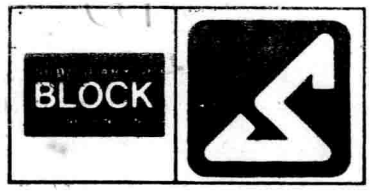
Standard Infrared Grating Spectra

Volume 49–50

48001 - 50000



SADTLER RESEARCH LABORATORIES, INC.

SADTLER STANDARD GRATING SPECTRA

UPDATE VOLUME -- REISSUED PRISM SPECTRA

CREATIVE CHEMISTS SINCE 1874

3316 SPRING GARDEN ST., PHILADELPHIA, PA.
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.

SADTLER RESEARCH LABORATORIES, INC. DOES NOT WARRANT MERCHANTABILITY OR FITNESS FOR ANY PARTICULAR PURPOSE, OR MAKE ANY OTHER WARRANTY OR AGREEMENT EXPRESS OR IMPLIED WITH RESPECT TO THE SPECTRA CONTAINED HEREIN. IF ANY MODEL OR SAMPLE WAS SHOWN TO BUYER, SUCH MODEL OR SAMPLE WAS USED MERELY TO ILLUSTRATE THE ARTICLE AND NOT TO REPRESENT THAT ANY SPECTRA CONTAINED HEREIN WOULD CONFORM TO THE MODEL OR SAMPLE.

SADTLER STANDARD GRATING SPECTRA

This 1976 supplement of 4,000 spectra to the Sadtler Standard Grating Spectra collection brings the total collection to almost 51,000 infrared reference spectrograms. Spectra numbered 49001K through 51000K were determined in the 2.5 - 40 micron region (4000 to ~ 200 cm^{-1}) and are presented on a linear frequency (or wavenumber) vs. transmittance format. Spectra numbered 39001P through 41000P are previously published infrared prism spectra which are now renumbered and re-issued to form an integral part of the Sadtler Standard Grating Spectra collection. Inclusion of the infrared prism spectra is intended to provide the widest available selection of spectral data to Grating Spectra subscribers, grating format spectra are not available at this time since many of the compounds are no longer obtainable.

Presently all grating spectra are prepared at Sadtler Research Laboratories on either a Perkin-Elmer 621 instrument or a Digilab FTS-14 Fourier transform instrument, using samples donated by scientists throughout the world, the source of each sample is shown next to the spectrogram.

Standard techniques have been developed in our laboratories to insure that the spectra published are of the best possible quality and reproducible for comparison and identification purposes. The preferred sample preparation methods are the capillary cell for liquids and the KBr wafer for solids, the spectra obtained are qualitative only. The KBr method is used for solids since it is a standard technique and requires a small sample amount for preparation of good spectra, leaving the remainder for further analytical investigation.

When the KBr method cannot be used for solids due to reaction with the sample, the Split Mull technique is used; the sample is mulled in mineral oil and the entire spectrum is scanned, then a perfluorinated hydrocarbon mull is prepared and scanned in the 3.0 - 3.8 and 6.6 - 7.4 micron regions where mineral oil gives interference from its own absorption. This provides a complete spectrum of the compound.

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

Each spectrum is clearly labelled with the sample preparation technique used.

Continuous updating of the collection is taking place to provide the best possible data. Although the spectra at the beginning of the collection, published over 15 years ago, do not always appear to be of optimum quality, it should be remembered that more recent advances in instrumentation and techniques have improved spectra quality. Earlier spectra are continuously reviewed and replaced when necessary, if a sample is available.

Samples of 98% pure compounds are continually being sought, it is only due to the generosity of those donors whose names appear as the "Source of Sample" that we can offer these spectra to scientists. Our continued thanks are expressed to these contributors.

The following five indexes accompany the Sadtler Standard Spectra:

- Alphabetical Index
- Molecular Formula Index
- Chemical Classes Index
- Numerical Index
- Spec-Finder

The first three are composite indexes containing entries for 51,000 prism spectra and corresponding spectrum numbers for the ∿ 51,000 Sadtler Standard Grating Spectra, the 40,000 Sadtler Ultraviolet Spectra and the 24,000 Sadtler Nuclear Magnetic Resonance Spectra. The last two indexes are specific to the Sadtler Standard Grating Spectra, the numerical index is according to the sequence of the publication and the Spec-Finder provides a means of identifying grating spectra of unknown compounds by comparison with the coded peaks of the references.

WE SUGGEST THAT THE INTRODUCTIONS TO THE VARIOUS INDEXES BE READ CAREFULLY TO ASSURE THE BEST UTILIZATION OF THEIR APPLICATIONS.

