

THE
SADTLER
HANDBOOK

OF

INFRARED
SPECTRA

Editor:
William W. Simons

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HANDBOOK**

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SPECTRA**

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Spectroscopist
Sadler Research Laboratories, Inc.**



SADTLER

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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.

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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.

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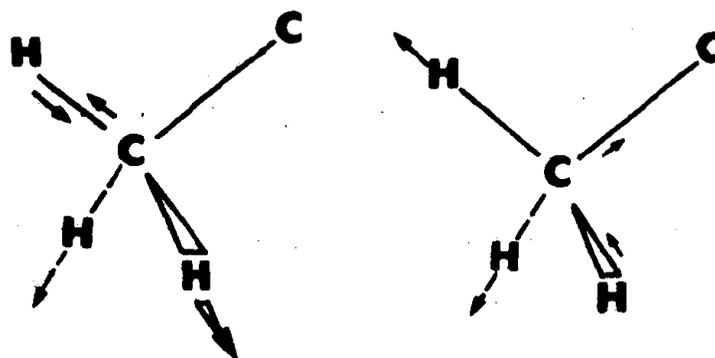
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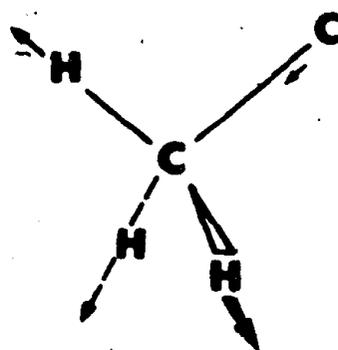
VIBRATIONS OF C-H LINKAGES IN CH₃, CH₂, AND CH GROUPS

Methyl Groups:

1. Stretching vibration (st)

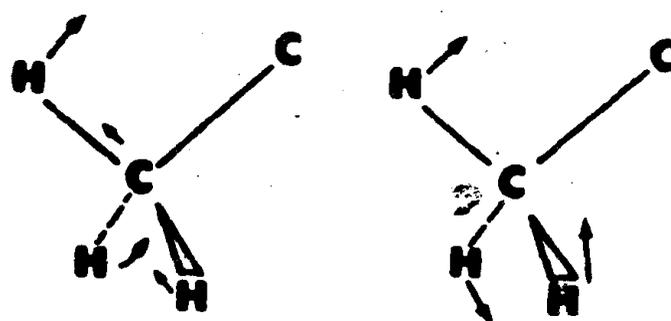


CH₃ asymmetric stretch (CH₃ st_a)

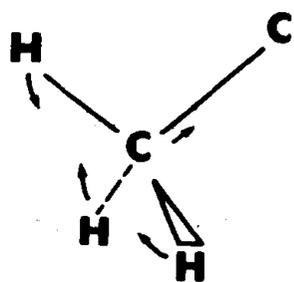


CH₃ symmetric stretch (CH₃ st_s)

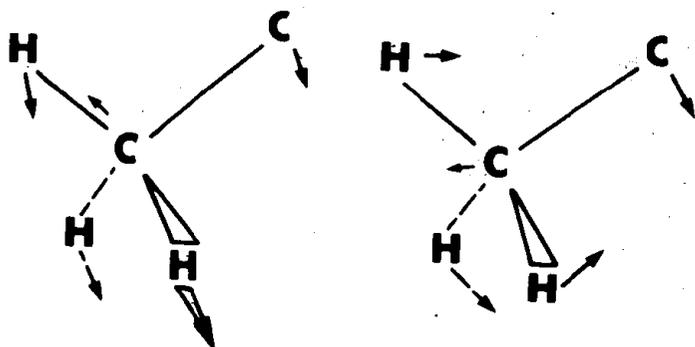
2. Deformation vibration (d)



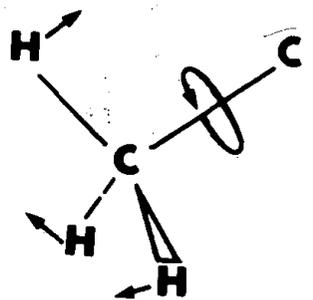
CH₃ asymmetric bend (CH₃ b_a)



