single drops over a period of two hours. The mixture was then allowed to stand overnight (with stirring), after which warm water was slowly added to the bath until the mixture began to reflux gently. The water bath was replaced by a heating

mantle and refluxing was continued for eight hours. The reaction mixture was cooled and transferred to another vessel (Figure 11) for the preparation of the dihydrochloride salt.

It was noted that when the reaction was initiated with the temperature of the solution at 25°C, considerable amounts of heat were evolved after the first half-hour, and ice had to be added to the bath to keep the temperature below 30°C; but if the solution of the amine were cooled below 15°C before beginning the addition of the epichlorohydrin, little change occurred in the temperature during the entire addition of the reagent. However, when such a mixture was then allowed to warm to 25°C, the evolution of heat became spontaneous and generally rather violent. Consequently, the reactions were usually run with the bath temperature maintained between 25°--30°C, until sufficient time had elapsed to permit safe refluxing.

Preparation of the Hydrochlorides

The classical procedure for preparing the hydrochlorides of amines involves passing a stream of anhydrous hydrogen chloride directly into a solution of the base in a non-polar solvent (e.g., ether or benzene), so that the highly-polar salt which is formed will precipitate (28). For the alkanolamines, Fuson recommends 1-propanol as a better solvent for the more polar bases (28); and it was found that the greatly enhanced polarity of the polyhydroxyamines required absolute ethanol (methanol was preferable for 2-amino-2-hydroxymethyl-1,3-propanediol) as the solvent for this reaction. A distinct disadvantage of these polar solvents, however, was that the hydrochlorides were generally sufficiently soluble to remain in solution. To force precipitation of the salts, small amounts of absolute

ether were added until a faint turbidity was produced in the solution. Then, the reaction vessel (Figure 11) was placed in an ice bath and the passage of the gas was resumed until crystals were formed.

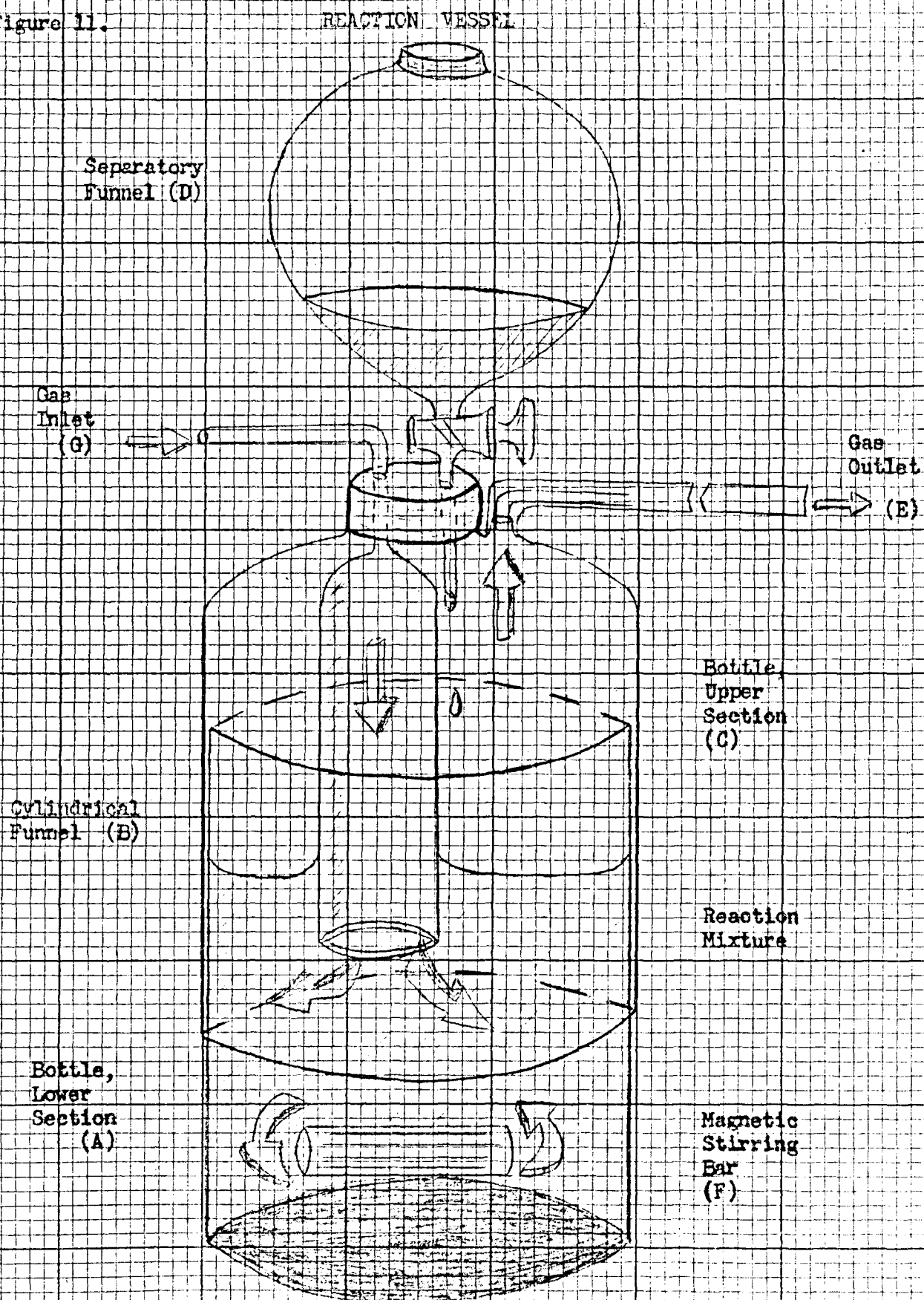
Since most of these salts were found to be quite hygroscopic, it was necessary to conduct this reaction with a minimum exposure to atmospheric moisture. The crystals, which showed a tendency to mat, were difficult to remove from an ordinary flask with a small neck; consequently, a closed vessel with a wide mouth was desired. An inexpensive, but highly satisfactory, vessel (Figure 11) was constructed from two 500 ml. polyethylene wash bottles (A) and (C), a cylindrical funnel (B), and a separatory funnel (D). The bottom was removed from one of the polyethylene bottles and the top from the other, so that the pair could be put together to form a closed vessel, which was easily opened to remove the salt.

When the reaction was complete, the product was filtered with suction through a fine sintered-glass disc. The crystals were washed rapidly with several portions of absolute ether and transferred to a vacuum desiccator for storage until recrystallization.

Purification of the Compounds

The hydrochlorides of the amines of Table II were recrystallized to constant melting point. The crude product from the reaction was dissolved in 2-butanol by boiling the mixture until all of the solid had gone into solution. The solution was chilled in an ice bath and the crystals which were obtained were filtered with suction through a fine sintered-glass disc and washed with several portions of absolute ether. The purified compounds were stored in a vacuum desiccator until the spectra were taken.

Figure 11.



B. INFRARED TECHNIQUE

The potassium bromide disc technique (30) was used to prepare samples of the hydrochlorides for infrared analysis. The discs were prepared by the following procedure.

One gram of spectroquality potassium bromide (powder) was weighed on an automatic electric balance and transferred to a stainless-steel ball-milling capsule. Five tenths of a milligram of the hydrochloride was added to the capsule, and the mixture was ground in a mechanical shaker for ten minutes. After grinding, 200.0 mg. of the mixture was transferred to the pellet die, and a high vacuum was applied for five minutes to remove volatile impurities (viz., water, ether, or 2-butanol). Without interrupting the vacuum, a pressure of 10,000 lbs./in.² was applied to the plunger of the die by means of a hydraulic press. After fifteen minutes the pressure was released, the vacuum was broken slowly, and the disc was placed on a special mount in the Perkin-Elmer Model 21 infrared spectrophotometer.

A distinct advantage of this technique is that the sample discs are permanent and can be stored conveniently. Nevertheless, it was found that even in an evacuated desiccator, the spectra of the more hygroscopic salts studied tended to lose their reproducibility after a month. However, these discs could be ground, dried in a vacuum oven to remove the sorbed water, and re-pressed, giving spectra which were essentially the same as the originals (taken before storage). Most of the discs can still be made to yield spectra which are good reproductions of those first taken.

C. CODING OF SPECTRAL DATA

The IBM 1620 digital computer was used to make a rapid examination of the experimental spectral data for each pertinent group frequency which was found in the literature. In this way, all of the experimental data could be examined for the presence of a specific group frequency, and many characteristic frequencies could be checked in a comparatively short period of time.

A system of coding the spectral data onto punched cards was needed, before the computer could produce the lists of the bands in the experimental spectra which were comparable to the literature group frequencies. The systems which are used by compilers of the spectral reference literature generally index only the major peaks in the absorption bands. However, since the bands of the experimental spectra were often composed of other points of significance (i.e., shoulders), it was decided to use a system of coding which could index all maxima (peaks and shoulders) which were found in the absorption bands. For each of the maxima indexed, the following specifications were recorded on an IBM data card:

1. The abscissa of the point--its spectral wavelength in microns. This variable (designated "A") was recorded as a four digit number, with a decimal point implied between the second and third digits. (The computer was instructed to insert a decimal point at this position.)
2. The ordinate of the point--its absorbance value in (logarithmic) absorbance units. This variable (designated "B") was recorded as a three digit number with the decimal point implied between the first and second digits.
3. The spectral width of the maximum. This variable (designated "C") was measured by counting the number of chart divisions which were

along a horizontal line segment that was 0.01 absorbance unit below the absorbance of the maximum and enclosed by the curve. The width in microns could be obtained, since each of the divisions represented 0.05 μ . However, a simplification was possible in reporting the value of this variable: it was observed that for most of the experimental maxima, the curve appeared Gaussian at this small distance from the peak. Therefore, the number of divisions was multiplied by 0.025 and reported as the abscissa of the maximum plus the spectral width, and the abscissa of the maximum minus the spectral width ($A \pm C$). The variable "C" is not intended to represent the accuracy or the precision of the measurement of the variable "A"; but the location of two additional points on the curve at a fixed distance below the peak. The absolute value of this variable is directly related to the spread of the curve in the region of the point of maximum absorbance, and it indicates the sharpness of the peak.

4. The type of maximum. Since the shoulder and the peak maxima of a band are recorded as separate points of significance (on different IBM data cards), an arbitrary classification system was devised in which the type of a particular maximum could be specified. Nine distinct types of maxima were idealized from the experimental spectra, each of these types being represented in the coding system by a different value (1--9) of a single digit variable, "I". The nine idealized types of maxima were defined as follows:

TYPE #1: A peak-maximum which has no shoulder-maxima associated with it and which is not a branch of a multiple-peak band. The Type #1 maximum is an isolated peak and it does not occur in a band with any other of the idealized

types. A Type #1 maximum is shown in Figure 12.

TYPE #2: A shoulder-maximum which lies on the low-wavelength (left) side of the peak and which has the lowest absorbance value of any of the shoulders on this side.

A Type #2 maximum is shown in Figures 13, 14, 15, and 20.

TYPE #3: A shoulder-maximum which lies on the low-wavelength (left) side of the peak and which has an absorbance value higher than that of the shoulder-maximum immediately preceding it. A Type #3 maximum is shown in Figures 14 and 20.

TYPE #4: A peak-maximum which has shoulder-maxima associated with it, but which is not a branch of a multiple-peak band.

A Type #4 maximum is shown in Figures 13--17.

TYPE #5: A shoulder-maximum which lies on the high-wavelength (right) side of the peak and which has an absorbance value higher than that of the shoulder-maximum immediately following it. A Type #5 maximum is shown in Figures 16 and 20.

TYPE #6: A shoulder-maximum which lies on the high-wavelength (right) side of the peak and which has the lowest absorbance value of any of the shoulders on this side.

A Type #6 maximum is shown in Figures 15--17, and 20.

TYPE #7: A peak-maximum which is the lowest-wavelength branch (left branch) of a multiple-peak band (i.e., a single absorption band in which several separate peaks can be distinguished clearly, but lie so close together that the "valley" between any two of them lies high above the

base line). A rule was made to distinguish between adjacent peaks which could be considered disjunct (in separate absorption bands) and those which could be considered conjunct (in the same absorption band). The rule states: If the minimum of the valley between a pair of adjacent peaks lies at a height which is less than half the height of the lower maximum, the pair is disjunct. The Type #7 maximum is shown in Figures 18 and 20.

TYPE #8: A peak-maximum which is an intermediate branch of a multiple-peak band, which has more than two peaks. The Type #8 maximum may either be shouldered or unshouldered. A Type #8 maximum is shown in Figures 19 and 20.

TYPE #9: A peak-maximum which is the highest-wavelength branch (right branch) of a multiple-peak band. The Type #9 maximum may either be shouldered or unshouldered. A Type #9 maximum is shown in Figures 18--20.

TYPE #0: An exceptional maximum which will not fit into one of the other type categories. (It has not been used in classifying any of the experimental maxima.)

5. The overall appearance of the curve in the region of the maximum. Although the spectral width was used to indicate the exact positions of two additional points on the curve at 0.01 absorbance unit below the indexed maximum, it was desirable to be able to describe the general appearance of the curve throughout this region. Six distinct

Figure 12. IDEALIZED BAND #1.
Showing Types of Maxima

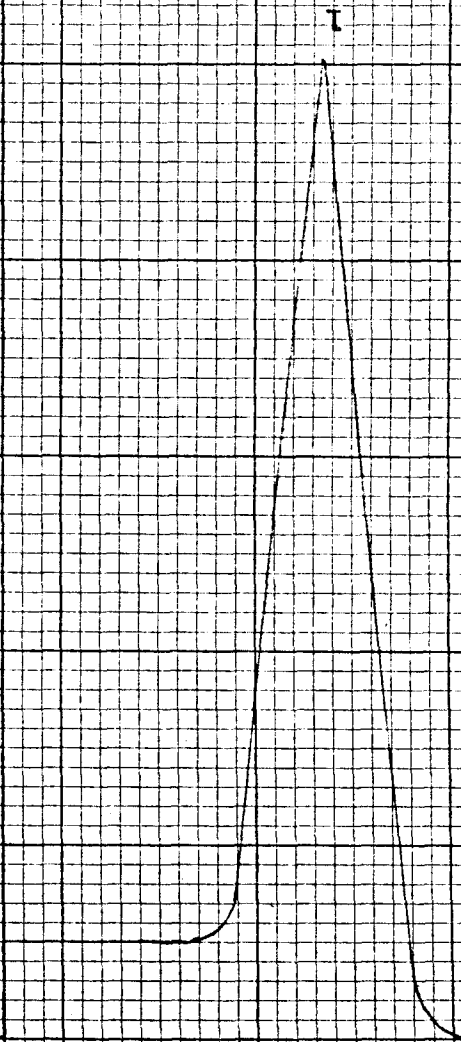


Figure 13. IDEALIZED BAND #2.
Showing Types of Maxima

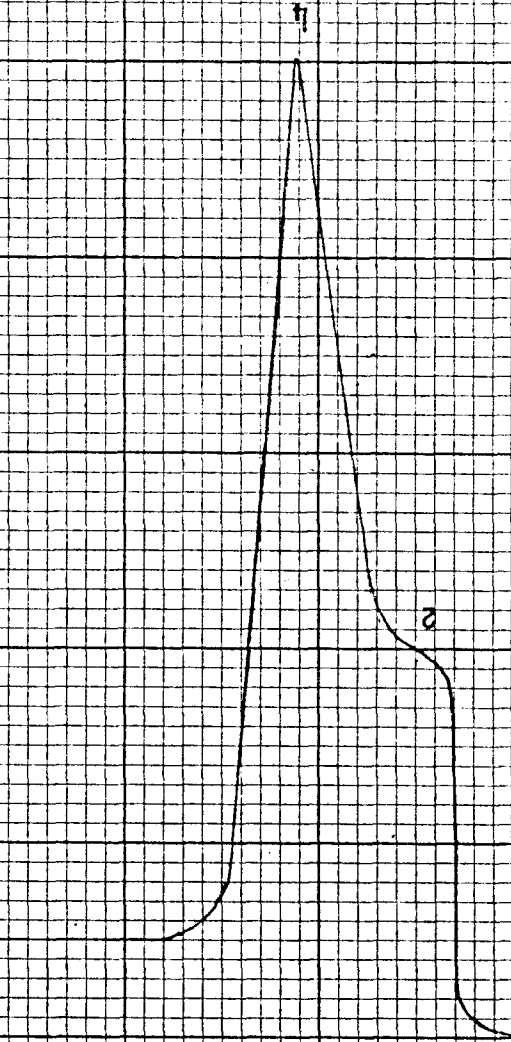


Figure 14. IDEALIZED BAND #3.
Showing Types of Maxima

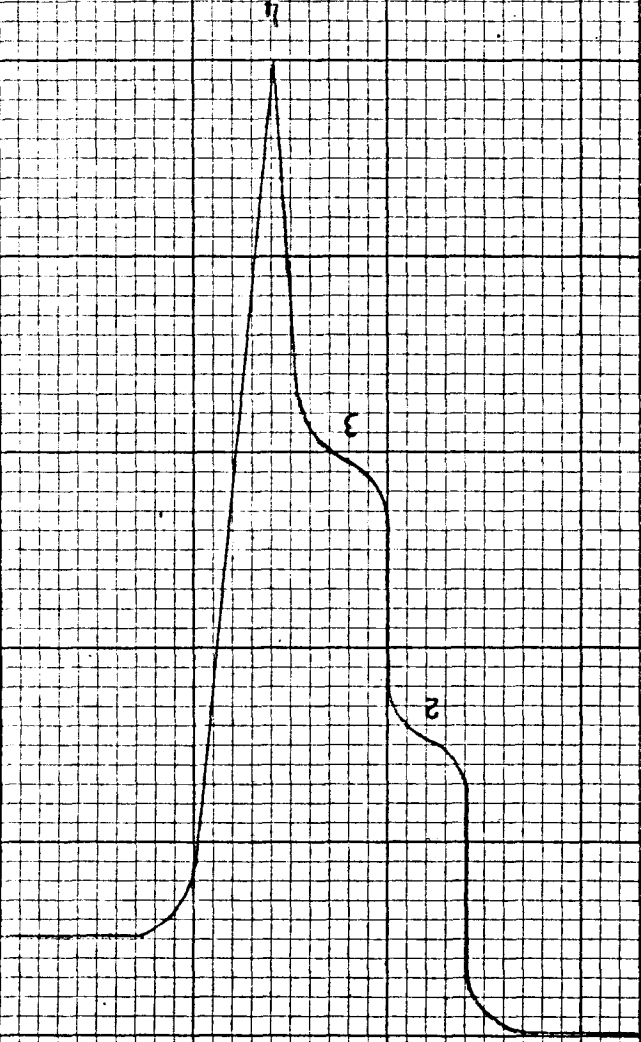


Figure 15. IDEALIZED BAND #1.
Showing Types of Maxima

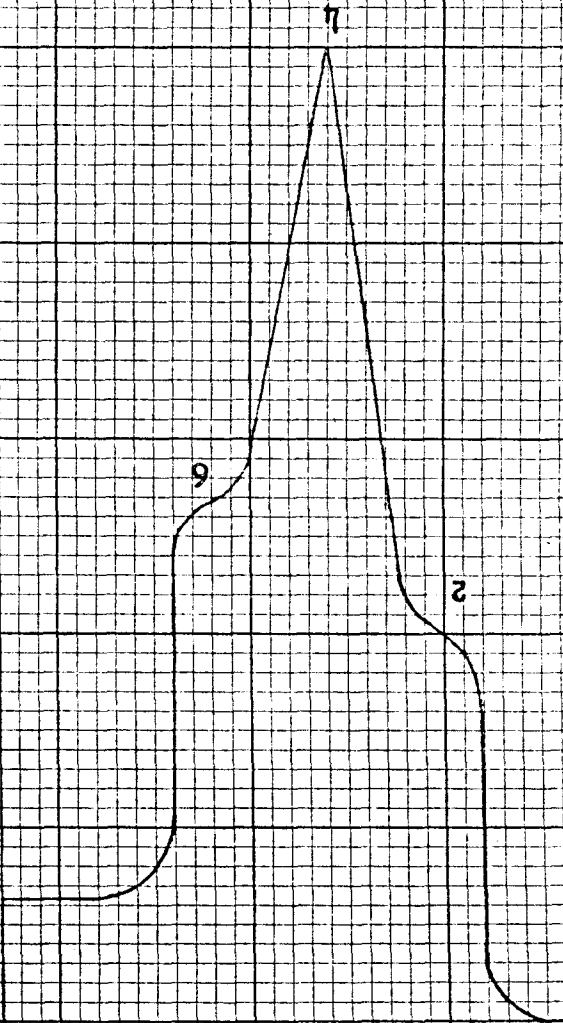


Figure 16. IDEALIZED BAND #5.
Showing Types of Maxima

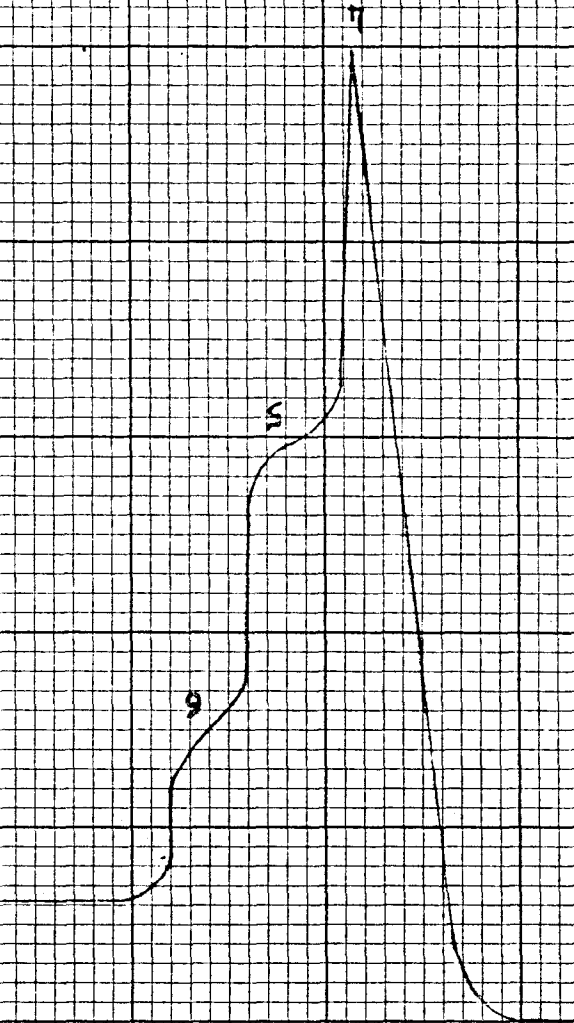


Figure 17. IDEALIZED BAND #6.
Showing Types of Maxima

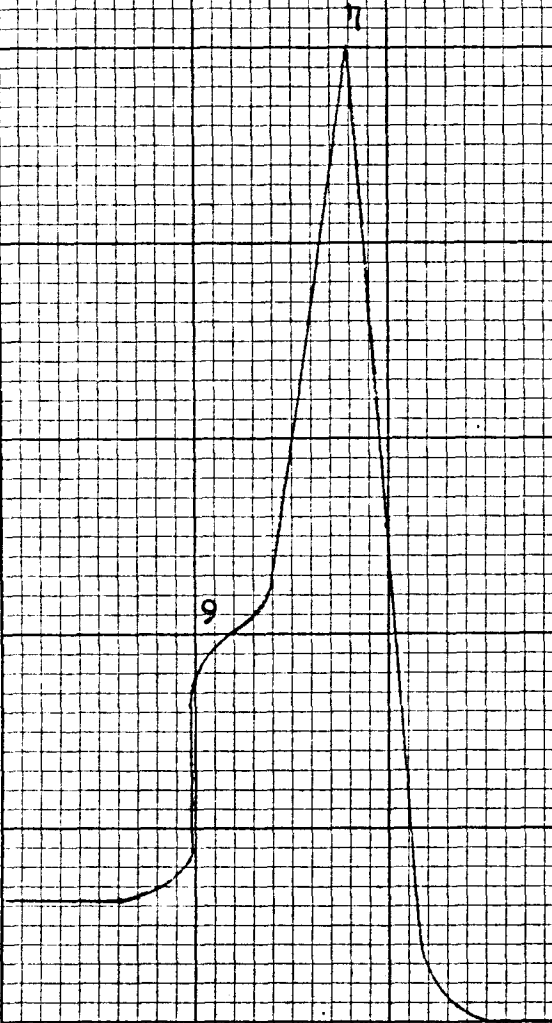


Figure 18. IDEALIZED BAND #7.