48001 P

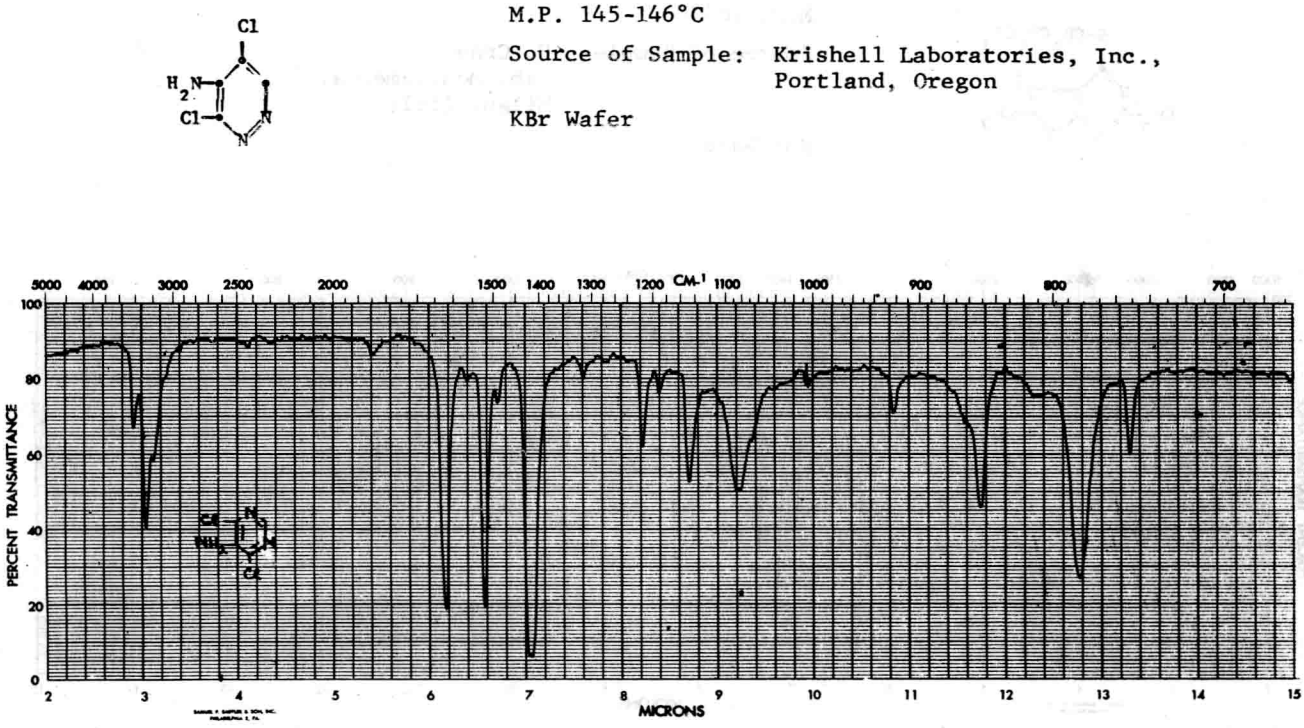
5-AMINO-4,6-DICHLOROPYRIMIDINE

$C_4H_3Cl_2N_3$ Mol. Wt. 164.00

M.P. 145-146°C

Source of Sample: Krishell Laboratories, Inc., Portland, Oregon

KBr Wafer



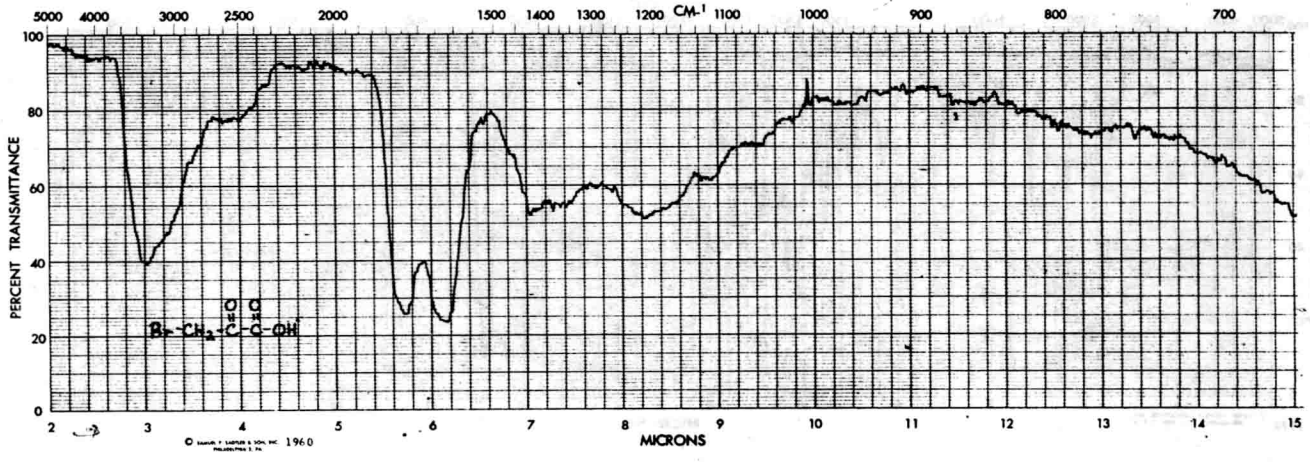
48002 P

BROMOPYRUVIC ACID

$C_3H_3BrO_3$ Mol. Wt. 166.96

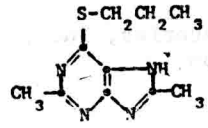
Source of Sample: Fluka AG, Buchs, Switzerland

KBr Wafer



48003 P

2,8-DIMETHYL-6-(PROPYLTHIO) PURINE

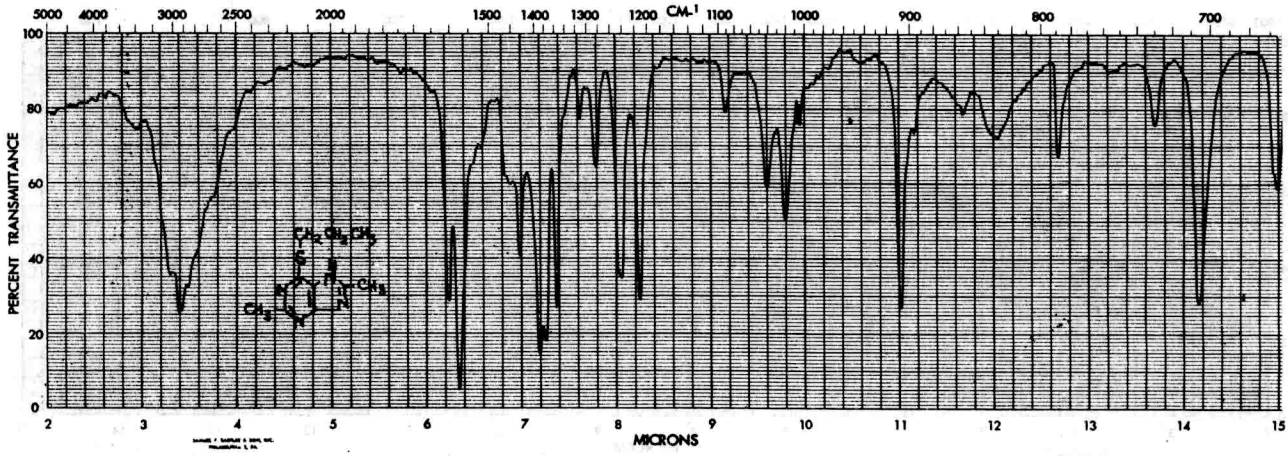


$C_{10}H_{14}N_4S$ Mol. Wt. 222.31

M.P. 168°C

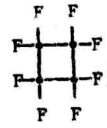
Source of Sample: F. Craveri,
Lab. Medicamenta,
Milan, Italy

