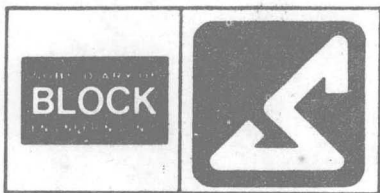


THE **SADTLER**

**STANDARD
SPECTRA**





SADTLER RESEARCH LABORATORIES, INC.

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RAMAN SPECTRA

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SADTLER STANDARD RAMAN SPECTRA

INTRODUCTION

This ongoing publication is intended to provide the spectroscopist with a central source of reliable data in the developing area of Raman spectroscopy.

Compounds for inclusion in the spectra collection were selected with the intention of providing simple compounds of representative functional groups at the beginning of the publication, progressing to more complex compounds in later volumes. The spectra in each volume are arranged according to the sequence of chemical functionality in the Sadtler Chemical Classes Index.

Sample Preparation

Every effort was made to obtain analytically pure samples for spectra preparation, however, many samples exhibited too much fluorescence in the initial rough Raman scan and further purification was necessary. Solid samples were recrystallized from a suitable solvent and liquid samples were stored over activated decolorizing charcoal for a prolonged time and the charcoal filtered off.

Instrumentation

All spectra contained in this publication were prepared on a Cary 83 Laser Raman Spectrophotometer. Solids were run in a single pass solid sample holder and with a spike filter placed between the laser and the sample. Liquids were run using a multi-pass cell.

The Cary 83 instrument utilizes the 4880⁰Å argon line, the laser power is a nominal 100 mW at the laser head and 30-60 mW at the sample. The nominal power was seldom achieved during preparation of the spectra, the actual power for each sample is indicated in the heading data on each spectrum. The source used in this volume of spectra was a Coherent Radiation model 59B Argon Ion laser and the detector is a bi-alkali cathode type photodetector. Sample geometry is 90⁰ in all cases. A Lexon model 75 Argon Ion laser is being used for the preparation of spectra in later volumes.

Sample Presentation

The spectra presentation format generally follows the recommendations for the presentation of Raman spectra by the Physical Chemistry Division of the Commission on Molecular Structure and Spectroscopy of The International Union of Pure and Applied Chemistry. Solid samples are represented by one non-polarized spectrum in every case. There are no spectra of solids in solution included. Liquid samples are represented by two spectra prepared at identical instrument settings; the parallel polarized scan and the perpendicular polarized scan. The infrared absorption spectrum for each compound is also included, in order to provide complimentary information. These absorption spectra have, in part, been taken from the previously published Sadtler Standard Grating Spectra publication and they were not necessarily prepared from the same sample as the Raman spectrum.

Data Presentation

Each spectrum shows the pertinent information as to compound name, molecular formula, molecular weight, structural formula, physical data (when available) and the source of the sample for the Raman scans. The instrumental parameters are also included.

The intensity values for those peaks which exceed the 100% intensity scale at high sensitivity on some spectra have been calculated according to the procedure shown on the following page and are shown in the data box labelled WAVELENGTH/INTENSITY on each spectrum.

Indexes

The indexes provided for location of spectra by chemical identity are as follows:

- the alphabetical index in chemical name sequence,
- the chemical classes index in chemical functionality sequence,
- the molecular formula index in increasing carbon atom sequence.

In each of the above indexes the Raman spectrum number of the compound is shown in the right hand column labelled RAMAN, with the numbers in the other columns referring to the location of that compound in the other Sadtler Standard Spectra publications.

The Raman Specfinder ® index provides a means of locating spectra by the position of intensity peaks, matching of peak locations of an unknown spectrum with this index will establish the spectrum numbers of comparable published spectra.

Comprehensive introductions to each of the above indexes are contained in the index section of the publication.

Instrumentation

All spectra contained in this publication were prepared on a Cary 83 Laser Raman Spectrophotometer. Solids were run in a single pass sample holder and with a spike filter placed between the laser and the sample. Liquids were run using a multi-pass cell.

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Sample Presentation

The spectra presentation format generally follows the recommendations for the presentation of Raman spectra by the Physical Chemistry Division of the Commission on Molecular Structure and Spectroscopy of The International Union of Pure and Applied Chemistry. Solid samples are represented by one non-polarized spectrum in every case. There are no spectra of solids in solution included. Liquid samples are represented by two spectra prepared at identical instrument settings: the parallel polarized scan and the perpendicular polarized scan. The infrared absorption spectrum for each compound is also included in order to provide complementary information. These absorption spectra have, in part, been taken from the previously published Sadtler Standard Grating Spectra publication and they were not necessarily prepared from the same sample as the Raman spectrum.

Data Presentation

Each spectrum shows the pertinent information as to compound name, molecular formula, molecular weight, structural formula (when available) and the source of the sample for the Raman scans. The instrumental parameters are also included.

Calculation of Intensities

Intensity values are derived by running a preliminary low sensitivity scan on each compound in which all peaks appear on the chart and the final higher sensitivity scan for publication in which some peaks may exceed the intensity scale. A single high, complete peak from the latter scan is selected and its intensity from the baseline is measured and compared with the intensity on the preliminary scan to obtain the ratio of intensity increase to sensitivity increase. This ratio is then applied to the peaks which exceed the intensity scale on the published spectrum and the wavelength/calculated intensity of each, together with the reference peak data is shown in the WAVELENGTH/INTENSITY data box.

The actual calculations for spectrum below are as follows:

