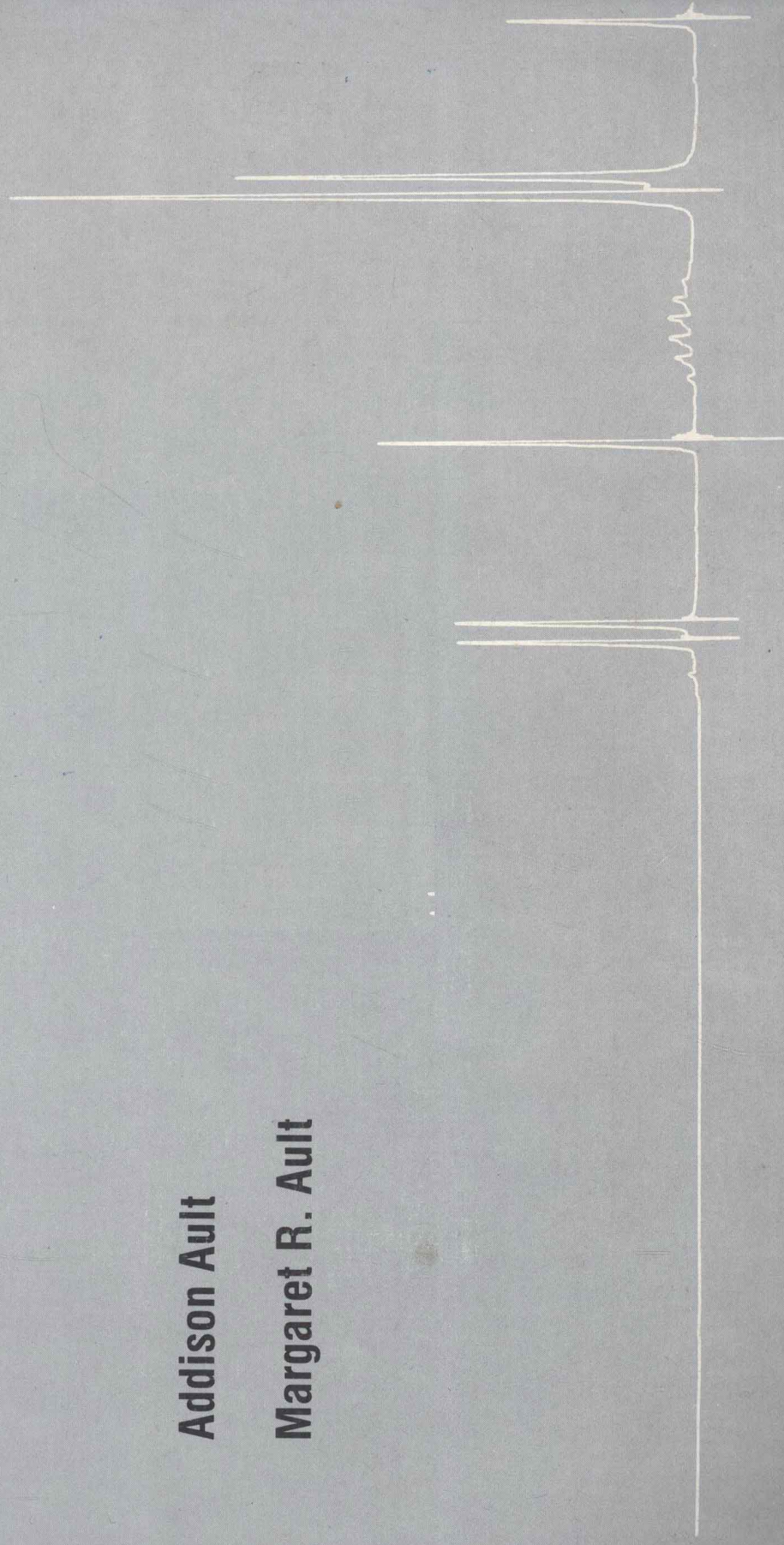


A Handy and Systematic Catalog of NMR Spectra

INSTRUCTION THROUGH EXAMPLES

Addison Ault

Margaret R. Ault



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A Handy and Systematic Catalog of NMR Spectra

