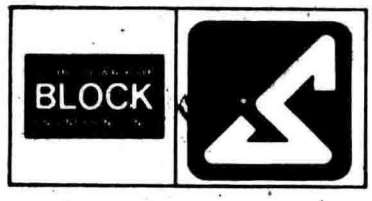
Standard Infrared Grating Spectra Volume 31–32

30001 - 32000



SADTLER RESEARCH LABORATORIES, INC.

STANDARD INFRARED PRISM SPECTRA

CREATIVE CHEMISTS SINCE 1874

3316 SPRING GARDEN ST., PHILADELPHIA, PA. 19104
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.

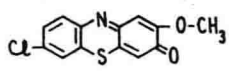
WE SUGGEST THAT THE PREFACES TO THE VARIOUS INDICES BE READ SINCE SEVERAL CHANGES AND ADDITIONS HAVE BEEN MADE.

7-CHLORO-2-METHOXY-3H-PHENOTHIAZIN-3-ONE

30001K

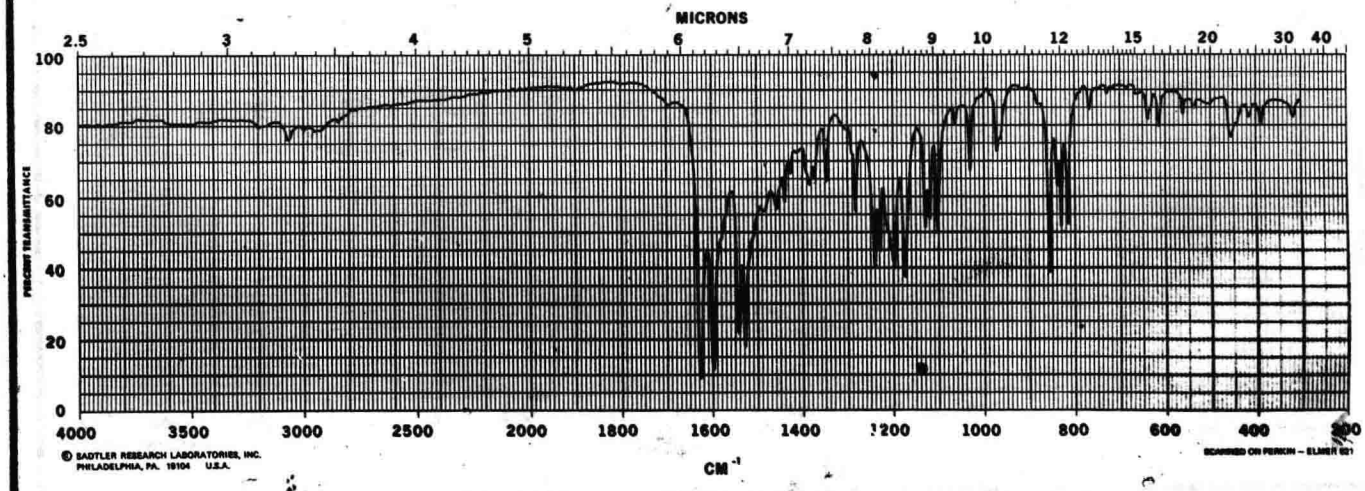
$C_{13}H_8ClNO_2S$ Mol. Wt. 277.73

M.P. 231°C



Source: S. K. Jain,
University of Rajasthan,
Jaipur, India

KBr Wafer

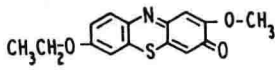


7-ETHOXY-2-METHOXY-3H-PHENOTHIAZIN-3-ONE

30002K

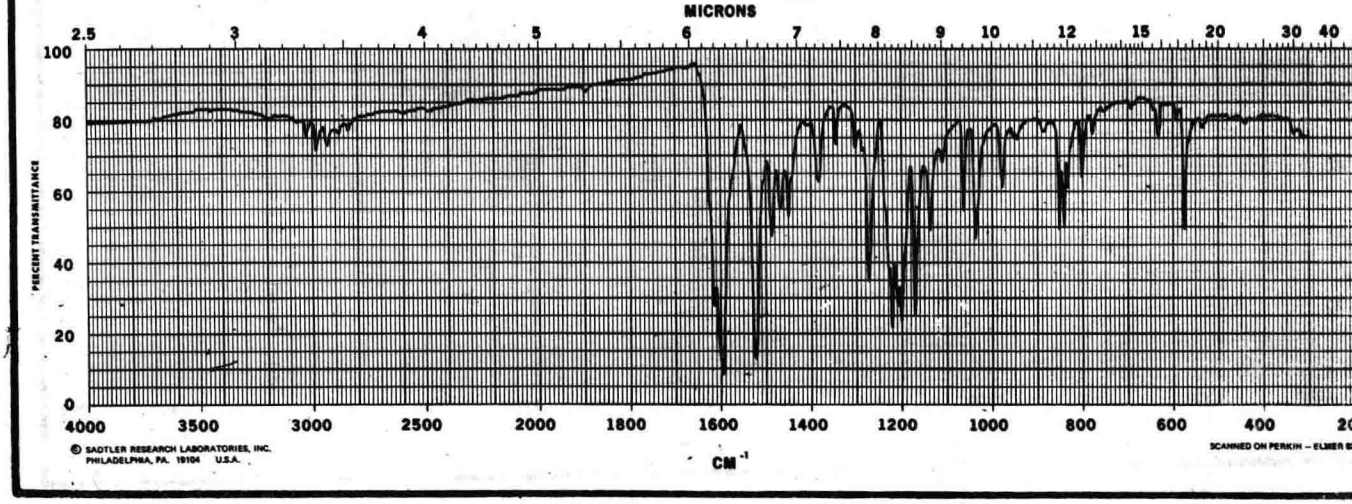
$C_{15}H_{13}NO_3S$ Mol. Wt. 287.34

M.P. 208°C



Source: S. K. Jain,
University of Rajasthan,
Jaipur, India

KBr Wafer

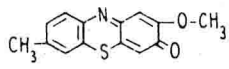


30003K

2-METHOXY-7-METHYL-3H-PHENOTHIAZIN-3-ONE

$C_{14}H_{11}NO_2S$ Mol. Wt. 257.31

M.P. 203°C



Source: S. K. Jain,
University of Rajasthan,
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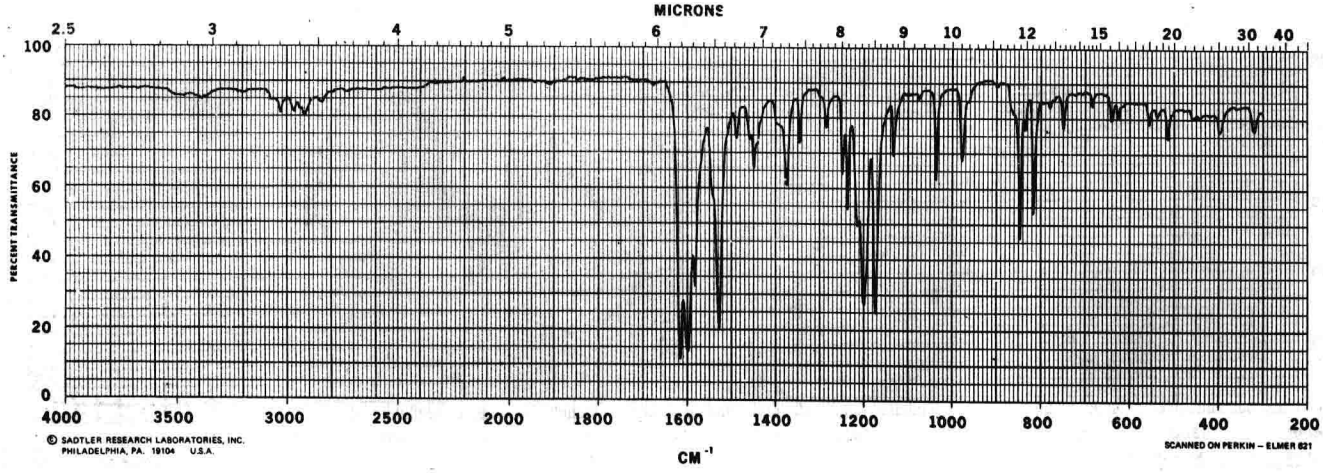
KBr Wafer

