

**THE
SADTLER
HANDBOOK**

OF

**INFRARED
SPECTRA**

**Editor:
William W. Simons**

**THE
SADTLER
HANDBOOK**

OF

**INFRARED
SPECTRA**

**Editor:
William W. Simons
Spectroscopist
Sadler Research Laboratories, Inc.**

Published by
Sadtler Research Laboratories, Inc.
Subsidiary of Block Engineering, Inc.
3316 Spring Garden Street
Philadelphia, Pennsylvania 19104

ISBN 0-8456-0034-6

Library of Congress Catalog Card Number: 77-95458

Co-published for exclusive distribution in Europe by
Heyden & Son Ltd.
Spectrum House, Hillview Gardens
London N.W. 4, England 2JQ

ISBN 0-85501-441-5

Copyright © 1978, by Sadtler Research Laboratories, Inc. All rights reserved. No part of this book may be reproduced or reformatted in any form, by photostat, microfilm, retrieval system, or any other means, without written permission from Sadtler Research Laboratories, Inc.

Printed in the United States of America

PREFACE

The purpose of this abridged edition of the Sadtler Standard Spectra, IR Grating, is twofold. It is intended to satisfy the academic need for a small convenient collection of infrared spectra of organic compounds relevant to college introductory courses on organic chemistry and the supplementary laboratory courses on experimental organic chemistry and qualitative organic analysis. To those who are employed in industry and resort to infrared spectroscopy for the identification of organic compounds, this collection of spectra is intended to serve as a reference when comprehensive collections are not available.

Approximately 3000 spectra are contained in the collection. They are arranged in the chemical class order of their respective organic compound. Each chemical class section has a table of correlations and absorption band locations. The listing of the correlations and absorption band locations are in decreasing order of diagnostic value. The first listed absorption feature is considered to be related to the most important atomic linkage in the particular functional group or structure. Absorption bands assigned the numbers 2, 3, ..., are considered to be of secondary importance, but necessary for confirming the identity of the primary absorption band and defining it as part of a specific functional group or carbon framework. Such information provides the means of identifying a compound as a member of a specific chemical class.

In addition to serving as a teaching aid, the collection of spectra affords convenient and easy access to the spectra of compounds having the desired functional group and which can be used to establish an identity through empirical comparison.

With regard to the spectra of the collection, consideration should be given to the manner in which the compound was prepared for examination. A compound prepared by most preparative procedures fails to yield an infrared absorption spectrum which is ideal in all respects. Although a compound prepared for examination by a particular procedure yields a reproducible spectrum, the same compound prepared by two different methods does not, necessarily, yield identical spectra. For most compounds, a change in physical state or a change in solvent for solution spectra cause shifts in absorption band locations, changes in absorption band contours, and a splitting or coalescence of absorption bands. Furthermore, the use of solvents for solution spectra and the use of liquid media for mulls tend to confound the spectrum of the compound with their own unique absorption characteristics. However, each method of preparing a sample for examination has certain advantages and merits. The information desired from a spectrum largely determines how the compound is to be prepared for examination.

A compound in the crystalline state generally yields a spectrum which has more absorption bands than the spectrum of the same compound when examined in the liquid state or in solvent solution. The absorption bands in the spectrum of a solid compound, examined in the crystalline state, or a liquid compound, examined in the pure concentrated form (neat), are found, usually, at lower frequencies than the absorption bands in the spectrum of the same compound when it is examined in the vapor state or in solvent solution. The degree of absorption band shifts depends upon the presence or absence of intermolecular and intramolecular forces.

For qualitative examinations involving empirical comparison of spectra, the spectrum of the sample should be obtained in a manner which is the same as that used for obtaining the spectrum of the reference compound. Identification established through empirical comparison of spectra should always be supported with physical or chemical data. The greatest obstacle to obtaining a spectrum of a sample which will match a reference spectrum of a pure compound is the lack of sameness in the composition of the sample.