Reference Peak at 384 cm^{-1}

Measured intensity 22.9 mm (preliminary scan) -- Sensitivity 2000

Measured intensity 71.0 mm (published scan) -- Sensitivity 6000

Ratio 3.1

Sample Peak at 2945 cm^{-1} -- Calculation Sample

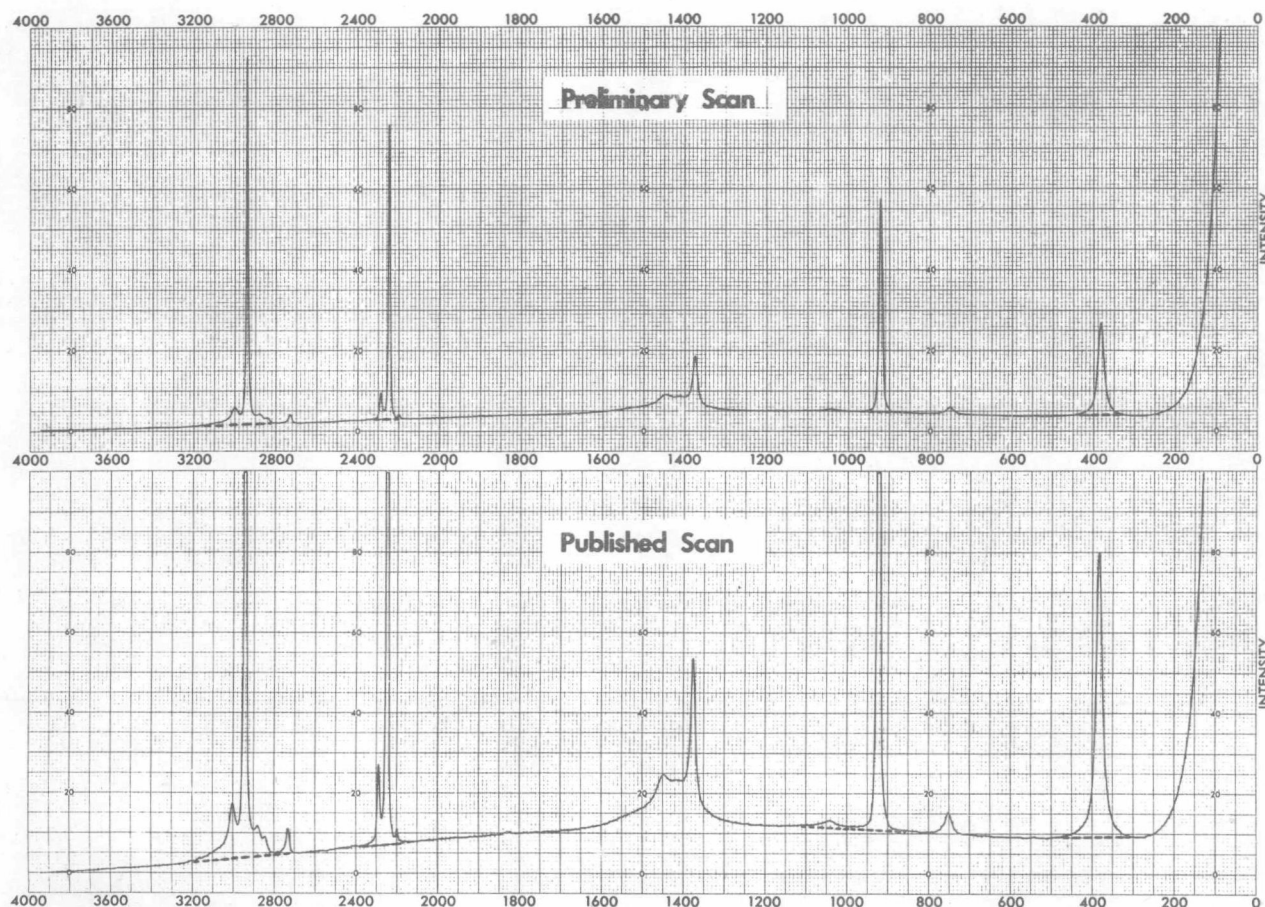
Measured intensity 91.1 mm (preliminary scan)

Calculated intensity 282.4 mm (published scan)

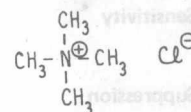
WAVENUMBER / INTENSITY

2945/282.4 2252/226.3 924/164.0

384/71.0



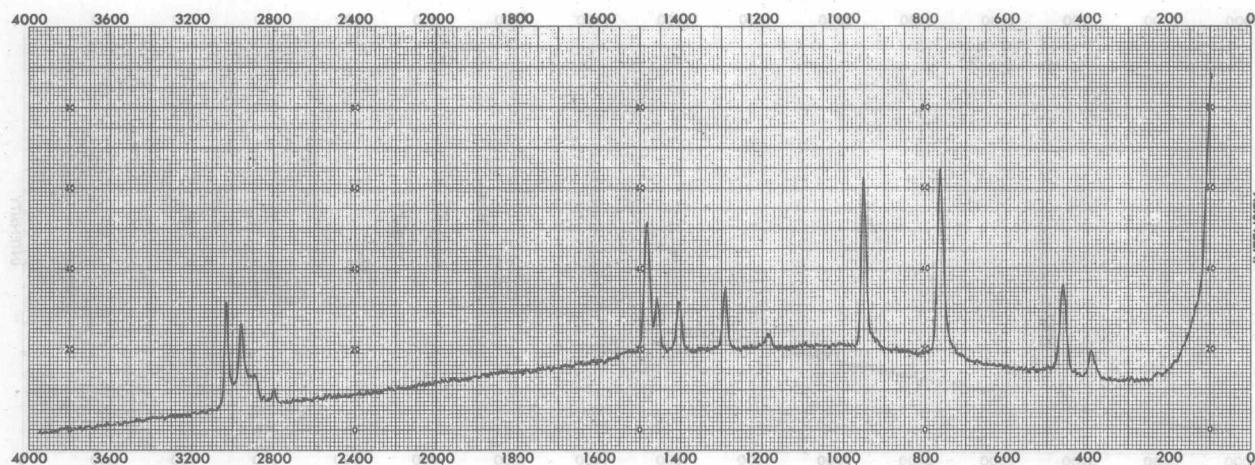
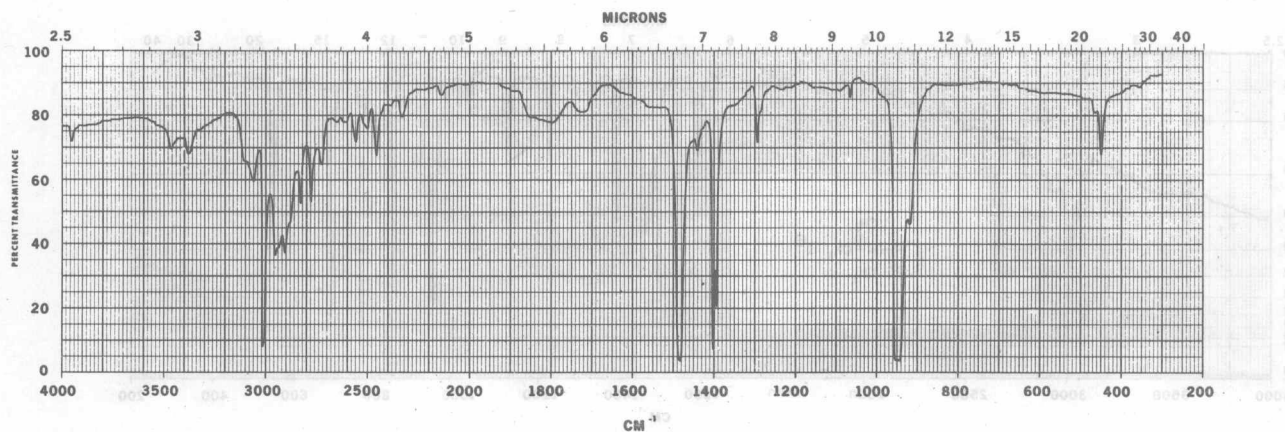
RAMAN DATA

Spectrophotometer Cary 83Sensitivity 50000Suppression 65Laser Power 11 mWSpectral Slitwidth 12 cm⁻¹ $C_4H_{12}ClN$ Mol. Wt. 109.60Source: Chem Service, Inc.,
West Chester, Pa.

WAVENUMBER / INTENSITY		
1485/60.3	951/79.8	764/87.7

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KBr Wafer



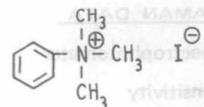
RAMAN DATA

Spectrophotometer Cary 83
Sensitivity 75000;
7500
Suppression 110;
0
Laser Power 11 mW
Spectral Slitwidth 12 cm⁻¹

$C_9H_{14}IN$ Mol. Wt. 263.12

M.P. 230°C (subl.)

Source: Chem Service, Inc.,
West Chester, Pa.