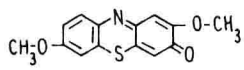


30004K

2,7-DIMETHOXY-3H-PHENOTHIAZIN-3-ONE

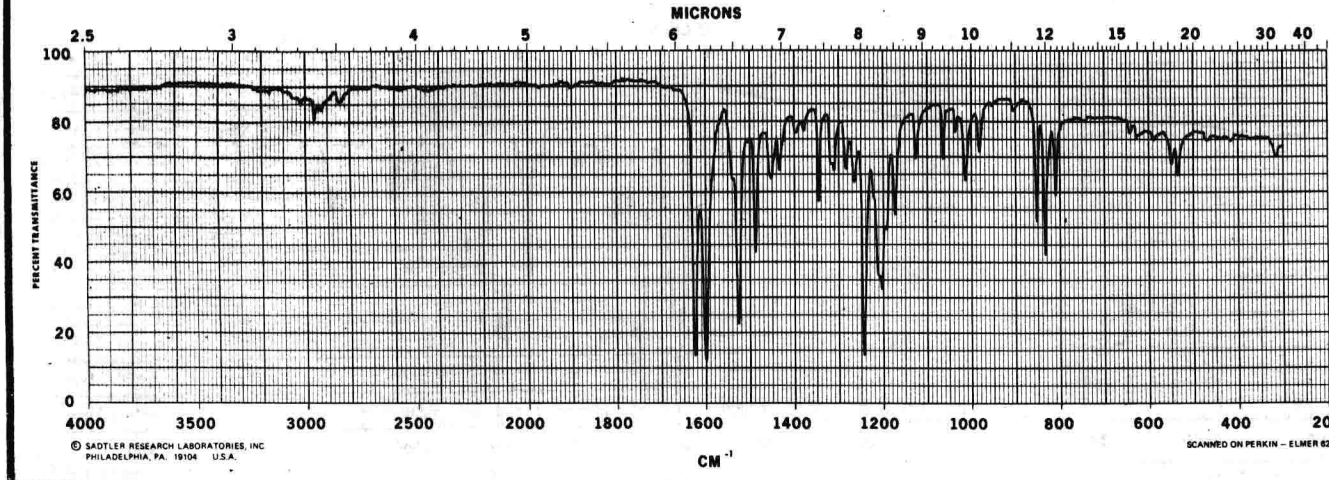
$C_{14}H_{11}NO_3S$ Mol. Wt. 273.31

M.P. 232°C



Source: S. K. Jain,
University of Rajasthan,
Jaipur, India

KBr Wafer

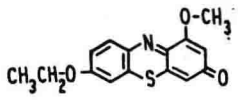


7-ETHOXY-1-METHOXY-3H-PHENOTHIAZIN-3-ONE

30005K

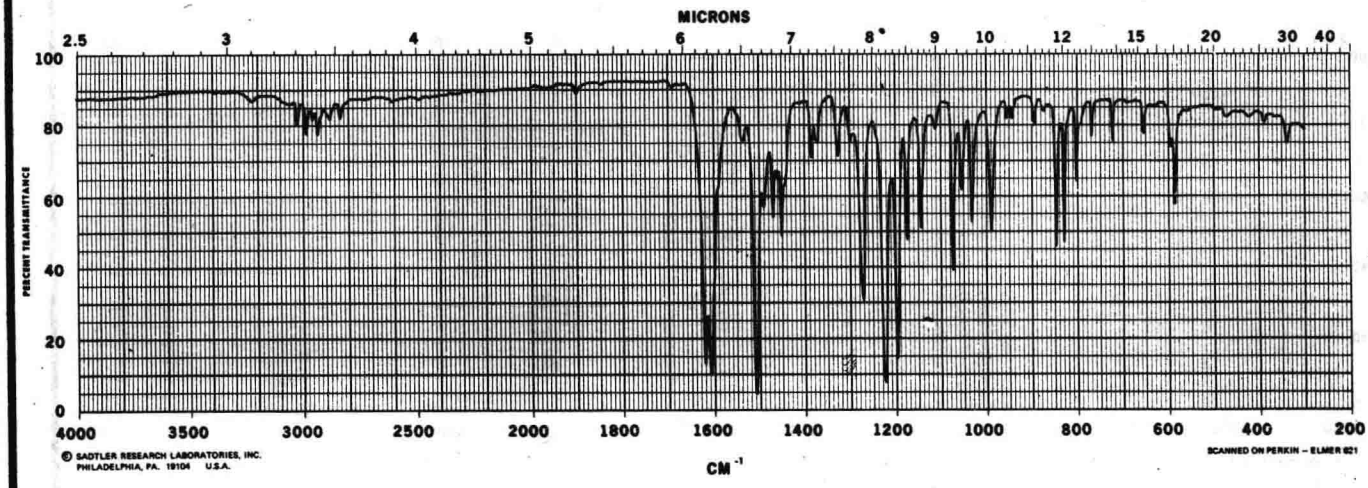
$C_{15}H_{13}NO_3S$ Mol. Wt. 287.34

M.P. 235°C



Source: S. K. Jain,
University of Rajasthan,
Jaipur, India

KBr Wafer

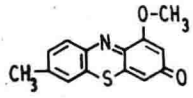


1-METHOXY-7-METHYL-3H-PHENOTHIAZIN-3-ONE

30006K

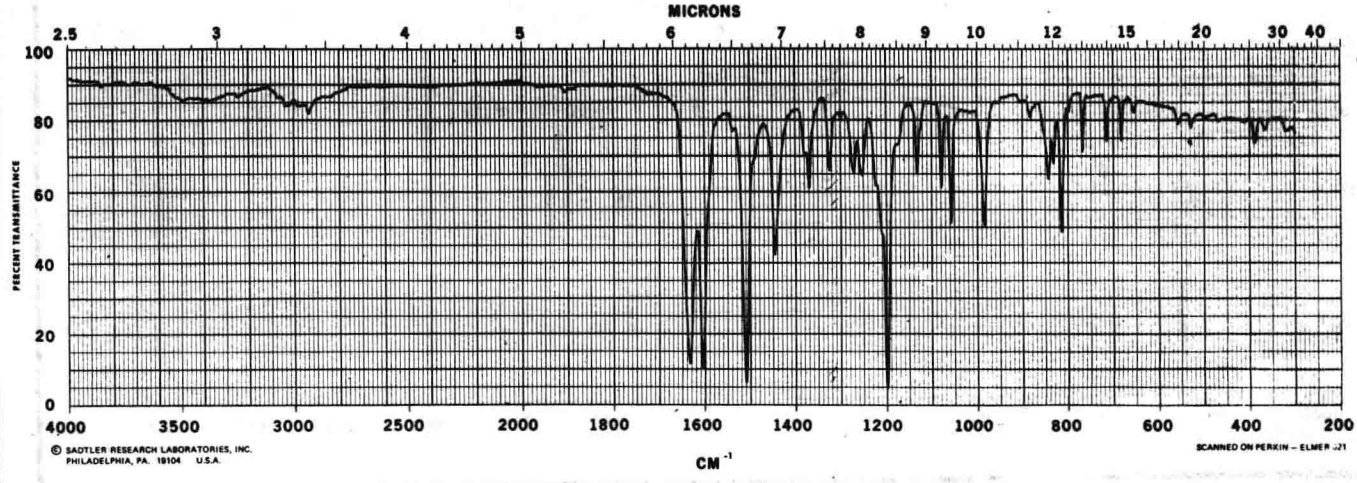