CH₃ symmetric bend (CH₃ b_s)



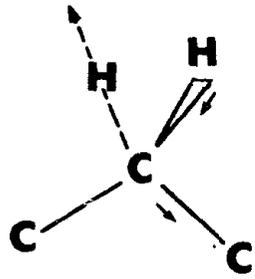
CH₃ rock (CH₃ r)



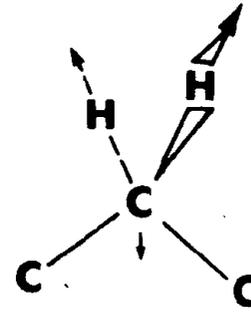
CH₃ twist (CH₃ t)

Methylene Groups:

1. Stretching vibration (st)

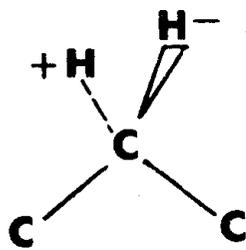


CH₂ asymmetric stretch
(CH₂ st_a)

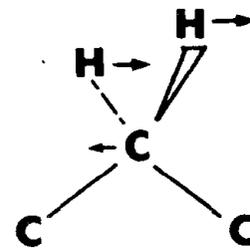


CH₂ symmetric stretch
(CH₂ st_s)

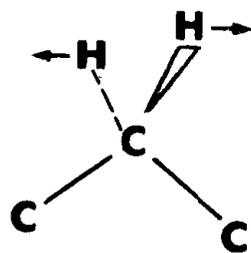
2. Deformation vibration (d)



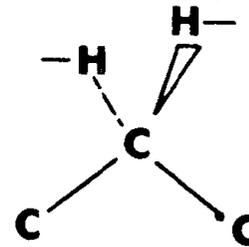
CH₂ bend (CH₂ b)



CH₂ wag (CH₂ w)



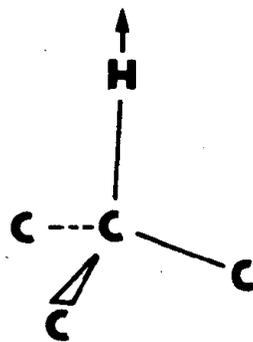
CH₂ twist (CH₂ t)



CH₂ rock (CH₂ r)

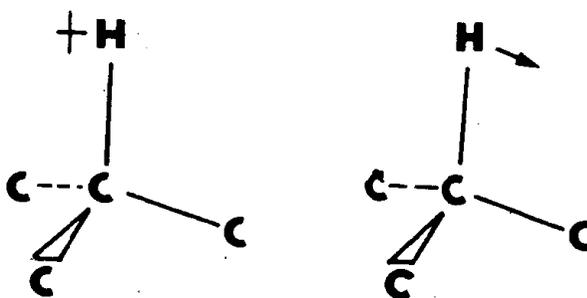
Methidyne Groups:

