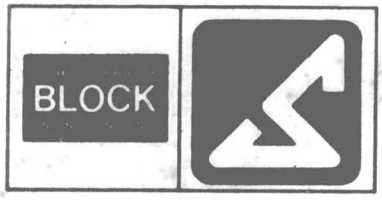
THE SADTLER STANDARD SPECTRA



SADTLER RESEARCH LABORATORIES, INC.

STANDARD GRATING SPECTRA

CREATIVE CHEMISTS SINCE 1874

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TEL. 215 382-7800 • TWX 710 - 670-1186 • CABLE SADTLABS

The publication of the physical data of the Sadtler Standard Spectra and the Sadtler Commercial Spectra is intended to be descriptive. The samples of the materials represented have come generally from other sources than our own laboratories and frequently without the donors' knowledge of their part in this publication.

On the other hand every effort is made by Sadtler Research Laboratories, Inc. to assure the reliability of the published spectra. When improved data is available or errors are called to our attention we revise and reissue the proper replacement spectra.

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SADTLER STANDARD GRATING SPECTRA

With this 1974 supplement of 4,000 spectra to the Sadtler Standard Grating Spectra collection, the catalog now contains 34,000 grating spectra determined in the region of 2.5 - 40 microns (4000 to $\sim$ 200 cm^{-1}).

All spectra are presently scanned in the Sadtler Research Laboratories on a Perkin-Elmer 621 instrument using samples donated by scientists in universities and in industry.

Standard techniques have been developed in our laboratories to insure spectra which are both of the best possible quality and reproducible by others for comparison.

The method most used is the KBr Wafer Technique which has been improved to remove the water which generally imposes a problem. A paper entitled Improved KBr Techniques by Traude and Philip Sadtler was presented at the 1965 Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy and copies are available from our laboratories.

The KBr method is employed because it is a standard method that can be used by all, and at the same time, the sample size can be kept to a minimum due to the small amount required in the preparation of a wafer. This then allows for the use of the remaining sample for further analyses such as UV and NMR. These additional spectral and thermogram data are also published and made available by Sadtler.

When a sample cannot be run as a KBr Wafer because of reaction, the Split Mull technique is used; the entire 2.5 - 40 micron region is scanned using a Mineral Oil Mull and the 3.0 - 3.8 and 6.6 - 7.4 micron regions using a Perfluorinated Hydrocarbon Mull.

Liquid samples and low melting solids are generally determined using capillary cells.

All spectra are clearly labelled with the method employed in their preparation.

Your comments and suggestions are always welcome as well as samples whose spectra require replacement. Samples of new 98% pure compounds (accompanied by structure and/or name, physical data, solubility, and journal reference) are continually being sought and it is only because of the generous contributions of those whose names appear as the "source" that we can offer these spectra to scientists. Our sincere thanks is always expressed to these donors.

Five indices accompany the Sadtler Standard Spectra as follows:

Alphabetical

Chemical Classes

Molecular Formula

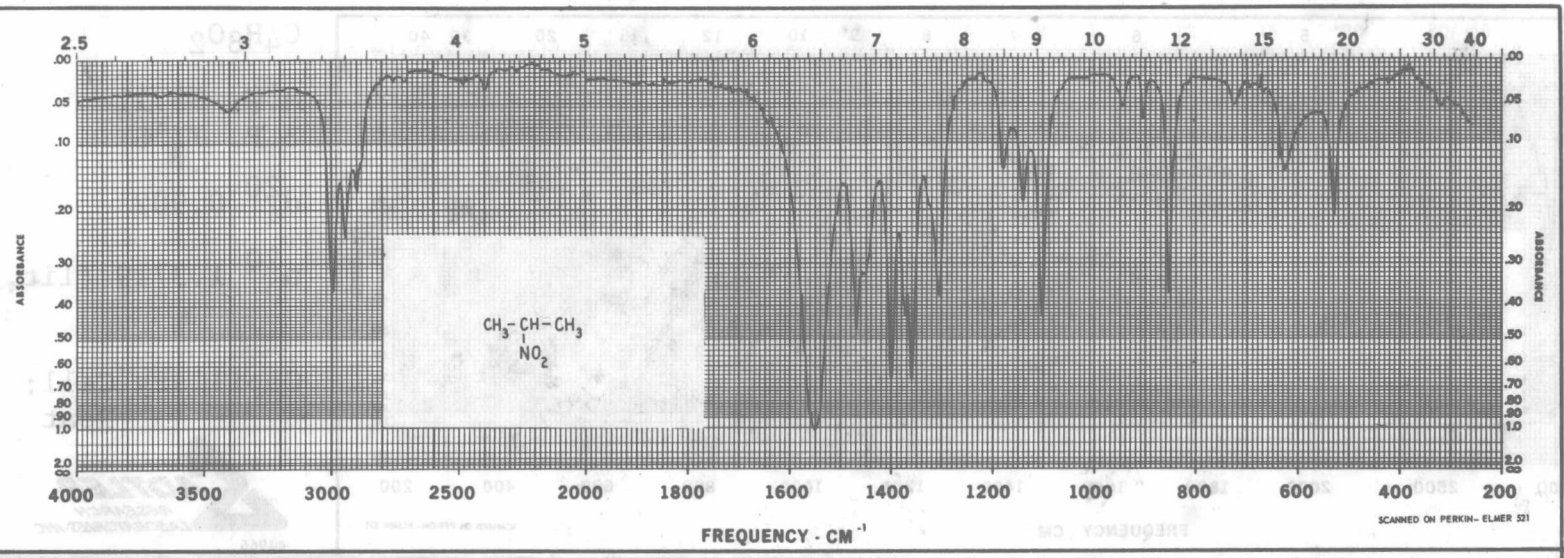
Numerical

Spec-Finder

The first four are composites containing entries for 47,000 prism spectra and corresponding numbers for the 34,000 Sadtler Standard Grating Spectra and the 36,000 Sadtler Ultraviolet Spectra. Also listed are the numbers for the 20,000 Sadtler Nuclear Magnetic Resonance Spectra, Sadtler DTA thermograms and the Varian High Resolution NMR Spectra and JEOL High Resolution NMR Spectra for those compounds which are included in both the prism and these collections. Appropriately labelled columns enable one to locate all data available for any compound.

WE SUGGEST THAT THE PREFACES TO THE VARIOUS INDICES BE READ SINCE SEVERAL CHANGES AND ADDITIONS HAVE BEEN MADE.

2-NITROPROPANE



$C_3H_7NO_2$

M.W. 89.10
B.P. 120.3°C

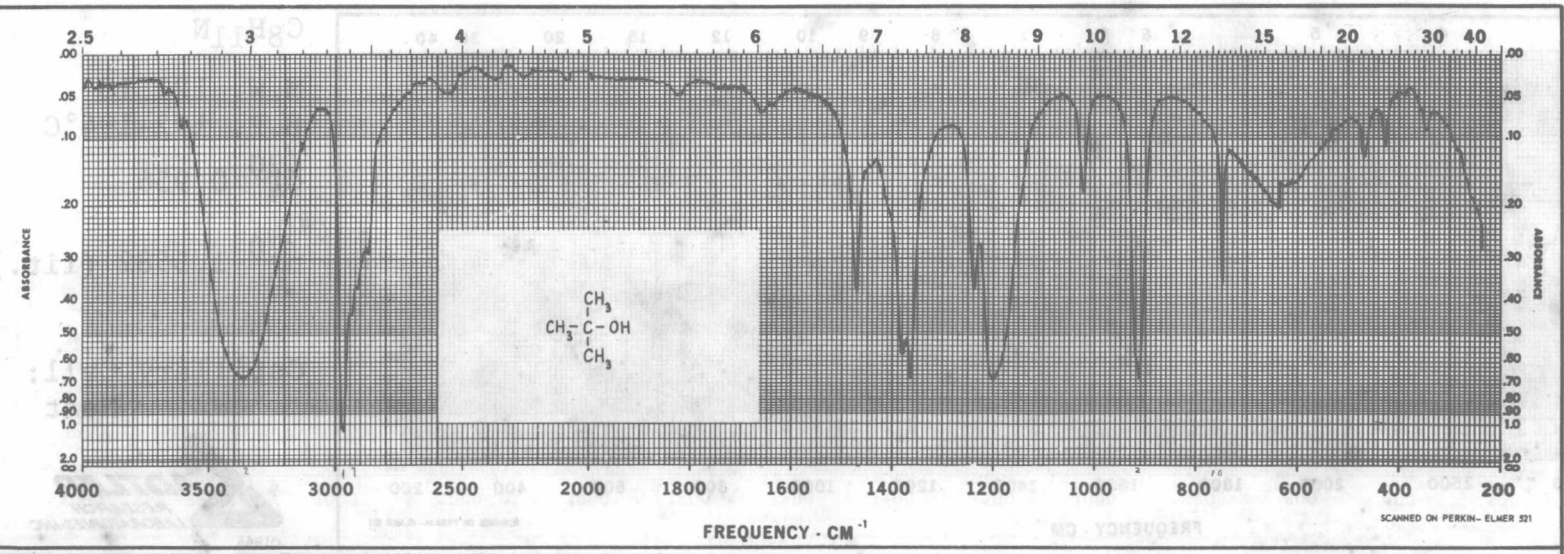
Capillary Cell:
Neat

SADTLER RESEARCH LABORATORIES INC

Source: Commercial Solvents Corp., New York, N.Y.

1 K

tert-BUTYL ALCOHOL



$C_4H_{10}O$

M.W. 74.12
M.P. 24.5-25.5°C
B.P. 82.8°C (lit.)