$C_{14}H_{11}NO_2S$ Mol. Wt. 257.31

M.P. 237°C



Source: S. K. Jain,
University of Rajasthan,
Jaipur, India

KBr Wafer

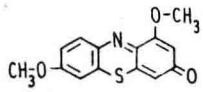


30007K

1,7-DIMETHOXY-3H-PHENOTHIAZIN-3-ONE

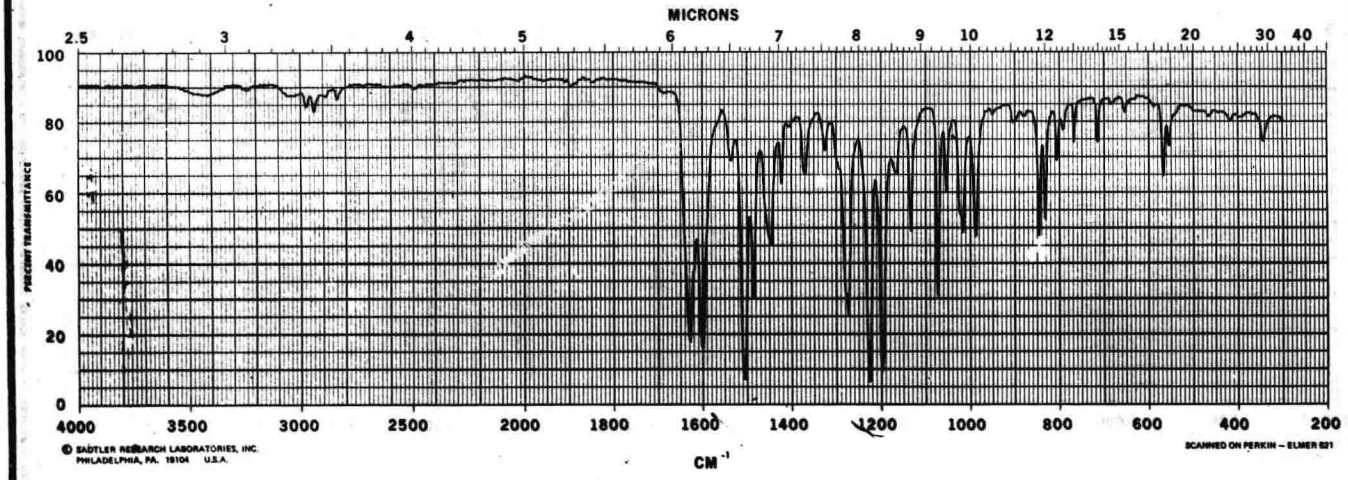
$C_{14}H_{11}NO_3S$ Mol. Wt. 273.31

M.P. 253°C



Source: S. K. Jain,
University of Rajasthan,
Jaipur, India

KBr Wafer

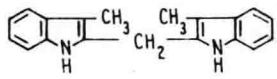


30008K

2,2'-METHYLENEBIS[3-METHYLINDOLE]

$C_{19}H_{18}N_2$ Mol. Wt. 274.37

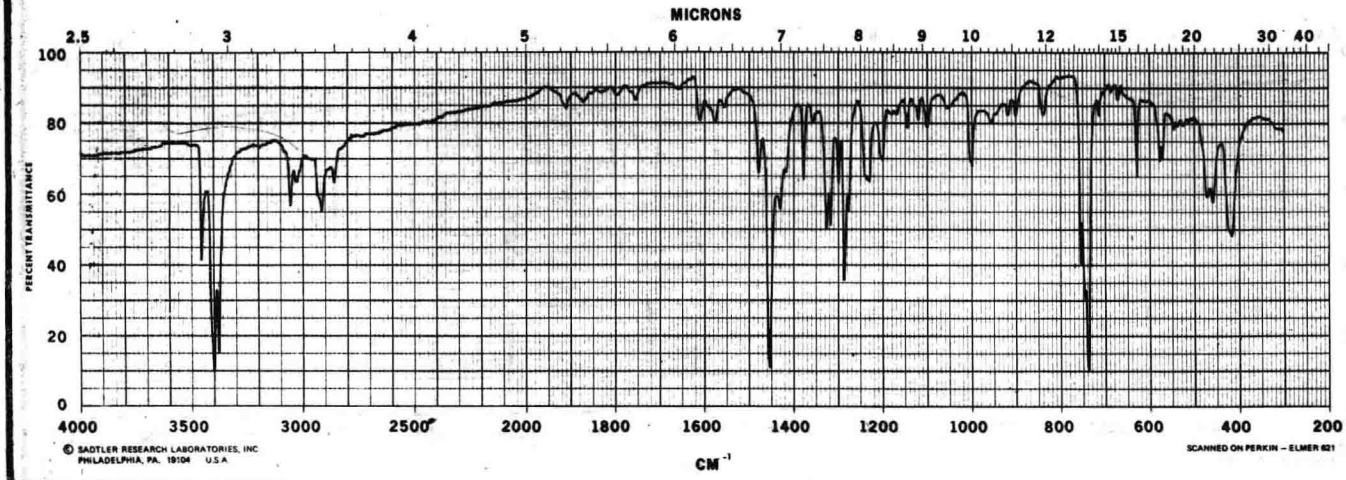
M.P. 130-132°C



Source: C. H. Brieskorn,
University of Wuerzburg,
Wuerzburg, Germany

Ref.: Chem. Abstr. 77, 5273(1972)