ORGANIC CHEMISTRY SERIES

Nicholas J. Turro, Editor

Preface

This book is a collection of 350 nuclear magnetic resonance (NMR) spectra. Two hundred ninety of the spectra are proton NMR spectra obtained at 60 MHz with a Varian T-60 spectrometer, and the remaining spectra include 10 examples of 270 MHz proton NMR spectra, 5 fluorine-19 spectra, and 45 carbon-13 spectra. The collection is intended to be of use both by those who teach NMR spectrometry, by providing appropriate and interesting examples in a format suitable for reproduction, and by those who wish to extend their experience in the interpretation of NMR spectra, by presenting the spectra of a variety of compounds of known structure organized according to spectral features and by type of compound.

After a set of 60 MHz proton NMR spectra that consist of one or more singlets (spectra 1-30) and a set of spectra that consist of singlets and/or one or more "ethyl resonances" (31-50), the spectra of members of several common classes of aliphatic compounds are presented (51-100), followed by the spectra of members of most of the common classes of aromatic compounds (101-230). The next sets of spectra (231-280) illustrate, among other phenomena, the effects of solvent, concentration, and acid on the spectra of alcohols, the effect of a shift reagent, the chemical shift non-equivalence of diastereotopic methyl groups and diastereotopic protons within a methylene group, C-13 satellites, virtual coupling, and the effects of fluorine and phosphorus on proton NMR spectra. The last sets of spectra include selected 270 MHz proton NMR spectra (281-287), selected F-19 spectra (288-290), a variety of C-13 NMR spectra (291-339), and calculated spectra of five common N+1 Rule spin systems (340-344). All of these sets of spectra are listed in the Table of Contents, on pages iii, iv, and v.

Within the catalog, each set of spectra is introduced by a list of the compounds whose spectra are in the set, and reference is made to each spectrum by number. Spectra that could logically be included in more than one set are listed in each set, but the spectrum appears only once in the book.

Two indexes are provided at the end of the catalog: a Compound Name Index and a Molecular Formula Index.

In order that spectra can be more easily reproduced for use in problems or for distribution with an unknown for qualitative organic analysis, the constitutional formula, the name, and the molecular formula are presented below the spectrum so that some or all of this information can be covered and thereby eliminated during duplication. Furthermore, spectra grouped according to the molecular constitution of the sample (for example, aromatic aldehydes, or phenols) are of relatively inexpensive compounds, which may therefore be more desirable for use as unknowns in qualitative organic analysis.

This catalog could not have been produced without the help that was provided by many other people. A list of those who assisted with this project would include Prof. Paul Bender, Dr. David Hillenbrand, Dr. Paul Schatz, Daniel Steffek, and Loretta Grezzo (all of the Department of Chemistry, University of Wisconsin, Madison, Wisconsin), William McGranahan and Tom Lyttle (Department of Chemistry, Iowa State University, Ames, Iowa), Barbara Erwine (Product Manager, Analytical NMR, Varian Associates, Palo Alto, California), Dr. Gerald A. Pearson (Department of Chemistry, University of Iowa, Iowa City, Iowa), and Bruce Armbruster, University Science Books, Mill Valley, California.