ACKNOWLEDGEMENTS

I wish to recognize the important contribution made to this endeavor by the late Harry T. Johnston, a friend, teacher and co-worker for more than ten years.

My personal appreciation goes to all the Sadtler personnel who have labored long and diligently to bring this volume to completion. My special thanks go to Bernadette Steiner, Mary Schimminger, Marsha Moore, Matthew Levin and John Selfridge, without whose help, the task would have been nearly impossible.

January 1978

W. W. S.

TABLE OF CONTENTS

	<i>Text Page</i>	<i>Spectra Page</i>
I. HYDROCARBONS		
A. SATURATED HYDROCARBONS		
1. NORMAL ALKANES	5	7
2. BRANCHED ALKANES	11	13
3. CYCLIC ALKANES	19	21
B. UNSATURATED HYDROCARBONS		
1. ACYCLIC ALKENES	25	27
2. CYCLIC ALKENES	39	41
3. ALKYNES	47	49
C. AROMATIC HYDROCARBONS		
1. MONOCYCLIC (BENZENES)	53	59
2. POLYCYCLIC		74
II. HALOGENATED HYDROCARBONS	81	
A. FLUORINATED HYDROCARBONS	82	
1. ALIPHATIC		83
2. AROMATIC		83
B. CHLORINATED HYDROCARBONS	87	
1. ALIPHATIC		88
2. OLEFINIC		97
3. AROMATIC		100
C. BROMINATED HYDROCARBONS	109	
1. ALIPHATIC		110
2. OLEFINIC		122
3. AROMATIC		123
D. IODINATED HYDROCARBONS	131	
1. ALIPHATIC AND OLEFINIC		132
2. AROMATIC		137
III. NITROGEN CONTAINING COMPOUNDS		
A. AMINES		
1. PRIMARY		
a. ALIPHATIC AND OLEFINIC	141	142
b. AROMATIC		152
2. SECONDARY		
a. ALIPHATIC AND OLEFINIC	169	171
b. AROMATIC		179
3. TERTIARY		
a. ALIPHATIC AND OLEFINIC	189	190
b. AROMATIC		196
B. PYRIDINES	207	209
C. QUINOLINES		218

TABLE OF CONTENTS

		Text Page	Spectra Page
D.	MISCELLANEOUS NITROGEN HETEROAROMATICS		220
E.	HYDRAZINES	227	228
F.	AMINE SALTS	231	232
G.	OXIMES (-CH=N-OH)	253	254
H.	HYDRAZONES (-CH=N-NH_2)		260
I.	AZINES (-CH=N-N=CH-)		262
J.	AMIDINES (-N=CH-N)		262
K.	HYDROXAMIC ACIDS		264
L.	AZO COMPOUNDS (-N=N-)	267	268
M.	TRIAZENES (-N=N-NH-)		270
N.	ISOCYANATES (-N=C=O)	271	272
O.	CARBODIIMIDES (-N=C=N-)		276
P.	ISOTHIOCYANATES (-N=C=S-)		277
Q.	NITRILES ($\text{-C}\equiv\text{N}$)	281	
	1. ALIPHATIC		282
	2. OLEFINIC		287
	3. AROMATIC		289
R.	CYANAMIDES ($\text{>N-C}\equiv\text{N}$)	297	298
S.	THIOCYANATES ($\text{-S-C}\equiv\text{N}$)		299
T.	NITROSO COMPOUNDS (-N=O)	303	304
U.	N-NITROSO COMPOUNDS (>N-N=O)		305
V.	NITRITES (-O-N=O)		307
W.	NITRO COMPOUNDS (-NO_2)	309	
	1. ALIPHATIC		310
	2. AROMATIC		311
X.	N-NITRO COMPOUNDS (>N-NO_2)		319
Y.	NITRATES (-O-NO_2)		320
IV.	SILICON CONTAINING COMPOUNDS (EXCEPT Si-O)	321	322
V.	PHOSPHORUS CONTAINING COMPOUNDS (EXCEPT P-O and P(=O)-O)	325	326
VI.	SULFUR CONTAINING COMPOUNDS		
	A. SULFIDES (R-S-R)	329	
	1. ALIPHATIC		330
	2. HETEROCYCLIC		335
	3. AROMATIC		342