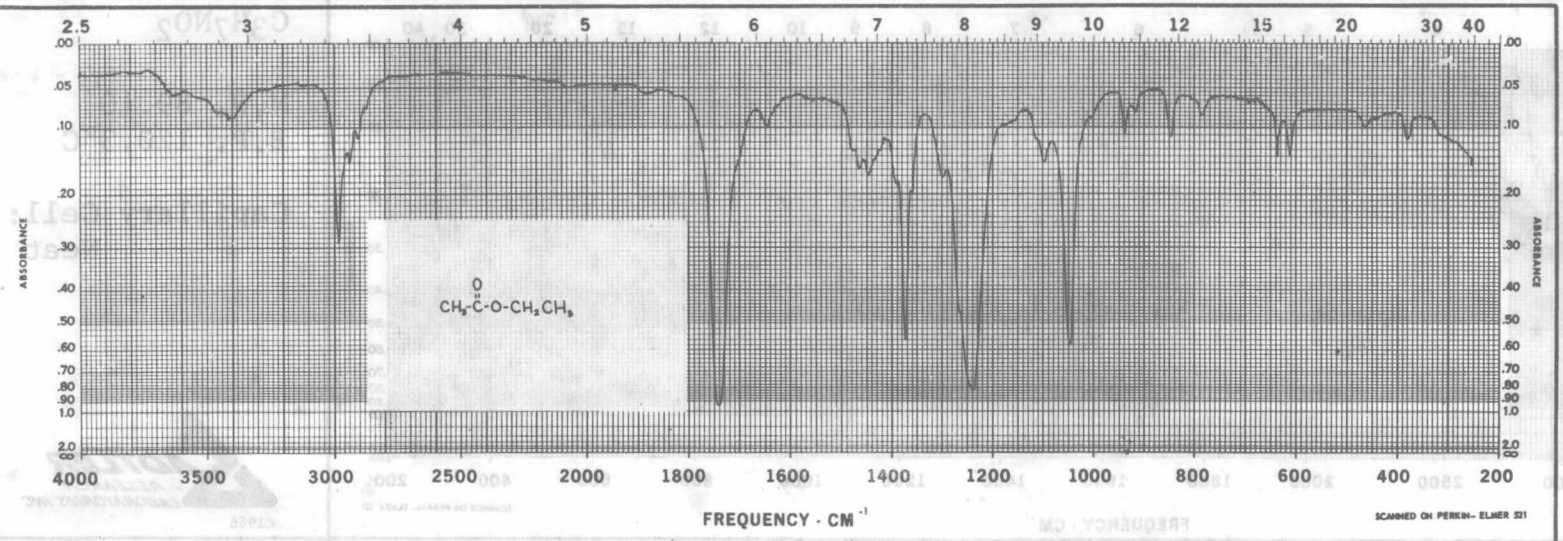
Capillary Cell:
Neat

SADTLER RESEARCH LABORATORIES INC

Source: The Matheson Co., Inc., E. Rutherford, N.J.

2 K

ETHYL ACETATE



$C_4H_8O_2$

M.W. 88.11
B.P. 77°C

d_4^{20} 0.902

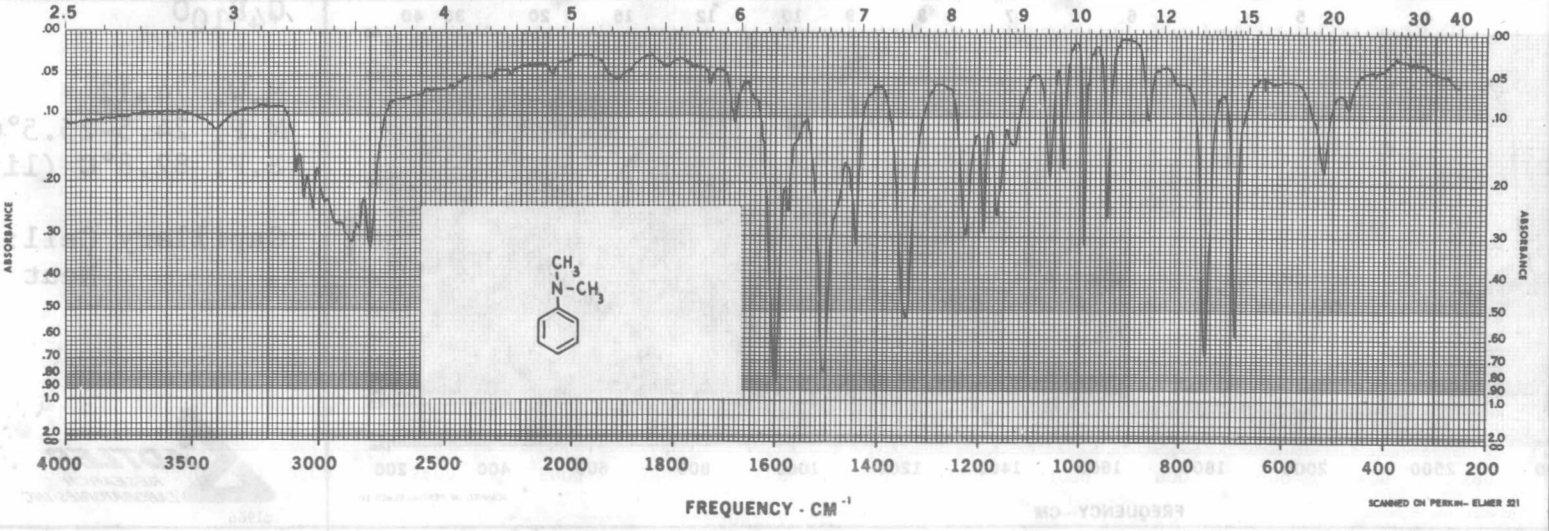
n_D^{20} 1.3719 (lit.)

Capillary Cell:
Neat

Source: Dodge & Olcott Inc., New York, N.Y.

3 K

N,N-DIMETHYLANILINE



$C_8H_{11}N$

M.W. 121.18
B.P. 192-194°C

d_4^{20} 0.956

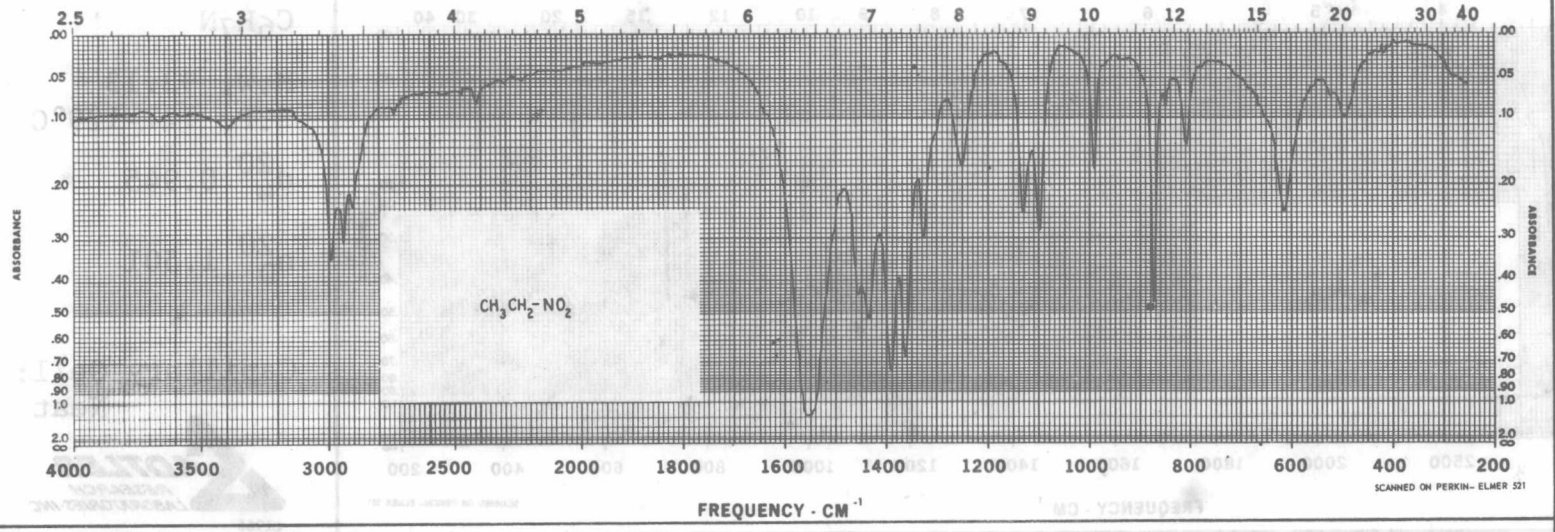
n_D^{20} 1.5582 (lit.)

Capillary Cell:
Neat

Source: E. I. duPont de Nemours & Co., Wilmington, Del.