1. Stretching vibration (st)



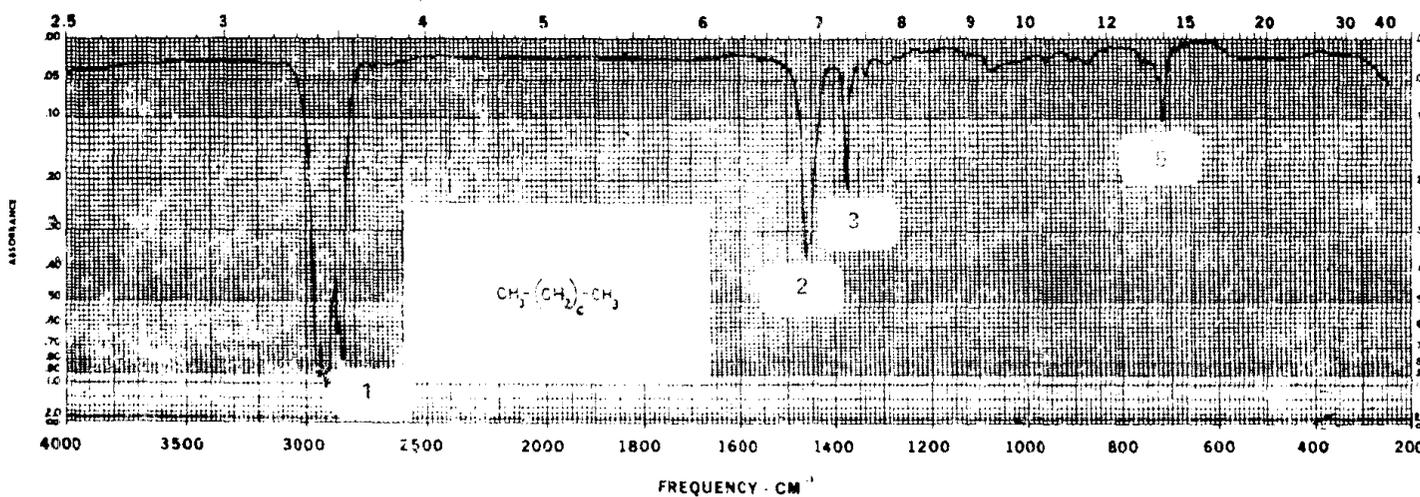
CH stretch (CH st)

2. Deformation vibration (d)



CH deformation (CH d)

SATURATED HYDROCARBONS
(Normal Alkanes)



CORRELATION AND LOCATION OF ABSORPTION BANDS

1. C-H stretching vibration:
 - CH₃ st_a, 2962 ± 10 cm⁻¹
 - CH₃ st_s, 2872 ± 10 cm⁻¹
 - CH₂ st_a, 2926 ± 10 cm⁻¹
 - CH₂ st_s, 2853 ± 10 cm⁻¹
2. C-H bending vibration:
 - CH₃ b_a, 1450 ± 20 cm⁻¹
 - CH₂ b_a, 1465 ± 20 cm⁻¹ (overlaps band due to CH₃ b_a)
3. C-H bending vibration:
 - CH₃ b_s, 1380 - 1365 cm⁻¹ (when CH₃ is attached to a C atom)
4. C-H wagging vibration:
 - CH₂ w_{op}, 1307 - 1303 cm⁻¹ (weak)
5. CH₂ rocking vibration:
 - (CH₂)₂ r_{ip}, 750 - 740 cm⁻¹
 - (CH₂)₃ r_{ip}, 740 - 730 cm⁻¹
 - (CH₂)₄ r_{ip}, 730 - 725 cm⁻¹
 - (CH₂)_{≥ 6} 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