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Contents

Spectra that consist of one or more singlets: 1-30

Spectra that consist of singlets and/or one or more ethyl resonances: 31-50

Spectra of aliphatic alkyl chlorides: 51-60

Spectra of aliphatic alcohols: 61-70

Spectra of aliphatic ketones: 71-80

Spectra of aliphatic esters: 81-90

Spectra of miscellaneous aliphatic compounds: 91-100

Spectra of selected monosubstituted aromatic compounds: 101-110

Spectra of aromatic hydrocarbons, halogen substituted aromatic hydrocarbons, and aromatic ethers: 111-130

Spectra of aromatic aldehydes: 131-140

Spectra of ketones that contain an aromatic ring: 141-150

Spectra of carboxylic acids that contain an aromatic ring: 151-160

Spectra of esters of carboxylic acids that contain an aromatic ring: 161-170

Spectra of amides and nitriles that contain an aromatic ring: 171-180

Contents, continued

Spectra of phenols: 181-190

Spectra of aromatic amines and benzylamine: 191-210

Spectra of miscellaneous aromatic compounds: 211-230

Spectra that illustrate the effects of concentration and the addition of acid on the proton NMR spectrum of ethanol: 231-233

Spectra that illustrate the effects of the addition of acid and of D₂O on the proton NMR spectrum of 1-octanol: 234-236

Spectra that illustrate the effects of solvent and concentration on the proton NMR spectrum of benzyl alcohol: 237-240

Spectra that illustrate the effect of a shift reagent: 241-244

Spectra that consist of exactly two N+1 Rule multiplets: 245-252

Spectra of compounds that contain diastereotopic methyl groups: 253-256

Spectra of compounds that contain diastereotopic protons within methylene groups: 257-261

Spectra that illustrate C-13 satellites: 262-267

A spectrum that illustrates virtual coupling: 268

Contents, continued

A spectrum that is recorded with its integral: 269

Spectra that illustrate the influence of fluorine on
proton NMR spectra: 270-272

Spectra that illustrate the influence of phosphorus on
proton NMR spectra: 273-275

Spectra of standards and of chloroform under different
experimental conditions: 276-280