4 K

NITROETHANE



$C_2H_5NO_2$

M.W. 75.07

B.P. 114-115°C

d_{25}^{25} 1.041

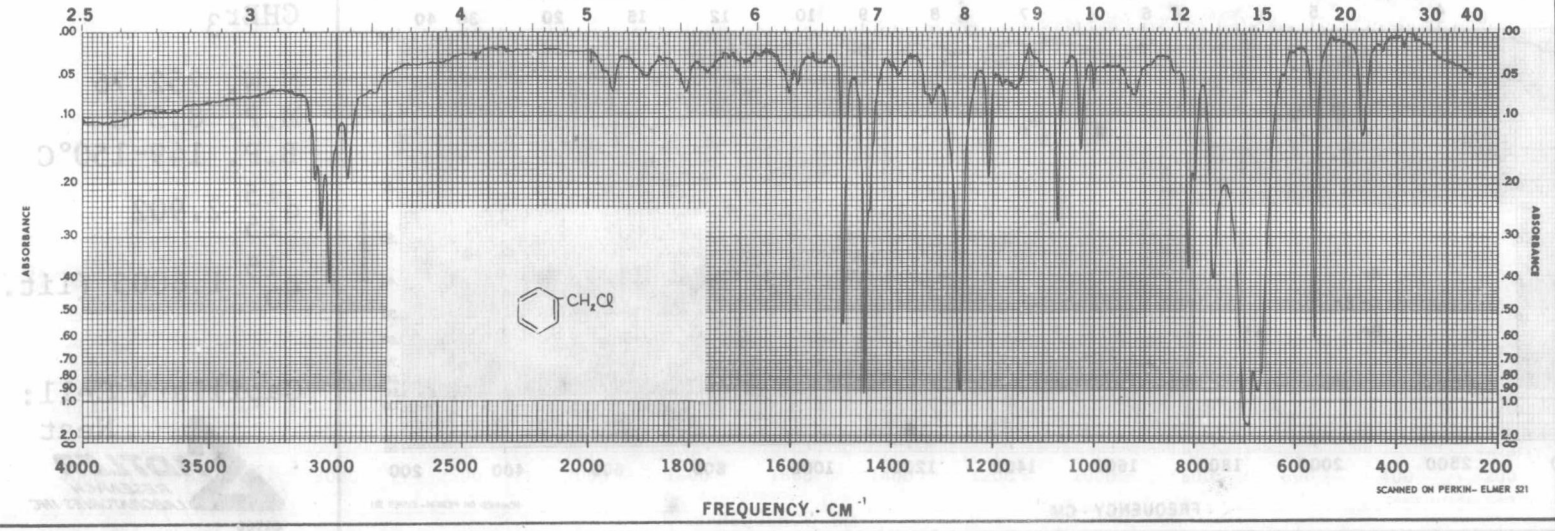
n_D^{20} 1.392 (lit.)

Capillary Cell:
Neat

Source: Fluka AG, Buchs, Switzerland

5 K

α-CHLOROTOLUENE



C_7H_7Cl

M.W. 126.59

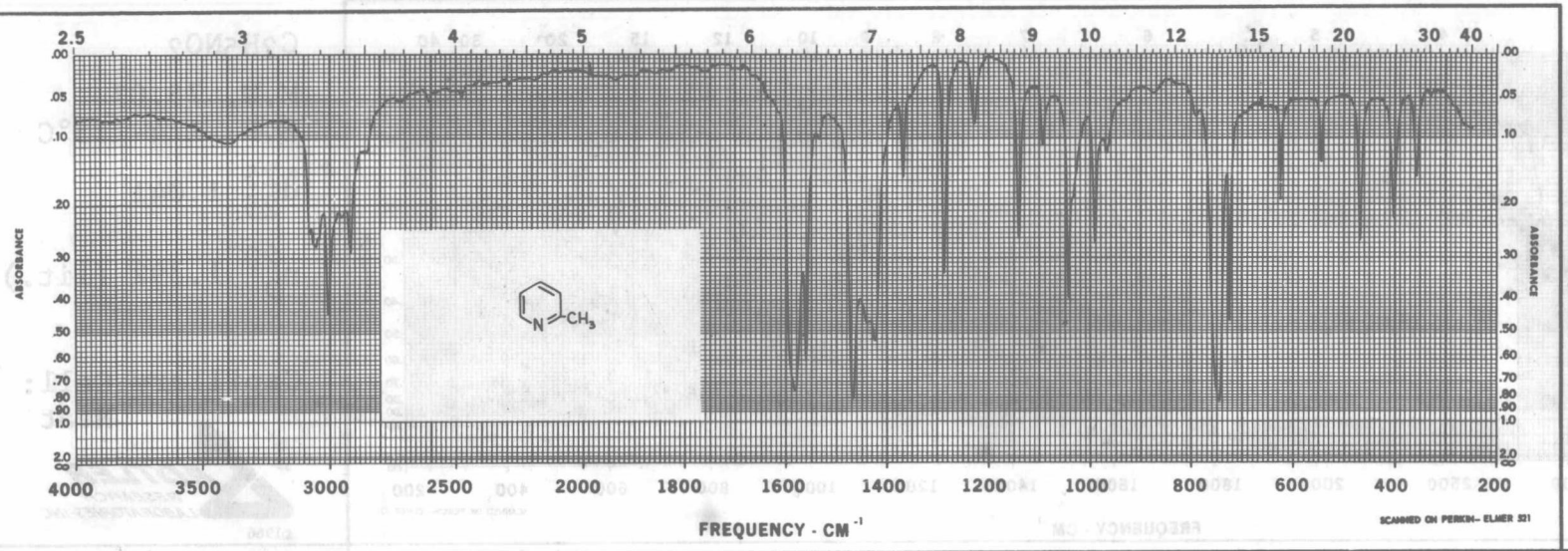
B.P. 72-74°C/20mm

Capillary Cell:
Neat

Source: The Matheson Co., Inc., E. Rutherford, N.J.

6 K

2-PICOLINE



C_6H_7N

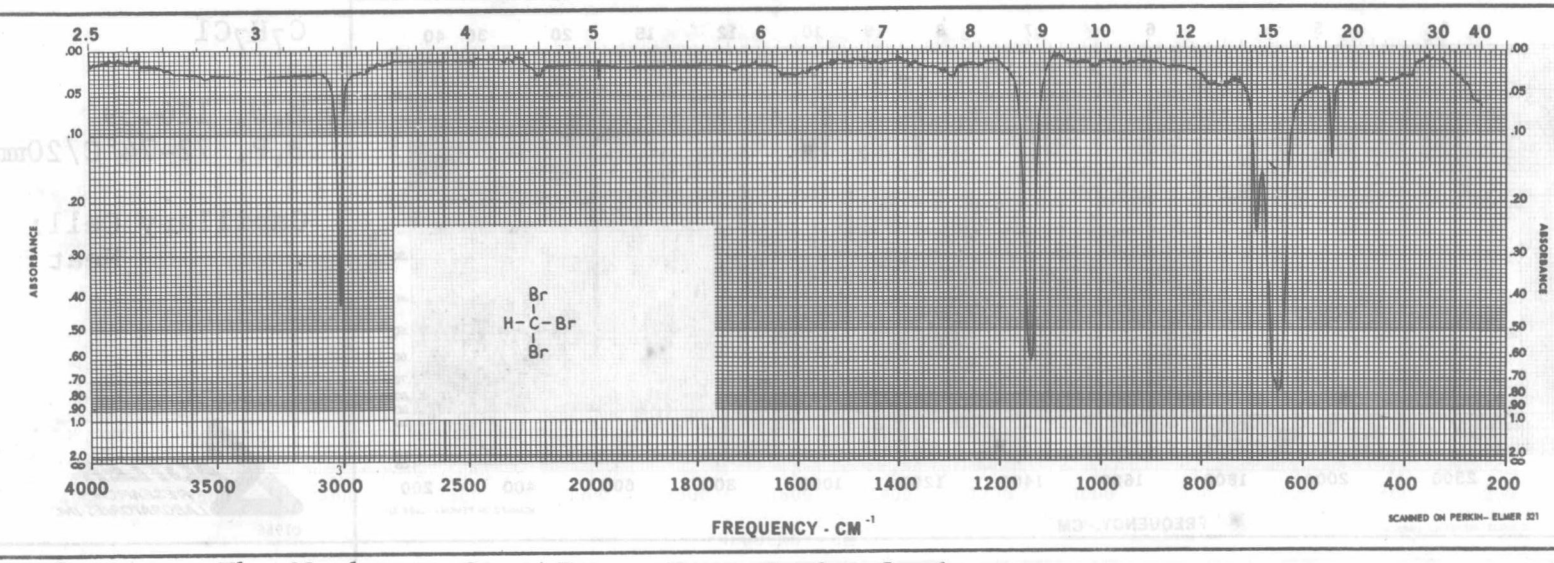
M.W. 93.13
B.P. 127-129°C
d_4^{20} 0.945
n_D^{20} 1.501