Showing Types of Maxima



Figure 19. IDEALIZED BAND #8.

Showing Types of Maxima

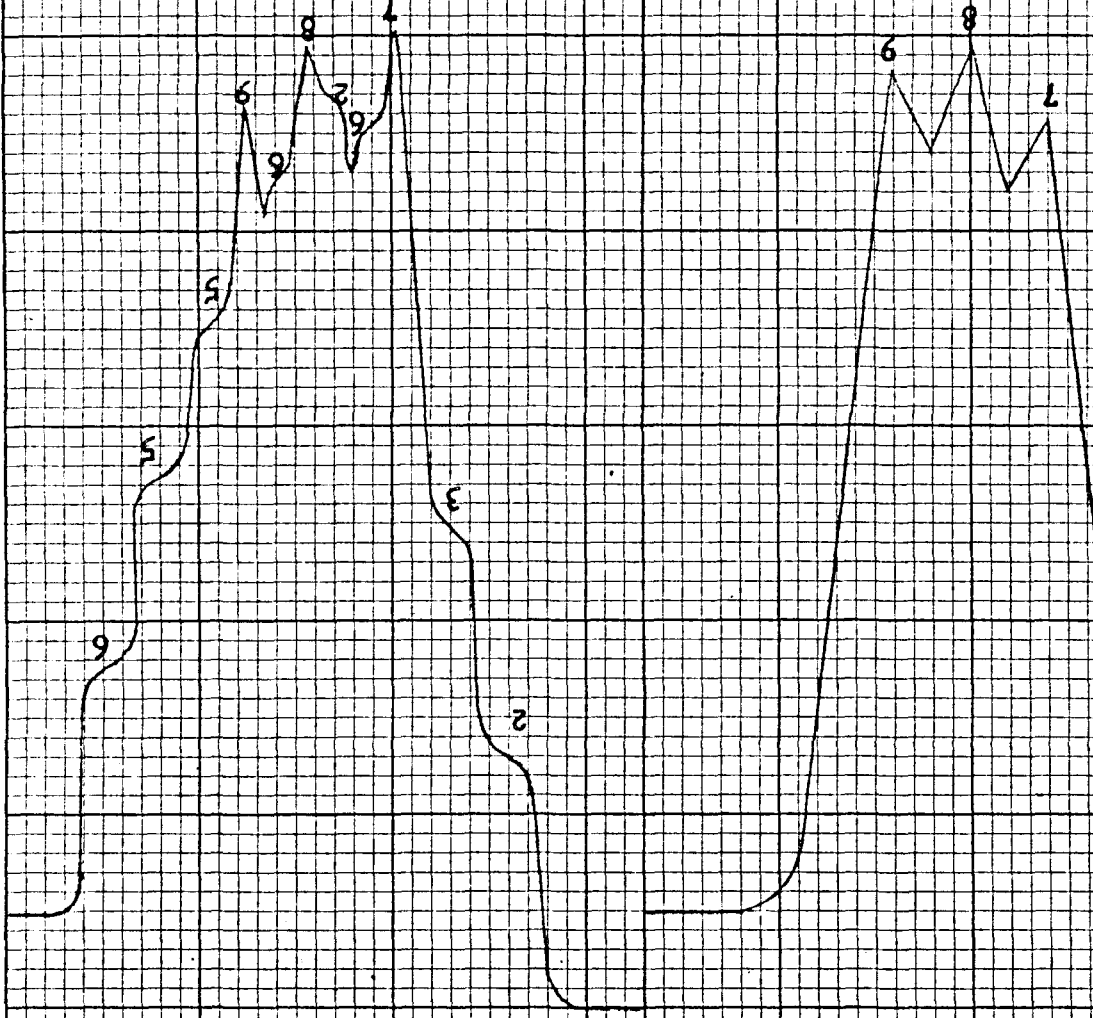
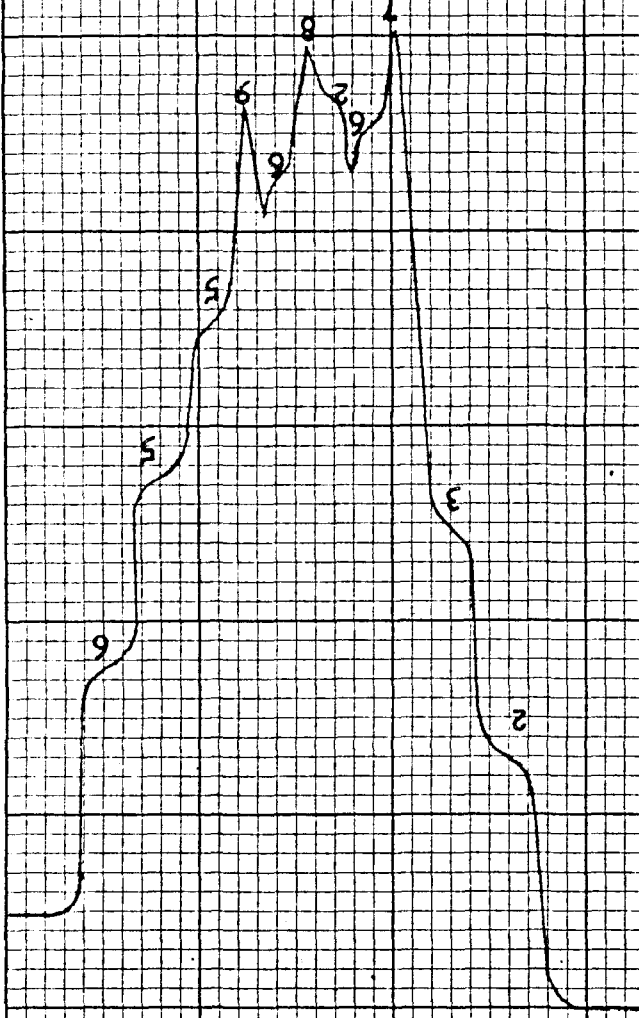


Figure 20. IDEALIZED BAND #9.

Showing Types of Maxima



shapes of maxima were idealized from the experimental curves, each different shape being represented in the coding system by a different value (1--6) of a single digit variable, "M". This classification is the most subjective indication of the data, but it is useful in being able to describe the appearance of the curve. The six idealized shapes are described as follows:

- SHAPE #1: The Inflection Point--a shoulder-maximum of very small spectral width. This shape of maximum (Figure 21) usually appears as a change in the slope of the vertical portion of the spectral curve. It is the least significant shape of maximum which was indexed.
- SHAPE #2: The Plateau--a peak, or a shoulder-maximum of rather large spectral width, which appears essentially flattened in the region of the maximum. (Figure 22)
- SHAPE #3: The Small Finger--a minor (low absorbance) peak, which appears distinctly rounded in the region of the maximum. (Figure 23)
- SHAPE #4: The Large Finger--a major (high absorbance) peak, which appears distinctly rounded in the region of the maximum. (Figure 24)
- SHAPE #5: The Small Spike--a minor (low absorbance) peak, which comes to a sharp point in the region of the maximum. (Figure 26)
- SHAPE #6: The Large Spike--a major (high absorbance) peak, which comes to a sharp point in the region of the maximum. (Figures 21, 22, 23-b, 25, 26-b)

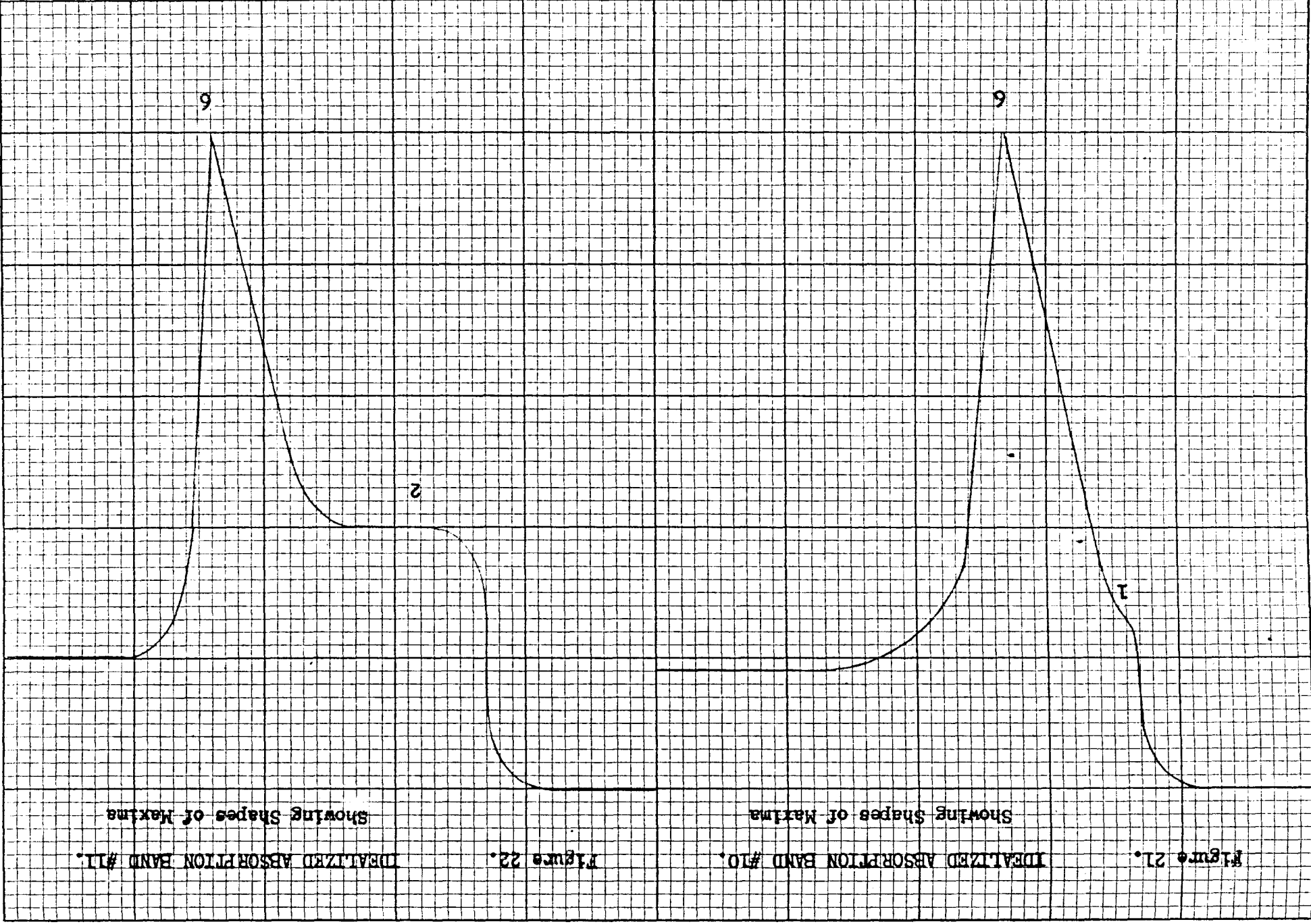


Figure 23 (a). IDEALIZED ABSORPTION BAND # 12.

Showing Shapes of Maxima

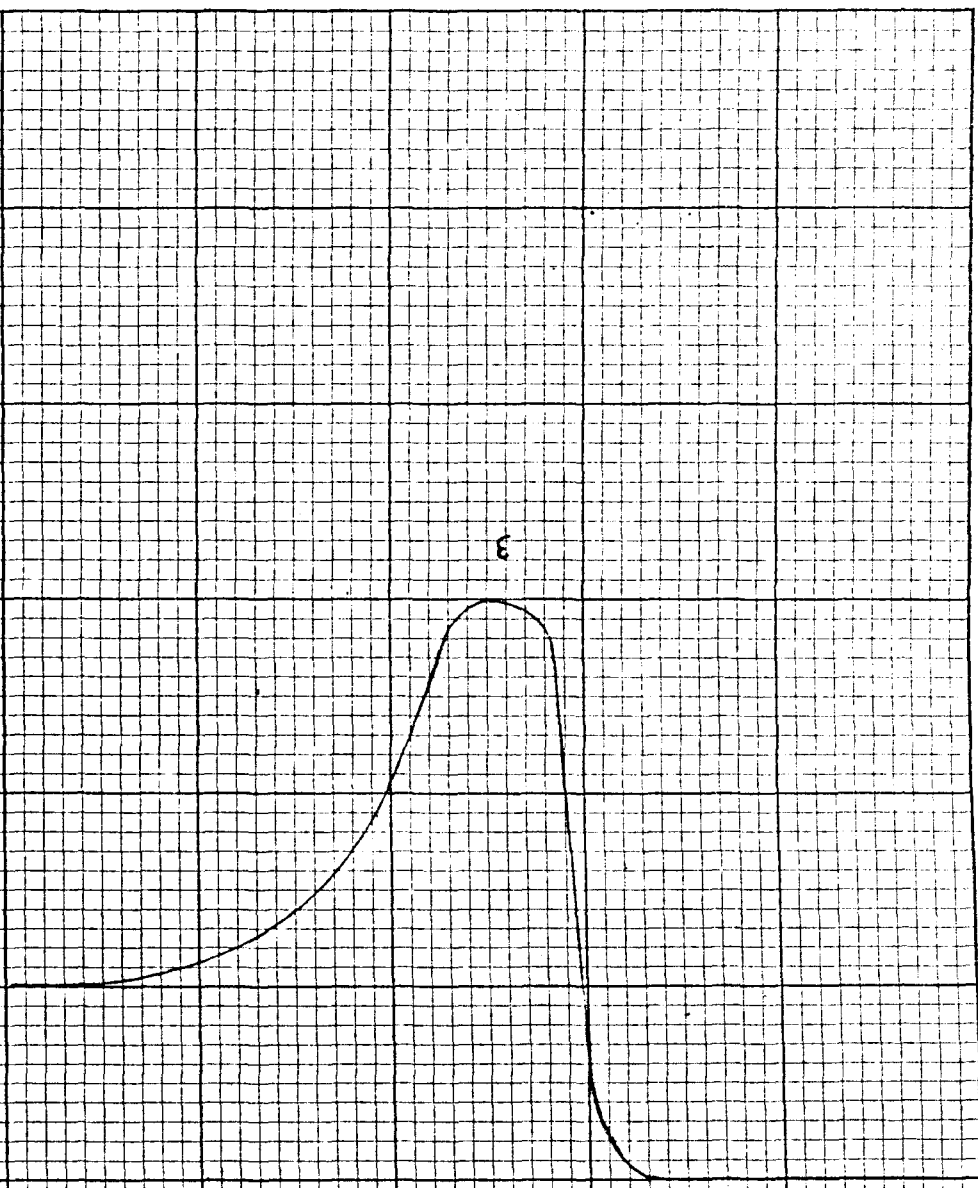


Figure 23 (b). IDEALIZED ABSORPTION BAND # 13.

Showing Shapes of Maxima

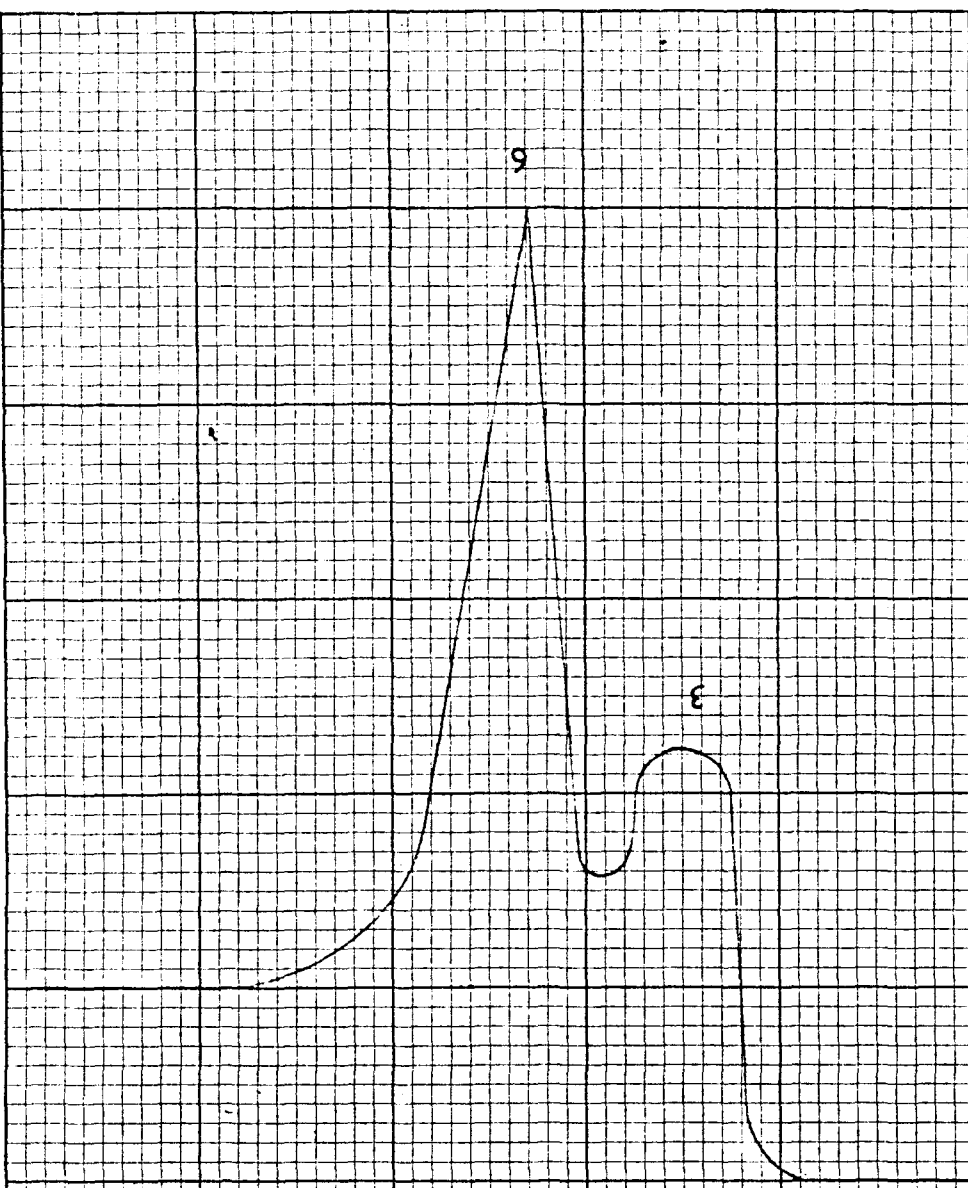


Figure 21. IDEALIZED ABSORPTION BAND #11.

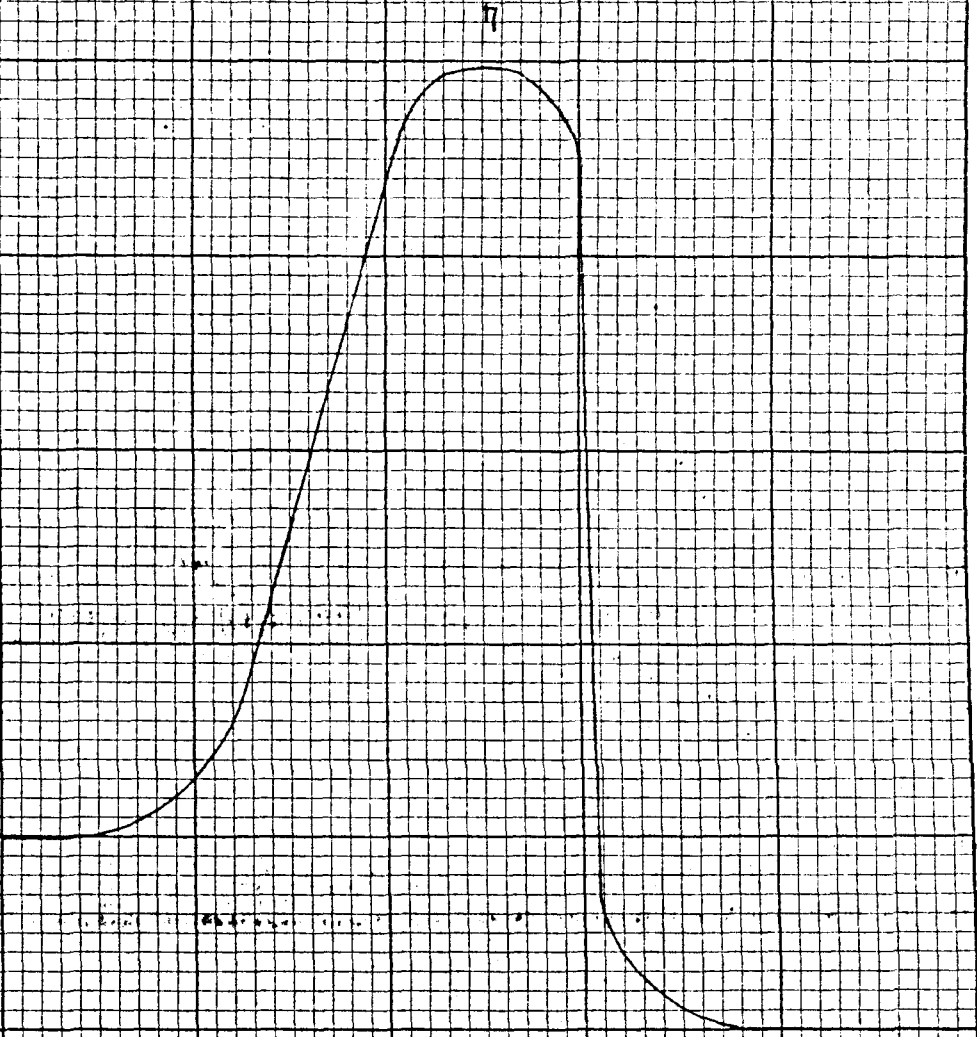


Figure 25.