KBr Wafer



48004 P

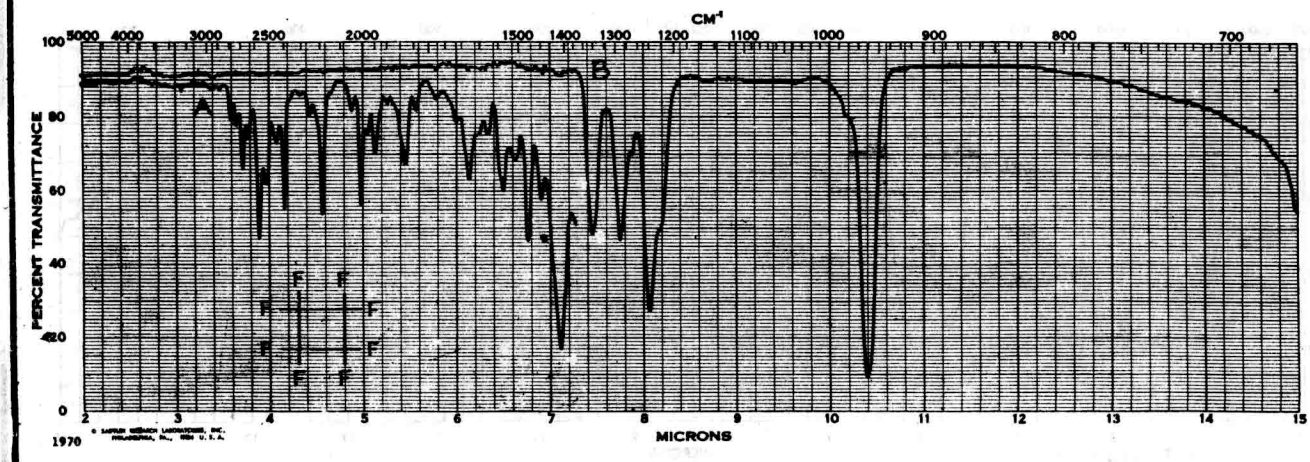
OCTAFLUOROCYCLOBUTANE



C_4F_8 Mol. Wt. 200.03

Source of Sample: Allied Chemical Corp.,
Morristown, New Jersey

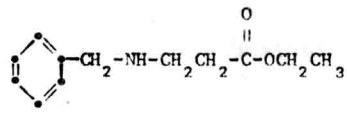
10cm Gas Cell: A=200mm Hg
B=2.8mm Hg



48005 P

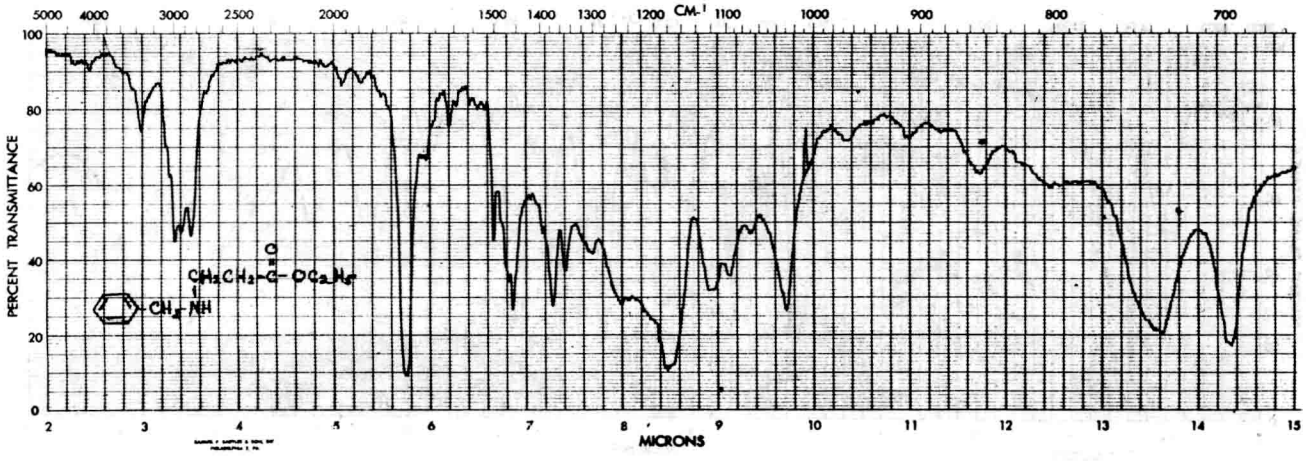
N-BENZYL-β-ALANINE, ETHYL ESTER

$C_{12}H_{17}NO_2$ Mol. Wt. 207.27



Source of Sample: C. Janssen Research Laboratories, Beerse, Belgium

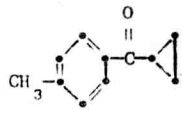
Capillary Cell: Neat



48006 P

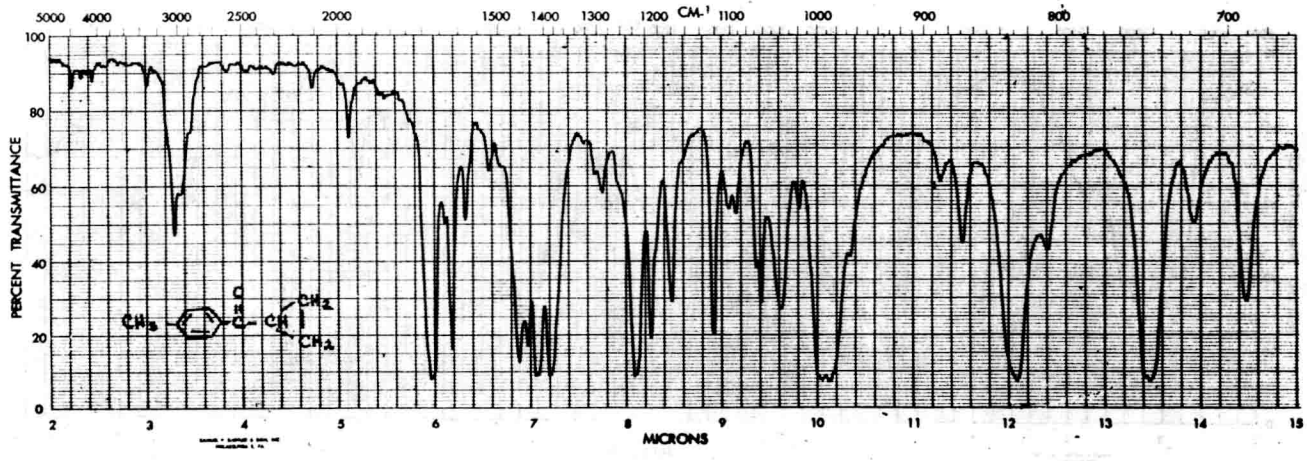
CYCLOPROPYL p-TOLYL KETONE

$C_{11}H_{12}O$ Mol. Wt. 160.22



Source of Sample: C. Janssen Research Laboratories, Beerse, Belgium

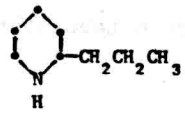
Capillary Cell: Neat



48007 P

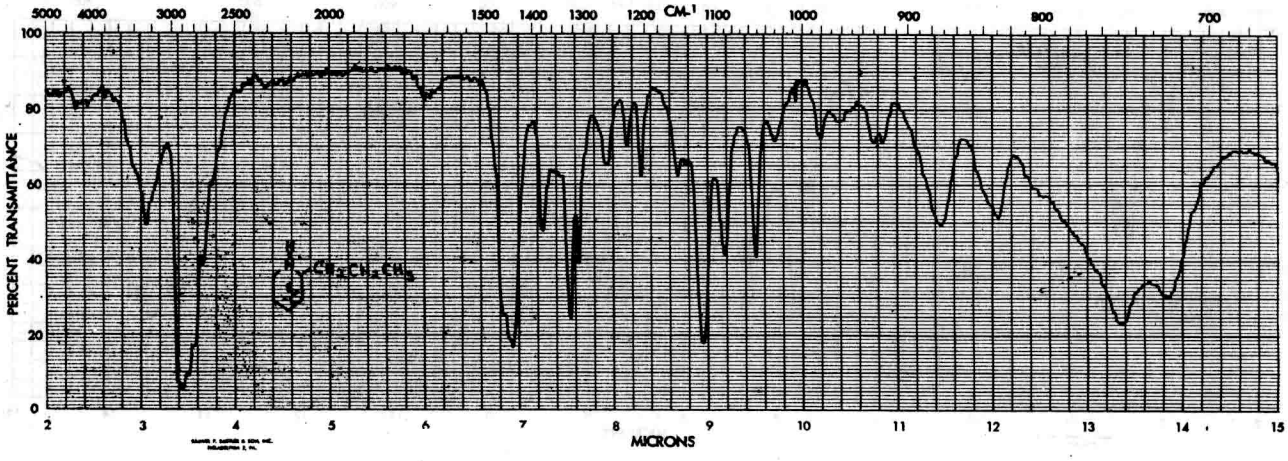