Capillary Cell:
Neat

Source: Fluka AG, Buchs, Switzerland

7 K

TRIBROMOMETHANE



$CHBr_3$

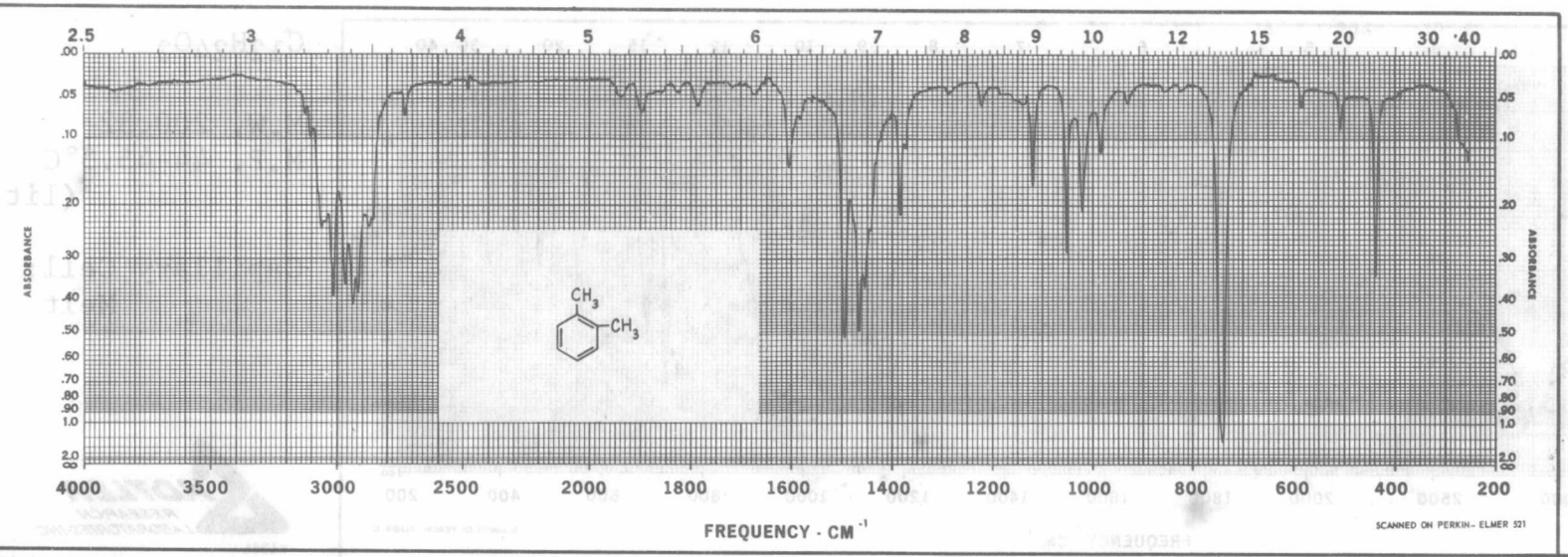
M.W. 252.76
M.P. 8.3°C
B.P. 149-150°C
d_{15}^{15} 2.902
n_D^{15} 1.6005 (lit.)

Capillary Cell:
Neat

Source: The Matheson Co., Inc., East Rutherford, N.J.

8 K

o-XYLENE



C_8H_{10}

M.W. 106.17
B.P. 143.5-144.5°C

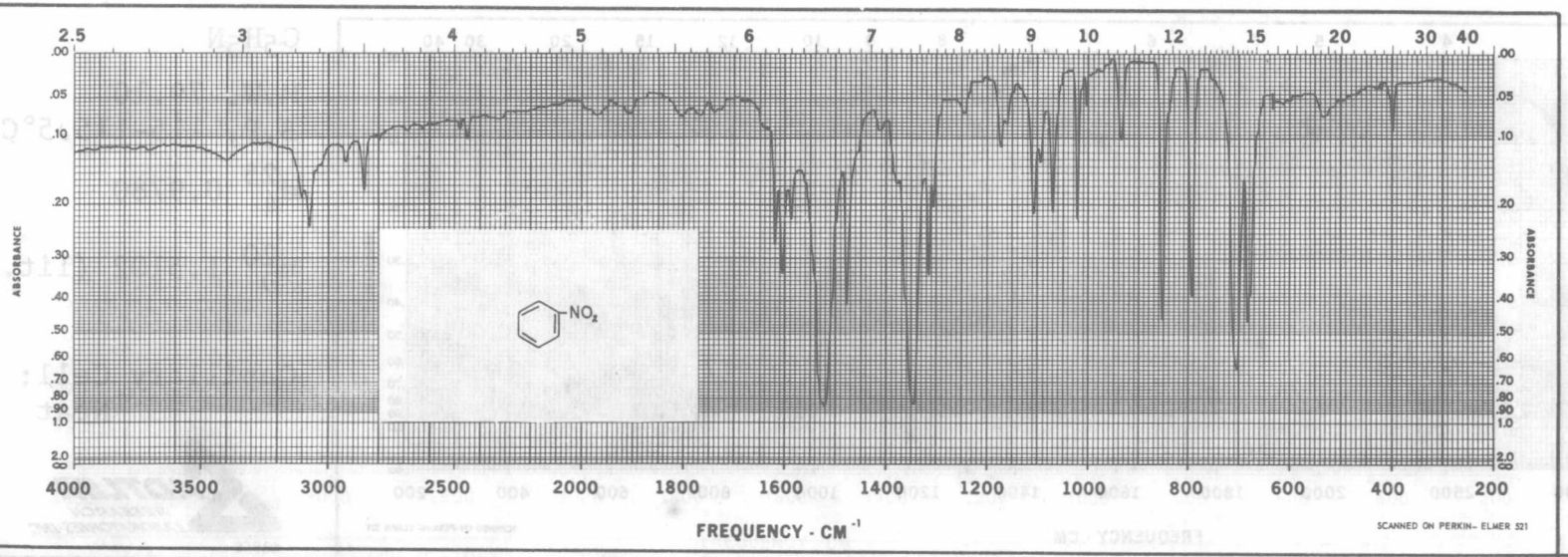
n_D^{20} 1.4998 (lit.)

Capillary Cell:
Neat

Source: The Matheson Co., Inc., E. Rutherford, N.J.

9 K

NITROBENZENE



$C_6H_5NO_2$

M.W. 123.11
B.P. 210-211°C

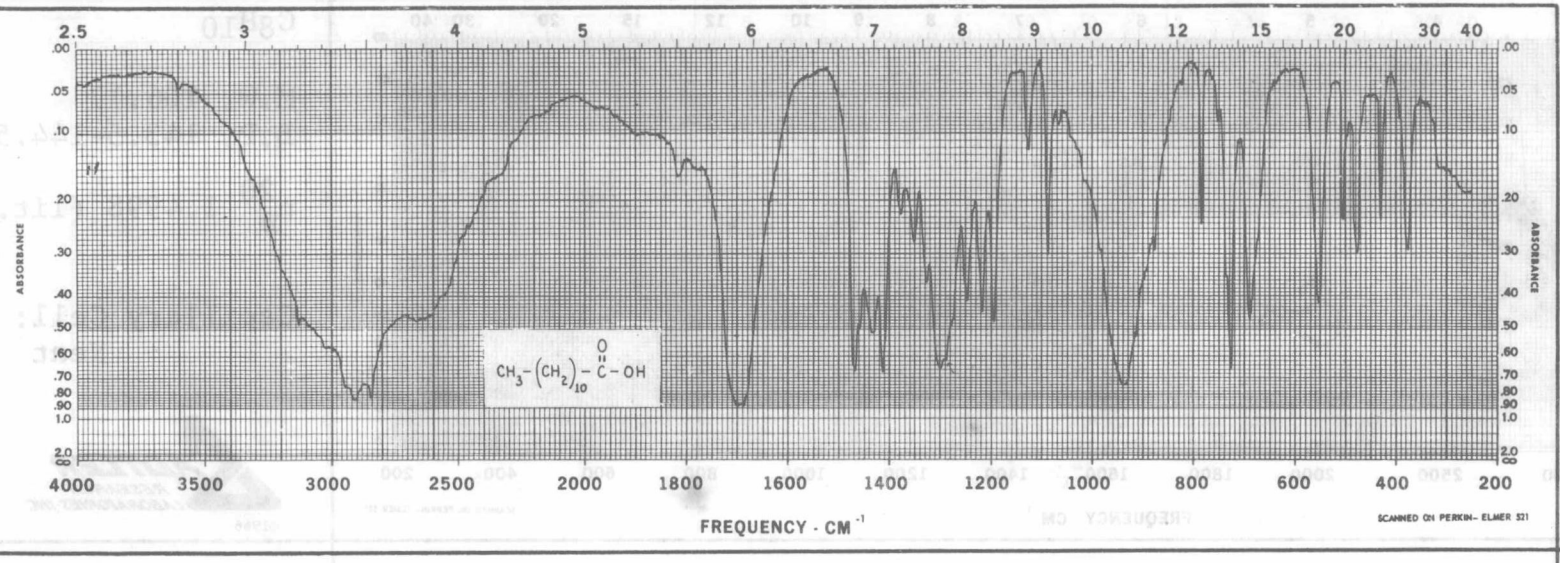
d_4^{15} 1.205

Capillary Cell:
Neat

Source: J. T. Baker Chemical Co., Phillipsburg, N.J.

10 K

LAURIC ACID



$C_{12}H_{24}O_2$

M.W. 200.32
M.P. 44-45.5°C (lit.)