TABLE OF CONTENTS

		<i>Text Page</i>	<i>Spectra Page</i>
VI.	SULFUR CONTAINING COMPOUNDS Continued		
B.	DISULFIDES (R-S-S-R)		349
C.	THIOLS	353	
1.	ALIPHATIC		354
2.	AROMATIC		360
D.	SULFOXIDES (R-S(=O)-R)	365	366
E.	SULFONES (R-SO ₂ -R)		368
F.	SULFONYL HALIDES (R-SO ₂ -X)		375
G.	SULFONIC ACIDS (R-SO ₂ -OH)	377	378
1.	SULFONIC ACID SALTS (R-SO ₂ -O-M)		379
2.	SULFONIC ACID ESTERS (R-SO ₂ -O-R)		385
3.	SULFURIC ACID ESTERS (R-O-S(=O)-O-R)		387
4.	SULFURIC ACID SALTS (R-O-S(=O)-O-M)		387
H.	THIOAMIDES (R-C(=S)-NH ₂)	389	390
I.	THIOUREAS (R-NH-C(=S)-NH ₂)		391
J.	SULFONAMIDES (R-SO ₂ -NH ₂)	397	398
K.	SULFAMIDES (R-NH-SO ₂ -NH-R)		402
VII.	OXYGEN CONTAINING COMPOUNDS (EXCEPT -C(=O)-)		
A.	ETHERS	403	
1.	ALIPHATIC ETHERS (R-O-R)		405
2.	ACETALS (R-CH(-O-R) ₂)		415
3.	ALICYCLIC ETHERS		419
4.	AROMATIC ETHERS		430
5.	FURANS		453
6.	SILICON ETHERS (R ₃ -Si-O-R)		458
7.	PHOSPHORUS ETHERS ((R-O) ₃ -P)		461
8.	PEROXIDES (R-O-O-R)		462
B.	ALCOHOLS (R-OH)	463	
1.	PRIMARY		
a.	ALIPHATIC AND ALICYCLIC		464
b.	OLEFINIC		482
c.	AROMATIC		486
d.	HETEROCYCLIC		493
2.	SECONDARY		
a.	ALIPHATIC AND ALICYCLIC	495	496
b.	OLEFINIC		507
c.	AROMATIC		509
3.	TERTIARY		
a.	ALIPHATIC	511	512
b.	OLEFINIC		516
c.	AROMATIC		517