KBr Wafer

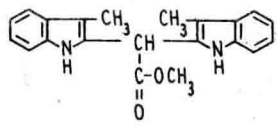


BIS(3-METHYLINDOL-2-YL)ACETIC ACID, METHYL ESTER

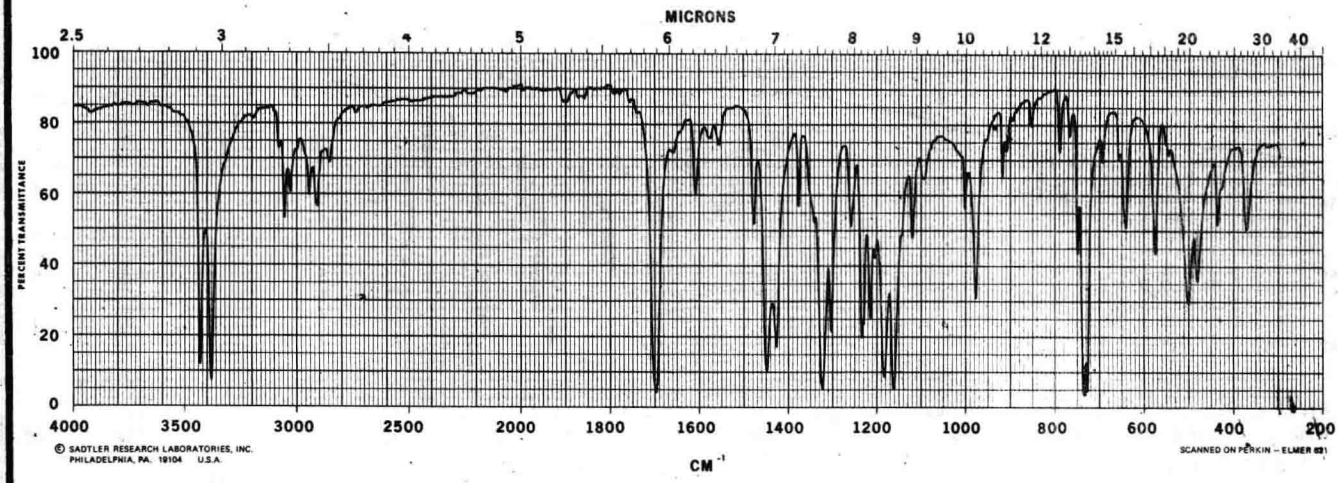
30009K

$C_{21}H_{20}N_2O_2$ Mol. Wt. 332.41

M.P. 203-204°C



Source: C. H. Brieskorn,
University of Wuerzburg,
Wuerzburg, Germany
Ref.: Chem. Abstr. 77, 5273(1972)
KBr Wafer

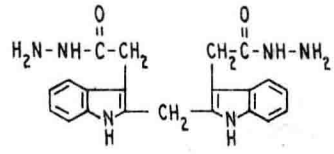


2,2'-METHYLENEDIINDOLE-3-ACETIC ACID, DIHYDRAZIDE

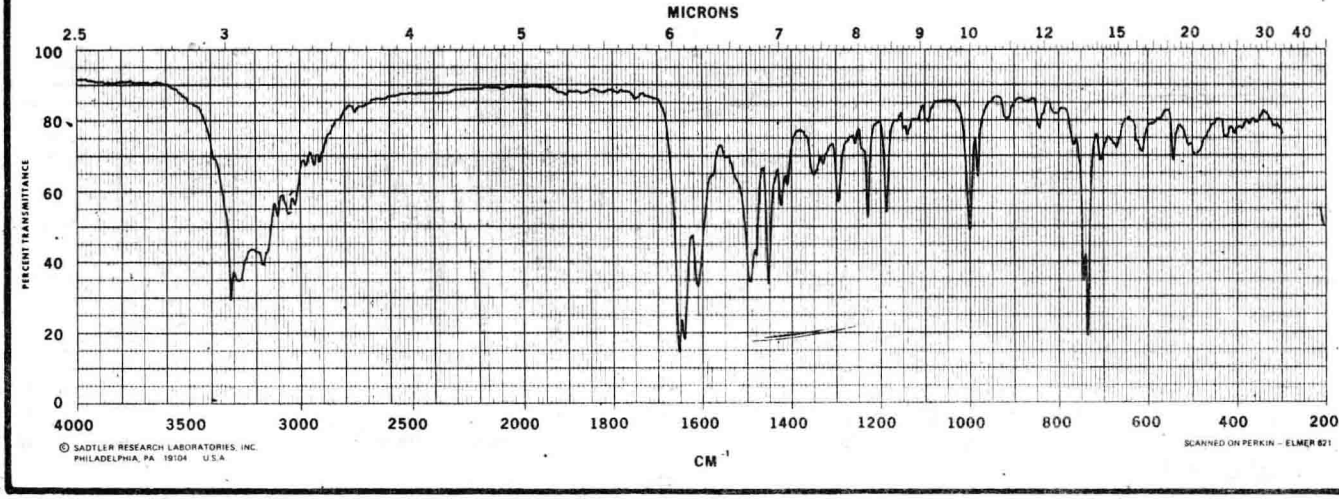
30010K

$C_{21}H_{22}N_6O_2$ Mol. Wt. 390.45

M.P. 264-268°C

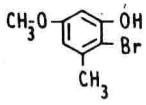


Source: C. H. Brieskorn,
University of Wuerzburg,
Wuerzburg, Germany
Ref.: Chem. Abstr. 77, 5273(1972)
KBr Wafer



30011K

2-BROMO-5-METHOXY-m-CRESOL



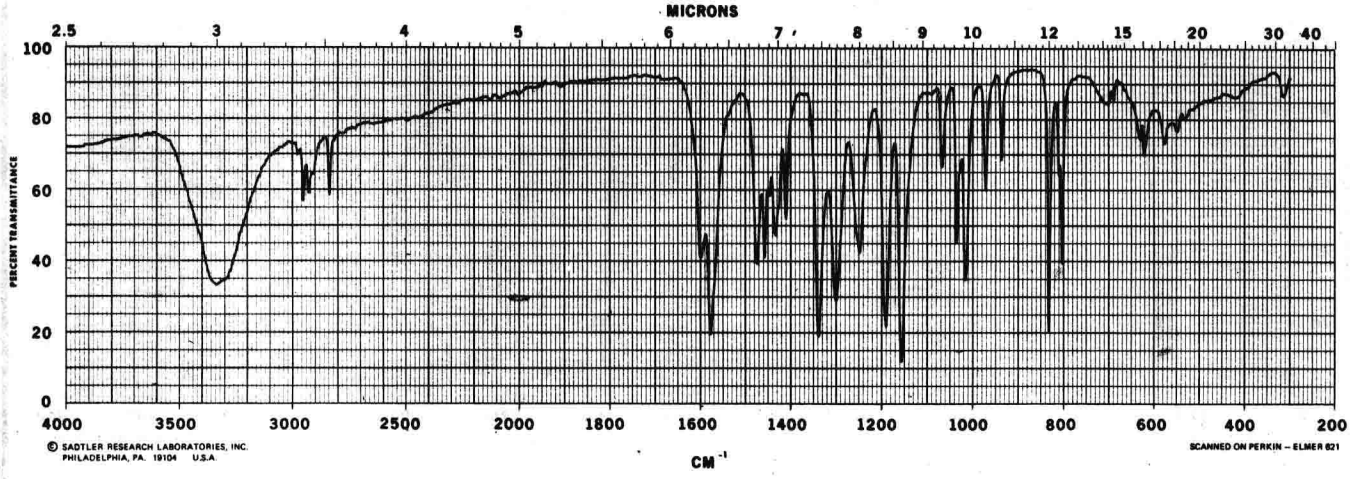
$C_8H_9BrO_2$ Mol. Wt. 217.07

M.P. 68-70°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

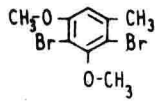
Ref.: J. Chem. Soc. (C), 3495(1971)

