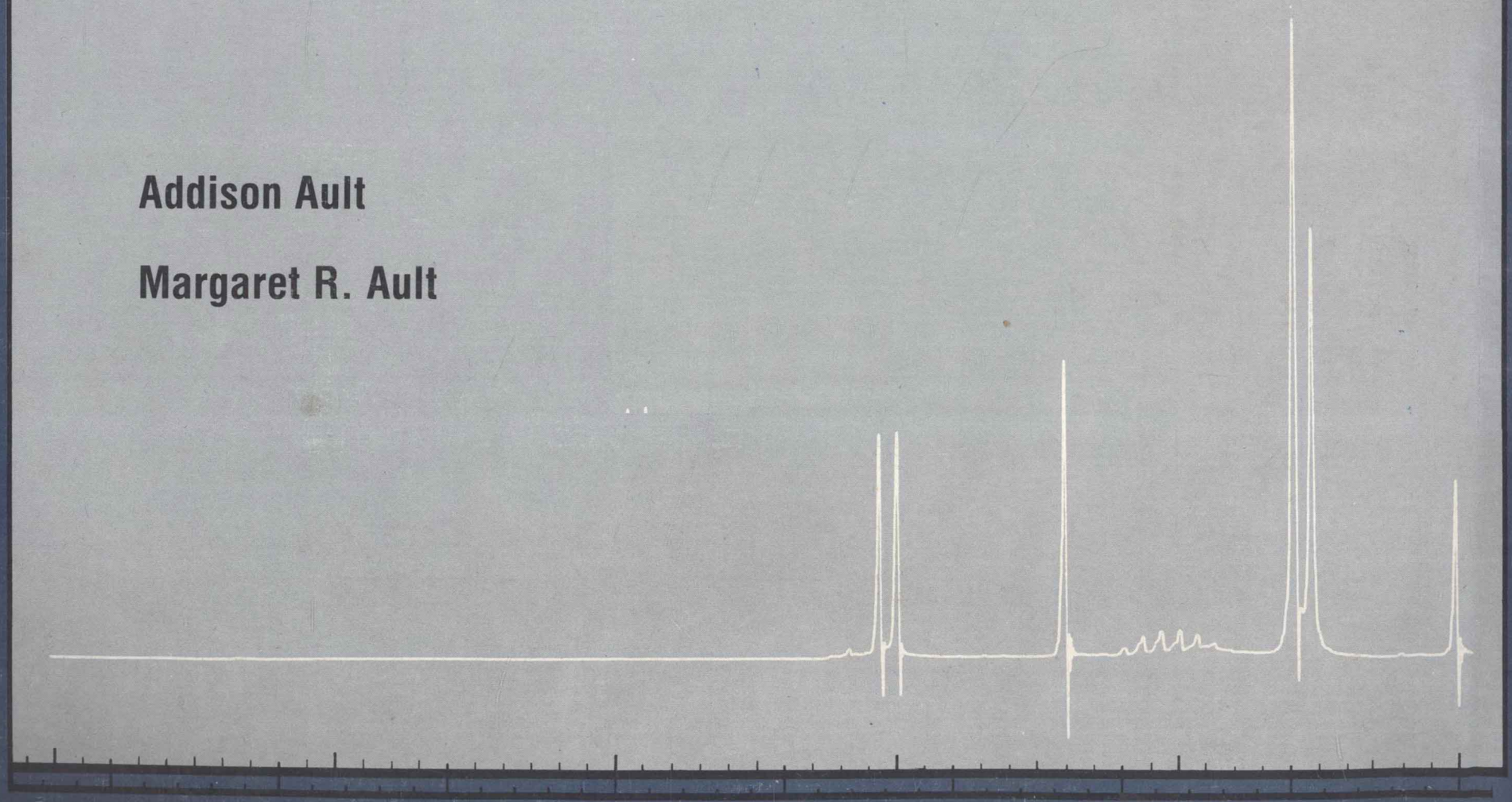
A Handy and Systematic Catalog of NMR Spectra

INSTRUCTION THROUGH EXAMPLES

Addison Ault

Margaret R. Ault



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University Science Books
Mill Valley, California