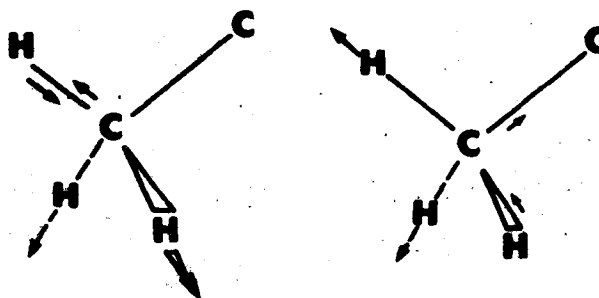
TABLE OF CONTENTS

	<i>Text Page</i>	<i>Spectra Page</i>
B. ALCOHOLS Continued		
4. DIOLS	519	520
5. CARBODHYDRATES		529
6. PHENOLS	533	534
VIII. COMPOUNDS CONTAINING CARBON TO OXYGEN DOUBLE BONDS		
A. KETONES (R-C(=O)-R)	557	
1. ALIPHATIC AND ALICYCLIC		558
2. OLEFINIC		570
3. AROMATIC		574
4. α -DIKETONES AND β -DIKETONES	599	600
B. ALDEHYDES (R-C(=O)-H)	605	606
C. ACID HALIDES (R-C(=O)-X)	615	616
D. ANHYDRIDES (R-C(=O)-O-C(=O)-R)	631	632
E. AMIDES		
1. PRIMARY (R-C(=O)-NH₂)	639	640
2. SECONDARY (R-C(=O)-NH-R)	645	646
3. TERTIARY (R-C(=O)-N-R₂)	659	660
F. IMIDES (R-C(=O)-NH-C(=O)-R)	667	668
G. HYDRAZIDES (R-C(=O)-NH-NH₂)	675	676
H. UREAS (R-NH-C(=O)-NH₂)	679	680
I. HYDANTOINS, URACILS, BARBITURATES	687	688
J. CARBOXYLIC ACIDS (R-C(=O)-OH)	695	
1. ALIPHATIC AND ALICYCLIC		696
2. OLEFINIC		707
3. AROMATIC		713
4. AMINO ACIDS	731	732
5. SALTS OF CARBOXYLIC ACIDS	741	742
K. ESTERS		
1. ALIPHATIC ESTERS OF ALIPHATIC ACIDS	753	754
2. OLEFINIC ESTERS OF ALIPHATIC ACIDS		780
3. ALIPHATIC ESTERS OF OLEFINIC ACIDS		782
4. AROMATIC ESTERS OF ALIPHATIC ACIDS	789	790
5. ESTERS OF AROMATIC ACIDS		794
6. CYCLIC ESTERS (LACTONES)		818
7. CHLOROFORMATES		822
8. ESTERS OF THIO-ACIDS		824
9. CARBAMATES		825
10. ESTERS OF PHOSPHORUS ACIDS		831

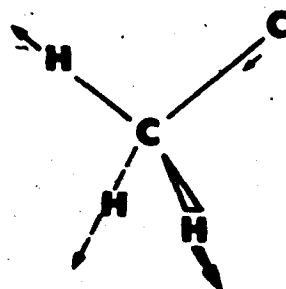
VIBRATIONS OF C-H LINKAGES IN CH₃, CH₂, AND CH GROUPS

Methyl Groups:

1. Stretching vibration (st)

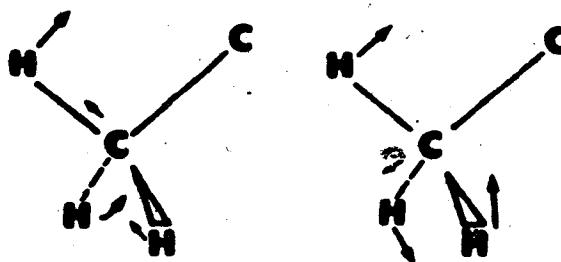


CH₃ asymmetric stretch (CH₃ st₂)

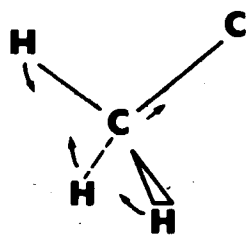


CH₃ symmetric stretch (CH₃ st₃)

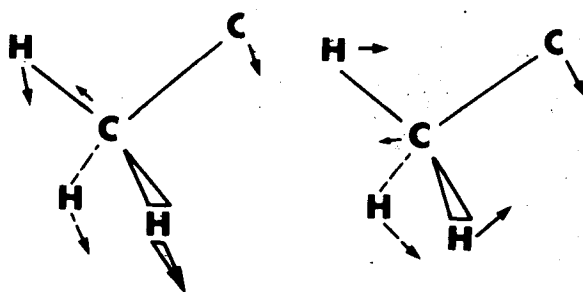
2. Deformation vibration (d)



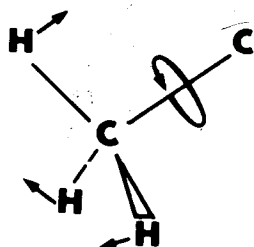
CH₃ asymmetric bend (CH₃ b_a)