KBr Wafer



30012K

2,4-DIBROMO-3,5-DIMETHOXYTOLUENE



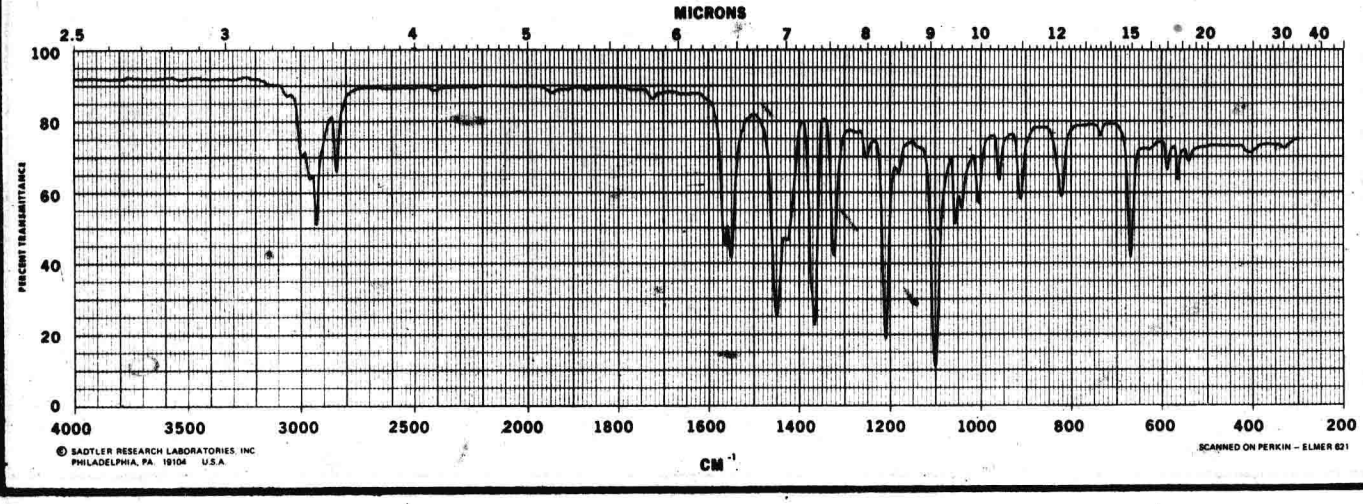
$C_9H_{10}Br_2O_2$ Mol. Wt. 310.00

M.P. 59-60°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

Ref.: J. Chem. Soc. (C), 3495(1971)

Film (Cast from $CHCl_3$)

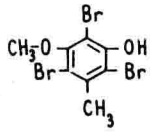


5-METHOXY-2,4,6-TRIBROMO-m-CRESOL

30013K

$C_8H_7Br_3O_2$ Mol. Wt. 374.87

M.P. 91-91.5°C

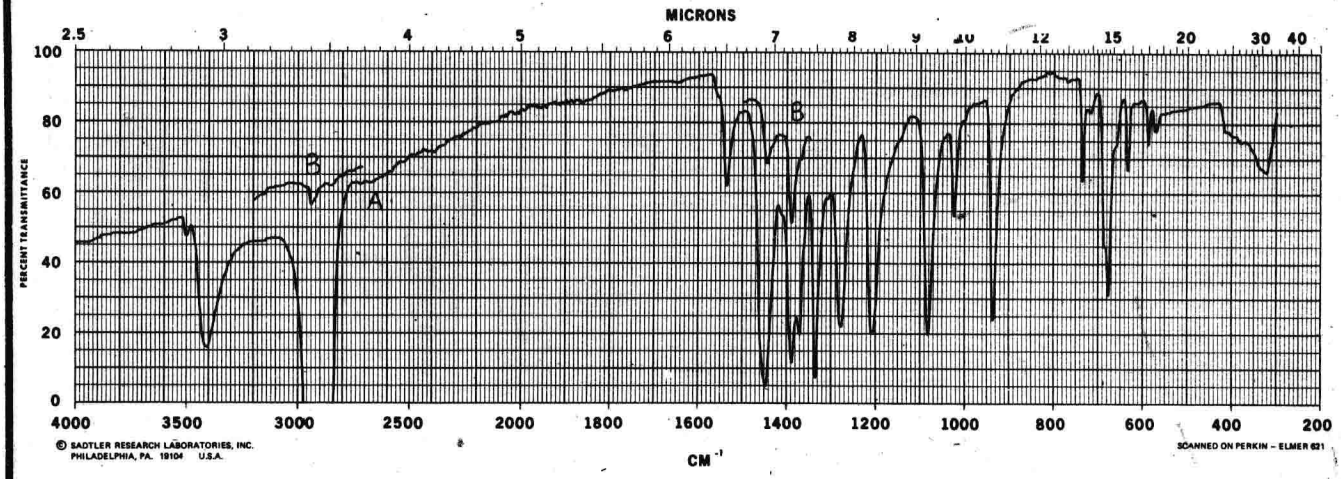


Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

Ref.: J. Chem. Soc. (C), 3495(1971)

A=Mulled in Mineral Oil

B=Mulled in Perfluorinated Hydrocarbon

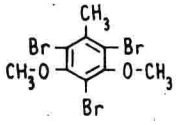


3,5-DIMETHOXY-2,4,6-TRIBROMOTOLUENE

30014K

$C_9H_9Br_3O_2$ Mol. Wt. 388.90

M.P. 103-103.5°C



Source: M. V. Sargent,
The University of Western
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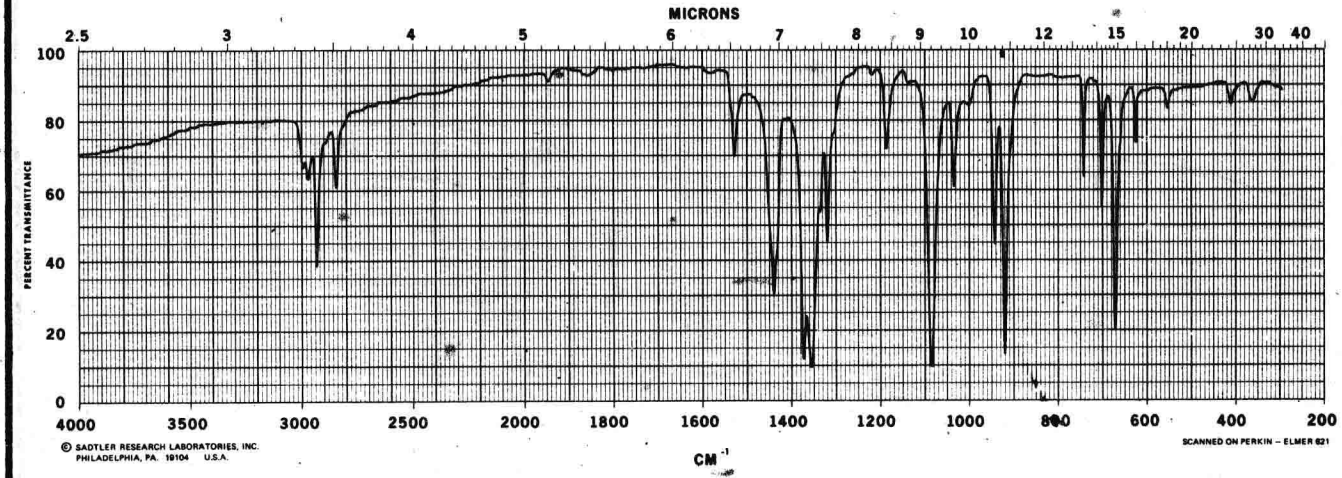
Nedlands, W. Australia

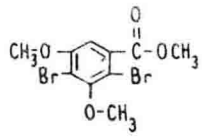
Ref.: J. Chem. Soc. (C), 3495(1971)