CONINE

$C_8H_{17}N$ Mol. Wt. 127.23



Source of Sample: Fluka AG,
Buchs, Switzerland

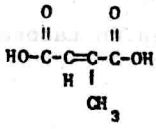
Capillary Cell: 0.01 mm



48008 P

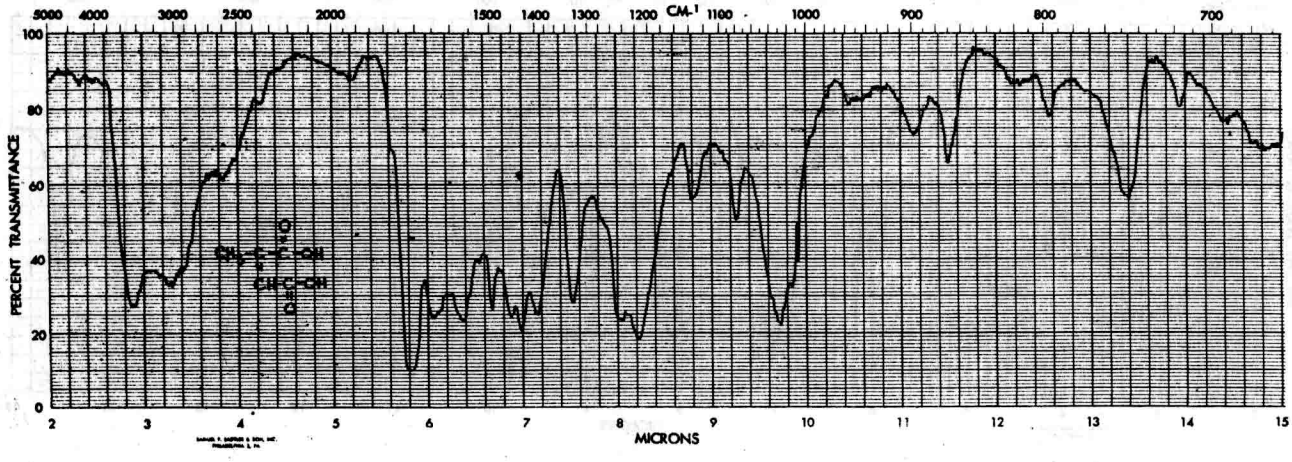
CITRACONIC ACID

$C_5H_6O_4$ Mol. Wt. 130.10



Source of Sample: Fluka AG,
Buchs, Switzerland

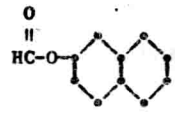
KBr Wafer



48009 P

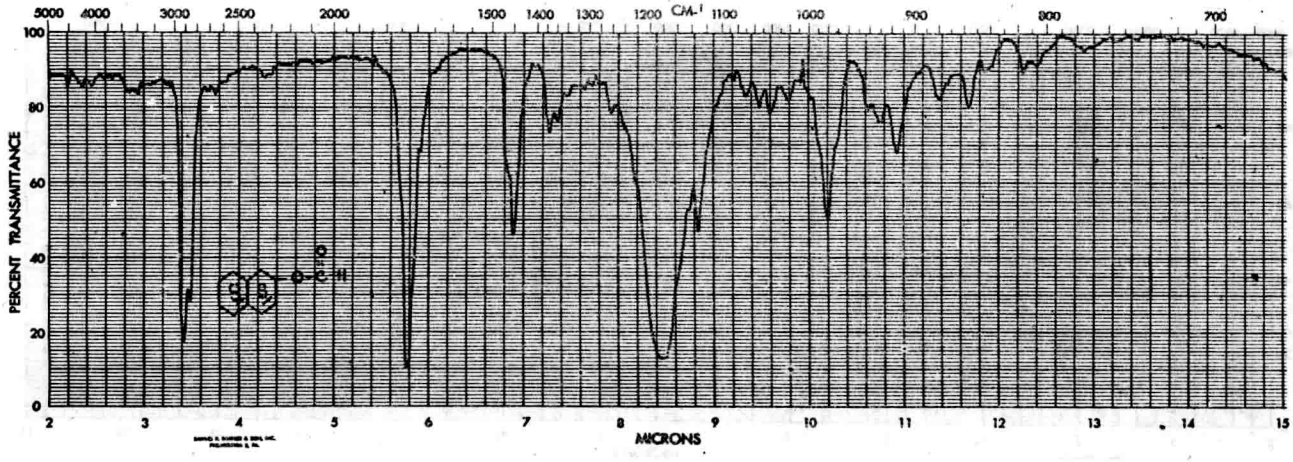
FORMIC ACID, DECAHYDRO-2-NAPHTHYL ESTER

$C_{11}H_{18}O_2$ Mol. Wt. 182.26



Source of Sample: Fluka AG,
Buchs, Switzerland

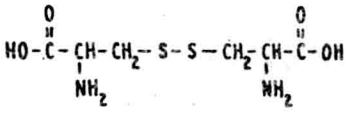
Capillary Cell: Neat



48010 P

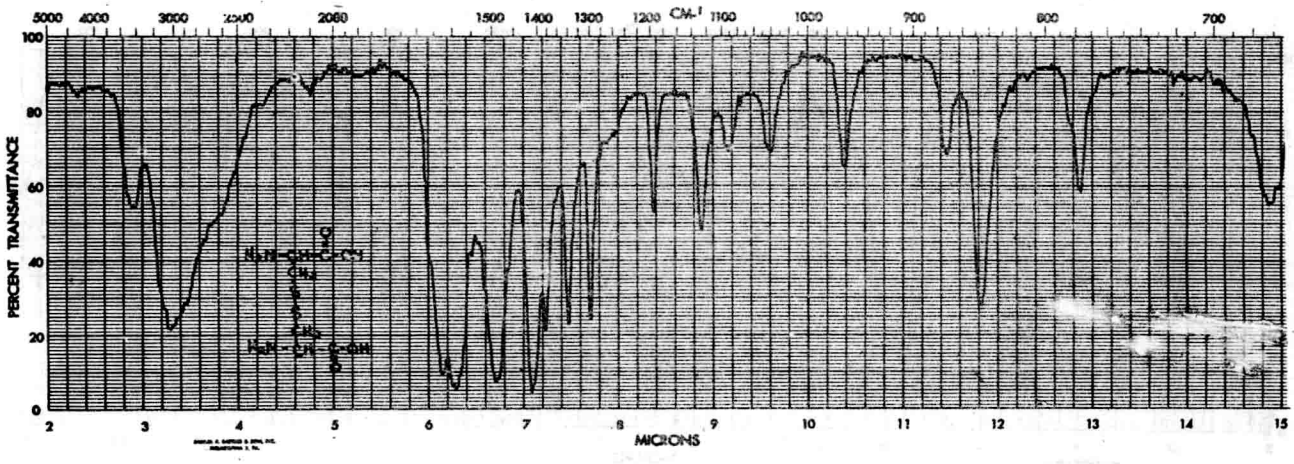
D-CYSTINE

$C_6H_{12}N_2O_4S_2$ Mol. Wt. 240.30



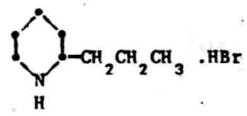
Source of Sample: Fluka AG,
Buchs, Switzerland