CH₃ symmetric bend (CH₃ b_s)



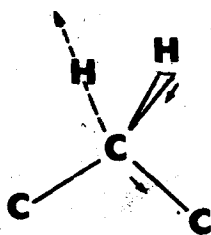
CH₃ rock (CH₃ r)



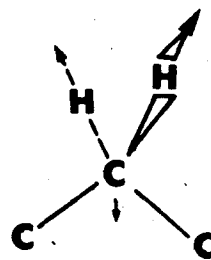
CH₃ twist (CH₃ t)

Methylene Groups:

1. Stretching vibration (st)

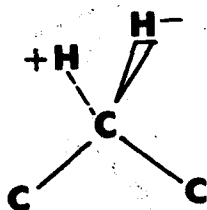


CH₂ asymmetric stretch
(CH₂ st_a)

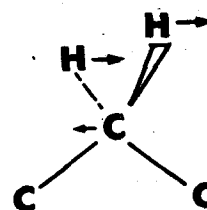


CH₂ symmetric stretch
(CH₂ st_s)

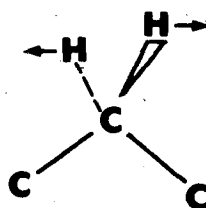
2. Deformation vibration (d)



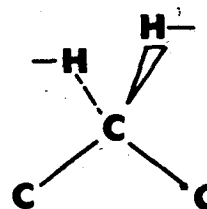
CH₂ bend (CH₂ b)



CH₂ wag (CH₂ w)



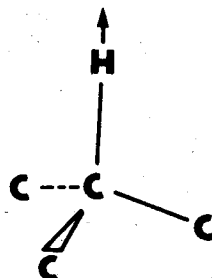
CH₂ twist (CH₂ t)



CH₂ rock (CH₂ r)

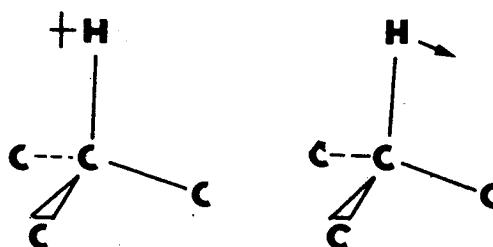
Methyldidyne Groups:

1. Stretching vibration (st)



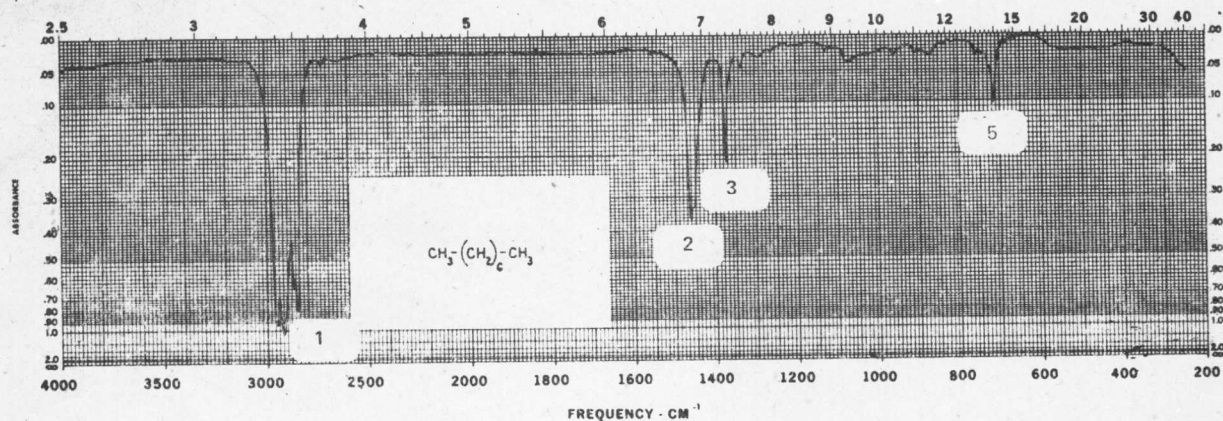
CH stretch (CH st)