Selected 270 MHz proton NMR spectra: 281-287

Selected 56.4 MHz fluorine NMR spectra: 288-290

22.5 MHz carbon-13 NMR spectra of aliphatic alcohols: 291-310

22.5 MHz carbon-13 NMR spectra of selected aliphatic
compounds: 311-320

22.5 MHz carbon-13 NMR spectra of selected aromatic
compounds: 321-330

22.5 MHz carbon-13 NMR spectra of miscellaneous aliphatic
compounds and natural products: 331-339

Computer-simulated spectra for five common N+1 Rule
spin systems: 340-344

60 MHz Proton NMR Spectra that Consist of One or More Singlets

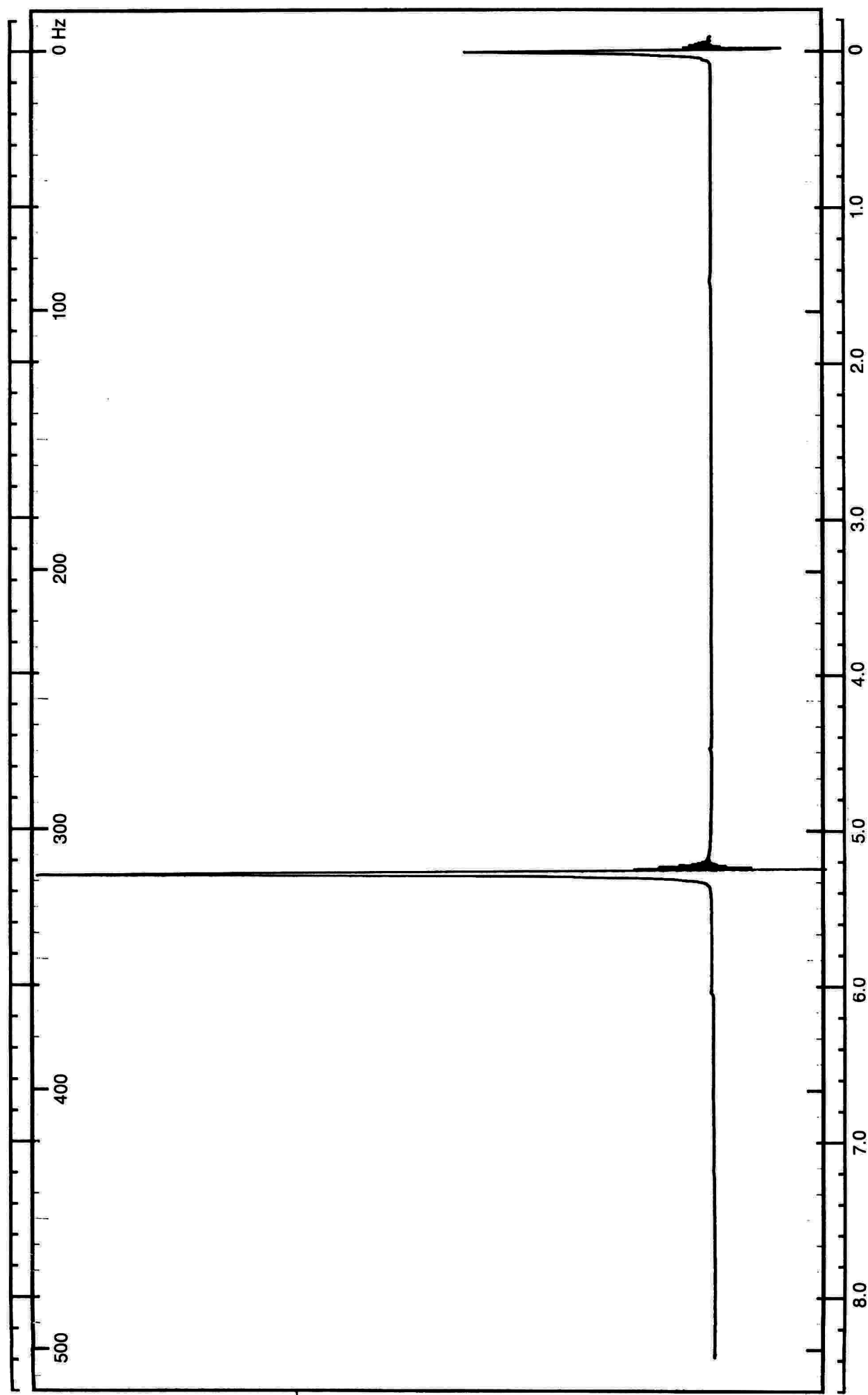
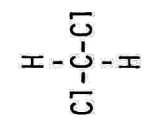
| Compound Name | Spectrum Number | Compound Name | Spectrum Number |
|---------------------------|-----------------|--|-----------------|
| Dichloromethane | 1 | 1,2-Dimethoxyethane | 16 |
| Methyl iodide | 2 | Hexane-2,5-dione | 17 |
| 1,1,1-Trichloroethane | 3 | Dimethyl succinate | 18 |
| Acetonitrile | 4 | 1,2-Diacetoxyethane | 19 |
| Acetone | 5 | tert.-Butyl chloride | 20 |
| Dimethyl carbonate | 6 | 1-Chloro-2,2-dimethylpropane | 21 |
| Dimethyl oxalate | 7 | tert.-Butyl alcohol | 22 |
| 2,2-Dimethoxypropane | 8 | tert.-Butyl acetate | 23 |
| Acetic acid | 9 | Methyl trimethylacetate; Methyl pivalate | 24 |
| Methyl formate | 10 | 3,3-Dimethyl-2-butanone; Pinacolone | 25 |
| Methyl acetate | 11 | Cyclohexane | 26 |
| Dimethyl maleate | 12 | Dioxane | 27 |
| Dimethyl terephthalate | 13 | Benzene | 28 |
| 1,1,2,2-Tetrachloroethane | 14 | p-Xylene | 29 |
| 1,2-Dichloroethane | 15 | Ethylene carbonate | 30 |

