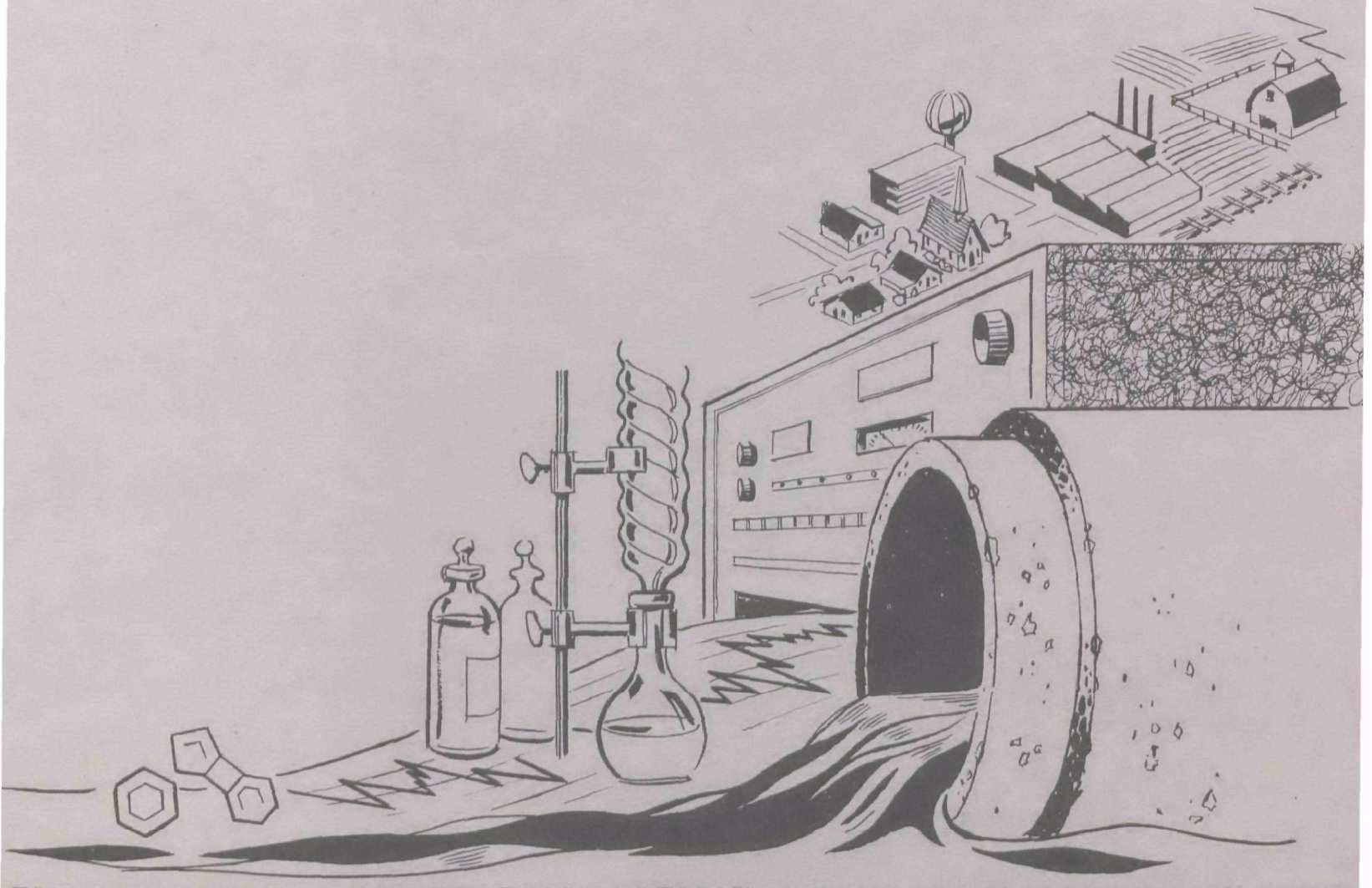
CLEAN WATER

WATER POLLUTION CONTROL RESEARCH SERIES • 16020 EWC 04/71

# Catalog of Pesticide NMR Spectra



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# CATALOG OF PESTICIDE

# NMR SPECTRA

by

Environmental Protection Agency
Southeast Water Laboratory
Athens, Georgia 30601

Project #16020 EWC
April 1971

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ABSTRACT

This catalog contains the 100-MHz NMR spectra of 114 organophosphorus, DDT, and carbamate pesticides and a brief discussion of their most important features. Chemical shifts and coupling constants are shown on each spectrum.

CONTENTS

# SECTION I

## INTRODUCTION

Pesticides are important sources of water contamination. Individual pesticides or their degradation products must often be identified if the water quality is to be protected and improved. Nuclear magnetic resonance (NMR) spectroscopy provides unique structural information (1) that cannot be obtained from infrared spectroscopy, mass spectrometry, and gas chromatography (the primary instrumental methods currently used to identify water contaminants).

Interpretation of NMR spectra is enhanced when spectra of known similar compounds are available for comparison. Since few pesticides have been included in NMR spectral catalogs, we recorded and interpreted spectra of three important classes of pesticides and some of their degradation products. Spectral interpretations were discussed in previous publications (2-5), but only a few spectra were included.

This catalog contains spectra of 114 compounds arranged according to molecular structures:

1. Organophosphorus pesticides
   a. Phosphomethoxy [$(CH_3O)_2$-P]
   b. Phosphoethoxy [$(C_2H_5O)_2$-P]
   c. Miscellaneous
2. DDT and related compounds -- pesticides and several known or proposed metabolites with the substitute diphenyl methane skeleton.
3. Carbamate pesticides.

Chemical names and sources of the compounds are listed in the Appendix in the order they appear in this publication. Section IV is an alphabetical index of the common names and trade names of all compounds in this catalog.

## SECTION II

## EXPERIMENTAL

The 100-MHz spectra were recorded with a Varian HA-100 NMR spectrometer equipped with a variable-temperature probe and a homonuclear spin decoupler. Solutions (300 mg/ml) were prepared in deuterochloroform, except when other solvents or less concentrated solutions had to be used, or when changing solvent or concentration produced a desirable chemical shift. Each spectrum shows chemical shifts ($\tau$ values with reference to the internal standard, tetramethylsilane). Sweep widths of 1000 Hz or 500 Hz were used, but portions of some spectra were expanded for more detailed analysis. In some cases homonuclear spin decoupling, integration, protonation with trifluoroacetic acid, $D_2O$ exchange, temperature, solvent and concentration variations, and supplemental 60-MHz spectra were needed for spectral interpretation.

## SECTION III

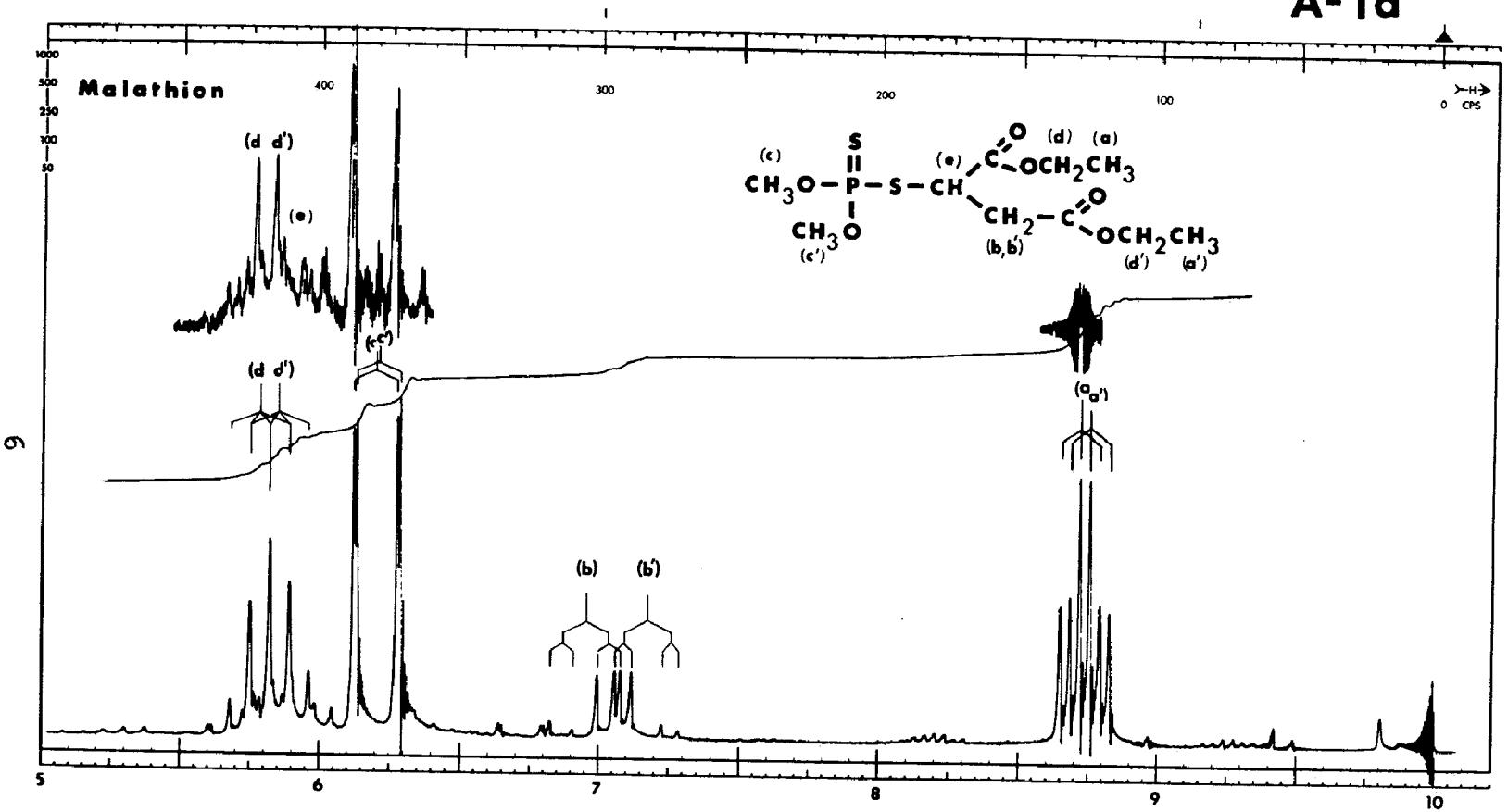
## DISCUSSION

### THE ORGANOPHOSPHORUS PESTICIDES

Signal splittings due to coupling of phosphorus with hydrogen complicate these spectra. Coupling constants, inversely proportional to the P-H distance, vary from 0.5 to 18 Hz. The aromatic proton signals of ronnel, dicapthon, Ruelene, Zytron, methyl parathion, ethyl parathion and paraoxon, have a small splitting due to P-H coupling through four and/or five bonds. The phosphoethoxy methyl signals ($\tau$ 8.59-8.67, J = 0.5-1.2 Hz) also show P-H coupling through four bonds.

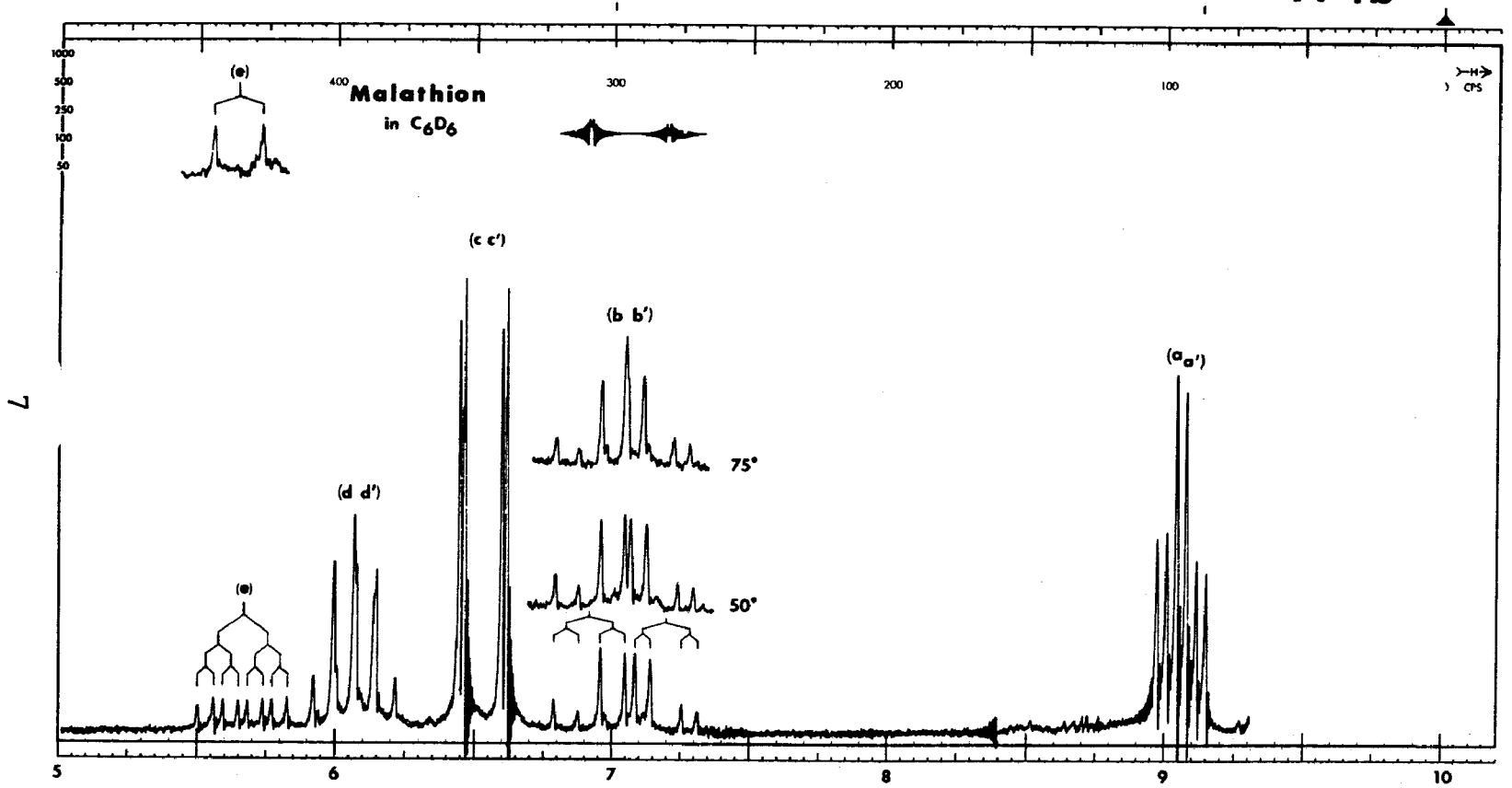
Each spectrum of the phosphomethoxy compounds exhibits a doublet (J = 11-16 Hz, $\tau$ 6.1-6.3) due to the $CH_3O$-P protons coupled through oxygen to phosphorus. In malathion, malaoxon, Dibrom, and Neguvon, each doublet exhibits a smaller splitting (<2Hz). Two methoxyl groups are attached to the phosphorus atom and an asymmetric carbon atom is present; therefore, this splitting is actually a chemical shift difference due to a small magnetic non-equivalence of the methoxyl groups. Similarly, methylene groups of several phosphoethoxy compounds (Thimet, Di-Syston, Trithion and ethion) produce 16, rather than the expected eight, peaks. Each non-equivalent methylene group is coupled with methyl protons to produce a quartet that is further split by phosphorus. The signals of the phosphoethoxy methylene protons appear at $\tau$5.65-5.91 with P-H coupling of 8-10 Hz.

# A-1a



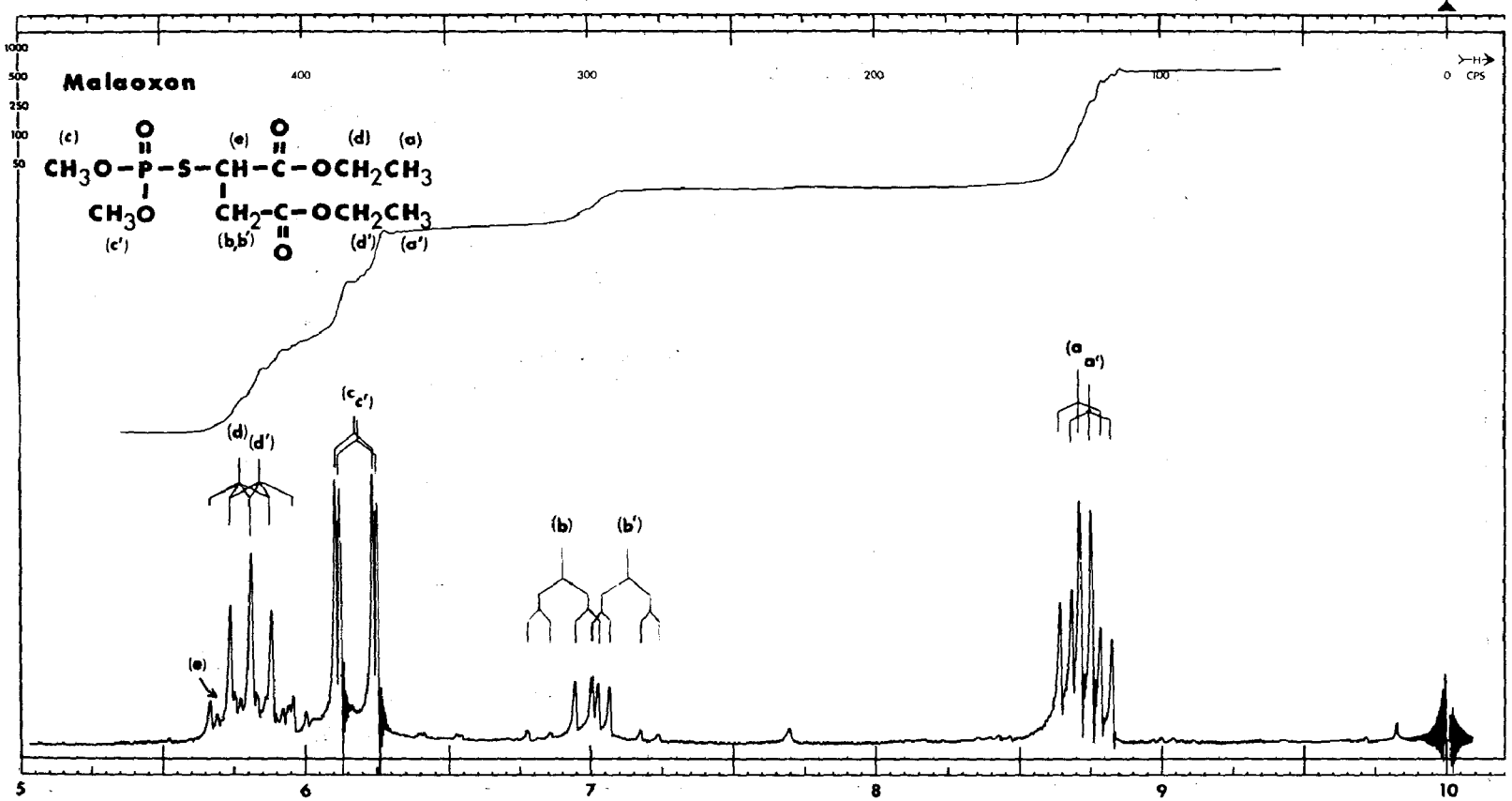

| | T | J |
|---|---|---|
| a | 8.71 | 7 |
| a' | 8.75 | 7 |
| b | *6.93 | < 9 (vic.) < 17 (gem.) |
| b' | *7.19 | < 6.0 (vic.) |
| c | 6.19 | 15.5 (P-H) |
| c' | 6.20 | 15.5 (P-H) |
| d | 5.78 | 7 |
| d' | 5.85 | 7 |
| e | 5.9 | |

# A-1b



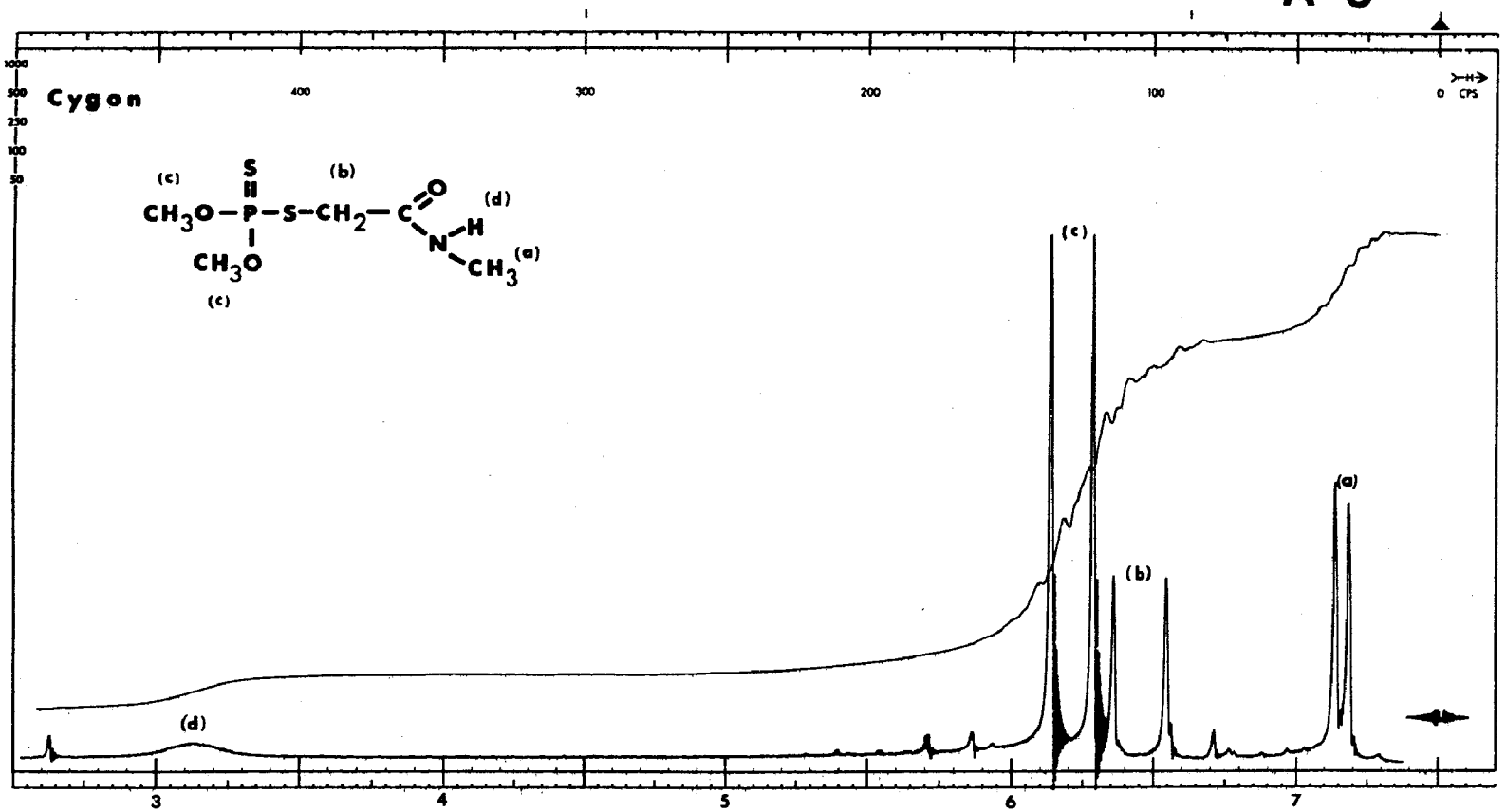

| | T | J |
|---|---|---|
| a | 9.04 | 7 |
| a' | 9.08 | 7 |
| b | *6.90 | 9 (vic.)<br>17 (gem.) |
| b' | *7.22 | 6 (vic.) |
| c | 6.52 | 15.5(P-H) |
| c' | 6.54 | 15.5(P-H) |
| d | 6.03 | 7 |
| d' | 6.10 | 7 |
| e | 5.67 | 17.5(P-H)<br>9 ($H-H_b$)<br>6 ($H-H_{b'}$) |

# A-2



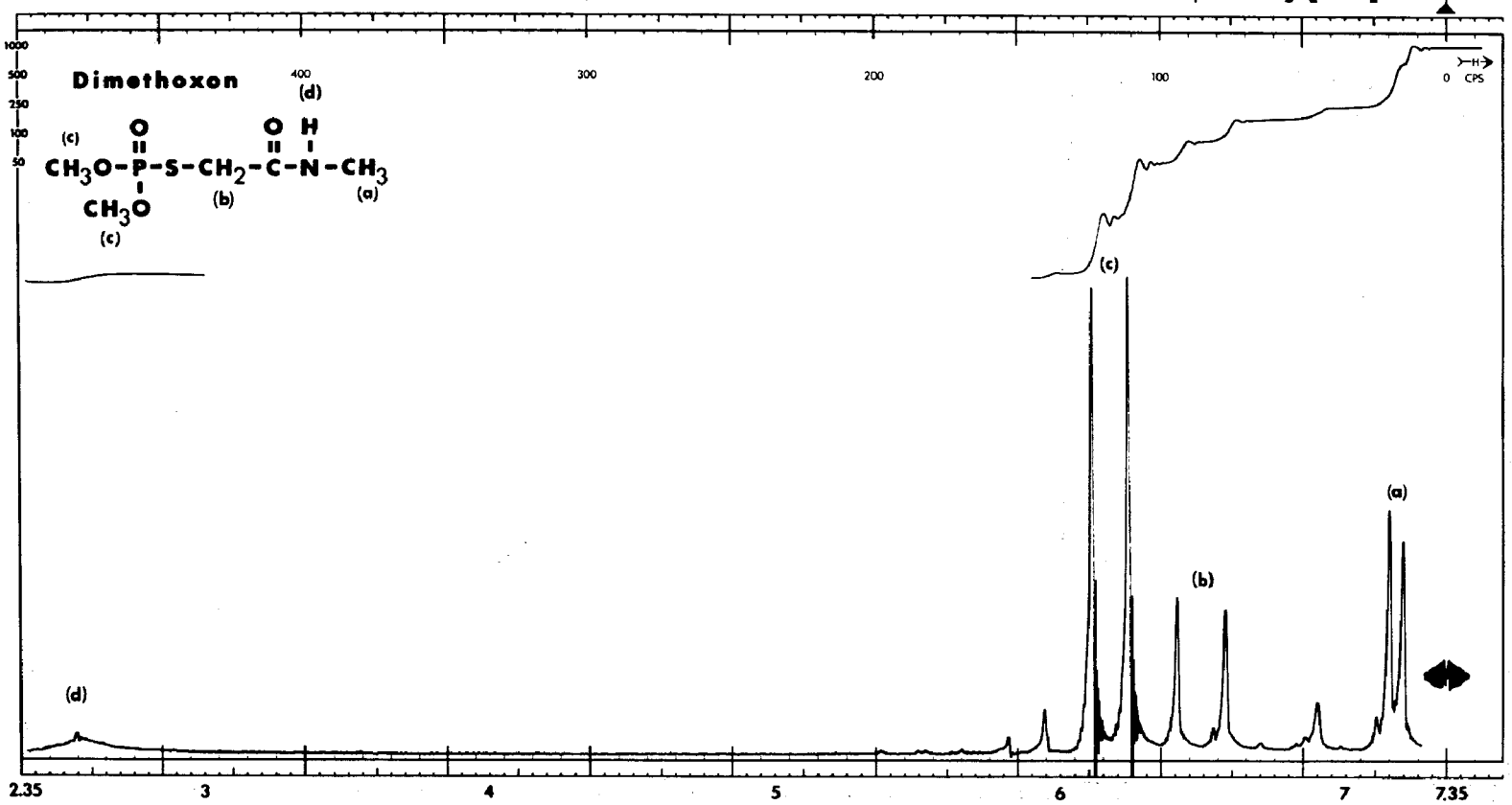

| | T | J |
|---|---|---|
| a | 8.71 | 7 |
| a' | 8.75 | 7 |
| b | *6.88 | 8 (vic.), 17 (gem.) |
| b' | *7.15 | 17 (gem.), 6 (vic.) |
| c | 6.17 | 13 |
| c' | 6.18 | 13 |
| d | 5.78 | 7 |
| d' | 5.85 | 7 |
| e | 5.9 | |

# A-3



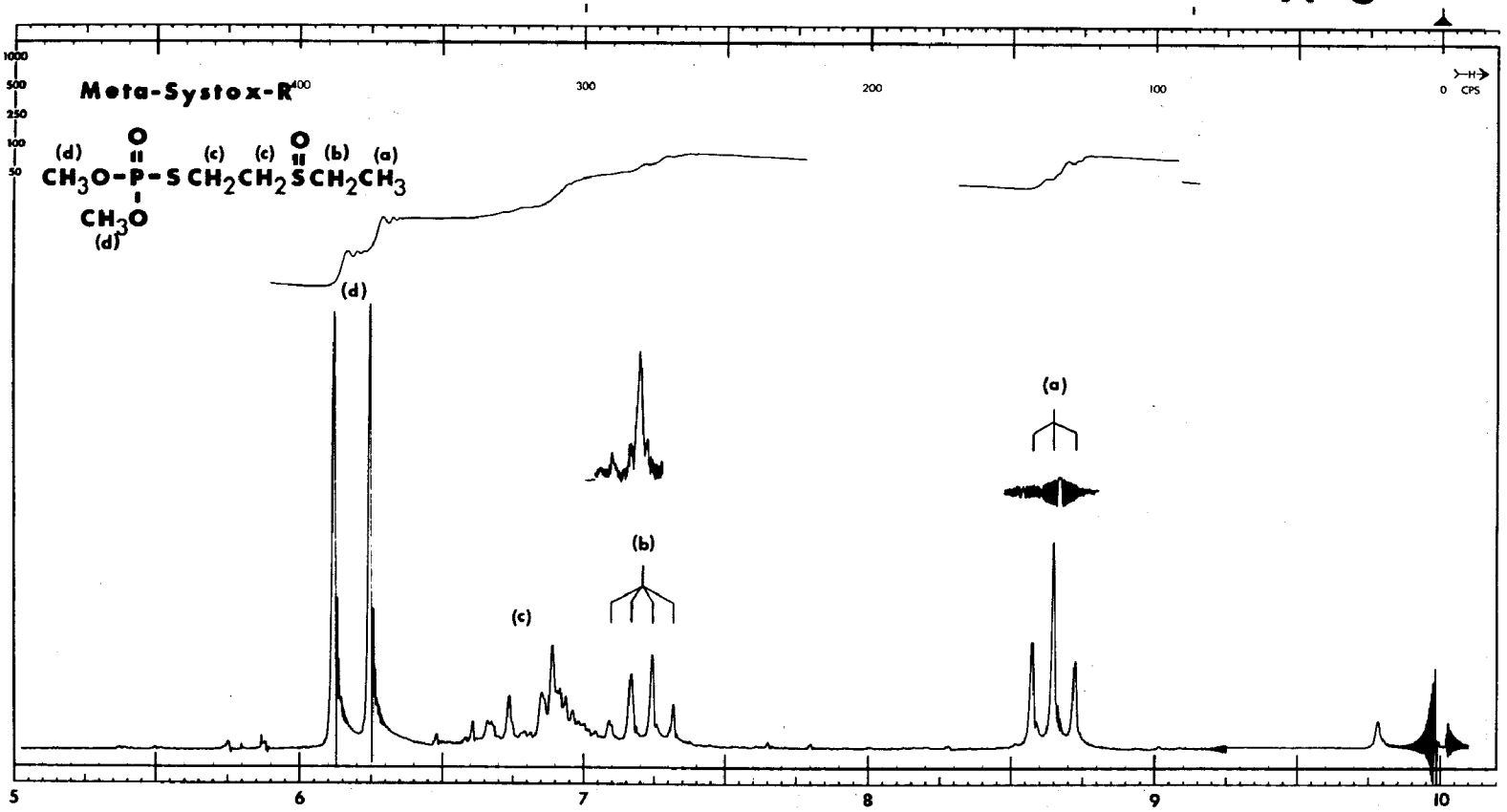

| | T | J |
|---|---|---|
| a | 7.15 | 4.5 |
| b | 6.44 | 18 |
| c | 6.20 | 15 |
| d | 3.13 | |

# A-4




| | T | J |
|---|---|---|
| a | 7.17 | 5 |
| b | 6.49 | 17 |
| c | 6.17 | 12.5 |
| d | 2.55 | |

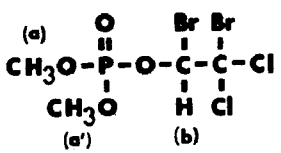
# A-5




| | T | J |
|---|---|---|
| a | 8.65 | 7 |
| b | 7.21 | 7 |
| c | 6.8 | |
| d | 6.18 | 13 |

# A-6

**Dibrom**

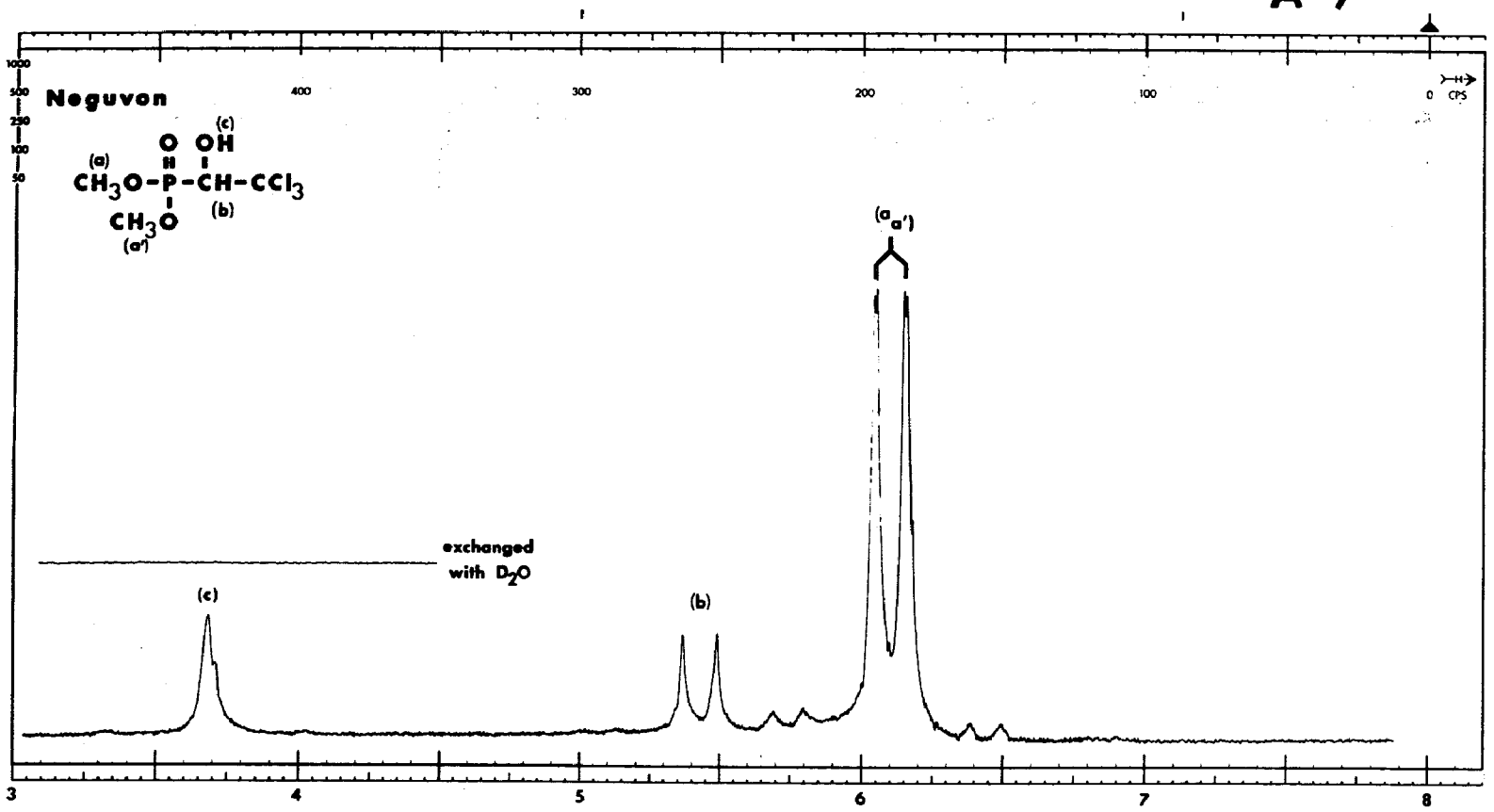






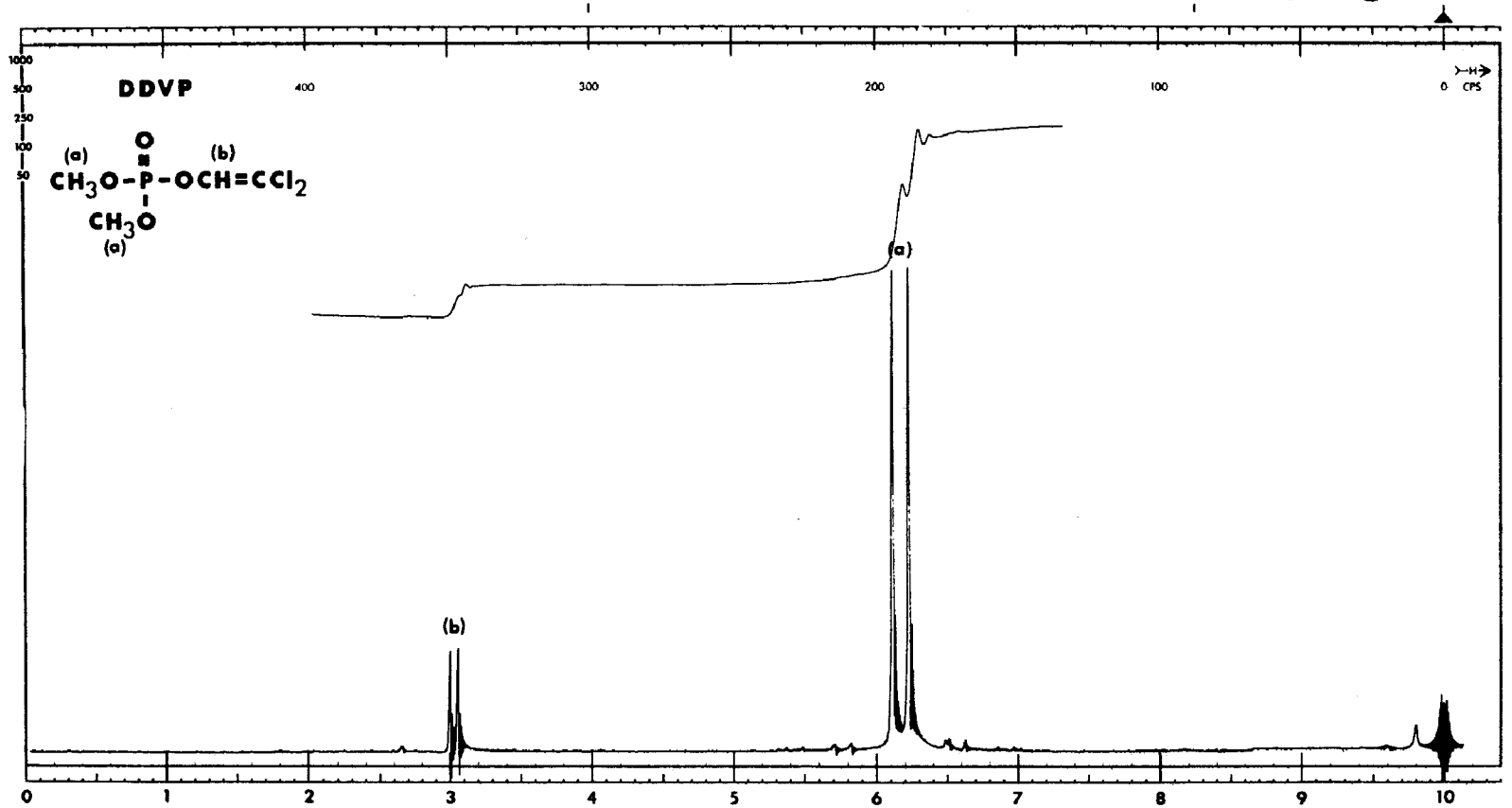
| | T | J |
|---|---|---|
| a | 6.08 | 12 (P-H) |
| a' | 6.09 | 12 (P-H) / 0.3 (H-H) |
| b | 3.30 | 9 |

# A-7



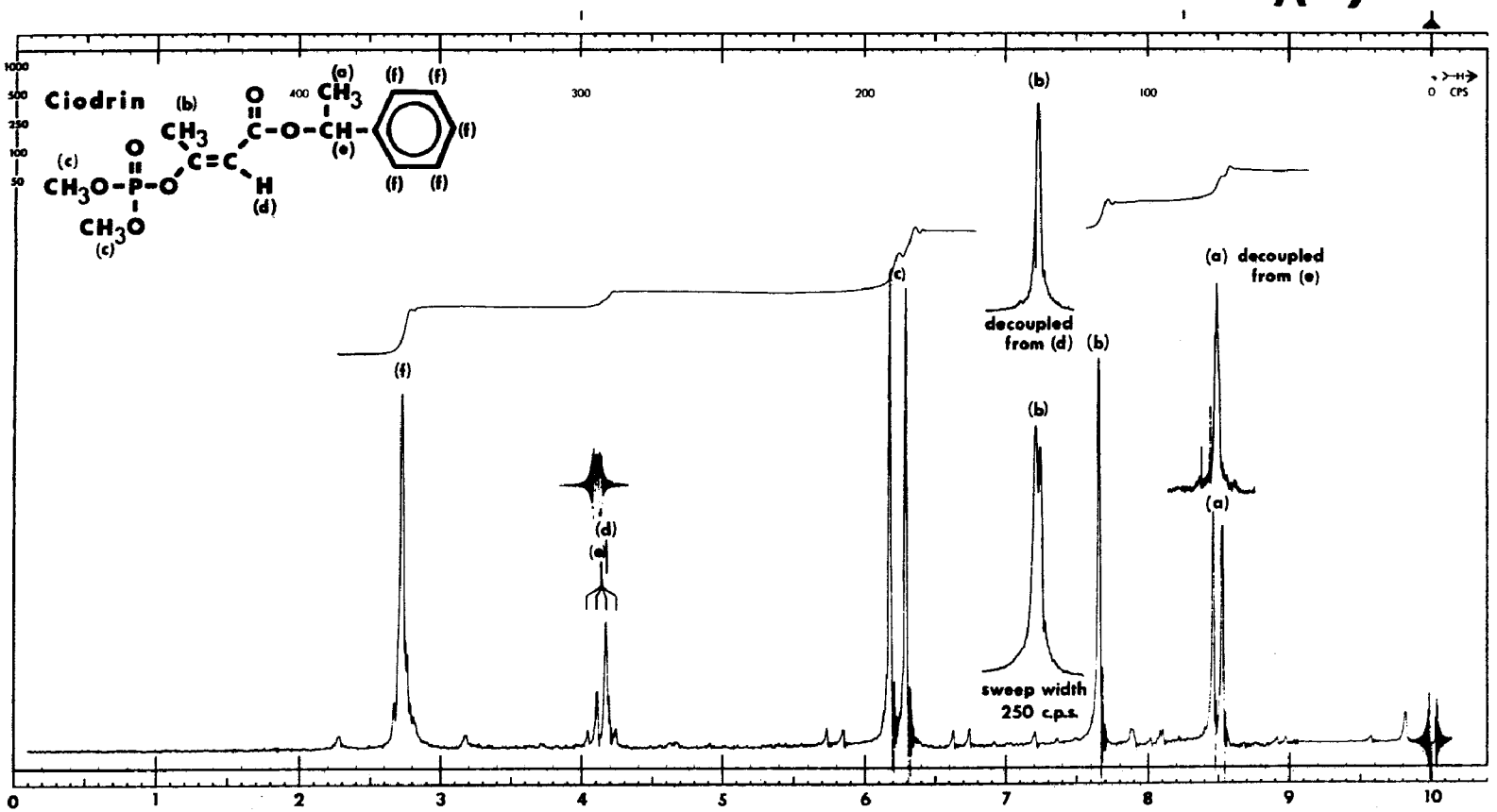

| | T | J |
|---|---|---|
| a | 6.09 | 11 (P-H) |
| a' | 6.10 | 11 (P-H) |
| b | 5.43 | 12 (P-H) |
| c | 3.69 | |