2. Deformation vibration (d)



CH deformation (CH d)

SATURATED HYDROCARBONS (Normal Alkanes)



CORRELATION AND LOCATION OF ABSORPTION BANDS

1. C—H stretching vibration:
 - $\text{CH}_3 \text{ st}_a$, $2962 \pm 10 \text{ cm}^{-1}$
 - $\text{CH}_3 \text{ st}_s$, $2872 \pm 10 \text{ cm}^{-1}$
 - $\text{CH}_2 \text{ st}_a$, $2926 \pm 10 \text{ cm}^{-1}$
 - $\text{CH}_2 \text{ st}_s$, $2853 \pm 10 \text{ cm}^{-1}$
2. C—H bending vibration:
 - $\text{CH}_3 \text{ b}_a$, $1450 \pm 20 \text{ cm}^{-1}$
 - $\text{CH}_2 \text{ b}_a$, $1465 \pm 20 \text{ cm}^{-1}$ (overlaps band due to $\text{CH}_3 \text{ b}_a$)
3. C—H bending vibration:
 - $\text{CH}_3 \text{ b}_s$, $1380 - 1365 \text{ cm}^{-1}$ (when CH_3 is attached to a C atom)
4. C—H wagging vibration:
 - $\text{CH}_2 \text{ w}_{op}$, $1307 - 1303 \text{ cm}^{-1}$ (weak)
5. CH_2 rocking vibration:
 - $(\text{CH}_2)_2 \text{ r}_{ip}$, $750 - 740 \text{ cm}^{-1}$
 - $(\text{CH}_2)_3 \text{ r}_{ip}$, $740 - 730 \text{ cm}^{-1}$
 - $(\text{CH}_2)_4 \text{ r}_{ip}$, $730 - 725 \text{ cm}^{-1}$
 - $(\text{CH}_2)_{\geq 6} \text{ r}_{ip}$, 722 cm^{-1}

Splitting of the absorption band occurs in most cases (730 and 720 cm^{-1}) when the long carbon-chain alkane is in the crystalline state (orthorhombic or monoclinic form).