IDEALIZED ABSORPTION BAND #15. Showing Shapes of Maxima

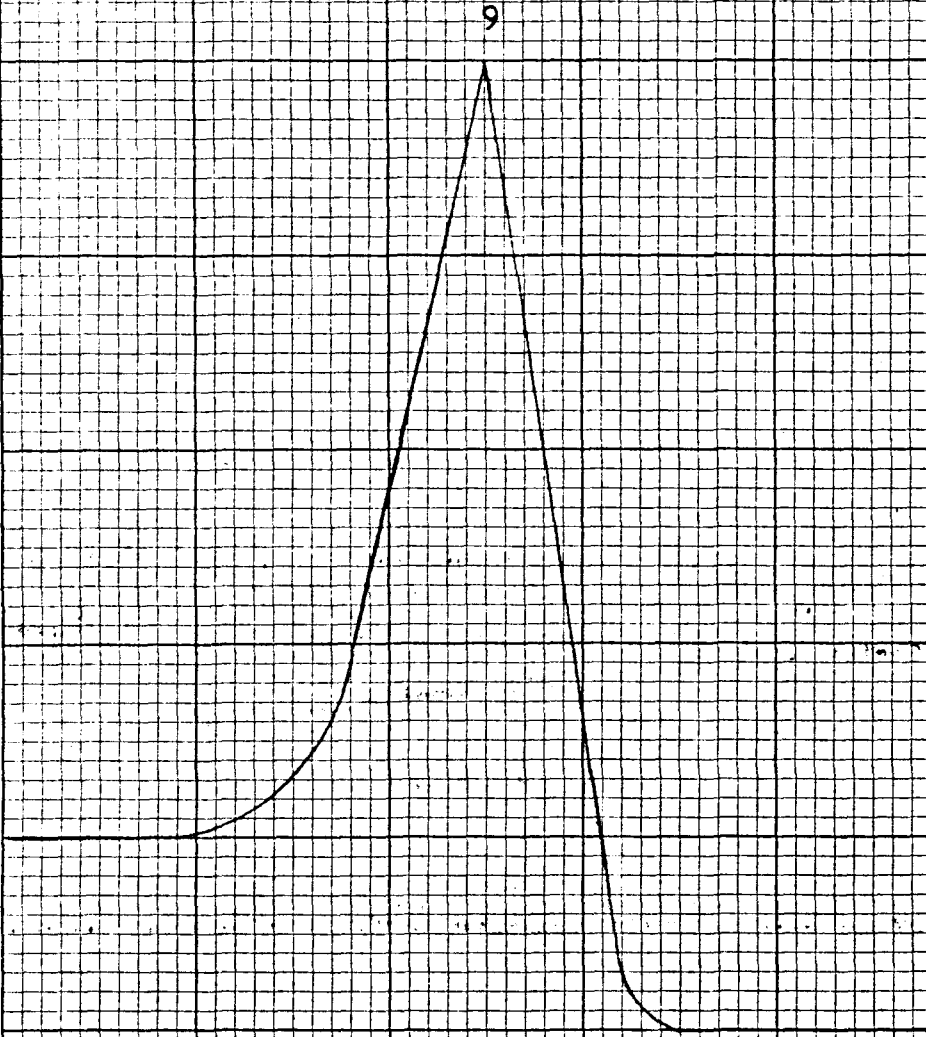


Figure 26 (a). IDEALIZED ABSORPTION BAND #16.

Showing Shapes of Maxima

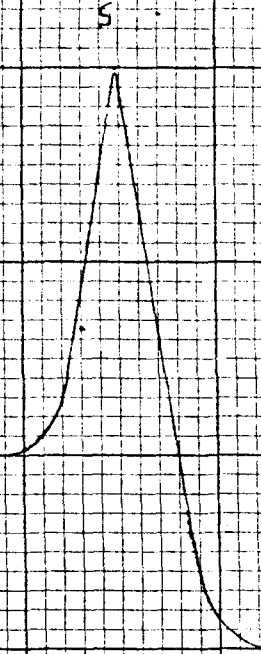
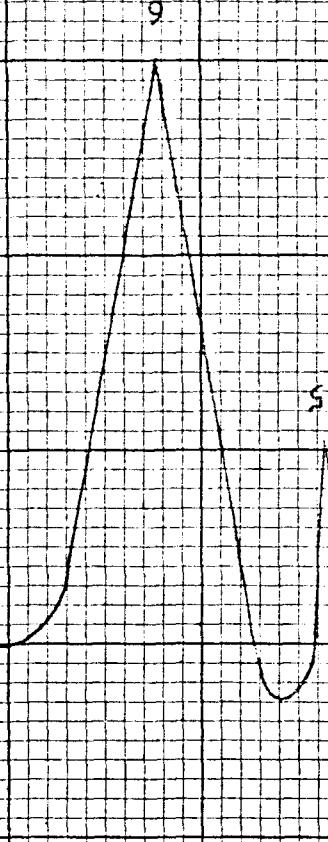


Figure 26 (b). IDEALIZED ABSORPTION BAND #17.

Showing Shapes of Maxima



6. The spectrum in which the maximum occurred was indicated by a combination of three variables, "I", "J", "K":

"I" indicated the code number of the compound (Tables I & II);

"J" indicated the number assigned to the specific spectral chart;

"K" indicated the number of a particular spectrum on the chart, counting down from the upper left corner of the sheet.

To indicate the beginning and end of the absorption bands, two single-digit variables were defined. If a band contained only an isolated peak, the particular combination of values for these variables ("LA" and "LB") was LA = 1, LB = 2. For the initial maximum of a band containing more than one peak, the combination was LA = 1; LB = 0; and each succeeding maximum in the band (except the last) was given the combination LA = 0, LB = 0 (unpunched). The last maximum of a band containing more than one peak was given the combination LA = 9, LB = 0.

To indicate the final maximum for each coded spectrum, the variable "N" was defined. For all maxima of a spectrum except the last, this variable had the value "0" (zero, unpunched); for the final maximum, the value of "N" was nine. In this way, the computer could detect the end of a spectrum when it occurred, which simplified the program considerably.

The Fortran source program, which was written to enable the IBM 1620 to correlate the positions of the absorption bands in the experimental spectra to the positions of the group frequencies found in the literature, appears on the next three pages. A block diagram of the interrelationships between the Fortran statements is shown in Figure 27.

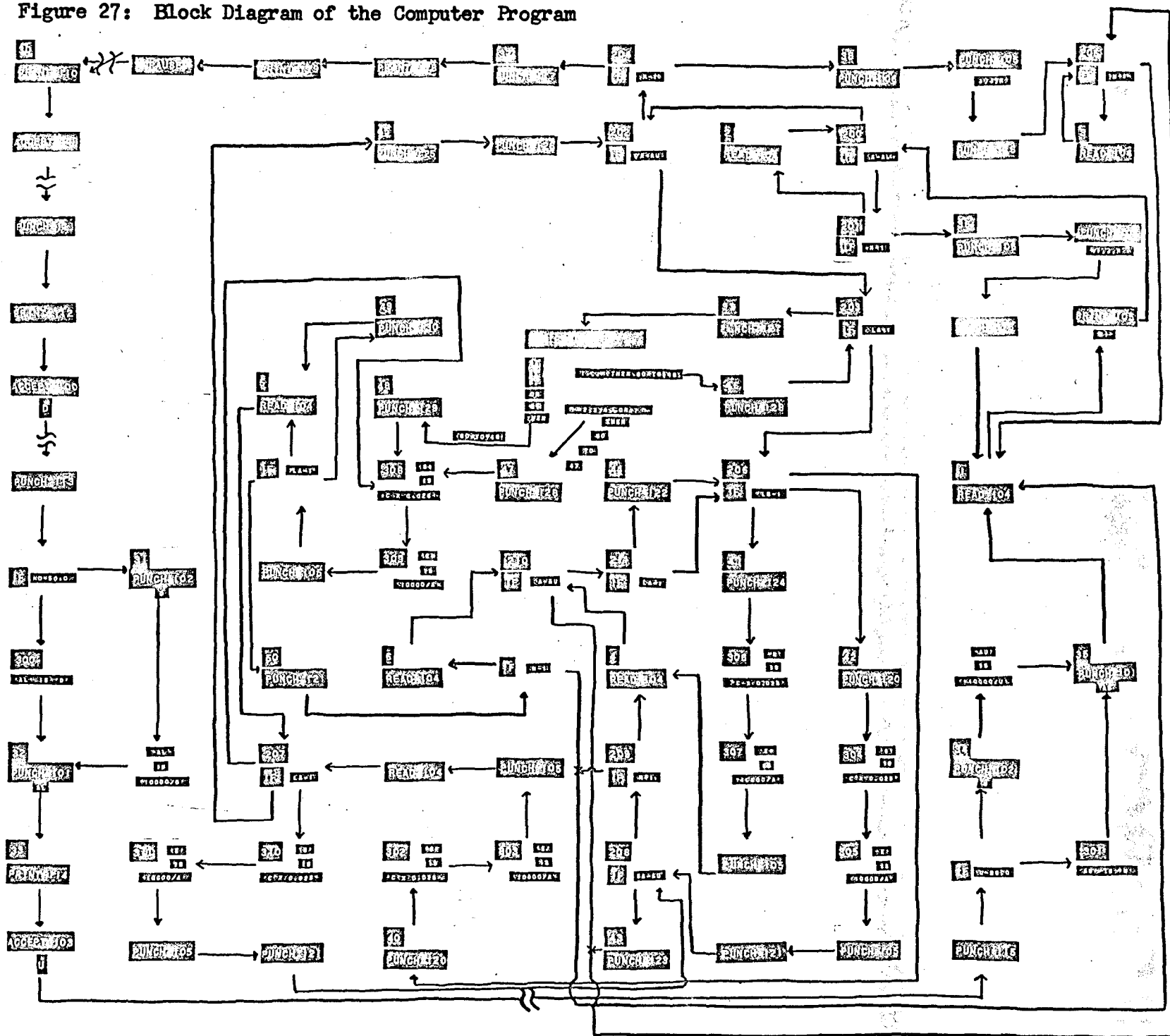
Fortran Source Program

```

30 PRINT 110
110 FORMAT(22HENTER FUNCTIONAL GROUP)
    ACCEPT 111
111 FORMAT(49H
    PUNCH 111
    PRINT 112
112 FORMAT(17HENTER LOWER LIMIT)
    ACCEPT 100, D
100 FORMAT (F8.2)
    PUNCH 113
113 FORMAT(40HLOWER LIMIT OF REGION BEING EXAMINED IS-)
    IF (D-50.) 300, 300, 31
    31 PUNCH 102, D
102 FORMAT (F8.1,6X,13H1/CENTIMETERS)
    AL=10.0**4/D
    GO TO 32
300 AL=D
    32 PUNCH 101, AL
101 FORMAT (F9.2,5X,07HMICRONS/)
    33 PRINT 114
114 FORMAT(17HENTER UPPER LIMIT)
    ACCEPT 103, U
103 FORMAT (F8.2)
    PUNCH 115
115 FORMAT(40HUPPER LIMIT OF REGION BEING EXAMINED IS-)
    IF (U-50.) 301, 301, 34
    34 PUNCH 102, U
    AU=10.0**4/U
    GO TO 35
301 AU=U
    35 PUNCH 101, AU
    1 READ 104, I,J,K,A,B,C,L,M,LA,LB,N
104 FORMAT(I4,I2,I1,3X,F4.2,F3.2,F2.1,I1,I1,8X,I1,I1,3X,I1)
    PRINT 105, I
105 FORMAT (I5,I3,I2,5X,F6.2,2X,F6.4,7X,F8.1,8X,F5.2,6X,I2,5X,I2)
200 IF (A-AL) 201, 202, 202
201 IF (N-1) 2, 2, 36
    2 READ 104, I,J,K,A,B,C,L,M,LA,LB,N
    GO TO 200
    36 PUNCH 106
106 FORMAT (/)
    PUNCH 105, I,J,K
    PUNCH 116
116 FORMAT (44HHAS NO PEAK, -S IN THE REGION BEING EXAMINED)
    GO TO 1
202 IF (A-AU) 203, 203, 204
204 IF (K-1) 37, 38, 38
    37 PUNCH 117
117 FORMAT(13HEND OF REGION//)
    PRINT 118
118 FORMAT (28HEND OF SEARCH IN THIS REGION)
    PRINT 119

```

Figure 27: Block Diagram of the Computer Program



IV. SPECTRA

Figure 28:
THE SPECTRUM OF
1,3-Diaminopropane dihydrochloride

Figure 29:
THE SPECTRUM OF
1,3-Diamino-2-propanol dihydrochloride
(002)

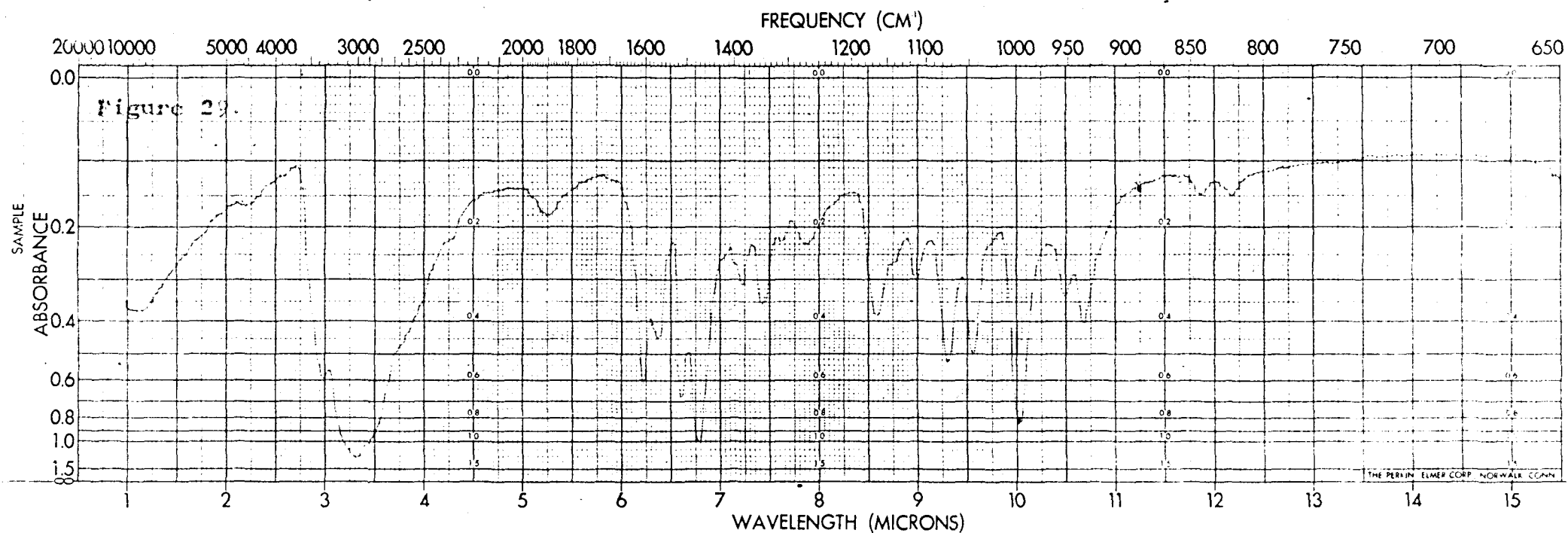
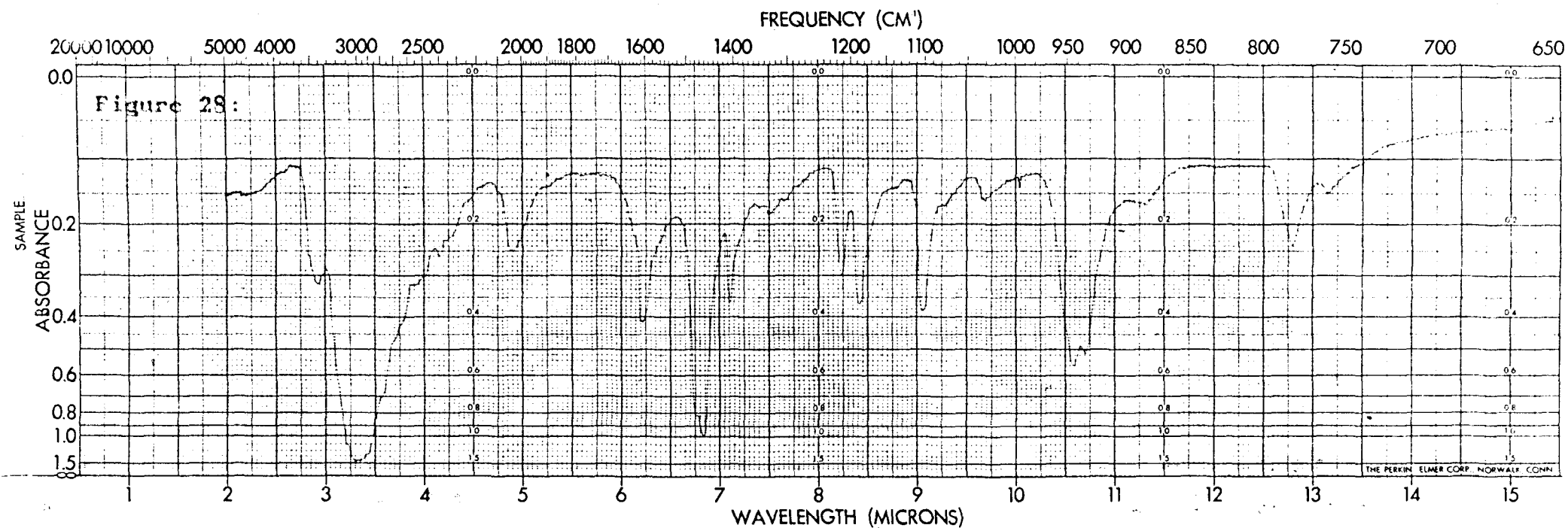


Figure 30:
THE SPECTRUM OF
2-Aminoethanol hydrochloride
(211)

Figure 31:
THE SPECTRUM OF
3,7-Diaza-1,5,9-nonanetriol dihydrochloride
(212)

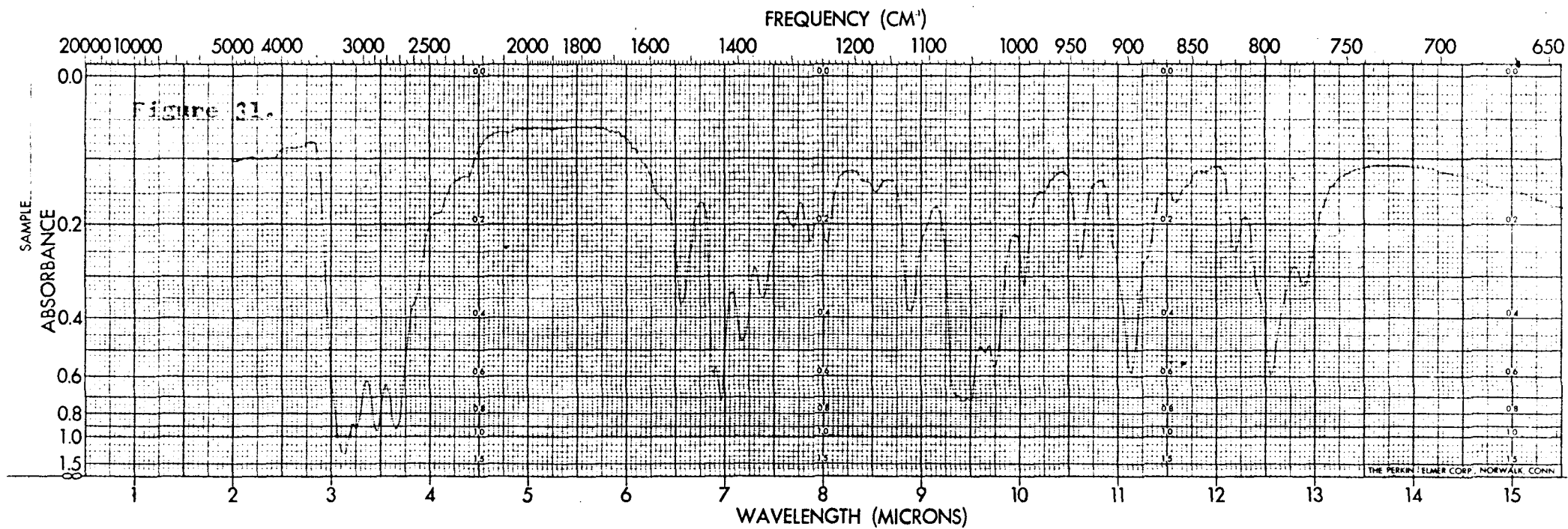
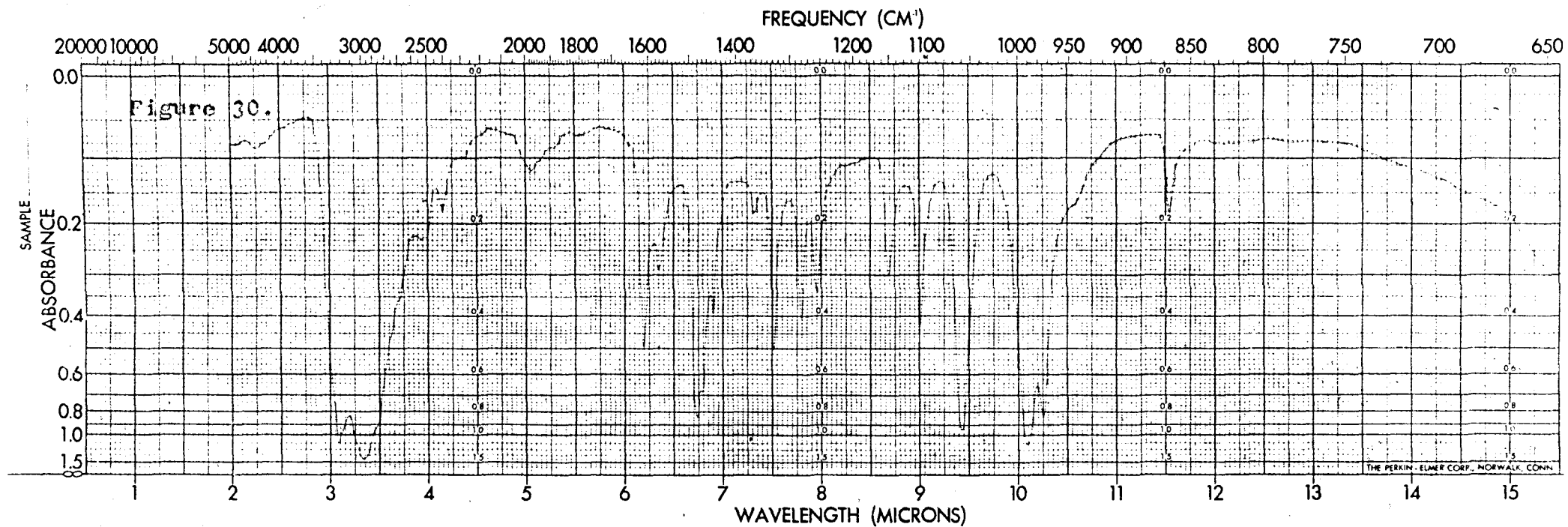


Figure 32:
THE SPECTRUM OF
2-Aminopropane hydrochloride
(301)

Figure 33:
THE SPECTRUM OF
2,8-Dimethyl-3,7-diaza-5-nonanol dihydrochloride
(302)