# A-8



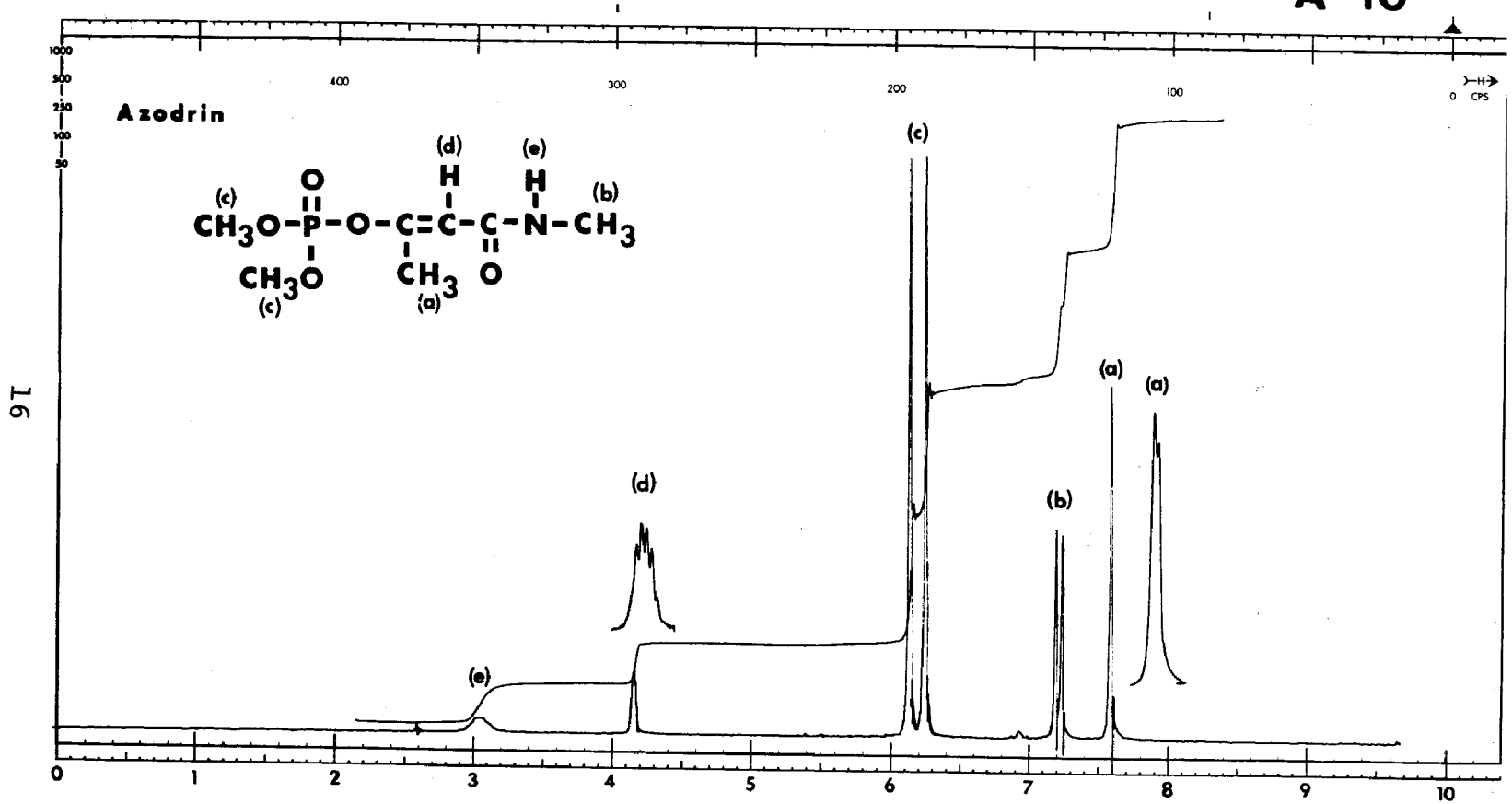

| | T | J |
|---|---|---|
| a | 6.14 | 11 |
| b | 3.00 | 5.5 |

# A-9



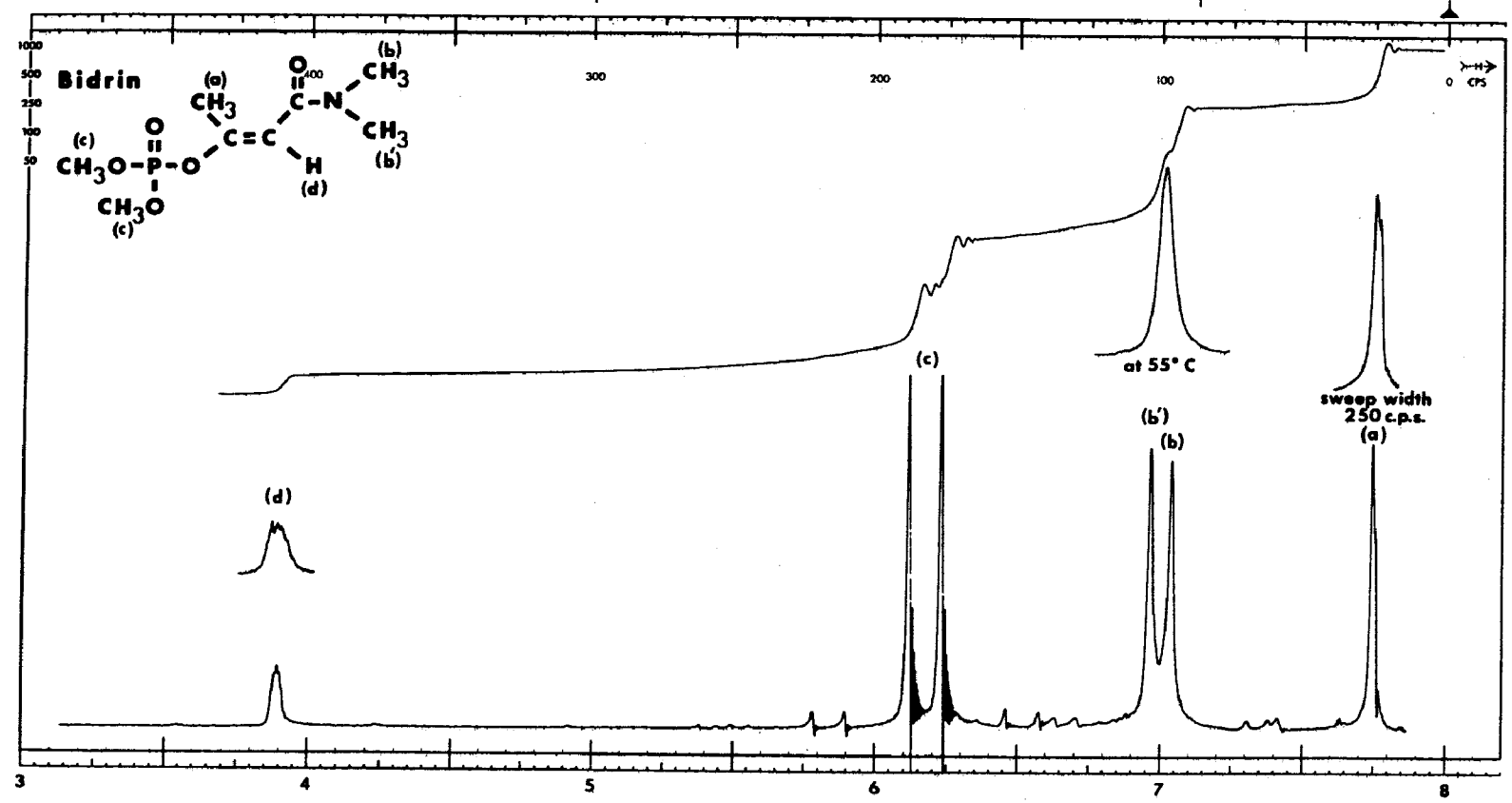

| | T | J |
|---|---|---|
| a | 8.48 | 7 |
| b | 7.63 | 0.8 |
| c | 6.20 | 11 (P-H) |
| d | 4.14 | |
| e | 4.10 | 7 |
| f | 2.70 | |

# A-10



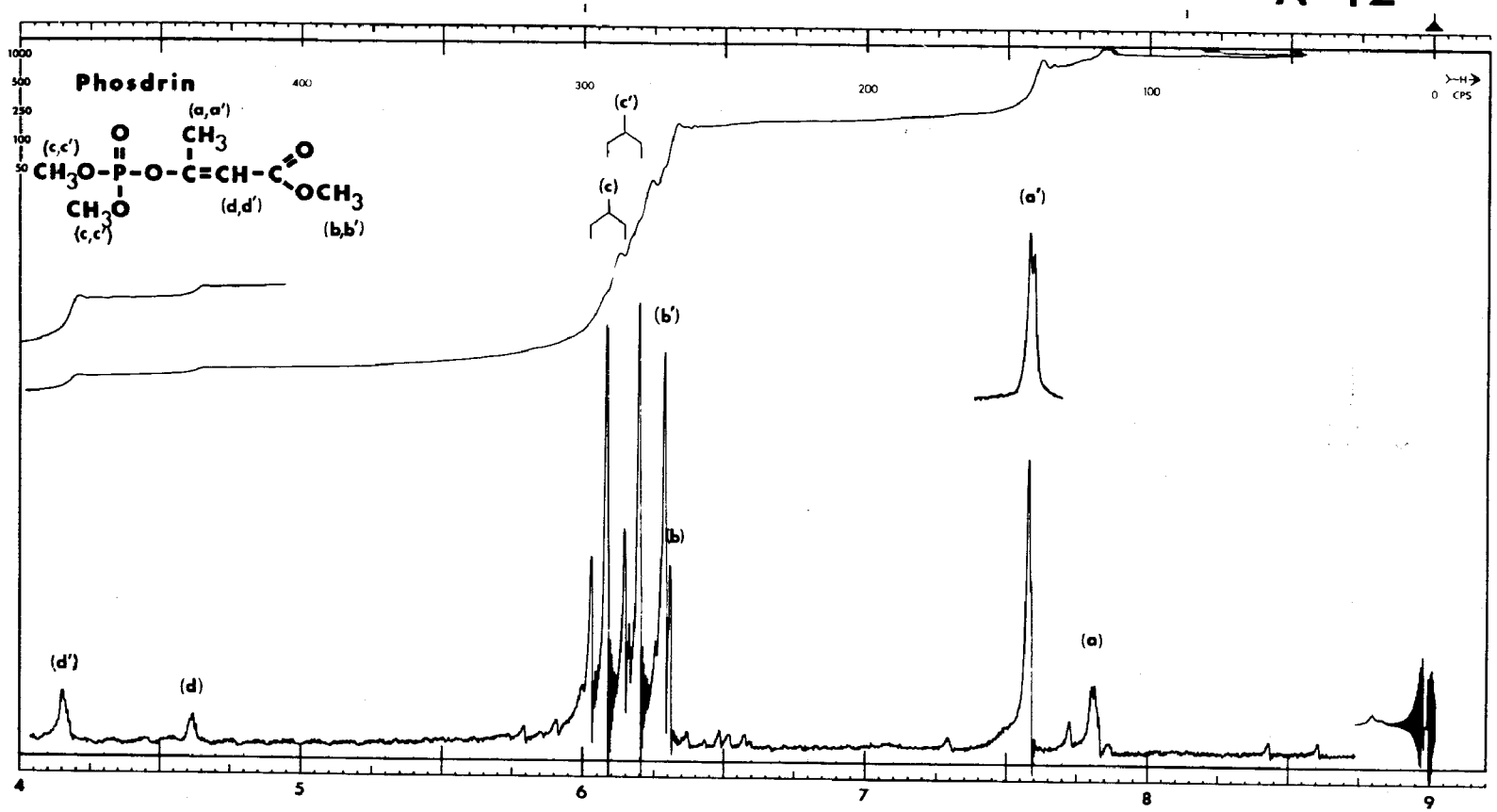

| | T | J |
|---|---|---|
| a | 7.58 | 0.9 |
| b | 7.21 | 5 |
| c | 6.16 | 11 (P-H) |
| d | 4.21 | 0.9 |
| e | 3.0 | |

# A-11




| | T | J |
|---|---|---|
| a | 7.74 | 0.5 |
| b | 7.03 | |
| b' | 6.96 | |
| c | 6.17 | 11 |
| d | 3.89 | |

# A-12

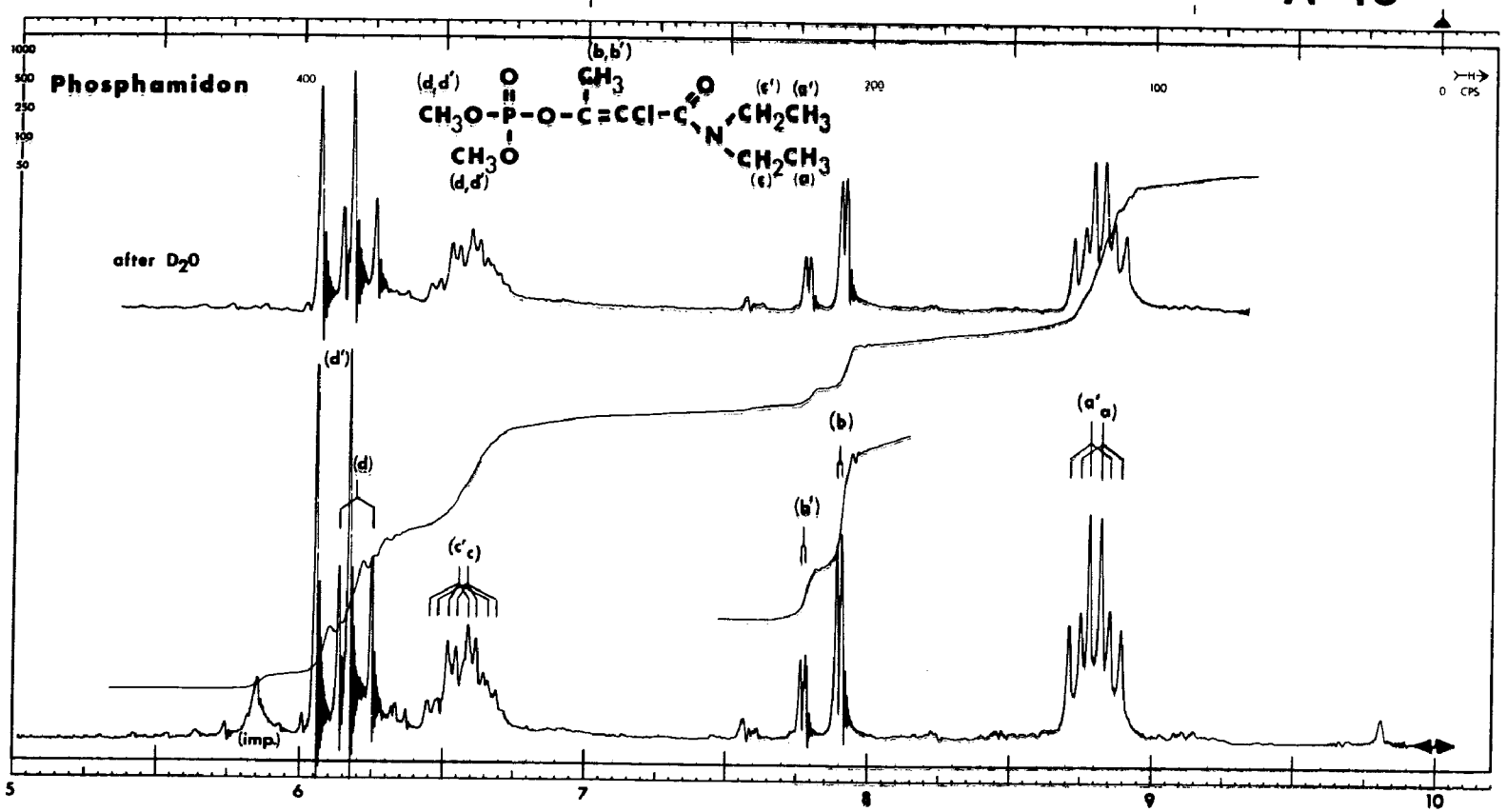



| | | T | J |
|---|---|---|---|
| a | trans | 7.81 | 1.0 |
| a' | cis | 7.58 | 0.7 |
| b | trans | 6.31 | |
| b' | cis | 6.29 | |
| c' | cis | 6.14 | 11.5 |
| c | trans | 6.09 | 11.5 |
| d | trans | 4.62 | |
| d' | cis | 4.15 | |

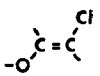
cis 

trans 

# A-13

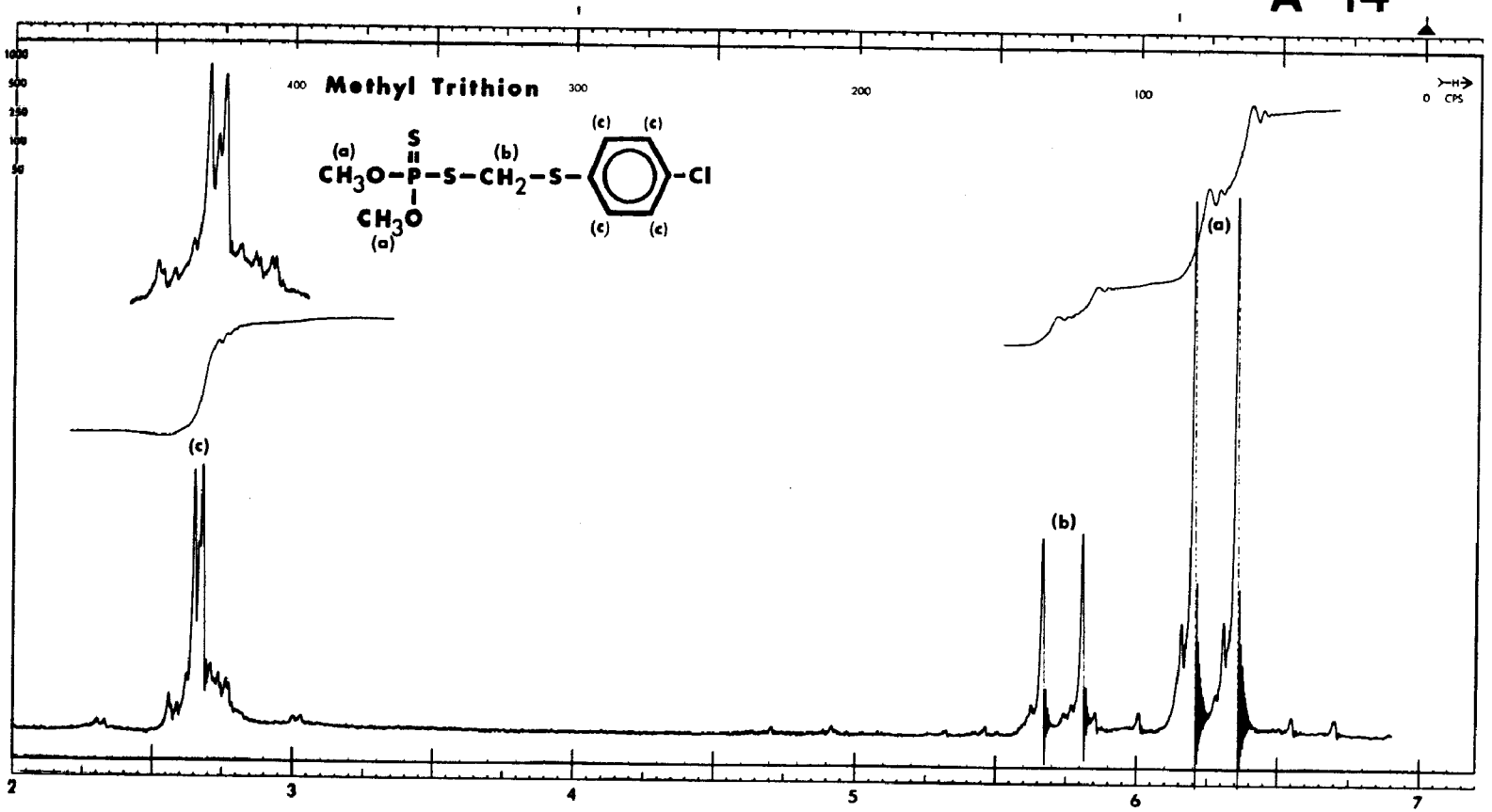



| | T | J |
|---|---|---|
| a | 8.83 | 7 |
| a' | 8.79 | 7 |
| b trans | 7.90 | 1.6 |
| b' cis | 7.78 | 1.6 |
| c | 6.59 | 7 |
| c' | 6.56 | 7 |
| d cis | 6.20 | 12 |
| d' trans | 6.12 | 12 |

trans 

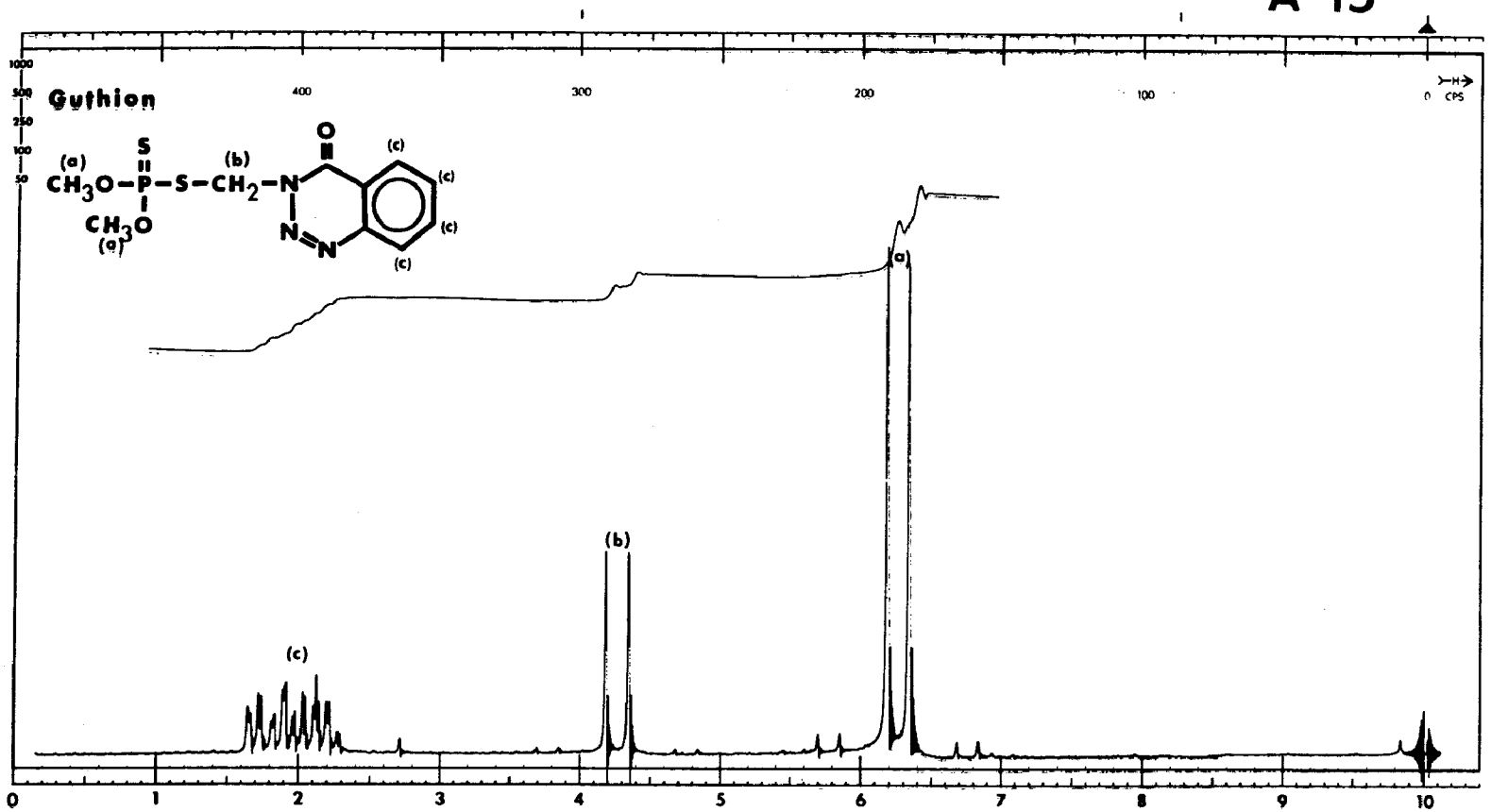
cis 

# A-14



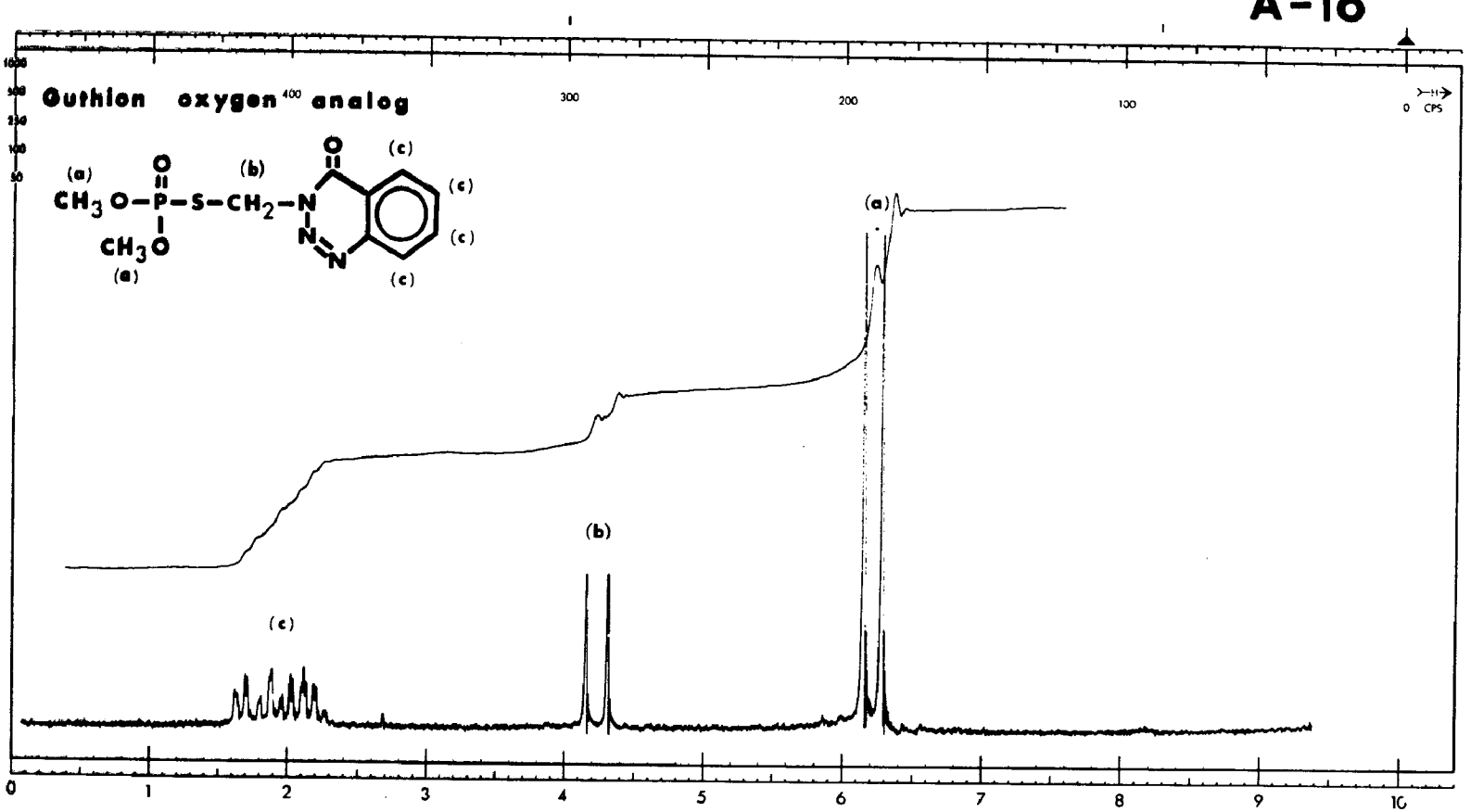

| | T | J |
|---|---|---|
| a | 6.28 | 15 |
| b | 5.74 | 14 |
| c | 2.67 | |

# A-15



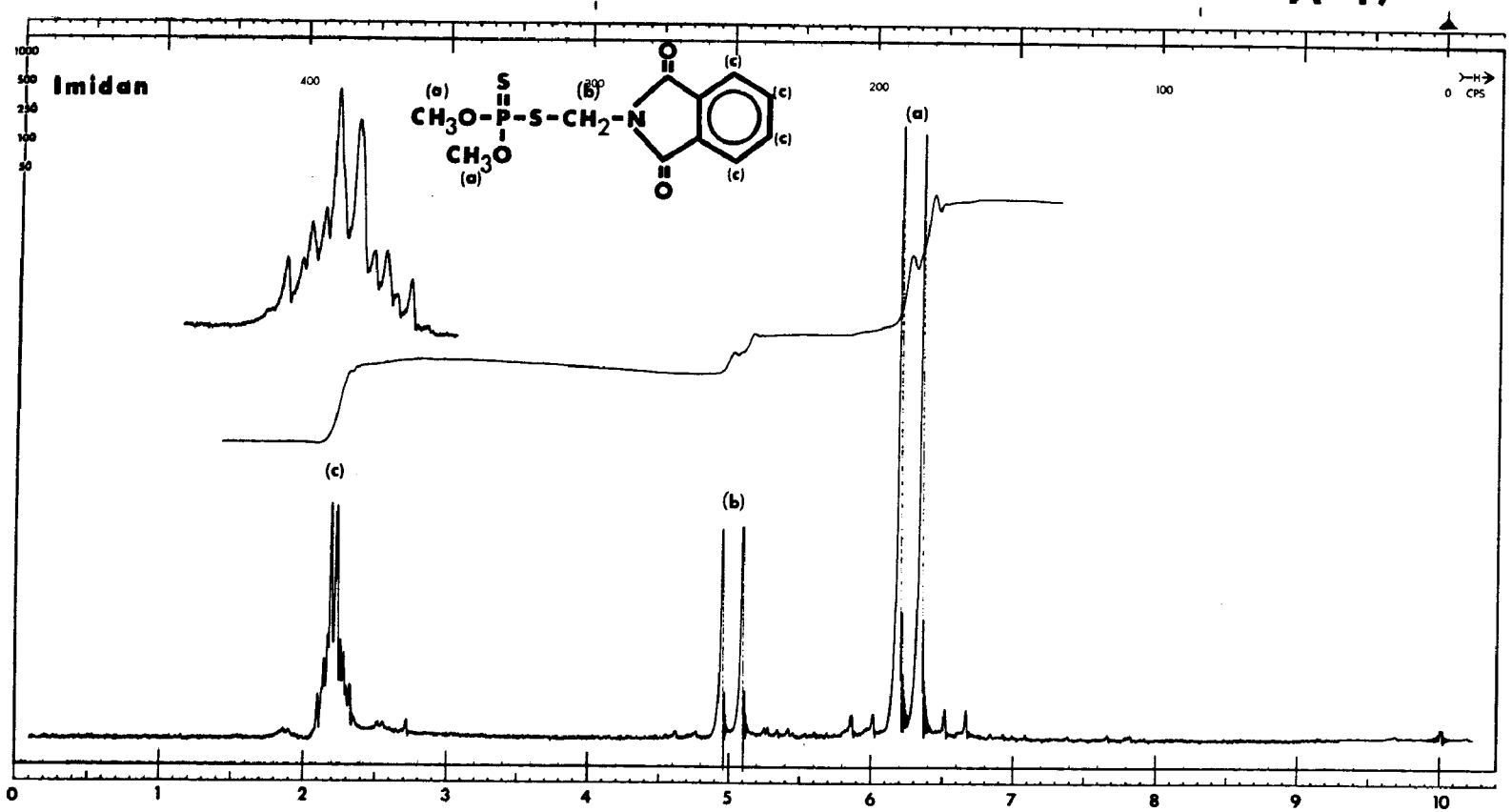

| | T | J |
|---|---|---|
| a | 6.24 | 15 |
| b | 4.23 | 16 |
| c | 1.9 | |

# A-16



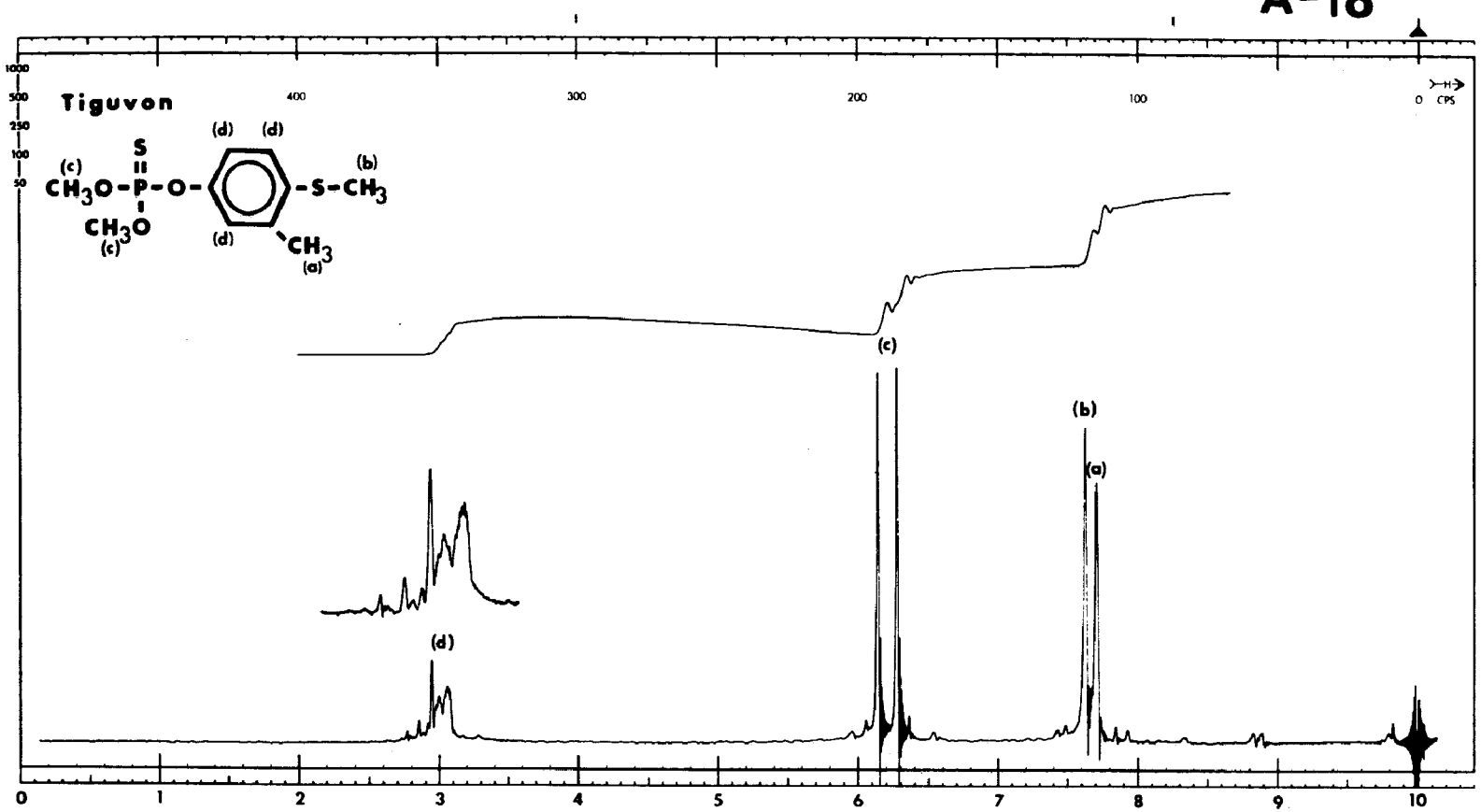

| | T | J |
|---|---|---|
| a | 6.19 | 13 |
| b | 4.20 | 15 |
| c | 2.0 | |

# A-17



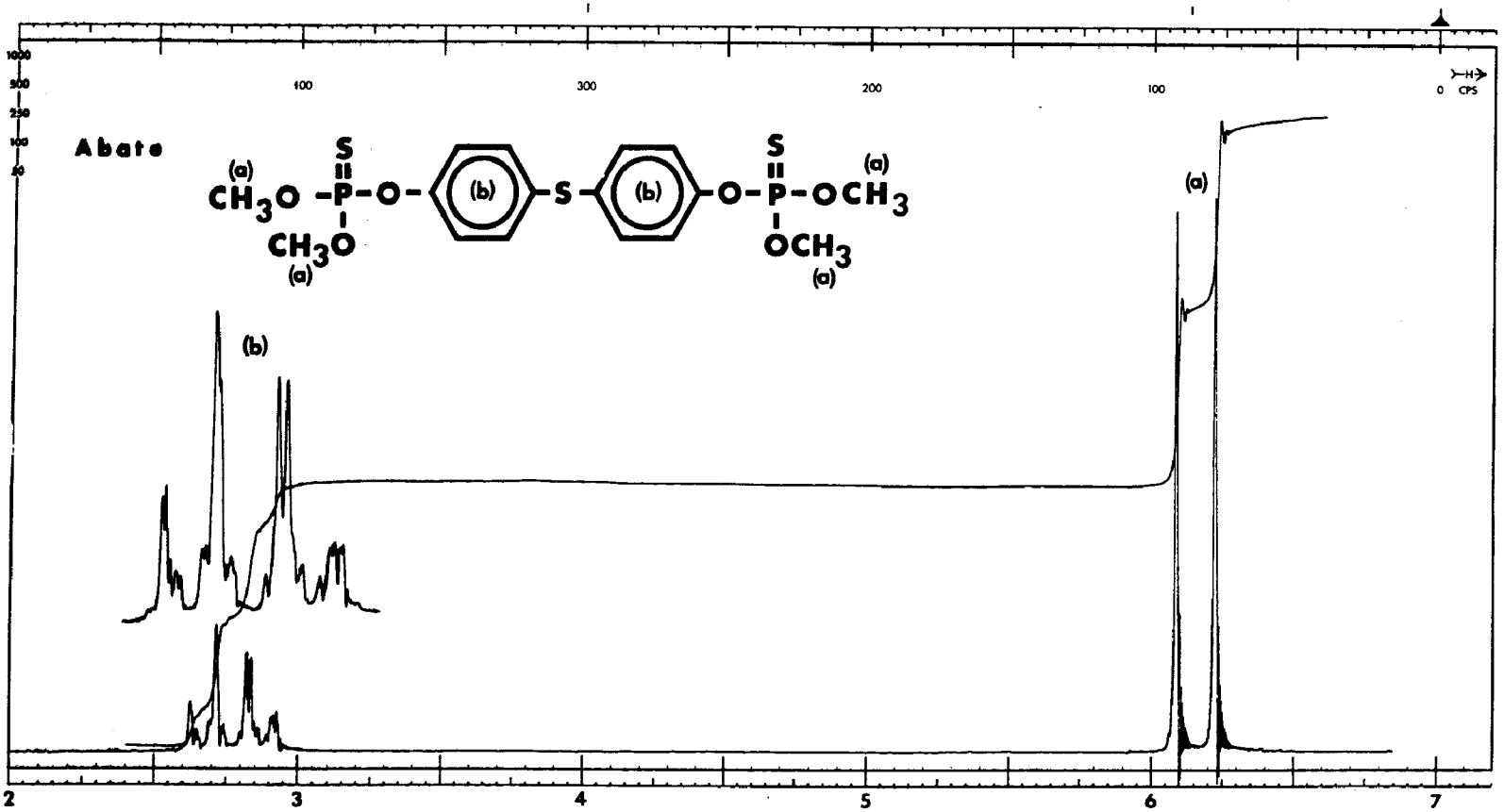

| | T | J |
|---|---|---|
| a | 6.23 | 15 |
| b | 4.98 | 15 |
| c | 2.18 | |

# A-18



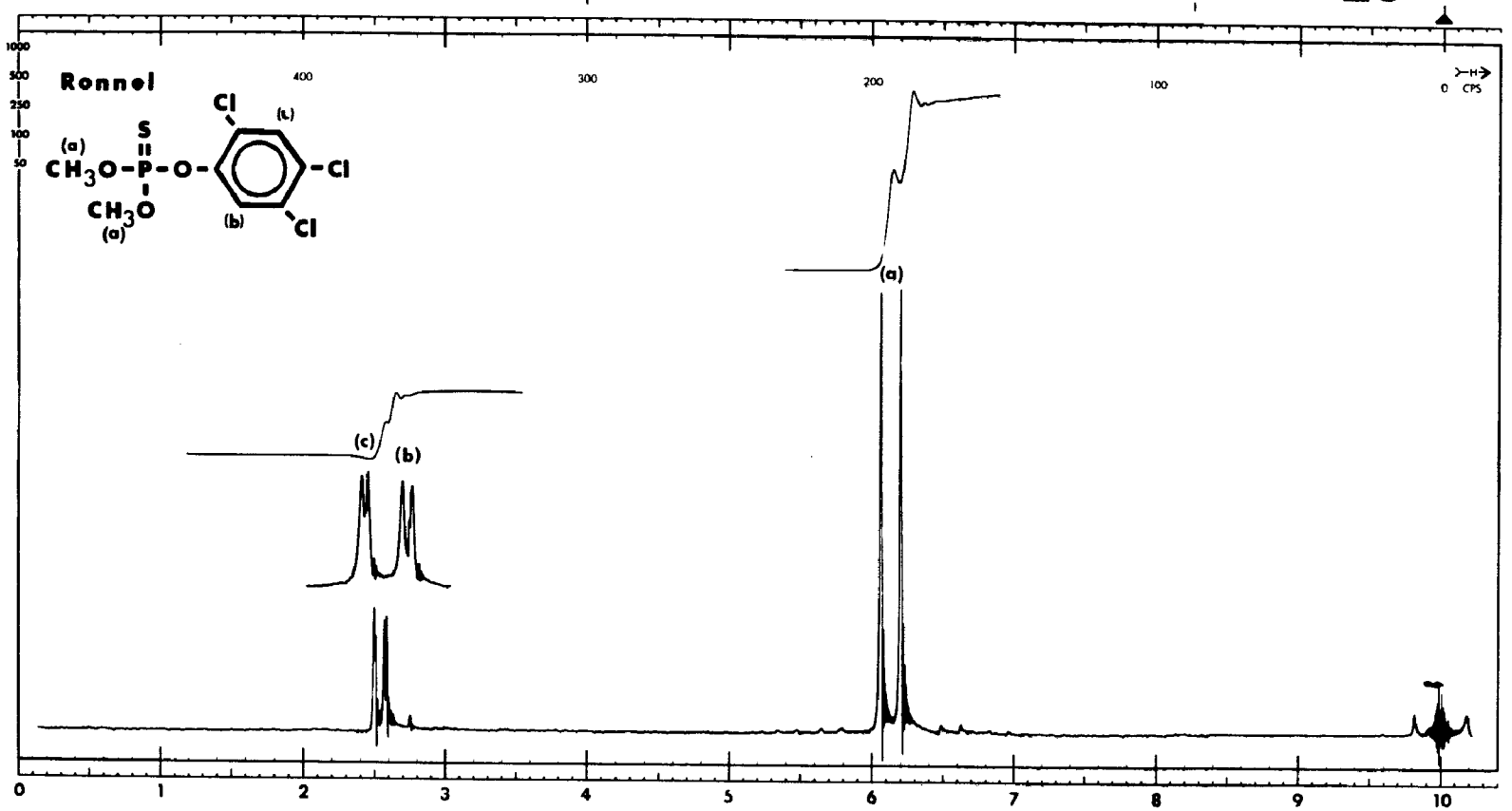

| | T | J |
|---|---|---|
| a | 7.68 | |
| b | 7.60 | |
| c | 6.19 | 14 |
| d | 3.0 | |

# A-19



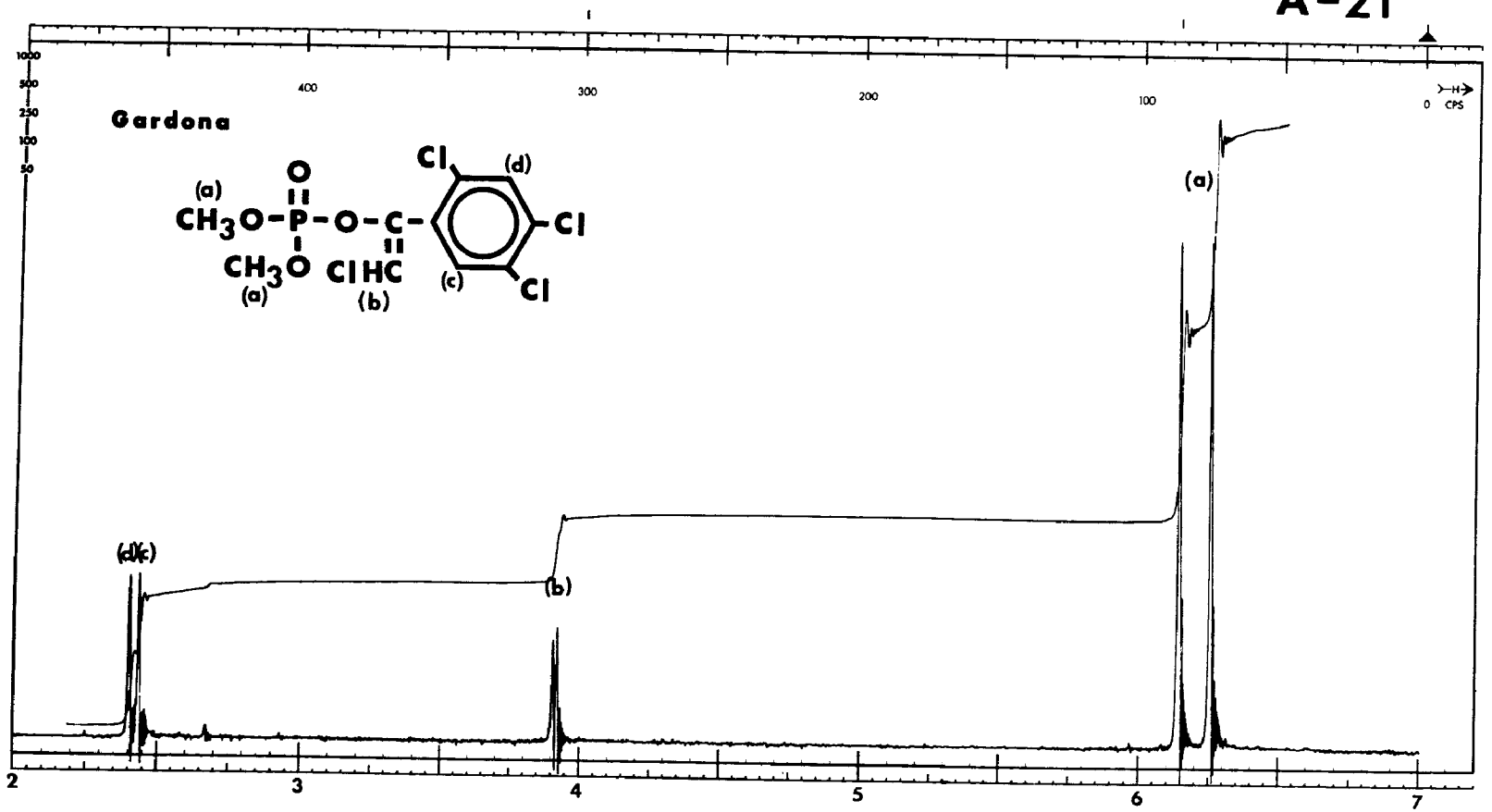

| | T | J |
|---|---|---|
| a | 6.17 | 14 (P-H) |
| b | 2.5 | |

# A-20



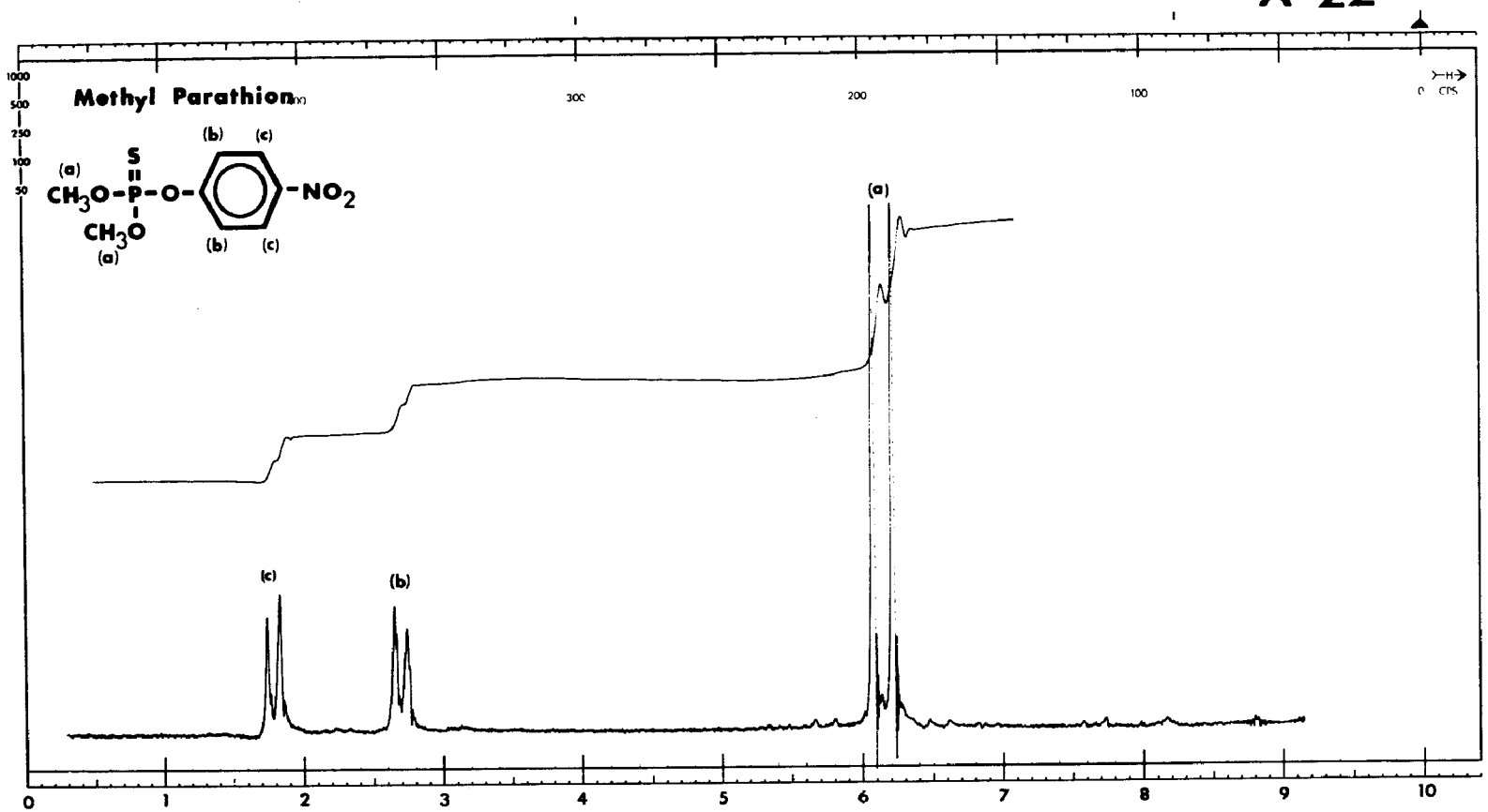

| | T | J |
|---|---|---|
| a | 6.10 | 14 |
| b | 2.55 | 1.8(P-H) |
| c | 2.47 | 1.0(P-H) |