ISBN 0 19 855701 9

Library of Congress Catalog Card Number: 79-57227

Printed in the United States of America
10 9 8 7 6 5 4 3 2 1

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 ninty 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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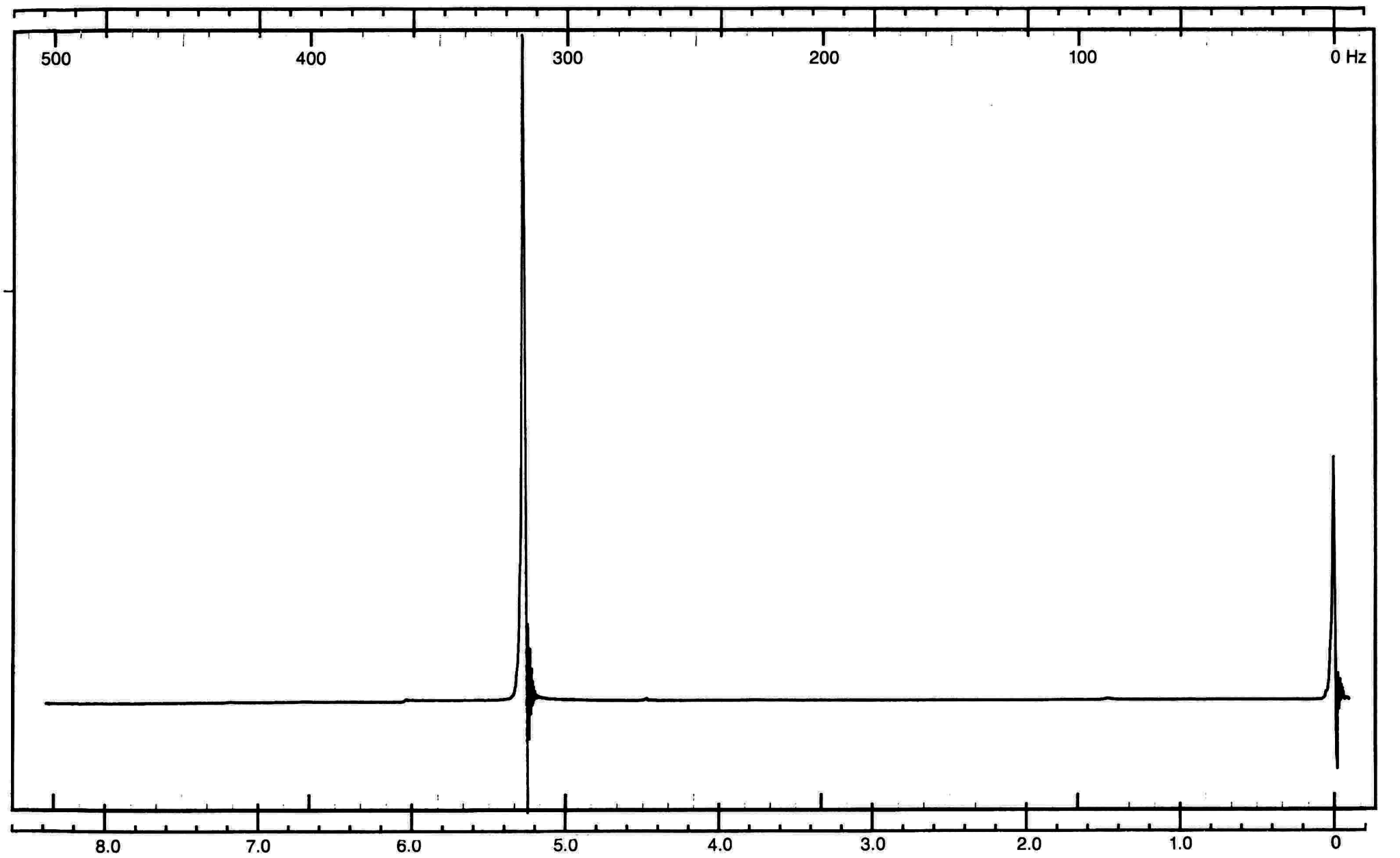
Contents