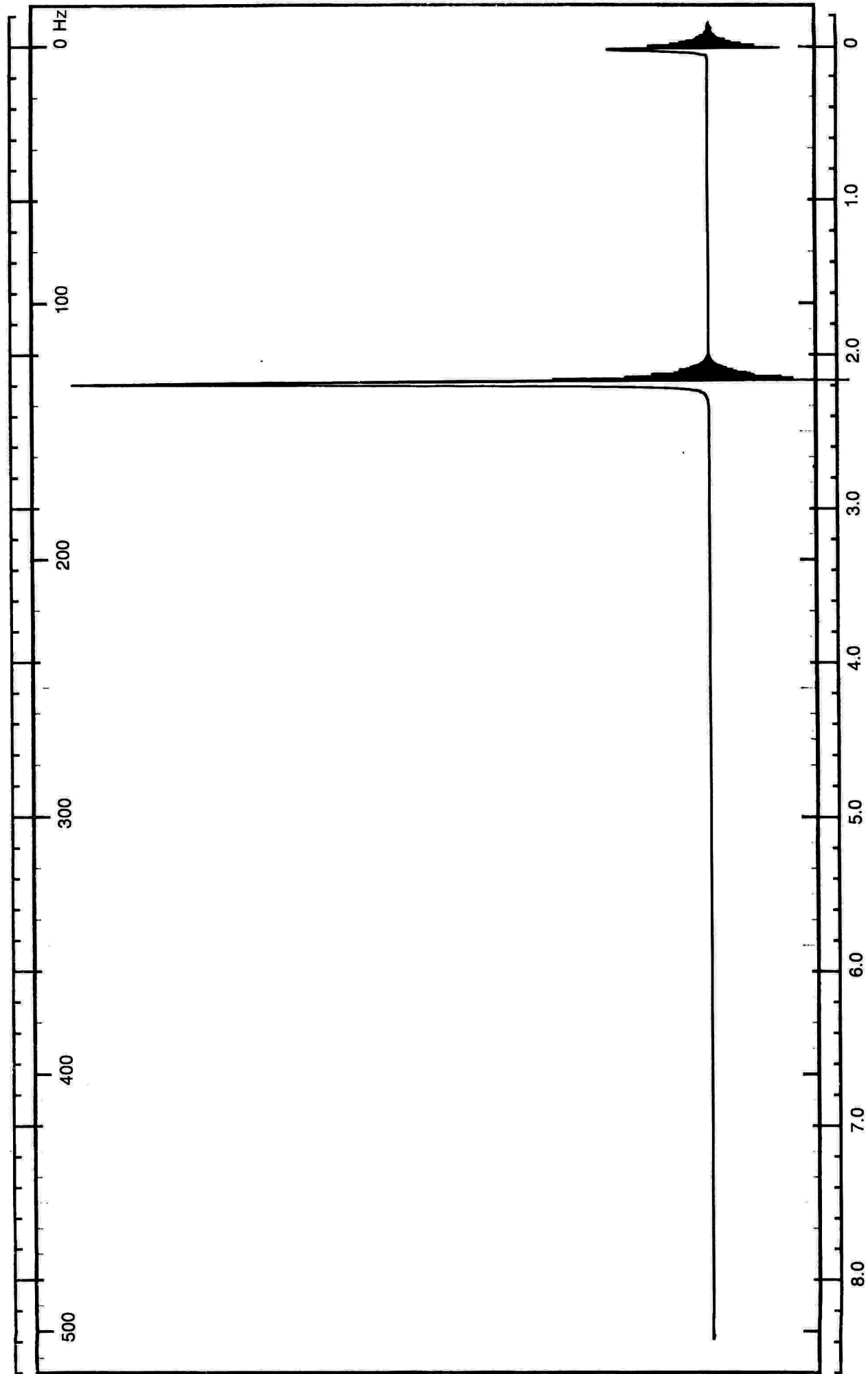
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