# A-21



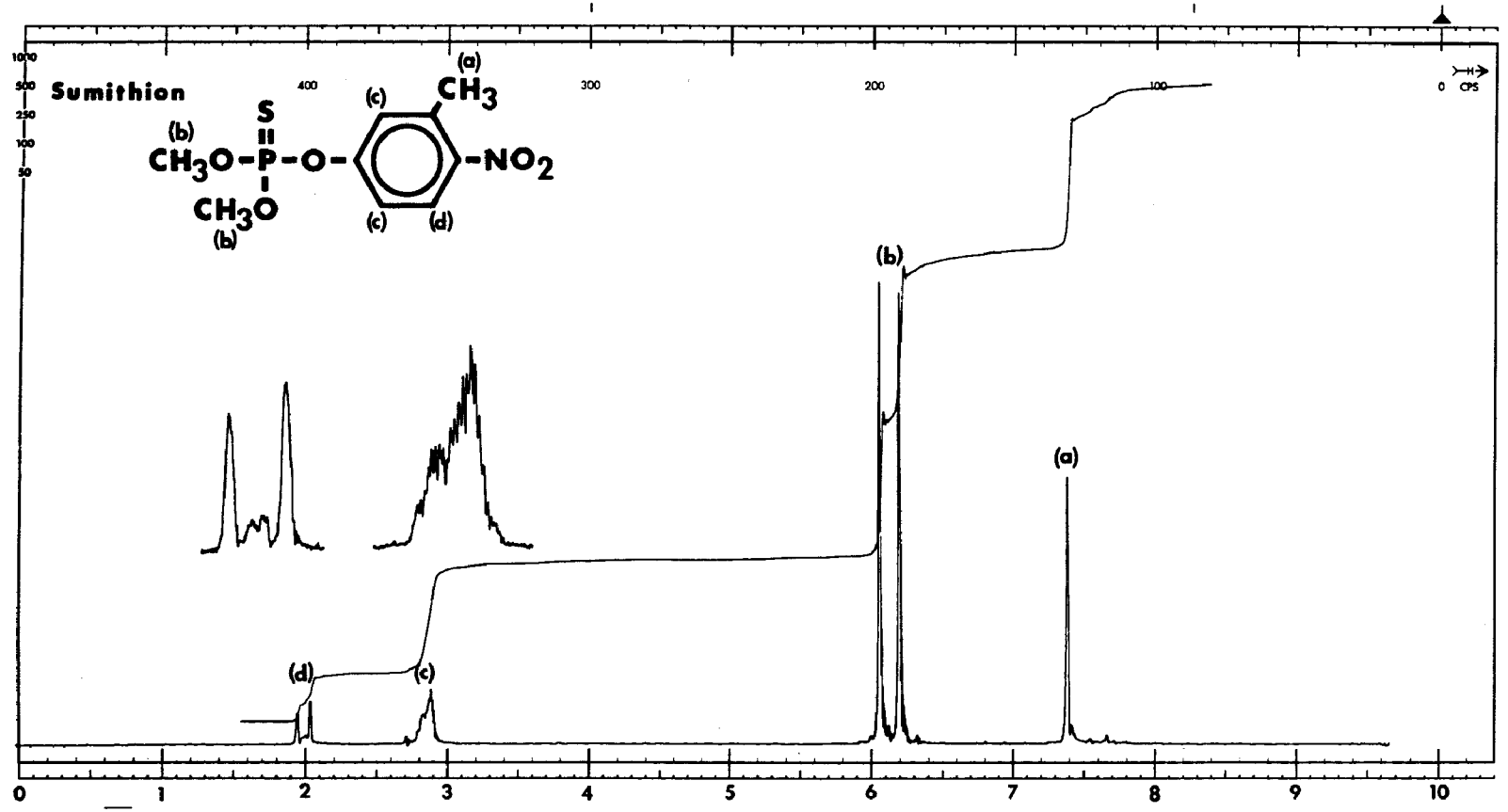

| | T | J |
|---|---|---|
| a | 6.21 | 11 (P-H) |
| b | 3.92 | 1.5 (P-H) |
| c | 2.46 | |
| d | 2.43 | |

# A-22



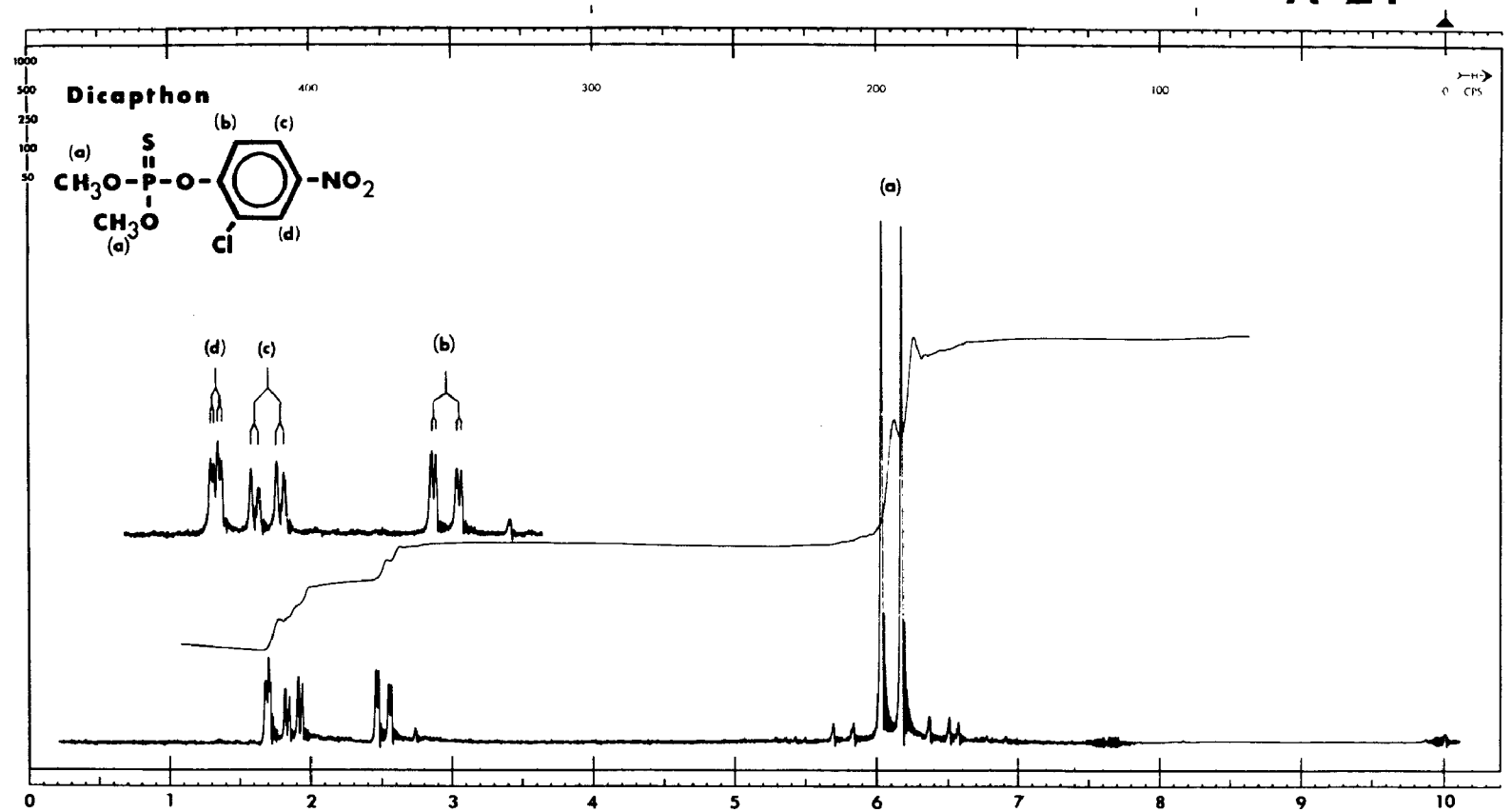

| | T | J |
|---|---|---|
| a | 6.13 | 14 |
| b | 2.70 | 9 |
| c | 1.78 | 9 |

# A-23



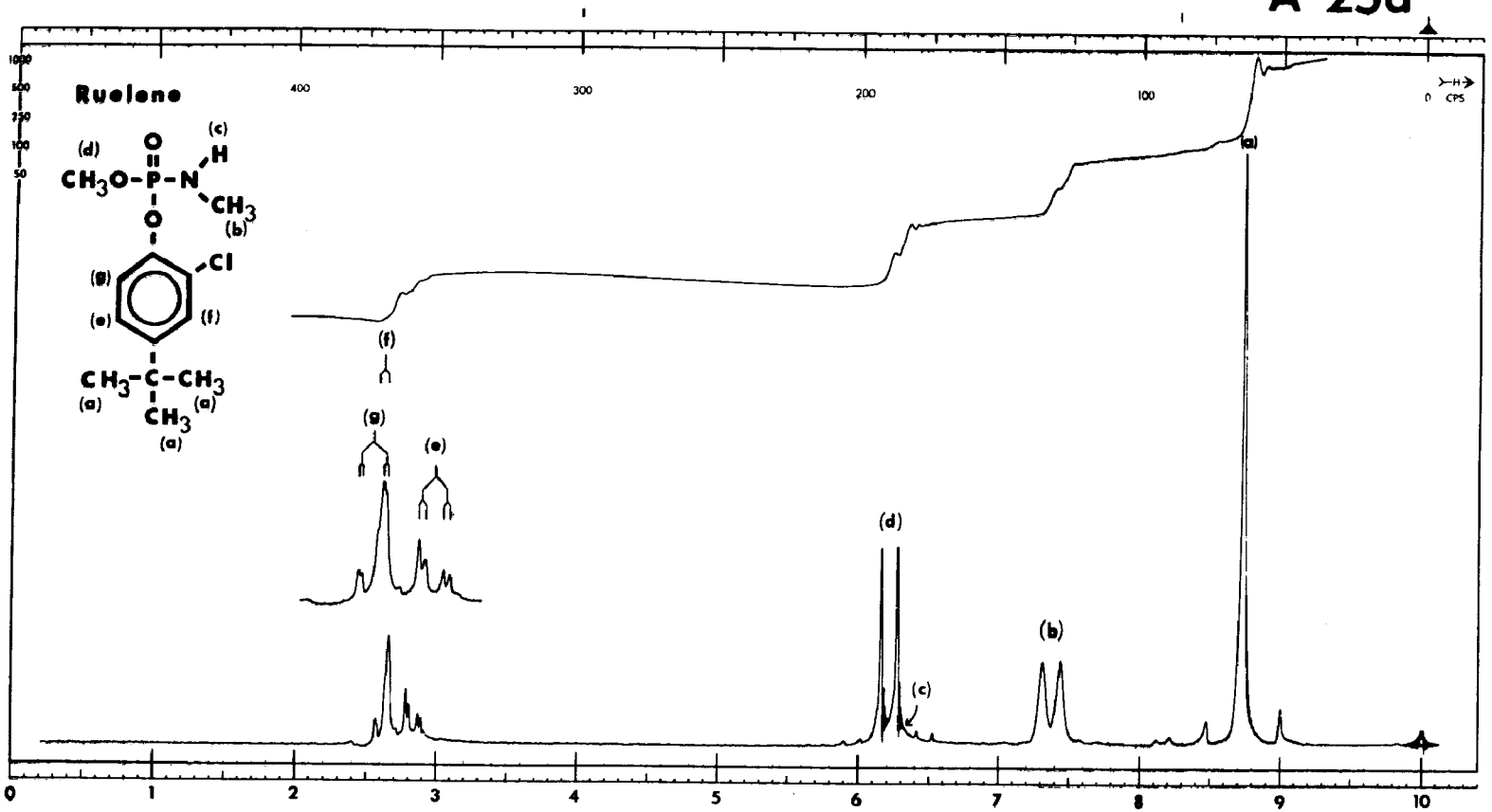

| | T | J |
|---|---|---|
| a | 7.38 | |
| b | 6.12 | 14 (P-H) |
| c | 2.84 | |
| d | 1.98 | |

# A-24

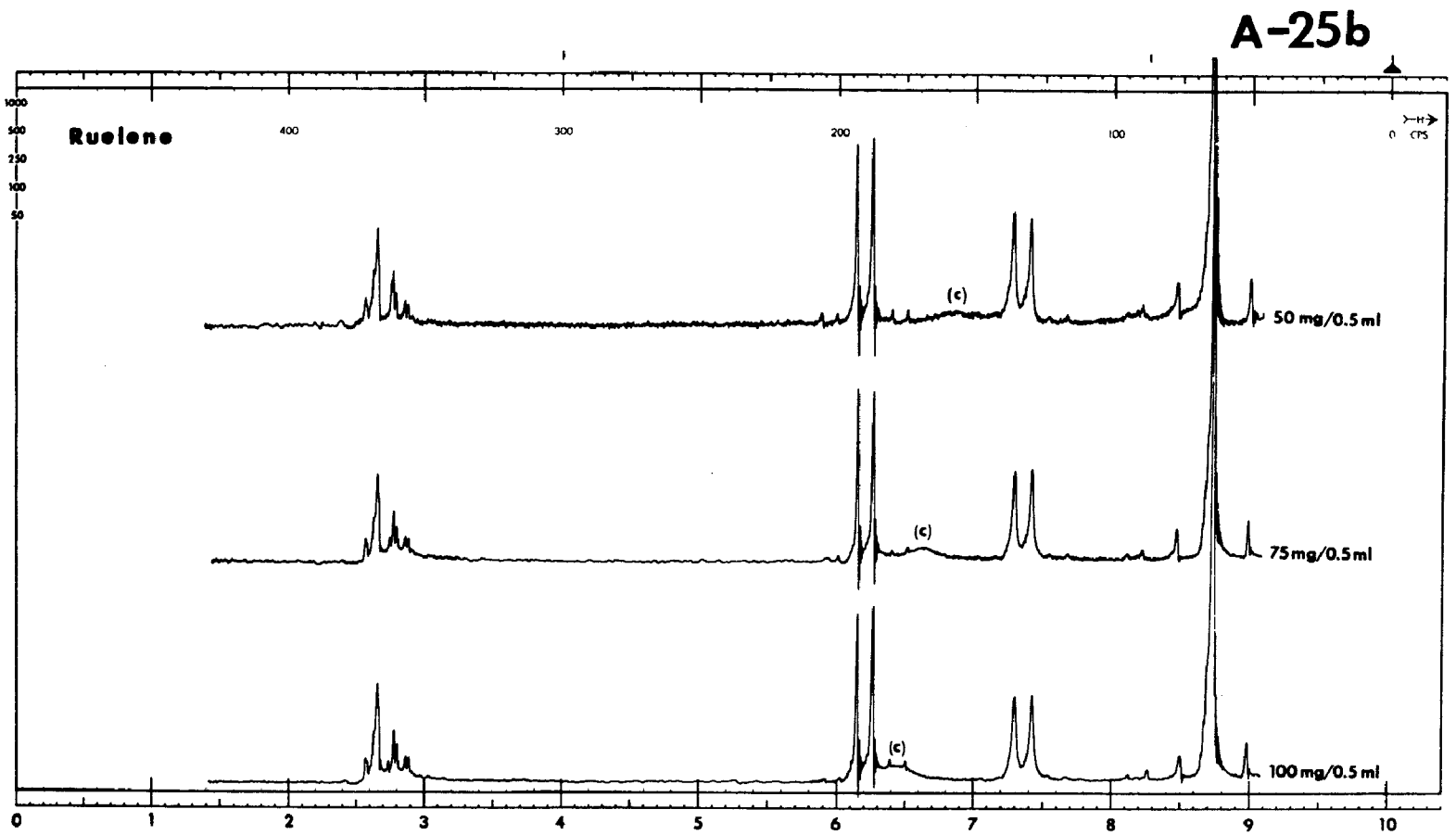


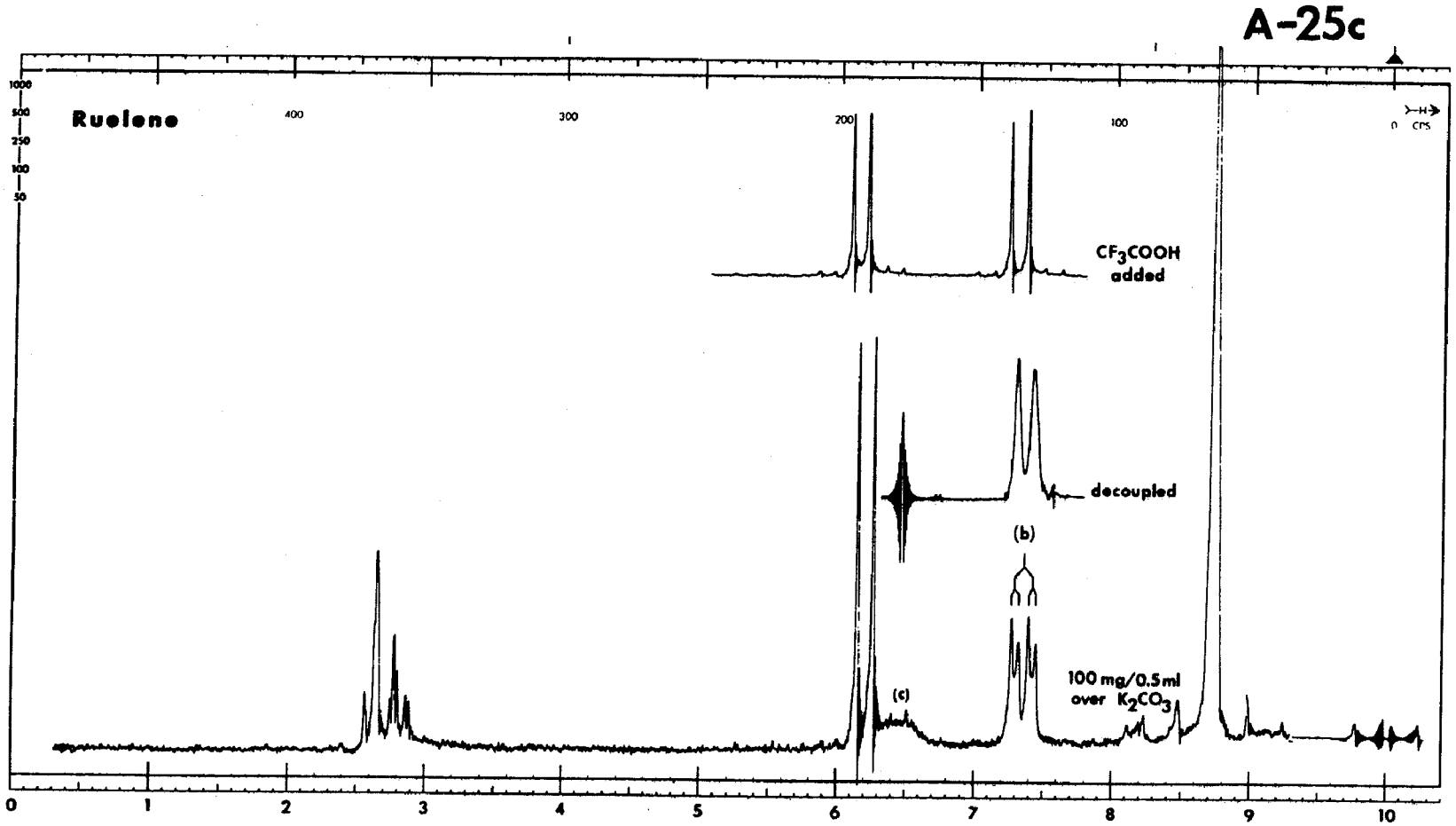

| | T | J |
|---|---|---|
| a | 6.08 | 14 |
| b | 2.49 | < 9 (H-H$_o$) / 1.5 (P-H) |
| c | 1.87 | < 9 (H-H$_o$) / 2.8 (H-H$_m$) |
| d | 1.68 | < 2.8 (H-H$_m$) / 1.2 (P-H) |

# A-25a

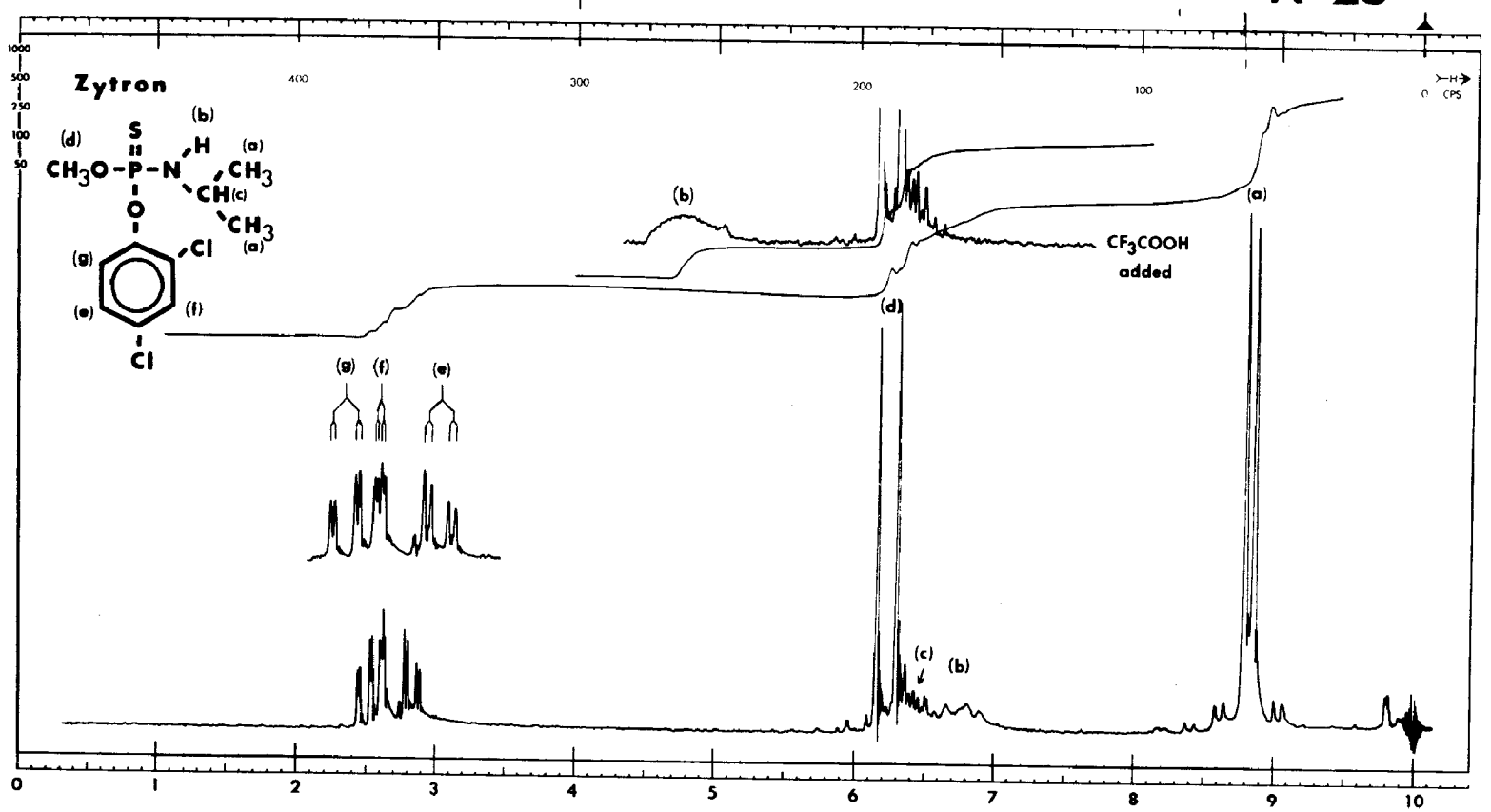



| | T | J |
|---|---|---|
| a | 8.72 | |
| b | 7.34 | < 13 (P-H) < 5 (H-H) |
| c | 6.2-6.7 | |
| d | 6.19 | 11 (P-H) |
| e | 2.80 | < 9 ($H-H_o$) < 2.5 ($H-H_m$) |
| f | 2.62 | 2.5 ($H-H_m$) |
| g | 2.57 | < 9 ($H-H_o$) < 1.0 (P-H) |

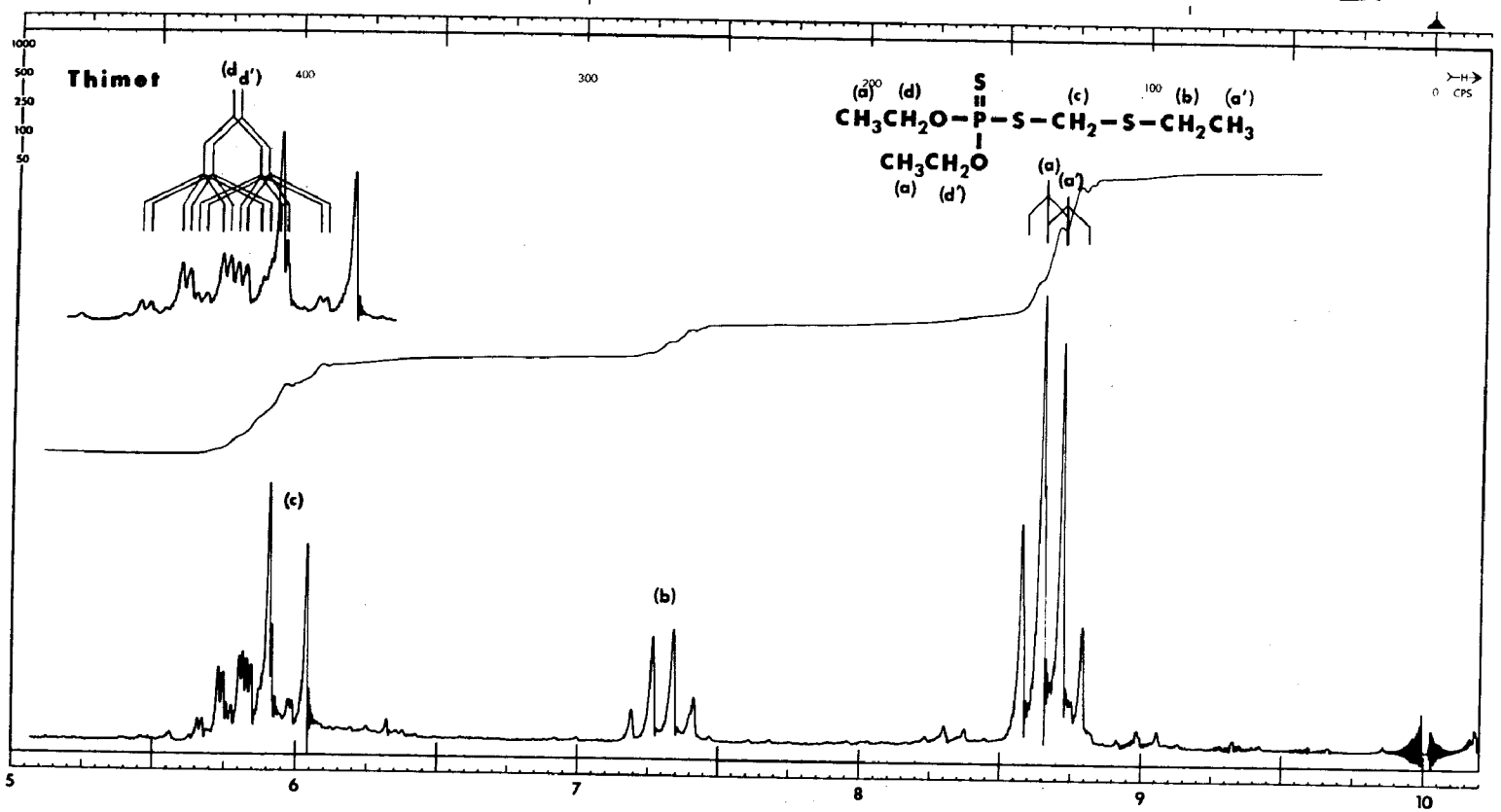

A-25b
Ruelene
400
300
200
100
0 CPS
(c)
50 mg/0.5 ml
(c)
75 mg/0.5 ml
(c)
100 mg/0.5 ml
0
1
2
3
4
5
6
7
8
9
10


A-25c
Ruelene
400
300
200
100
0 CPS
1000
500
250
100
50
$CF_3COOH$ added
decoupled
(b)
(c)
100 mg/0.5 ml over $K_2CO_3$
0
1
2
3
4
5
6
7
8
9
10

# A-26

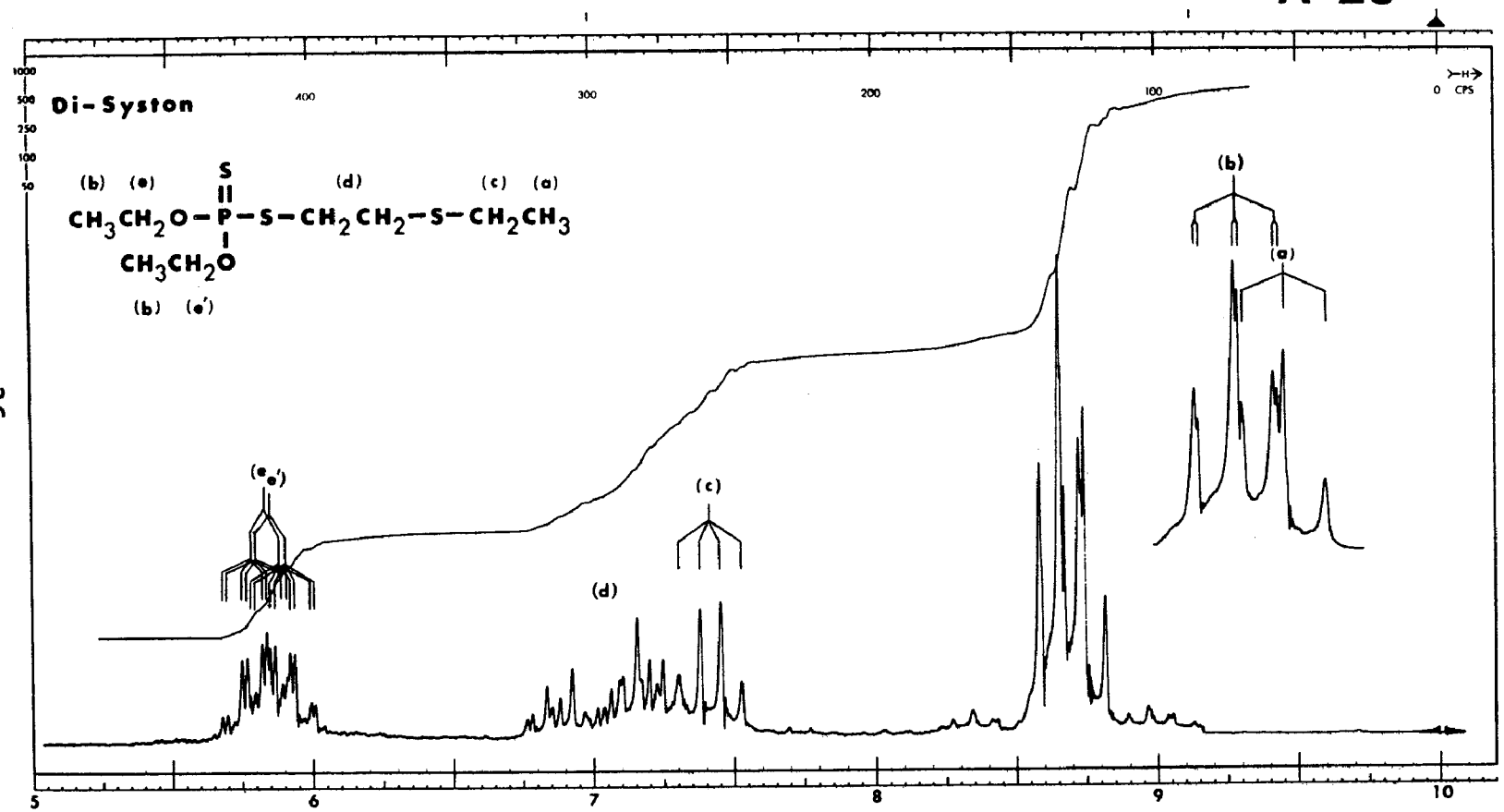



| | T | J |
|---|---|---|
| a | 8.81 | 6.5 |
| b | 6.8 | |
| c | 6.3 | |
| d | 6.20 | 14 |
| e | 2.81 | $< \frac{9\ (H\text{-}H_o)}{2.5\ (H\text{-}H_m)}$ |
| f | 2.59 | $< \frac{2.5\ (H\text{-}H_m)}{1.0\ (P\text{-}H^{-})}$ |
| g | 2.46 | $< \frac{9\ (H\text{-}H_o)}{1.3\ (P\text{-}H^{-})}$ |



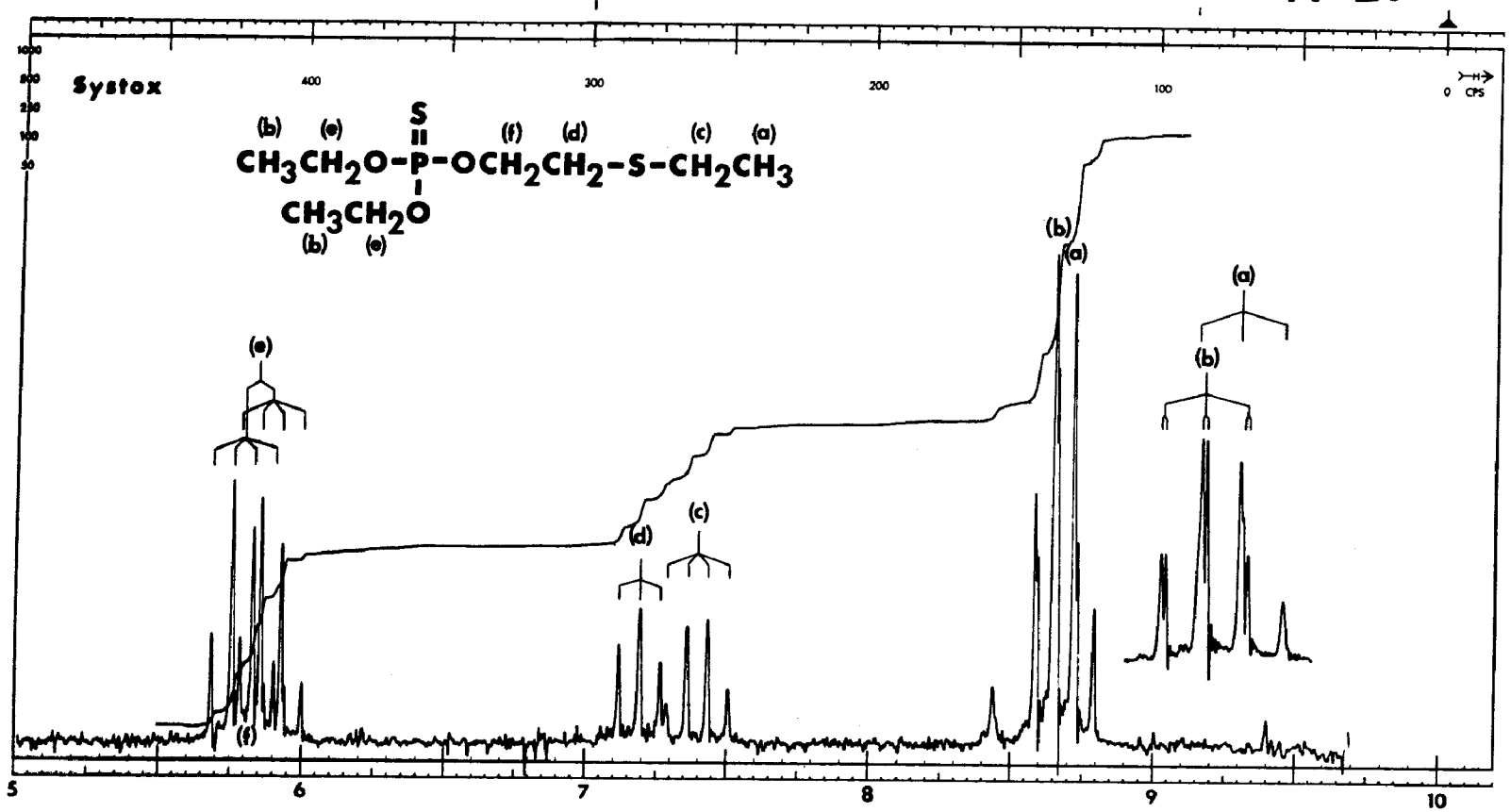

| | T | J |
|---|---|---|
| a | 8.64 | 7 (H-H) / 0.8 (P-H) |
| a' | 8.71 | 7 |
| b | 7.30 | 7 |
| c | 5.97 | 13 (P-H) |
| d | 5.815 | 10 (P-H) / 7 (H-H) |
| d' | 5.83 | |

# A-28



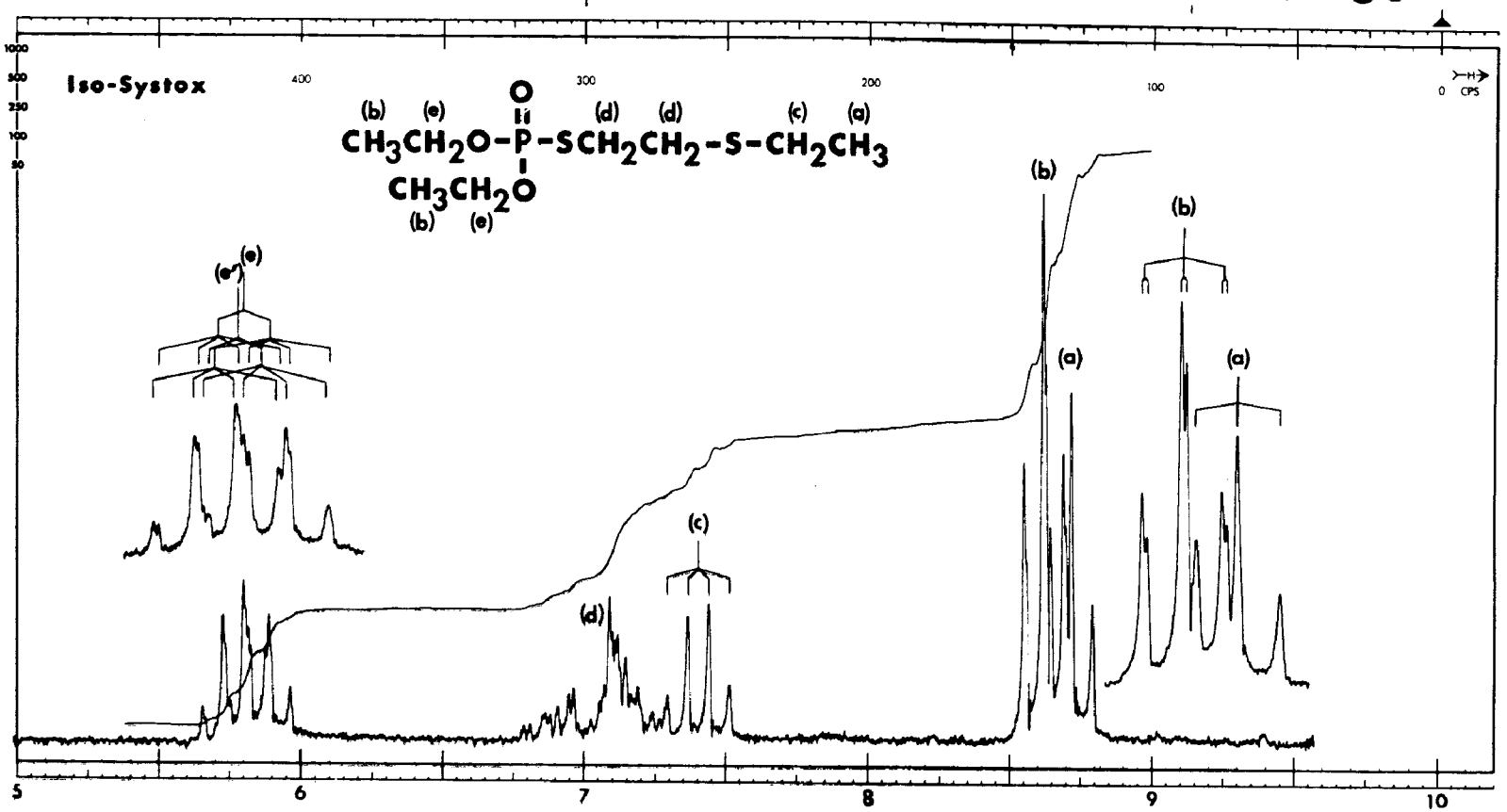

| | T | J |
|---|---|---|
| a | 8.73 | 7.5 |
| b | 8.65 | 7 (H-H), 0.7 (P-H) |
| c | 7.40 | 7.5 |
| d | 6.5-7.5 | |
| e | 5.83 | 10 (P-H) |
| e' | 5.85 | 7 (H-H) |

# A-29



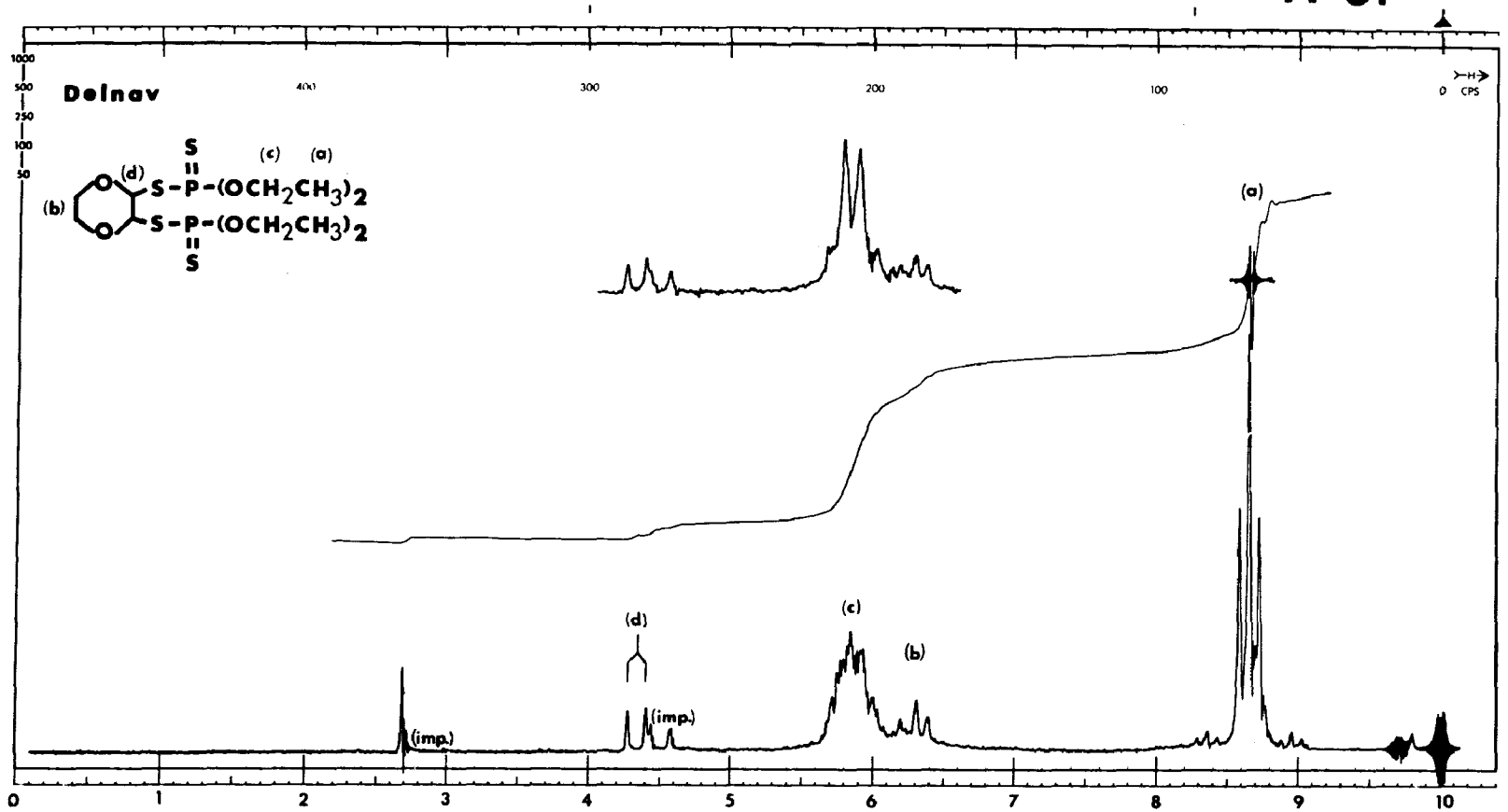

| | T | J |
|---|---|---|
| a | 8.73 | 7.5 |
| b | 8.67 | 7 (H-H), 0.9 (P-H) |
| c | 7.41 | 7.5 |
| d | 7.20 | 7 |
| e | 5.86 | 7 (H-H), 10 (P-H) |
| f | 5.8 | |