KBr Wafer



30015K

2,4-DIBROMO-3,5-DIMETHOXYBENZOIC ACID, METHYL ESTER



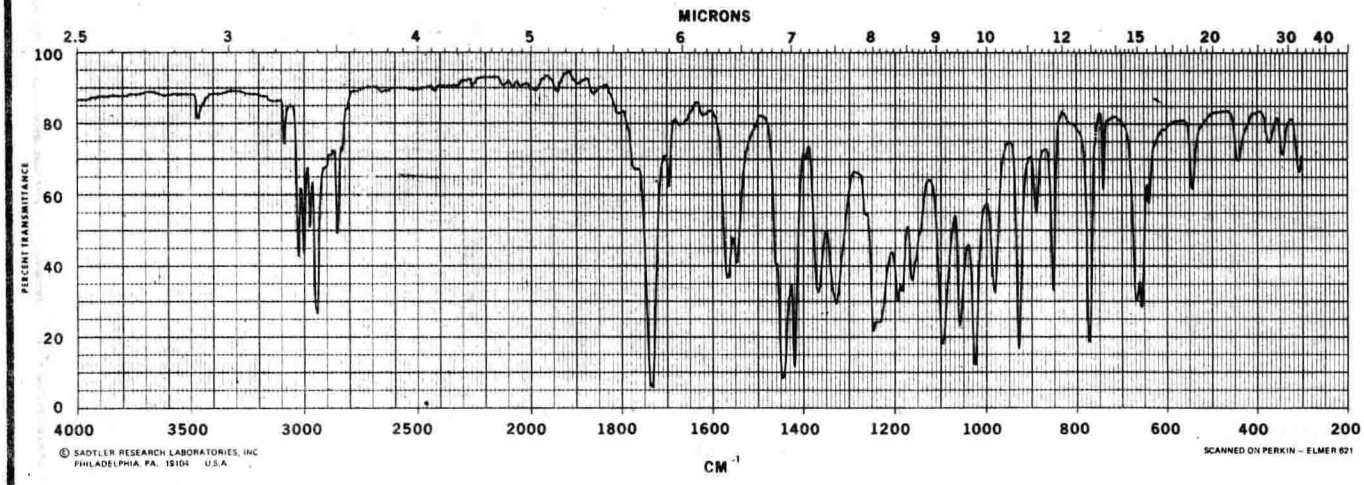
$C_{10}H_{10}Br_2O_4$ Mol. Wt. 354.01

M.P. 65-66°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

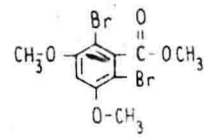
Ref.: J. Chem. Soc. (C), 3495(1971)

Capillary Cell: Melt (Crystallized)



30016K

2,6-DIBROMO-3,5-DIMETHOXYBENZOIC ACID, METHYL ESTER



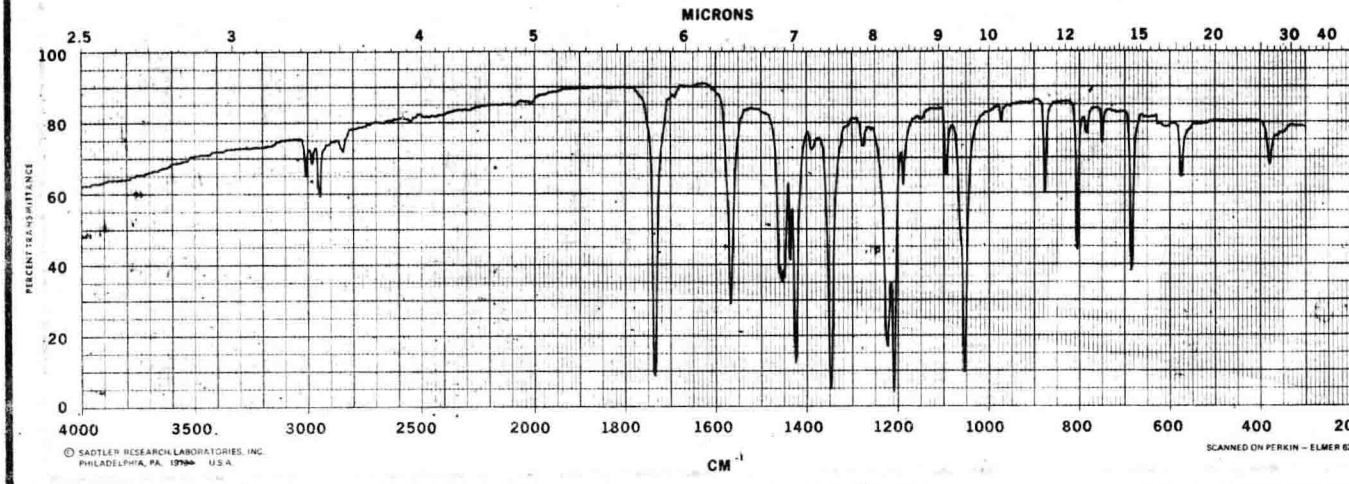
$C_{10}H_{10}Br_2O_4$ Mol. Wt. 354.01

M.P. 145-147°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

Ref.: J. Chem. Soc. (C), 3495(1971)

KBr Wafer

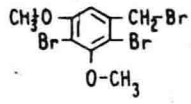


3,5-DIMETHOXY-α,2,4-TRIBROMOTOLUENE

30017K

$C_9H_9Br_3O_2$ Mol. Wt. 388.90

M.P. 136-136.5°C



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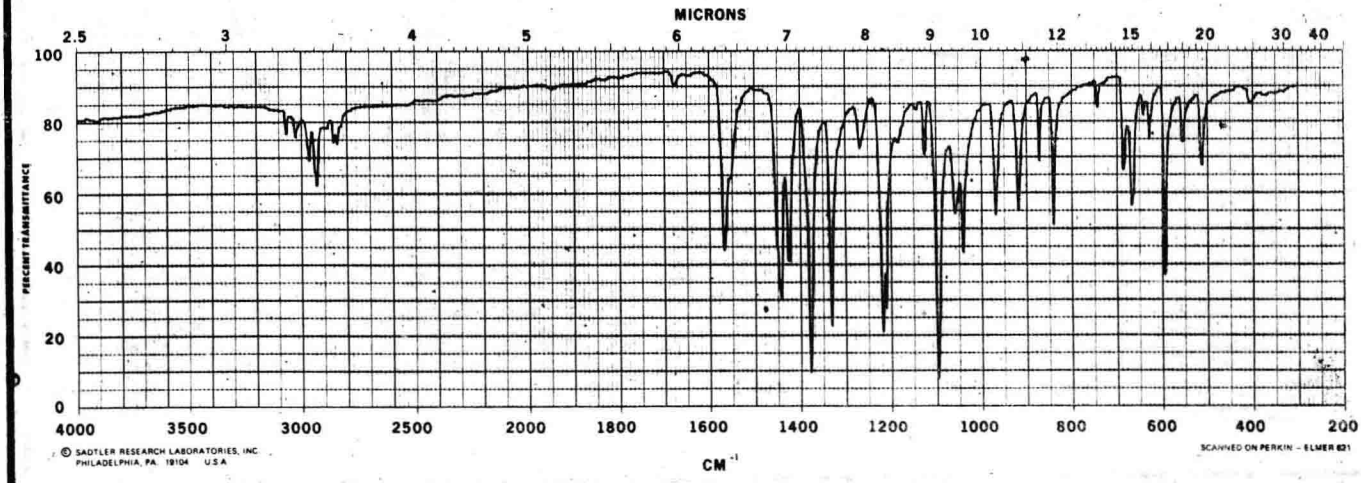
Nedlands, W. Australia

Ref.: J. Chem. Soc. (C), 3495(1971)