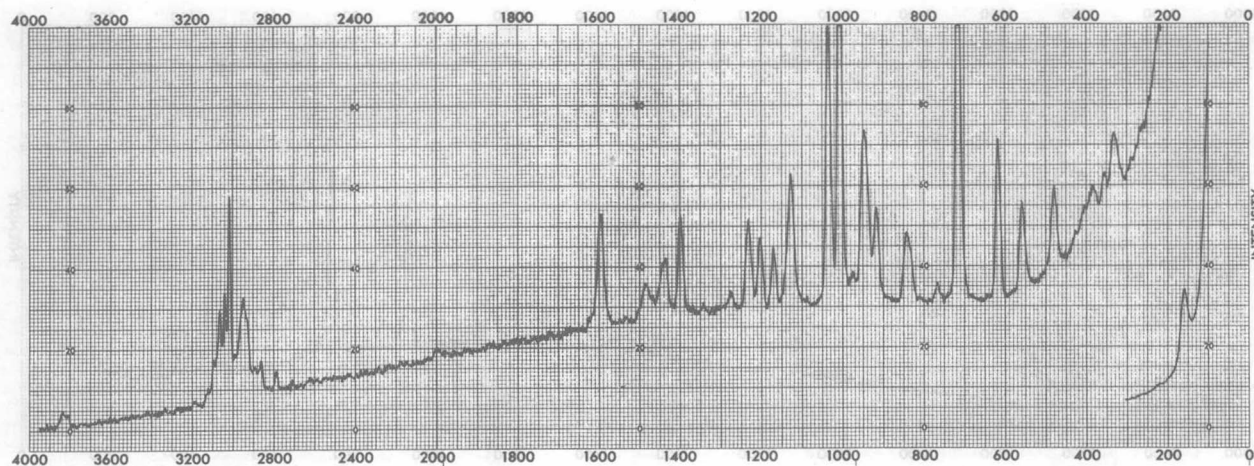
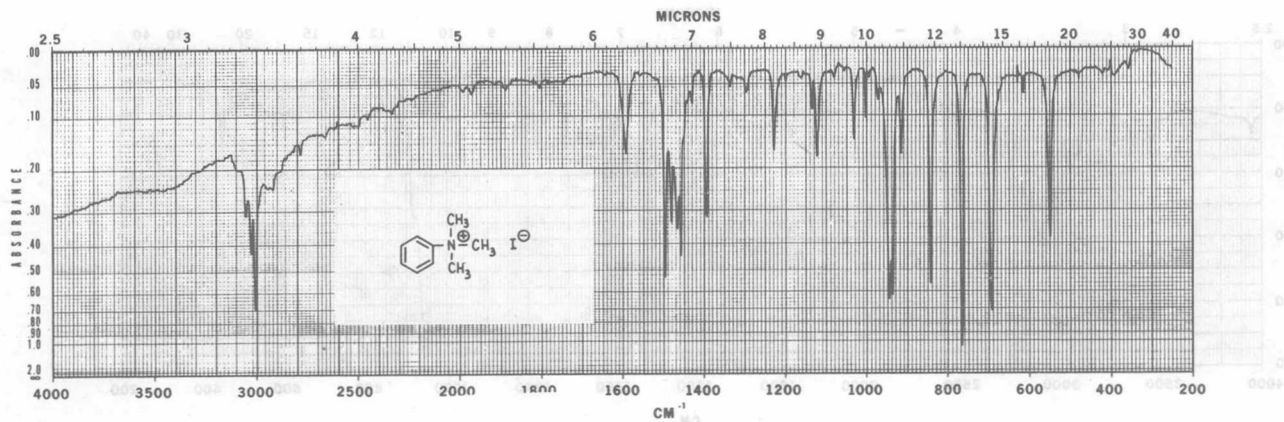


WAVENUMBER / INTENSITY

3020/50.2 1035/71.4 1006/103.9
715/98.6 160/137.0

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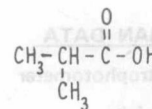
ISOBUTYRIC ACID

3 R

RAMAN DATA

Spectrophotometer Cary 83Sensitivity 100000Suppression 183Laser Power 22 mWSpectral Slitwidth 6 cm⁻¹ $C_4H_8O_2$ Mol. Wt. 88.11

B.P. 153-154°C

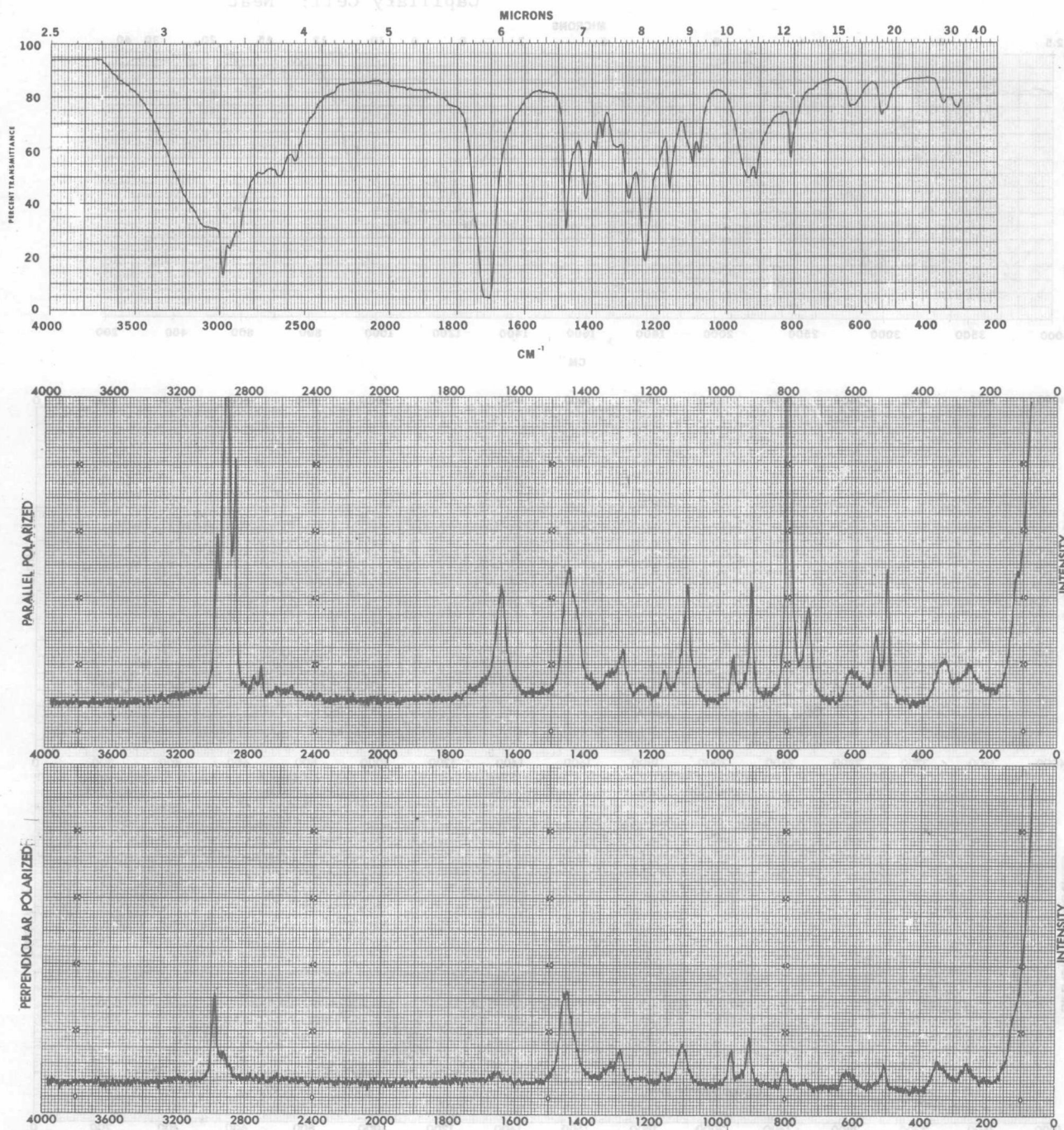
Source: Chem Service, Inc.,
West Chester, Pa.