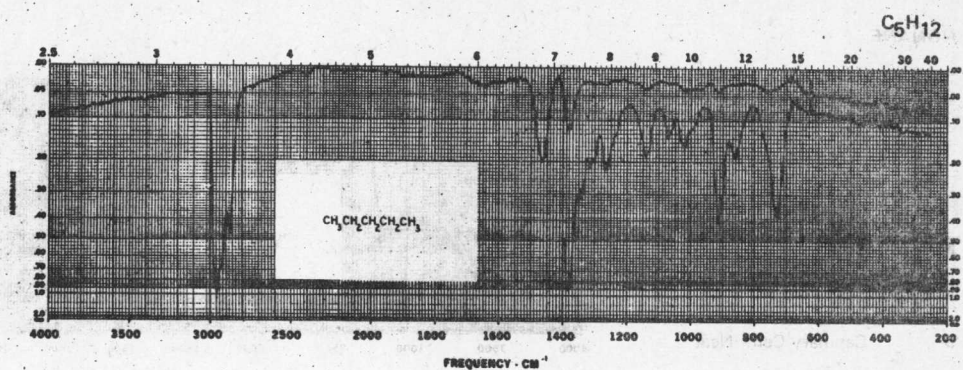
NOTES

PENTANE

Mol. Wt. 72.15

B.P. 36.1° C

1 Capillary Cell: Neat

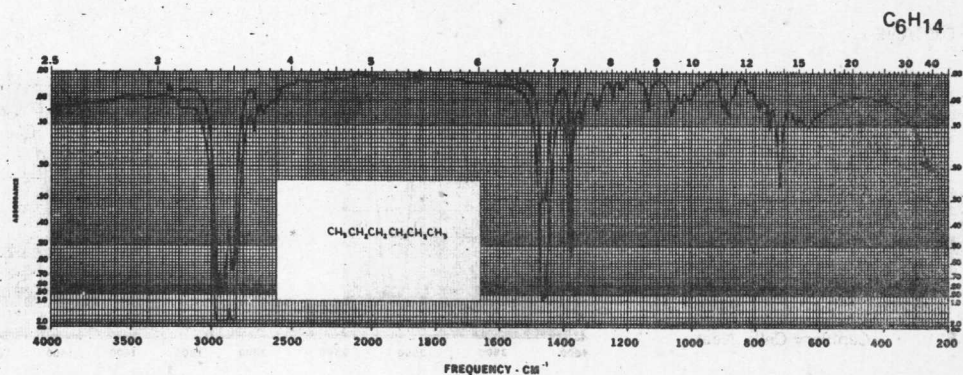


HEXANE

Mol. Wt. 86.18

B.P. 68.8° C

2 Capillary Cell: Neat

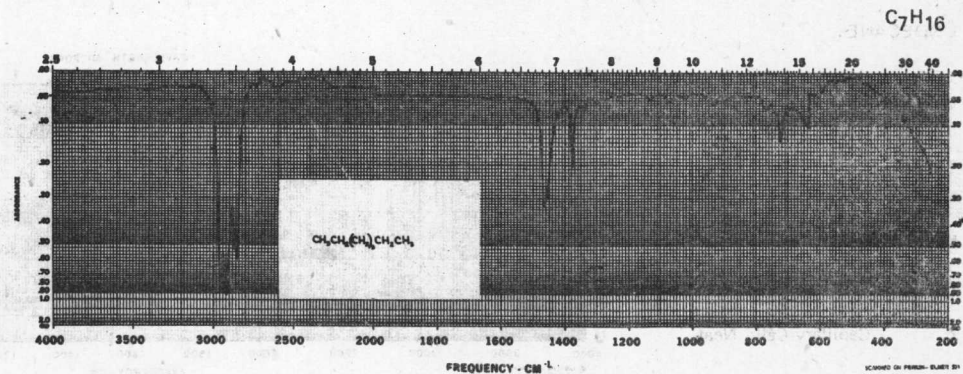


HEPTANE

Mol. Wt. 100.21

B.P. 98-99° C

3 Capillary Cell: Neat

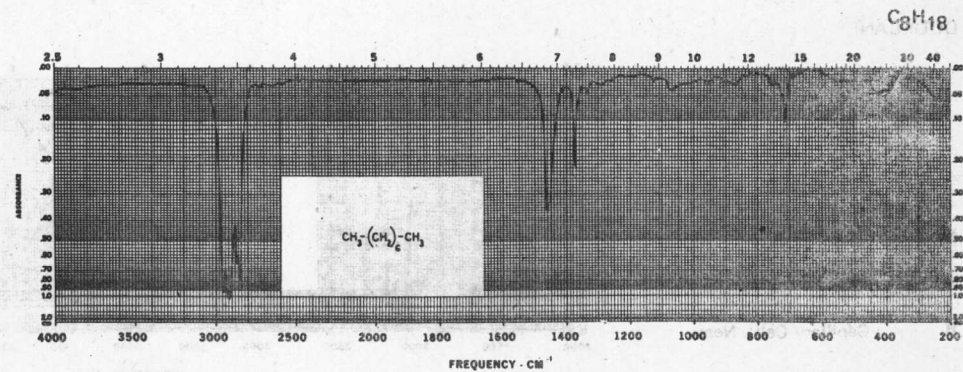


OCTANE

Mol. Wt. 114.23

B.P. 124-126° C

4 Capillary Cell: Neat