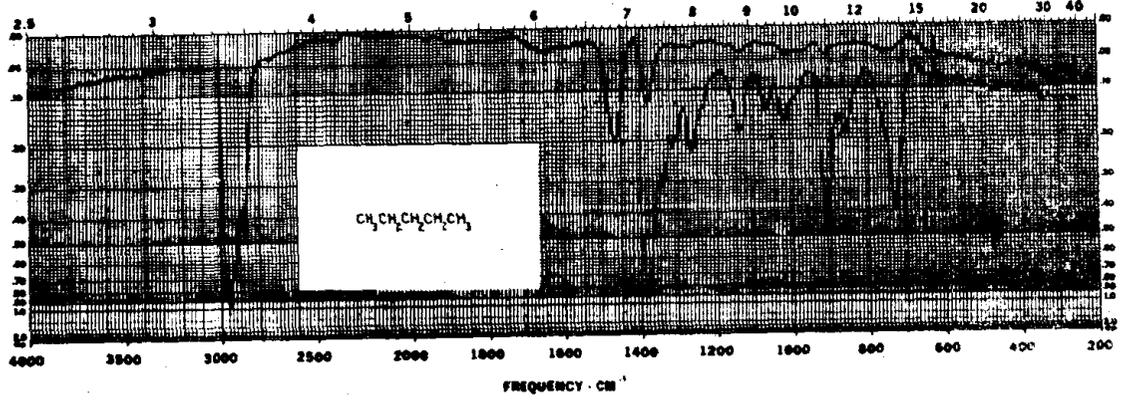
PENTANE

C₅H₁₂

Mol. Wt. 72.15

B.P. 36.1° C

1 Capillary Cell: Neat



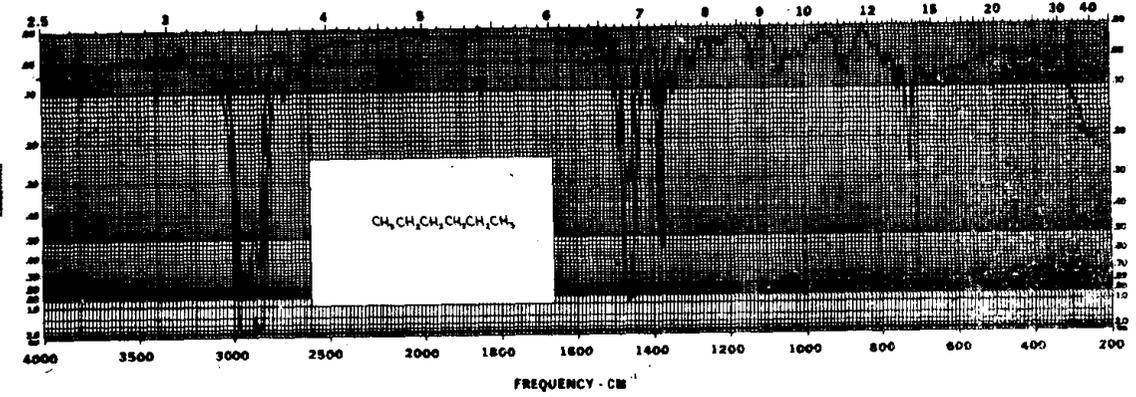
HEXANE

C₆H₁₄

Mol. Wt. 86.18

B.P. 68.8° C

2 Capillary Cell: Neat



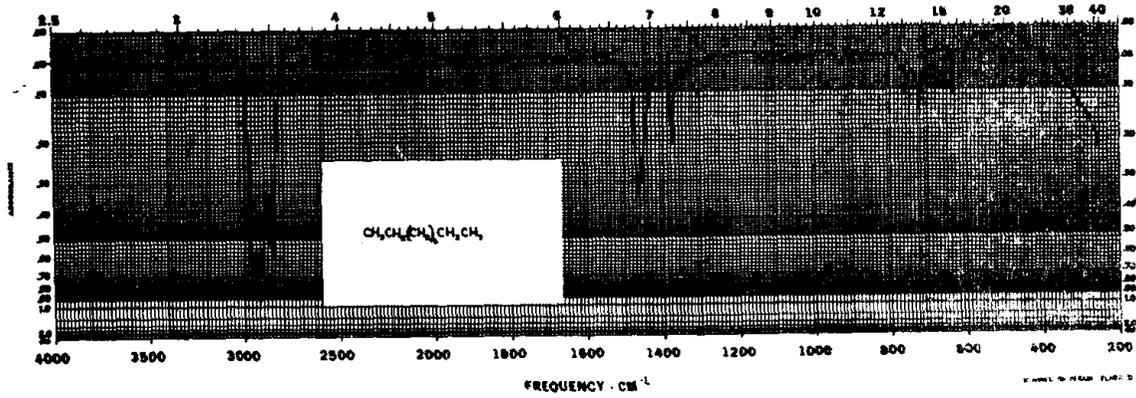
HEPTANE

C₇H₁₆

Mol. Wt. 100.21

B.P. 98-99° C

3 Capillary Cell: Neat



OCTANE

C₈H₁₈

Mol. Wt. 114.23

B.P. 124-126° C

4 Capillary Cell: Neat