KBr Wafer



48011 P

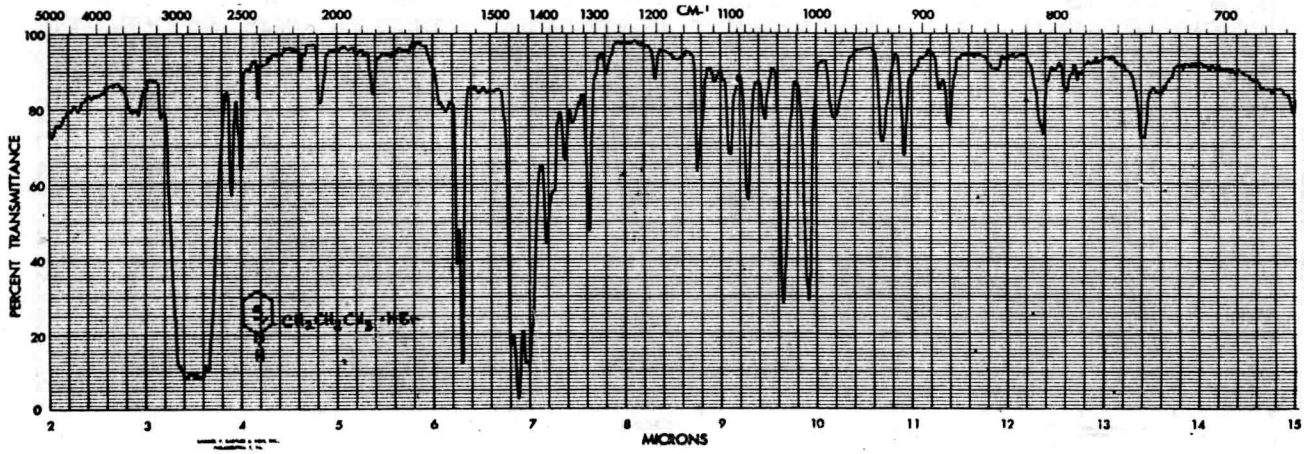
DL-CONINE, HYDROBROMIDE



$C_8H_{17}N \cdot HBr$ Mol. Wt. 208.15

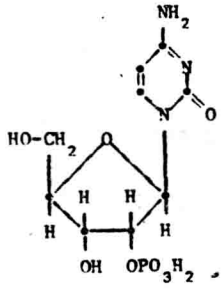
Source of Sample: Fluka AG,
Buchs, Switzerland

KBr Wafer



48012 P

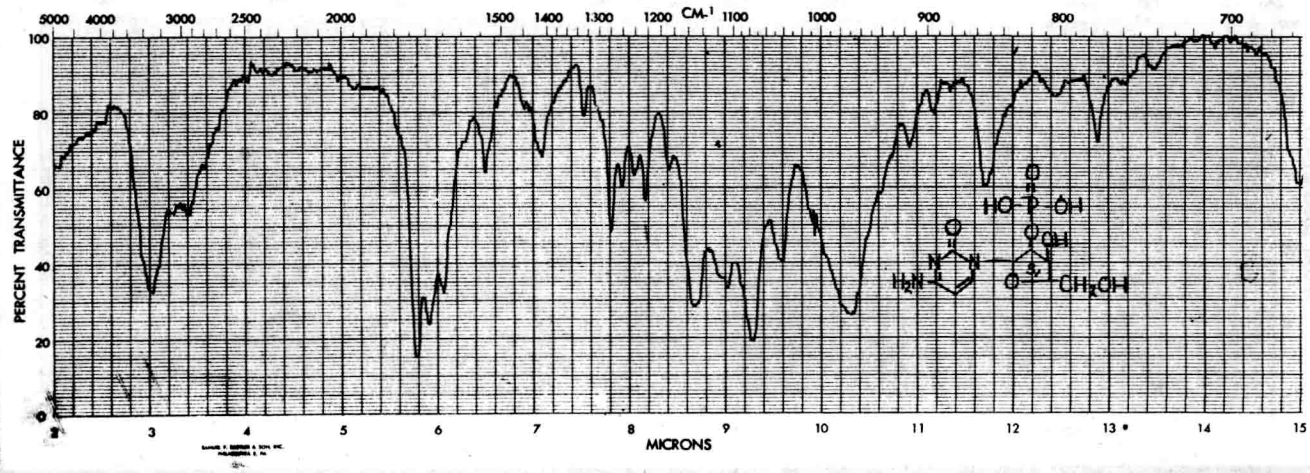
2'-CYTIDYLIC ACID



$C_9H_{14}N_3O_8P$ Mol. Wt. 323.20

Source of Sample: Fluka AG,
Buchs, Switzerland

KBr Wafer



48013 P

2-AMINOETHANETHIOL

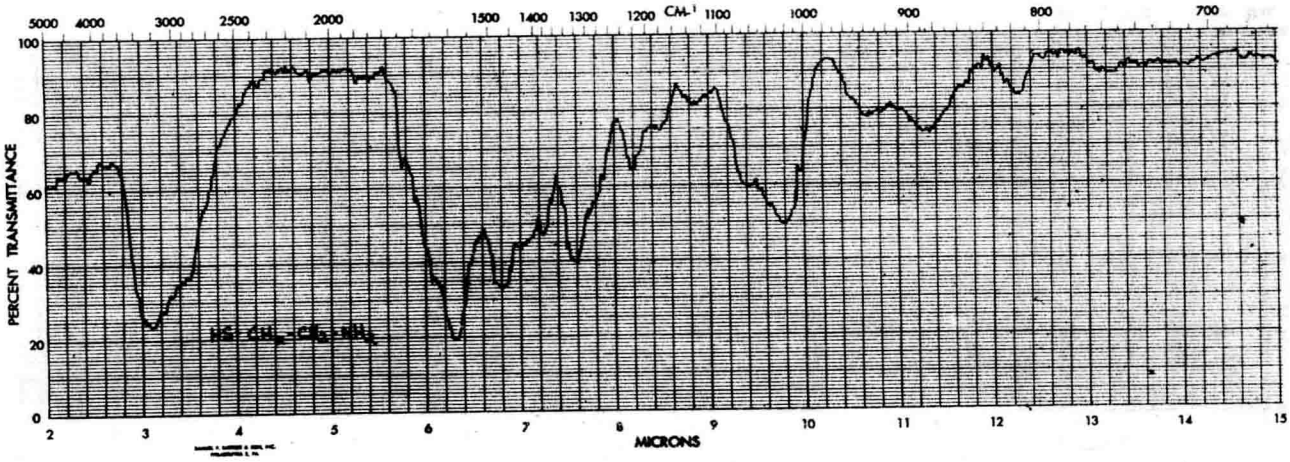
C_2H_7NS Mol. Wt. 77.15

M.P. 95-97°C

Source of Sample: Fluka AG,
Buchs, Switzerland

$H_2N-CH_2CH_2-SH$

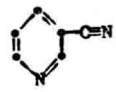
KBr Wafer



48014 P

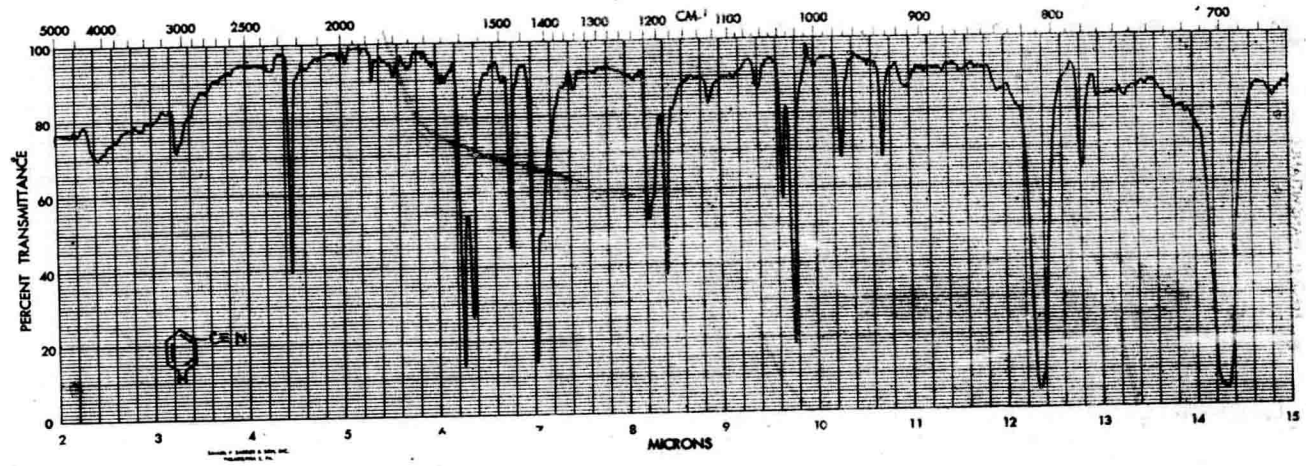
NICOTINONITRILE

$C_6H_4N_2$ Mol. Wt. 104.11



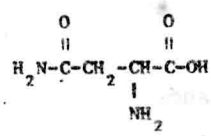
Source of Sample: Fluka AG,
Buchs, Switzerland