# A-30



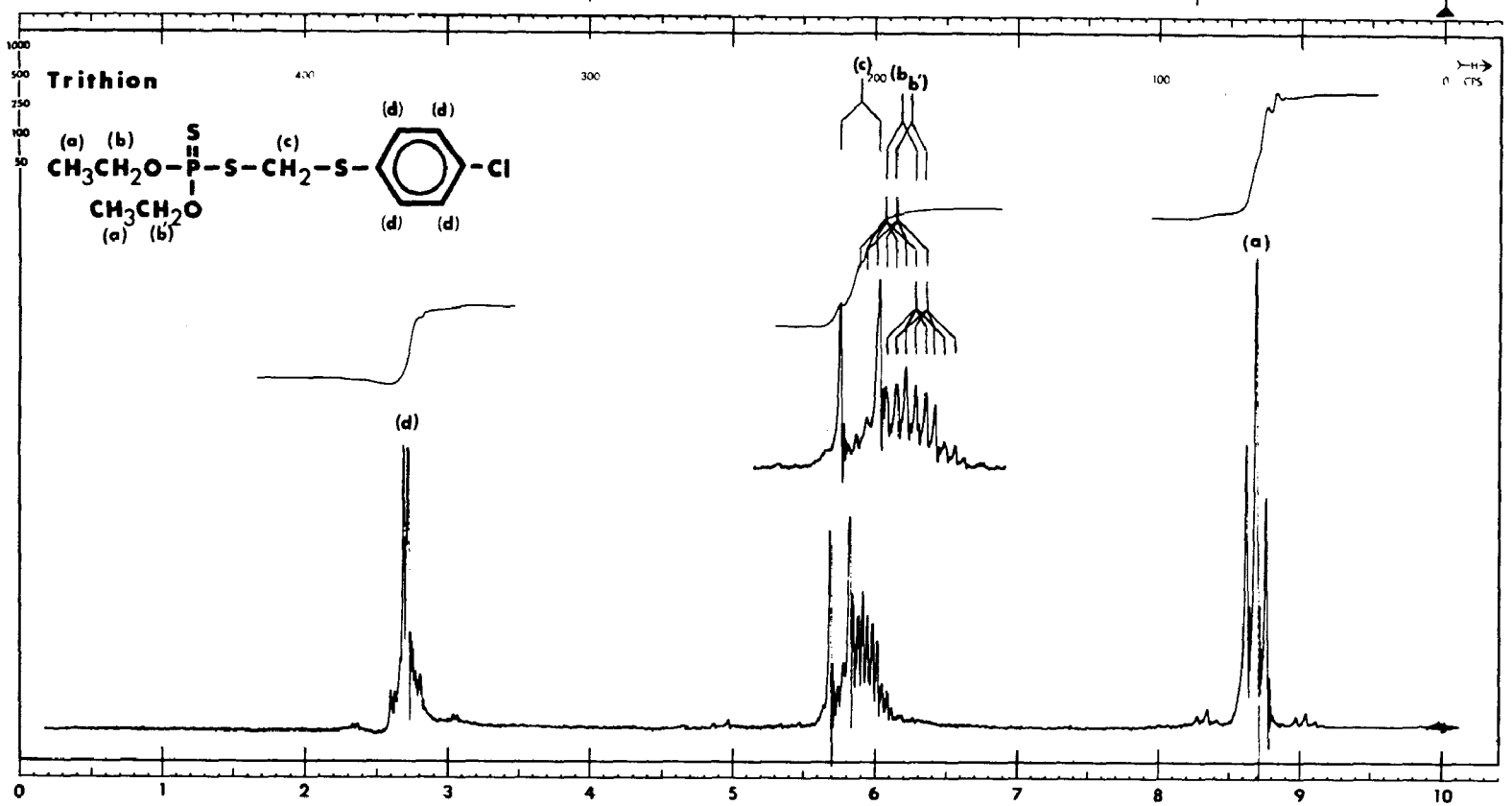

| | T | J |
|---|---|---|
| a | 8.73 | 7.5 |
| b | 8.62 | 7 (H-H), 0.9 (P-H) |
| c | 7.40 | 7.5 |
| d | 7.0 | |
| e | 5.82 | 7 (H-H), 9 (P-H) |
| e | 5.81 | |

# A-31



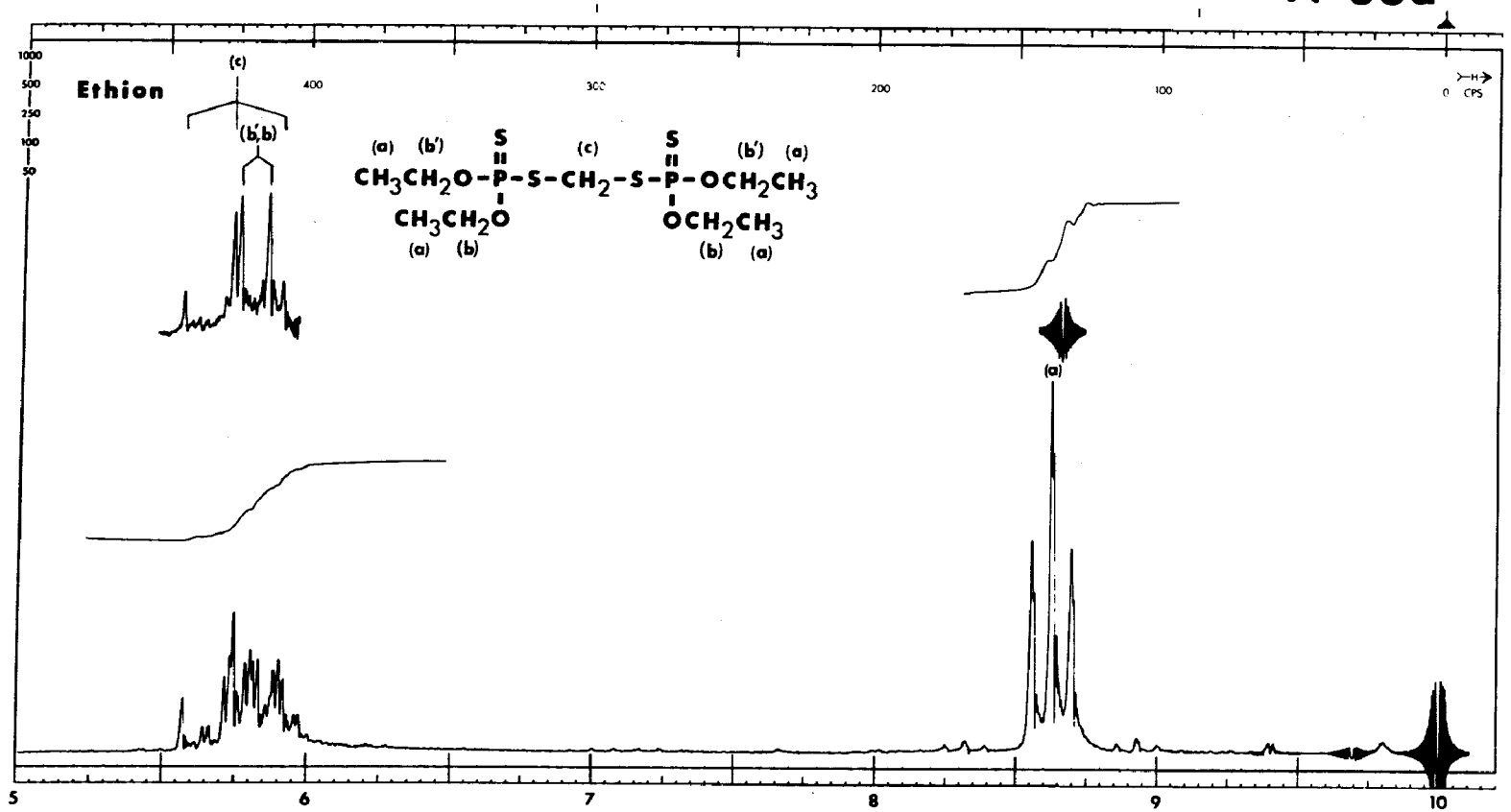

| | T | J |
|---|---|---|
| a | 8.64 | 7 |
| b | 6.3 | |
| c | 5.83 | 10 (P-H) |
| d | 4.32 | 13 |

# A-32



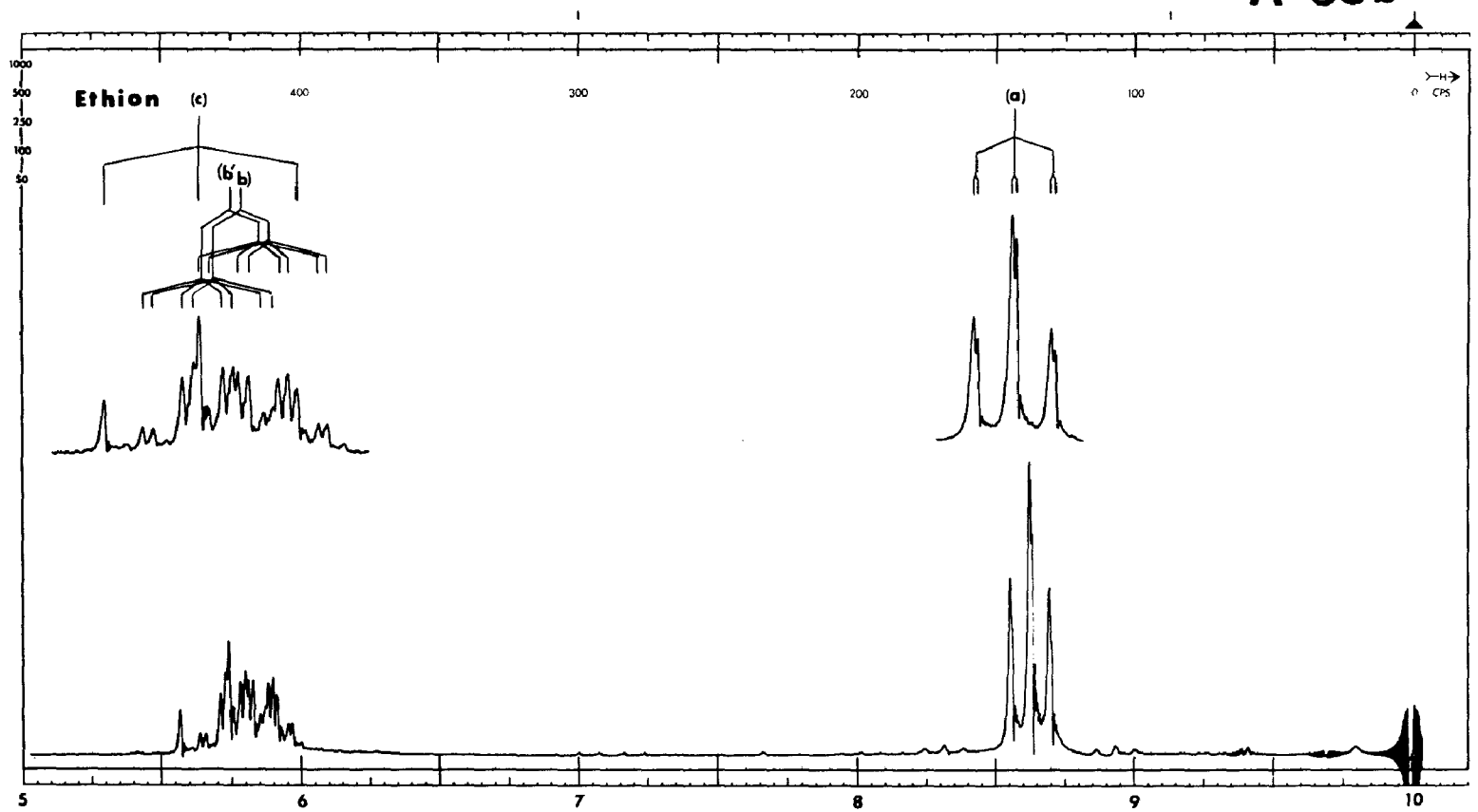

| | T | J |
|---|---|---|
| a | 8.67 | 7 |
| b | 5.88 | 10(P-H) |
| b | 5.91 | 7 (H-H) |
| c | 5.72 | 13.5(P-H) |
| d | 2.68 | |

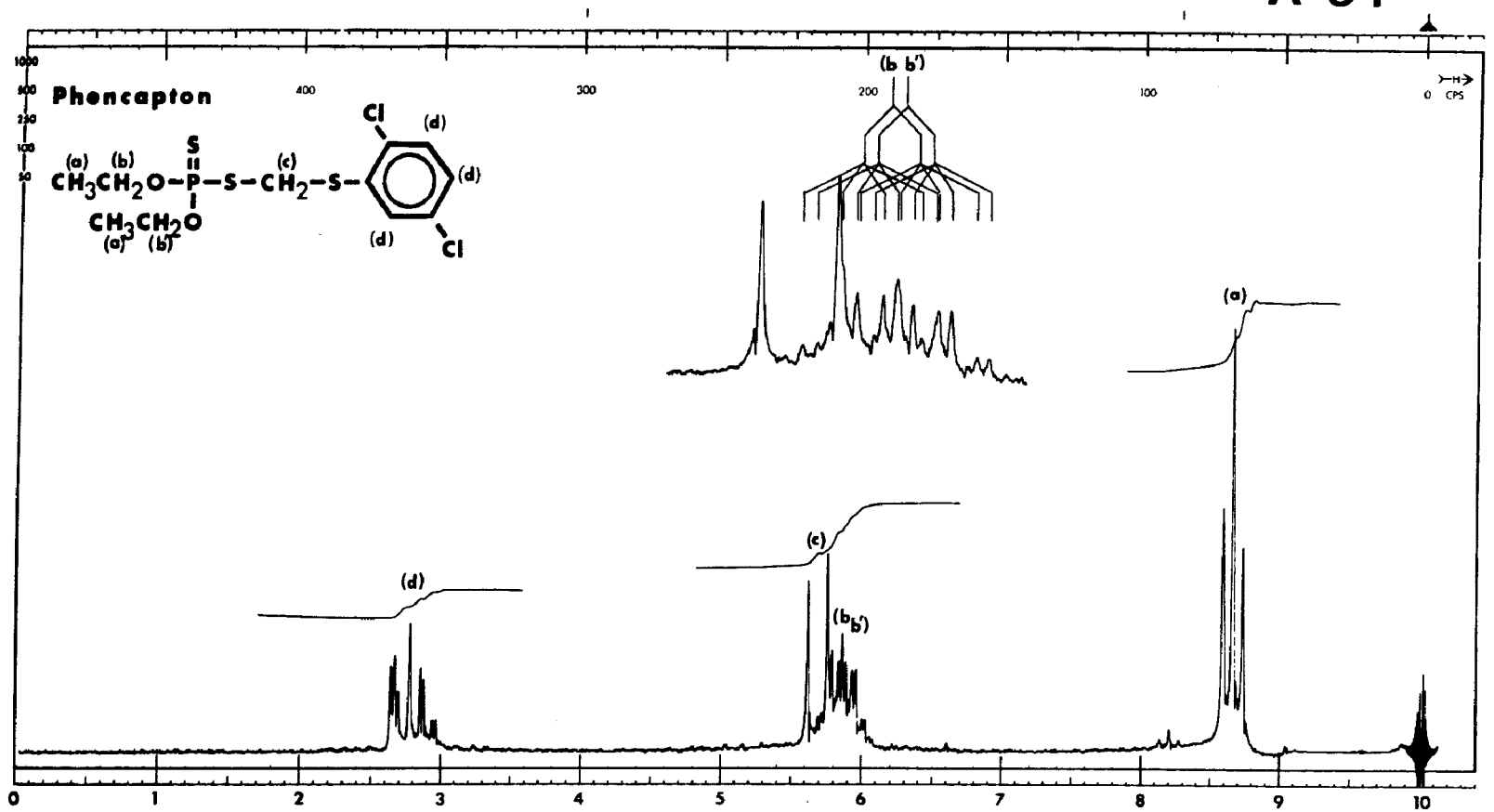
# A-33a




| | T | J |
|---|---|---|
| a | 8.62 | < 7 (H-H), 0.8 (P-H) |
| b | 5.82 | < 7 (H-H), 10 (P-H) |
| b' | 5.80 | < 7 (H-H), 10 (P-H) |
| c | 5.74 | 17 (P-H) |

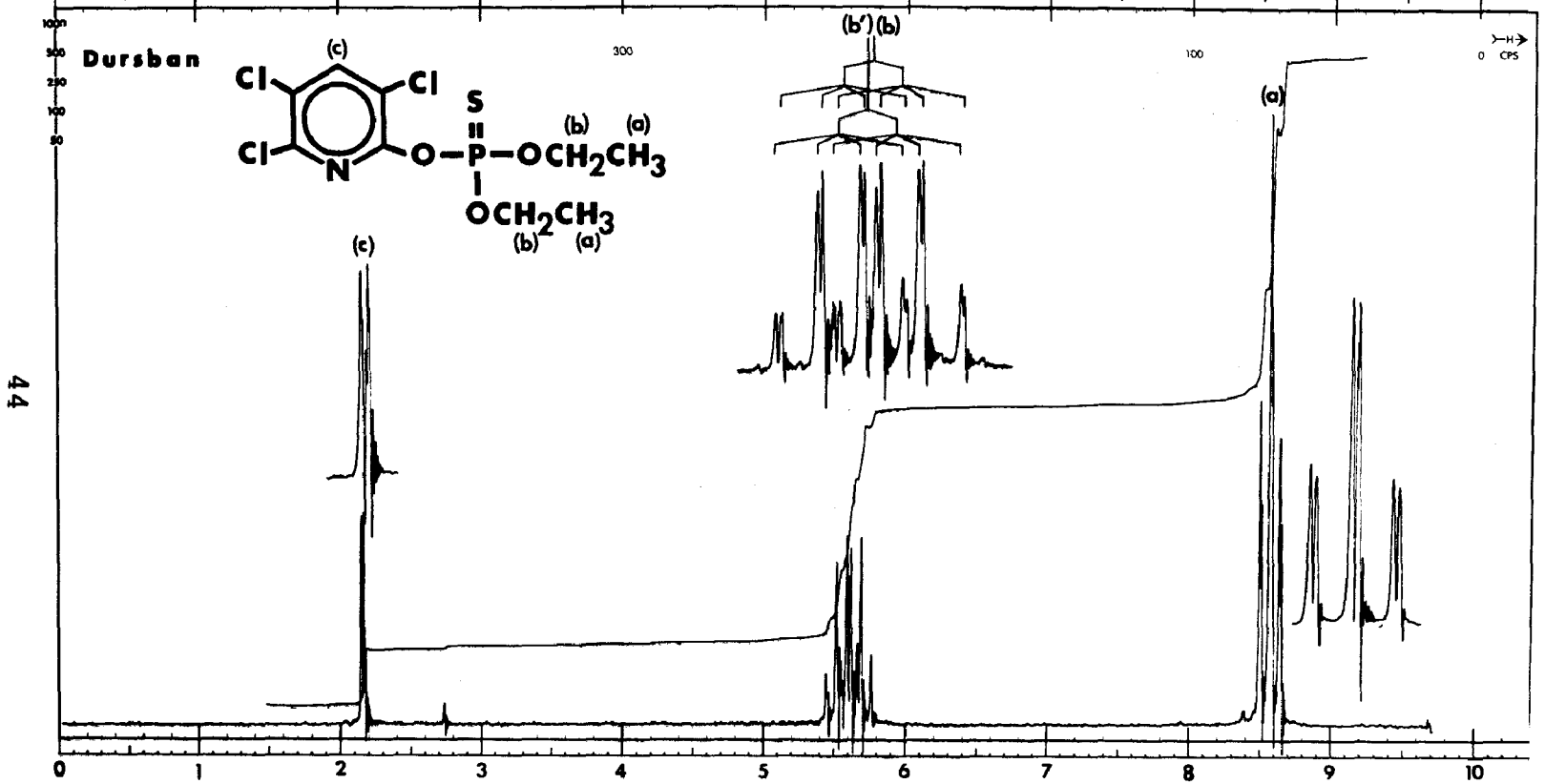
A-33b





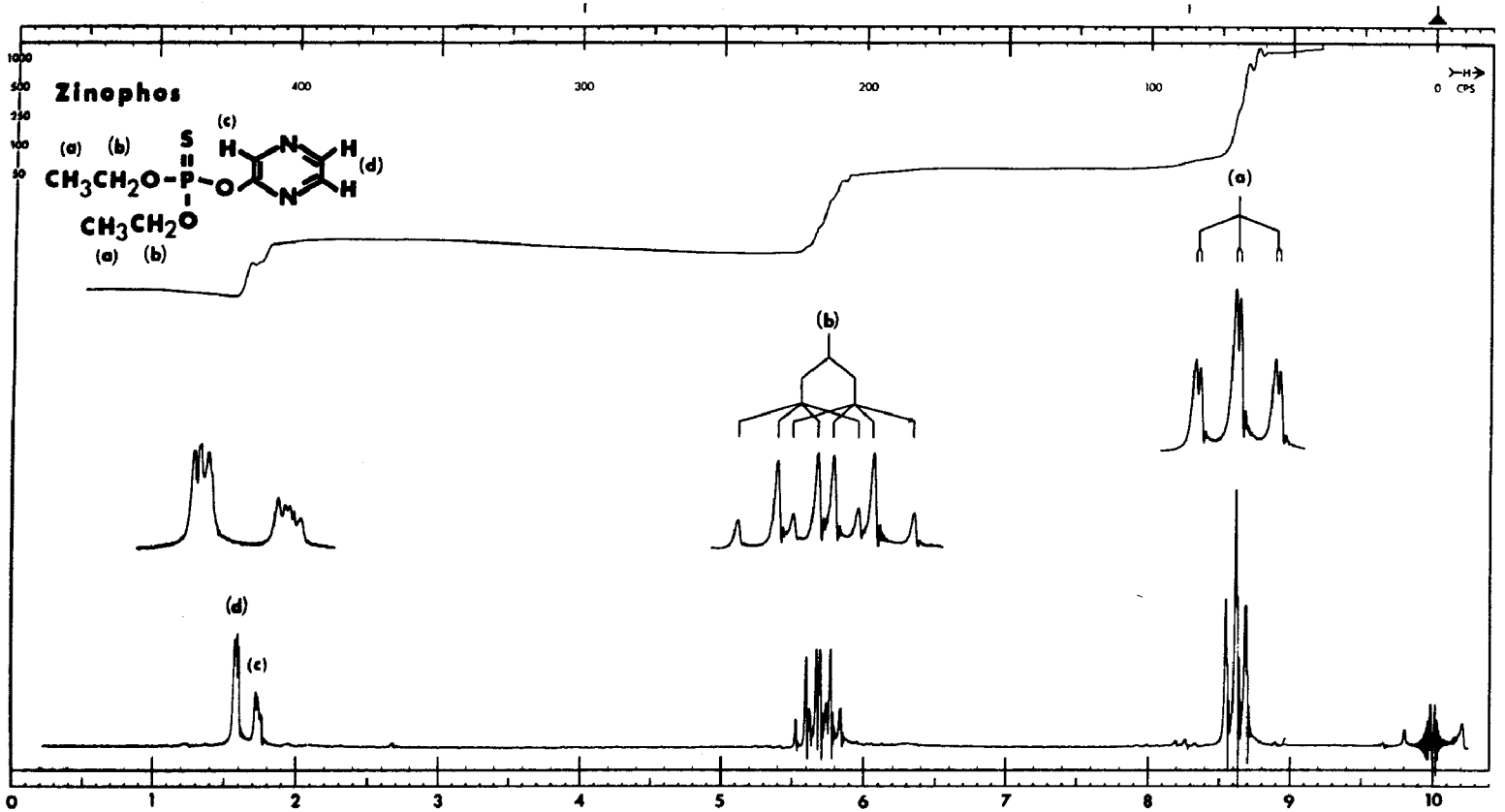

| | T | J |
|---|---|---|
| a | 8.64 | 7 |
| b | 5.82 | 10 (P-H) |
| b' | 5.84 | 7 (H-H) |
| c | 5.66 | 14 |
| d | 2.8 | |

# A-35

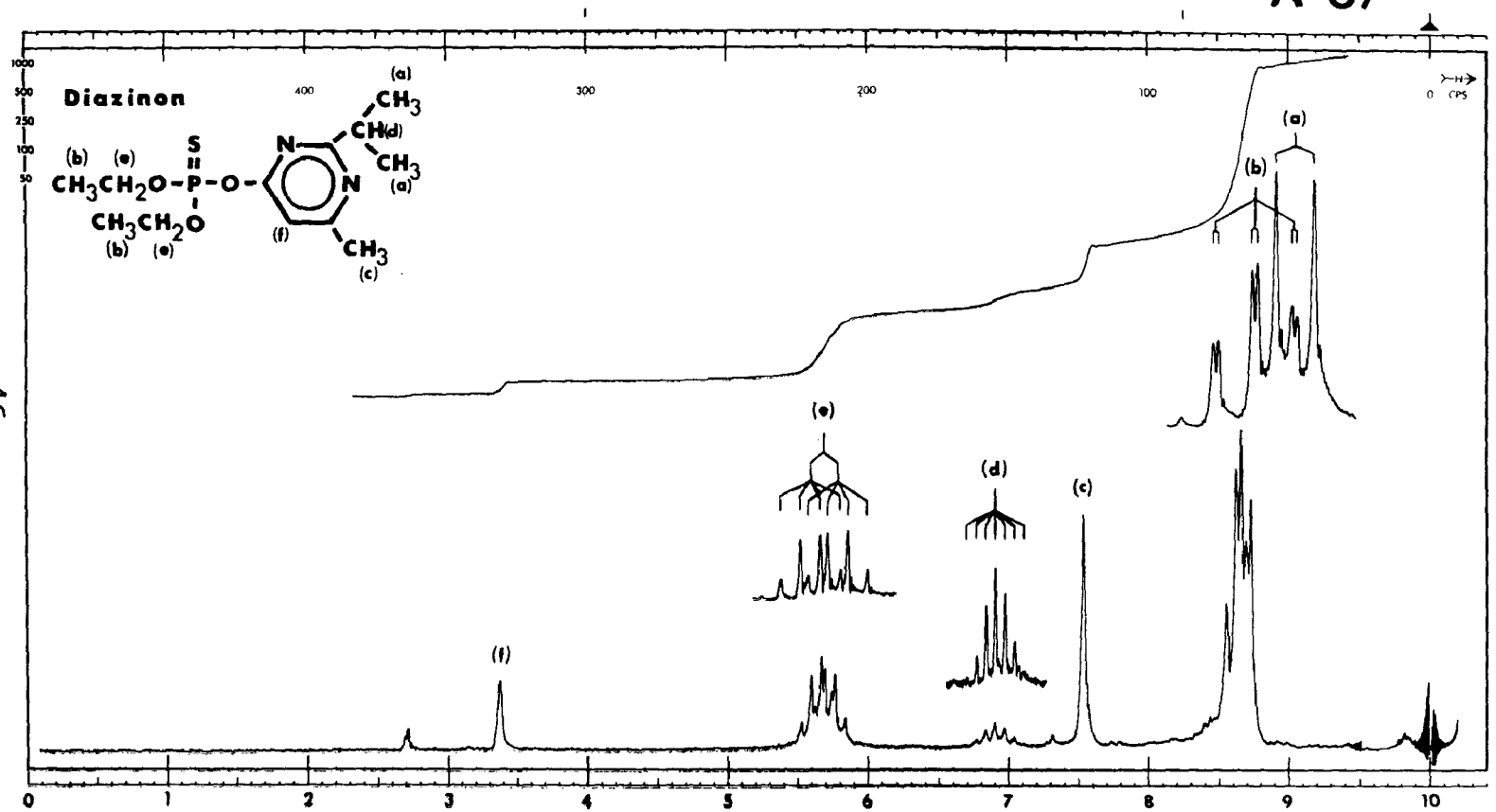



| | T | J |
|---|---|---|
| a | 8.59 | 7 (H-H), 1 (P-H) |
| b | 5.61 | 7 (H-H), 10 (P-H) |
| b′ | 5.60 | |
| c | 2.16 | 1.2 (P-H) |

# A-36

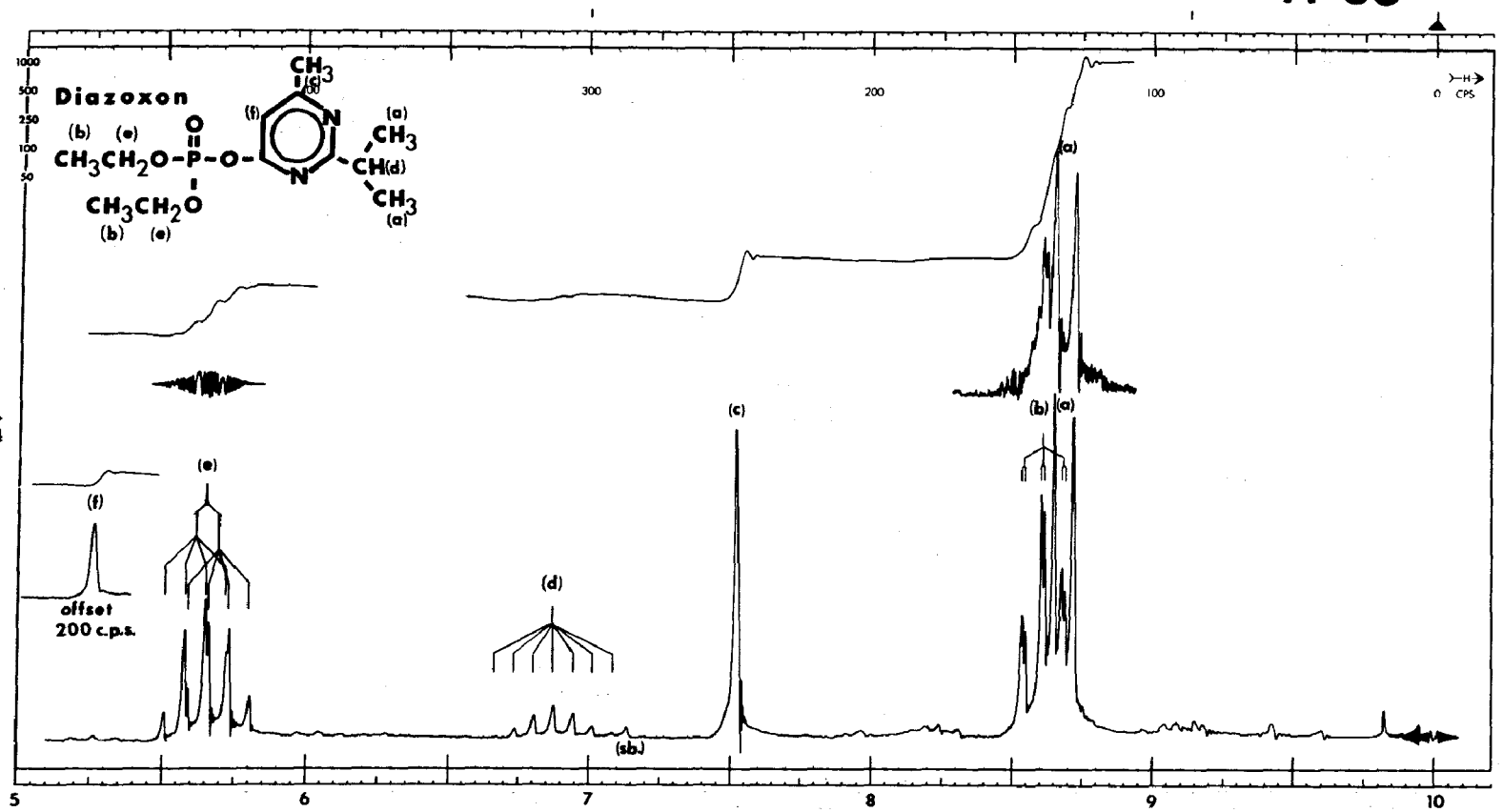



| | T | J |
|---|---|---|
| a | 8.59 | 7 (H-H), 0.8 (P-H) |
| b | 5.65 | 9 (P-H), 7 (H-H) |
| c | 1.72 | |
| d | 1.67 | |



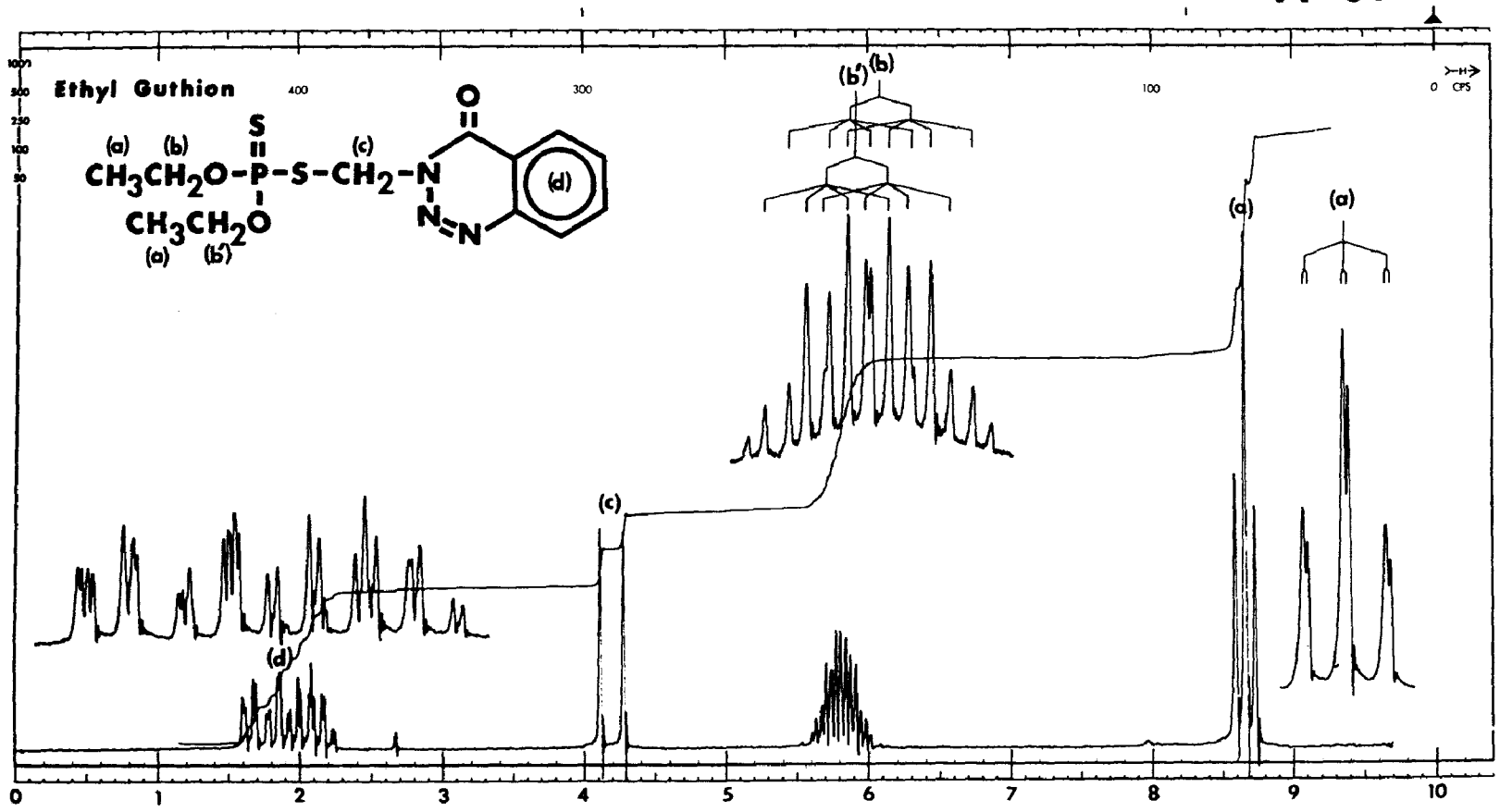

| | T | J |
|---|---|---|
| a | 8.68 | 7 |
| b | 8.62 | ≃ 7 (H-H) ≃ 0.8 (P-H) |
| c | 7.51 | |
| d | 6.88 | 7 |
| e | 5.66 | ≃ 9.5 (P-H) ≃ 7 (H-H) |
| f | 3.34 | |

# A-38



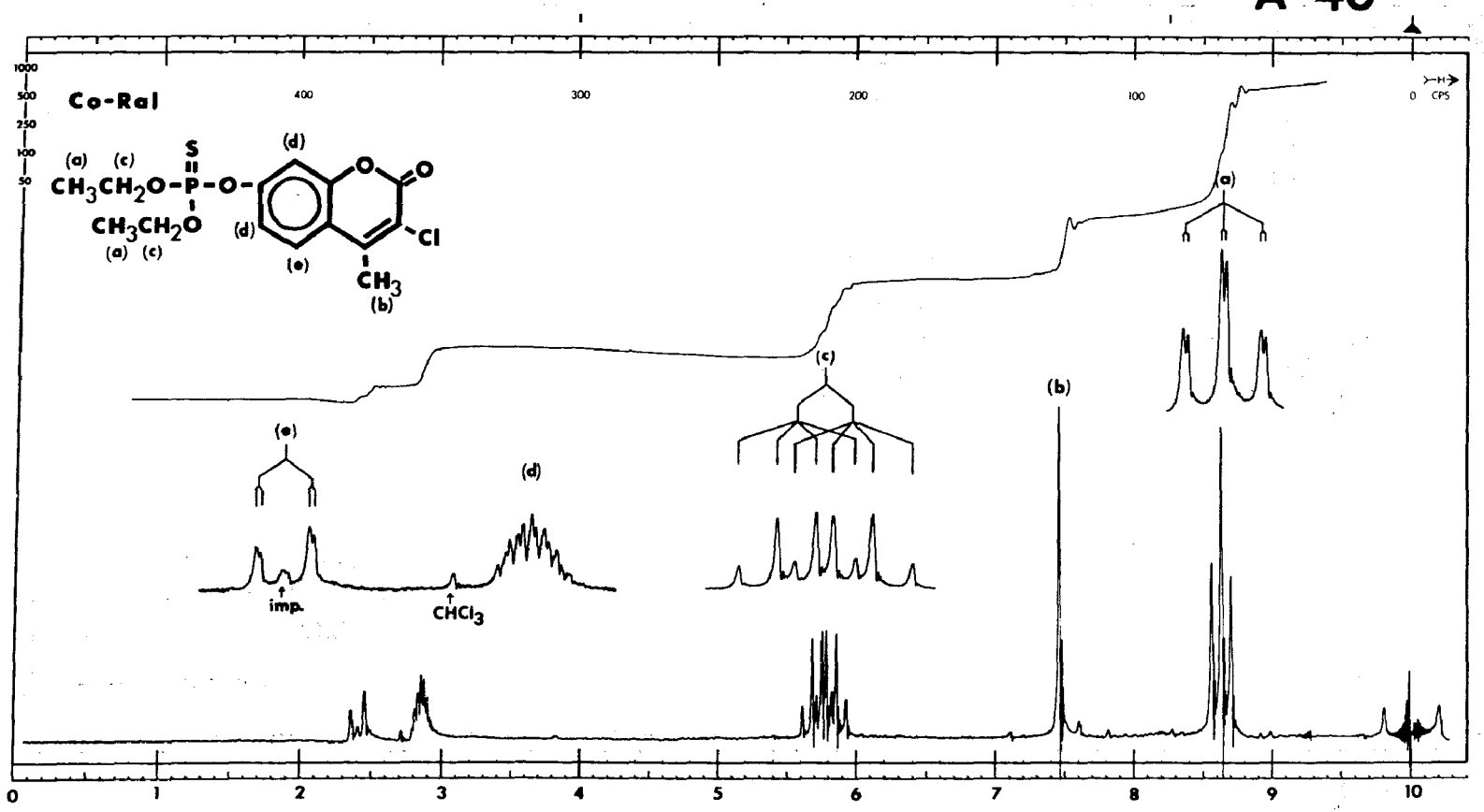

| | T | J |
|---|---|---|
| a | 8.68 | 7 |
| b | 8.61 | < 7 (H-H) < 1.2 (P-H) |
| c | 7.51 | |
| d | 6.87 | 7 |
| e | 5.65 | < 7 (H-H) < 8 (P-H) |
| f | 3.26 | |

# A-39



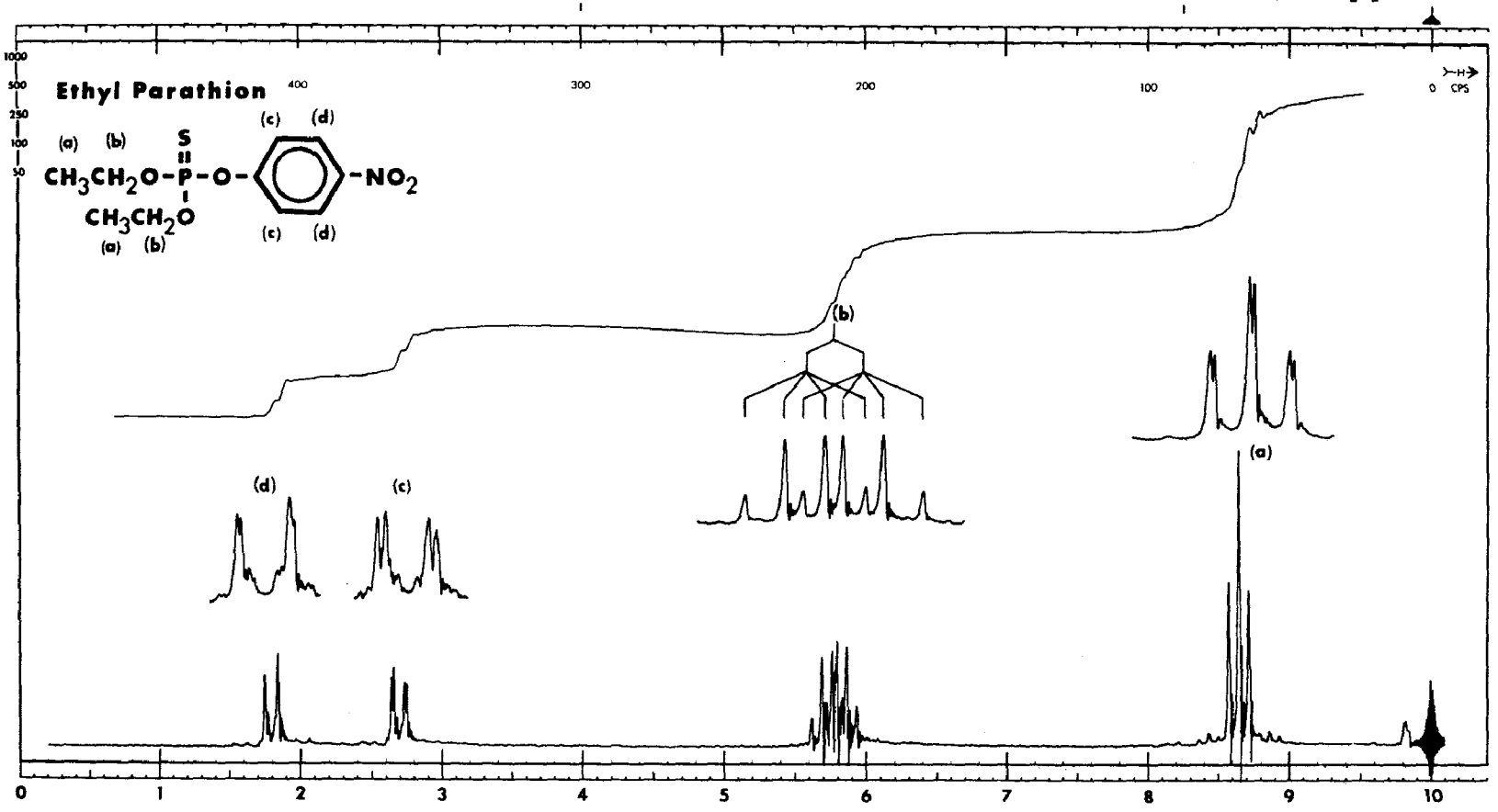

| | T | J |
|---|---|---|
| a | 8.66 | 0.8 (P-H), 7 (H-H) |
| b | 5.84 | 10.5 (P-H), 7 (H-H) |
| b' | 5.80 | |
| c | 4.19 | 16 (P-H) |
| d | 1.9 | |

# A-40




| | T | J |
|---|---|---|
| a | 8.60 | 7.0 (H-H) / 0.8 (P-H) |
| b | 7.43 | |
| c | 5.75 | 7.0 (H-H) / 10.0 (P-H) |
| d | 2.83 | |
| e | 2.37 | 9.5 ($H-H_o$) / 0.8 |