Capillary Cell: Melt

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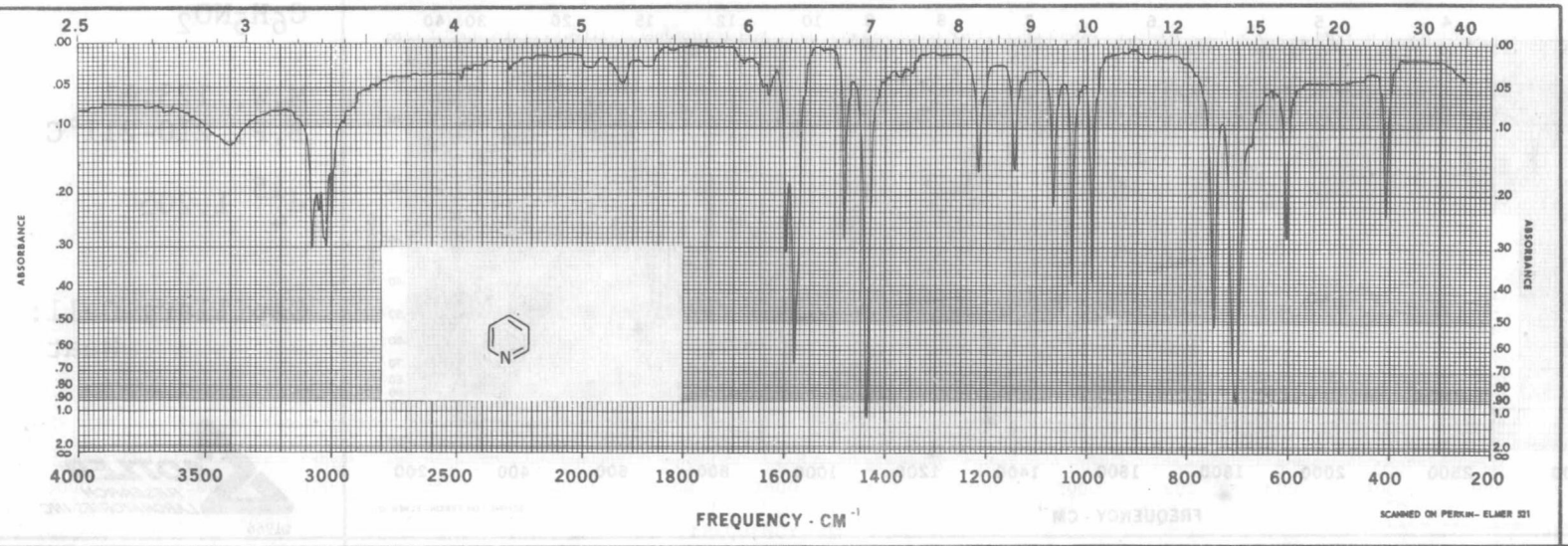
©1966

Source: The Matheson Co., Inc., E. Rutherford, N.J.

11 K

PYRIDINE



C_5H_5N

M.W. 79.10
B.P. 115-115.5°C

d_4^{25} 0.9780

n_D^{20} 1.5102 (lit.)

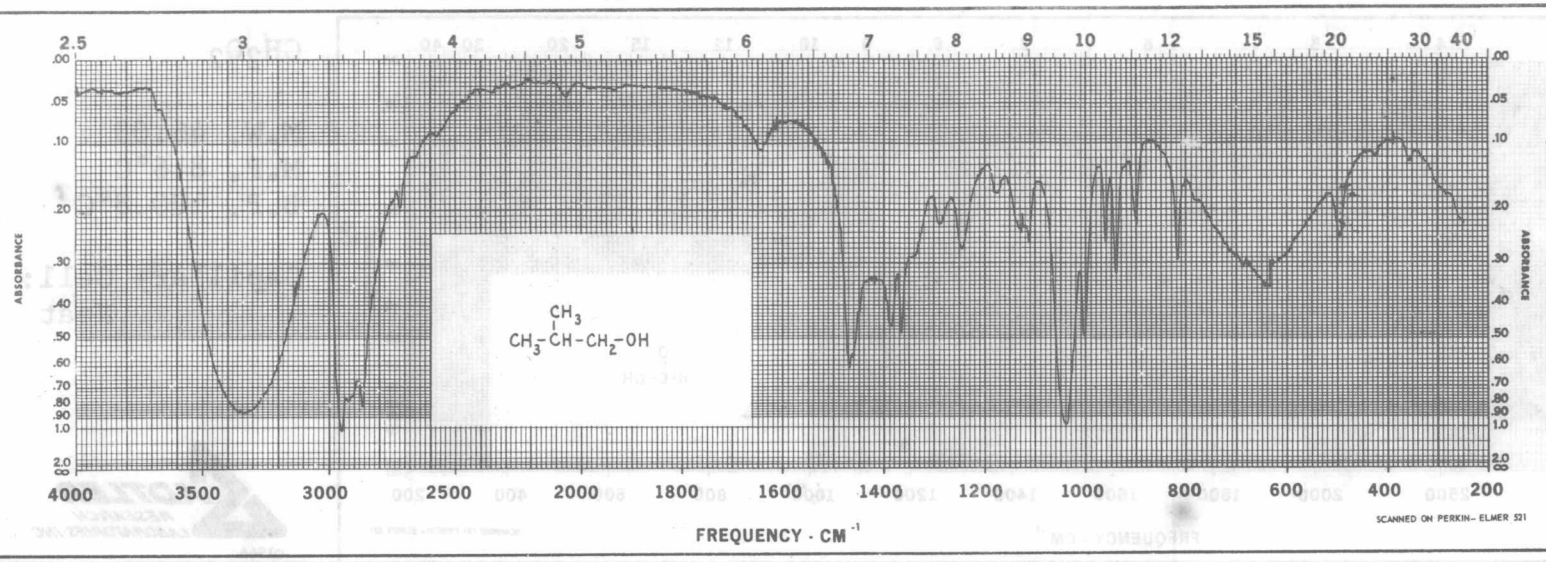
Capillary Cell: Neat

SADTLER RESEARCH LABORATORIES INC
©1966

Source: The Matheson Co., Inc. E. Rutherford, N.J.

12 K

ISOBUTYL ALCOHOL



$C_4H_{10}O$

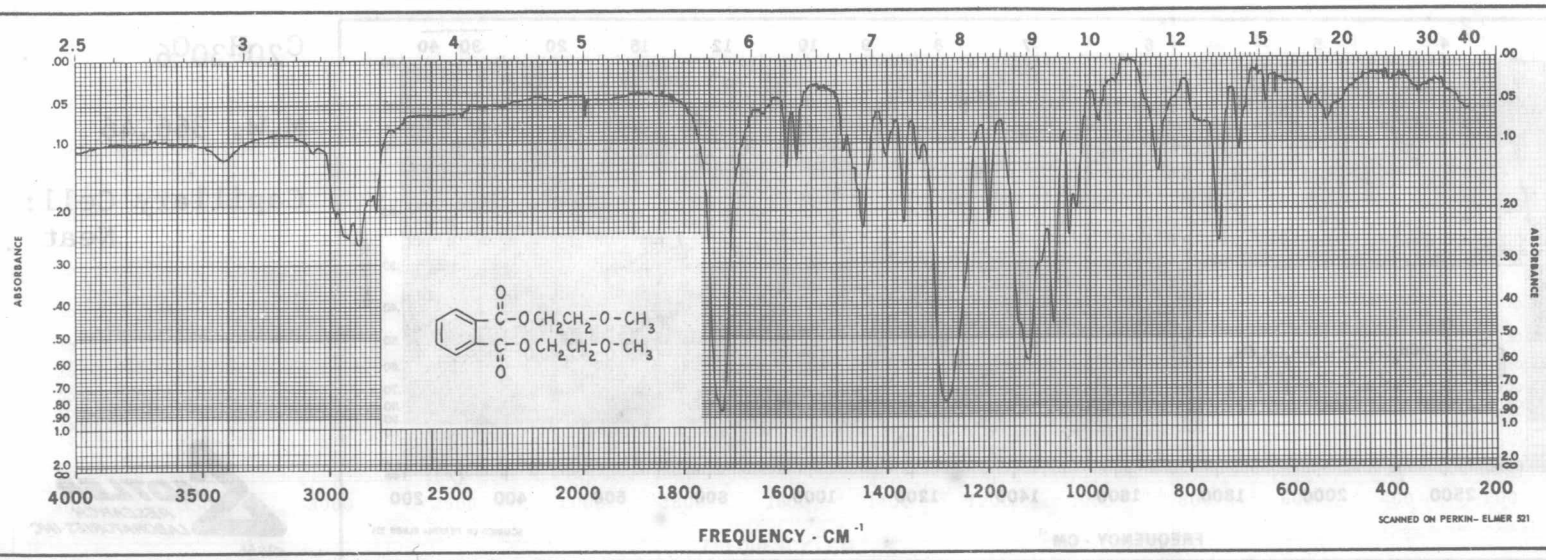
M.W. 74.12
B.P. 107.4°C (lit.)

Capillary Cell: Neat

Source: Eastman Chemical Products, Inc., Kingsport, Tennessee

13 K

PHTHALIC ACID, BIS(2-METHOXYETHYL) ESTER



$C_{14}H_{18}O_6$

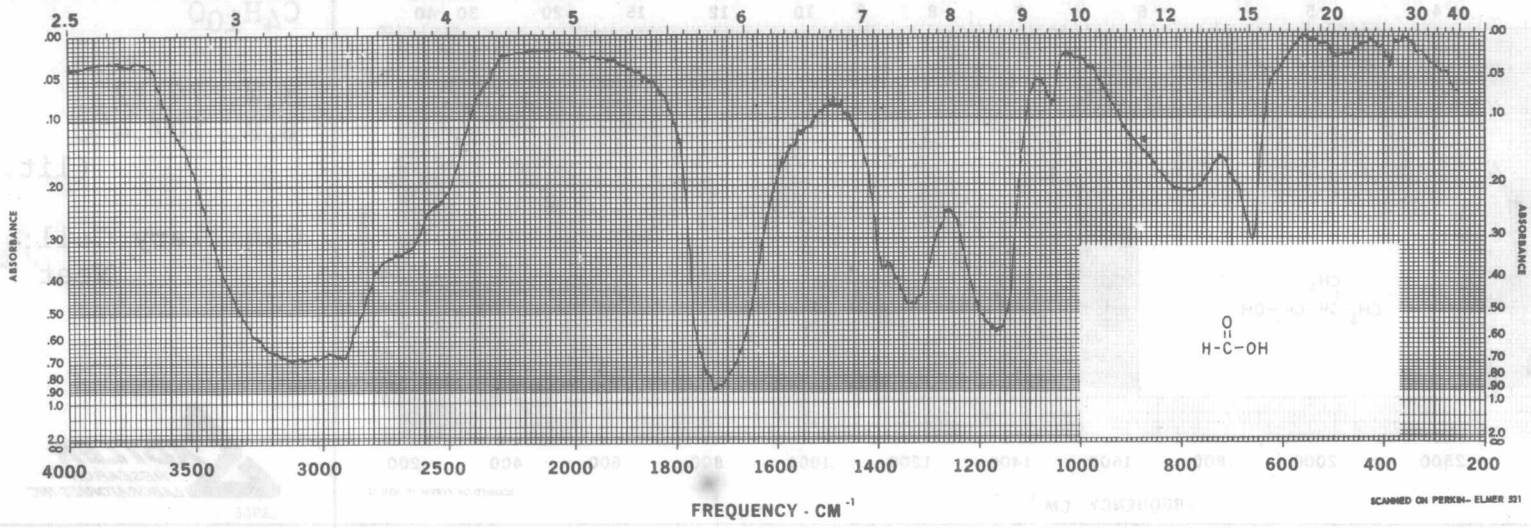
M.W. 282.30

Capillary Cell: Neat

Source: Ohio Apex, Inc., Nitro, W. Va.