WAVENUMBER / INTENSITY

2930/99.9 2875/71.9 799/314.4

© 1973 Sadtler

Capillary Cell: Neat



4 R

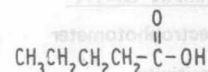
VALERIC ACID

RAMAN DATA

Spectrophotometer Cary 83
Sensitivity 100000;
10000
Suppression 46;
0
Laser Power 12 mW
Spectral Slitwidth 6 cm⁻¹

 $C_5H_{10}O_2$ Mol. Wt. 102.13

B.P. 186-187°C

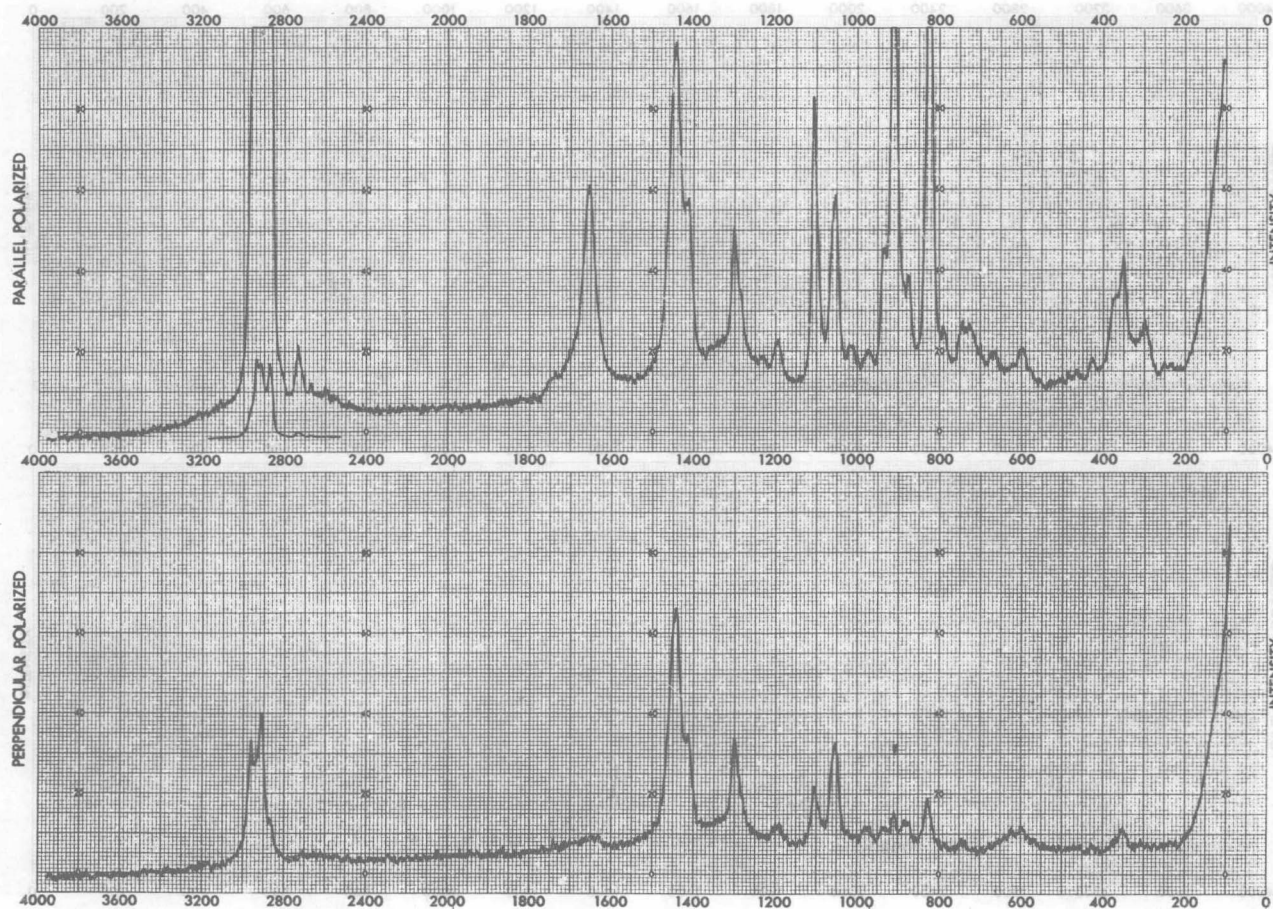
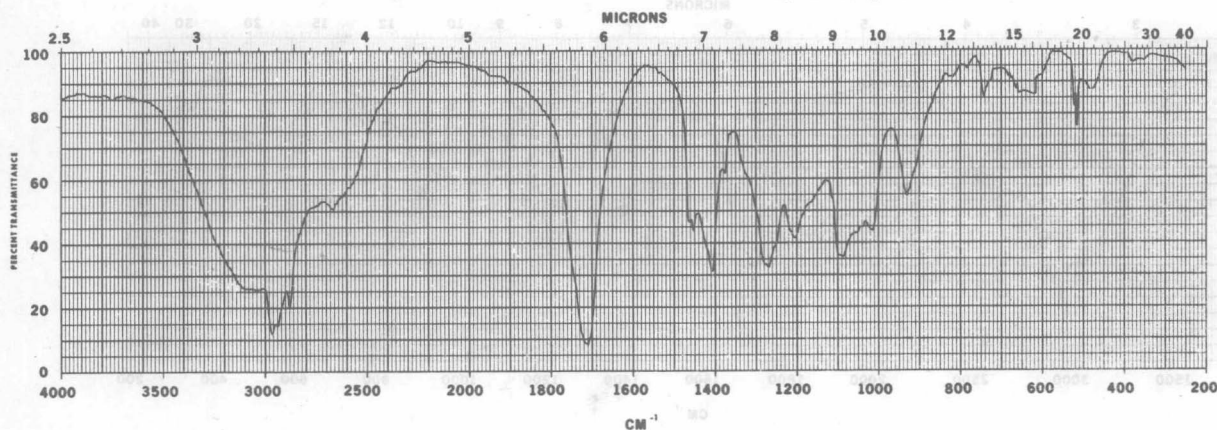
Source: Chem Service, Inc.,
West Chester, Pa.

WAVENUMBER / INTENSITY

2940/205.0	2920/189.6	2875/186.7
1107/20.0	911/109.3	824/138.7

© 1973 Sadtler

Capillary Cell: Neat



ISOVALERIC ACID

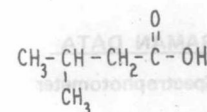
5 R

RAMAN DATA

Spectrophotometer Cary 83
Sensitivity 120000;
24000
Suppression 28;
0
Laser Power 12 mW
Spectral Slitwidth 6 cm⁻¹