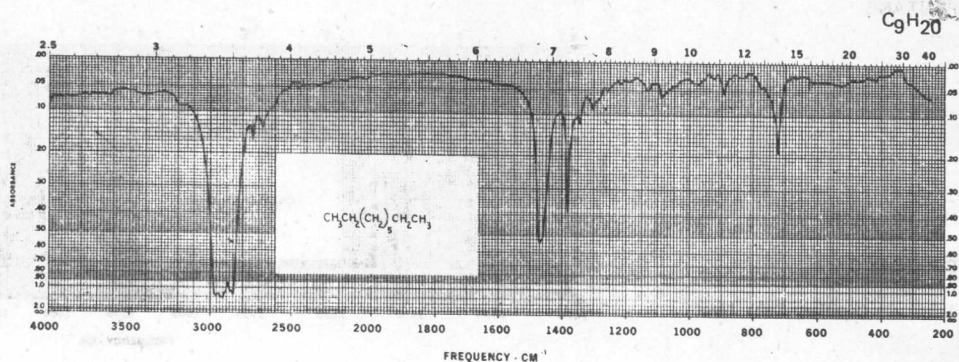


NONANE

Mol. Wt. 128.26

B.P. 150.7° C

5 Capillary Cell: Neat

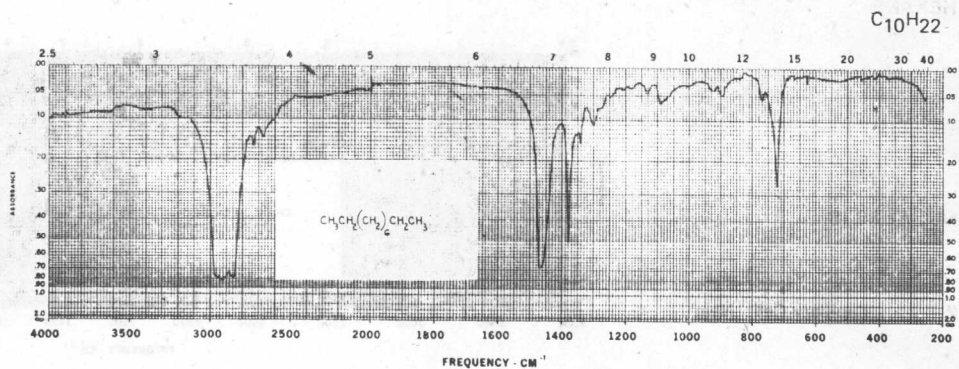


DECANE

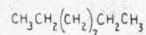
Mol. Wt. 142.29

B.P. 174° C

6 Capillary Cell: Neat



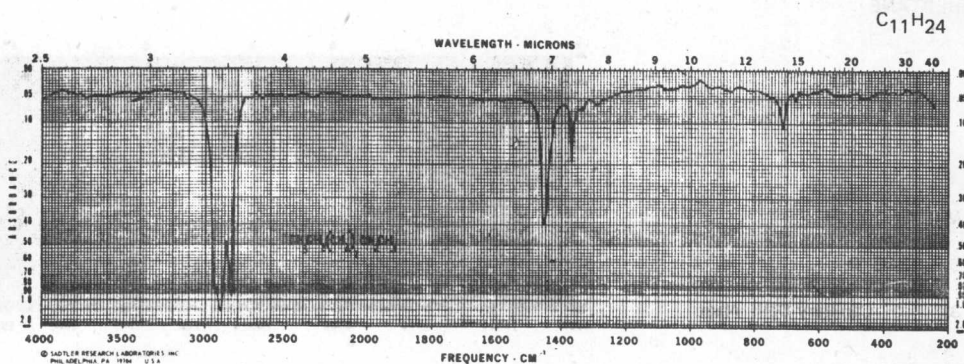
UNDECANE



Mol. Wt. 156.31

B.P. 19.6° C

7 Capillary Cell: Neat



DODECANE

Mol. Wt. 170.34

B.P. 212.8° C

8 Capillary Cell: Neat