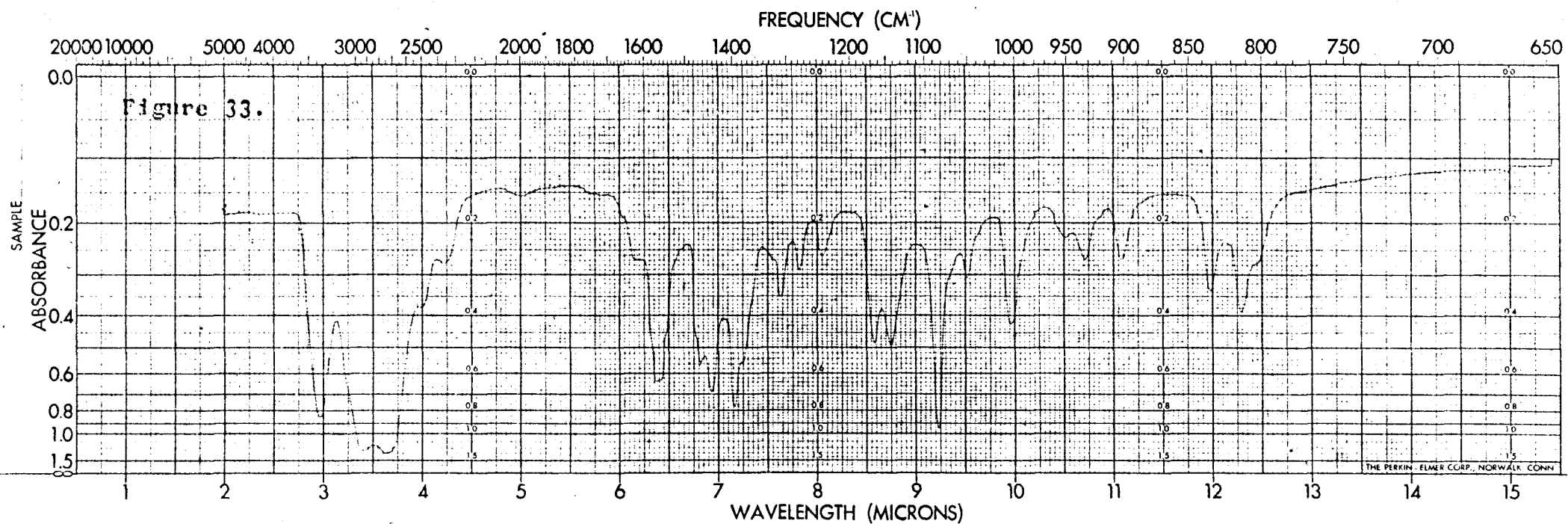
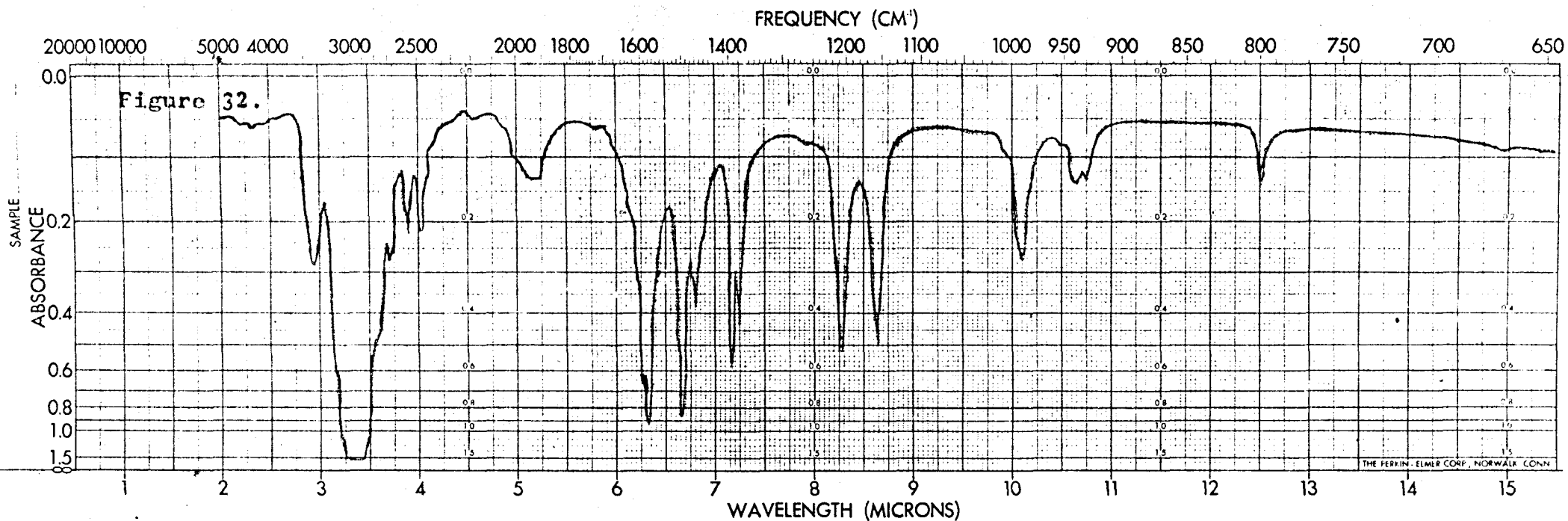


Figure 34:
THE SPECTRUM OF
2-Amino-1-propanol hydrochloride
(311)

Figure 35:
THE SPECTRUM OF
2,8-Dimethyl-3,7-diaza-1,5,9-nonanetriol dihydrochloride
(312)

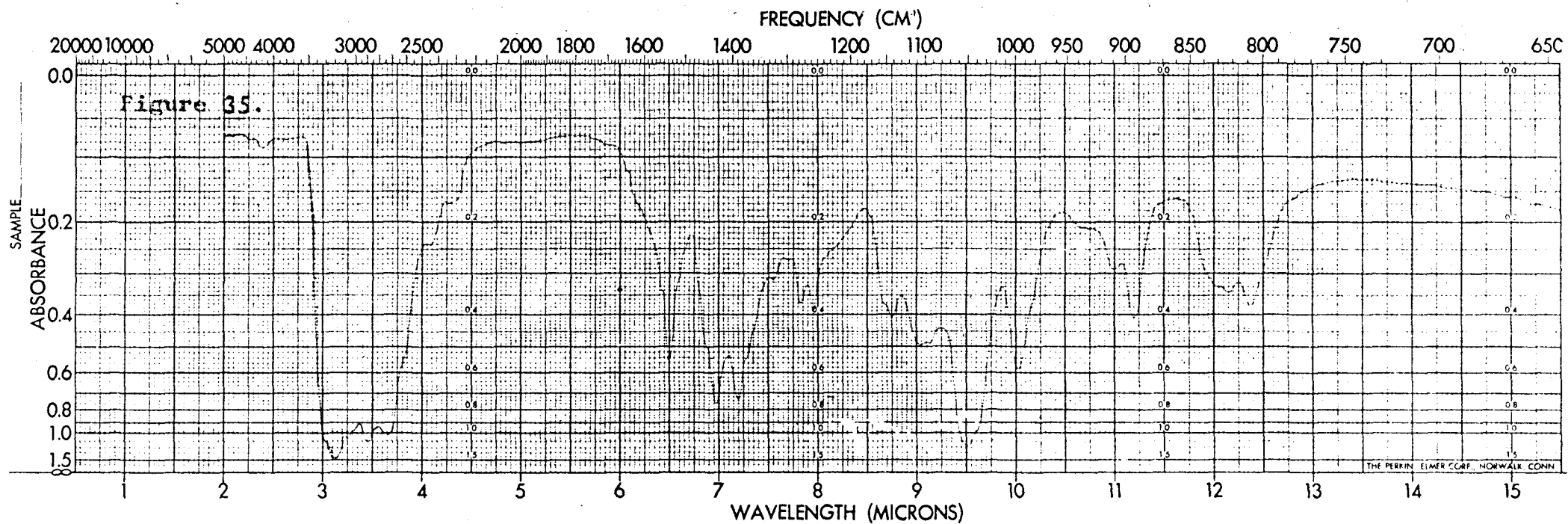
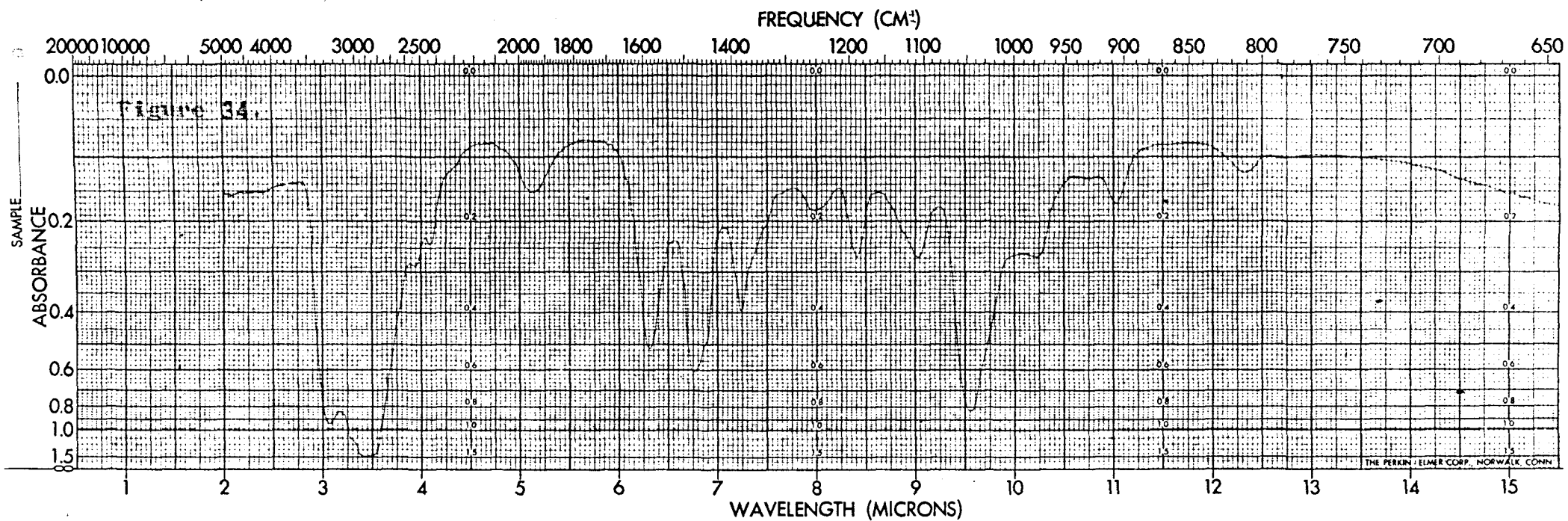


Figure 36:
THE SPECTRUM OF
2-Amino-1,3-propanediol hydrochloride
(321)

Figure 37:
THE SPECTRUM OF
3-Aza-6-chloro-2-hydroxymethyl-1,5-hexanediol hydrochloride

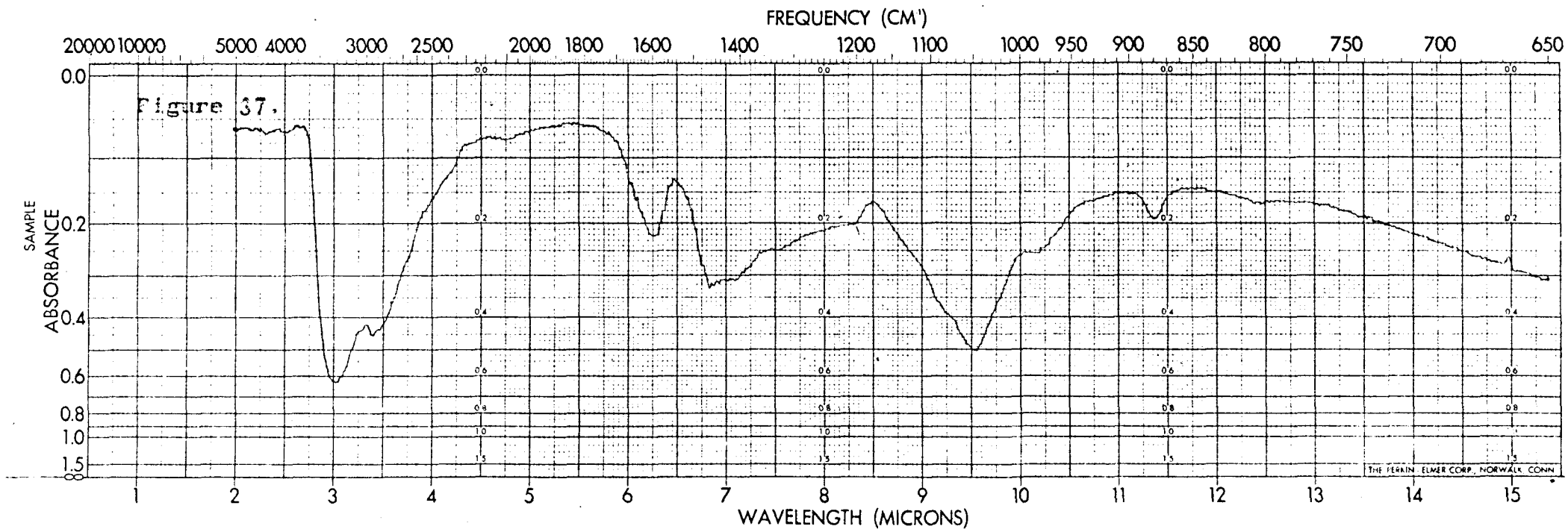
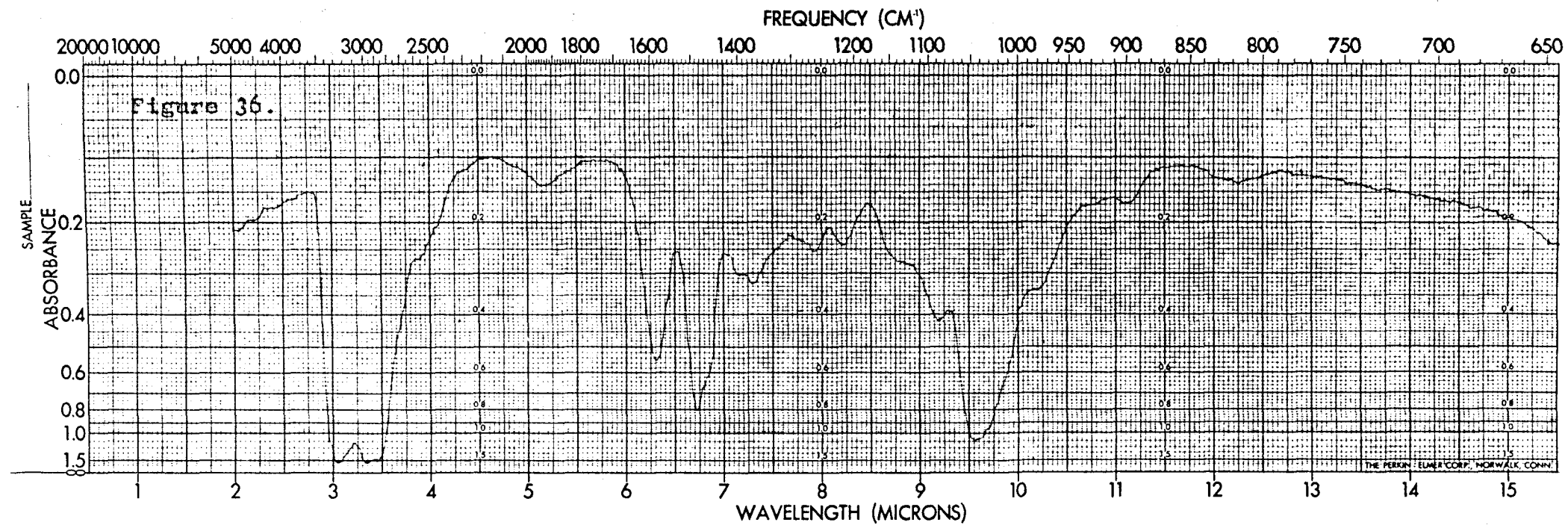


Figure 38:
THE SPECTRUM OF
2-Amino-2-methylpropane hydrochloride
(401)

Figure 39:
THE SPECTRUM OF
2,2,8,8-Tetramethyl-3,7-diaza-5-nonanol dihydrochloride
(402)

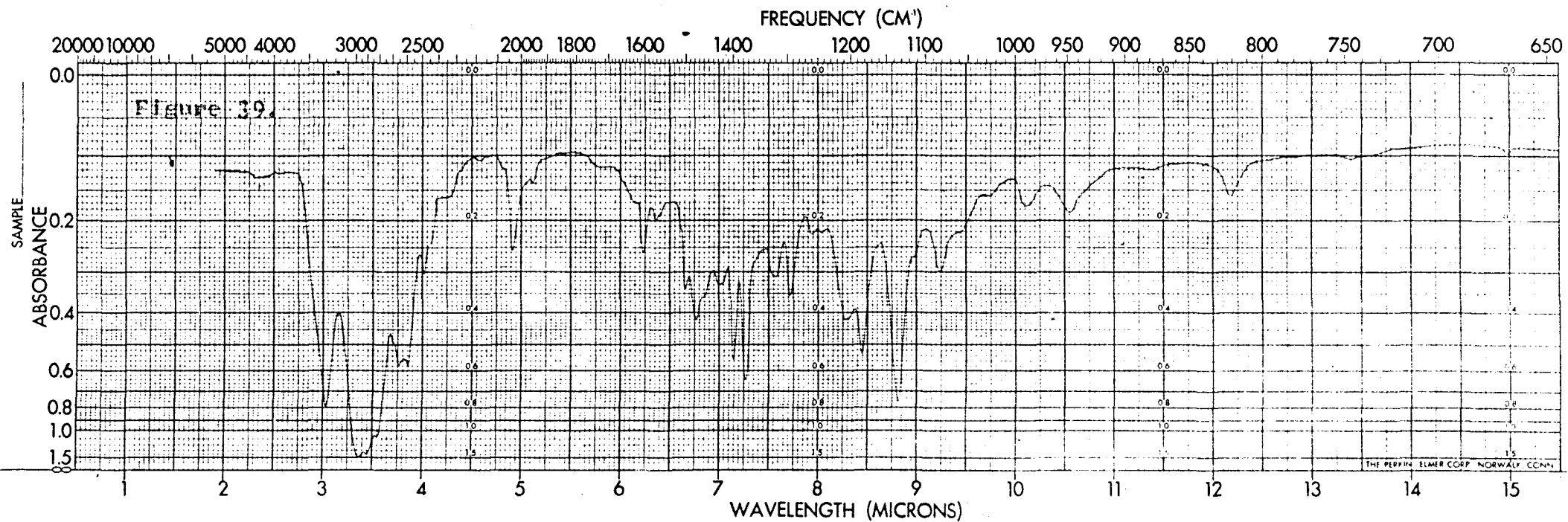
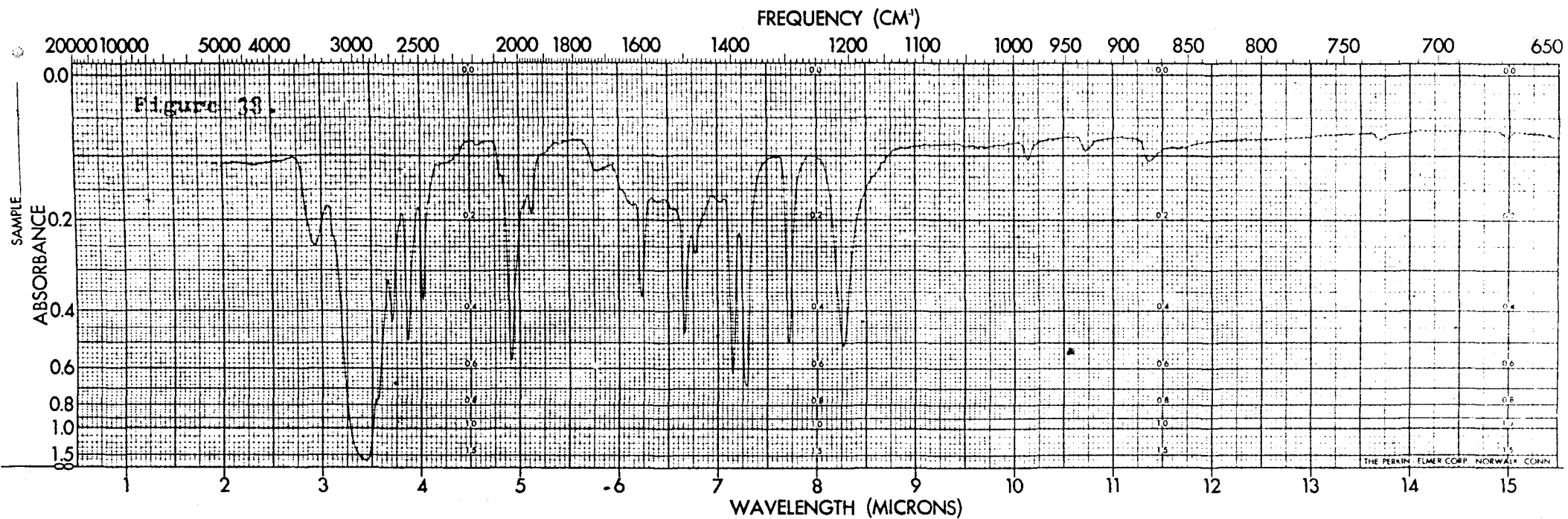


Figure 40:
THE SPECTRUM OF
2-Amino-2-methyl-1-propanol hydrochloride
(411)

Figure 41:
THE SPECTRUM OF
2,2,8,8-Tetramethyl-3,7-diaza-1,5,9-nonanetriol dihydrochloride
(412)