 $C_5H_{10}O_2$ Mol. Wt. 102.13

B.P. 173-175°C

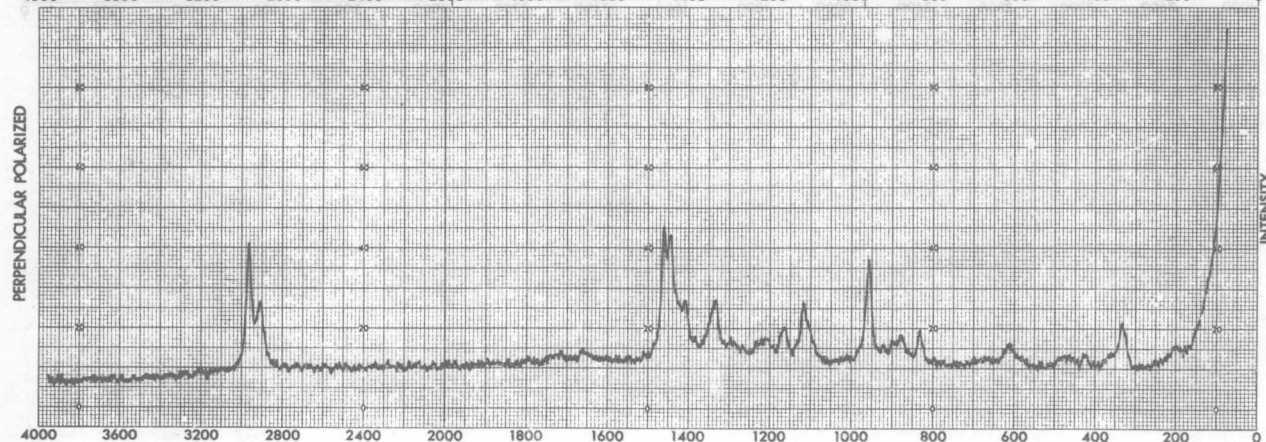
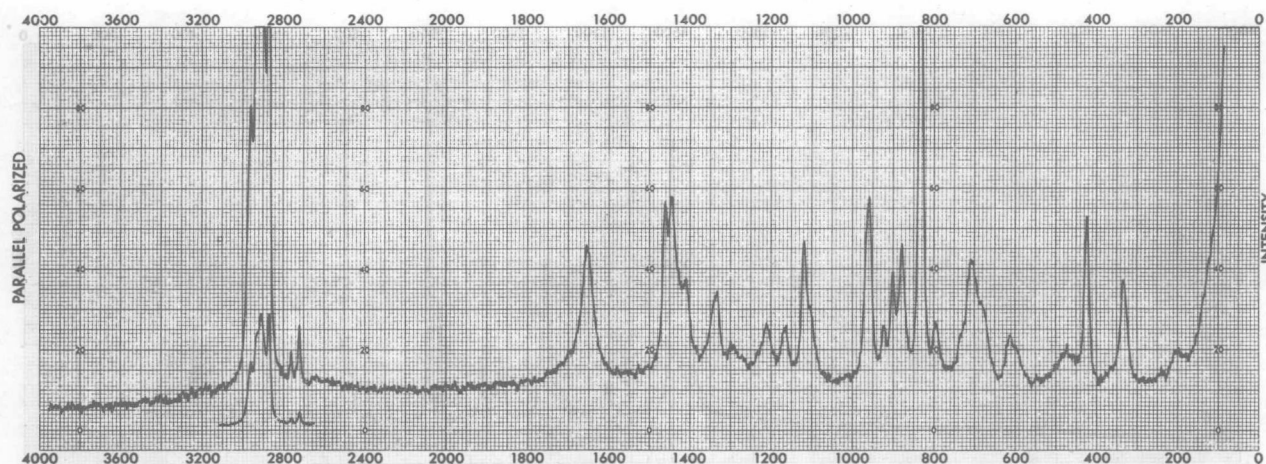
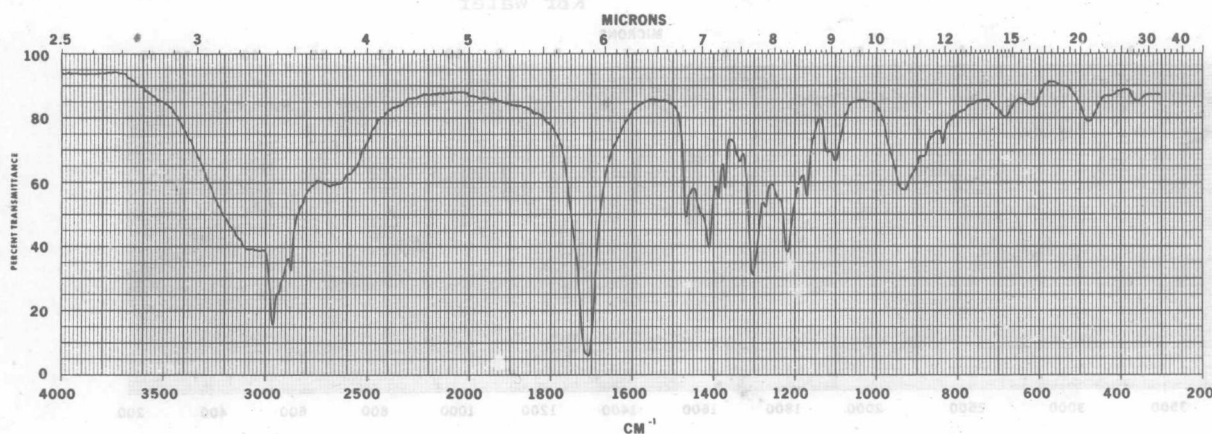
Source: Chem Service, Inc.,
West Chester, Pa.

WAVENUMBER / INTENSITY

2920/112.3	2910/131.9	2870/128.4
833/158.3	424/41.0	

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Capillary Cell: Neat



6 R

BENZOIC ACID

RAMAN DATA

Spectrophotometer

Sensitivity

Suppression

Laser Power

Spectral Slitwidth

Cary 83

50000;

8125

43;

0

10 mW

6 cm⁻¹

Mol. Wt. 122.12

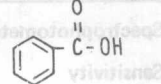
M.P. 123-125°C

Source: Chem Service, Inc.,
West Chester, Pa.

WAVENUMBER / INTENSITY

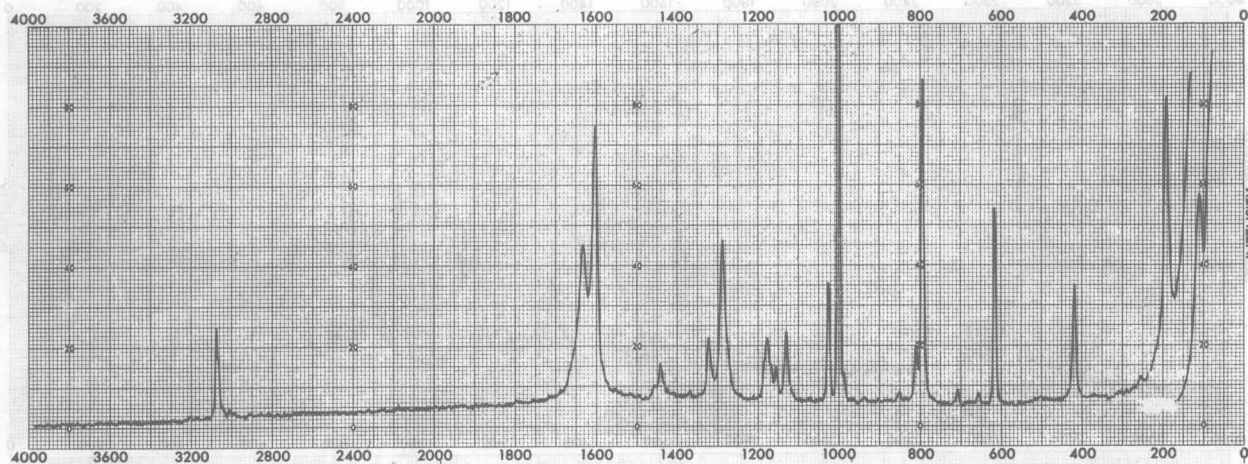
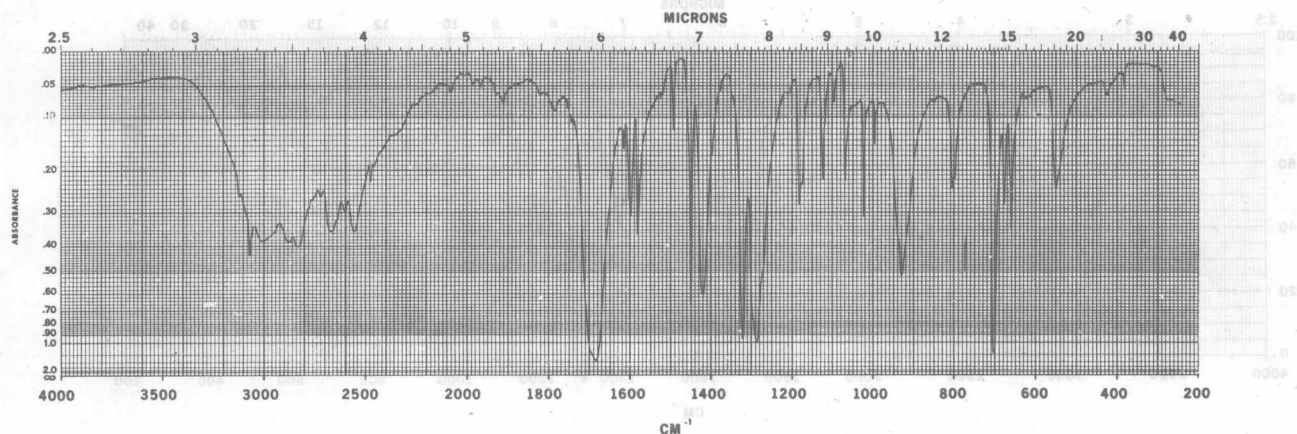
1000/208.1 795/80.8 110/175.1