KBr Wafer



48015 P

L-ASPARAGINE

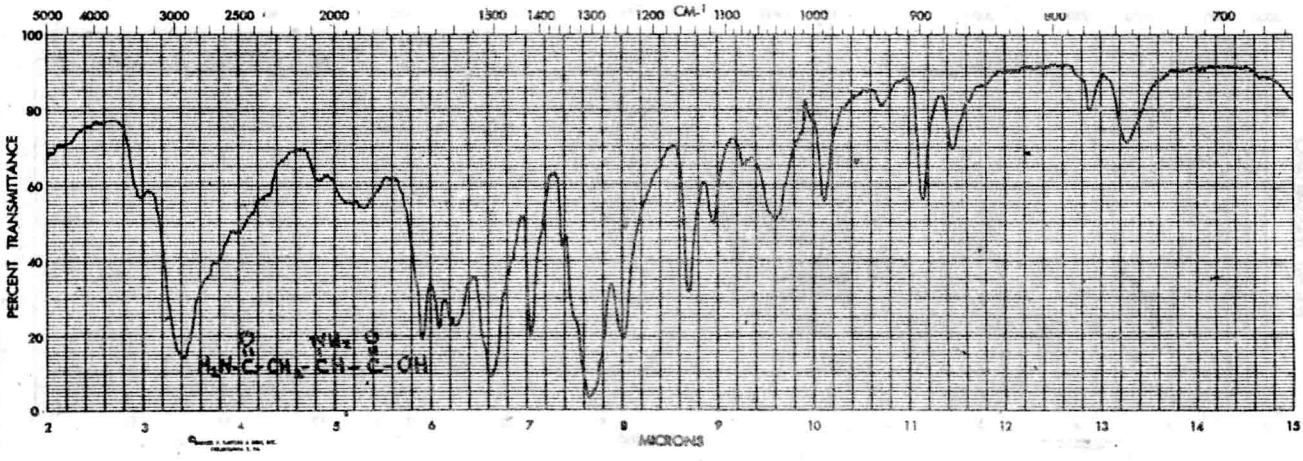


$C_4H_8N_2O_3$ Mol. Wt. 132.12

α_D^{25} 36.10

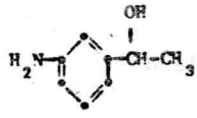
Source of Sample: Fluka AG,
Buchs, Switzerland

KBr Wafer



48016 P

m-AMINO-α-METHYLBENZYL ALCOHOL

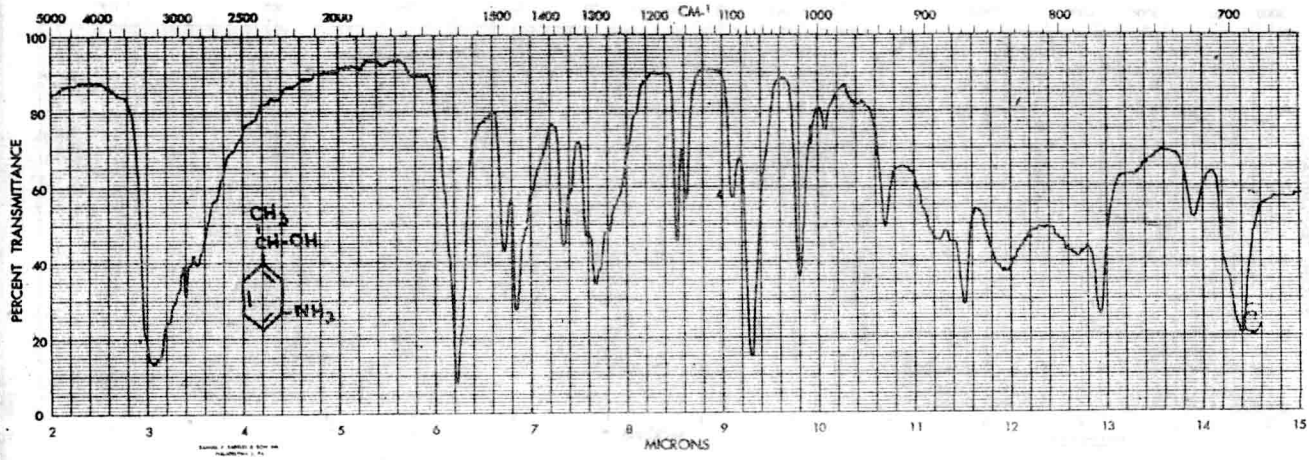


$C_8H_{11}NO$ Mol. Wt. 137.18

B.P. 160.5°C/10 mm

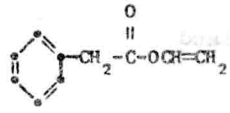
Source of Sample: MCB Manufacturing Chemists,
Norwood, Ohio

KBr Wafer



48017 P

PHENYLACETIC ACID, VINYL ESTER

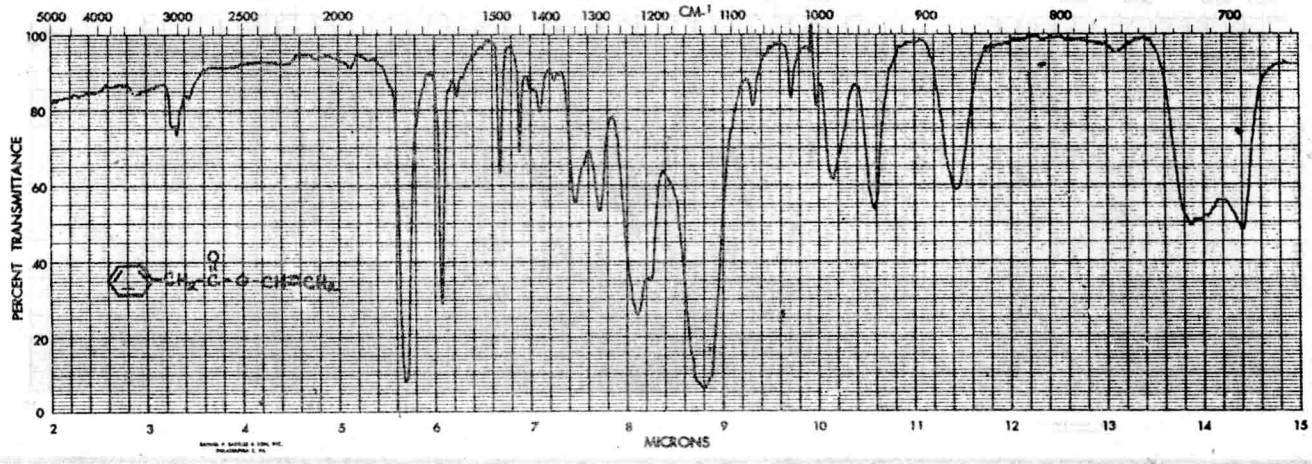


$C_{10}H_{10}O_2$ Mol. Wt. 162.19

B.P. 88-90°C/4 mm

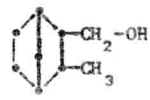
Source of Sample: Monomer-Polymer Labs., Borden, Inc., Philadelphia, Pennsylvania