14 K

FORMIC ACID



CH_2O_2

M.W. 46.03
M.P. 8.6°C
B.P. 100.8°C

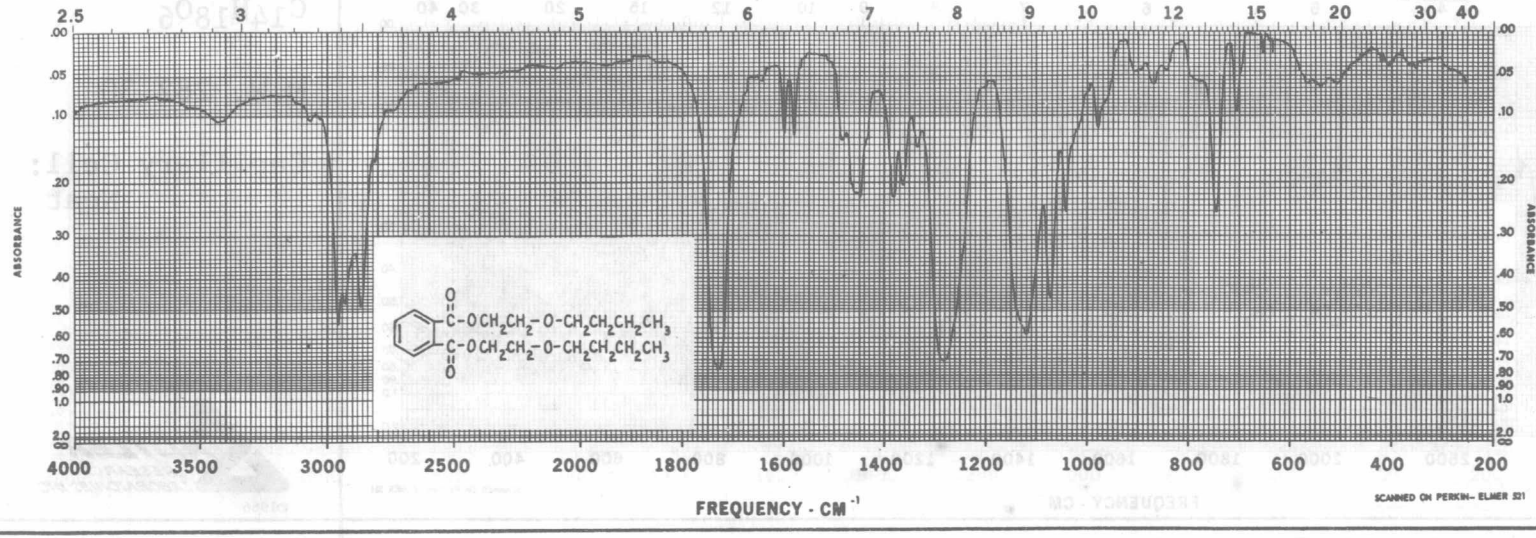
Capillary Cell:
Neat

SADTLER RESEARCH LABORATORIES, INC

Source: The Matheson Co., Inc., E. Rutherford, N.J.

15 K

PHTHALIC ACID, BIS(2-BUTOXYETHYL) ESTER



$C_{20}H_{30}O_6$

M.W. 366.46

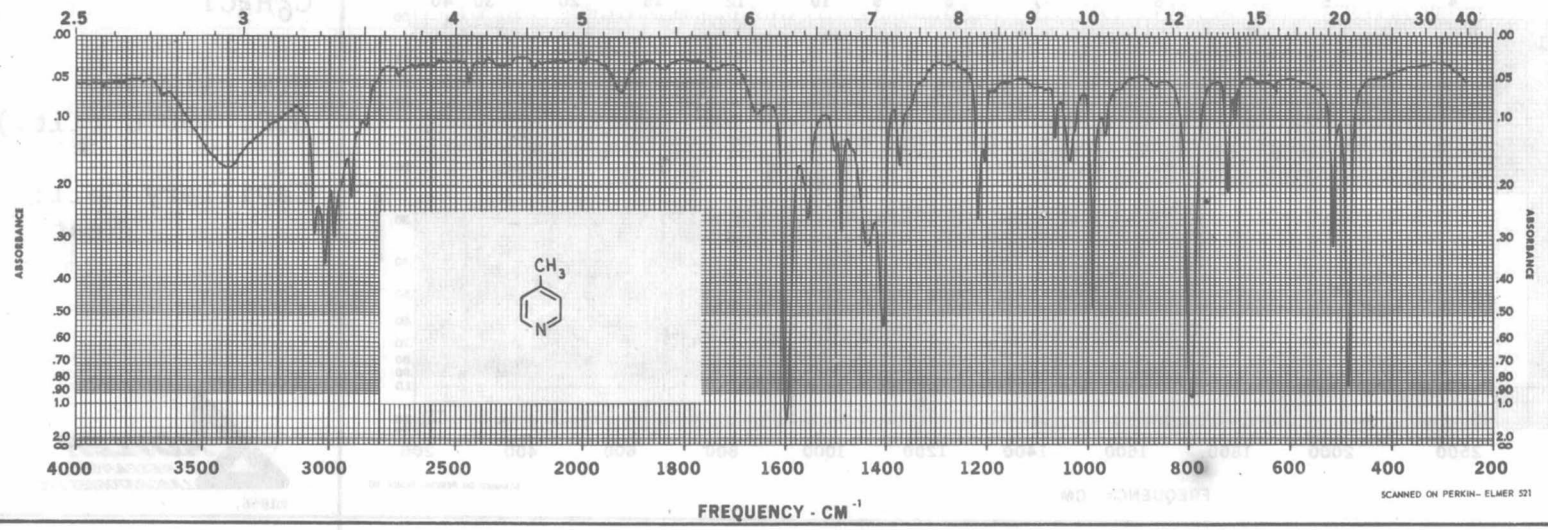
Capillary Cell:
Neat

SADTLER RESEARCH LABORATORIES, INC

Source: Kessler Chemical Co., Inc., Philadelphia, Penna.

16 K

4-PICOLINE



C_6H_7N

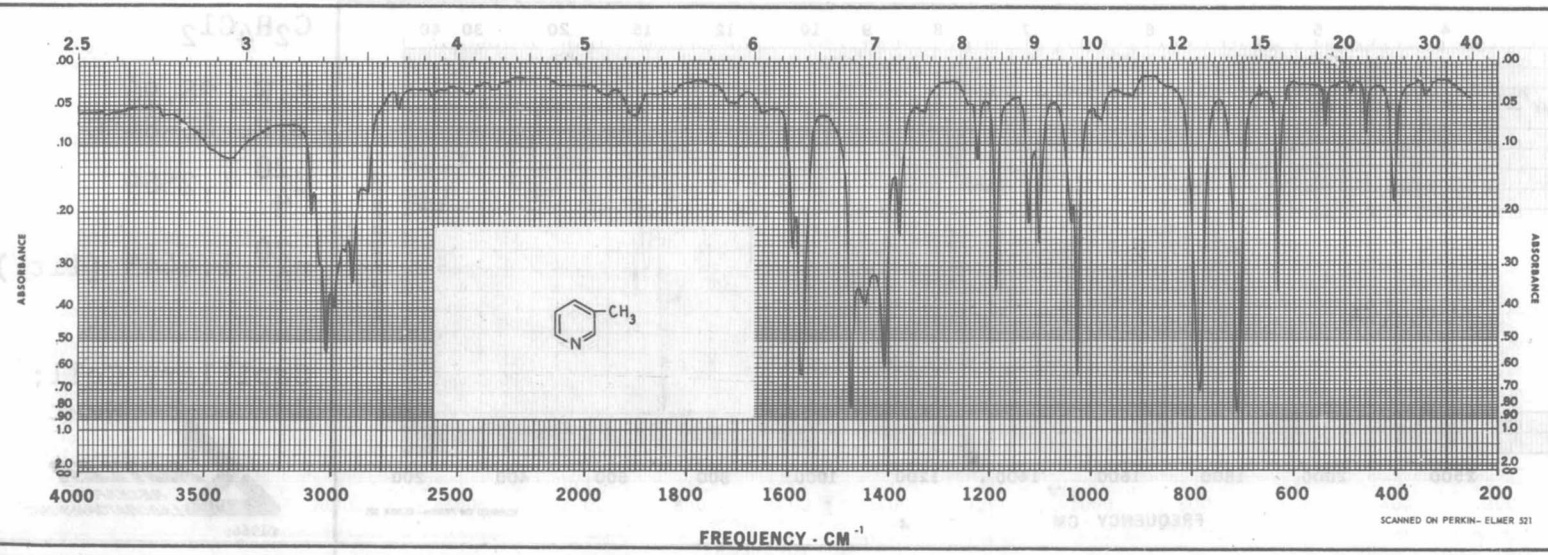
M.W. 93.13
B.P. 142-145°C
d_4^{20} 0.956
n_D^{20} 1.506