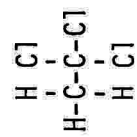
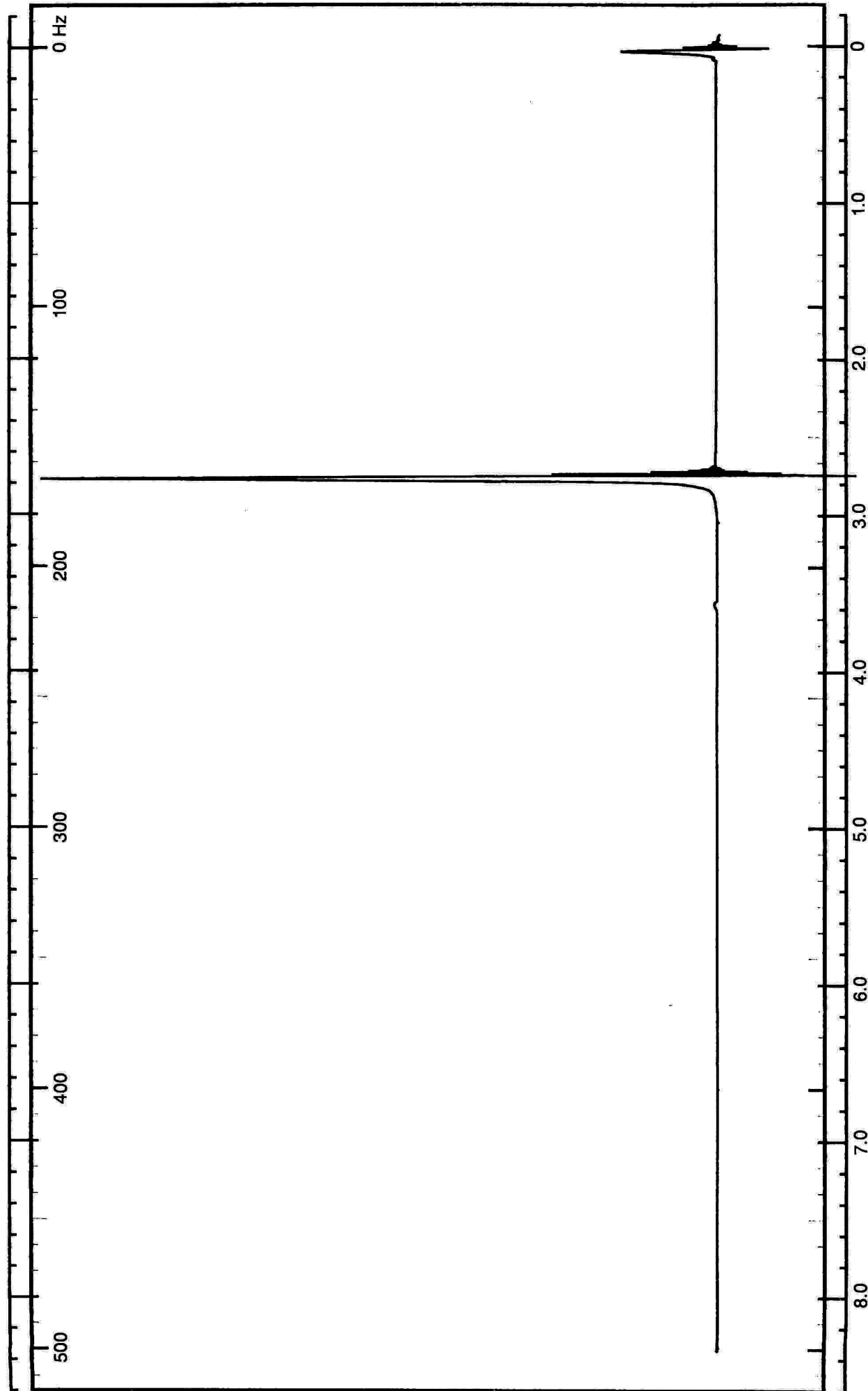
CH_2Cl_2