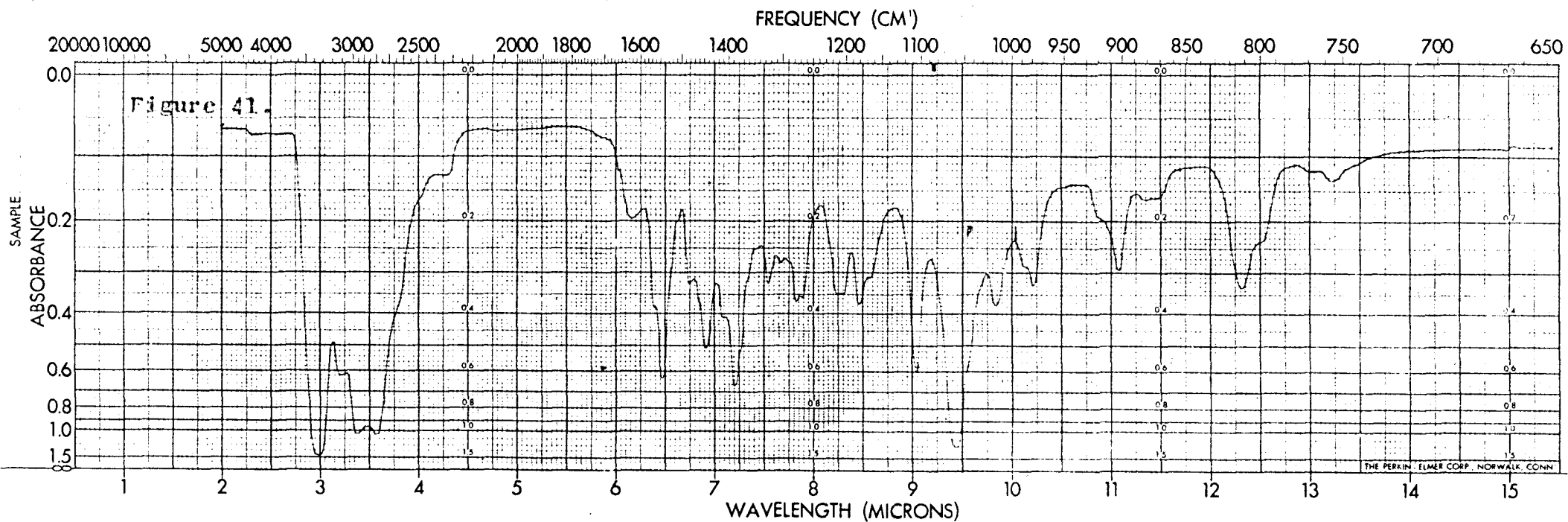
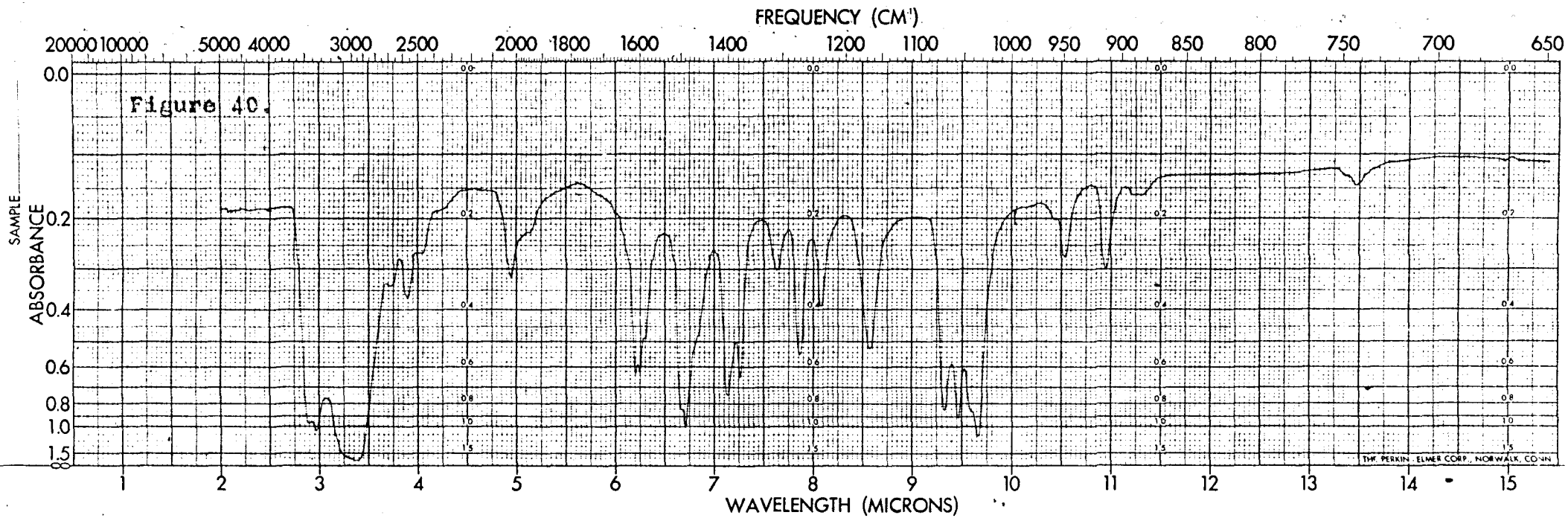


Figure 42:
THE SPECTRUM OF
2-Amino-2-methyl-1,3-propanediol hydrochloride
(421)

Figure 43:
THE SPECTRUM OF
2,8-Bis(hydroxymethyl)-2,8-dimethyl-3,7-diaza-1,5,9-nonanetriol dihydrochloride
(422)

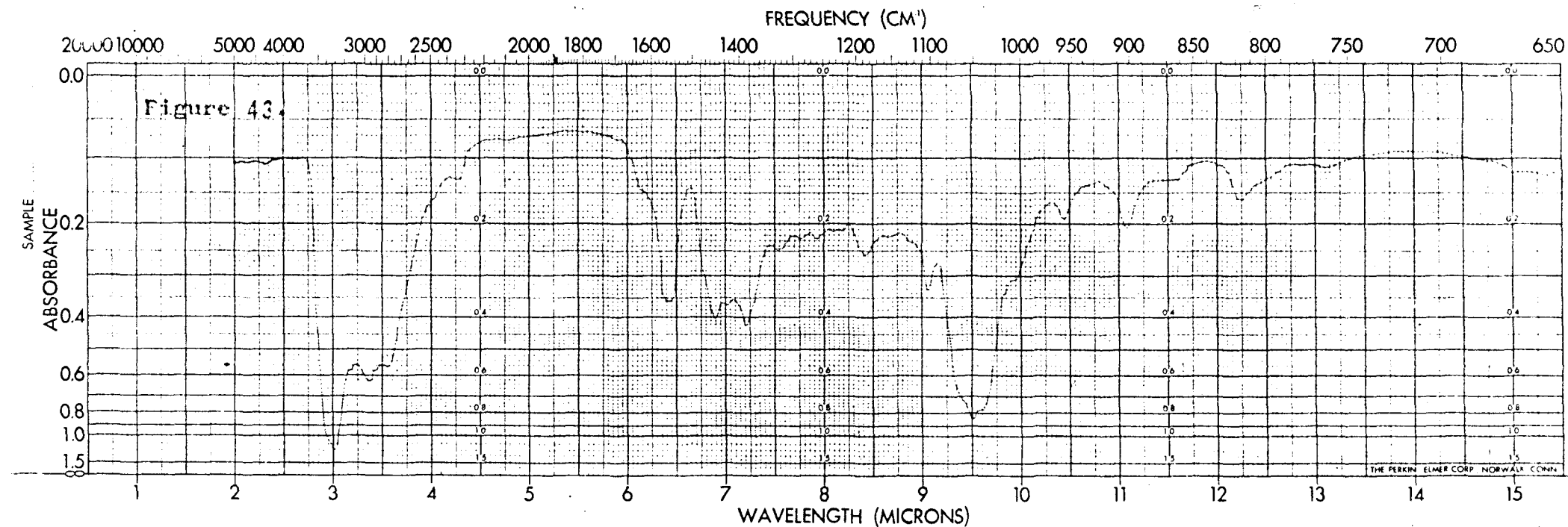
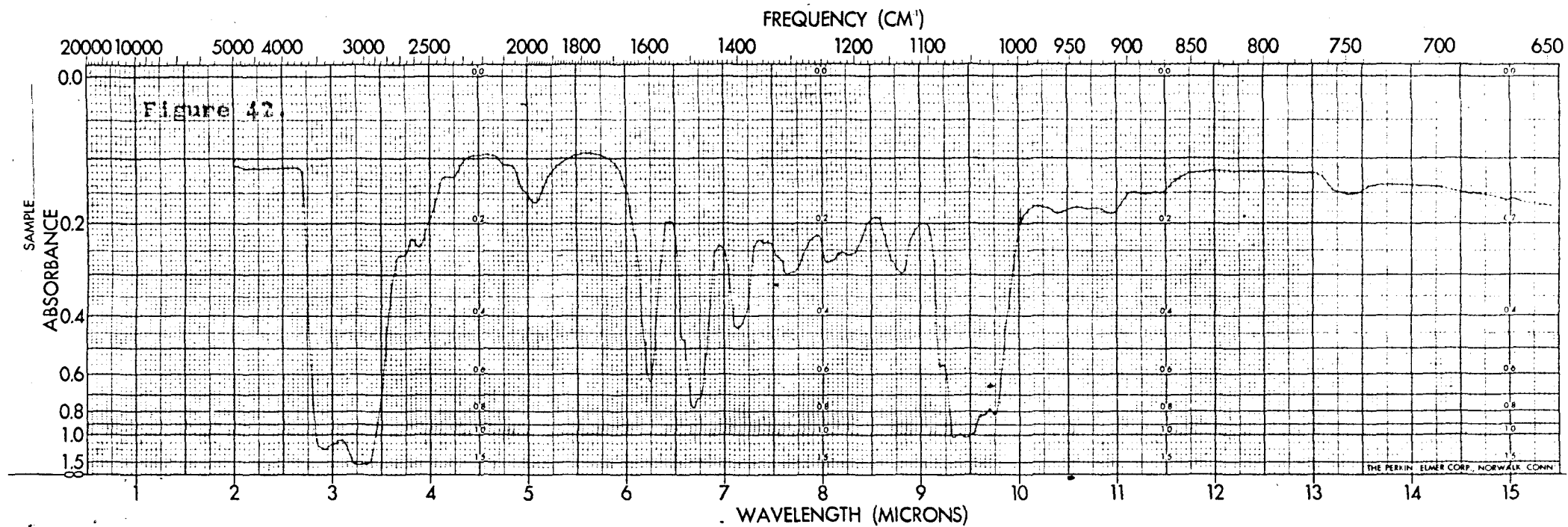


Figure 44:

THE SPECTRUM OF

2-Amino-2-hydroxymethyl-1,3-propanediol hydrochloride

(431)

Figure 45:

THE SPECTRUM OF

2,2,8,8-Tetrakis(hydroxymethyl)-3,7-diaza-1,5,9-nonanetriol dihydrochloride

(432)

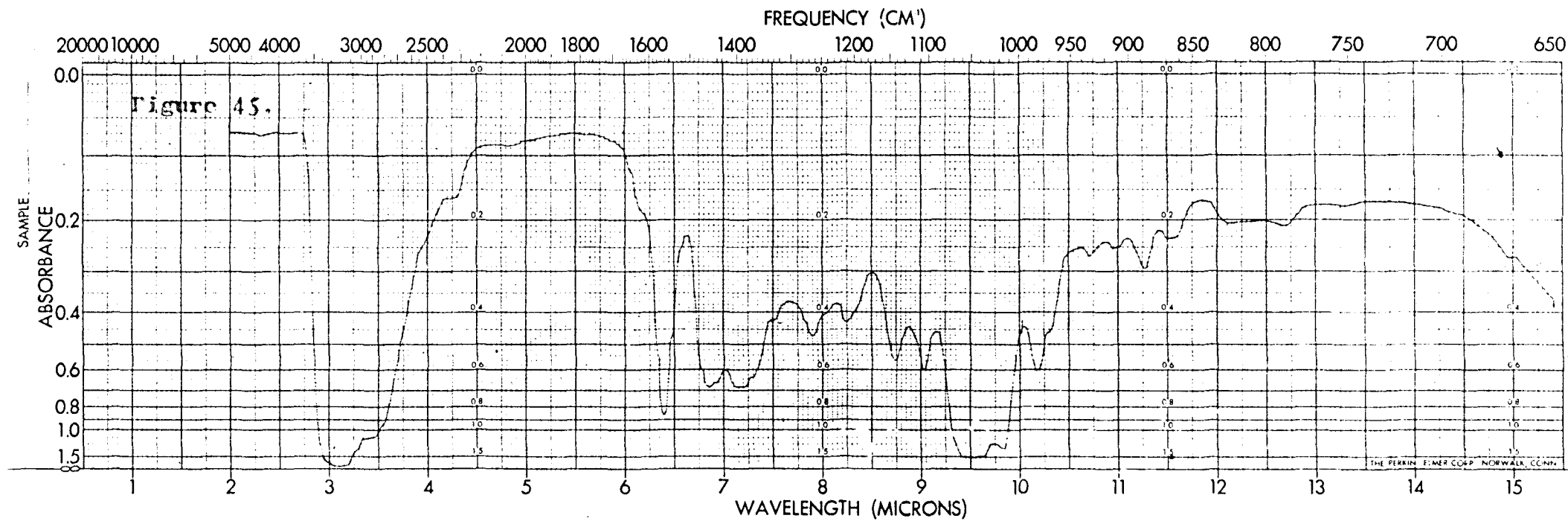
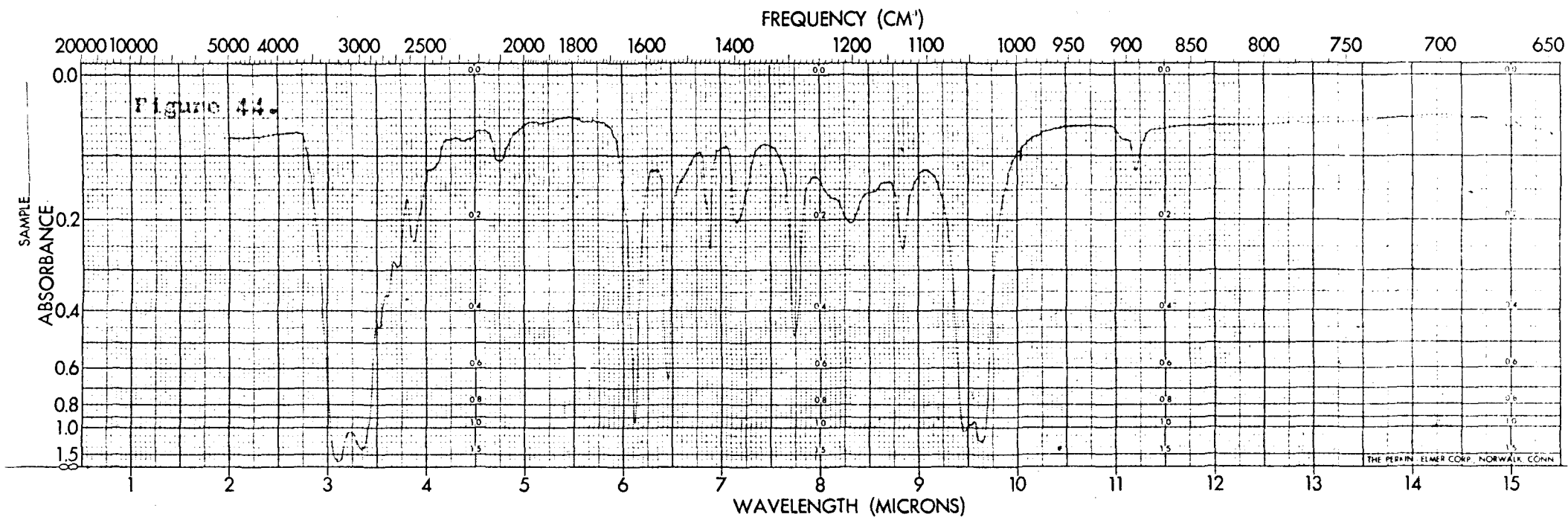
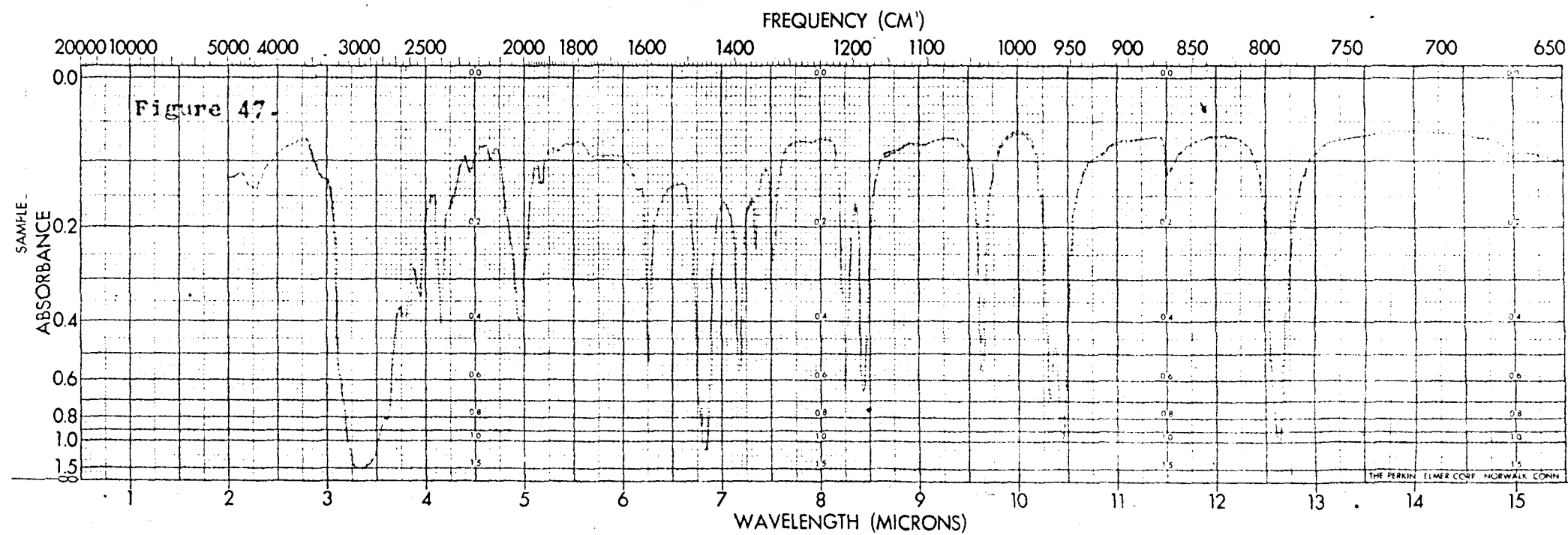
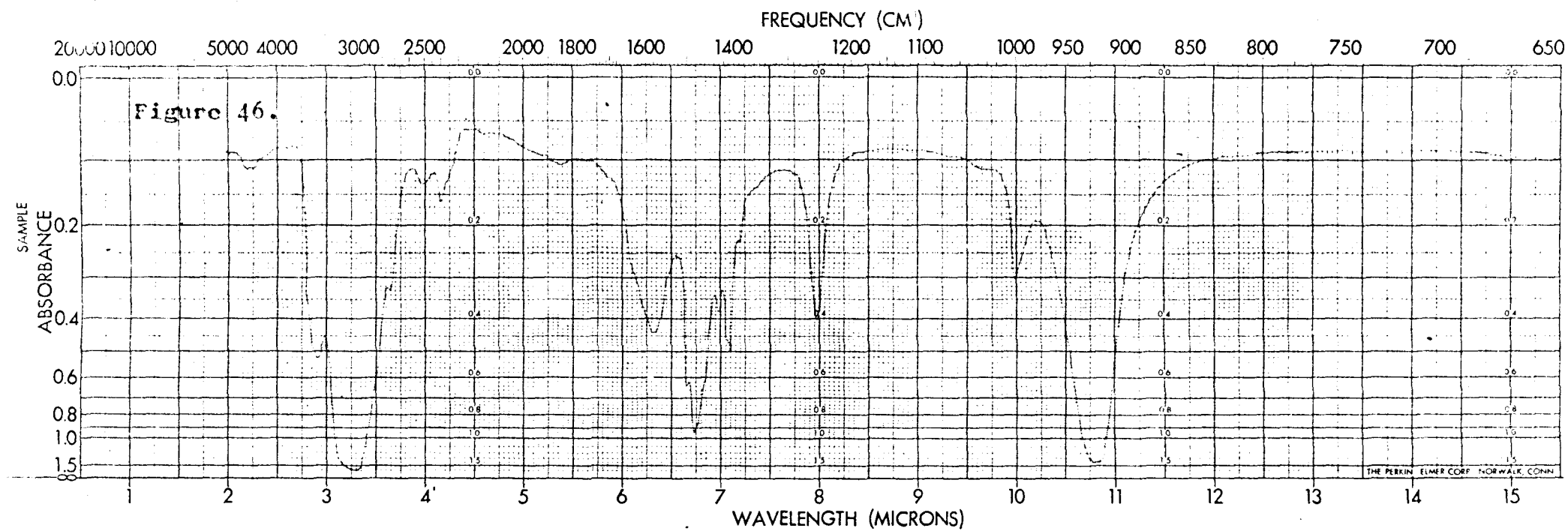


Figure 46:
THE SPECTRUM OF
Aminomethane hydrochloride
(101)

Figure 47:
THE SPECTRUM OF
Aminomethane hydrochloride
(201)



V. TABLES OF RESULTS

Correlations between the positions of the absorption bands in the experimental spectra and those of pertinent structural group frequencies are summarized in Tables III -- XXII. These tables are presented in the same order as the preceeding spectra (i.e., Table III corresponds to Figure 28, Table IV to Figure 29, etc.), and they are designed to show the positions of the absorption bands and those reported for structural units which have corresponding group frequencies in the same region of the spectrum.

The information is tabulated in the following units:

1. Peak Wavelength -- microns
(The spectral width function is listed with the abscissa of each maximum. The symbol "+" is used to indicate plus and minus, " \pm ".
2. Wavenumber -- reciprocal centimeters
3. Absorbance -- logarithmic absorbance units
4. Type and Shape -- these numbers refer to the code categories which were defined on pages 11--17.
5. Band Position -- microns
6. Literature Positions of (corresponding) Group Frequencies -- reciprocal centimeters

If a pertinent structural unit was not found for a band position, this column was left blank. The notation "(unspecified)" indicates that the Vibrational Mode of the Structural Group was not specified in the reference literature.

TABLE III.
THE ABSORPTION BANDS OF
1,3-Diaminopropane dihydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Position of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	2.93 + 0.020	3413	0.32	7	3	2.83 - 4.46	3200 - 2955	-NH ₃ ⁺ (unspecified)
	3.30 + 0.008	3030	1.50	8	3		2967 - 2873	-CH ₂ stretching (asym.)
	4.16 + 0.022	2404	0.26	9	5		2898 - 2810	-CH ₂ scissors (sym.)
							2820 - 2760	-N-CH ₂ - stretching
						2700 - 2480	-NH ₃ ⁺ (unspecified)	
2	4.91 + 0.008	2037	0.25	4	3	4.73 - 5.10	2050 - 1800	-NH ₃ ⁺ (unspecified)
3	6.23 + 0.008	1605	0.42	4	3	6.03 - 6.50	1650 - 1590	-NH ₂ deformation
4	6.83 + 0.022	1464	1.00	4	4	6.65 - 6.95	1480 - 1420	-CH ₂ scissors (sym.)
							1460 - 1430	-N-CH ₂ deformation
5	7.11 + 0.015	1406	0.36	4	6	7.09 - 7.28	1400 - 1350	-CH ₂ scissors (sym.)
6	7.50 + 0.025	1333	0.18	4	3	7.38 - 7.84	1340	-C-H bending
7	8.24 + 0.015	1214	0.30	1	6	8.23 - 8.25	1220 - 1020	-C-N (unspecified)
8	8.42 + 0.020	1180	0.37	4	6	8.40 - 8.81	1220 - 1020	-C-N (unspecified)
9	9.06 + 0.025	1104	0.38	4	4	8.96 - 9.30	1096	N-C-C-C-N (unspecified)
							1090 - 1067	-NH ₂ (pri.) stretching

TABLE III. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
10	9.69 + 0.005	1032	0.16	4	3	9.62 - 9.74	1023 995	N-C-C-C-N (unspecified) -N-CH ₂ stretching (sym.)
11	10.58 + 0.022	945	0.56	7	4	10.36 - 10.98	950 - 905	-CH ₂ -CH ₂ - (unspecified)
	10.70 + 0.010	935	0.51	9	5			
12	11.33 + 0.050	882	0.17	1	2	11.28 - 11.38	900 - 840	-CH ₂ -CH ₂ - (unspecified)
13	12.80 + 0.018	781	0.24	7	6	12.69 - 13.26	745 - 715	-CH ₂ -CH ₂ - rocking
	13.16 + 0.038	760	0.15	9	3			

TABLE IV.