Capillary Cell: Neat



48018 P

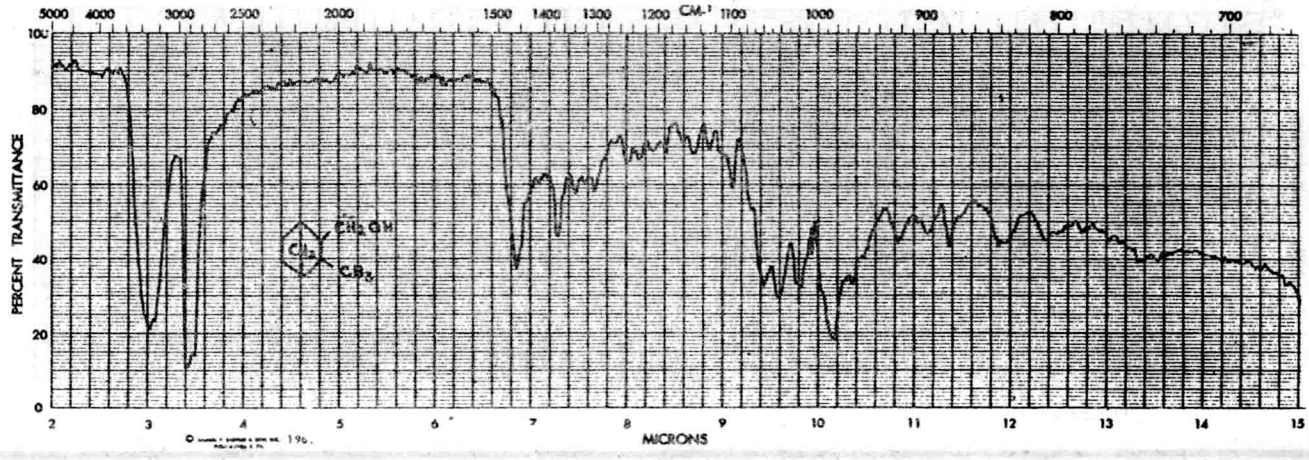
3-METHYL-2-NORBORNANEMETHANOL



$C_9H_{16}O$ Mol. Wt. 140.23

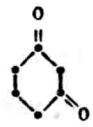
Source of Sample: Eastman Chemical Products, Inc. Kingsport, Tennessee

Capillary Cell: Neat



48019 P

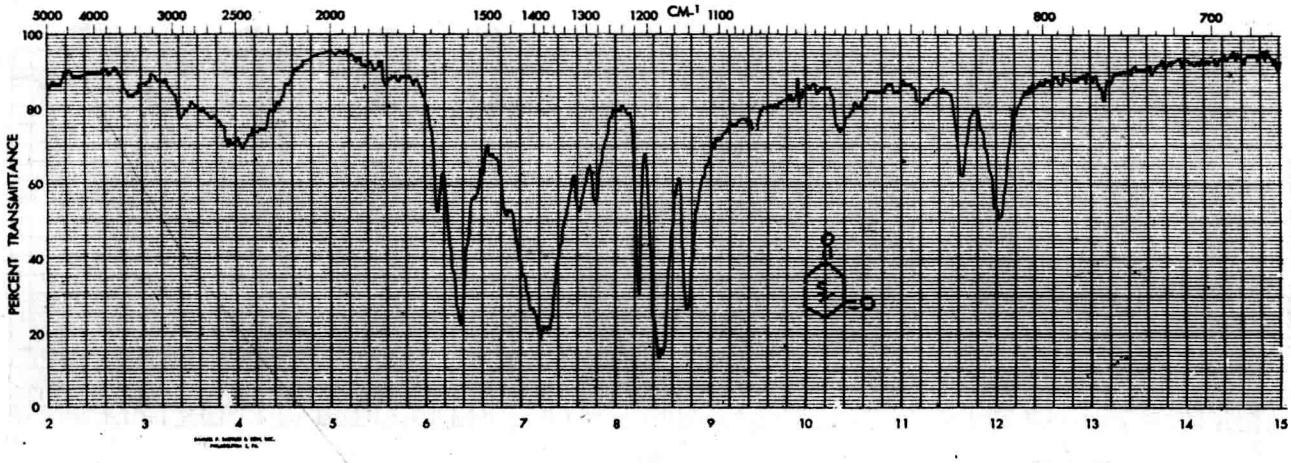
1,3-CYCLOHEXANEDIONE



$C_6H_8O_2$ Mol. Wt. 112.13

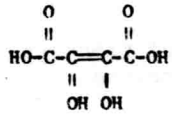
Source of Sample: Fluka AG,
Buchs, Switzerland

KBr Wafer



48020 P

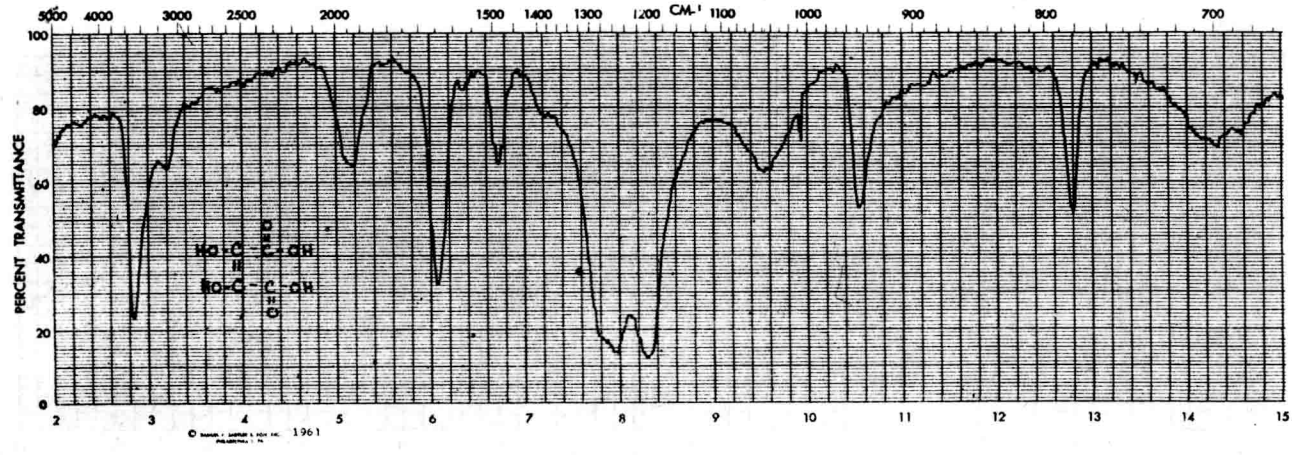
DIHYDROXYMALEIC ACID



$C_4H_4O_6$ Mol. Wt. 148.07

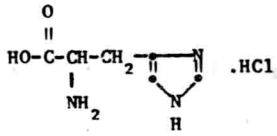
Source of Sample: Fluka AG,
Buchs, Switzerland