Dichloromethane

CDCl_3





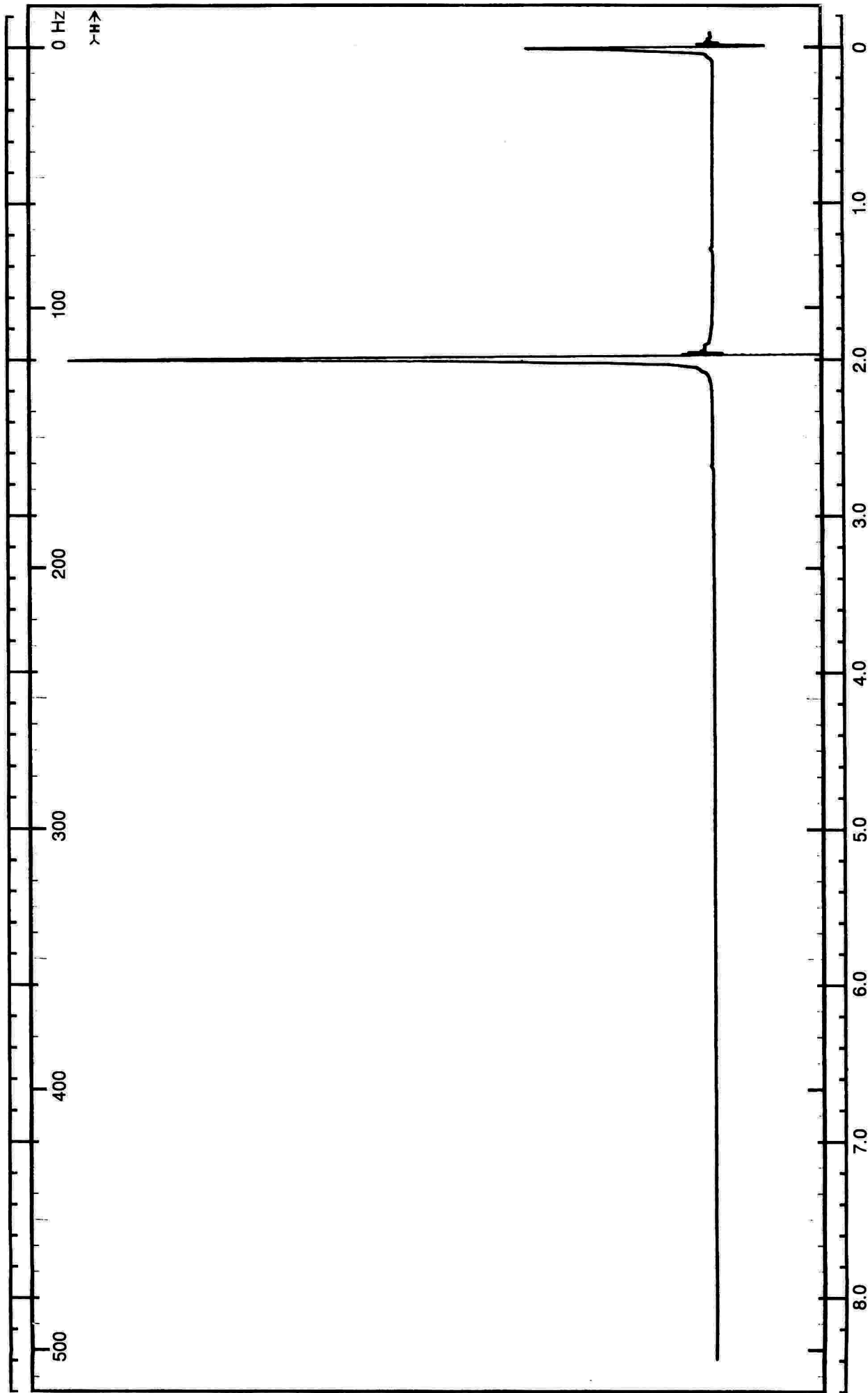


1,1,1-Trichloroethane

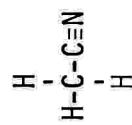
CCl_4