THE ABSORPTION BANDS OF

1,3-Diamino-2-propanol dihydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	2.98 + 0.020	3355	0.60	7	3	2.94 - 4.30	3500 - 3300	-N-H stretching (asym)
	3.53 + 0.010	3003	1.22	9	3			-N-H stretching (sym.)
							3476 - 3484	-O-H stretching (sec.)
							3200 - 2955	-NH ₃ ⁺ (unspecified)
							2967 - 2873	-CH ₂ stretching (asym.)
							2898 - 2810	-CH ₂ scissors (sym.)
							2820 - 2760	-N-CH ₂ stretching
							2700 - 2480	-NH ₃ ⁺ (unspecified)
2	5.25 + 0.080	1905	0.18	1	4	5.17 - 5.33	2050 - 1800	-NH ₃ ⁺ (unspecified)
3	6.22 + 0.008	1608	0.62	7	6	6.03 - 6.47	1650 - 1590	-NH ₂ (pri.) deformation
	6.37 + 0.025	1570	0.45	9	3			
4	6.60 + 0.020	1515	0.68	7	5	6.57 - 7.08	1480 - 1420	-CH ₂ scissors (sym.)
	6.78 + 0.020	1475	1.00	9	6		1460 - 1430	-N-CH ₂ - deformation
							1433 - 1375	-OH (sec.) (unspecified)
5	7.24 + 0.025	1381	0.31	4	3	7.14 - 7.28	1400 - 1350	-CH ₂ scissors (sym.)
6	7.43 + 0.012	1346	0.36	7	4	7.42 - 7.64	1350 - 1260	-OH (sec.) (unspecified)
	7.62 + 0.025	1312	0.22	9	3			
7	7.88 + 0.050	1269	0.23	1	3	7.83 - 7.93	1350 - 1260	-OH (sec.) (unspecified)

TABLE IV. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
8	8.59 + 0.030	1164	0.38	4	4	8.56 - 8.82	1220 - 1020 1164 - 1052 1147 - 1118	-N-C- (unspecified) -OH (sec.) (unspecified) N-C-C-C-N (unspecified)
9	8.99 + 0.300	1112	0.30	1	6	8.96 - 9.02	1125 - 1025	-OH (sec.) (unspecified)
10	9.32 + 0.015	1073	0.53	1	6	9.30 - 9.34	1125 - 1025 1090 - 1067	-OH (sec.) (unspecified) -NH ₂ (pri.) stretching
11	9.56 + 0.012	1046	0.50	1	6	9.55 - 9.57	1125 - 1025	-OH (sec.) (unspecified)
12	10.04 + 0.025	996	0.84	1	6	10.01 - 10.07	995	-N-CH ₂ stretching (sym.)
13	10.49 + 0.018 10.68 + 0.022	953 936	0.34 0.40	7 9	3 4	10.45 - 11.00	995	-N-CH ₂ stretching (sym.)
14	11.85 + 0.008	844	0.15	4	3	11.80 - 11.95	900 - 840	-CH ₂ -CH ₂ - (unspecified)
15	12.18 + 0.038	821	0.15	4	3	12.04 - 12.34	840 - 790	-C-C- stretching

TABLE V.
THE ABSORPTION BANDS OF
2-Aminoethanol hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.10 ± 0.010	3226	1.10	7	5	3.09 - 4.45	3650 - 2500	-O-H stretching
	3.36 ± 0.030	2976	1.45	8	4		3500 - 3300	-NH ₂ (pri.) stretching
	4.16 ± 0.008	2404	0.18	9	5		3200 - 2955	-NH ₃ ⁺ (unspecified)
							2994 - 2900	-CH ₂ -CH ₂ stretching (asym.)
							2967 - 2874	-CH ₂ -CH ₂ stretching (sym.)
							2820 - 2760	-N-CH ₂ - stretching
2700 - 2480	-NH ₃ ⁺ (unspecified)							
2	5.06 ± 0.050	1976	0.12	4	3	4.95 - 5.35	2050 - 1800	-NH ₃ ⁺ (unspecified)
3	6.20 ± 0.078	1613	0.48	7	6	6.05 - 6.50	1650 - 1590	-NH ₂ (pri.) deformation
	6.36 ± 0.015	1572	0.29	9	3		1642 - 1525	-NH ₃ ⁺ (unspecified)
4	6.74 ± 0.005	1484	0.82	7	6	6.65 - 6.96	1572 - 1493	-NH ₃ ⁺ (unspecified)
	6.91 ± 0.002	1447	0.40	9	5		1477 - 1420	-CH ₂ -CH ₂ - scissors (sym.)
							1466 - 1400	-OH (pri.) (unspecified)
							1460 - 1430	-N-CH ₂ - deformation
5	7.33 ± 0.010	1364	0.18	1	3	7.31 - 7.35	1397 - 1351	-CH ₂ -CH ₂ - scissors (sym.)
6	7.53 ± 0.005	1328	0.50	1	6	7.52 - 7.54	1350 - 1260	-OH (Pri.) deformation
								-C-O stretching
7	7.80 ± 0.002	1282	0.39	1	6	7.79 - 7.82	1350 - 1260	-OH (pri.) deformation
								-C-O stretching

TABLE V. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
8	7.96 + 0.010	1256	0.34	1	6	7.95 - 7.97	1350 - 1260	-OH (pri.) deformation -C-O stretching
9	8.70 + 0.012	1149	0.29	1	6	8.69 - 8.71	1178 - 1000 1220 - 1020	-OH (pri.) (unspecified) -C-N (unspecified)
10	9.02 + 0.010	1109	0.42	1	6	9.01 - 9.03	1100 - 1000	-CH ₂ -CH ₂ - (unspecified)
11	9.44 + 0.008	1059	0.94	1	6	9.43 - 9.45	1075 - 1000	-OH (pri.) deformation -C-O stretching
12	10.10 + 0.038 10.26 + 0.015	990 975	1.09 0.82	7 9	4 5	10.08 - 10.60	995	-N-CH ₂ - stretching (sym.)
13	11.54 + 0.015	867	0.20	1	6	11.53 - 11.55	900 - 840	-CH ₂ -CH ₂ - (unspecified)

TABLE VI.

THE ABSORPTION BANDS OF

3,7-Diaza-1,5,9-nonanetriol dihydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.14 + 0.110	3185	1.22	7	4	3.11 - 4.41	3650 - 2500	-O-H stretching
	3.25 + 0.015	3077	0.92	8	3		3500 - 3100	-N-H ₂ (sec.) (unspecified)
	3.46 + 0.012	2890	0.95	8	3		3200 - 2955	-NH ₂ ⁺ (unspecified)
	3.66 + 0.015	2732	0.92	9	4		2994 - 2900	-CH ₂ -CH ₂ - (unspecified)
							2967 - 2874	-CH ₂ -CH ₂ - stretching (asym)
2	6.56 + 0.012	1524	0.36	4	6	6.05 - 6.65	2898 - 2810	-CH ₂ -CH ₂ - stretching (symm)
							2890 - 2833	-CH ₂ -CH ₂ - scissors (sym.)
							2820 - 2760	-N-CH ₂ - stretching
							2700 - 2480	-NH ₃ ⁺ (unspecified)
3	6.89 + 0.010	1451	0.57	7	3	6.81 - 7.41	1650 - 1550	-NH ₂ (sec.) deformation
	6.96 + 0.008	1437	0.72	8	6		1620 - 1560	-NH ₂ ⁺ deformation
	7.18 + 0.008	1393	0.47	8	4			
	7.39 + 0.015	1353	0.34	9	4			
4	7.87 + 0.020	1271	0.22	7	3	7.86 - 8.06	1480 - 1420	-CH ₂ scissors (symm.)
	8.05 + 0.012	1242	0.23	9	3		1460 - 1430	-N-CH ₂ - deformation
							1433 - 1375	-OH (sec.) rocking def.
							1397 - 1351	-CH ₂ -CH ₂ - (unspecified)
							1350 - 1260	-OH (pri., sec.) deformation
5	8.54 + 0.045	1171	0.15	4	3	8.40 - 8.57		-C-O stretching
6							1350 - 1260	-OH (pri., sec.) deformation
								-C-O stretching
7							1350 - 1260	-OH (pri., sec.) deformation
								-C-O stretching
8							1178 - 1000	-OH (pri.) (unspecified)

TABLE VI. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
7	8.90 + 0.005	1124	0.38	4	4	8.88 - 9.09	1125 - 1025	-OH (sec.) deformation -C-O stretching
8	9.42 + 0.030	1062	0.72	7	3	9.35 - 10.25	1125 - 1025	-OH (sec.) deformation -C-O stretching
	9.51 + 0.023	1061	0.71	8	3			
	9.65 + 0.023	1036	0.52	8	3		1075 - 1000	-OH (pri.) deformation -C-O stretching
	9.75 + 0.018	1026	0.56	8	5			
	10.05 + 0.020	995	0.31	9	6			
9	10.62 + 0.020	942	0.25	1	4	10.60 - 10.64		
10	11.14 + 0.020	898	0.58	4	6	10.95 - 11.30	900 - 840	-CH ₂ -CH ₂ - (unspecified)
11	11.60 + 0.030	862	0.16	4	3	11.57 - 11.92	900 - 840	-CH ₂ -CH ₂ - (unspecified)
12	12.20 + 0.020	820	0.24	7	3	12.18 - 12.93	840 - 790	-CH ₂ -CH ₂ - (unspecified)
	12.56 + 0.010	796	0.58	8	6			
	12.90 + 0.040	775	0.32	9	3			

TABLE VII.
THE ABSORPTION BANDS OF
2-Aminopropane hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	2.95 ± 0.022	3390	0.22	1	5	2.92 - 2.98	3500 - 3300	-N-H (pri.) stretching (asy) -N-H (pri.) stretching (asy)
2	3.42 ± 0.078 3.71 ± 0.005	2924 2695	1.28 0.24	7 9	4 5	3.25 - 3.72	2994 - 2899 2967 - 2874 2890 - 2833 2857 - 2800 2700 - 2480	(CH ₃) ₂ CH- stretching (asy) (CH ₃) ₂ CH- stretching (sym) (CH ₃) ₂ CH- stretching (asy) (CH ₃) ₂ CH- stretching (sym) -NH ₃ ⁺ (unspecified)
3	3.90 ± 0.005	2564	0.19	1	5	3.89 - 3.91	2700 - 2480	-NH ₃ ⁺ (unspecified)
4	4.04 ± 0.020	2475	0.19	1	3	4.03 - 4.05	2700 - 2480	-NH ₃ ⁺ (unspecified)
5	5.25 ± 0.080	1905	1.04	4	3	4.90 - 5.35	2050 - 1800	-NH ₃ ⁺ (unspecified)
6	6.33 ± 0.005	1580	0.68	4	6	6.02 - 6.48	1642 - 1625 1572 - 1493 1650 - 1590	-NH ₃ ⁺ (unspecified) -NH ₃ ⁺ (unspecified) -NH ₂ (pri.) deformation
7	6.66 ± 0.008 6.81 ± 0.005	1502 1468	0.62 0.32	7 9	6 5	6.62 - 6.86	1479 - 1420	(CH ₃) ₂ CH- scissors (asy)
8	7.16 ± 0.005 7.25 ± 0.005	1397 1379	0.45 0.35	7 9	6 6	7.15 - 7.26	1397 - 1364 1375 - 1345	(CH ₃) ₂ CH- scissors (sym) (CH ₃) ₂ CH- scissors (sym)
9	8.28 ± 0.020	1208	0.43	1	4	8.27 - 8.29	1220 - 1020	-C-N (unspecified)

TABLE VII. (CONTINUED)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
10	8.65 + 0.010	1156	0.40	1	6	8.64 -- 8.66	1200 - 1150 1155 - 1100	(CH ₃) ₂ CH- skeletal scissors (CH ₃) ₂ CH- skeletal scissors
11	10.11 + 0.012	989	0.24	4	4	9.90 - 10.30	995 980 - 908	-N-CH stretching (sym) (CH ₃) ₂ CH- skeletal deformation
12	10.66 + 0.018 10.76 + 0.025	938 929	0.14 0.13	7 9	3 3	10.64 - 10.78	980 - 908	(CH ₃) ₂ CH- skeletal deformation
13	12.52 + 0.020	799	0.13	1	3	12.50 - 12.54	840 - 790	(CH ₃) ₂ CH- skeletal deformation

TABLE VIII.

THE ABSORPTION BANDS OF

2,8-Dimethyl-3,7-diaza-5-nonanol dihydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	2.97 + 0.025	3367	0.86	4	6	2.83 - 2.99	3650 - 3496 3500 - 3300 3484 - 3476	-O-H (sec.) stretching (asy) -N-H (sec.) stretching (asy) -N-H (sec.) stretching (sym) -O-H (sec.) stretching (sym)
2	3.40 + 0.050 3.63 + 0.030 4.23 + 0.035	2941 2755 2364	1.48 1.48 0.28	7 8 9	4 4 3	3.25 - 4.26	3200 - 2955 2994 - 2899 2967 - 2874 2890 - 2833 2857 - 2800 2700 - 2480	-NH ₂ ⁺ (unspecified) (CH ₃) ₂ CH- stretching (asy) (CH ₃) ₂ CH- stretching (sym) (CH ₃) ₂ CH- stretching (asy) (CH ₃) ₂ CH- stretching (sym) -NH ₂ ⁺ (unspecified)
3	5.03 + 0.075	1988	0.16	1	2	4.95 - 5.11	2050 - 1800	-NH ₂ ⁺ (unspecified)
4	6.37 + 0.025	1570	0.52	4	3	6.02 - 6.67	1650 - 1550 1642 - 1525 1620 - 1560 1572 - 1493	-NH- (sec.) deformation -NH ₂ ⁺ (sec.) (unspecified) -NH ₂ ⁺ (sec.) (unspecified) -NH ₂ ⁺ (sec.) (unspecified)
5	6.82 + 0.023 6.93 + 0.020	1466 1443	0.56 0.68	7 9	3 5	6.78 - 6.95	1477 - 1420	(CH ₃) ₂ CH- scissors (asy)
6	7.16 + 0.020	1397	0.78	4	6	7.14 - 7.33	1433 - 1300 1397 - 1364 1375 - 1345	-OH (sec.) rocking def. (CH ₃) ₂ CH- scissors (sym) (CH ₃) ₂ CH- scissors (sym)

TABLE VIII. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
Peak Wavelength	Wavenumber	Abs.	Type	Shape				
7	7.63 + 0.025	1311	0.35	4	3	7.50 - 7.65	1350 - 1260 1345 - 1321	-OH (sec.) deformation -C-O stretching (CH ₃) ₂ CH- bending
8	7.82 + 0.023	1279	0.29	1	3	7.80 - 7.84	1350 - 1260	-OH (sec.) deformation -C-O stretching
9	8.05 + 0.040	1242	0.26	4	3	8.01 - 8.12		
10	8.58 + 0.020 8.75 + 0.013	1166 1143	0.48 0.49	7 9	5 5	8.56 - 8.76	1200 - 1150 1164 - 1052 1155 - 1100 1150 - 1085	(CH ₃) ₂ CH- skeletal scissors -OH (sec.) (unspecified) (CH ₃) ₂ CH- skeletal scissors -NH- (sec.) (unspecified)
11	9.23 + 0.018	1083	0.94	7	6	9.21 - 9.60	1164 - 1052 1155 - 1100 1150 - 1085 1125 - 1025	-OH (sec.) (unspecified) (CH ₃) ₂ CH- skeletal scissors -NH- (sec.) (unspecified) -OH (sec.) deformation
12	9.96 + 0.032	1004	0.42	4	4	9.93 - 10.08	1000	-C-C- stretching
13	10.53 + 0.038 10.72 + 0.030	950 933	0.23 0.26	7 9	3 3	10.49 - 10.83	980 - 908	(CH ₃) ₂ CH- skeletal deformation
14	11.03 + 0.028	907	0.27	1	4	11.05 - 11.11	980 - 908	(CH ₃) ₂ CH- skeletal deformation
15	11.99 + 0.023 12.29 + 0.025	834 814	0.34 0.39	7 9	4 6	11.97 - 12.49	840 - 790	(CH ₃) ₂ CH- skeletal deformation

TABLE IX.
THE ABSORPTION BANDS OF
2-Amino-1-propanol hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.10 ± 0.043	3226	1.01	7	4	3.00 - 4.15	3650 - 2500	-O-H stretching
	3.45 ± 0.050	2899	1.45	8	4		3500 - 3300	-N-H (pri.) stretching (asy)
	4.08 ± 0.020	2451	0.23	9	3			-N-H (pri.) stretching (sym)
							3200 - 2955	-NH ₃ ⁺ (unspecified)
							2994 - 2899	(CH ₃) ₂ CH- stretching (asy)
							2967 - 2874	(CH ₃) ₂ CH- stretching (sym)
							2890 - 2833	(CH ₃) ₂ CH- stretching (asy)
2						5.00 - 5.25	2857 - 2800	(CH ₃) ₂ CH- stretching (sym)
							2700 - 2480	-NH ₃ ⁺ (unspecified)
	5.13 ± 0.070	1949	0.15	1	4		2050 - 1800	-NH ₃ ⁺ (unspecified)
3	6.30 ± 0.025	1587	0.52	4	3	6.03 - 6.45	1650 - 1590	-NH ₂ (pri.) deformation
							1642 - 1625	-NH ₃ ⁺ (unspecified)
							1572 - 1493	-NH ₃ ⁺ (unspecified)
4	6.75 ± 0.038	1481	0.61	4	3	6.60 - 6.90	1572 - 1493	-NH ₃ ⁺ (unspecified)
							1480 - 1420	(CH ₃) ₂ CH- scissors (asy)
							1466 - 1400	-OH (pri.) (unspecified)
5	7.24 ± 0.013	1381	0.40	4	6	7.18 - 7.50	1400 - 1300	-OH (pri.) rocking def.
							1397 - 1364	(CH ₃) ₂ CH- scissors (sym)
							1375 - 1345	(CH ₃) ₂ CH- scissors (sym)
							1350 - 1260	-OH (pri.) deformation
								-C-O stretching
6	7.96 ± 0.073	1256	0.18	1	3	7.85 - 8.15	1345 - 1321	(CH ₃) ₂ CH- (-C-H) bending
							1350 - 1260	-OH (pri.) deformation
							1305 - 1275	-C-O stretching (CH ₃) ₂ CH- (CH ₃ -) wagging

TABLE IX. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
7	8.41 + 0.030	1189	0.27	1	3	8.26 - 8.52	1220 - 1020 1200 - 1180 1200 - 1150 1178 - 1000	-C-N (unspecified) CH ₃ - twisting (CH ₃) ₂ CH- skeletal scissors -OH (pri.) (unspecified)
8	9.04 + 0.033	1106	0.27	4	3	8.85 - 9.15	1220 - 1020 1178 - 1000 1155 - 1100 1140 - 1130	-C-N (unspecified) -OH (pri.) (unspecified) (CH ₃) ₂ CH- skeletal scissors CH ₃ - rocking deformation
9	9.55 + 0.050	1047	0.83	4	4	9.45 - 10.25	1075 - 1000 1038 - 1022 1000	-OH (pri.) (unspecified) -C=O stretching -N-C (pri.) -C-C stretching
10	11.03 + 0.050	907	0.17	4	3	10.92 - 11.08	980 - 908	(CH ₃) ₂ CH- skeletal deformation
11	12.33 + 0.083	811	0.13	1	3	12.20 - 12.50	840 - 790	(CH ₃) ₂ CH- skeletal deformation

TABLE I. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
4	7.83 + 0.018	1277	0.36	7	3	7.80 - 8.00	1350 - 1260	-OH (pri. & sec.) deformation
	7.91 + 0.013	1264	0.38	9	3		1305 - 1275	-C-O stretching -CH ₂ - wagging deformation
5	8.76 + 0.015	1142	0.40	7	3	8.66 - 10.18	1200 - 1150	(CH ₃) ₂ CH- skeletal scissors
	9.05 + 0.033	1105	0.49	8	4		1178 - 1000	-OH (pri.) (unspecified)
	9.54 + 0.020	1048	1.22	8	4		1164 - 1052	-OH (sec.) (unspecified)
	10.04 + 0.025	996	0.57	9	4		1155 - 1100	(CH ₃) ₂ CH- skeletal scissors
							1150 - 1085	-NH- (sec.) (unspecified)
							1140 - 1130	CH ₂ - rocking deformation
							1125 - 1025	-OH (sec.) deformation
							1119 - 1105	-OH (sec.) deformation
								-C-O stretching
							1075 - 1000	-OH (pri.) deformation
6	11.00 + 0.050	909	0.29	7	3	10.90 - 11.25	980 - 908	-C-O stretching
	11.20 + 0.043	893	0.40	9	4			(CH ₃) ₂ CH- skeletal deformation
7	12.18 + 0.053	821	0.34	7	3	11.90 - 12.53	840 - 790	(CH ₃) ₂ CH- skeletal deformation
	12.37 + 0.035	808	0.37	9	4			

TABLE XI.
THE ABSORPTION BANDS OF

2-Amino-1,3-propanediol hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band			Band Position		Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape		
1	3.05 + 0.045	3279	1.60	7	4	2.97 - 4.07	3650 - 2500
	3.34 + 0.050	2994	1.60	9	4		3500 - 3300
							-O-H (pri.) stretching
							-N-H (pri.) stretching (asy)
							-N-H (pri.) stretching (sym)
							-NH ₃ ⁺ (unspecified)
							(CH ₃) ₂ CH- stretching (asy)
							(CH ₃) ₂ CH- stretching (sym)
							(CH ₃) ₂ CH- stretching (asy)
							(CH ₃) ₂ CH- stretching (sym)
2	5.16 + 0.125	1938	0.14	1	4	5.04 - 5.28	2050 - 1800
							-NH ₃ ⁺ (unspecified)
3	6.32 + 0.020	1582	0.55	4	5	6.10 - 6.50	1650 - 1590
							-NH ₂ deformation
							1642 - 1525
							-NH ₃ ⁺ (unspecified)
							1572 - 1493
							-NH ₃ ⁺ (unspecified)
4	6.73 + 0.025	1486	0.80	4	6	6.58 - 6.84	1642 - 1525
							-NH ₃ ⁺ (unspecified)
							1572 - 1493
							-NH ₃ ⁺ (unspecified)
							1477 - 1420
							(CH ₃) ₂ CH- scissors (asy)
							1466 - 1400
							-OH (pri.) (unspecified)
5	7.30 + 0.040	1370	0.32	4	3	7.12 - 7.34	1433 - 1300
							-OH (pri.) rocking deformation
							1397 - 1364
							(CH ₃) ₂ CH- scissors (sym)
							1375 - 1345
							(CH ₃) ₂ CH- scissors (sym)
6	7.92 + 0.025	1263	0.25	1	3	7.92 - 7.94	1350 - 1260
							-OH (pri.) deformation
							-C-O stretching
7	8.24 + 0.025	1214	0.24	4	3	8.22 - 8.40	1220 - 1020
							-C-N (unspecified)
							1200 - 1180
							-CH ₂ - twisting deformation
							1200 - 1150
							(CH ₃) ₂ CH- skeletal scissors

TABLE XI. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
8	9.20 + 0.045	1087	0.42	7	3	8.75 - 10.26	1178 - 1000	-OH (pri.) (unspecified)
	9.59 + 0.078	1043	1.08	9	4		1155 - 1100	(CH ₃) ₂ CH- skeletal scissors
							1075 - 1000	-OH (pri.) deformation
								-C-O stretching
							1043 - 1037	-C-N stretching
							1000	-C-C stretching
							980 - 908	(CH ₃) ₂ CH- skeletal deformation
9	11.00 + 0.125	909	0.17	1	3	10.88 - 11.12	980 - 908	(CH ₃) ₂ CH- skeletal deformation
10	12.24 + 0.150	817	0.14	1	2	12.09 - 12.39	840 - 790	(CH ₃) ₂ CH- skeletal deformation

TABLE XII.