Contents, continued

Contents, continued

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

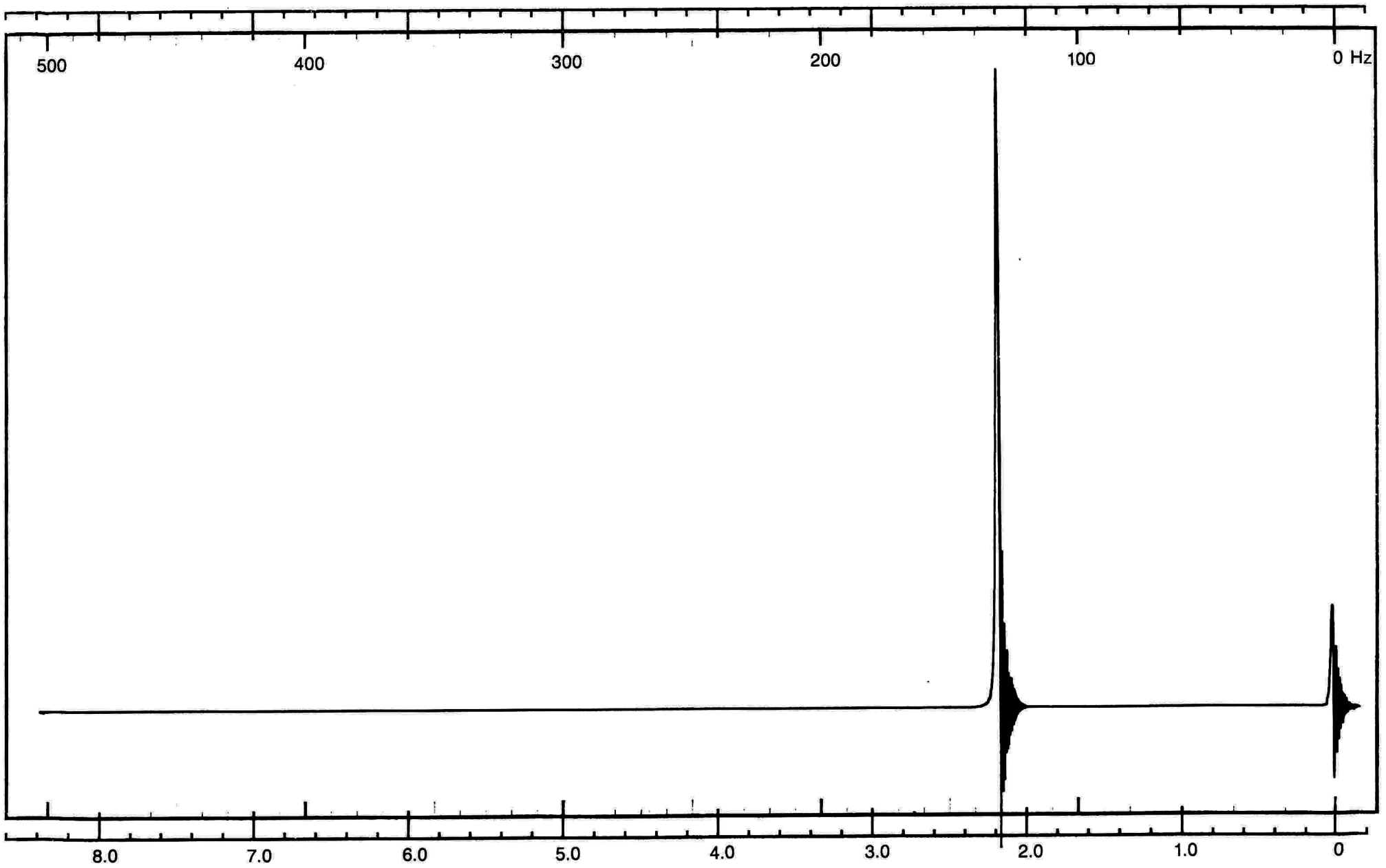


H