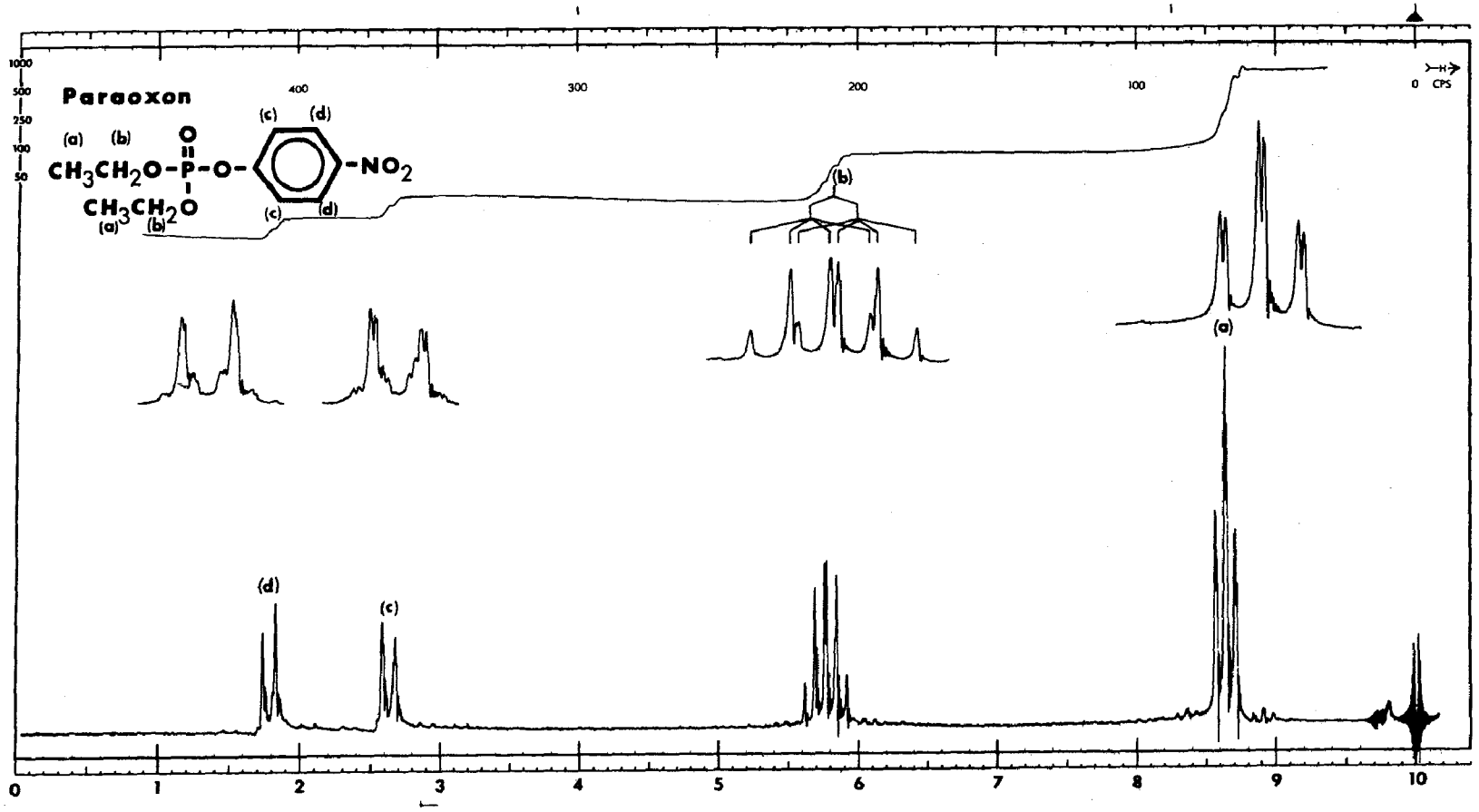
# A-41




| | T | J |
|---|---|---|
| a | 8.63 | 0.8 (P-H), 7 (H-H) |
| b | 5.75 | 10 (P-H), 7 (H-H) |
| c | 2.67 | 9 (H-H), 1.3 (P-H) |
| d | 1.77 | 9 (H-H), 0.7 (P-H) |

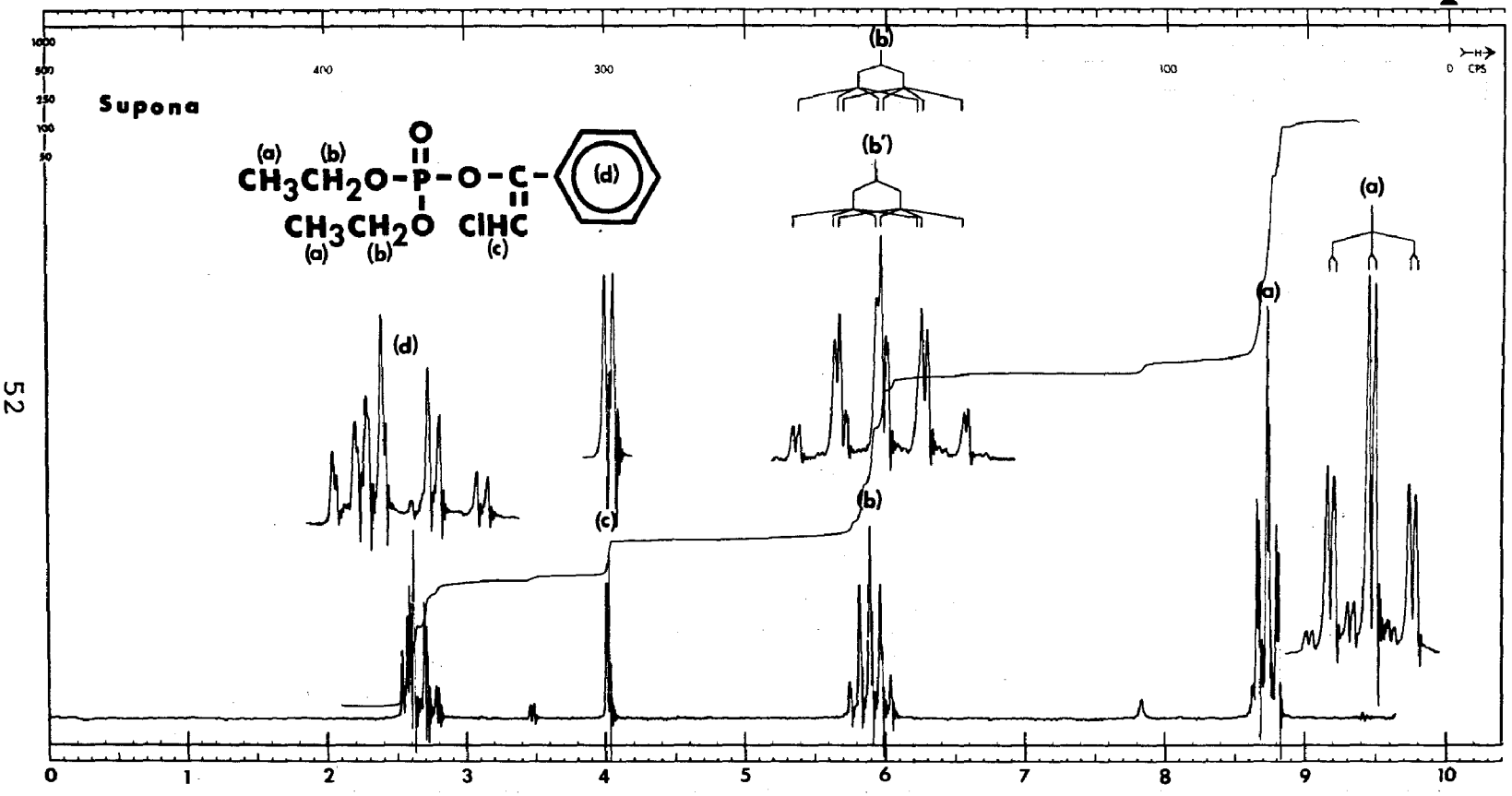
50

# A-42



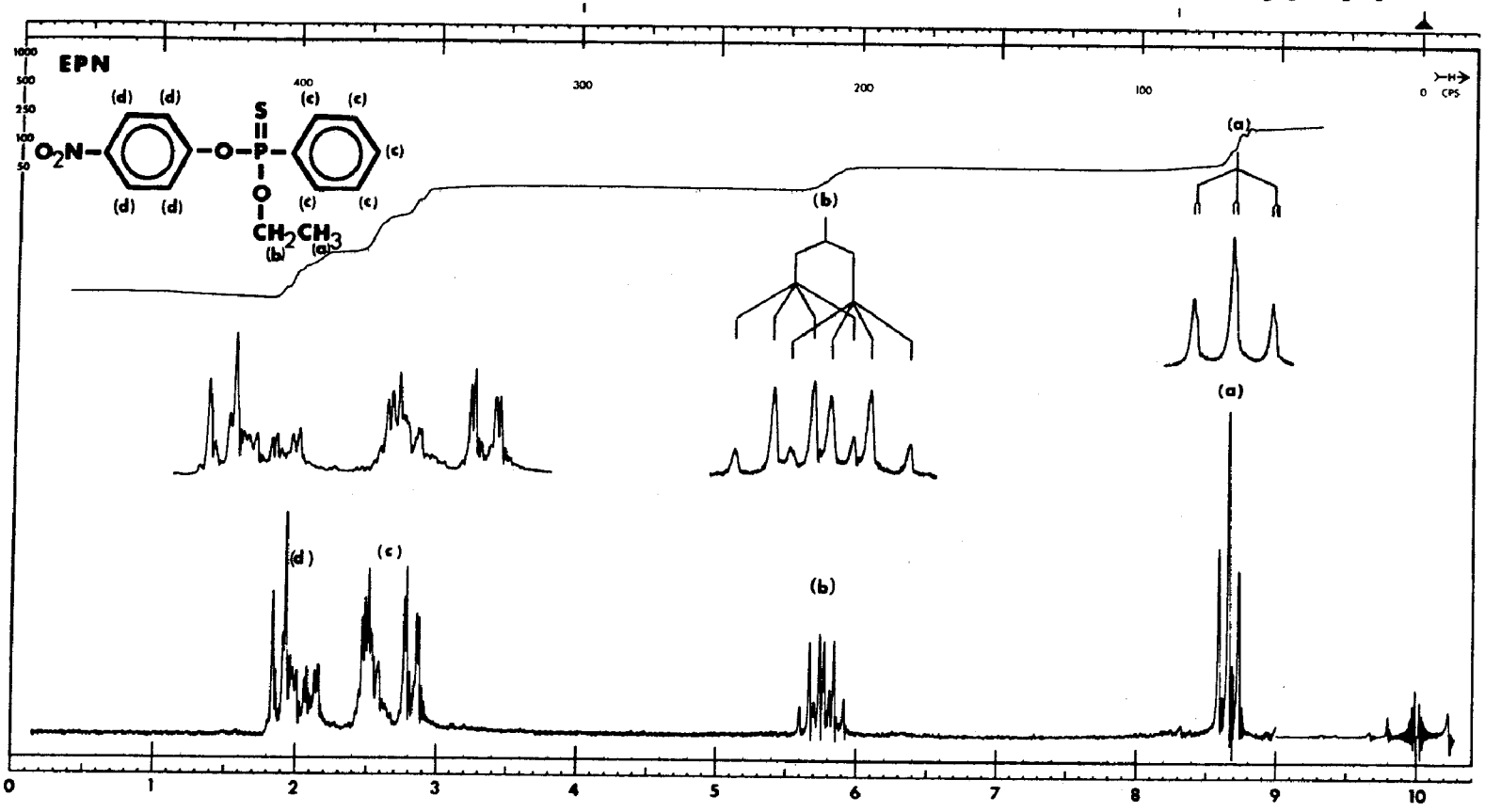

| | T | J |
|---|---|---|
| a | 8.61 | 7 (H-H), 0.9 (P-H) |
| b | 5.74 | 8.5 (P-H), 7 (H-H) |
| c | 2.60 | 9 (H-H), 1.0 (P-H) |
| d | 1.76 | 9 (H-H), 0.7 (P-H) |

# A-43



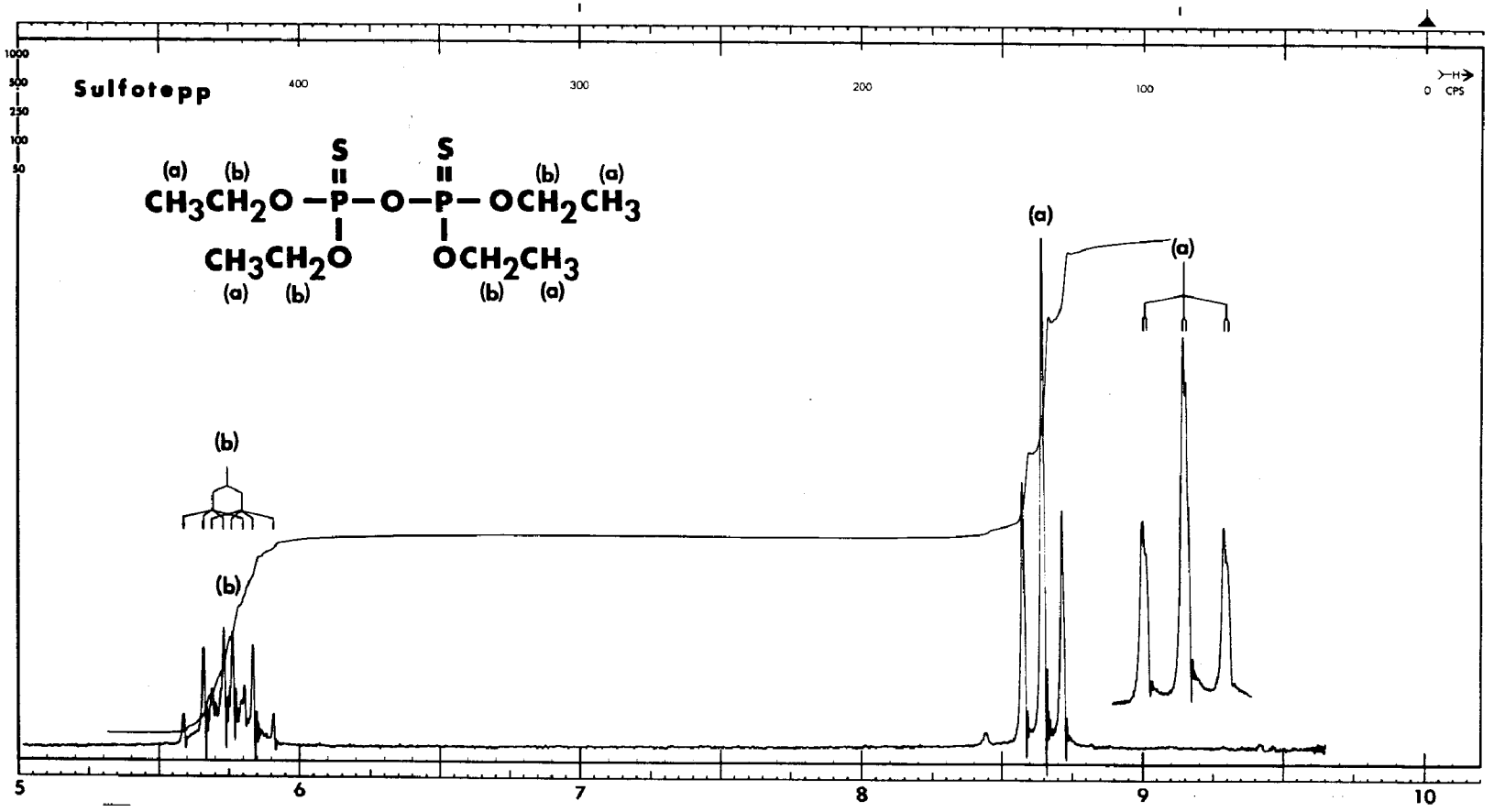

| | T | J |
|---|---|---|
| a | 8.74 | 7 / 1.2 (P-H) |
| b | 5.89 | 7 |
| b' | 5.88 | 7 |
| c | 4.00 | 1.5 (P-H) |
| d | 2.65 | |

# A-44



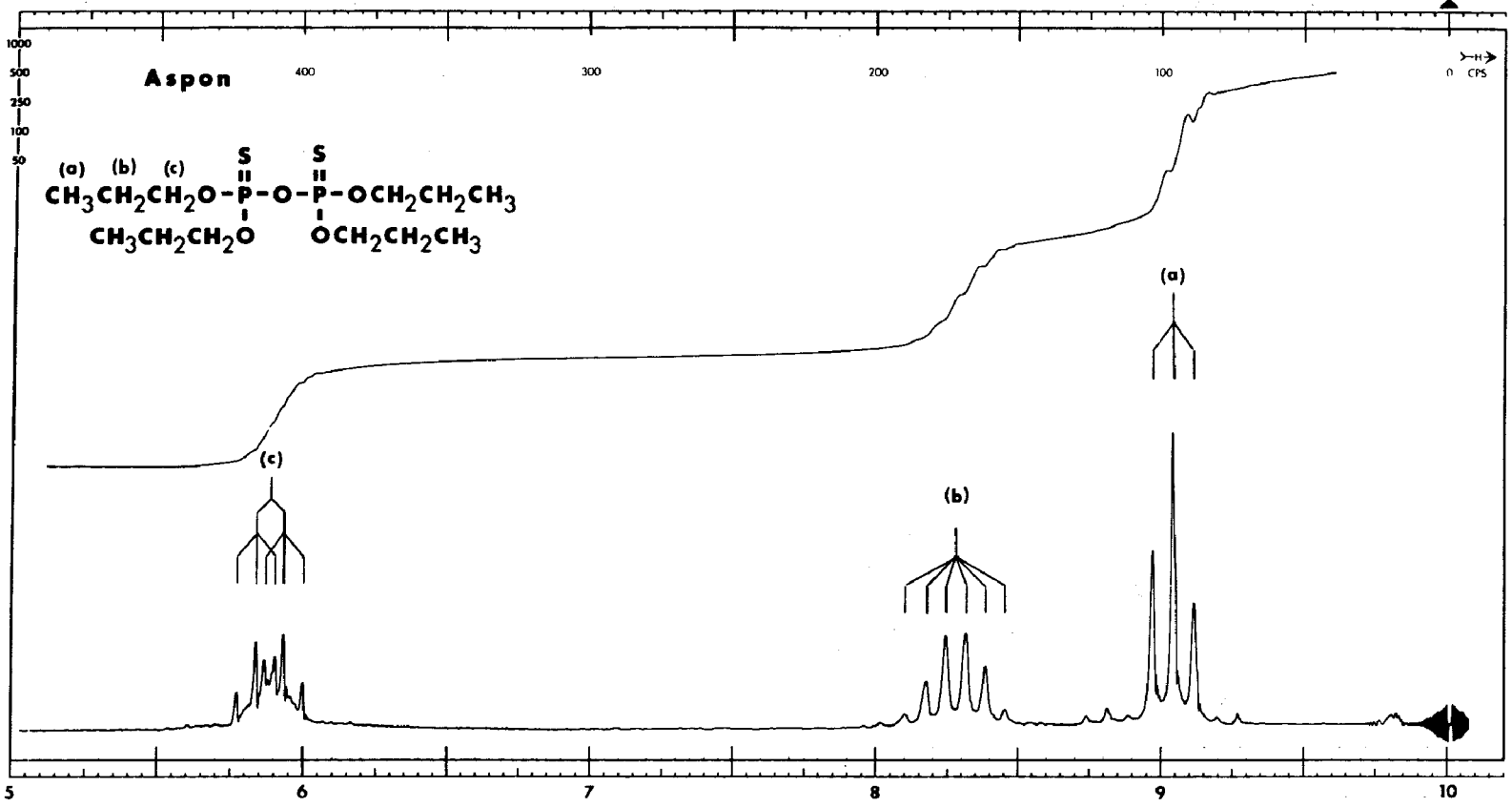

| | T | J |
|---|---|---|
| a | 8.64 | 7 (H-H), 0.5 (P-H) |
| b | 5.73 | 7 (H-H), 10 (P-H) |
| c | 2.64 | |
| d | 1.96 | |

# A-45



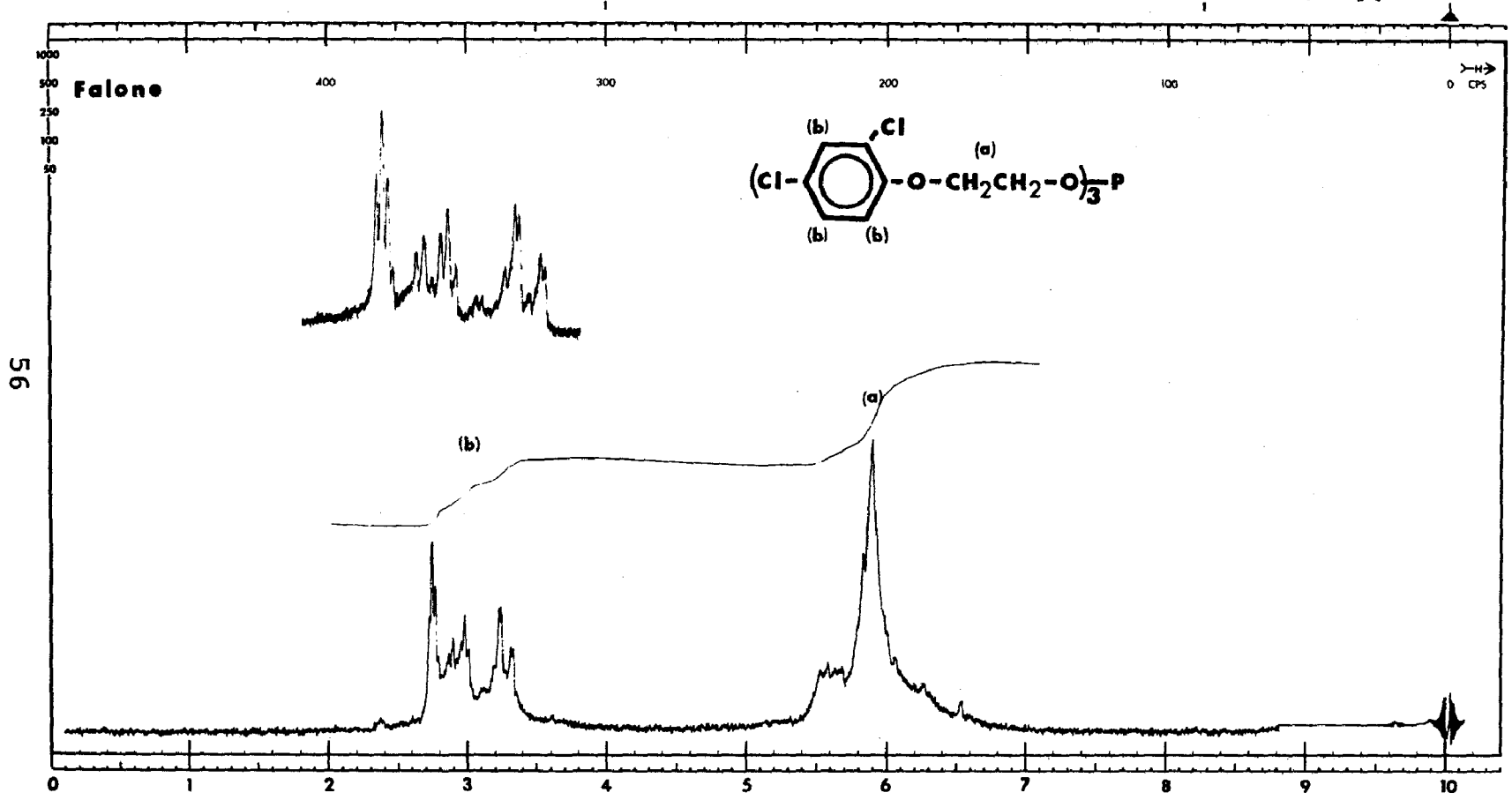

| | T | J |
|---|---|---|
| a | 8.65 | 7 (H-H), 0.5 (P-H) |
| b | 5.76 | 7 (H-H), 10 (P-H) |

# A-46



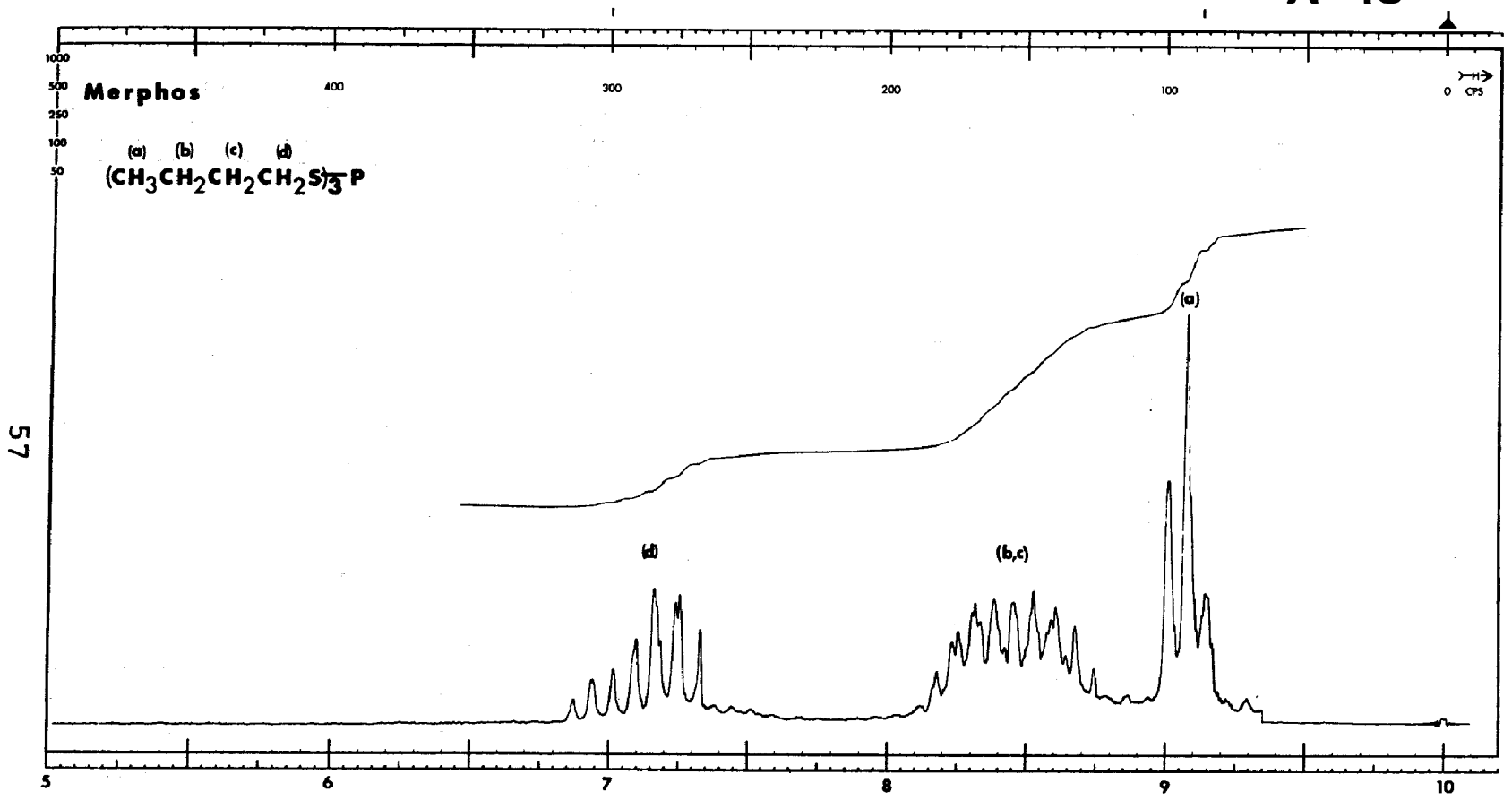

| | T | J |
|---|---|---|
| a | 9.03 | 7 |
| b | 8.27 | 7 |
| c | 5.88 | 9.5 (P-H) / 7 (H-H) |

# A-47



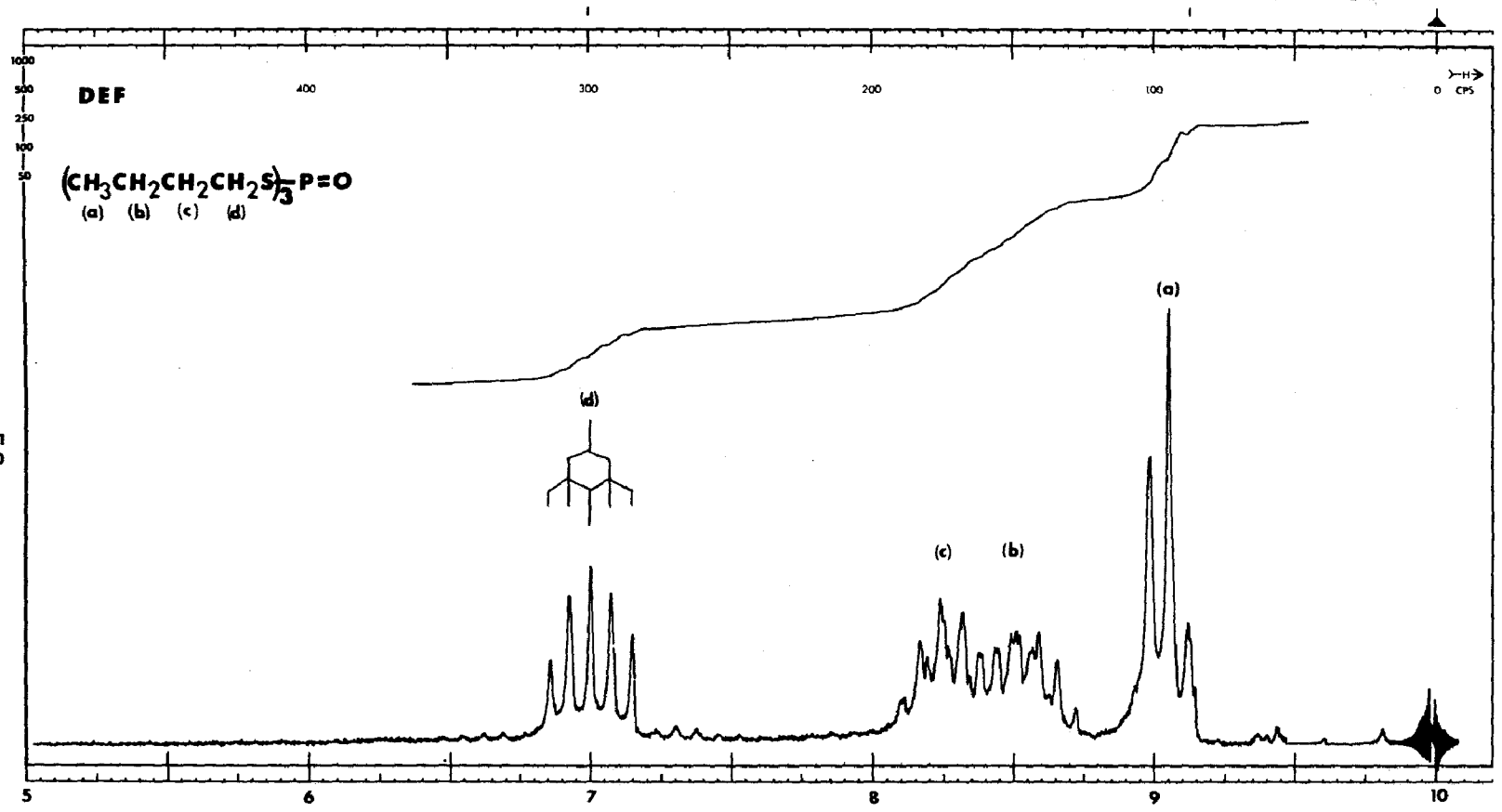

| | T |
|---|---|
| a | 5.4-6.7 |
| b | 2.6-3.4 |

# A-48



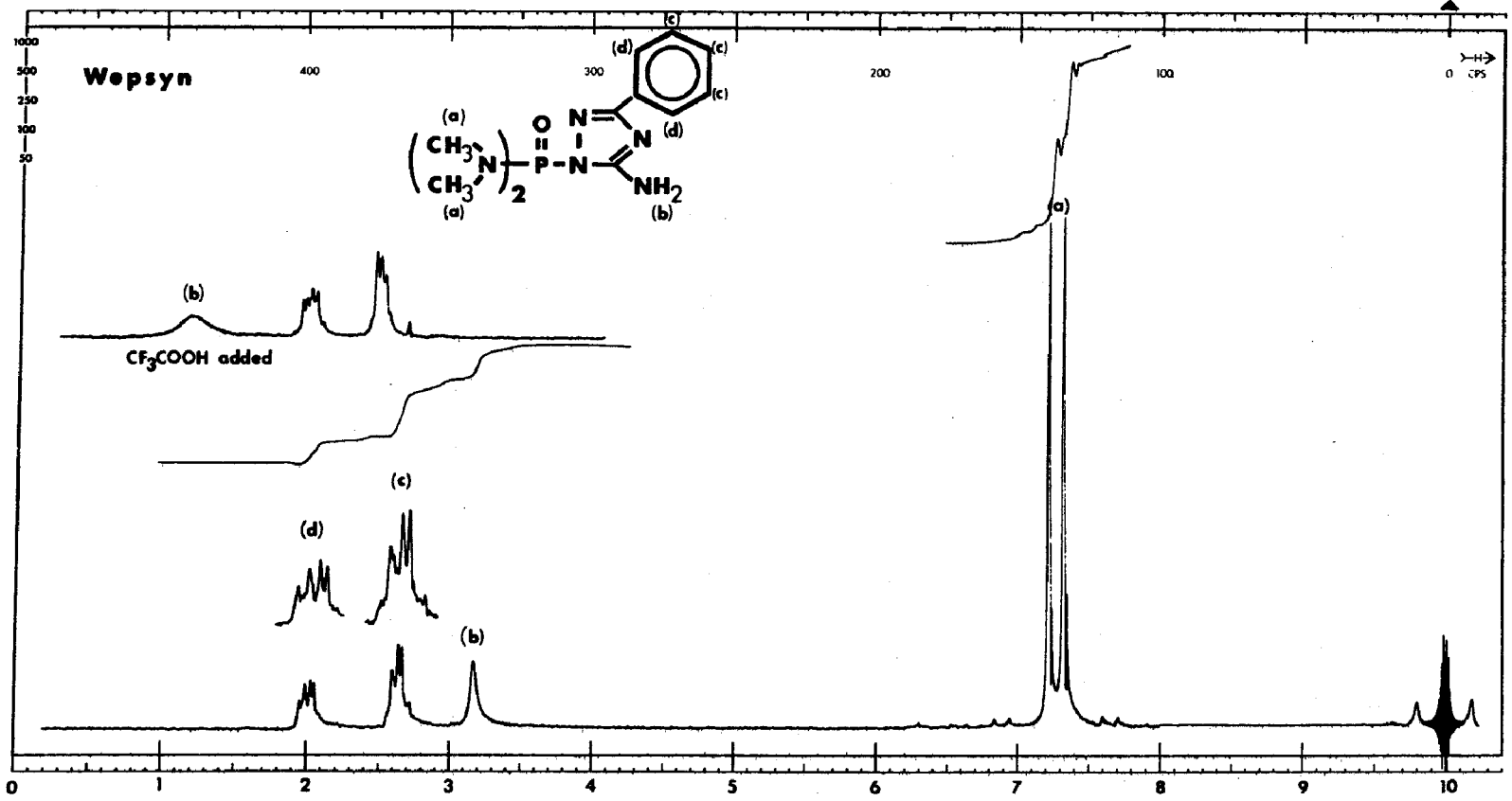

| | T | J |
|---|---|---|
| a | 9.08 | 7 |
| b,c | 8.1-8.8 | |
| d | 7.2 | |

# A-49




| | T | J |
|---|---|---|
| a | 9.05 | 6.5 |
| b | 8.5 | |
| c | 8.25 | |
| d | 7.01 | ≺ 7(H-H)<br>≺ 15(P-H) |

# A-50




| | T | J |
|---|---|---|
| a | 7.24 | 10.5 |
| b | 3.14 | |
| c | 2.61 | |
| d | 1.98 | |

THE DDT-TYPE COMPOUNDS

Most DDT-type compounds contain para-disubstituted benzene rings whose protons produce complex multiplets. Each benzene ring contains four magnetically non-equivalent protons that form two pairs of equivalent nuclei with a chemical shift difference approximately equal to the coupling constants involved. This is defined as an AA'BB' system (6). The complex spectrum prevents interpretation by visual inspection, but an approximation of the ortho coupling constants and aromatic proton chemical shifts was obtained as described in a previous publication (4).

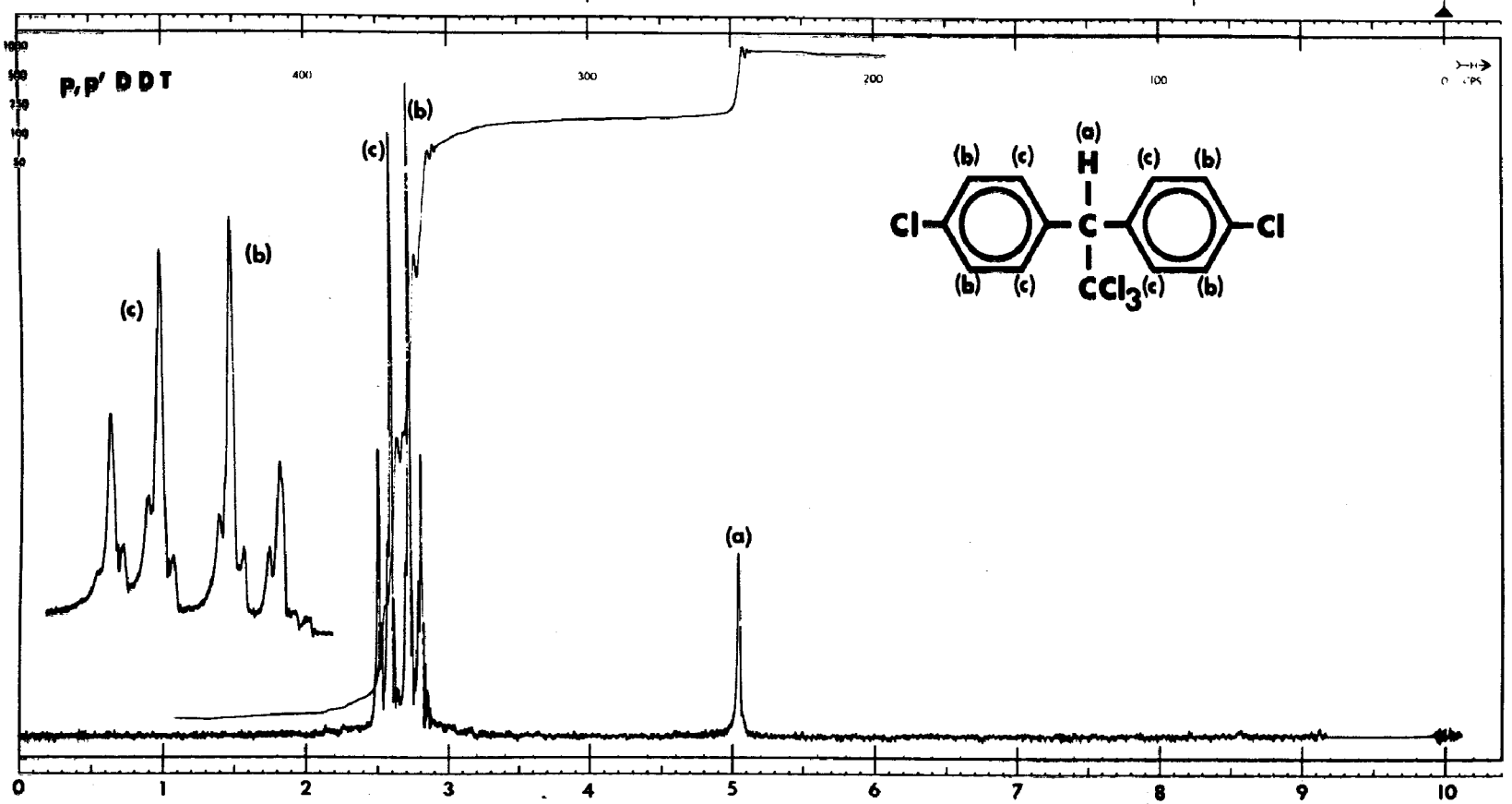
The ortho protons of compounds with the $CCl_3$ moiety on the α-carbon resonate at a significantly lower field (τ2.42-2.52) than ortho protons of compounds with other functional groups on the α-carbon (τ2.72-2.90). This large deshielding effect of the $CCl_3$ moiety may be explained by considering the molecular stereochemistry as observed in Leybold models. When three chlorines are substituted on the β-carbon, the ortho aromatic protons cannot escape the deshielding effect of the chlorine atoms. However, if only one chlorine atom is removed, the ortho protons are no longer forced into close proximity to the chlorine atoms. The deshielding effect of the $CCl_3$ group is greatest when chlorine substitution on one of the aromatic rings occurs in the ortho position. Examination of a Leybold model shows that a chlorine in the ortho position of a ring causes rotation of that ring around the aromatic-aliphatic C-C bond to be energetically unfavorable. The most favorable conformation places the remaining ortho proton near the β-carbon chlorines and the ortho chlorine as far as possible from the $CCL_3$ moiety.

The meta protons of the aromatic rings with para chlorine substituents resonate in a range from τ2.68-2.76. As expected, the benzylic

proton signals (τ5.06-6.0) are deshielded more by an ortho than a para chlorine on an aromatic ring.

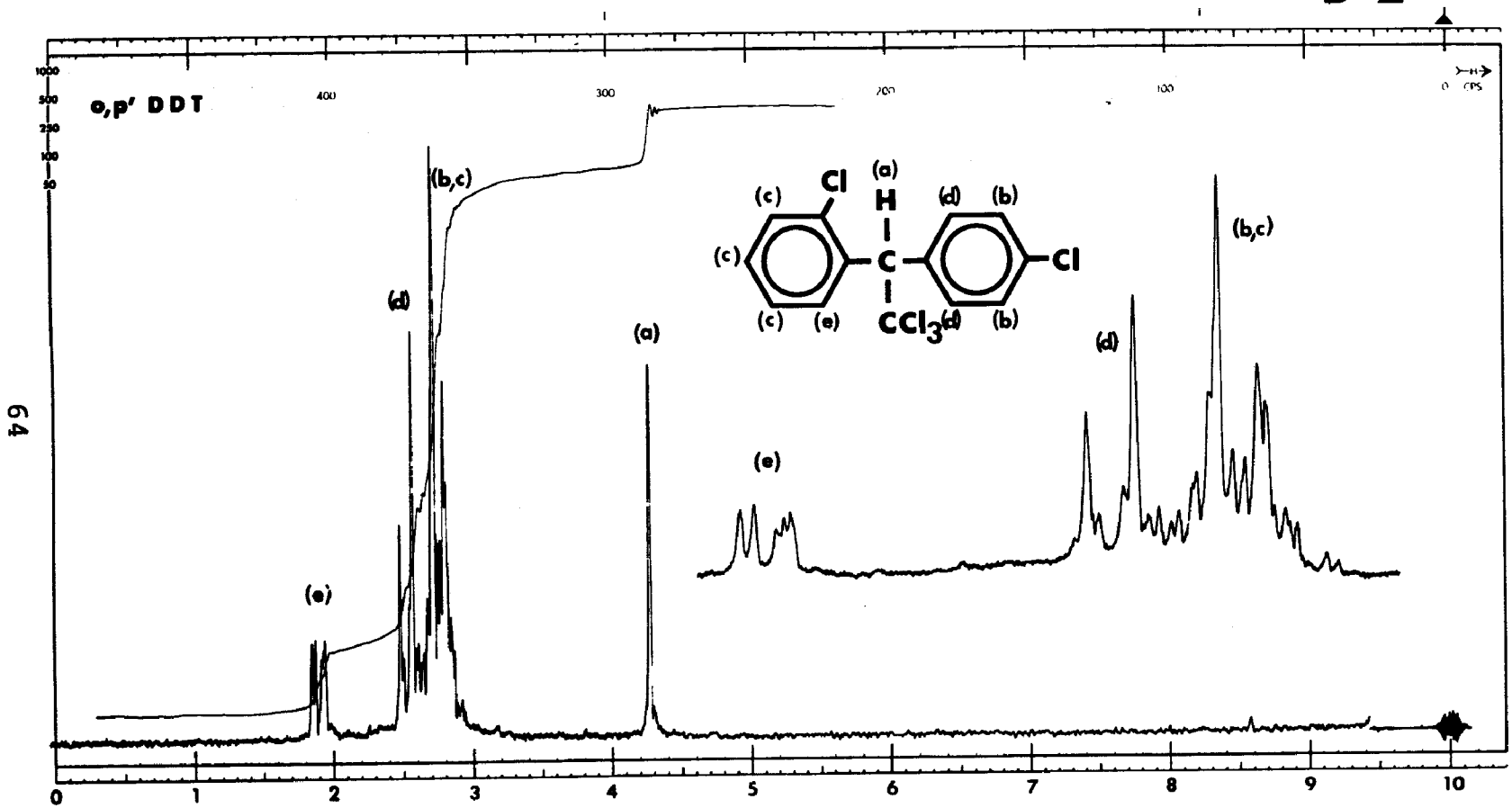
Technical DDT is a mixture of p,p'-DDT and o,p'-DDT. Peak area measurements by electronic integration of the part of the spectrum containing the signals of the benzylic protons (p,p'-DDT, τ5.00; o,p'-DDT, τ4.25) provide the isomeric composition of the sample (80% p,p'-DDT, 20% o,p'-DDT). The spectrum of Dilan, a mixture of Bulan and Prolan, contains only one benzylic peak but has two methyl signals with significantly different chemical shifts (triplet, τ9.11; doublet, τ8.54). The integration of these methyl signals provides the percentage of each compound in the mixture (62% Bulan, 38% Prolan).