RAMAN DATA



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KBr Wafer



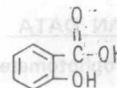
SALICYLIC ACID

7 R

RAMAN DATA

Spectrophotometer Cary 83Sensitivity 20000;10000Suppression 0;0Laser Power 13 mWSpectral Slitwidth 6 cm⁻¹ $C_7H_6O_3$ Mol. Wt. 138.12

M.P. 159-161°C

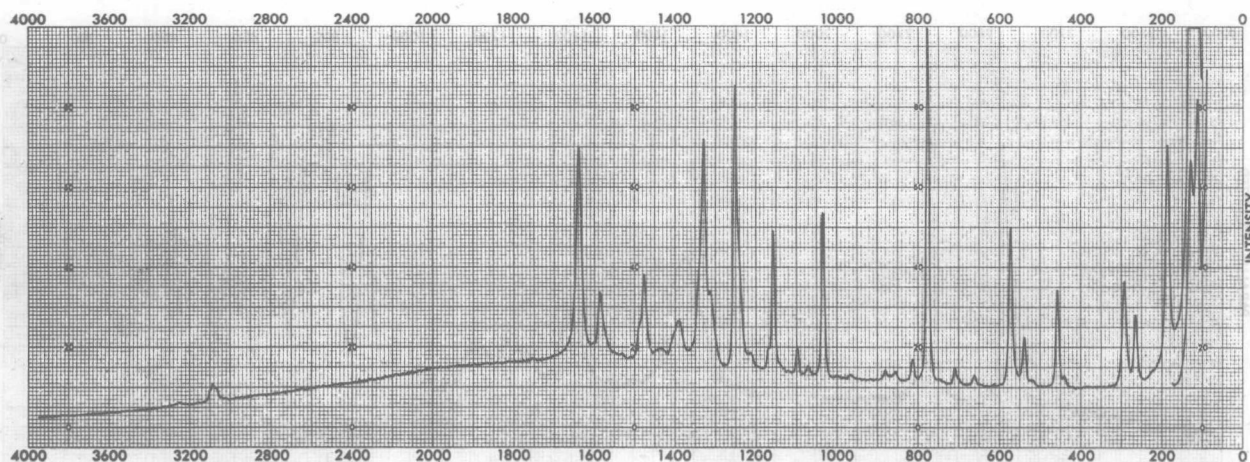
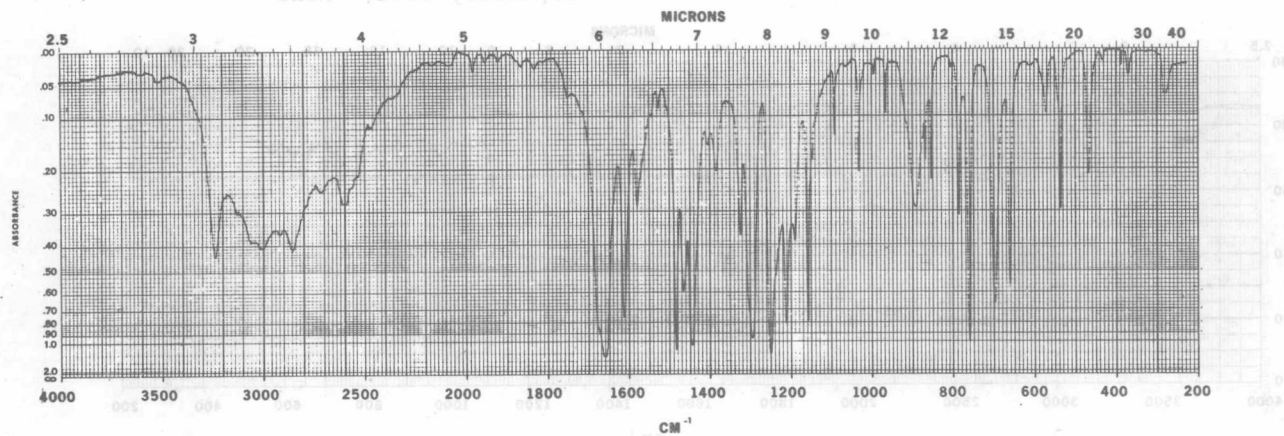
Source: Chem Service, Inc.,
West Chester, Pa.

WAVENUMBER / INTENSITY

Wavenumber (cm ⁻¹)	Intensity	
1252/70.3	778/87.6	130/79.4
112/87.8		

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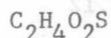
KBr Wafer



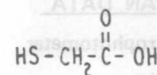
8 R

THIOGLYCOLIC ACID

RAMAN DATA

Spectrophotometer Cary 83Sensitivity 80000Suppression 98Laser Power 22 mWSpectral Slitwidth 8 cm⁻¹

Mol. Wt. 92.12

Source: Chem Service, Inc.,
West Chester, Pa.