KBr Wafer

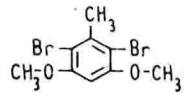


2,6-DIBROMO-3,5-DIMETHOXYTOLUENE

30018K

$C_9H_{10}Br_2O_2$ Mol. Wt. 310.00

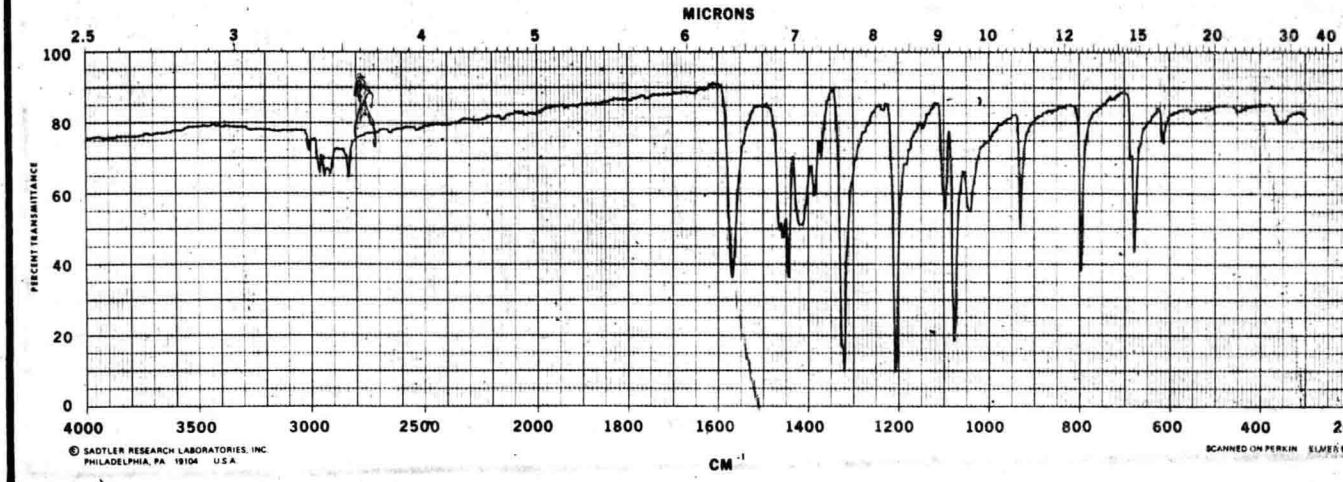
M.P. 171-172°C



Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

Ref.: J. Chem. Soc. (C), 3495(1971)

KBr Wafer



30019K

3,5-DIMETHOXY-α,2,4,6-TETRABROMOTOLUENE

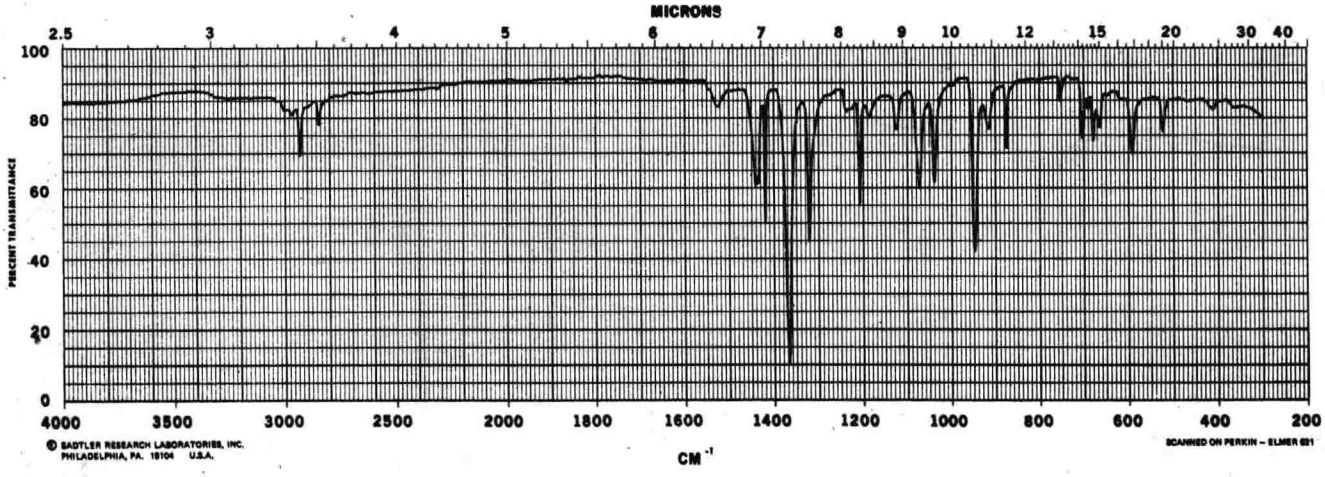
$C_9H_8Br_4O_2$ Mol. Wt. 467.80

M.P. 121-122°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

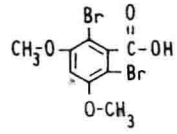
Ref.: J. Chem. Soc. (C), 3495(1971).

KBr Wafer



30020K

2,6-DIBROMO-3,5-DIMETHOXYBENZOIC ACID



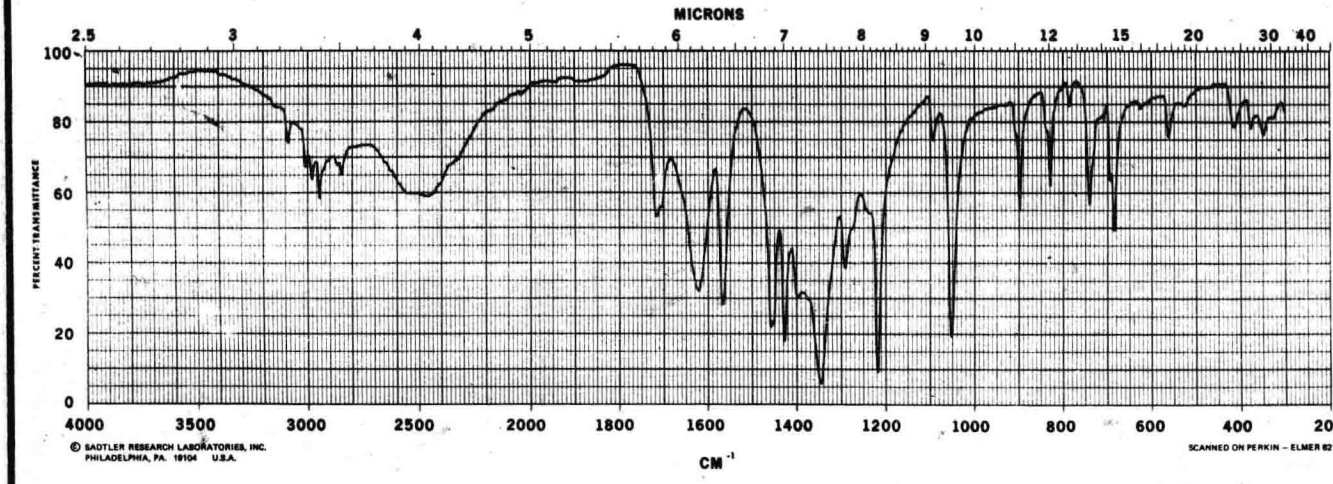
$C_9H_8Br_2O_4$ Mol. Wt. 340.00

M.P. 276-277°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

Ref.: J. Chem. Soc. (C), 3495(1971)