Cl-C-Cl
H

Dichloromethane

$CDCl_3$

CH_2Cl_2



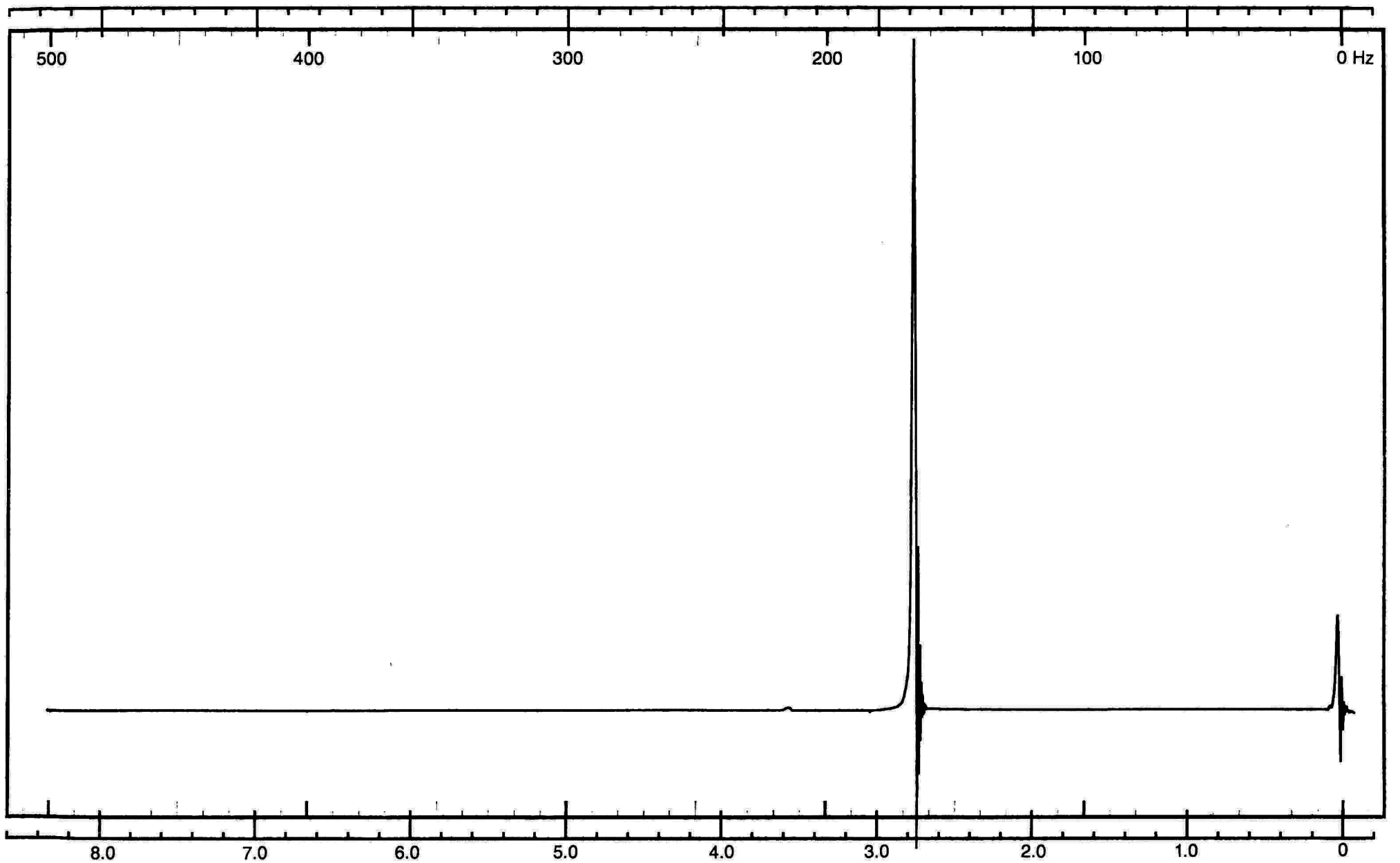
H
H-C-I
H

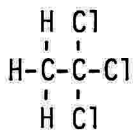