Capillary Cell:
Neat

Source: Fluka AG, Buchs, Switzerland

17 K

3-PICOLINE



C_6H_7N

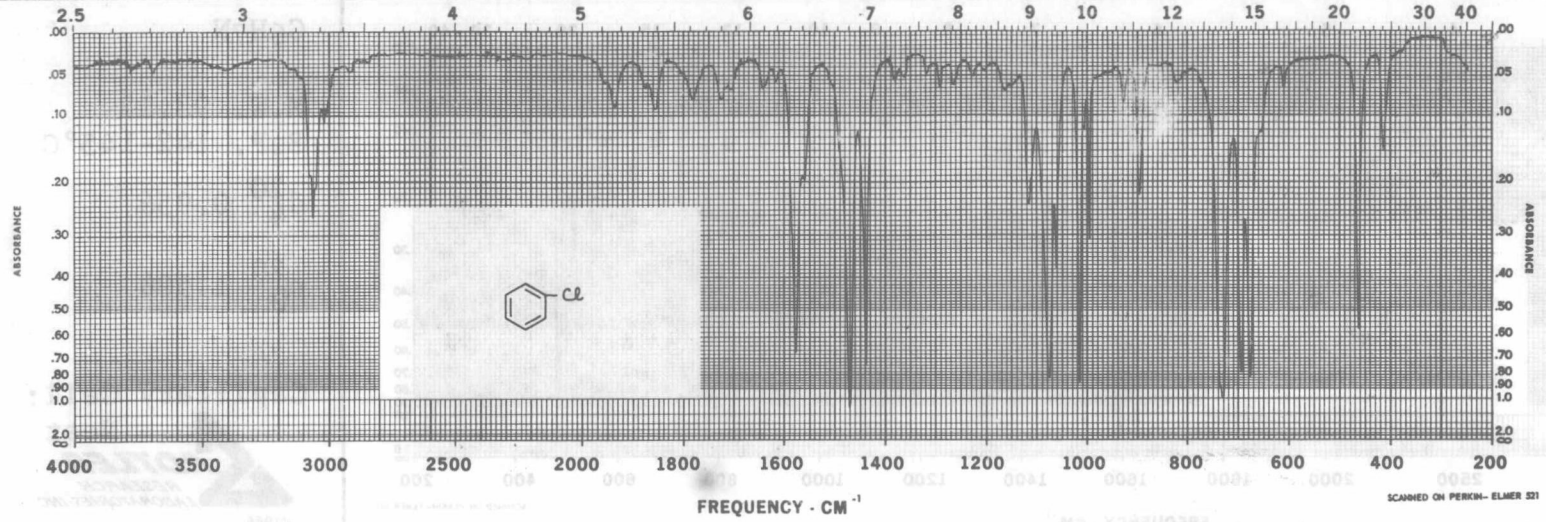
M.W. 93.13
B.P. 141-144°C
d_4^{20} 0.957
n_D^{20} 1.506

Capillary Cell:
Neat

Source: Fluka AG, Buchs, Switzerland

18 K

CHLOROBENZENE



C_6H_5Cl

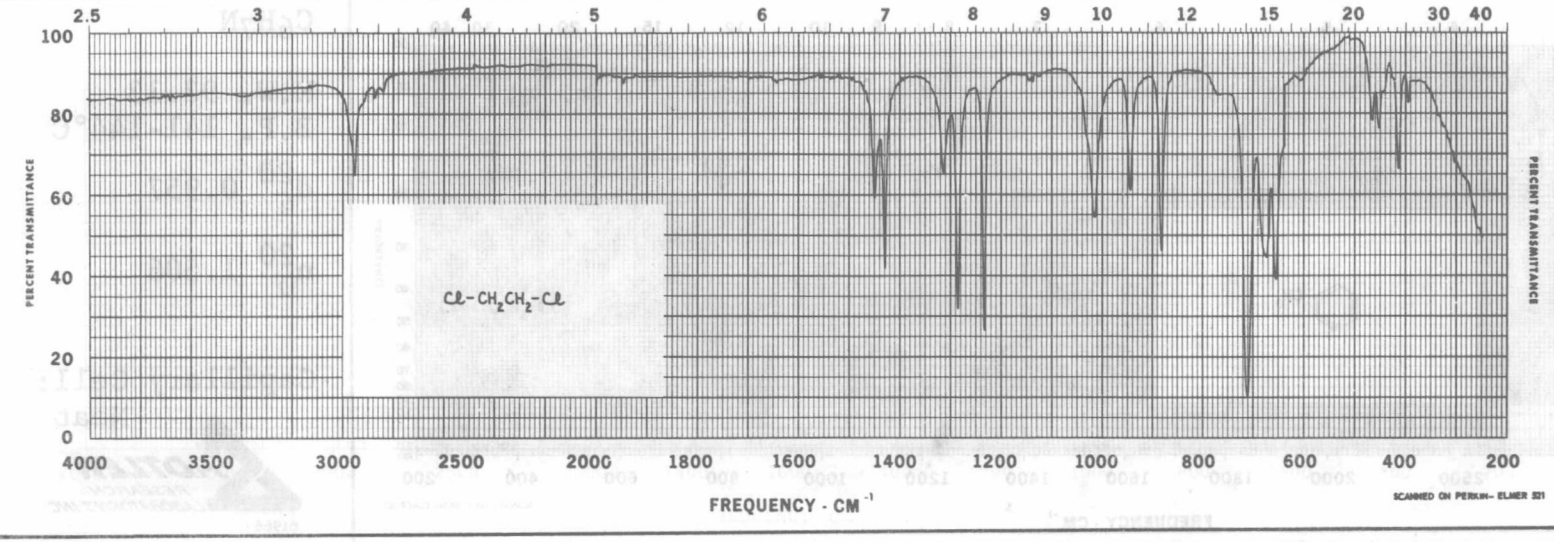
M.W. 112.56
B.P. 130°C (lit.)

Capillary Cell:
Neat

Source: Hooker Electrochemical Co., Niagara Falls, N.Y.

19 K

1,2-DICHLOROETHANE



$C_2H_4Cl_2$

M.W. 98.96
B.P. 83-84°C
d_4^{20} 1.2569

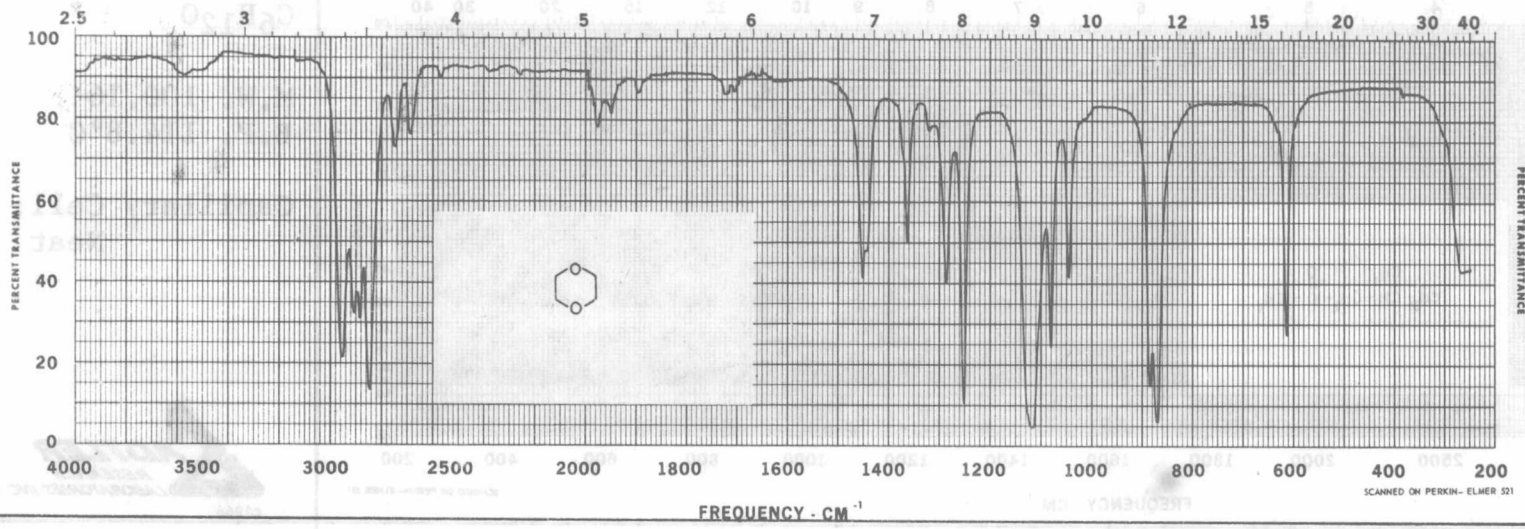
n_D^{20} 1.4443 (lit.)