KBr Wafer



3-(BENZYLOXY)-2-BROMO-5-METHOXYTOLUENE

30021K

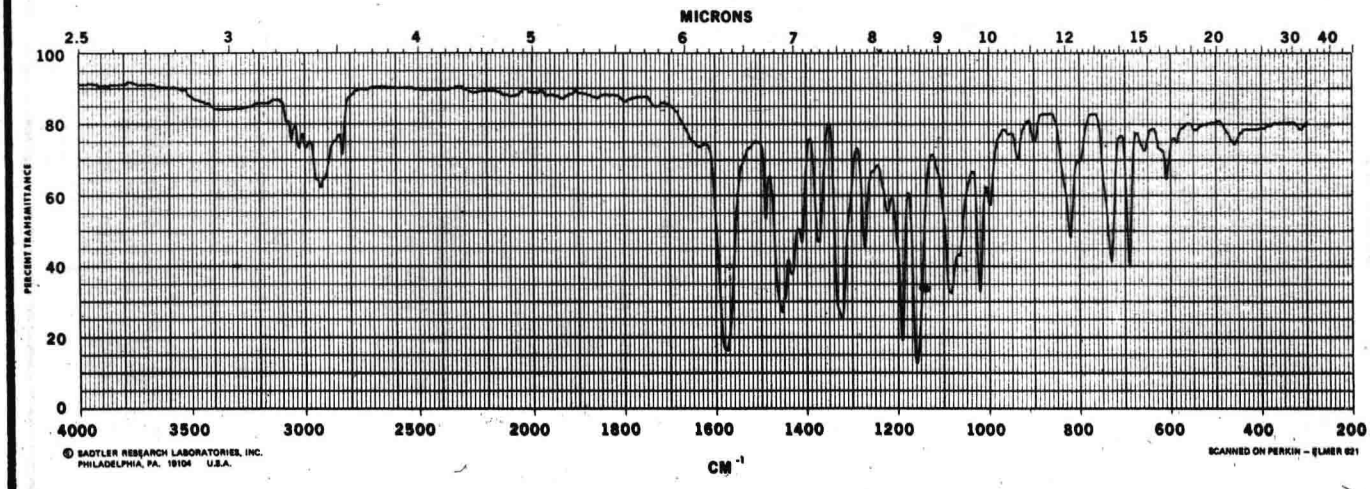
$C_{15}H_{15}BrO_2$ Mol. Wt. 307.19

B.P. 185°C/1 mm

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

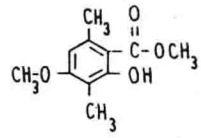
Ref.: J. Chem. Soc., Perkin Trans. (I),
1200(1972)

Capillary Cell: Neat



3,6-DIMETHYL-2-HYDROXY-p-ANISIC ACID, METHYL ESTER

30022K



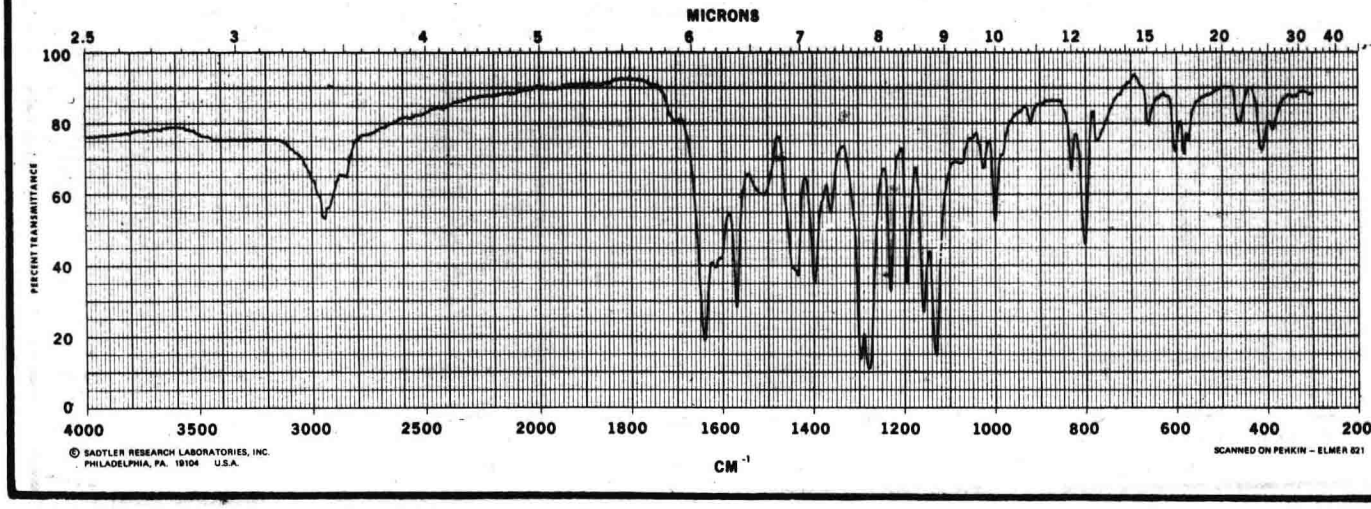
$C_{11}H_{14}O_4$ Mol. Wt. 210.23

M.P. 101-102.5°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

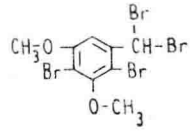
Ref.: Austral. J. Chem. 25, 2167(1972)

KBr Wafer



30023K

3,5-DIMETHOXY-[illegible],2,4-TETRABROMOTOLUENE



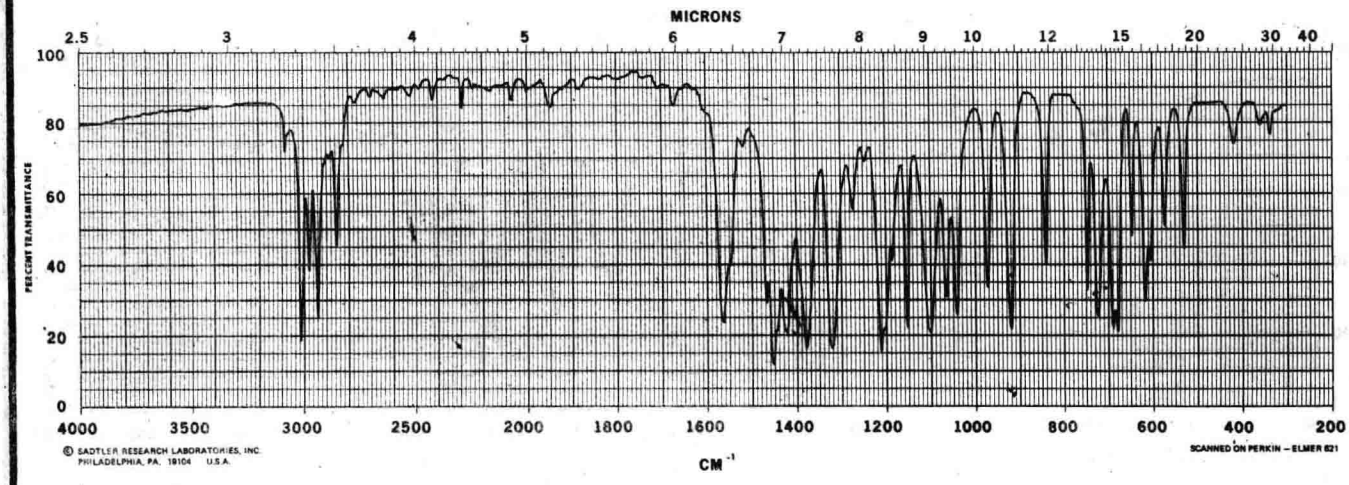
$C_9H_8Br_4O_2$ Mol. Wt. 467.80

M.P. 77-78°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

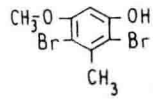
Ref.: J. Chem. Soc. (C), 3495(1971)

Capillary Cell: Melt (Crystallized)



30024K

2,4-DIBROMO-5-METHOXY-m-CRESOL



$C_8H_8Br_2O_2$ Mol. Wt. 295.97

M.P. 108.5-109.5°C

Source: M. V. Sargent,
The University of Western
Australia,
Nedlands, W. Australia

Ref.: J. Chem. Soc. (C), 3495(1971)

KBr Wafer