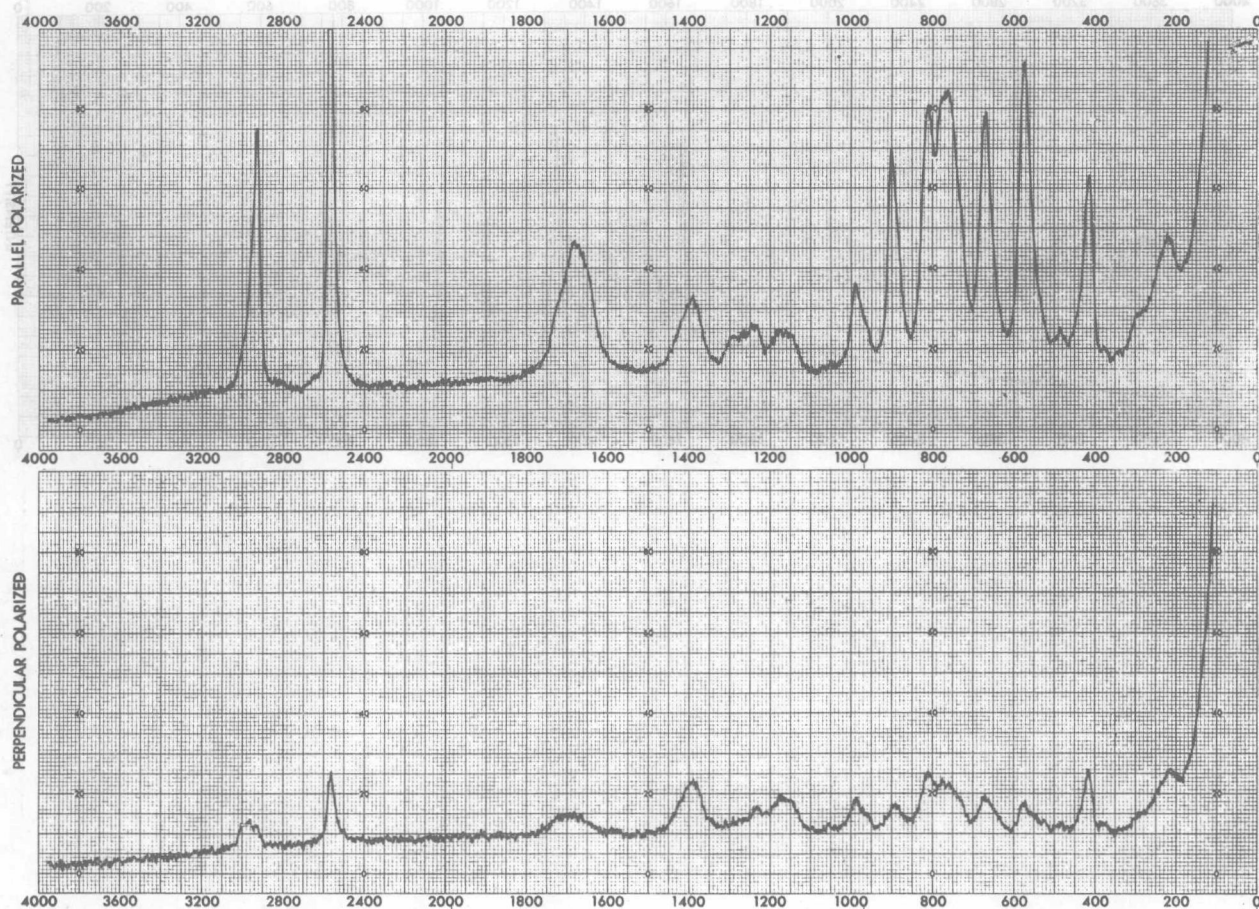
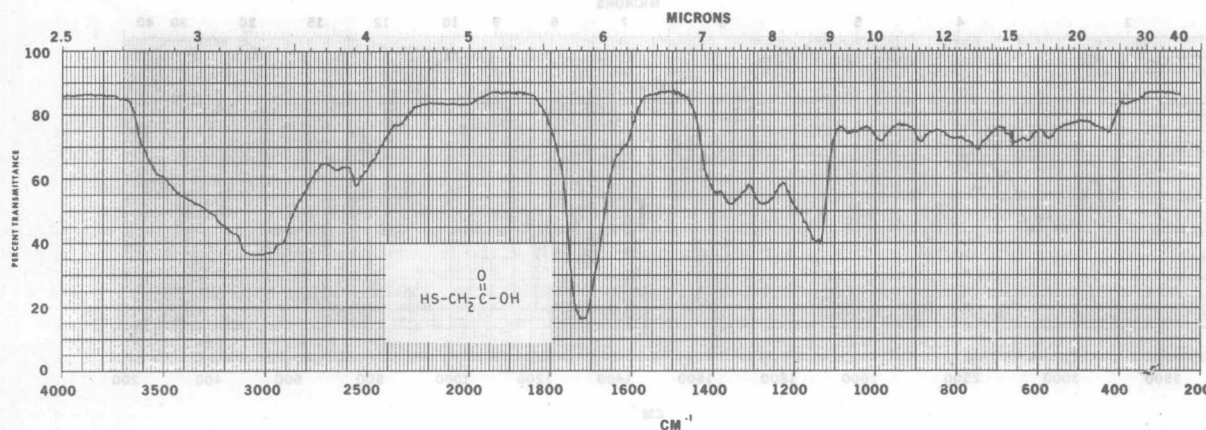
WAVENUMBER / INTENSITY

2930/65.3

2570/140.6

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Capillary Cell: Neat



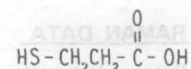
3-MERCAPTOPROPIONIC ACID

9 R

RAMAN DATA

Spectrophotometer Cary 83Sensitivity 100000Suppression 100Laser Power 12 mWSpectral Slitwidth 6 cm⁻¹ $C_3H_6O_2S$ Mol. Wt. 106.14

M.P. 17-19°C

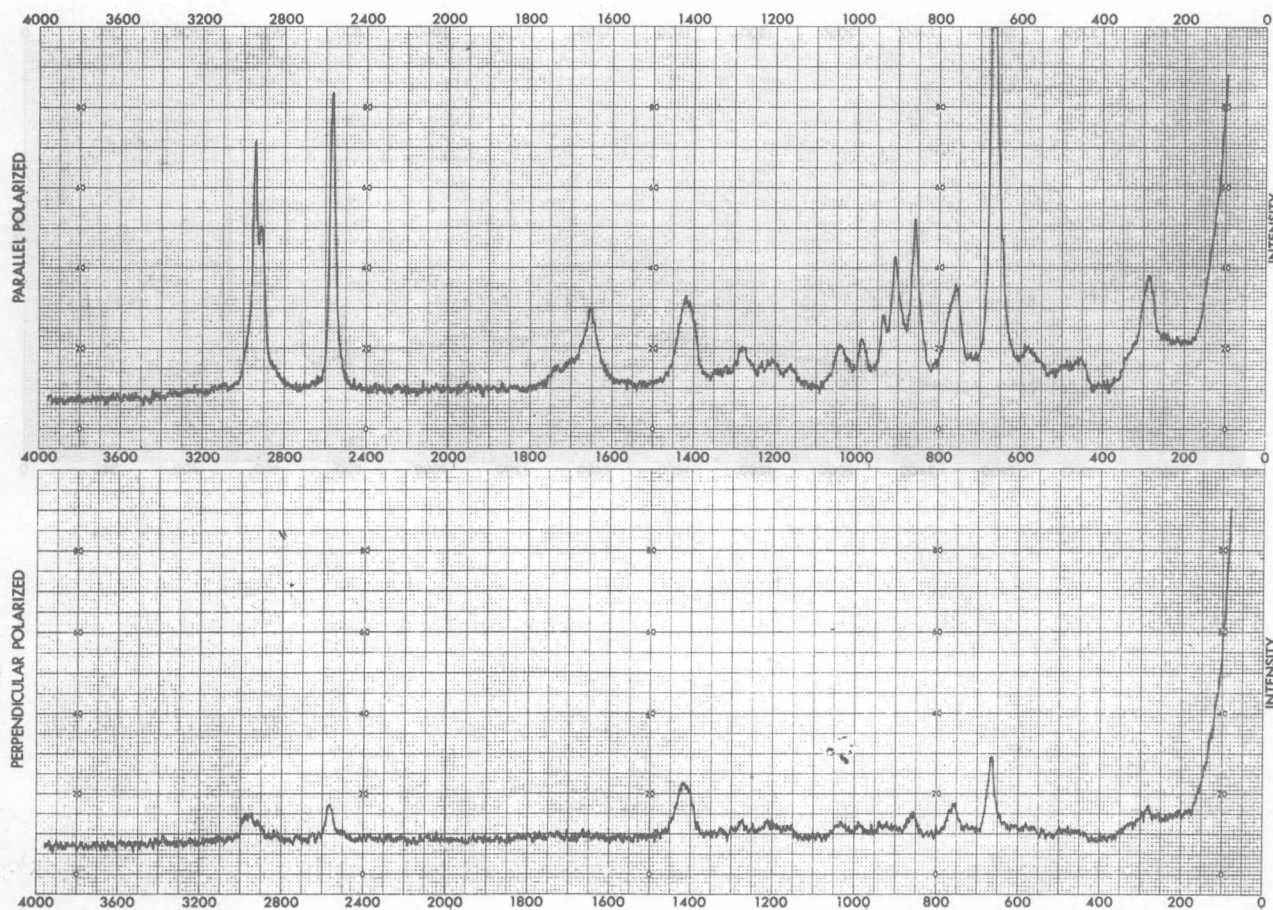
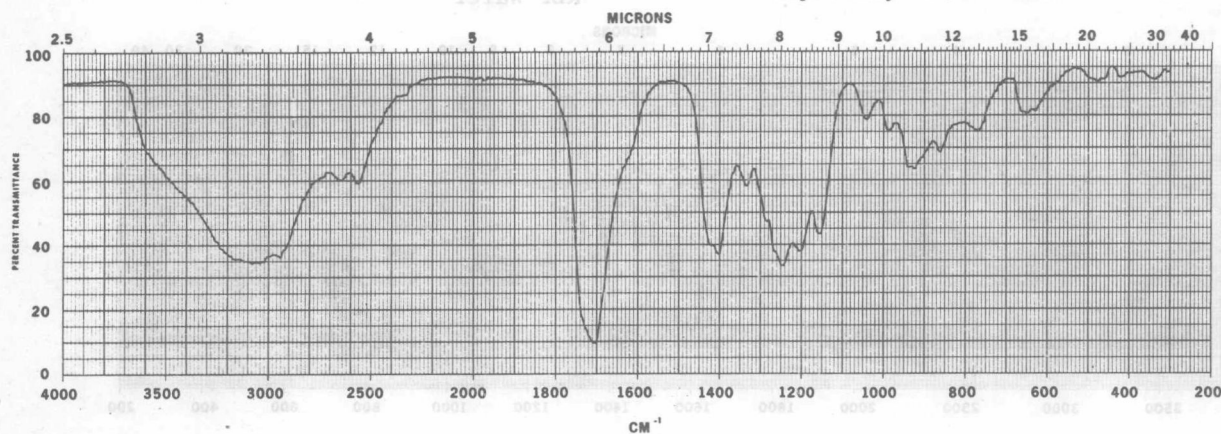
Source: Chem Service, Inc.,
West Chester, Pa.