Capillary Cell:
Neat

Source: United States Testing Co., Inc., Hoboken, N.J.

20 K

p-DIOXANE



$C_4H_8O_2$

M.W. 88.11
M.P. 11°C
B.P. 101°C

d_4^{20} 1.030

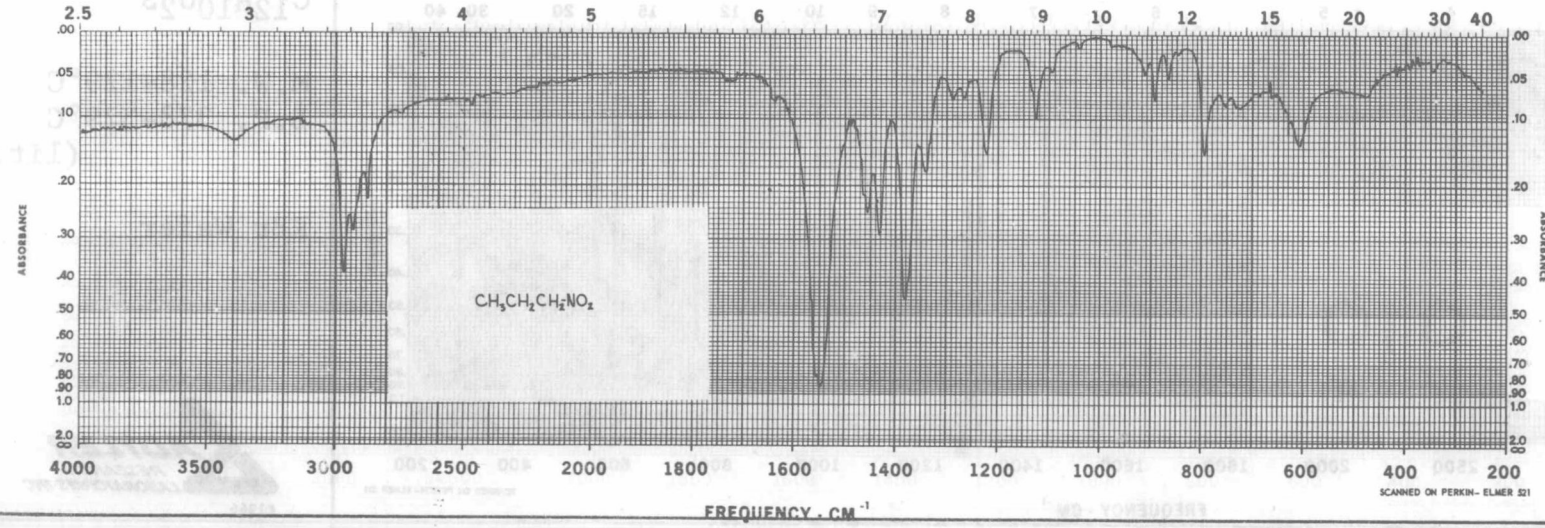
n_D^{20} 1.4232 (lit.)

Capillary Cell:
Neat

Source: The Matheson Co., Inc., E. Rutherford, N.J.

21 K

1-NITROPROPANE



$C_3H_7NO_2$

M.W. 89.09
B.P. 131.6°C/760mm

d_4^{25} 0.9934

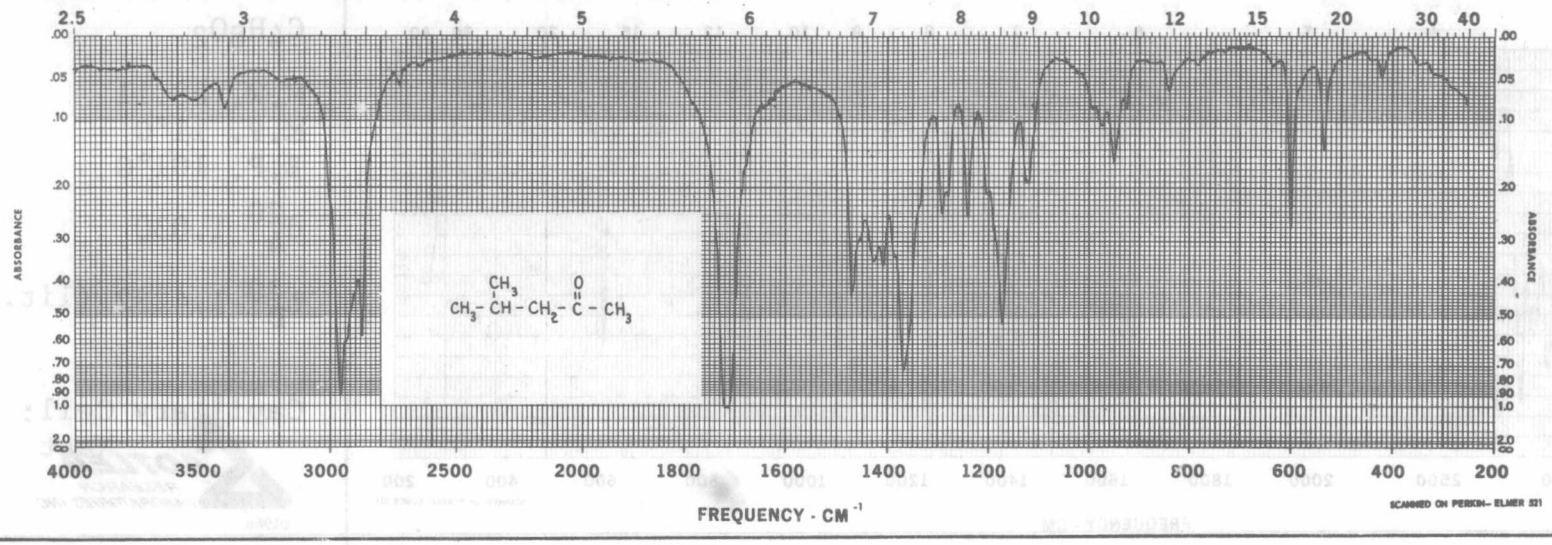
n_D^{20} 1.4018 (lit.)

Capillary Cell:
Neat

Source: Fluka AG, Buchs, Switzerland

22 K

4-METHYL-2-PENTANONE



$C_6H_{12}O$

M.W. 100.16
B.P. 114.8°C

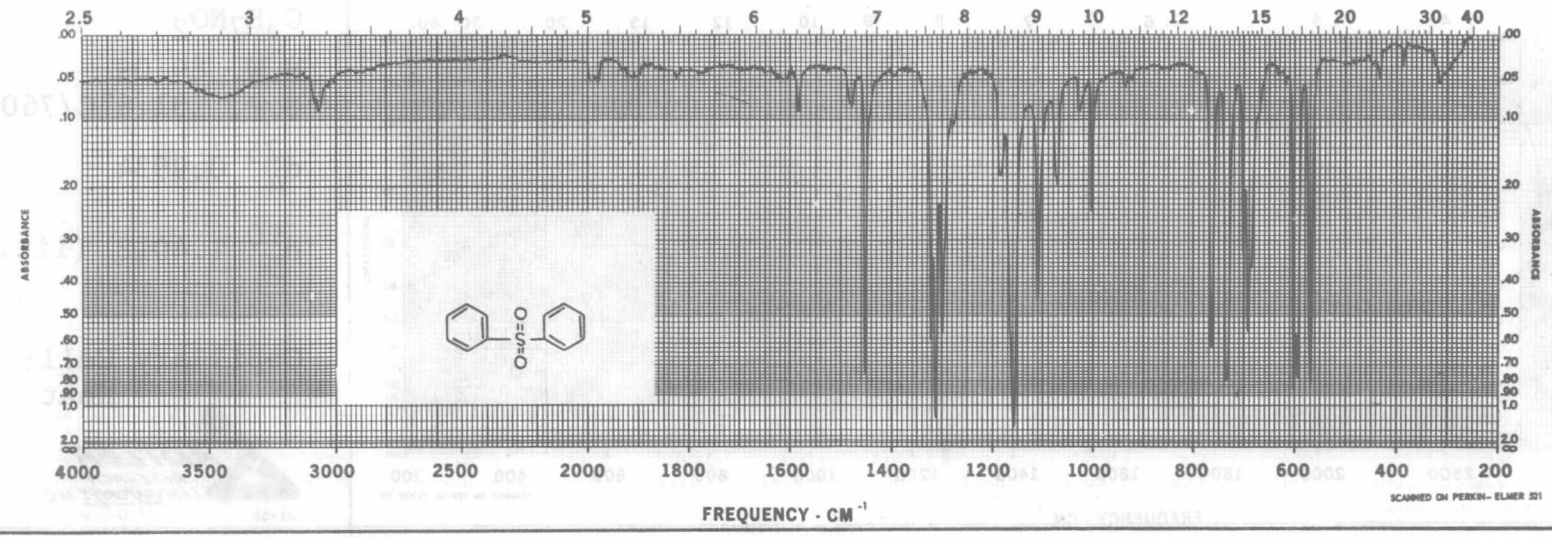
Capillary Cell:
Neat

SADTLER RESEARCH LABORATORIES INC

Source: The Matheson Co., Inc., E. Rutherford, N.J.

23 K

PHENYL SULFONE



$C_{12}H_{10}O_2S$

M.W. 128-129°C
B.P. 378-379°C
(lit.)

KBr Wafer

SADTLER RESEARCH LABORATORIES INC

Source: Aceto Chemical Co., Flushing, N.Y.

24 K