# B-1



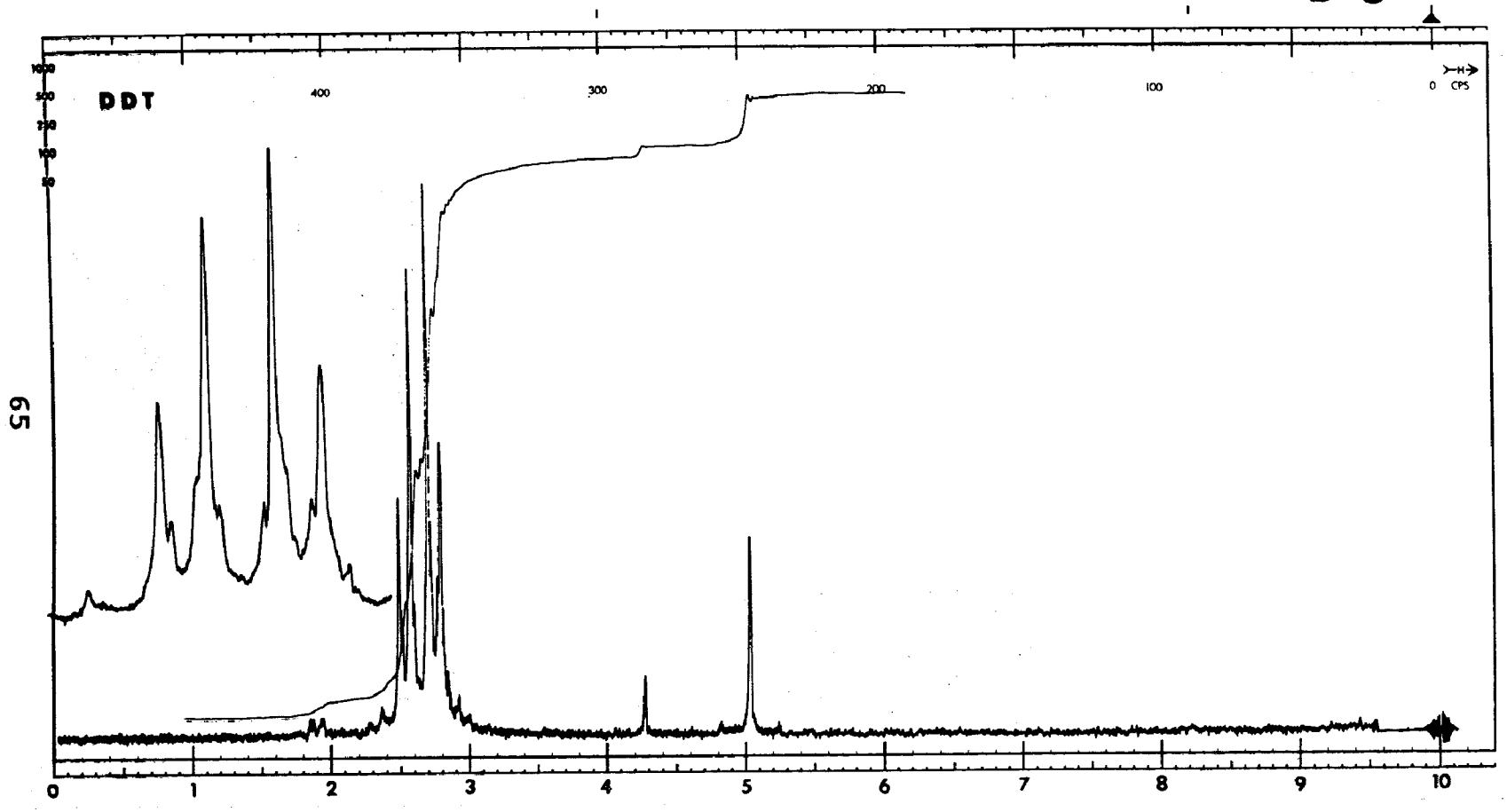

| | T | J |
|---|---|---|
| a | 5.00 | |
| b | 2.72 | 8.5 |
| c | 2.53 | 8.5 |

# B-2




| | T | J |
|---|---|---|
| a | 4.25 | |
| b | 2.74 | 8.5 |
| c | 2.6-2.9 | |
| d | 2.52 | 8.5 |
| e | 1.88 | |

B-3

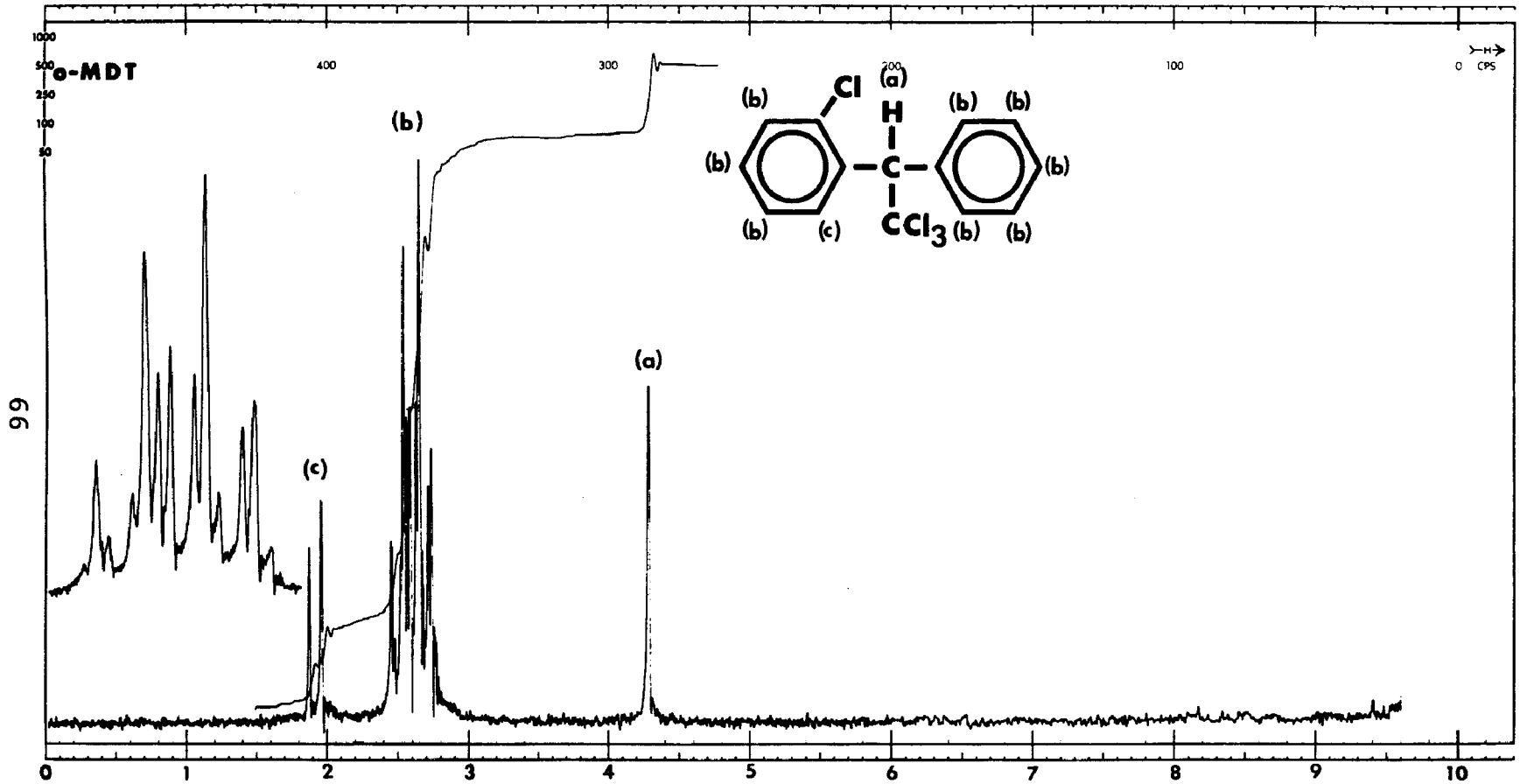



65

**Technical DDT**

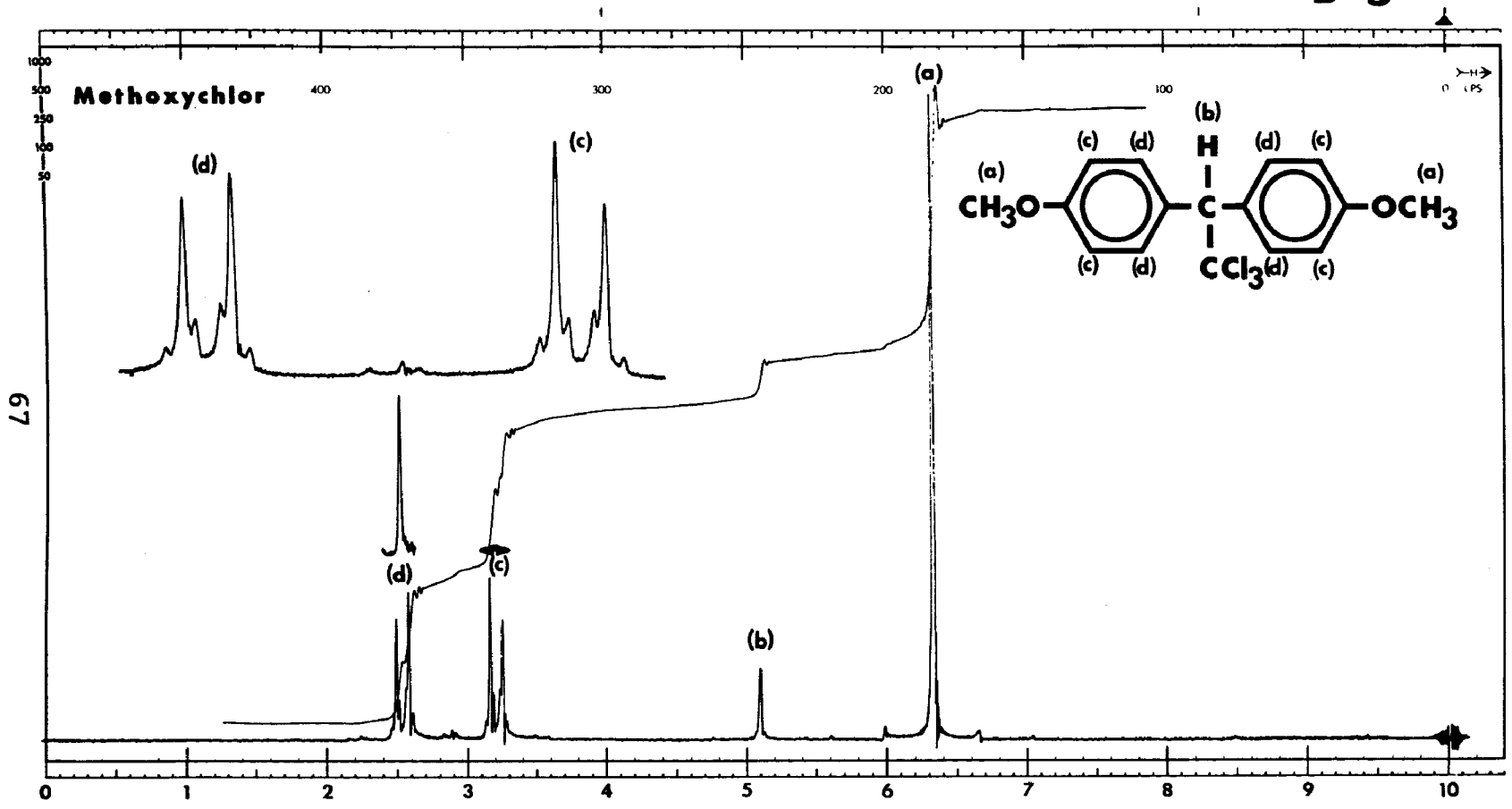
Mixture of
o,p' DDT
and
p,p' DDT

# B-4



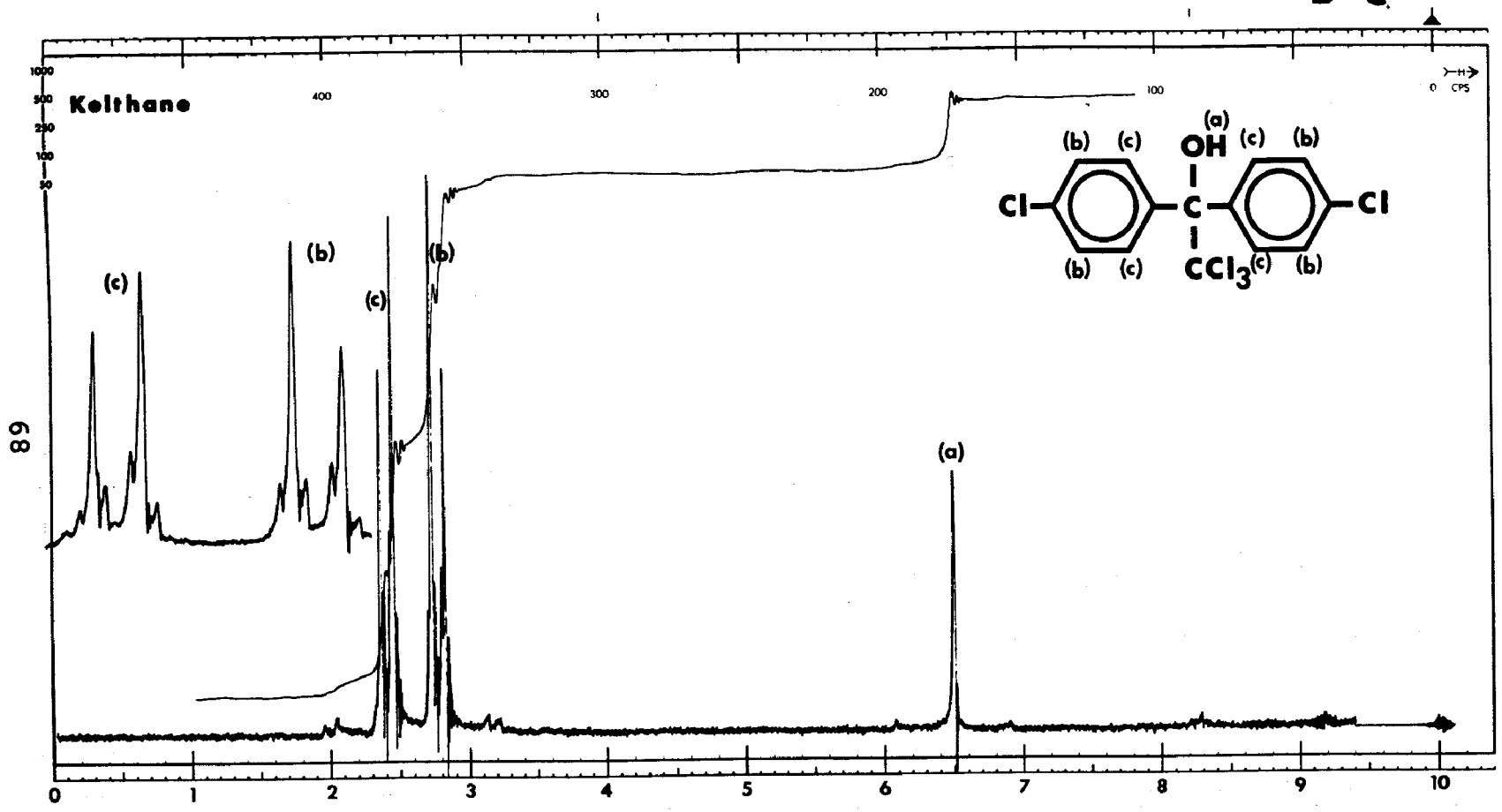

| T | |
|---|---|
| a | 4.28 |
| b | 2.4-2.8 |
| c | 1.84-1.98 |

# B-5



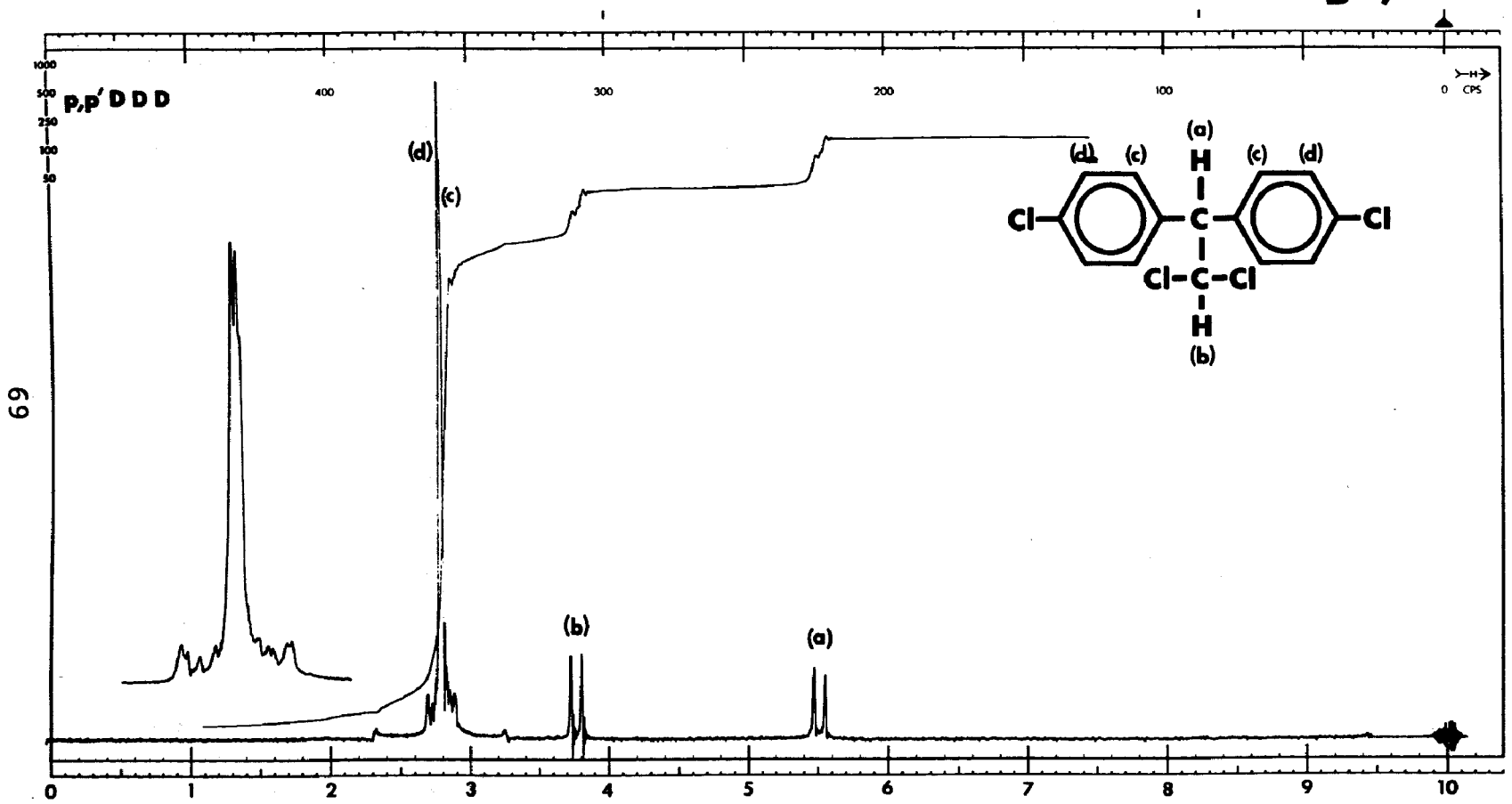

| | T | J |
|---|---|---|
| a | 6.29 | |
| b | 5.06 | |
| c | 3.18 | 9 |
| d | 2.52 | 9 |

# B-6




| | T | J |
|---|---|---|
| a | 6.48 | |
| b | 2.76 | 9 |
| c | 2.42 | 9 |

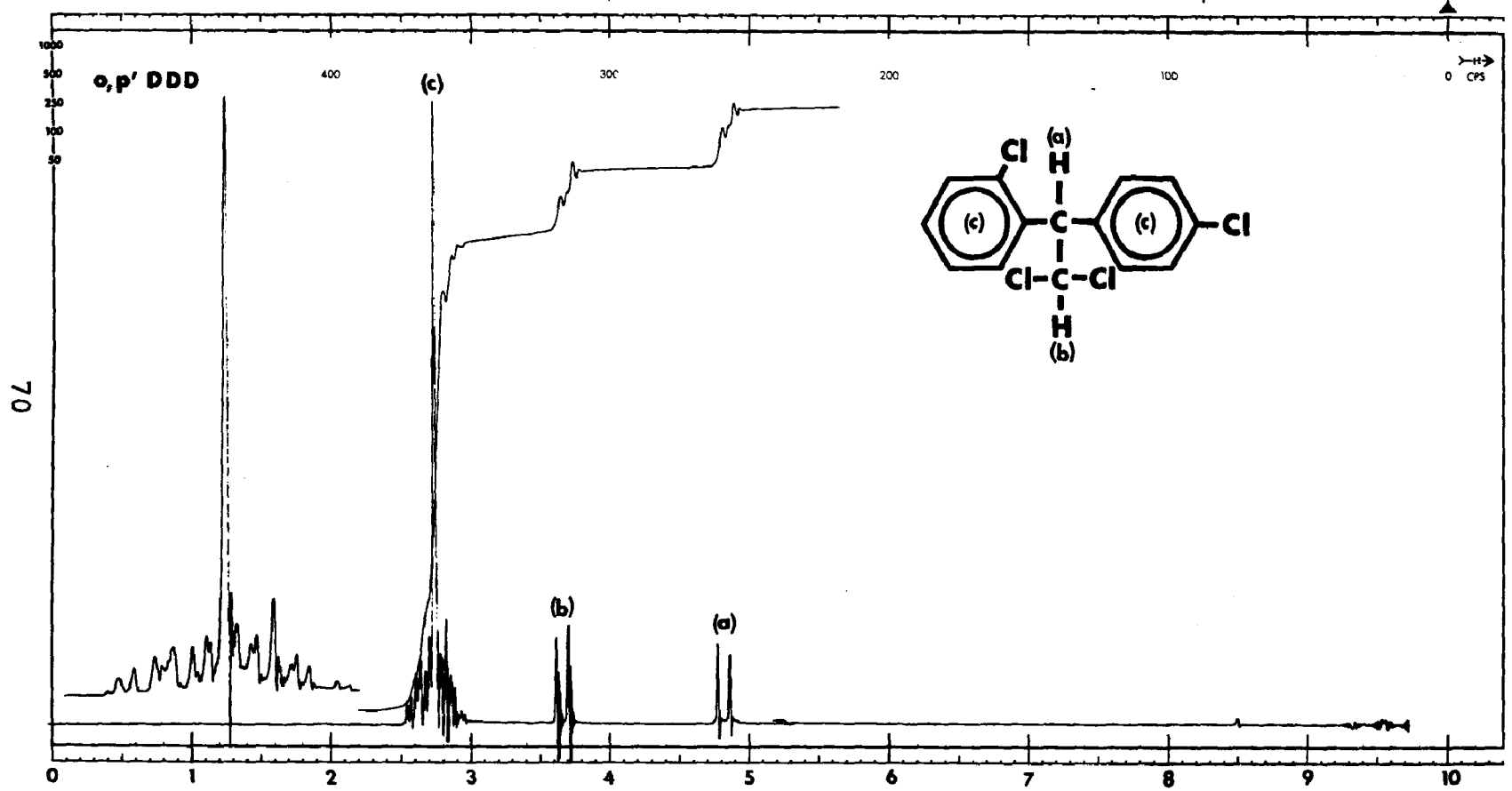
# B-7




69

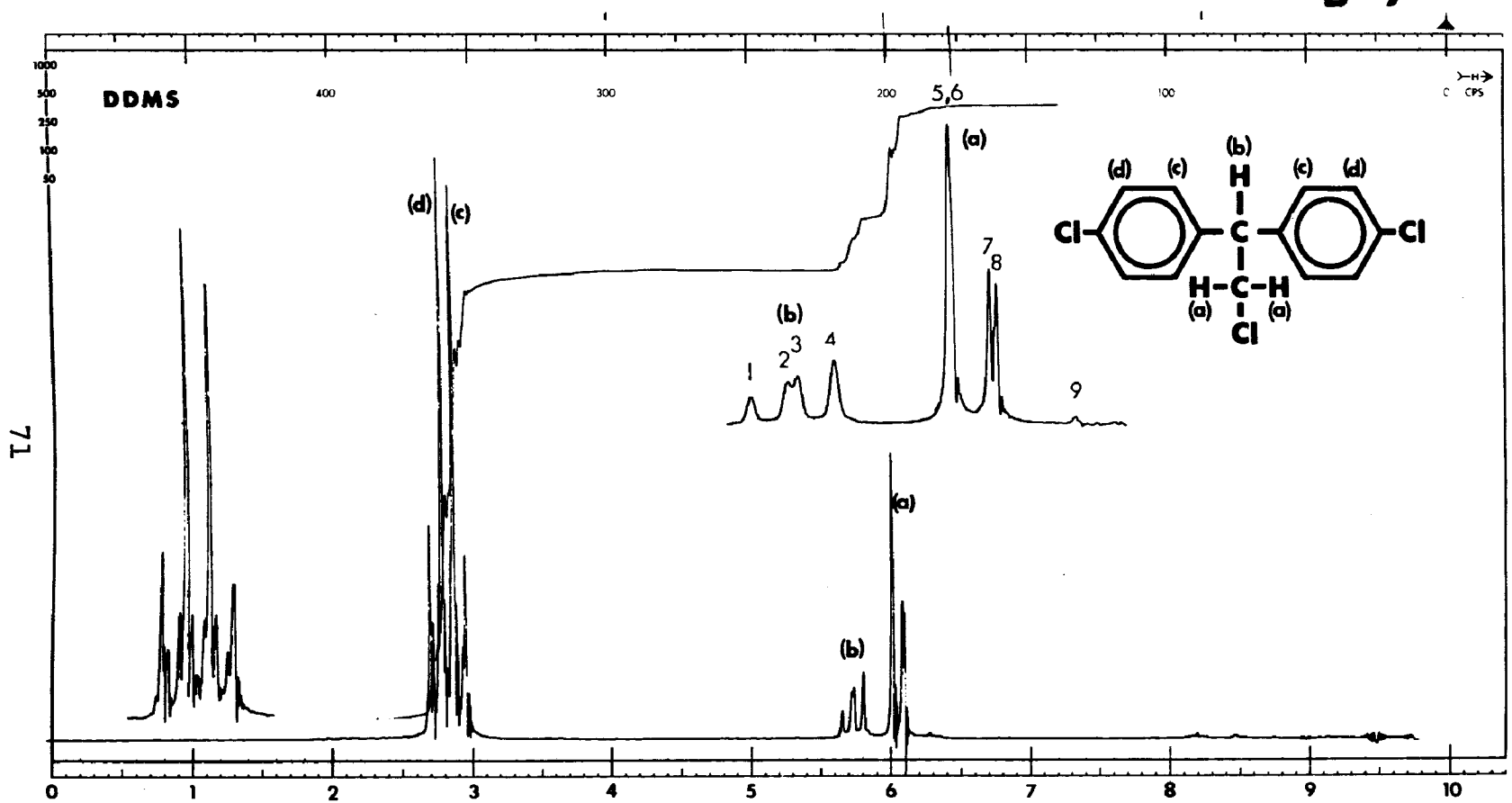
| | T | J |
|---|---|---|
| a | 5.49 | 8 |
| b | 3.74 | 8 |
| c | 2.78 | 9 |
| d | 2.74 | 9 |

# B-8



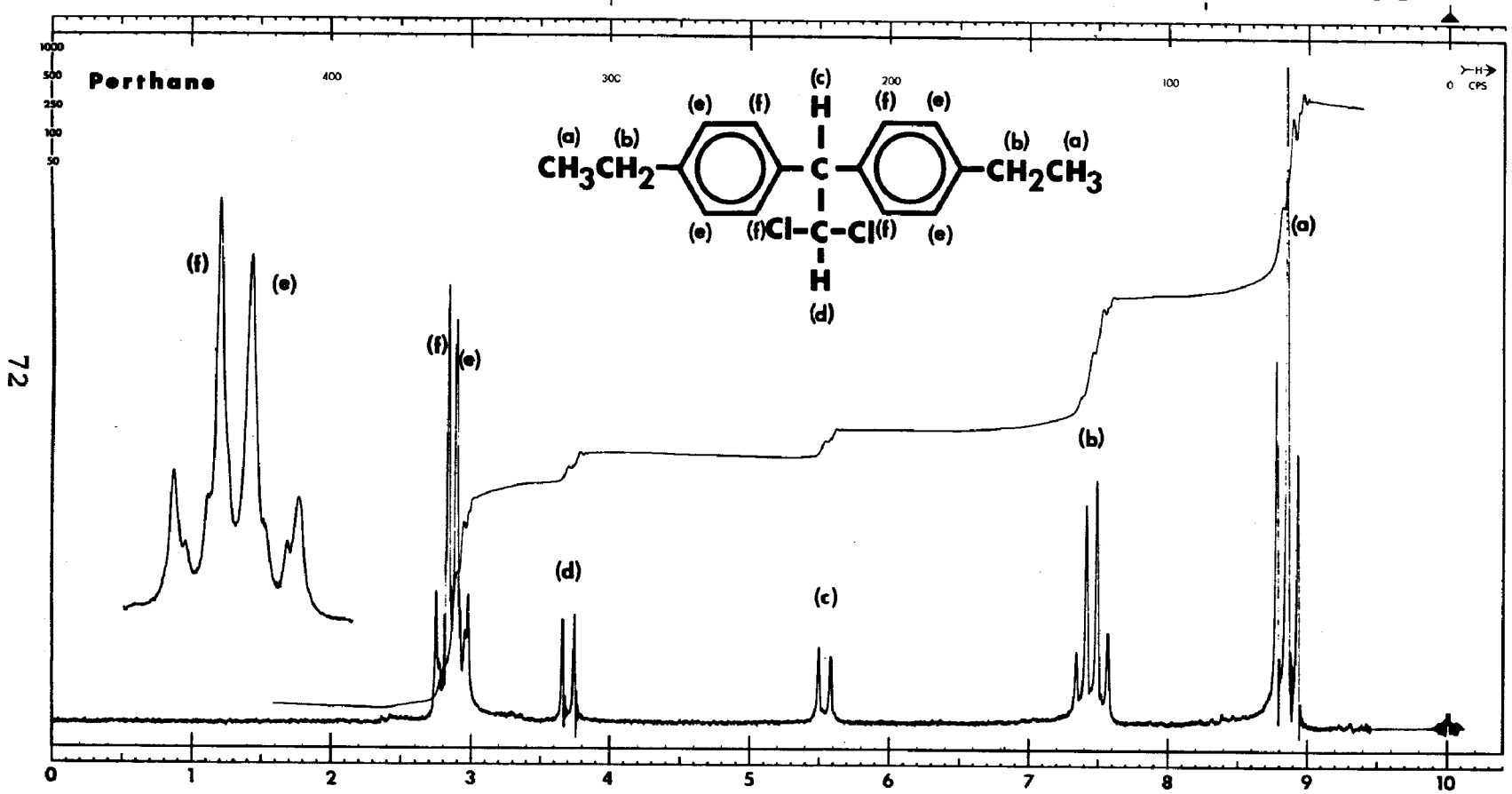

| | T | J |
|---|---|---|
| a | 4.82 | 8.5 |
| b | 3.64 | 8.5 |
| c | 2.5-2.9 | |

# B-9



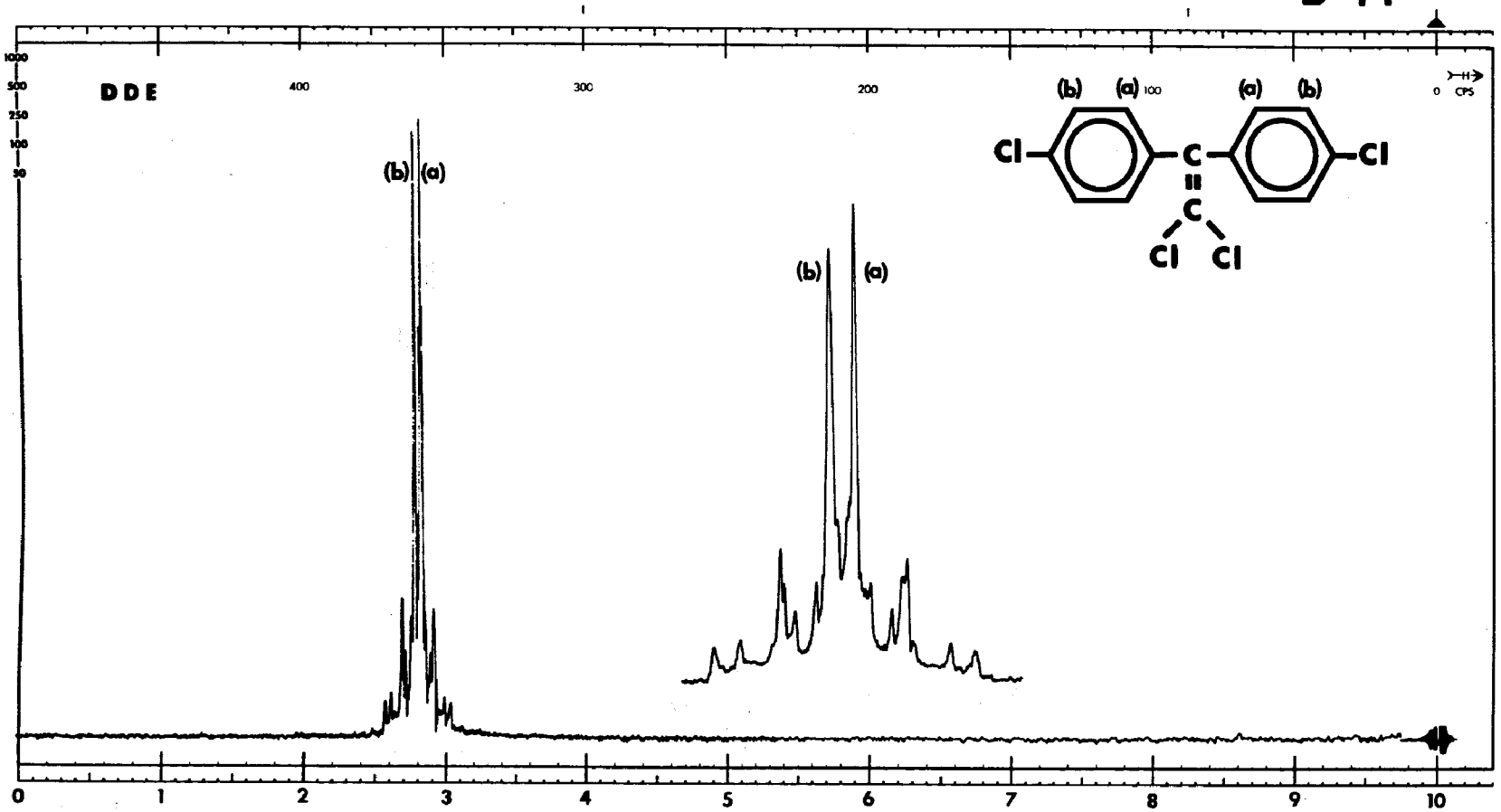

| | T | J |
|---|---|---|
| a | 6.05 | 8 |
| b | 5.75 | 8 |
| c | 2.88 | 8.5 |
| d | 2.74 | 8.5 |

# B-10



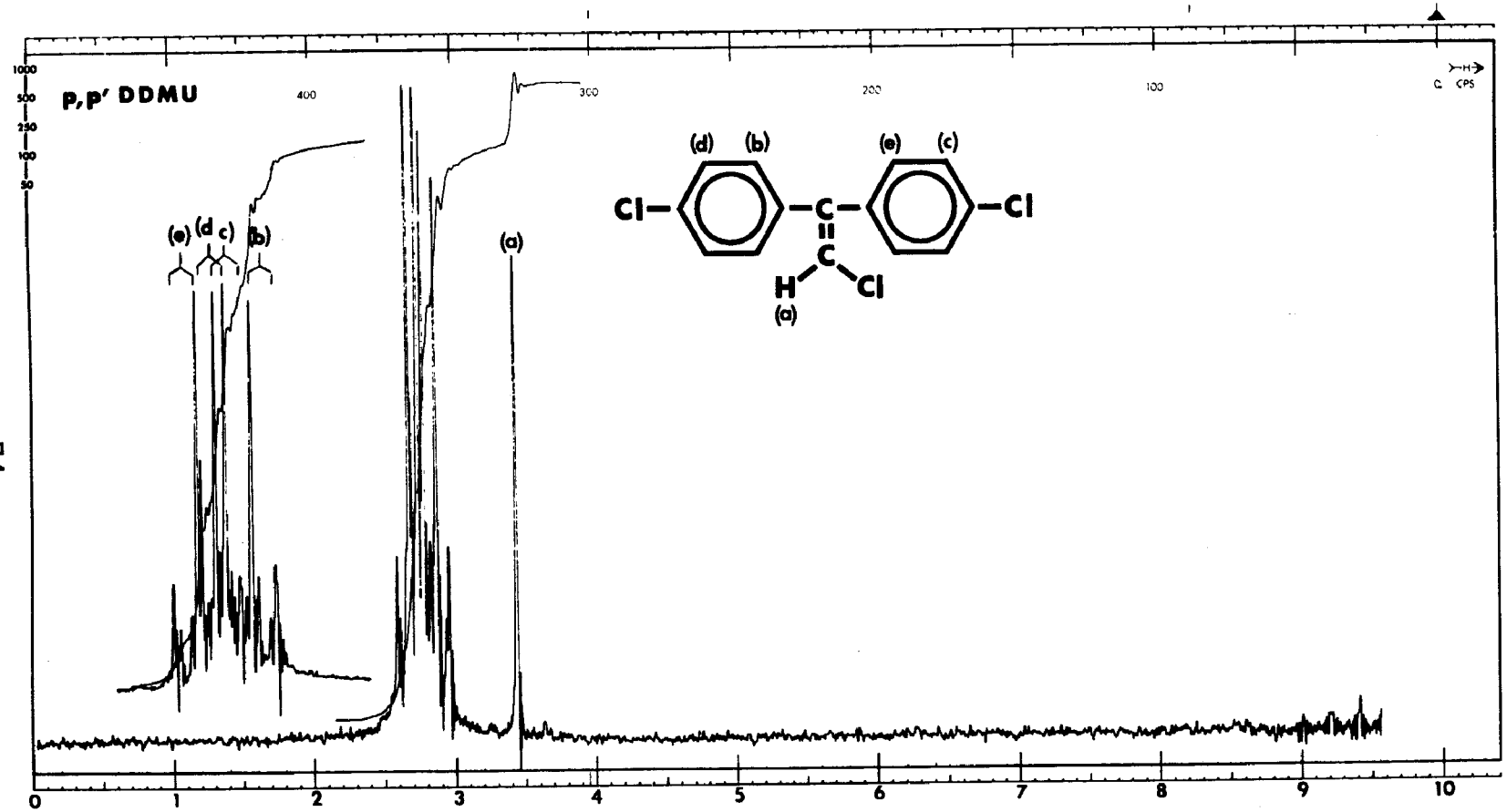

72

| | T | J |
|---|---|---|
| a | 8.84 | 7 |
| b | 7.43 | 7 |
| c | 5.50 | 8.5 |
| d | 3.68 | 8.5 |
| e | 2.92 | 9 |
| f | 2.80 | 9 |



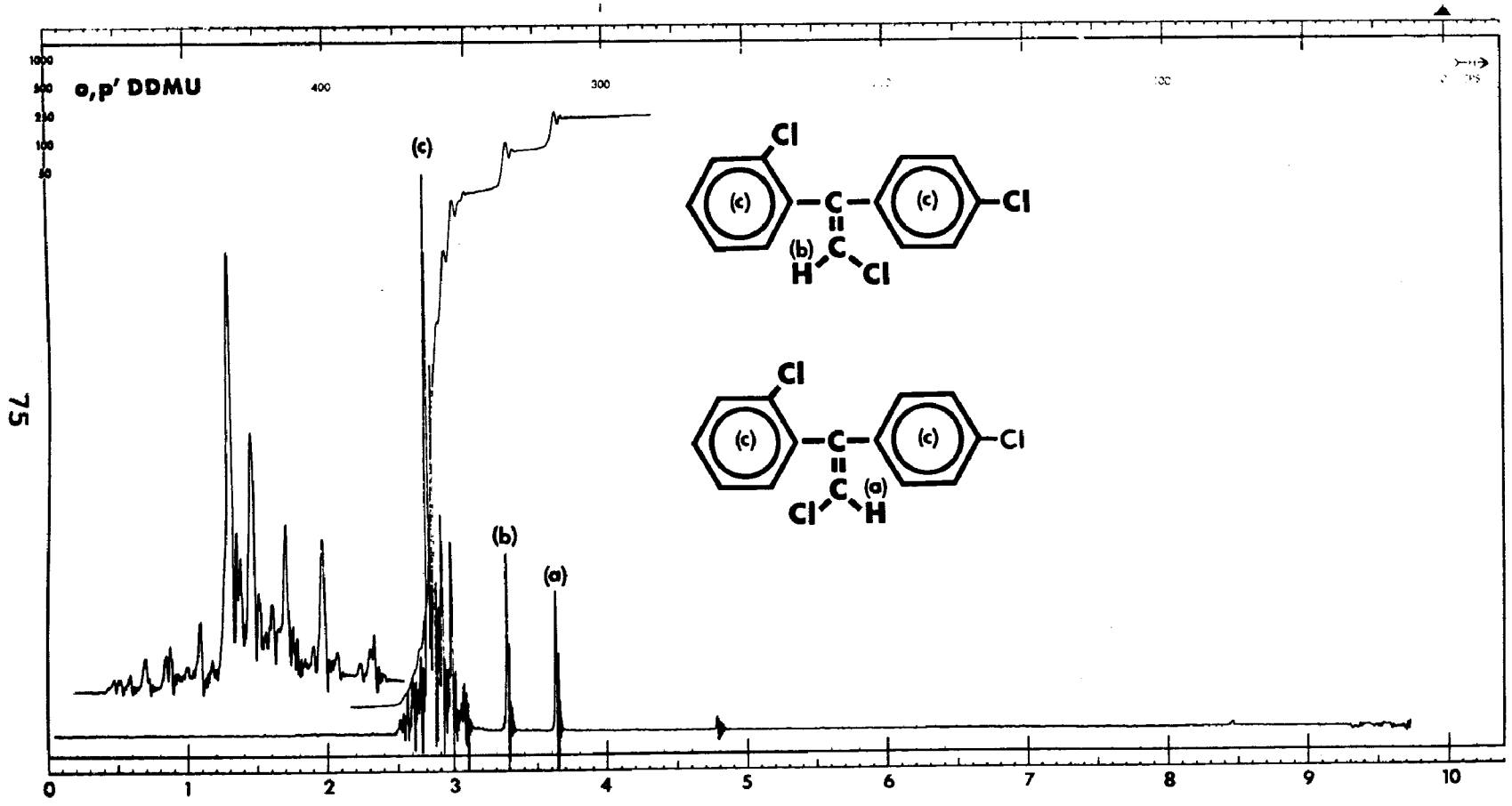

| | T | J |
|---|---|---|
| a | 2.88 | 9 |
| b | 2.75 | 9 |

# B-12




| | T | J |
|---|---|---|
| a | 3.45 | |
| b | 2.91 | 8.5 |
| c | 2.77 | 8.5 |
| d | 2.75 | 8.5 |
| e | 2.65 | 8.5 |