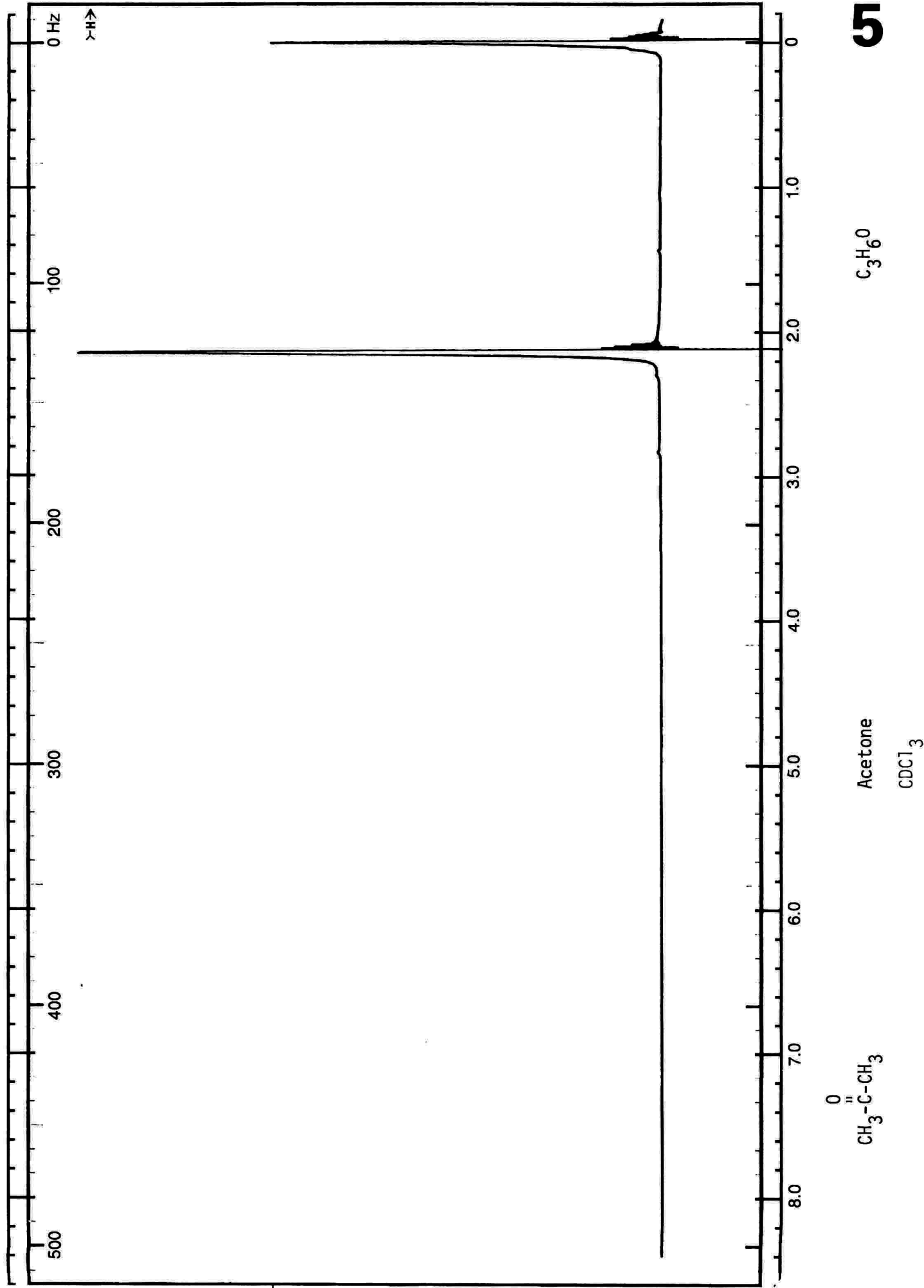
$\text{C}_2\text{H}_3\text{Cl}_3$

3

 $\text{C}_2\text{H}_3\text{N}$

Acetonitrile

 CDCl_3 



$C_3H_6O_3$

Dimethyl carbonate

CDCl₃