THE ABSORPTION BANDS OF

3-Aza-6-chloro-2-hydroxymethyl-1,5-hexanediol hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.00 + 0.050	3333	0.82	7	4	2.92 - 4.94	3650 - 2500	-O-H (pri. & sec.) stretching
	3.36 + 0.025	2976	0.58	9	5		3500 - 3300	-N-H (sec.) stretching (asy)
								-N-H (sec.) stretching (sym)
							3200 - 2955	-NH ₂ ⁺ (sec.) (unspecified)
							2994 - 2899	(CH ₃) ₂ CH- stretching (asy)
							2962 - 2874	(CH ₃) ₂ CH- stretching (sym)
							2890 - 2833	(CH ₃) ₂ CH- stretching (asy)
							2857 - 2800	(CH ₃) ₂ CH- stretching (sym)
							2700 - 2480	-NH ₂ ⁺ (unspecified)
							2050 - 1800	-NH ₂ ⁺ (unspecified)
2	6.26 + 0.050	1597	0.28	4	4	6.02 - 6.43	1650 - 1550	-NH- (sec.) deformation
							1620 - 1560	-NH ₂ ⁺ deformation
							1572 - 1493	-NH ₂ ⁺ deformation
3	6.82 + 0.020	1466	0.42	7	5	6.58 - 8.47	1572 - 1493	-NH ₂ ⁺ deformation
	6.87 + 0.020	1453	0.41	8	5		1477 - 1420	(CH ₃) ₂ CH- scissors (asy)
	7.05 + 0.125	1418	0.40	9	3		1466 - 1400	-OH (pri.) deformation
							1433 - 1300	-OH (sec.) rocking deformation
							1397 - 1364	(CH ₃) ₂ CH- scissors (sym)
							1375 - 1345	(CH ₃) ₂ CH- scissors (sym)
							1350 - 1260	-OH (pri. & sec.) deformation
								-C-O stretching
							1345 - 1321	(CH ₃) ₂ CH- (-C-H) bending def.
							1305 - 1275	-CH ₂ - wagging deformation
							1220 - 1020	-C-N (unspecified)
							1200 - 1180	-CH ₂ - twisting deformation
							1200 - 1150	(CH ₃) ₂ CH- skeletal scissors
							1191 - 1171	-C-N stretching (asy)

TABLE XII. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
4	9.54 + 0.063	1048	0.62	4	6	8.50 - 10.35	1220 - 1020	-C-N (unspecified)
							1191 - 1171	-C-N stretching (asy)
							1178 - 1000	-OH (pri.) (unspecified)
							1164 - 1052	-OH (sec.) (unspecified)
							1155 - 1100	(CH ₃) ₂ CH- skeletal scissors
							1125 - 1025	-OH (sec.) deformation
							1119 - 1105	-OH (sec.) deformation
								-C-O stretching
							1075 - 1000	-OH (pri.) deformation
								-C-O stretching
5	11.37 + 0.050	880	0.24	1	3	11.34 - 11.40	1038 - 1022	-C-N stretching
							1000	-C-C stretching
							980 - 908	(CH ₃) ₂ CH- skeletal deformation
							980 - 908	(CH ₃) ₂ CH- skeletal deformation

TABLE XIII.

THE ABSORPTION BANDS OF
2-Amino-2-methylpropane hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	2.93 + 0.023	3413	0.33	1	4	2.91 - 2.95	3500 - 3300	-N-H (pri.) stretching (asy) -N-H (pri.) stretching (sym)
2	3.44 + 0.050	2907	1.60	7	4	3.12 - 3.71	3200 - 2955	-NH ₃ ⁺ (unspecified)
	3.55 + 0.005	2817	0.77	8	5		2985 - 2890	(CH ₃) ₃ C- stretching (asy)
	3.70 + 0.005	2703	0.41	9	5		2967 - 2874	(CH ₃) ₃ C- stretching (sym)
							2890 - 2825	(CH ₃) ₃ C- stretching (asy)
						2700 - 2480	-NH ₃ ⁺ (pri.) (unspecified)	
3	3.86 + 0.005	2591	0.43	1	6	3.85 - 3.87	2700 - 2480	-NH ₃ ⁺ (pri.) (unspecified)
4	4.02 + 0.005	2488	0.34	1	6	4.01 - 4.03	2700 - 2480	-NH ₃ ⁺ (pri.) (unspecified)
5	4.91 + 0.008	2037	0.58	7	6	4.82 - 5.14	2050 - 1800	-NH ₃ ⁺ (pri.) (unspecified)
	5.13 + 0.010	1949	0.18	9	3			
6	6.23 + 0.005	1605	0.34	4	6	5.75 - 6.24	1650 - 1590	-NH ₂ deformation
							1642 - 1625	-NH ₃ ⁺ (pri.) (unspecified)
7	6.66 + 0.008	1502	0.40	7	6	6.65 - 6.82	1572 - 1493	-NH ₃ ⁺ (pri.) (unspecified)
	6.77 + 0.013	1480	0.25	9	3		1477 - 1420	(CH ₃) ₃ C- scissors (asy)
8	7.02 + 0.038	1425	0.17	1	3	6.98 - 7.06	1477 - 1420	(CH ₃) ₃ C- scissors (asy)
9	7.15 + 0.005	1399	0.52	7	6	7.14 - 7.30	1397 - 1364	(CH ₃) ₃ C- scissors (sym)
	7.29 + 0.008	1372	0.62	9	6		1375 - 1345	(CH ₃) ₃ C- scissors (sym)

TABLE XIII. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
10	7.72 + 0.005	1295	0.47	1	6	7.71 - 7.73	1305 - 1275	-CH ₂ - wagging deformation
11	8.26 + 0.020	1211	0.51	4	4	8.24 - 8.60	1250 - 1200 1220 - 1020 1200 - 1180	(CH ₂) ₃ C- skeletal scissors -C-N (unspecified) CH ₃ - twisting deformation
12	10.14 + 0.033	986	0.10	1	3	10.10 - 10.18		
13	10.72 + 0.025	933	0.09	1	3	10.70 - 10.74	950 - 860	(CH ₃) ₃ C- skeletal deformation
14	11.36 + 0.058	880	0.11	1	2	11.33 - 11.79	950 - 860	(CH ₃) ₃ C- skeletal deformation
15	13.71 + 0.073	729	0.09	1	3	13.63 - 13.69		

TABLE XIV.

THE ABSORPTION BANDS OF

2,2,8,8-Tetramethyl-3,7-diaza-1,5,9-nonanetriol dihydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.04 + 0.013	3289	0.80	1	6	3.03 - 3.05	3600 - 2500 3500 - 3300	-O-H (sec.) stretching -N-H (sec.) stretching (asy) -N-H (sec.) stretching (sym)
2	3.37 + 0.030 3.45 + 0.020	2967 2899	1.50 1.40	7 9	3 3	3.34 - 3.56	3200 - 2955 2985 - 2890 2967 - 2874 2890 - 2825	-NH ₂ ⁺ - (sec.) (unspecified) (CH ₃) ₃ C- stretching (asy) (CH ₃) ₃ C- stretching (sym) (CH ₃) ₃ C- stretching (asy)
3	3.76 + 0.008 3.86 + 0.005 4.02 + 0.008	2660 2591 2488	0.58 0.58 0.30	7 8 9	5 5 5	3.71 - 4.32	2700 - 2480	-NH ₂ ⁺ - (sec.) (unspecified)
4	4.92 + 0.010 5.12 + 0.015	2033 1954	0.26 0.14	7 9	6 5	4.80 - 5.14	2050 - 1800	-NH ₂ ⁺ - (sec.) (unspecified)
5	6.25 + 0.008 6.36 + 0.020	1603 1572	0.26 0.20	7 9	6 3	6.02 - 6.41	1650 - 1550 1642 - 1560 1572 - 1493	-NH- (sec.) deformation -NH ₂ ⁺ - (sec.) deformation -NH ₂ ⁺ - (sec.) (unspecified)
6	6.66 + 0.008 6.76 + 0.018	1502 1479	0.34 0.42	7 9	5 6	6.61 - 6.86	1572 - 1493 1477 - 1420	-NH ₂ ⁺ - (sec.) (unspecified) (CH ₃) ₃ C- scissors (asy)
7	7.02 + 0.038	1425	0.33	1	4	6.98 - 7.06	1477 - 1420 1433 - 1375 1433 - 1300	(CH ₃) ₃ C- scissors (asy) -OH ³ (sec.) (unspecified) -OH (sec.) rocking deformation
8	7.14 + 0.010	1401	0.53	1	6	7.13 - 7.15	1433 - 1300	-OH (sec.) rocking deformation

TABLE XIV. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
Peak Wavelength	Wavenumber	Abs.	Type	Shape				
9	7.27 + 0.020	1376	0.62	1	6	7.25 - 7.29	1397 - 1364 1375 - 1345	(CH ₃) ₃ C- scissors (sym) (CH ₃) ₃ C- scissors (sym)
10	7.57 + 0.010	1321	0.31	4	3	7.53 - 7.58	1350 - 1260	-OH (sec.) deformation -C-O stretching
11	7.72 + 0.008	1295	0.35	1	6	7.71 - 7.73	1350 - 1260	-OH (sec.) deformation -C-O stretching
12	7.93 + 0.025 8.04 + 0.015	1261 1244	0.22 0.22	7 9	3 3	7.91 - 8.06	1350 - 1260 1275 - 1225	-OH (sec.) deformation -C-O stretching (CH ₃) ₃ C- skeletal scissors
13	8.28 + 0.040 8.44 + 0.010	1208 1185	0.42 0.53	7 9	3 6	8.24 - 8.45	1220 - 1175 1220 - 1020	(CH ₃) ₃ C- skeletal scissors -C-N (unspecified)
14	8.82 + 0.010	1134	0.86	4	6	8.81 - 8.99	1164 - 1052 1150 - 1085 1140 - 1130 1125 - 1025	-OH (sec.) (unspecified) -NH- (sec.) (unspecified) CH ₃ - rocking deformation -OH (sec.) deformation
15	9.24 + 0.025	1082	0.30	4	5	9.22 - 9.79	1164 - 1052 1125 - 1025 1038 - 1022	-OH (sec.) (unspecified) -OH (sec.) deformation -C-N stretching
16	10.12 + 0.050	988	0.18	1	4	10.07 - 10.17		
17	10.56 + 0.043	947	0.19	1	4	10.52 - 10.60	950 - 860	(CH ₃) ₃ C- skeletal deformation
18	12.18 + 0.035	821	0.16	1	4	12.14 - 12.22		

THE ABSORPTION BANDS OF

Band No.	Characteristics of the Peak Maxima in the Band						Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape				
1	2.88 + 0.025	3472	1.08	7	3	2.85 - 4.29	3700 - 3496	-O-H (pri.) stretching (asy)	
	2.96 + 0.020	3378	1.09	8	3		3650 - 2500	-O-H (pri.) stretching	
	3.34 + 0.075	2994	1.80	8	4		3500 - 3300	-N-H (pri.) stretching (asy)	
	3.72 + 0.030	2688	0.33	8	3			-N-H (pri.) stretching (sym)	
	3.88 + 0.028	2577	0.37	9	4		3200 - 2955	-NH ₃ ⁺ (pri.) (unspecified)	
							2985 - 2890	(CH ₃) ₃ C- stretching (asy)	
							2967 - 2874	(CH ₃) ₃ C- stretching (sym)	
							2890 - 2825	(CH ₃) ₃ C- stretching (asy)	
							2700 - 2480	-NH ₃ ⁺ (pri.) (unspecified)	
2	4.93 + 0.023	2028	0.33	4	6	4.91 - 5.15	2050 - 1800	-NH ₃ ⁺ (unspecified)	
3	6.19 + 0.005	1616	0.66	7	5	6.02 - 6.39	1650 - 1590	-NH ₂ (pri.) deformation	
	6.24 + 0.005	1603	0.64	8	5		1642 - 1525	-NH ₃ ⁺ (pri.) (unspecified)	
	6.28 + 0.005	1592	0.48	9	3		1572 - 1493	-NH ₃ ⁺ (pri.) (unspecified)	
4	6.70 + 0.005	1493	1.00	4	5	6.58 - 6.87	1572 - 1493	-NH ₃ ⁺ (pri.) (unspecified)	
							1477 - 1420	(CH ₃) ₃ C- scissors deformation	
							1466 - 1400	-OH (pri.) (unspecified)	
5	7.13 + 0.018	1402	0.79	7	4	7.11 - 7.27	1466 - 1400	-OH (pri.) (unspecified)	
	7.26 + 0.008	1377	0.66	9	6		1433 - 1300	-OH (pri.) rocking deformation	
							1397 - 1364	(CH ₃) ₃ C- scissors def. (sym)	
6	7.62 + 0.025	1312	0.30	1	4	7.60 - 7.64	1350 - 1260	-OH (pri.) deformation -C-O stretching	

TABLE XV. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
7	7.81 + 0.018	1280	0.56	1	6	7.80 - 7.82	1350 - 1260 1275 - 1225	-OH (pri.) deformation -C-O stretching (CH ₃) ₃ C- skeletal scissors
8	8.07 + 0.020	1239	0.41	1	6	8.05 - 8.09	1275 - 1200	(CH ₃) ₃ C- skeletal scissors
9	8.57 + 0.025	1167	0.54	1	4	8.55 - 8.59	1220 - 1020 1178 - 1000	-C-N (unspecified) -OH (pri.) (unspecified)
10	9.32 + 0.013	1073	0.88	7	6	9.31 - 9.68	1220 - 1020	-C-N (unspecified)
	9.46 + 0.008	1057	0.96	8	6		1178 - 1000	-OH (pri.) (unspecified)
	9.66 + 0.015	1053	1.12	9	6		1075 - 1000	-OH (pri.) deformation -C-O stretching
11	10.54 + 0.020	949	0.28	4	4	10.40 - 10.56	950 - 860	(CH ₃) ₃ C- skeletal deformation
12	10.94 + 0.013	914	0.32	1	6	10.93 - 10.95	950 - 860	(CH ₃) ₃ C- skeletal deformation
13	11.27 + 0.070	887	0.16	1	2	11.20 - 11.35	950 - 860	(CH ₃) ₃ C- skeletal deformation
14	13.48 + 0.053	742	0.15	4	3	13.36 - 13.53		

TABLE XVI.

THE ABSORPTION BANDS OF

2,2,8,8-Tetramethyl-3,7-diaza-1,5,9-nonanetriol dihydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.00 + 0.040	3333	1.40	4	4	2.93 - 3.05	3600 - 2500 3500 - 3300	-O-H (pri. & sec.) stretching -N-H (sec.) stretching (asy) -N-H (sec.) stretching (sym)
2	3.36 + 0.043 3.57 + 0.030	2976 2801	1.05 1.09	7 9	3 3	3.24 - 4.83	3200 - 2955 2985 - 2890 2967 - 2874 2890 - 2825 2855 2700 - 2480	-NH ₂ ⁺ (sec.) (unspecified) (CH ₃) ₃ C- stretching (asy) (CH ₃) ₃ C- stretching (sym) (CH ₃) ₃ C- stretching (asy) -CH ₂ - scissors (sym) -NH ₂ ⁺ scissors
3	6.18 + 0.050	1618	0.18	4	3	6.02 - 6.25	1650 - 1550 1645 - 1560	-NH- (sec.) deformation -NH ₂ ⁺ (sec.) deformation
4	6.48 + 0.023	1543	0.62	4	4	6.32 - 6.62	1650 - 1550 1642 - 1560 1572 - 1493	-NH- (sec.) deformation -NH ₂ ⁺ (sec.) deformation -NH ₂ ⁺ (sec.) (unspecified)
5	6.75 + 0.023 6.92 + 0.023	1481 1445	0.34 0.52	7 9	3 4	6.73 - 6.94	1480 - 1420 1477 - 1420 1470 1466 - 1400	-CH ₂ - scissors (asy) (CH ₃) ₃ C- scissors (asy) -CH ₂ - scissors (sym) -OH ⁺ (pri.) (unspecified)
6	7.22 + 0.018	1385	0.67	4	4	7.08 - 7.35	1466 - 1400 1433 - 1375 1400 - 1300 1397 - 1364 1375 - 1345	-OH (pri.) (unspecified) -OH (sec.) (unspecified) -OH (pri. & sec.) rocking def. (CH ₃) ₃ C- scissors (sym) (CH ₃) ₃ C- scissors (sym)

TABLE XVI. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
7	7.55 ± 0.008	1324	0.33	1	5	7.54 - 7.56	1400 - 1300 1350 - 1260	-OH (pri. & sec.) rocking def. -OH (sec.) deformation -C-O stretching
8	7.66 ± 0.025	1305	0.29	1	3	7.64 - 7.68	1350 - 1260 1305 - 1275	-OH (sec.) deformation -C-O stretching -CH ₂ - wagging deformation
9	7.82 ± 0.013 7.88 ± 0.008	1279 1269	0.36 0.35	7 9	3 3	7.81 - 7.89	1350 - 1260 1305 - 1275 1275 - 1225 1250 - 1200	-OH (sec.) deformation -C-O stretching -CH ₂ - wagging deformation (CH ₃) ₃ C- skeletal scissors (CH ₃) ₃ C- skeletal scissors
10	8.27 ± 0.043	1209	0.35	1	2	8.23 - 8.31	1220 - 1175 1220 - 1020	(CH ₃) ₃ C- skeletal scissors -C-N (unspecified)
11	8.47 ± 0.015	1181	0.38	4	5	8.45 - 8.49	1220 - 1175 1220 - 1020 1200 - 1180 1178 - 1000	(CH ₃) ₃ C- skeletal scissors -C-N (unspecified) -CH ₂ - twisting deformation -OH (pri.) (unspecified)
12	9.05 ± 0.010	1105	0.60	1	6	9.04 - 9.06	1220 - 1020 1178 - 1000 1164 - 1052 1150 - 1085 1125 - 1025	-C-N (unspecified) -OH (pri.) (unspecified) -OH (sec.) (unspecified) -NH- (sec.) (unspecified) -OH (sec.) deformation -C-O stretching

TABLE XVI. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
13	9.45 ± 0.040	1058	1.20	7	4	9.38 - 10.24	1220 - 1020	-C-N (unspecified)
	9.84 ± 0.020	1016	0.38	8	3		1178 - 1000	-OH (pri.) (unspecified)
	10.22 ± 0.020	978	0.32	9	3		1164 - 1052	-OH (sec.) (unspecified)
							1125 - 1025	-OH (sec.) deformation
								-C-O stretching
14	11.07 ± 0.023	903	0.30	4	4	10.85 - 11.09	950 - 860	(CH ₃) ₃ C- skeletal deformation
15	11.40 ± 0.100	877	0.16	1	2	11.30 - 11.55	950 - 860	(CH ₃) ₃ C- skeletal deformation
16	12.33 ± 0.038	811	0.33	4	4	12.29 - 12.55		
17	13.23 ± 0.033	756	0.13	4	3	13.00 - 13.35		

THE ABSORPTION BANDS OF

2-Amino-2-methyl-1,3-propanediol hydrochloride

Band No.	Characteristics of the Peak	Maxima in the Band	Abs.	Type	Shape	Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
1	2.93 + 0.065 3.27 + 0.032 3.28 + 0.038	3413 3058 2577	1.20 1.60 0.24	7 8 9	3 3 3	2.82 - 4.26	3700 - 3496 3650 - 2500 3500 - 3300 3200 - 2955 2985 - 2890 2967 - 2874 2890 - 2825 2700 - 2480	-O-H (pri.) stretching (asy) -O-H (pri.) stretching -N-H (pri.) stretching (asy) -N-H (pri.) stretching (sym) -NH ₃ ⁺ (pri.) (unspecified) (CH ₃) ₃ C- stretching (asy) (CH ₃) ₃ C- stretching (sym) (CH ₃) ₃ C- stretching (asy) -NH ₃ ⁺ (pri.) (unspecified)
2	5.08 + 0.040	1969	0.17	4	3	4.74 - 5.12	2050 - 1800	-NH ₃ ⁺ (pri.) (unspecified)
3	6.24 + 0.015	1603	0.62	4	4	6.01 - 6.30	1650 - 1590 1642 - 1560	-NH ₂ (pri.) deformation -NH ₃ ⁺ deformation
4	6.68 + 0.025	1497	0.78	4	3	6.56 - 6.82	1572 - 1493 1477 - 1420 1466 - 1400	-NH ₃ ⁺ (unspecified) (CH ₃) ₃ C- scissors (asy) -OH (pri.) (unspecified)
5	7.14 + 0.038	1401	0.46	4	4	7.10 - 7.21	1466 - 1400 1400 - 1300 1397 - 1364	-OH (pri.) (unspecified) -OH (pri.) rocking def. (CH ₃) ₃ C- scissors (sym)
6	7.63 + 0.025	1311	0.30	4	3	7.53 - 7.72	1350 - 1260	-OH (pri.) deformation -C=O stretching

TABLE XVII. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
7	8.06 + 0.038	1241	0.28	7	3	8.02 - 8.35	1275 - 1225	(CH ₃) ₃ C- skeletal scissors
	8.26 + 0.028	1211	0.26	9	3		1220 - 1175	(CH ₃) ₃ C- skeletal scissors
							1220 - 1020	-C-N (unspecified)
							1200 - 1180	-CH ₂ - twisting deformation
8	8.82 + 0.033	1134	0.30	4	4	8.72 - 8.85	1220 - 1020	-C-N (unspecified)
							1178 - 1000	-OH (pri.) (unspecified)
							1150 - 1080	-NH ₃ ⁺ (unspecified)
9	9.34 + 0.015	1071	0.13	7	3	9.19 - 9.79	1220 - 1020	-C-N (unspecified)
	9.47 + 0.043	1056	0.13	8	3		1075 - 1000	-OH (pri.) deformation
	9.75 + 0.020	1026	0.82	9	5			-C-O stretching
10	10.41 + 0.050	961	0.18	1	3	10.36 - 10.46		
11	10.95 + 0.050	913	0.18	1	3	10.90 - 11.00	950 - 860	(CH ₃) ₃ C- skeletal deformation
12	13.38 + 0.175	747	0.15	1	2	13.20 - 13.56		

TABLE XVIII.