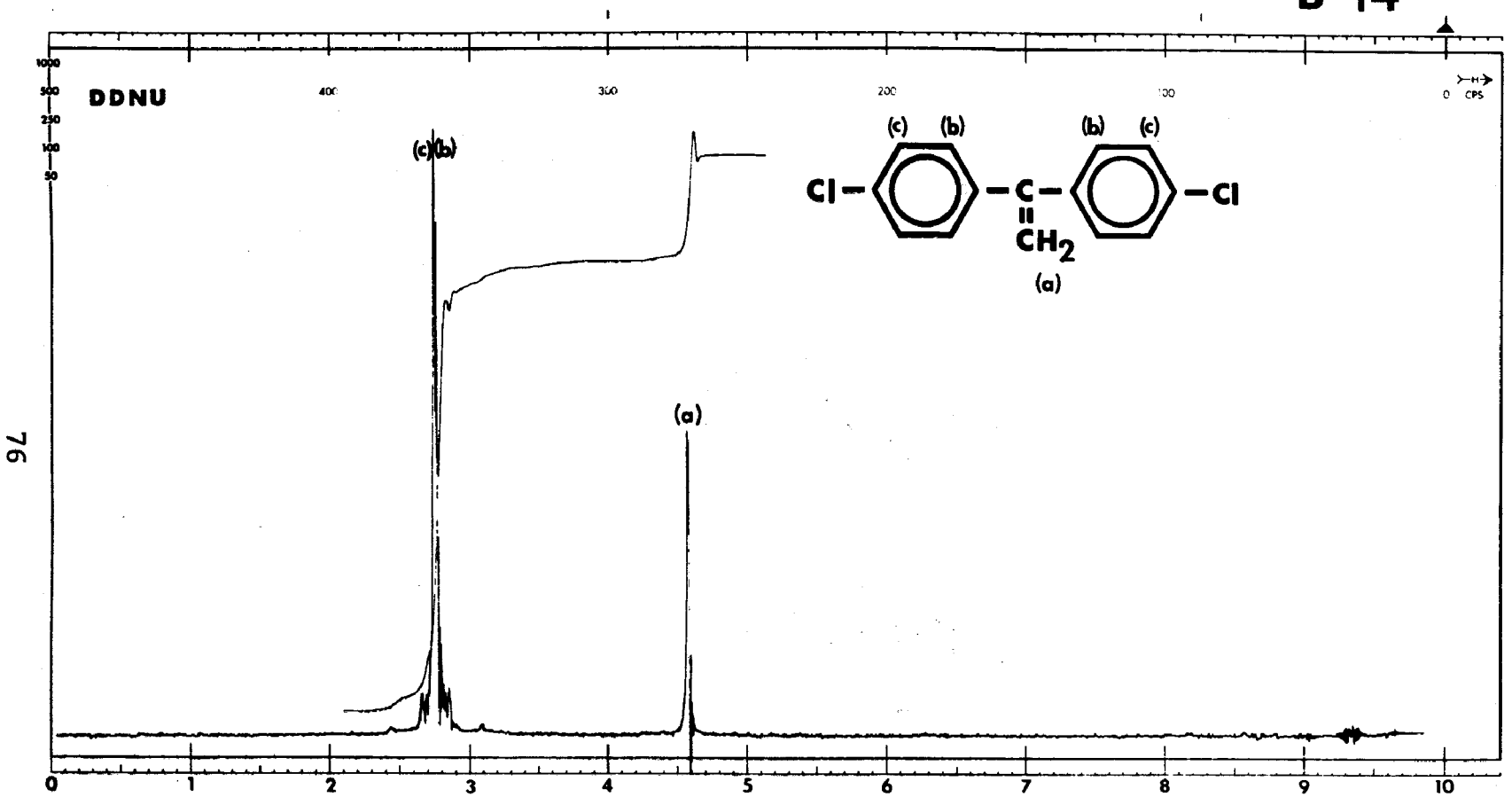
# B-13




75

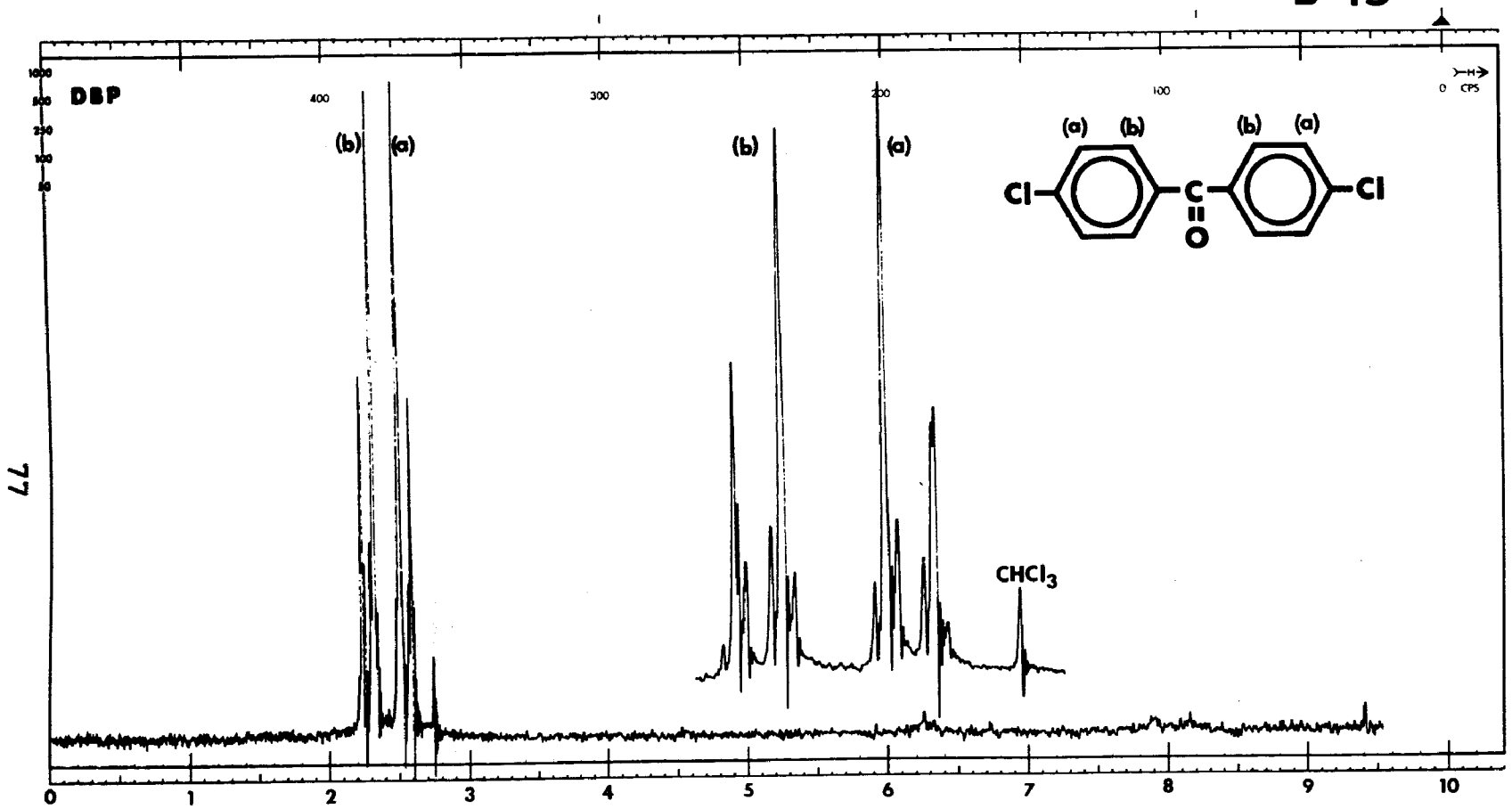
| | T |
|---|---|
| a | 3.62 |
| b | 3.28 |
| c | 2.5-3.0 |

# B-14



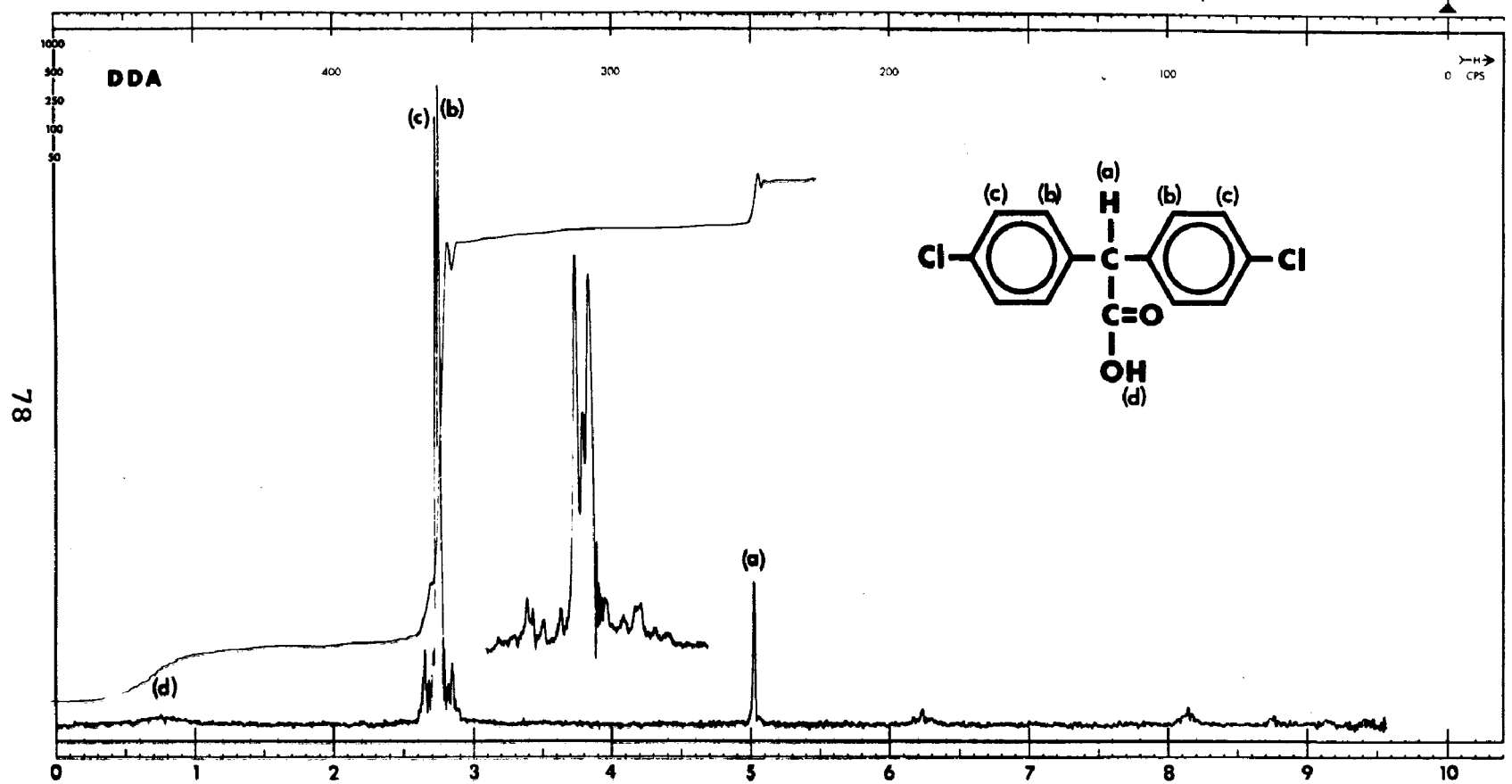

| | T | J |
|---|---|---|
| a | 4.59 | |
| b | 2.80 | 9 |
| c | 2.74 | 9 |

# B-15



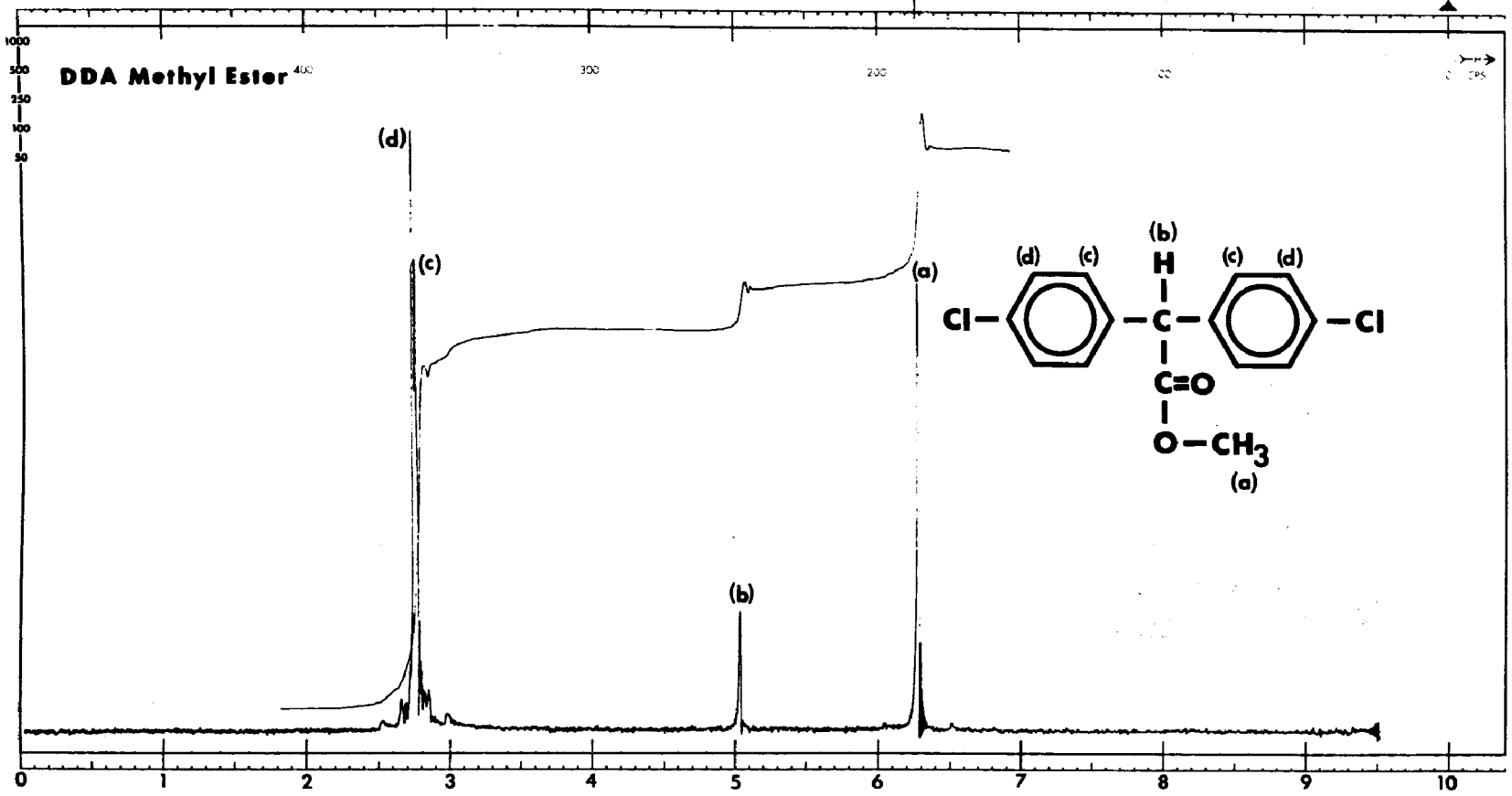

| | T | J |
|---|---|---|
| a | 2.55 | 8.5 |
| b | 2.29 | 8.5 |

# B-16



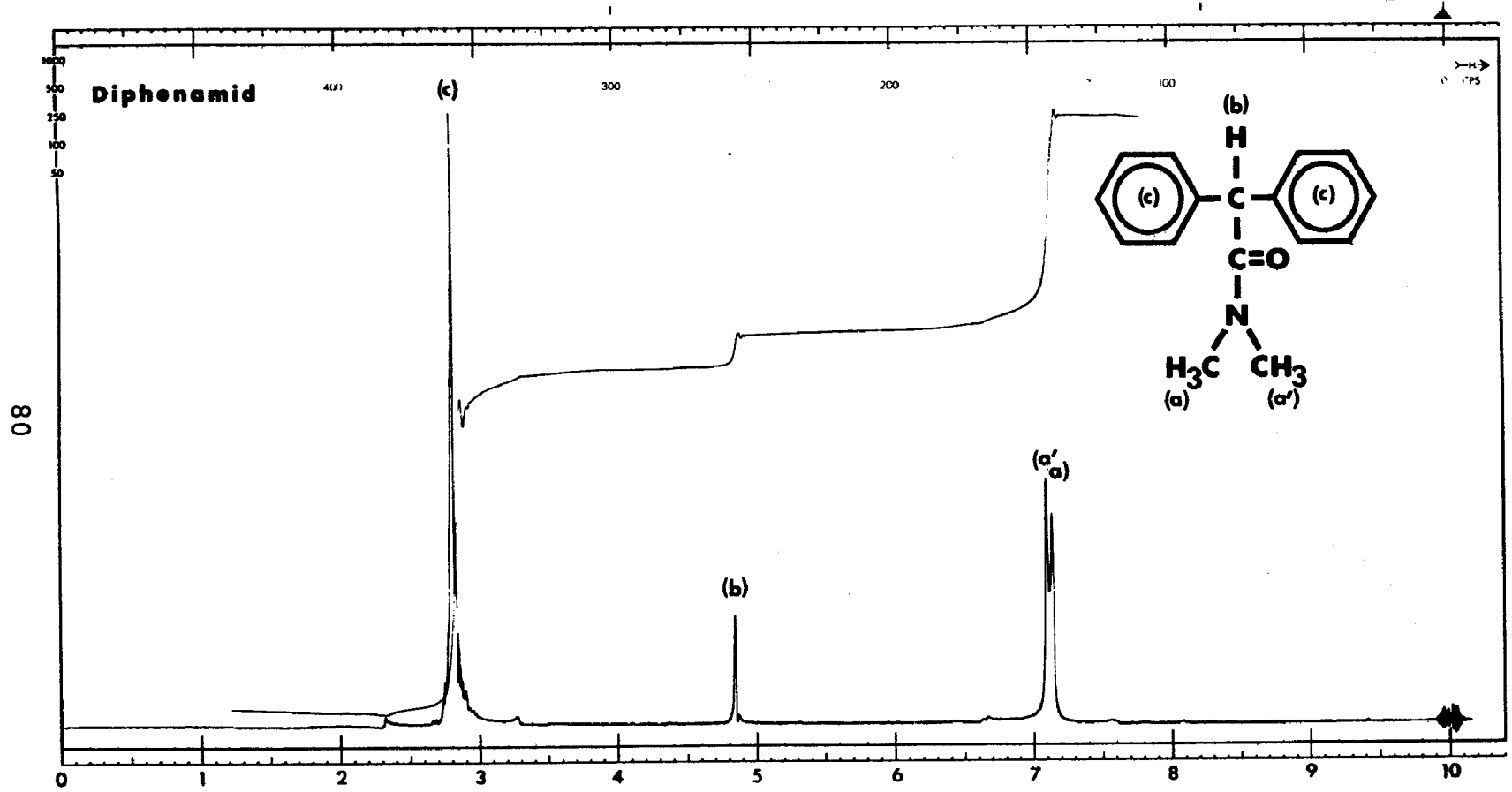

78

| | T | J |
|---|---|---|
| a | 5.03 | |
| b | 2.77 | 9 |
| c | 2.71 | 9 |
| d | 0.8 | |




| | T | J |
|---|---|---|
| a | 6.29 | |
| b | 5.06 | |
| c | 2.79 | 9 |
| d | 2.73 | 9 |

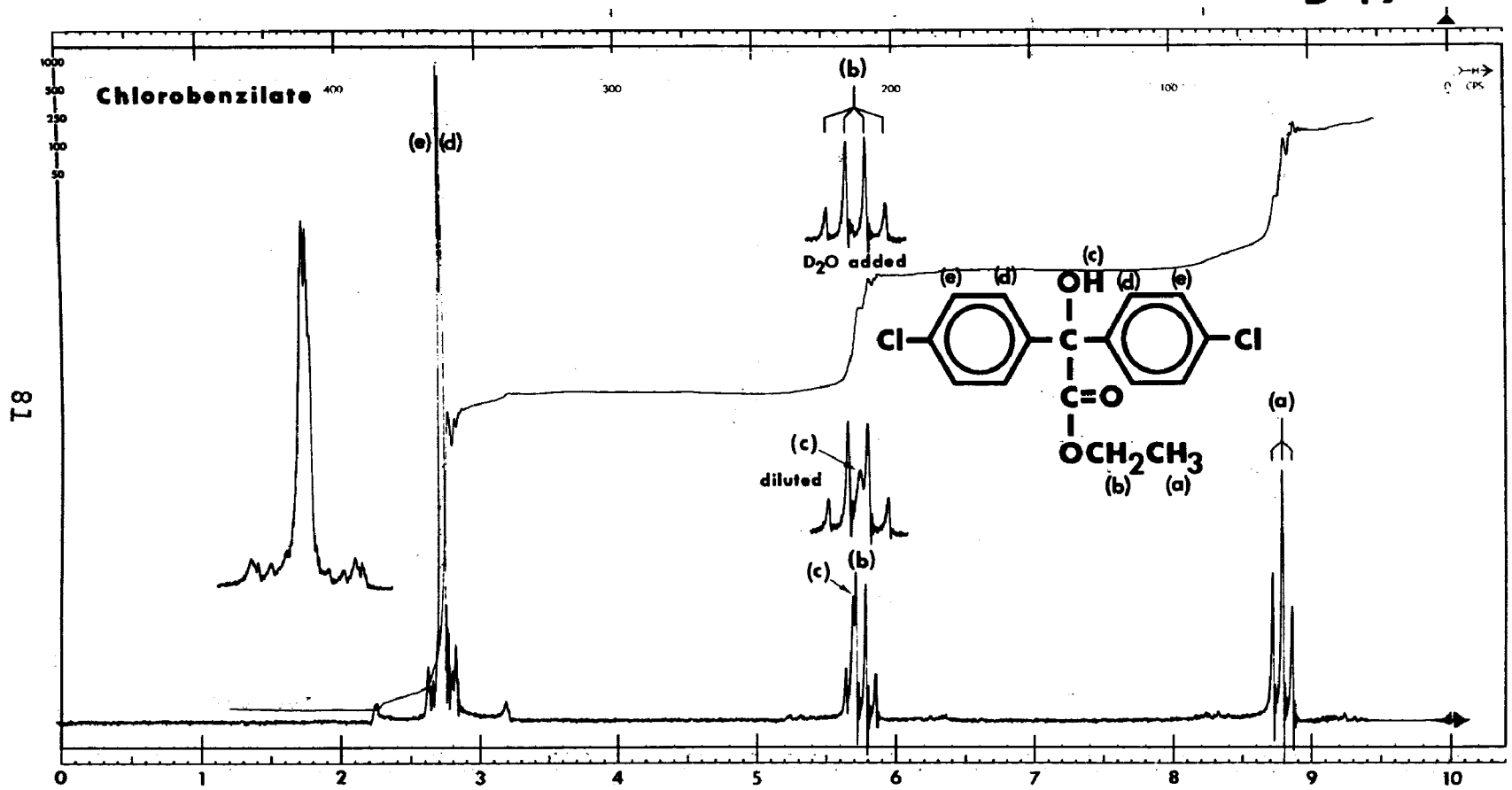
# B-18




80

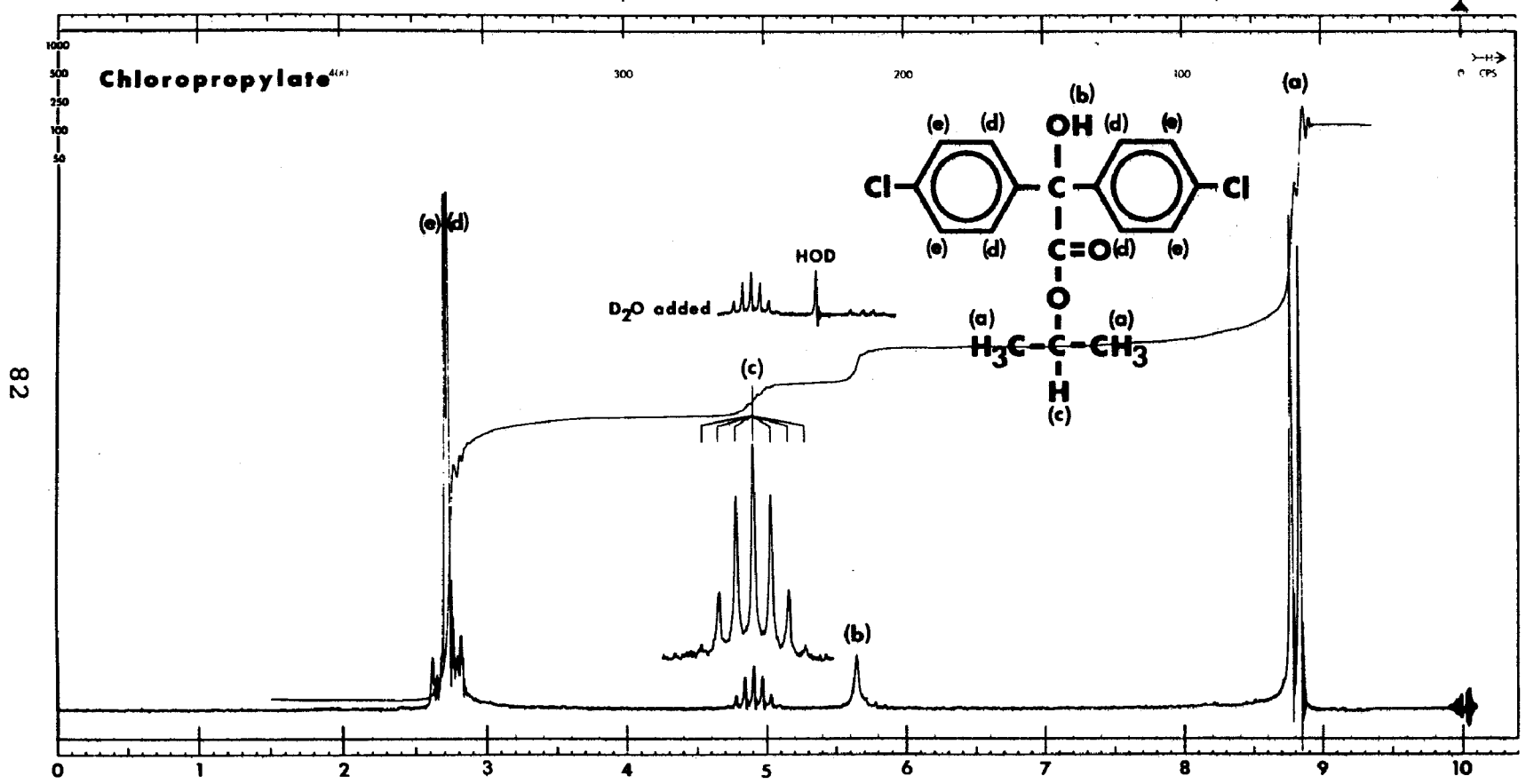
| | T |
|---|---|
| a | 7.12 |
| a' | 7.08 |
| b | 4.82 |
| c | 2.79 |

# B-19




| | T | J |
|---|---|---|
| a | 8.78 | 7 |
| b | 5.73 | 7 |
| c | 5.68 | |
| d | 2.72 | 9 |
| e | 2.68 | 9 |

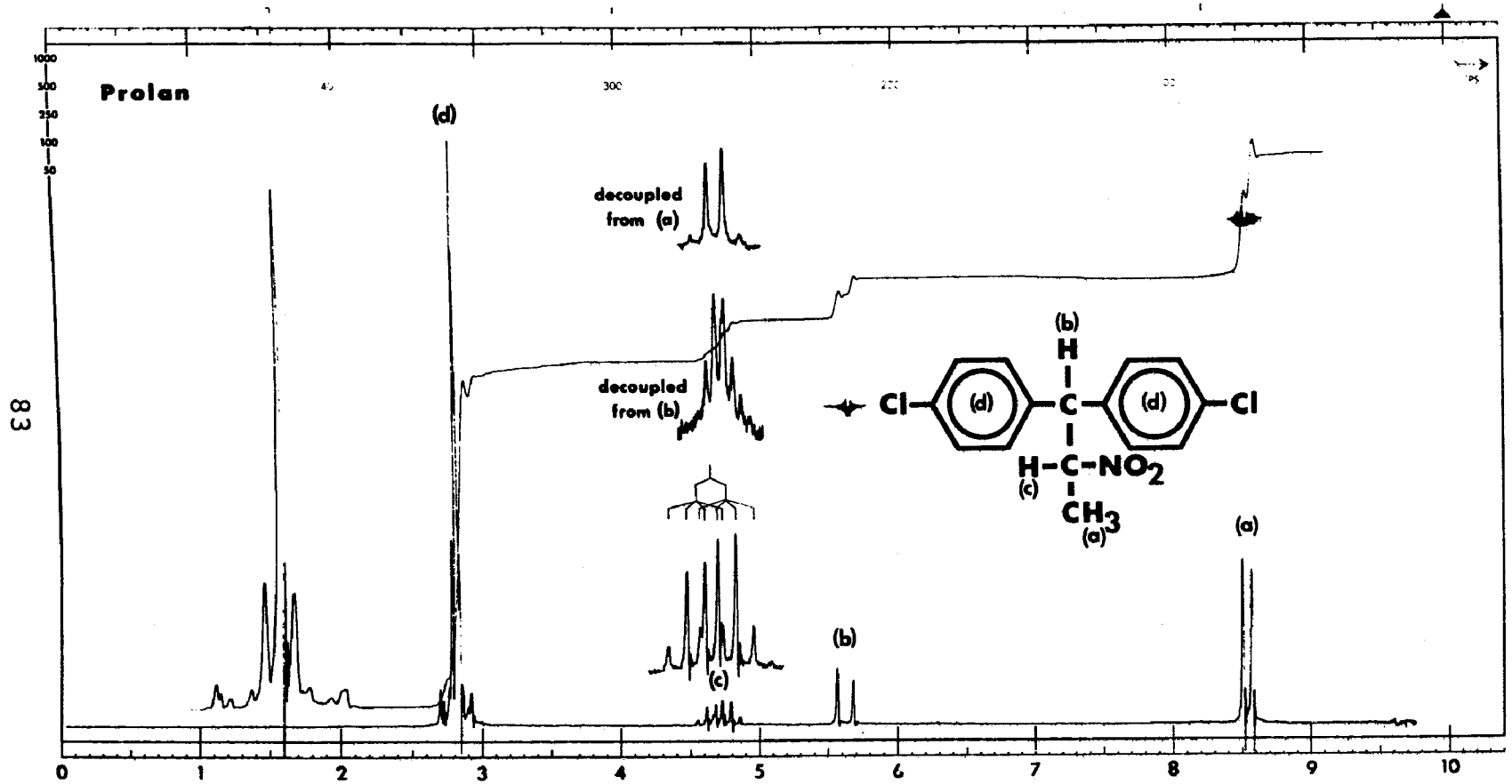
# B-20




82

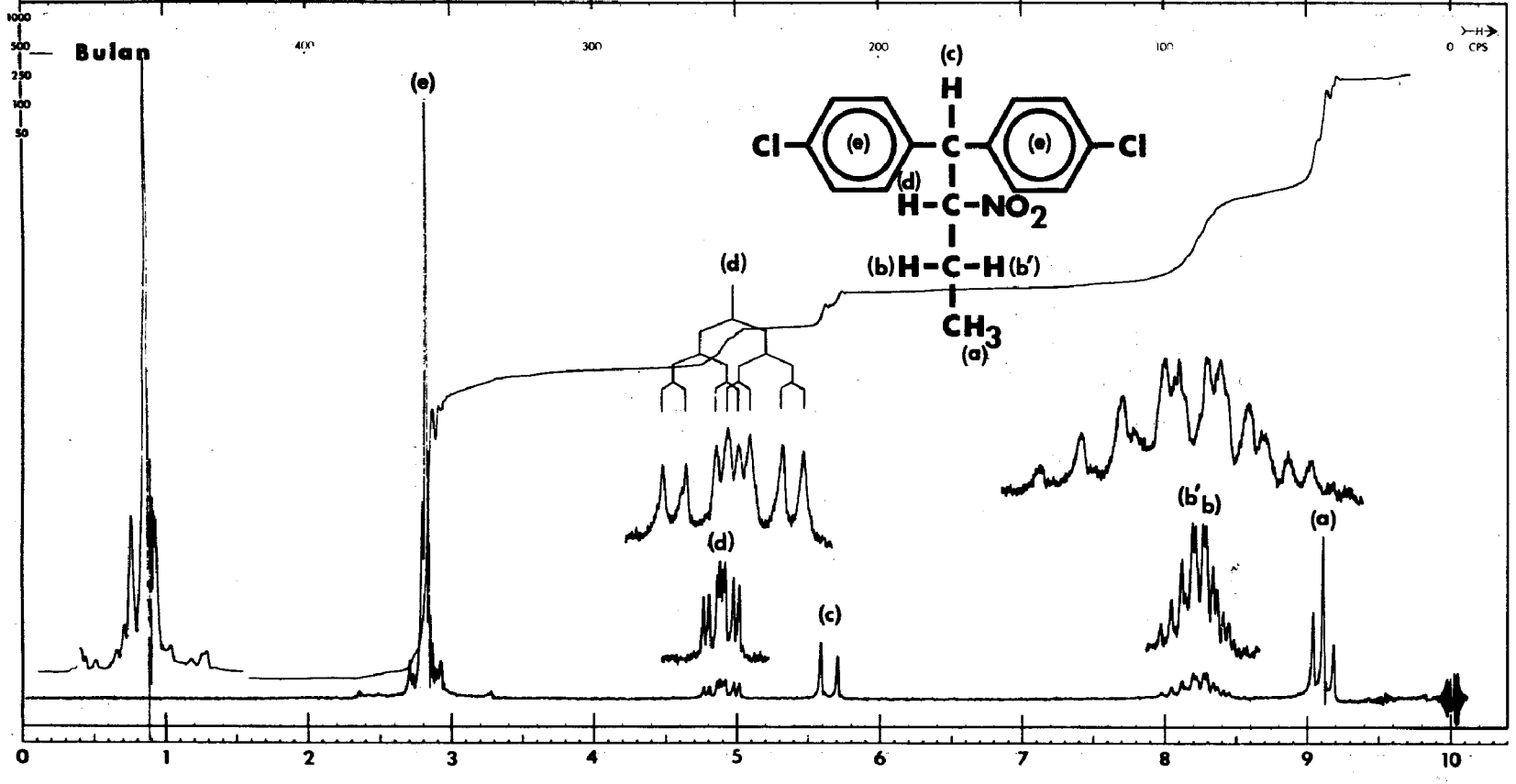
| | T | J |
|---|---|---|
| a | 8.79 | 6 |
| b | 5.63 | |
| c | 4.89 | 6 |
| d | 2.73 | 9 |
| e | 2.70 | 9 |

# B-21



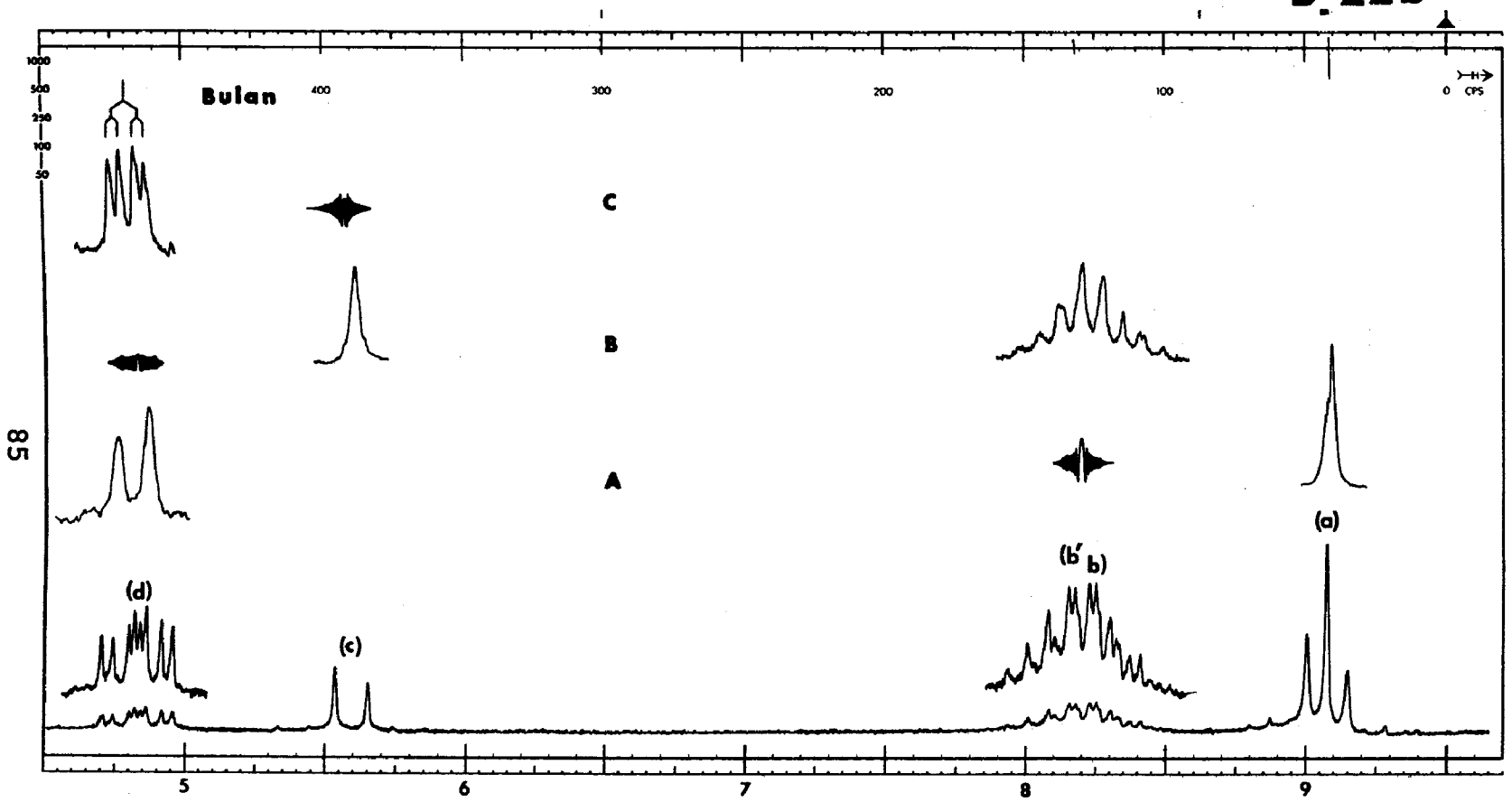

| | T | J |
|---|---|---|
| a | 8.54 | 6 |
| b | 5.62 | 12 |
| c | 4.70 | $\prec$ 6($H_c$-$H_a$) $\prec$ 12($H_c$-$H_b$) |
| d | 2.78 | |

# B-22a




| | T | J |
|---|---|---|
| a | 9.11 | 7 |
| b | 8.23 | |
| b′ | 8.25 | |
| c | 5.62 | 11.5 |
| d | 4.86 | 11.5($H_d$-$H_c$) |
| | | 9.5($H_d$-$H_b$) |
| | | 4 ($H_d$-$H_{b'}$) |
| e | 2.80 | |

# B-22b



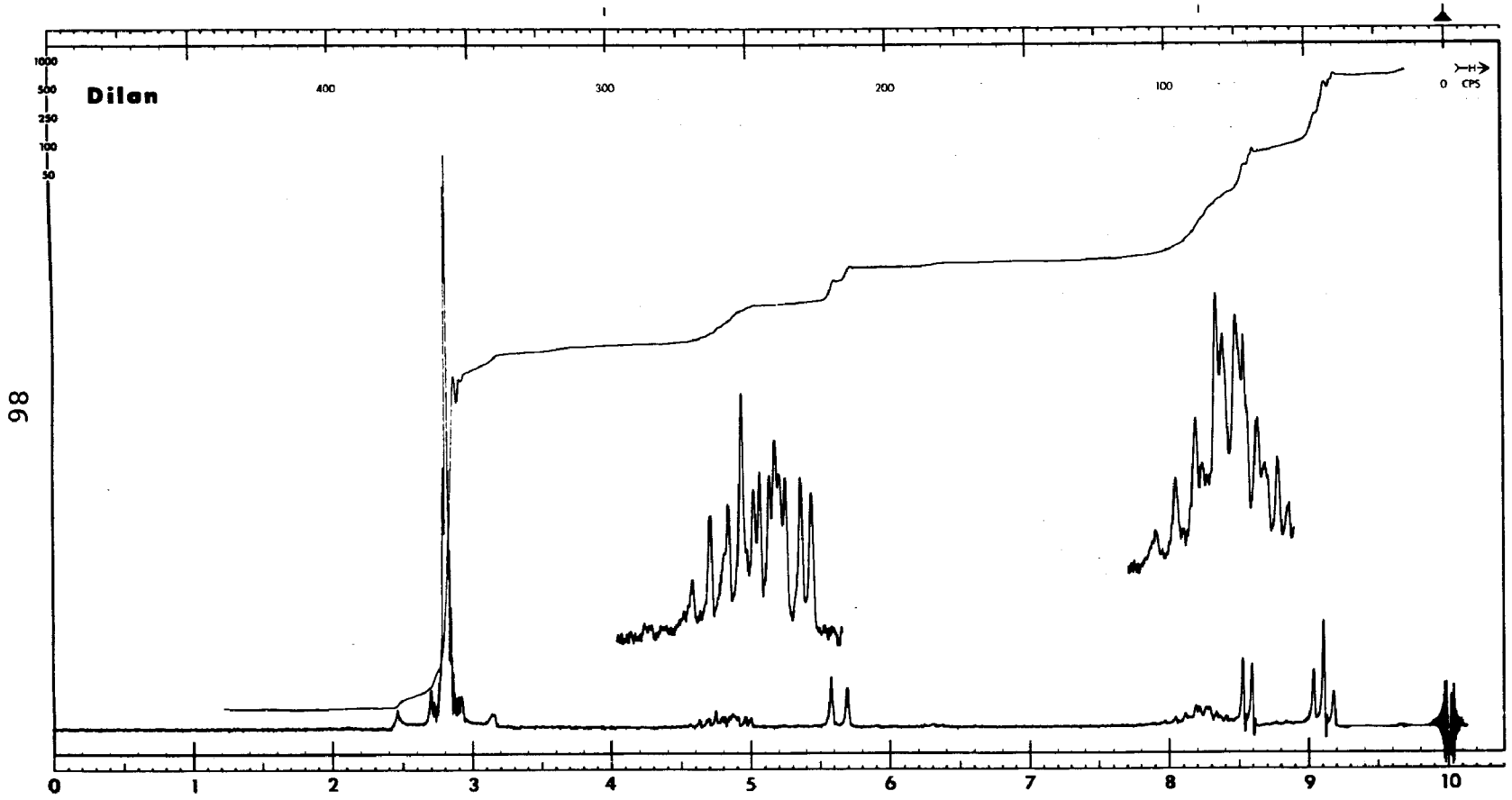

A $H_a$ & $H_d$ decoupled from $H_b$ & $H_{b'}$

B $H_c$, $H_b$ & $H_{b'}$ decoupled from $H_d$

C $H_d$ decoupled from $H_c$

Sweep Width 500 cps

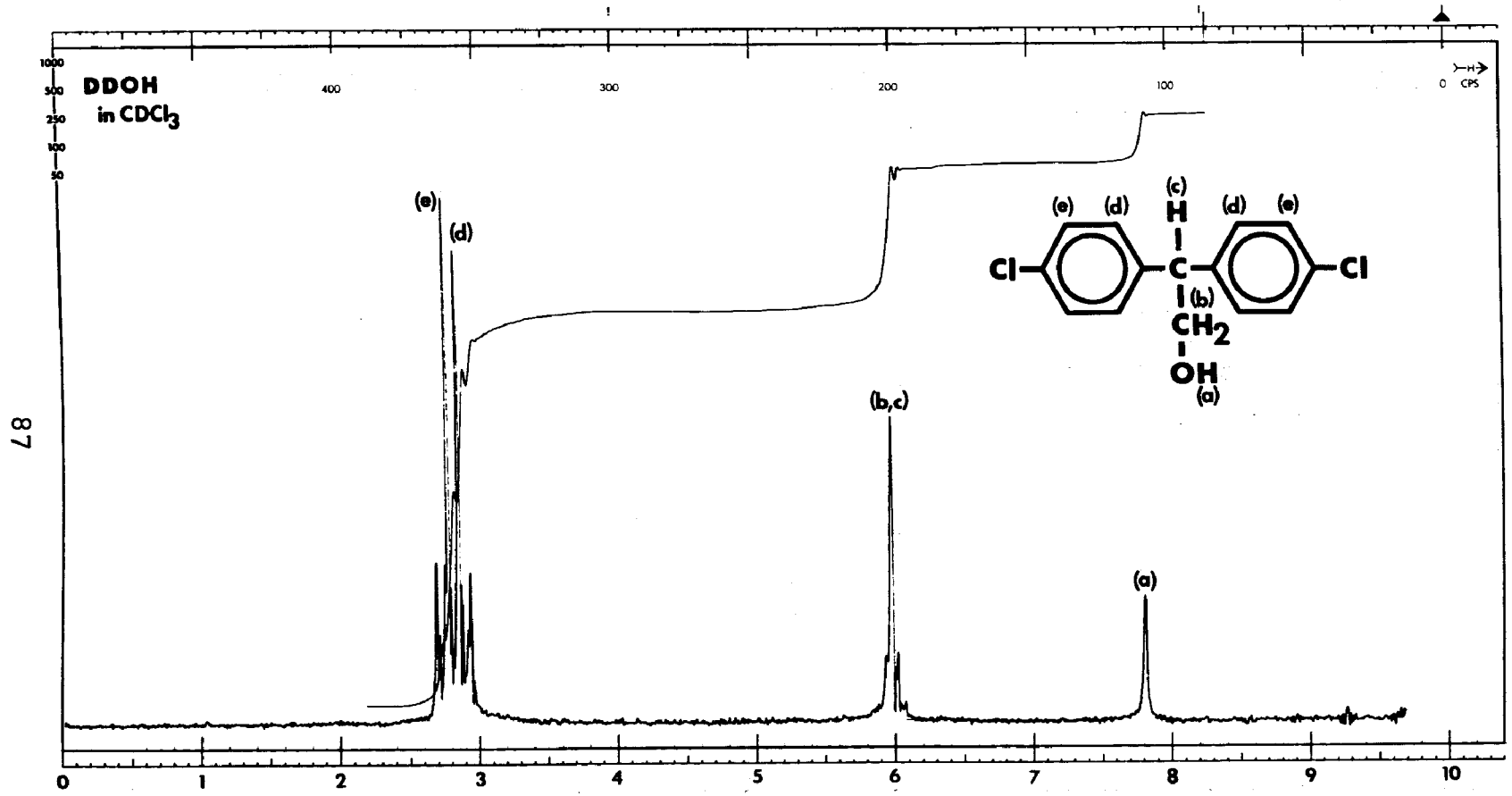
# B-23




**Mixture of**

**Prolan and Bulan**

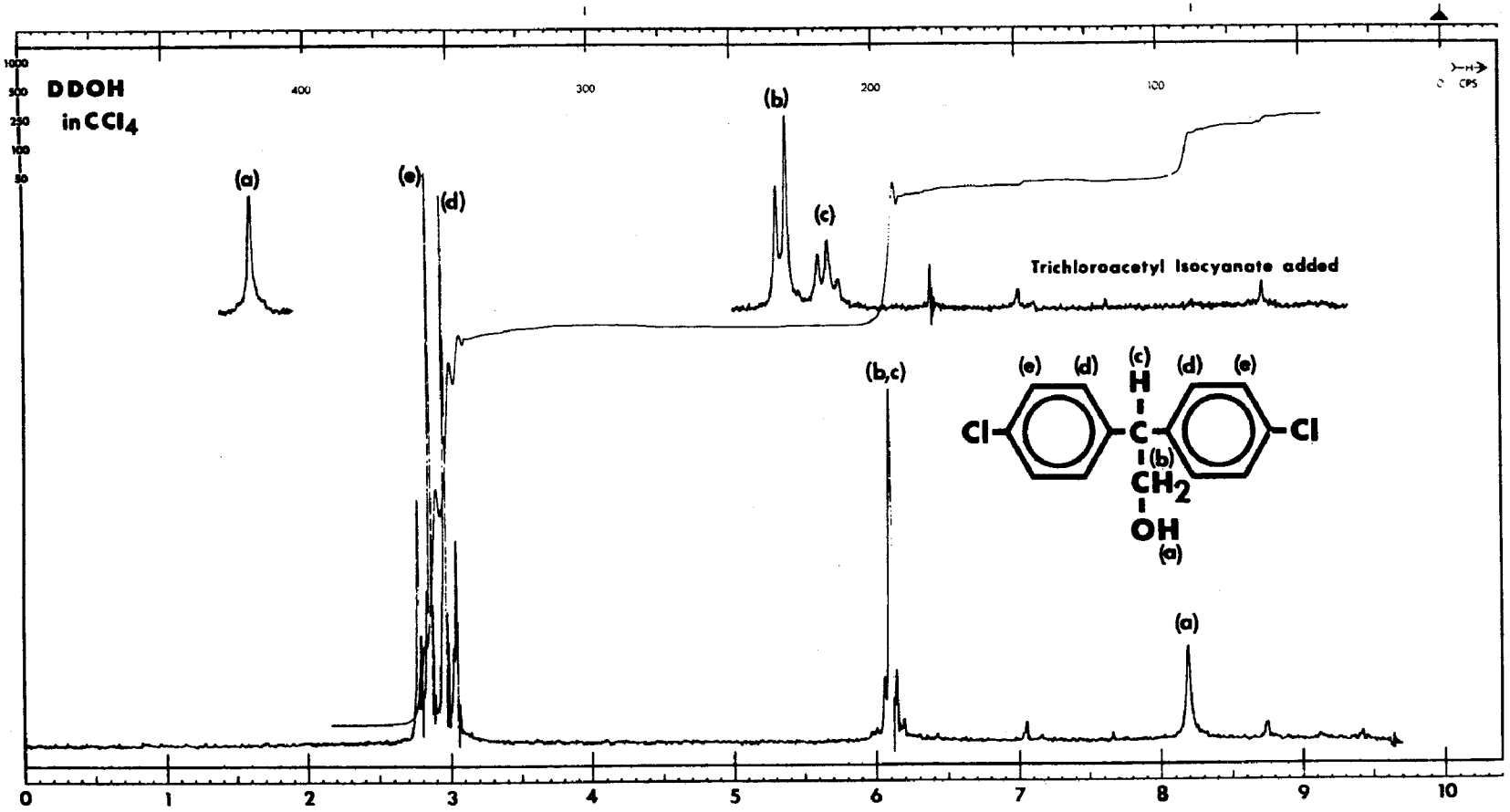
# B-24a



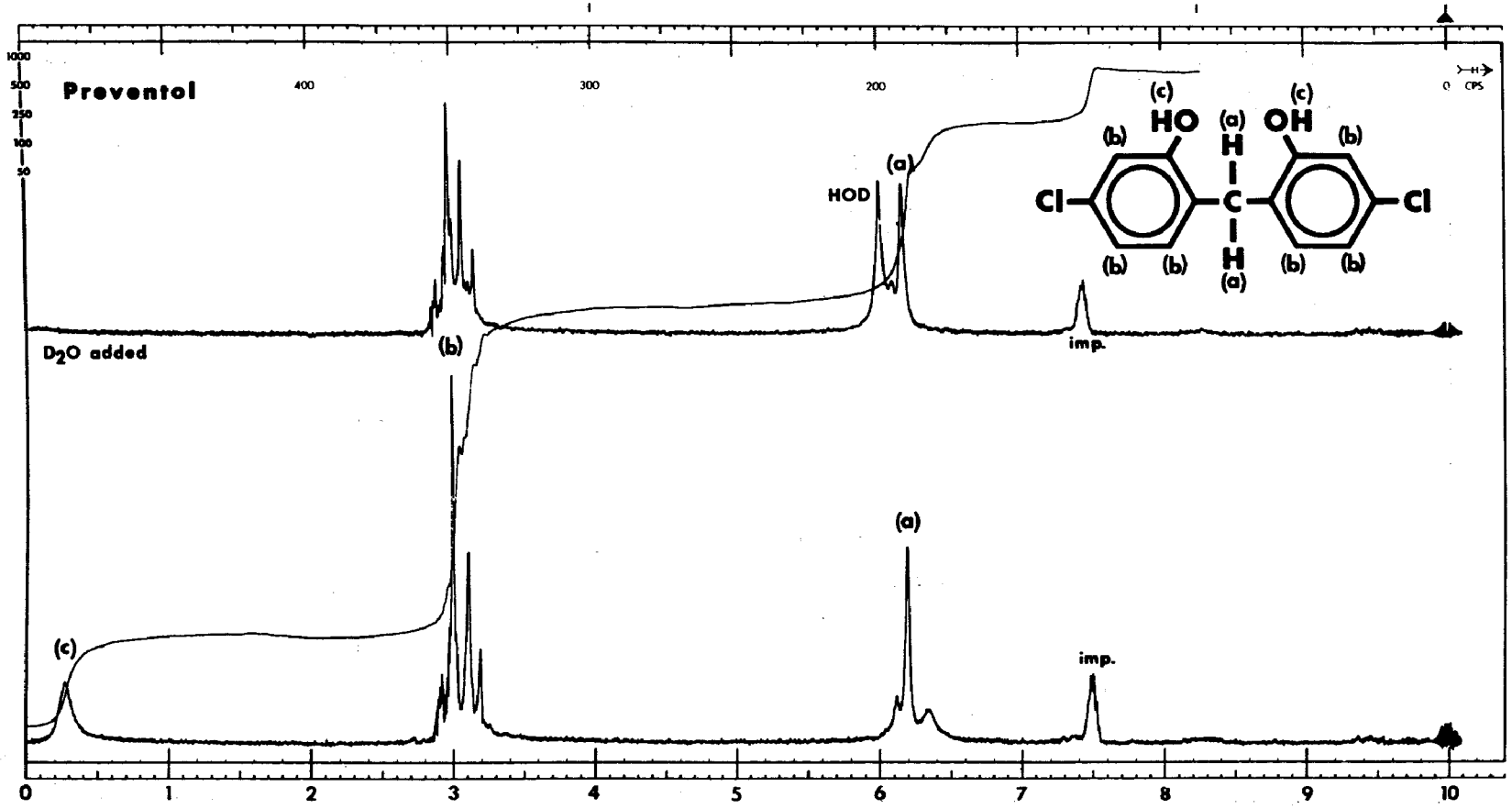

87

| | T | J |
|---|---|---|
| a | 7.82 | |
| b,c | 6.0 | |
| d | 2.90 | 9 |
| e | 2.75 | 9 |