KBr Wafer



48021 P

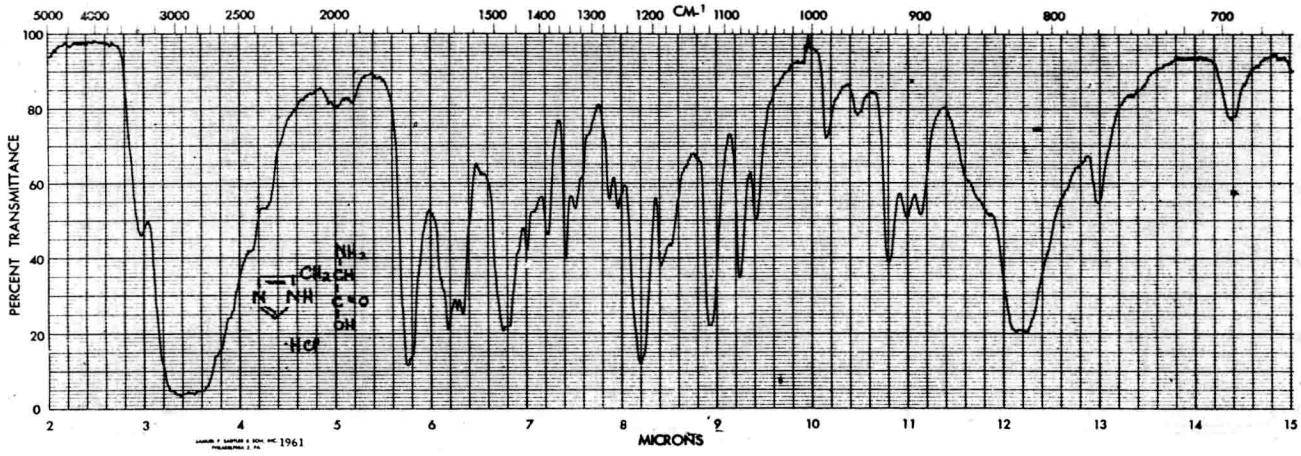
DL-HISTIDINE, MONOHYDROCHLORIDE



$C_6H_9N_3O_2 \cdot HCl$ Mol. Wt. 191.62

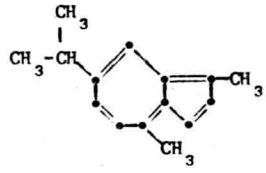
Source of Sample: Fluka AG,
Buchs, Switzerland

KBr Wafer



48022 P

1,4-DIMETHYL-7-ISOPROPYLAZULENE

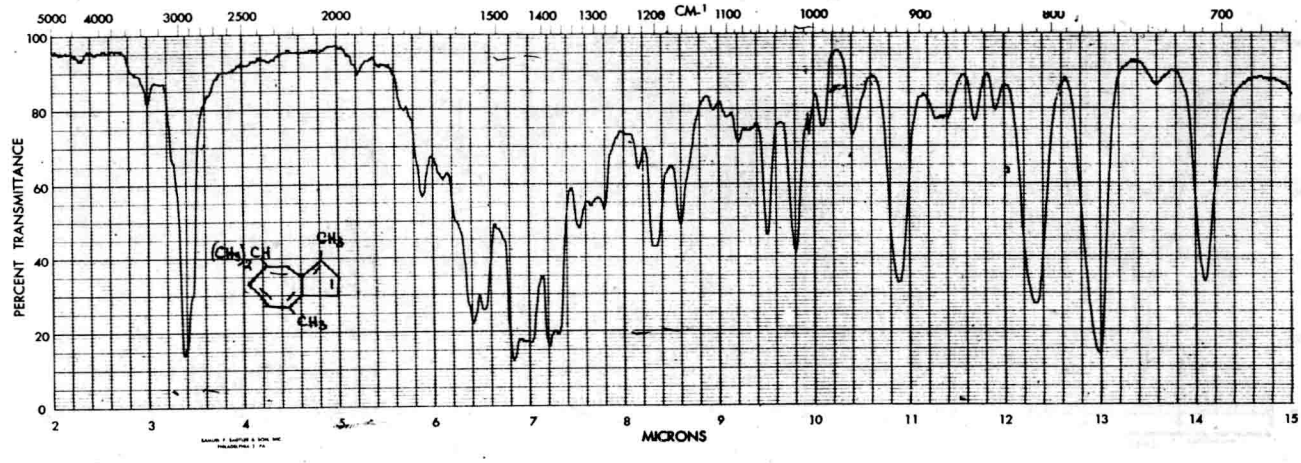


$C_{15}H_{18}$ Mol. Wt. 198.31

M.P. 28-30°C

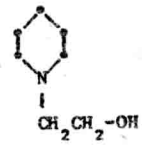
Source of Sample: Fluka AG,
Buchs, Switzerland

Capillary Cell: 0.025 mm



48023 P

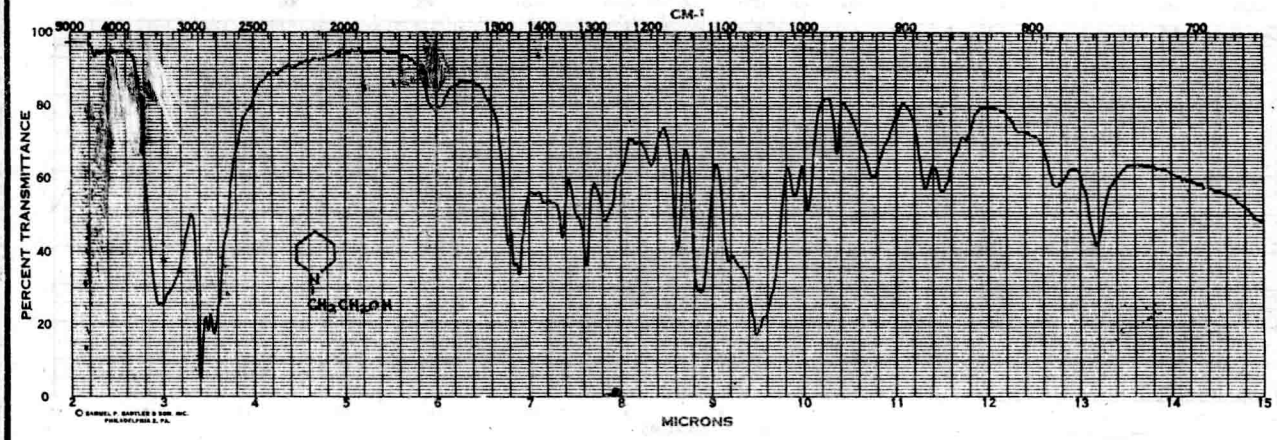
1-PIPERIDINEETHANOL



$C_7H_{15}NO$ Mol. Wt. 129.20

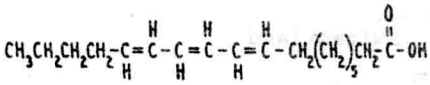
Source of Sample: Fluka AG,
Buchs, Switzerland

Capillary Cell: 0.01 mm



48024 P

trans,trans,trans-9,11,13-OCTADECATRIENOIC ACID



$C_{18}H_{30}O_2$ Mol. Wt. 278.44

M.P. 70.5-72°C (lit.)

Source of Sample: Fluka AG,
Buchs, Switzerland

Capillary Cell: Melt