Methyl iodide

$CDCl_3$

CH_3I

2



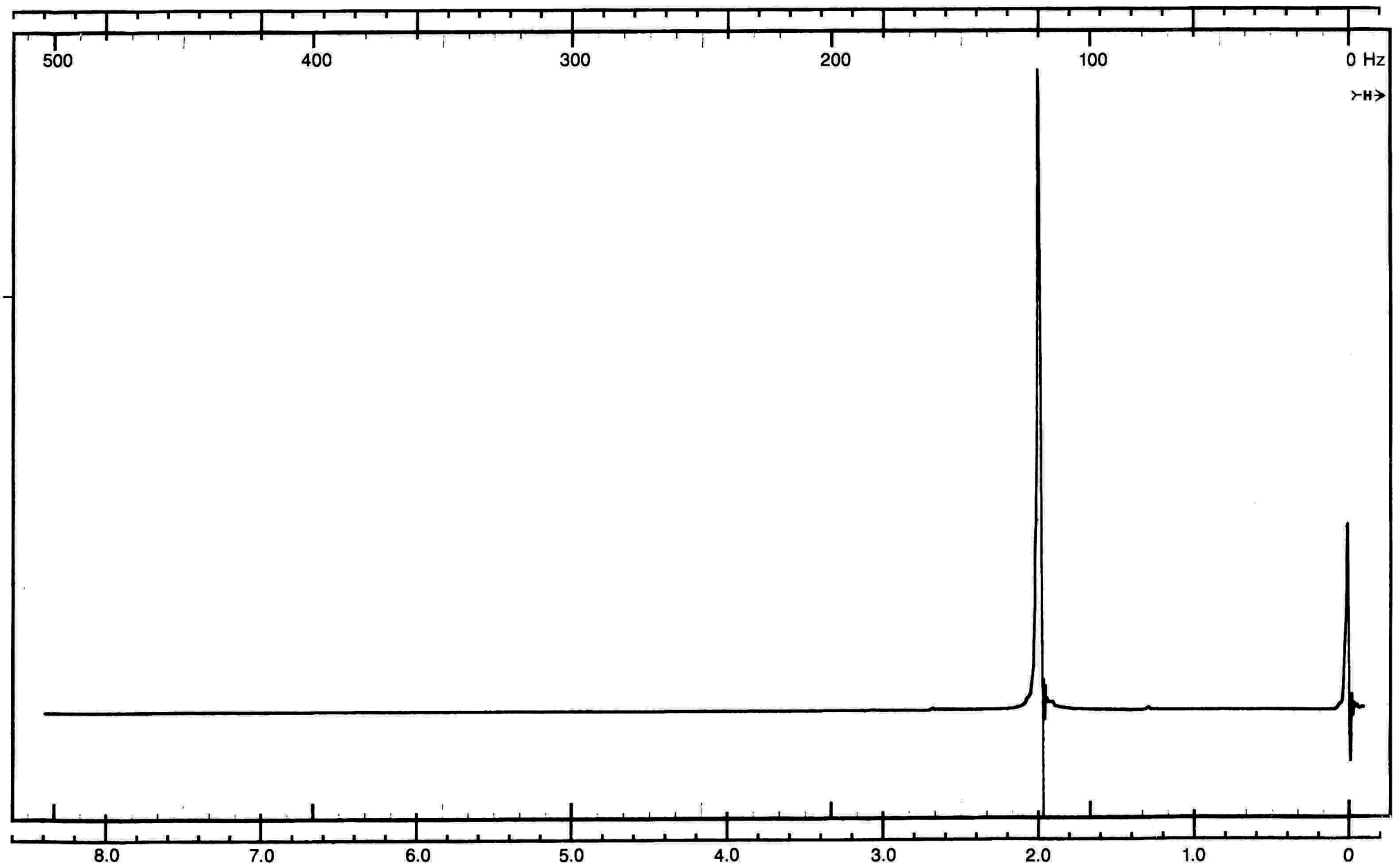


1,1,1-Trichloroethane

CCl_4

$C_2H_3Cl_3$

3