WAVENUMBER / INTENSITY

2565/73.6 666/119.5

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Capillary Cell: Neat



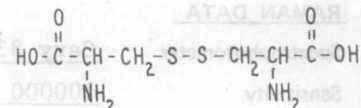
10 R

L-(-)-CYSTINE

RAMAN DATA

Spectrophotometer Cary 83Sensitivity 45000Suppression 60Laser Power 9 mWSpectral Slitwidth 6 cm⁻¹ $C_6H_{12}N_2O_4S_2$ Mol. Wt. 240.30

M.P. 260-261°C (dec.)

Source: Chem Service, Inc.,
West Chester, Pa.

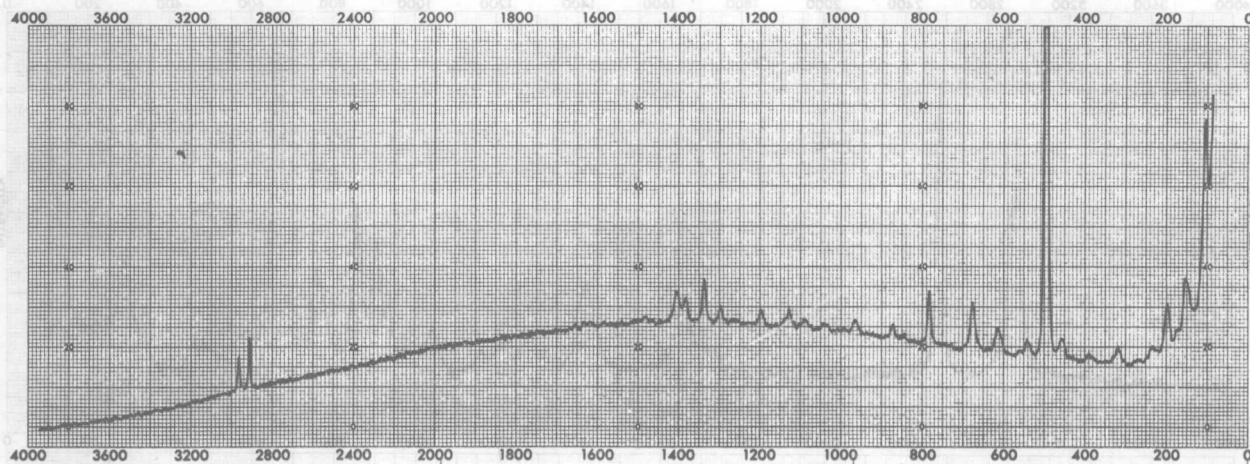
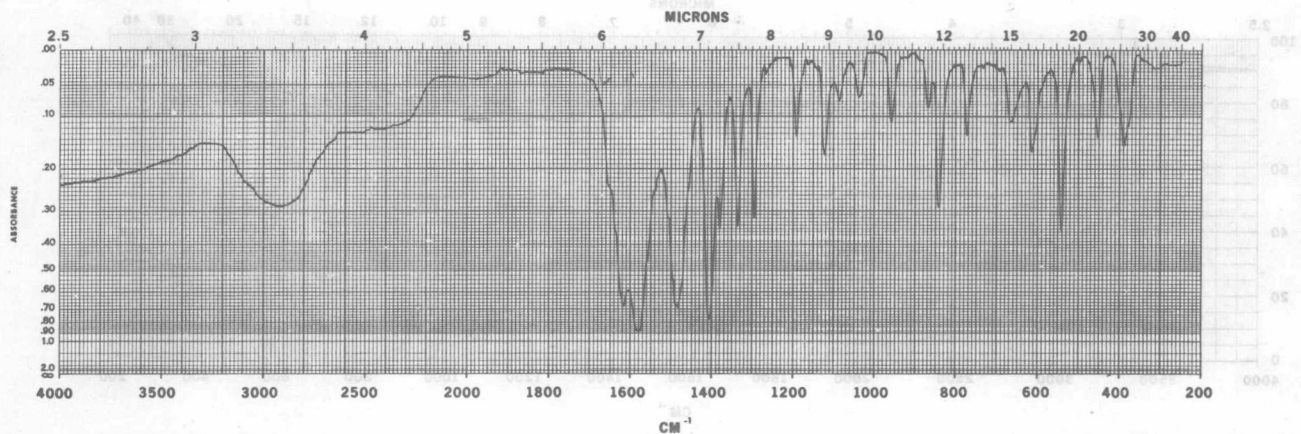
WAVENUMBER / INTENSITY

783/13.3

498/170.9

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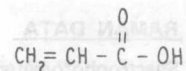
KBr Wafer



RAMAN DATA

Spectrophotometer Cary 83Sensitivity 30000Suppression 22Laser Power 22 mWSpectral Slitwidth 6 cm⁻¹ $C_3H_4O_2$ Mol. Wt. 72.06

M.P. 12-14°C

Source: Chem Service, Inc.,
West Chester, Pa.

WAVENUMBER / INTENSITY

1663/68.7 1640/158.8 867/81.9

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