THE ABSORPTION BANDS OF

2,8-Bis(hydroxymethyl)-2,8-dimethyl-3,7-diaza-1,5,9-nonanetriol dihydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.01 ± 0.023	3322	1.13	7	3	2.95 - 4.31	3600 - 2500	-O-H (pri. & sec.) stretching
	3.36 ± 0.043	2976	0.64	8	3		3500 - 3300	-N-H (sec.) stretching (asy)
	3.56 ± 0.035	2809	0.57	9	3			-N-H (sec.) stretching (sym)
							3200 - 2955	-NH ₂ ⁺ (sec.) (unspecified)
							2985 - 2890	(CH ₃) ₃ C- stretching (asy)
							2967 - 2874	(CH ₃) ₃ C- stretching (sym)
							2890 - 2825	(CH ₃) ₃ C- stretching (asy)
2	6.38 ± 0.020	1567	0.36	4	3	6.02 - 6.56	2700 - 2480	-NH ₂ ⁺ (sec.) (unspecified)
							1650 - 1550	-NH- (sec.) deformation
							1642 - 1560	-NH ₂ ⁺ deformation
3	6.88 ± 0.025	1453	0.40	7	3	6.70 - 7.62	1572 - 1493	-NH ₂ ⁺ (unspecified)
	7.21 ± 0.025	1387	0.42	9	3			
								(CH ₃) ₃ C- scissors (asy)
							1477 - 1420	-OH (pri.) (unspecified)
							1466 - 1400	-OH (pri. & sec.) rocking def.
							1433 - 1400	(CH ₃) ₃ C- scissors (sym)
							1397 - 1364	(CH ₃) ₃ C- scissors (sym)
4	7.76 ± 0.055	1289	0.23	7	3	7.70 - 7.97	1375 - 1345	-OH (pri. & sec.) def.
	7.93 ± 0.038	1261	0.23	9	3		1350 - 1260	-C-O stretching
							1350 - 1260	-OH (pri. & sec.) deformation
								-C-O stretching
5	8.42 ± 0.050	1188	0.26	1	4	8.37 - 8.47	1305 - 1275	-CH ₂ - wagging deformation
							1275 - 1225	(CH ₃) ₃ C- skeletal scissors
							1220 - 1175	(CH ₃) ₃ C- skeletal scissors
							1220 - 1020	-C-H (unspecified)
							1200 - 1180	-CH ₂ - twisting deformation

TABLE XVIII. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
Peak Wavelength	Wavenumber	Abs.	Type	Shape				
6	9.06 + 0.025	1104	0.33	4	5	8.88 - 9.13	1220 - 1020 1178 - 1000 1150 - 1085 1125 - 1025	-C-N (unspecified) -OH (pri. & sec.)(unspecified) -N-H (sec.) (unspecified) -OH (pri. & sec.) deformation -C-O stretching
7	9.52 + 0.045	1050	0.84	4	3	9.38 - 9.96	1220 - 1020 1178 - 1000 1125 - 1025 1038 - 1022	-C-N (unspecified) -OH (pri. & sec.)(unspecified) -OH (pri. & sec.) deformation -C-O stretching -C-N stretching
8	10.44 + 0.025	958	0.19	1	3	10.42 - 10.46		
9	11.08 + 0.038	903	0.22	4	4	10.86 - 11.59	950 - 860	(CH ₃) ₃ C- skeletal deformation
10	12.24 + 0.050	817	0.16	1	4	12.19 - 12.29		

TABLE XIX.

THE ABSORPTION BANDS OF

2-Amino-2-hydroxymethyl-1,3-propanediol hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.10 + 0.045	3226	1.70	7	4	3.00 - 4.20	3650 - 2500	-O-H (pri.) stretching
	3.35 + 0.050	2985	1.40	8	4		3500 - 3300	-N-H (pri.) stretching (asy)
	3.85 + 0.030	2597	0.29	9	3			-N-H (pri.) stretching (sym)
							3200 - 2995	-NH ₃ ⁺ (pri.) (unspecified)
							2985 - 2890	(CH ₃) ₃ C- stretching (asy)
							2967 - 2874	(CH ₃) ₃ C- stretching (sym)
							2890 - 2825	(CH ₃) ₃ C- stretching (asy)
2	4.78 + 0.070	2092	0.17	4	3	4.65 - 4.95	2700 - 2480	-NH ₃ ⁺ (pri.) (unspecified)
3	6.12 + 0.008	1634	0.80	4	6	6.02 - 6.13	2050 - 1800	-NH ₃ ⁺ (pri.) (unspecified)
4	6.33 + 0.020	1580	0.27	1	3	6.31 - 6.35	1650 - 1590	-NH ₂ (pri.) deformation
							1642 - 1525	-NH ₃ ⁺ (pri.) (unspecified)
5	6.43 + 0.005	1552	0.67	1	6	6.42 - 6.44	1642 - 1525	-NH ₃ ⁺ (unspecified)
							1572 - 1493	-NH ₃ ⁺ (unspecified)
6	6.66 + 0.025	1502	0.28	4	3	6.60 - 6.73	1572 - 1493	-NH ₃ ⁺ (unspecified)
7	6.85 + 0.005	1460	0.31	4	5	6.80 - 6.90	1477 - 1420	(CH ₃) ₃ C- scissors (asy)
							1466 - 1400	-OH (pri.) (unspecified)
8	7.15 + 0.020	1399	0.30	4	3	7.13 - 7.30	1466 - 1400	-OH (pri.) (unspecified)
							1433 - 1300	-OH (pri.) rocking deformation
							1397 - 1364	(CH ₃) ₃ C- scissors (sym)
							1375 - 1345	(CH ₃) ₃ C- scissors (sym)

TABLE XIX. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
9	7.74 + 0.005	1292	0.54	1	6	7.73 - 7.75	1350 - 1260	-OH (pri.) deformation -C-O stretching
10	8.33 + 0.050	1200	0.26	4	3	8.15 - 8.45	1250 - 1200 1220 - 1175 1220 - 1020	(CH ₃) ₃ C- skeletal scissors (CH) ⁻ C- skeletal scissors -C-N (unspecified)
11	8.85 + 0.023	1130	0.30	1	3	8.83 - 8.87	1220 - 1020 1178 - 1000	-C-N (unspecified) -OH (pri.) (unspecified)
12	9.54 + 0.030 9.67 + 0.018	1048 1034	1.05 1.30	7 9	3 4	9.48 - 9.75	1220 - 1020 1178 - 1000 1075 - 1000	-C-N (unspecified) -OH (pri.) (unspecified) -OH (pri.) deformation -C-O stretching
13	11.07 + 0.025 11.20 + 0.038	903 893	0.15 0.14	7 9	3 3	11.00 - 11.35	950 - 860	(CH ₃) ₃ C- skeletal deformation

TABLE XI.

THE ABSORPTION BANDS OF

2,2,8,8-Tetrakis(hydroxymethyl)-3,7-diaza-1,5,9-nonanetriol dihydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.10 + 0.125	3226	1.80	4	4	2.90 - 4.32	3600 - 2500 3500 - 3300 3200 - 2955 2985 - 2890 2967 - 2874 2890 - 2825 2700 - 2480	-O-H (sec.) stretching -N-H (sec.) stretching (asy) -N-H (sec.) stretching (sym) -NH ₂ ⁺ (sec.) (unspecified) (CH ₃) ₃ C- stretching (asy) (CH ₃) ₃ C- stretching (sym) (CH ₃) ₃ C- stretching (asy) -NH ₂ ⁺ (unspecified)
2	6.40 + 0.020	1563	0.86	4	6	6.02 - 6.50	1650 - 1550 1642 - 1560 1572 - 1493	-NH- (sec.) deformation -NH ₂ ⁺ (sec.) deformation -NH ₂ ⁺ (sec.) (unspecified)
3	6.85 + 0.075 7.18 + 0.075	1460 1393	0.66 0.68	7 9	4 4	6.70 - 7.60	1477 - 1420 1466 - 1400 1433 - 1300 1397 - 1364 1375 - 1345 1350 - 1260	(CH ₃) ₃ C- scissors (asy) -OH (pri.) (unspecified) -OH (sec.) rocking deformation (CH ₃) ₃ C- scissors (sym) (CH ₃) ₃ C- scissors (sym) -OH (pri. & sec.) deformation -C-O stretching
4	7.90 + 0.045 8.25 + 0.045	1266 1212	0.47 0.43	7 9	3 3	7.80 - 8.35	1350 - 1260 1275 - 1225 1220 - 1175 1220 - 1020	-OH (pri. & sec.) deformation -C-O stretching (CH ₃) ₃ C- skeletal scissors (CH ₃) ₃ C- skeletal scissors -C-N (unspecified)

TABLE IX. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
5	8.73 + 0.038	1145	0.56	7	4	8.20 - 9.07	1220 - 1175	(CH ₃) ₃ C- skeletal scissors
	9.04 + 0.030	1106	0.59	9	3		1220 - 1020	-C-N ₃ (unspecified)
							1178 - 1000	-OH (pri.) (Unspecified)
							1164 - 1052	-OH (sec.) (unspecified)
							1150 - 1085	-NH- (sec.) (unspecified)
							1119 - 1105	-OH (sec.) deformation
								-C-O stretching
6	9.53 + 0.130	1049	1.50	7	4	9.35 - 9.90	1078 - 1000	-OH (pri.) (unspecified)
	9.84 + 0.033	1016	1.30	9	4		1075 - 1000	-OH (pri.) deformation
								-C-O stretching
7	10.18 + 0.025	982	0.62	4	4	10.10 - 10.40		
8	10.72 + 0.050	933	0.26	1	3	10.67 - 10.77	950 - 860	(CH ₃) ₃ C- skeletal deformation
9	10.98 + 0.050	911	0.24	1	3	10.93 - 11.03	950 - 860	(CH ₃) ₃ C- skeletal deformation
10	11.28 + 0.030	887	0.29	1	3	11.25 - 11.31	950 - 860	(CH ₃) ₃ C- skeletal deformation
11	11.55 + 0.075	866	0.23	1	3	11.47 - 11.63	950 - 860	(CH ₃) ₃ C- skeletal deformation

TABLE XXI.

THE ABSORPTION BANDS OF
Aminomethane hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	2.90 + 0.013	3448	0.54	4	3	2.85 - 2.97	3500 - 3300	-N-H (pri.) stretching (asy) -N-H (pri.) stretching (sym)
2	3.26 + 0.078	3067	1.60	4	4	3.00 - 3.80	3500 - 3300 3200 - 2955 2985 - 2890 2700 - 2480	-N-H (pri.) stretching (asy) -N-H (pri.) stretching (sym) -NH ₃ ⁺ (unspecified) CH ₃ - stretching (asy. & sym.) -NH ₃ ⁺ (unspecified)
3	3.97 + 0.038 4.16 + 0.013	2519 2404	0.13 0.15	7 9	3 5	3.92 - 4.25	2700 - 2480	-NH ₃ ⁺ (unspecified)
4	5.38 + 0.125	1859	0.10	1	2	5.25 - 5.51	2050 - 1800	-NH ₃ ⁺ (unspecified)
5	6.31 + 0.008	1585	0.45	4	3	6.02 - 6.47	1650 - 1590 1642 - 1625 1572 - 1493	-NH ₂ (pri.) deformation -NH ₃ ⁺ (pri.) (unspecified) -NH ₃ ⁺ (pri.) (unspecified)
6	6.65 + 0.020 6.73 + 0.008 6.98 + 0.020	1504 1486 1433	0.58 0.94 0.38	7 8 9	3 5 5	6.60 - 7.01	1572 - 1493 1479 - 1420 1460 - 1430	-NH ₃ ⁺ (pri.) (unspecified) CH ₃ - scissors (asy.) CH ₃ -N- deformation
7	7.10 + 0.005	1408	0.50	4	5	7.04 - 7.23	1400 - 1351	CH ₃ - scissors (sym.)
8	7.97 + 0.018	1255	0.40	1	6	7.93 - 8.01		
9	9.99 + 0.015	1001	0.30	4	6	9.95 - 10.10	995	-C-N stretching
10	10.78 + 0.020	928	1.40	4	3	10.34 - 11.04		

TABLE XXII.

THE ABSORPTION BANDS OF
Aminoethane hydrochloride

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
1	3.34 + 0.085	2994	1.50	7	4	2.95 - 3.95	3500 - 3300	-N-H (pri.) stretching (asy)
	3.80 + 0.013	2632	0.39	8	3			-N-H (pri.) stretching (sym)
	3.95 + 0.005	2531	0.34	9	5		3200 - 2955	-NH ₃ ⁺ (pri.) (unspecified)
							2994 - 2900	CH ₃ CH ₂ - stretching (asy)
							2967 - 2874	CH ₃ CH ₂ - stretching (sym)
							2890 - 2833	CH ₃ CH ₂ - stretching (asy)
							2700 - 2480	-NH ₃ ⁺ (pri.) (unspecified)
2	4.16 + 0.005	2404	0.40	1	6	4.15 - 4.17		
3	4.46 + 0.025	2242	0.11	1	3	4.44 - 4.48		
4	4.66 + 0.018	2146	0.10	1	3	4.64 - 4.68		
5	4.96 + 0.013	2016	0.40	7	4	4.81 - 5.25	2050 - 1800	-NH ₃ ⁺ (pri.) (unspecified)
	5.18 + 0.008	1931	0.13	9	3			
6	6.22 + 0.003	1597	0.52	1	6	6.02 - 6.27	1650 - 1590	-NH ₂ (pri.) deformation
							1642 - 1525	-NH ₃ ⁺ (pri.) (unspecified)
7	6.84 + 0.013	1462	1.10	4	4	6.65 - 6.97	1572 - 1493	-NH ₃ ⁺ (pri.) (unspecified)
							1477 - 1420	CH ₃ -CH ₂ - scissors (asy)
8	7.18 + 0.003	1393	0.56	7	6	7.10 - 7.37	1397 - 1351	CH ₃ -CH ₂ - scissors (sym)
	7.35 + 0.005	1361	0.23	9	5			
9	7.53 + 0.005	1328	0.27	1	6	7.52 - 7.54		

TABLE XXII. (Continued)

Band No.	Characteristics of the Peak Maxima in the Band					Band Position (microns)	Lit. Positions of Group Freq.	Structural Group and Vibrational Mode
	Peak Wavelength	Wavenumber	Abs.	Type	Shape			
10	8.25 + 0.003	1212	0.64	1	6	8.24 - 8.26	1220 - 1020	-C-N (unspecified)
11	8.44 + 0.005	1185	0.64	1	6	8.43 - 8.45	1200 - 1180	-CH ₂ - twisting deformation
12	9.64 + 0.005	1037	0.56	1	6	9.62 - 9.66		
13	10.33 + 0.008	968	0.67	7	5	10.32 - 10.46		
	10.45 + 0.005	957	1.00	9	6			
14	11.53 + 0.028	867	0.12	4	3	11.51 - 11.65		
15	12.64 + 0.015	791	1.00	4	6	12.63 - 12.92		

VI. DISCUSSION

The general similarities which were noted in the experimental spectra and in the tables of correlation can be summarized as follows:

- (1) The strongest, and often the widest absorption band occurs between 2.80 and 4.25 microns (3570 to 2350 cm^{-1}). It is usually a multiple-peak band with a number of minor shoulders. The position of this band corresponds to positions reported in the literature (3, 4, 5, 13, 17, 18, 19, 22, 26, 29, 31, 32) for a number of different vibrational modes of structural groups containing three basis units: the -O--H group, the -N--H group, and the -C--H group. It has been stated (4, 22, 32) that structural groups containing a hydrogen atom generally show these characteristic frequencies because (1) the vibration is not mass sensitive; and (2) the hydrogen atom is a terminal group.
- (2) The compounds of both series (Tables I & II) exhibit a fairly strong band in the region from 6.00 to 6.80 microns (1667 to 1470 cm^{-1}) which generally corresponds to the position of an amine salt deformation ($-\text{NH}_3^+$ and $-\text{NH}_2^+-$) in the region from 1650 to 1550 cm^{-1} .
- (3) The compounds which contain hydroxyl groups exhibit a fairly strong peak in the region from 8.75 to 9.50 microns (1145 to 1050 cm^{-1}), which corresponds to the positions reported for the C--O stretching and O--H deformational modes that are characteristic of the alcohols (4). The moderately strong peak at $9.06\text{ }\mu$ (1104 cm^{-1}) in the spectrum of 1,3-diaminopropane appears to be an exception, but this peak may be due to the trimethylene diamine skeletal vibration at 1096 cm^{-1} . (Table III)
The compounds which do not contain hydroxyl groups (Compounds 101, 201, 301, and 401) generally do not exhibit a strong peak in this region,

and their spectra have narrower bands and sharper peaks than those which have a hydroxyl group attached to the same alkane skeleton. (Figures 32 and 34; Figures 38 and 40) For the compounds which have more than one hydroxyl group attached to the same alkane skeleton, the bands appear broader and the peaks more rounded as the number of hydroxyl groups becomes larger. (Figures 32, 34, & 36; Figures 38, 40, & 42) The unusually sharp peaks in the spectrum of compound 431 (Figure 44) are an exception to this general trend.

- (4) The symmetrical diamines generally exhibit a peak in the region from 9.25 to 10.25 μ , which corresponds to the positions reported (4,22) for the C--O stretching and O--H deformational vibrations of the secondary alcohol group (1125 to 1025 cm^{-1}). The spectrum of 1,3-diamino-2-propanol dihydrochloride (Figure 29) shows three peaks in this region which do not appear in the spectrum of 1,3-diaminopropane dihydrochloride (Figure 28).
- (5) The symmetrical diamines and their corresponding parent monoamines, which have hydroxyl groups attached to the alkane skeleton as primary alcohol structures, exhibit a strong peak in the region from 9.30 μ to 10.00 μ . This region corresponds to the positions reported (4,22) for the C--O stretching and O--H deformational vibrations of the primary alcohol group (1075 to 1000 cm^{-1}).
- (6) The intensities of the bands in the region from 11.00 to 15.50 μ (909 to 645 cm^{-1}) generally decrease, as branching at the alpha carbon increases. (Figures 47, 32, 38) It is interesting to note, however, that for the symmetrical diamines, which contain the unbranched methylene chain in the 2-propanol bridging structure, the intensities of the bands in this region are greater than the intensities of the corresponding bands in

their parent monoamines.

- (7) The isopropyl and tertiary-butyl skeletons of the parent monoamines are characterized in some of the spectra (Figures 32, 33, 34, 35, 38, 39, 40, 41, 42, 43, 44, & 45) by a series of minor peaks in the region from 10.00 μ to 12.65 μ (1000 to 790 cm^{-1}). In the spectra of the symmetrical diamines (Figures 33, 35, 39, 41, 43, & 45), the methylene units in the 2-propanol bridging structure contribute to the absorption in this region.

Structural group frequencies must always be used with caution, since the vibrational modes which give rise to the infrared absorption bands are determined by (1) the masses of the atoms of a molecule, (2) the force constants of the bonds between the atoms, (3) the symmetry of the molecule, and (4) the interaction of vibrations. Whenever correlations are made for a series of compounds, it is usually assumed that the masses of the atoms, force constants of the bonds, and vibrational interactions will remain constant, or will vary in a linear relationship from the simplest structure to the most complex. (32) The experimental spectra appear to exhibit general similarities which do vary in an approximately linear fashion among the compounds of each series, and the symmetrical diamines of Table I show a distinct similarity in the position of their absorption bands to those of their respective parent monoamines (Table II).

However, the absorption bands of one of the compounds which was studied appeared quite unusual and distinctly different from corresponding bands in the other spectra (Figure 37). This compound had been synthesized by an earlier worker and it was thought to be 2,8-bis(hydroxymethyl)-3,7-diaza-1,5,9-nonanetriol dihydrochloride (Compound 322). It was the only one of the twenty compounds which failed to crystallize, and the spectrum was obtained for this viscous oil by a "smear technique" (32). Mass spectrometric analysis

of this compound revealed that the molecular weight (220) corresponded to that of the propylene chlorohydrin derivative of the parent monoamine (Compound 321). The spectral data, supported by the mass spectrometric analysis, suggests that the original synthesis reaction did not proceed to completion (i.e., the coupling of two moles of the amine by each mole of epichlorohydrin), but had stopped after the first step, in which an epoxyamine was formed. When this product was treated with anhydrous hydrogen chloride, the epoxide ring was broken and the propylene chlorohydrin derivative of 321 (3-aza-6-chloro-2-hydroxymethyl-1,5-hexanediol hydrochloride) was formed. Since the supply of 321 (2-amino-1,3-propanediol) was extremely limited, no attempt was made in this work to resynthesize the symmetrical diamine (Compound 322), and no spectra for it were obtained.

It is hoped that the reference spectra and the tables of correlation of the absorption bands for these compounds will prove valuable in the interpretation of the infrared spectra of the chelates, and in clarifying the role of the hydroxyl groups in the coordinating properties of these ligands.

VII. SUMMARY

The infrared spectra of twenty amine hydrochlorides were recorded and studied, so that they could be used as reference spectra for further research. The positions of the absorption bands were compared with corresponding literature values for the characteristic frequencies of the molecular structural units. A code was devised for transferring this spectral data to IBM cards, and a Fortran source program was written to enable a digital computer (the IBM 1620) to make these comparisons for an unlimited number of group frequencies and a very large number of spectra; and the system should prove quite useful in the search of a large number of spectra for corresponding bands.

Of the ten symmetrical diamines which were studied, six contained the primary alcohol group. Two similar compounds without this group, 2,8-dimethyl-3,7-diaza-5-nonanol dihydrochloride and 2,2,8,8-Tetramethyl-3,7-diaza-5-nonanol dihydrochloride, were prepared in this work. A search of the literature did not yield any information about either of these two, and it is possible that they have not been prepared previously.

One of the compounds which was studied was a viscous oil. This compound had been synthesized by an earlier worker and was thought to be 2,8-Bis(hydroxymethyl)-3,7-diaza-1,5,9-nonanetriol dihydrochloride. However, the absorption bands in its spectrum (Figure 37) appeared unusually broad and distinctly different from corresponding bands in the other spectra. Mass spectrometric analysis revealed that the molecular weight of this compound corresponded to that of the propylene chlorohydrin derivative of the parent monoamine (2-amino-1,3-propanediol hydrochloride), and it is now suspected that the original synthesis reaction did not proceed to completion.

When purified, many of these amine hydrochlorides were found to be very hygroscopic, making them quite difficult to wash, even with anhydrous solvents. The powdered potassium bromide is also hygroscopic and the most transparent discs were obtained when the KBr had been dried overnight in a vacuum oven (100°C). It was found to be essential to evacuate the die for at least five minutes before applying pressure, to remove moisture from the mixture to the point where it had no significant effect on the spectra.

If the sample discs were exposed to the atmosphere for more than an hour, they became cloudy and the spectra lost their reproducibility. However, when they were no longer useable, they could be ground, dried in a vacuum oven, and re-pressed; and the spectra which were obtained were essentially the same as the originals.

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IX. AUTOBIOGRAPHY

I, Lawrence Ingram Briel, II, was born on February 1, 1940, in Richmond, Virginia. I attended local elementary and junior high schools and graduated from Thomas Jefferson High School in June 1958.

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