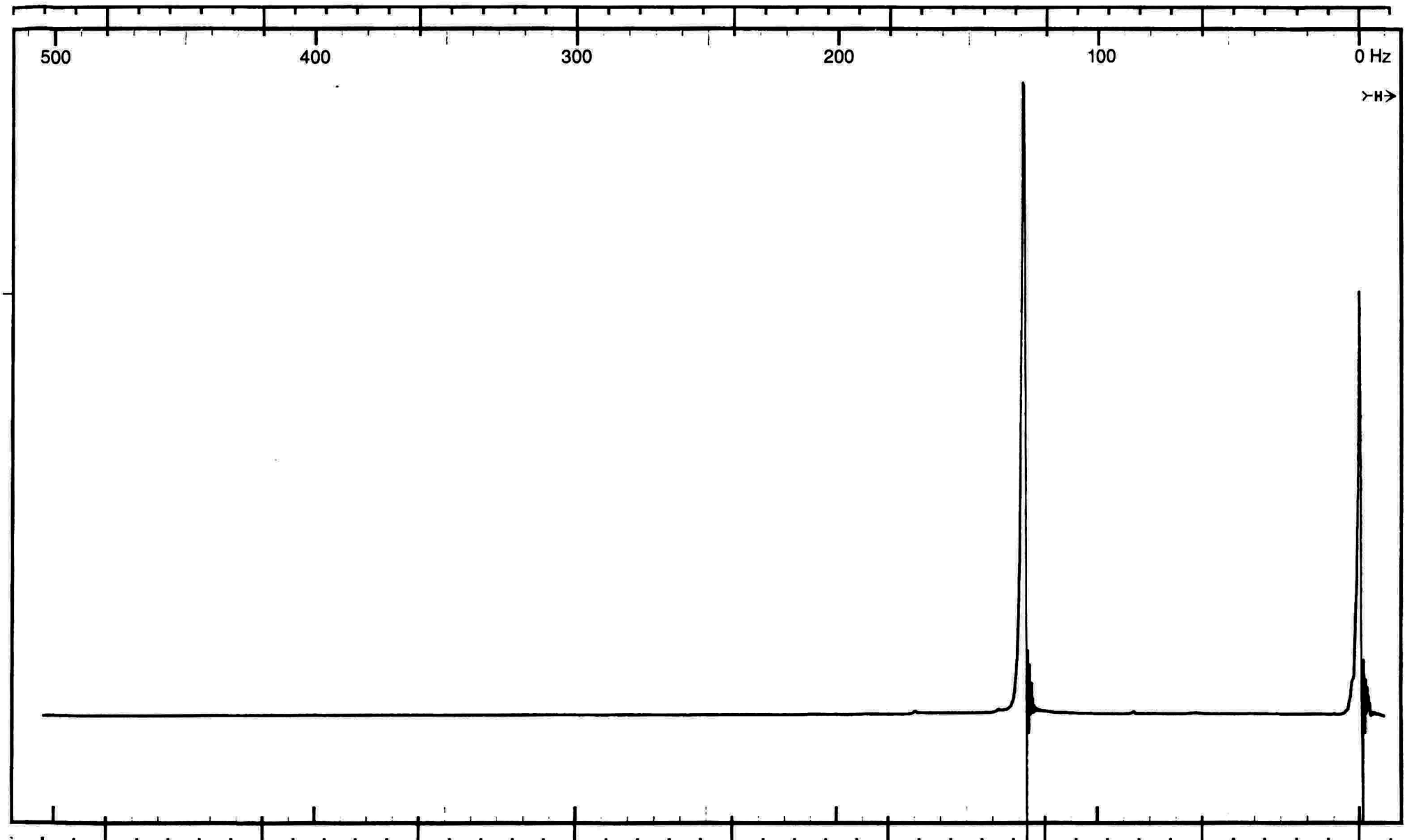


H
H-C-C≡N
H

Acetonitrile

C_2H_3N

$CDCl_3$



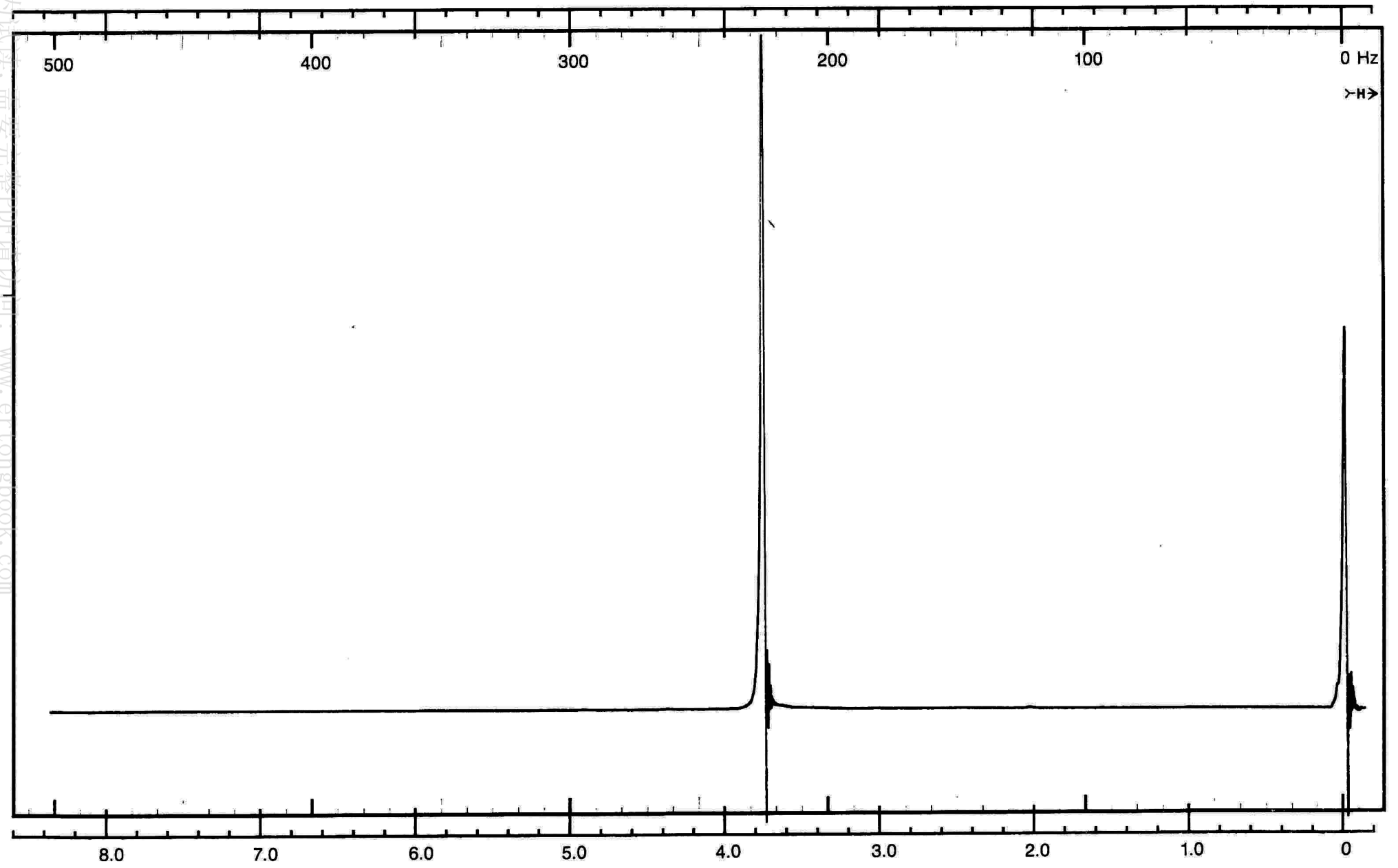
$CH_3-\overset{\overset{O}{\|}}{C}-CH_3$

Acetone

$CDCl_3$

C_3H_6O

5



$CH_3-O-\overset{\overset{O}{\|}}{C}-O-CH_3$

Dimethyl carbonate

$CDCl_3$

$C_3H_6O_3$

6