# B-24b

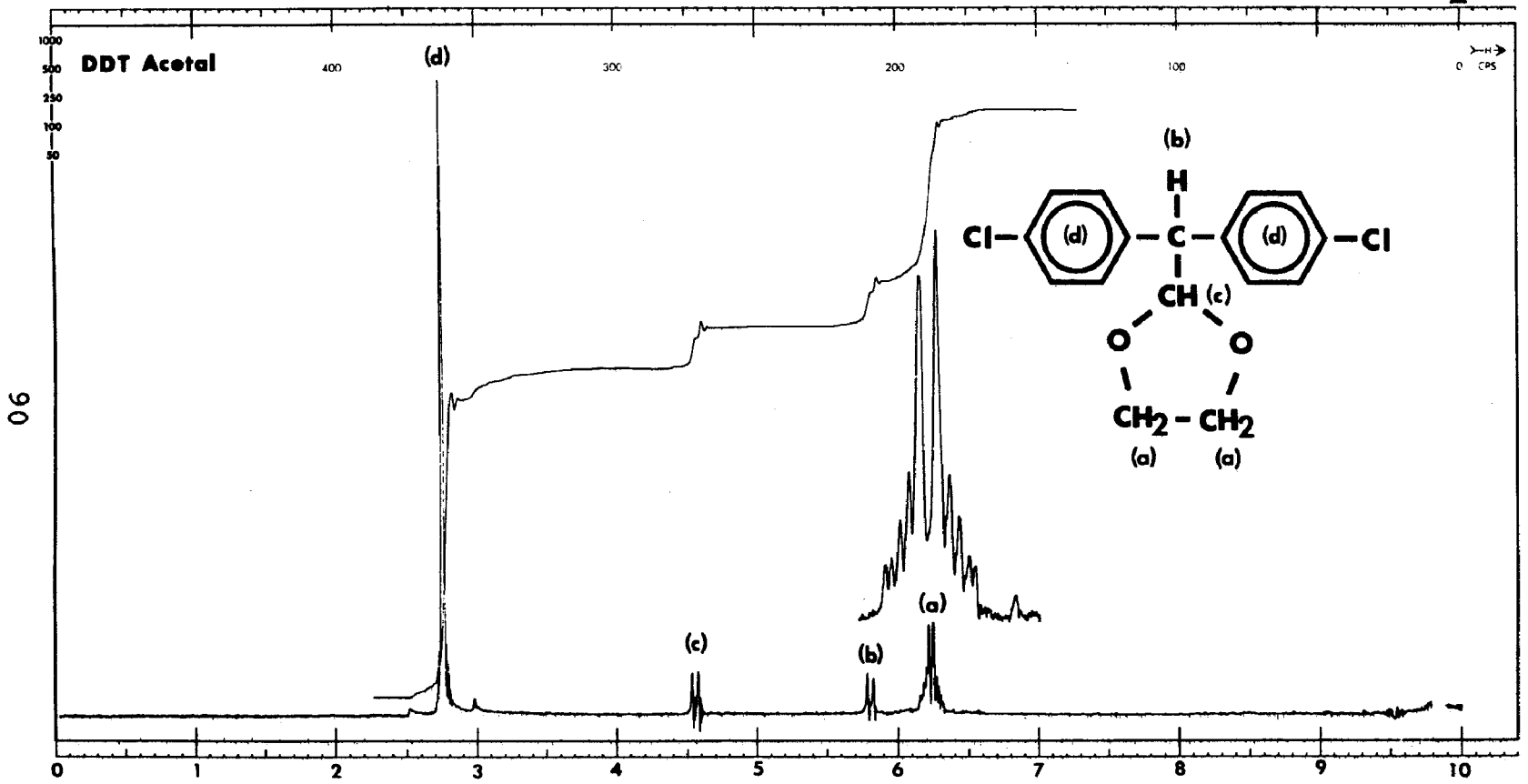



| | T | J |
|---|---|---|
| a | 8.19 | |
| b,c | 6.1 | |
| d | 2.97 | 9 |
| e | 2.81 | 9 |

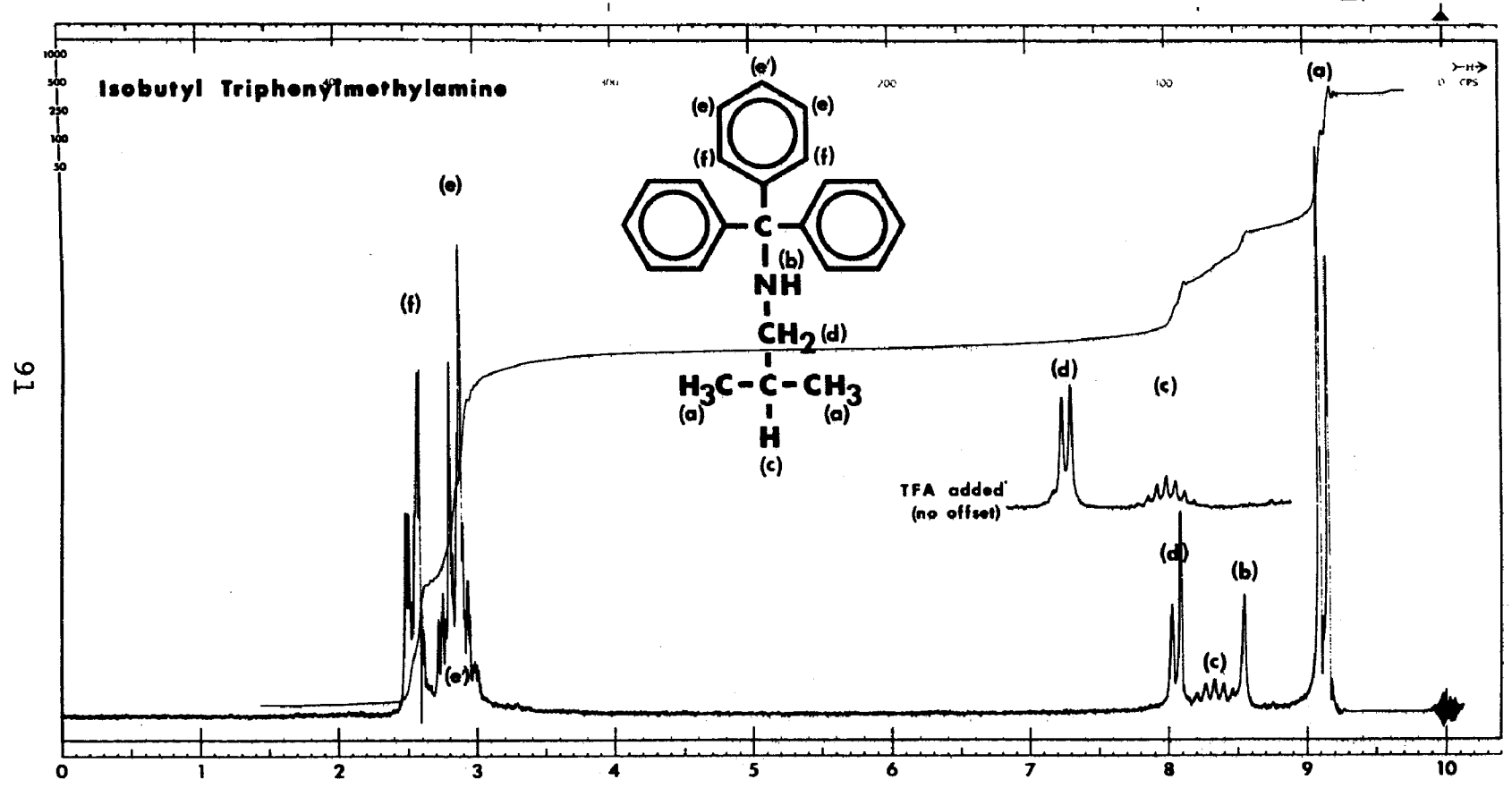



| T | |
|---|---|
| a | 6.17 |
| b | 2.9-3.1 |
| c | 0.3 |

# B-26



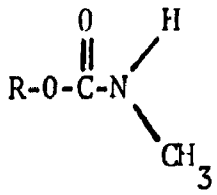

| | T | J |
|---|---|---|
| a | 6.24 | |
| b | 5.82 | 4 |
| c | 4.57 | 4 |
| d | 2.77 | |




| | T | J |
|---|---|---|
| a | 9.11 | 7 |
| b | 8.54 | |
| c | 8.33 | |
| d | 8.05 | 6 |
| e,e' | 2.7-3.0 | |
| f | 2.4-2.6 | |

THE CARBAMATE PESTICIDES

Thirteen carbamate pesticides included in this study have the general structure:



In all cases, the methyl protons resonate in a narrow range from τ7.20-7.29 and produce a doublet (J = 5 Hz) due to coupling of the methyl protons with the amide proton.

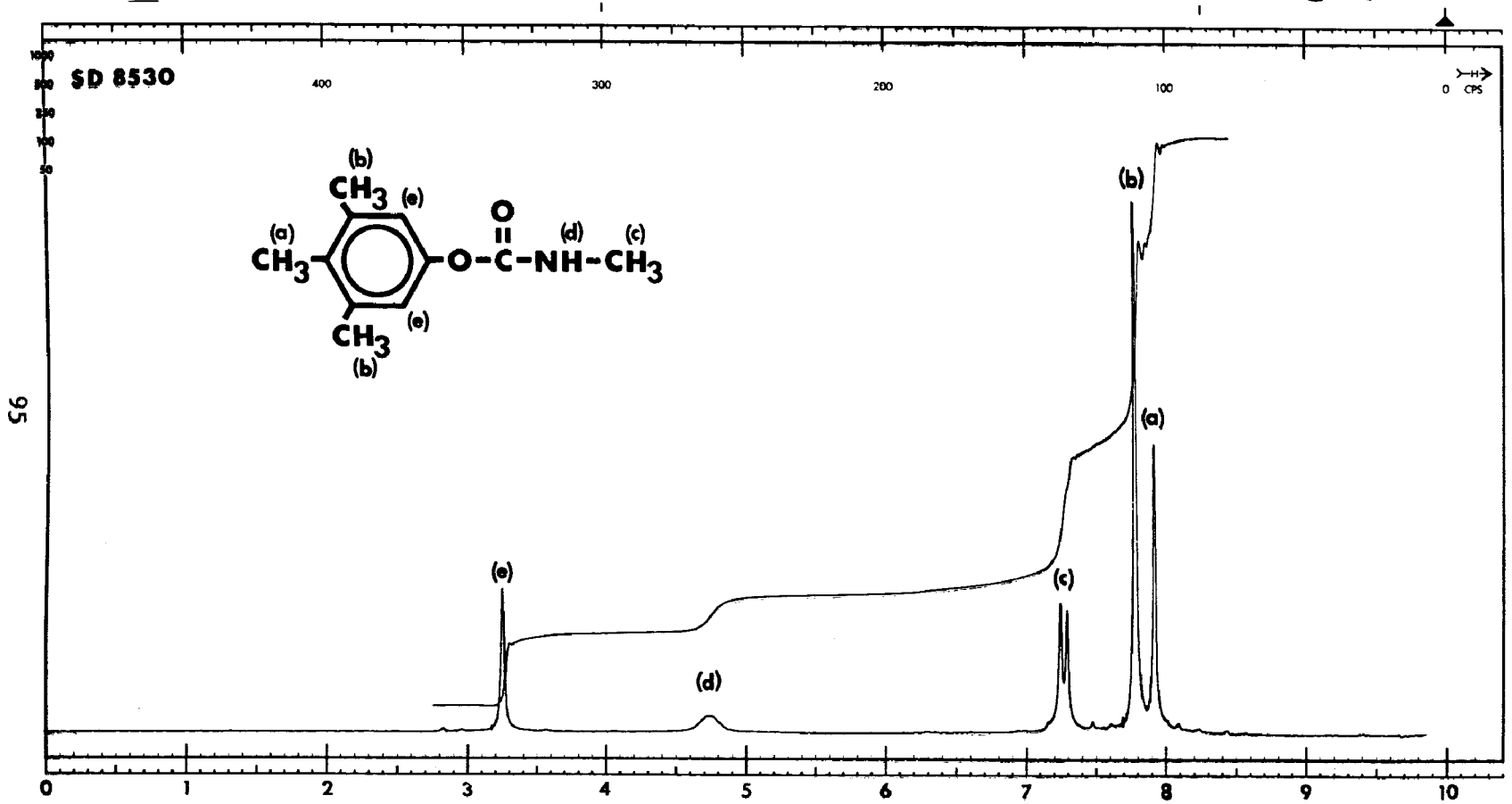
Although hindered rotation about the N-C=O bond of amides is quite common and produces both the cis and trans isomers, this phenomenon is observed at ambient temperature in only one of the N-monosubstituted carbamates, Azak. Other investigators (7,8) have also reported hindered rotation about the N-C=O bond in carbamates at low temperature but essentially free rotation at higher temperatures. In Azak, the bulky t-butyl groups substituted on the benzene ring in the ortho positions must sterically hinder rotation -- a signal is observed for each isomeric form at ambient temperature. Both N,N-dimethyl carbamates included in this study (Dimetilan and isolan) exhibit hindered rotation at ambient temperature and produce signals for both rotomer forms.

The chemical shifts of both the NH and $NCH_3$ proton signals of Zectran are dependent on solvent and concentration. Various concentrations of Zectran in three different solvents were used to study the effects of solute-solute and solute-solvent association (5).

The signals of the protons near or adjacent to nitrogen in many of these compounds show broadening due to the quadrupole moment of the nitrogen

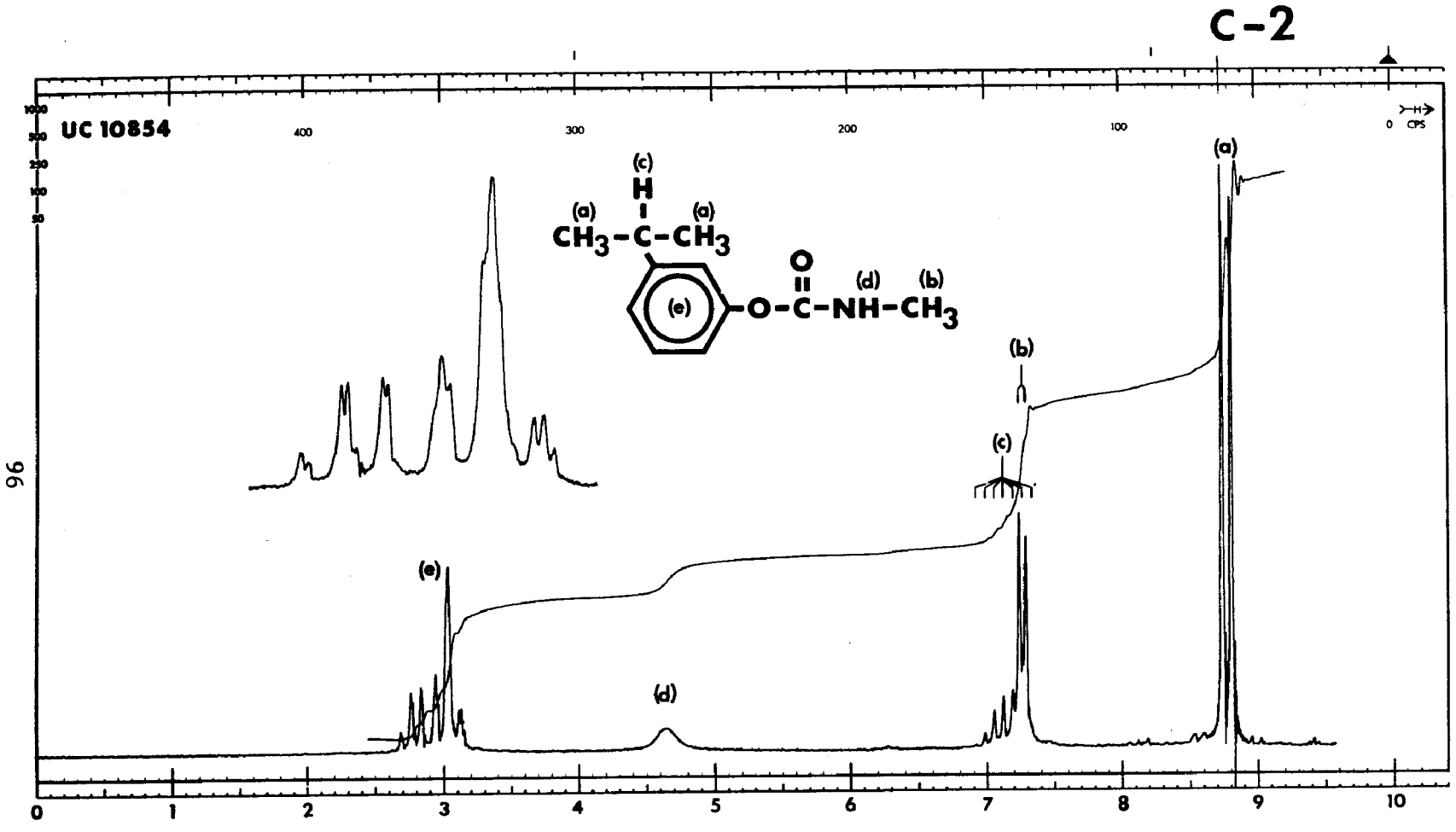
nucleus as well as some hindrance to rotation (7, 9). Increasing the sample temperature sharpens peaks that are broadened due to one or both effects (10, 11). Low temperature studies (5) confirmed that rotation is hindered in both the thiolcarbamates (example: sutan) and the dithiocarbamates (example: Vegadex).

# C-1




| | T | J |
|---|---|---|
| a | 7.91 | |
| b | 7.76 | |
| c | 7.26 | 5 |
| d | 4.7 | |
| e | 3.25 | |

# C-2

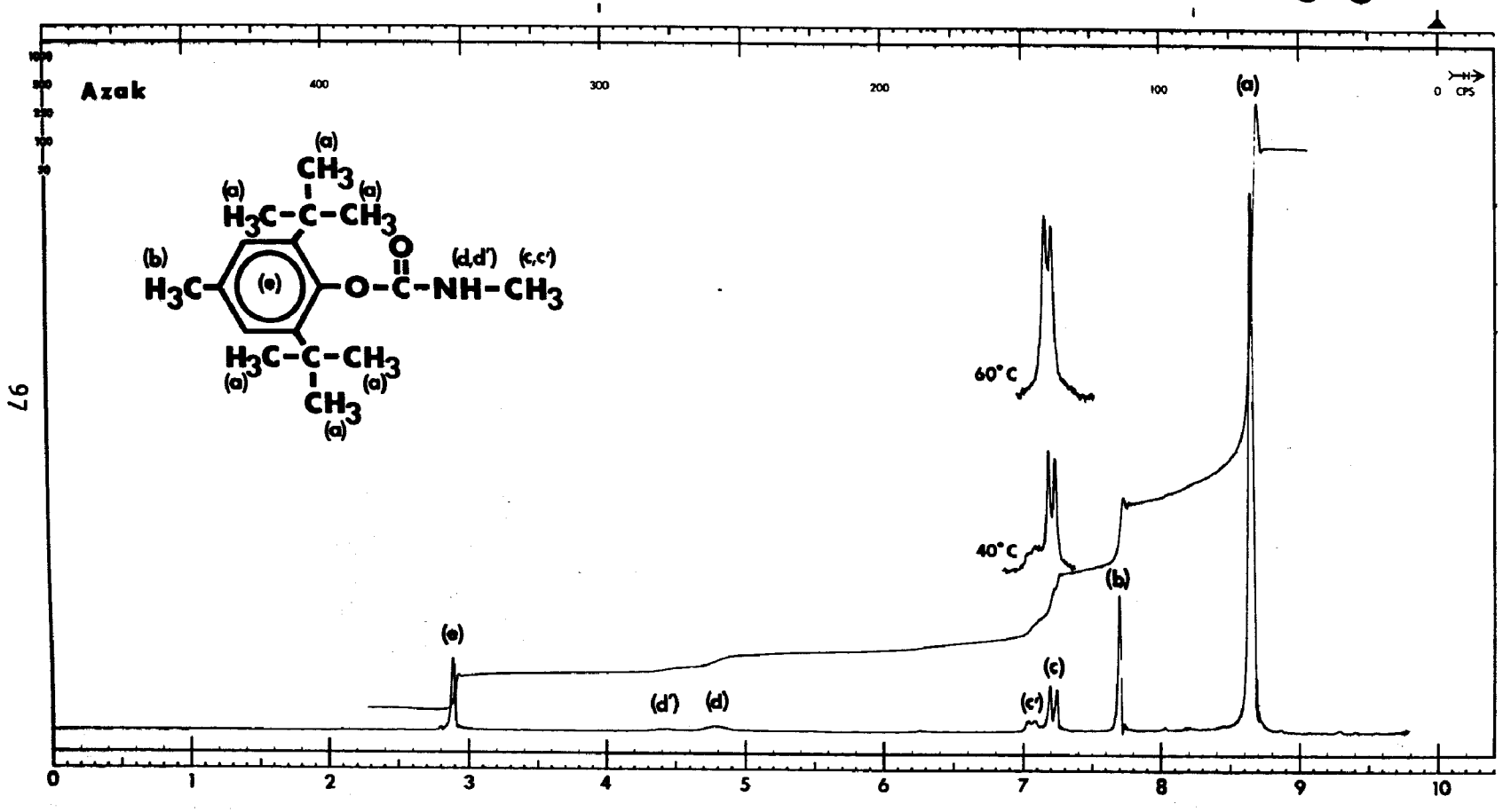






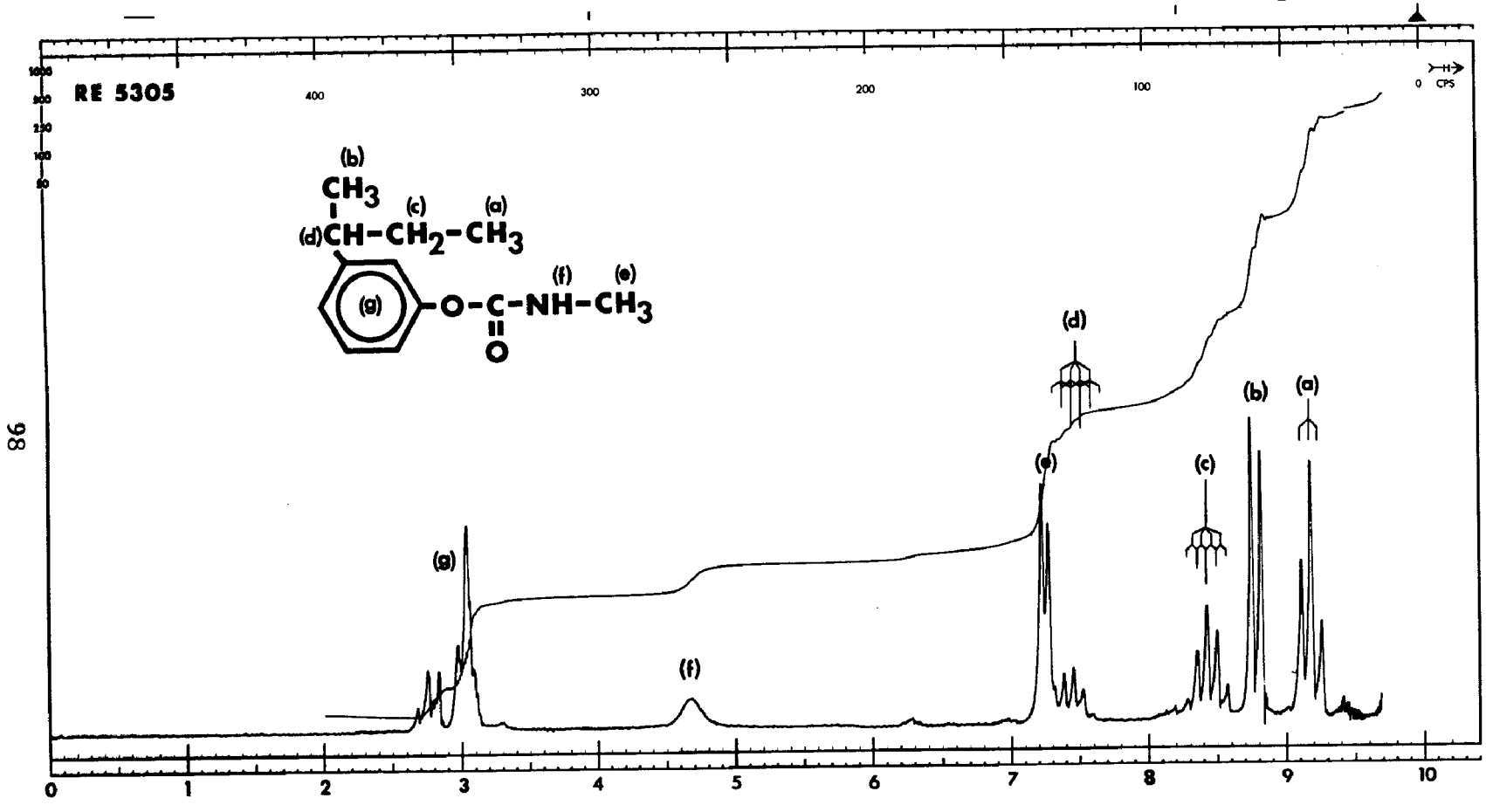
| | T | J |
|---|---|---|
| a | 8.77 | 7 |
| b | 7.26 | 5 |
| c | 7.12 | 7 |
| d | 4.6 | |
| e | 2.6-3.2 | |

# C-3



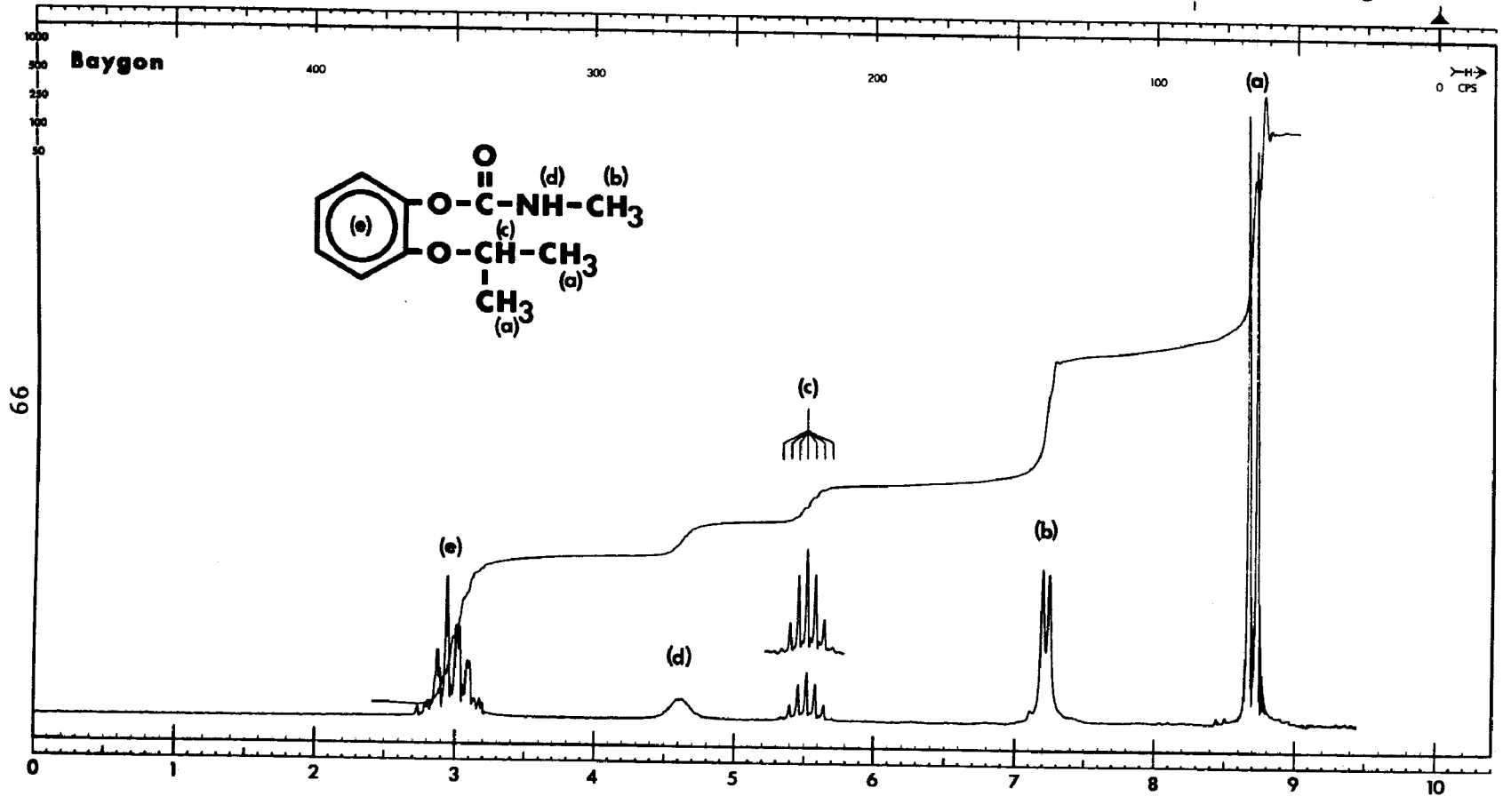

| | T | J |
|---|---|---|
| a | 8.64 | |
| b | 7.65 | |
| c | 7.22 | 5 |
| c' | 7.06 | 5 |
| d' | 4.8 | |
| d | 4.4 | |
| e | 2.88 | |

# C-4



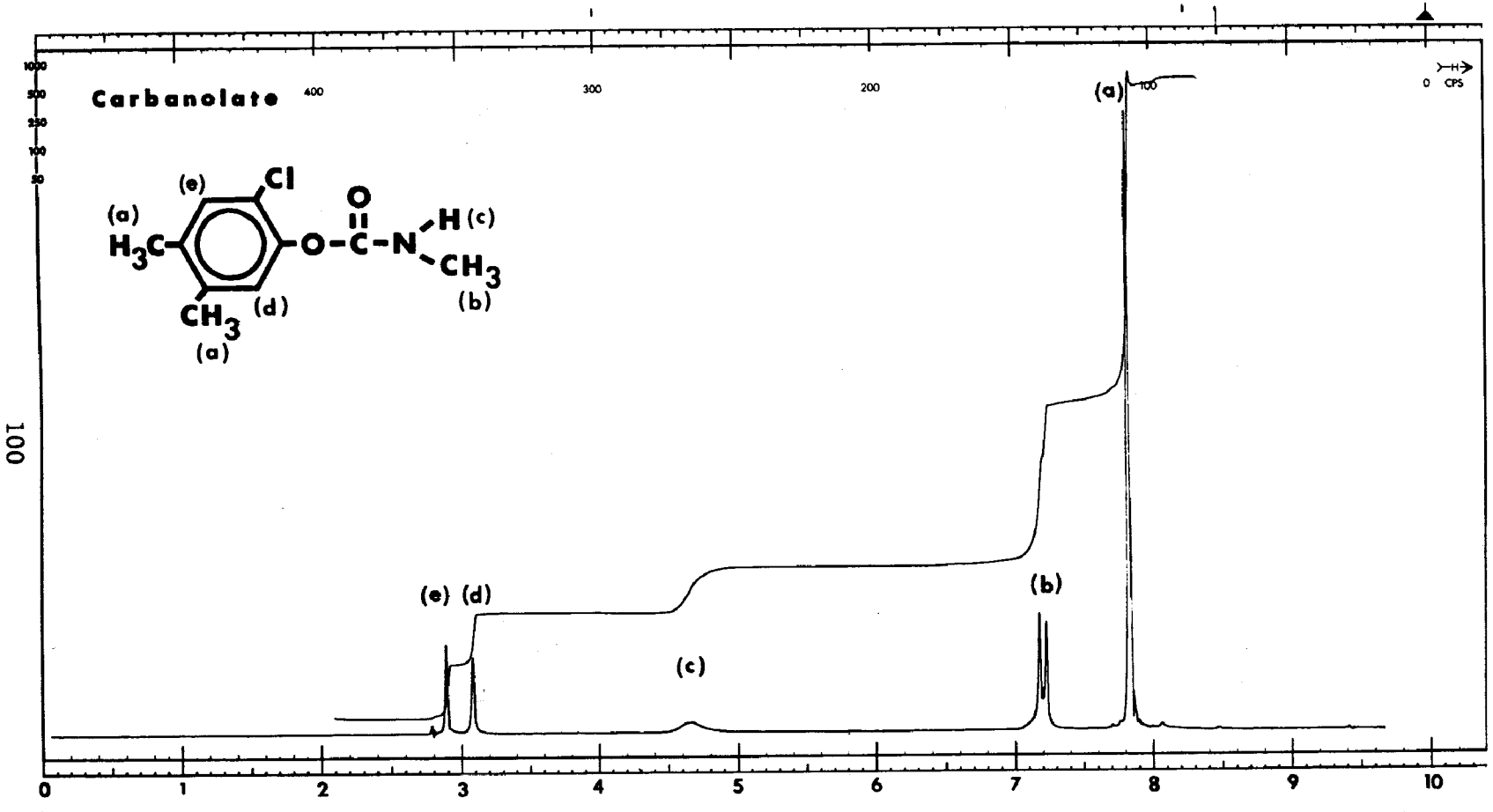

| | T | J |
|---|---|---|
| a | 9.19 | 7 |
| b | 8.78 | 7 |
| c | 8.43 | 7 |
| d | 7.50 | 7 |
| e | 7.25 | 5 |
| f | 4.5 | |
| g | 2.7-3.1 | |

# C-5



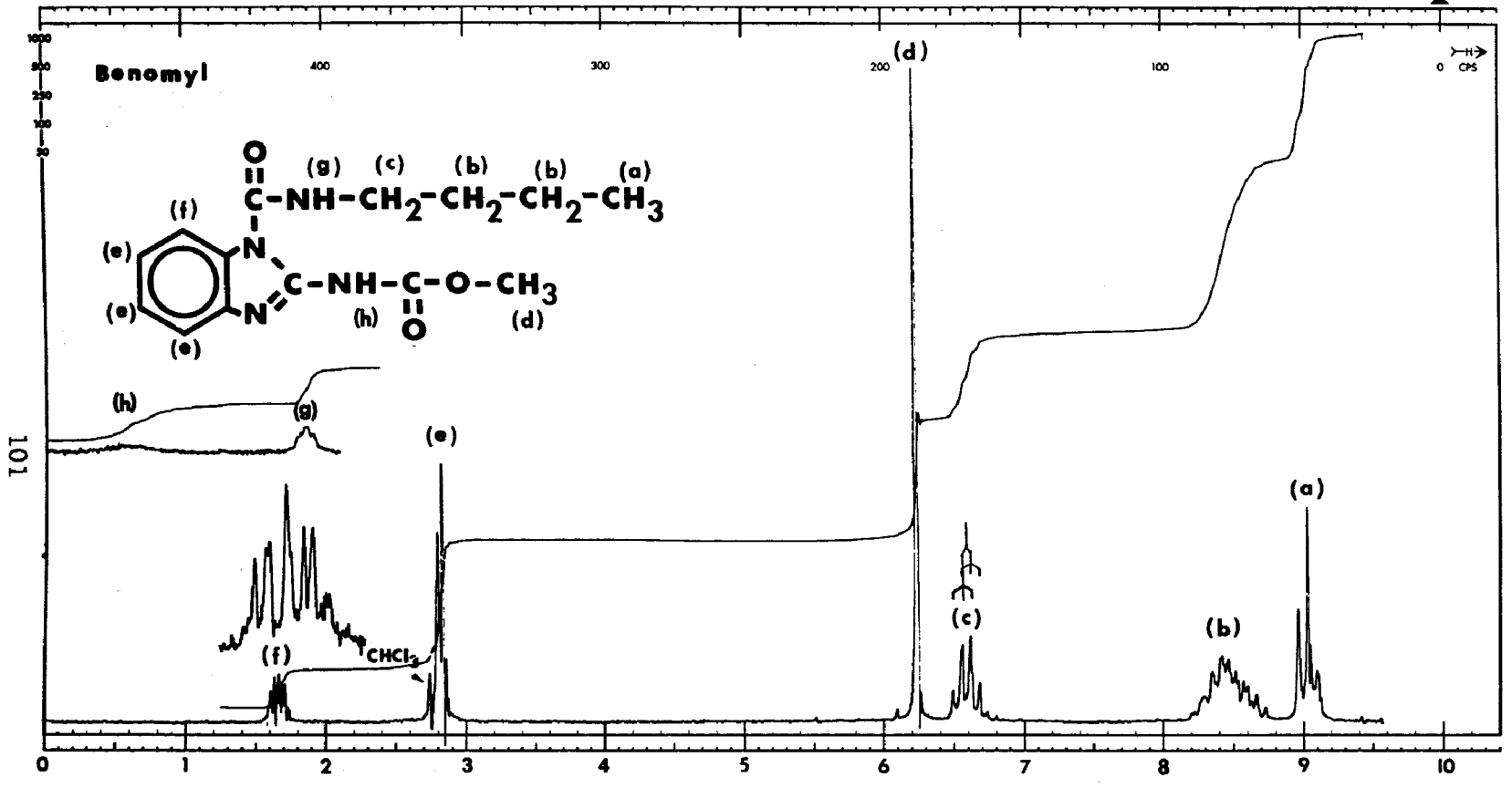

| | T | J |
|---|---|---|
| a | 8.70 | 6 |
| b | 7.22 | 5 |
| c | 5.52 | 6 |
| d | 4.6 | |
| e | 2.7-3.2 | |

# C-6



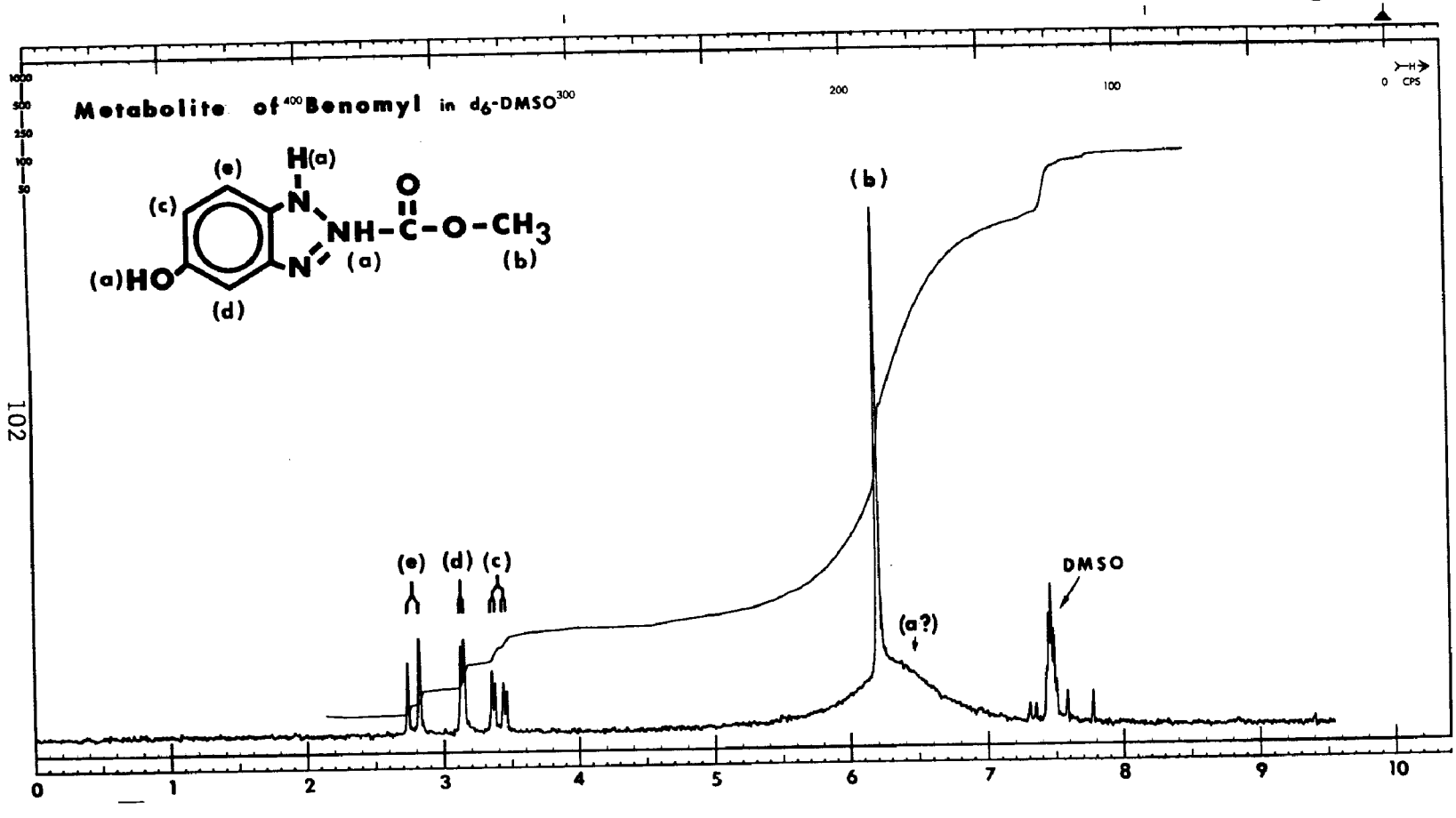

| | T | J |
|---|---|---|
| a | 7.83 | |
| b | 7.20 | 5 |
| c | 4.70 | |
| d | 3.07 | |
| e | 2.87 | |

# C-7



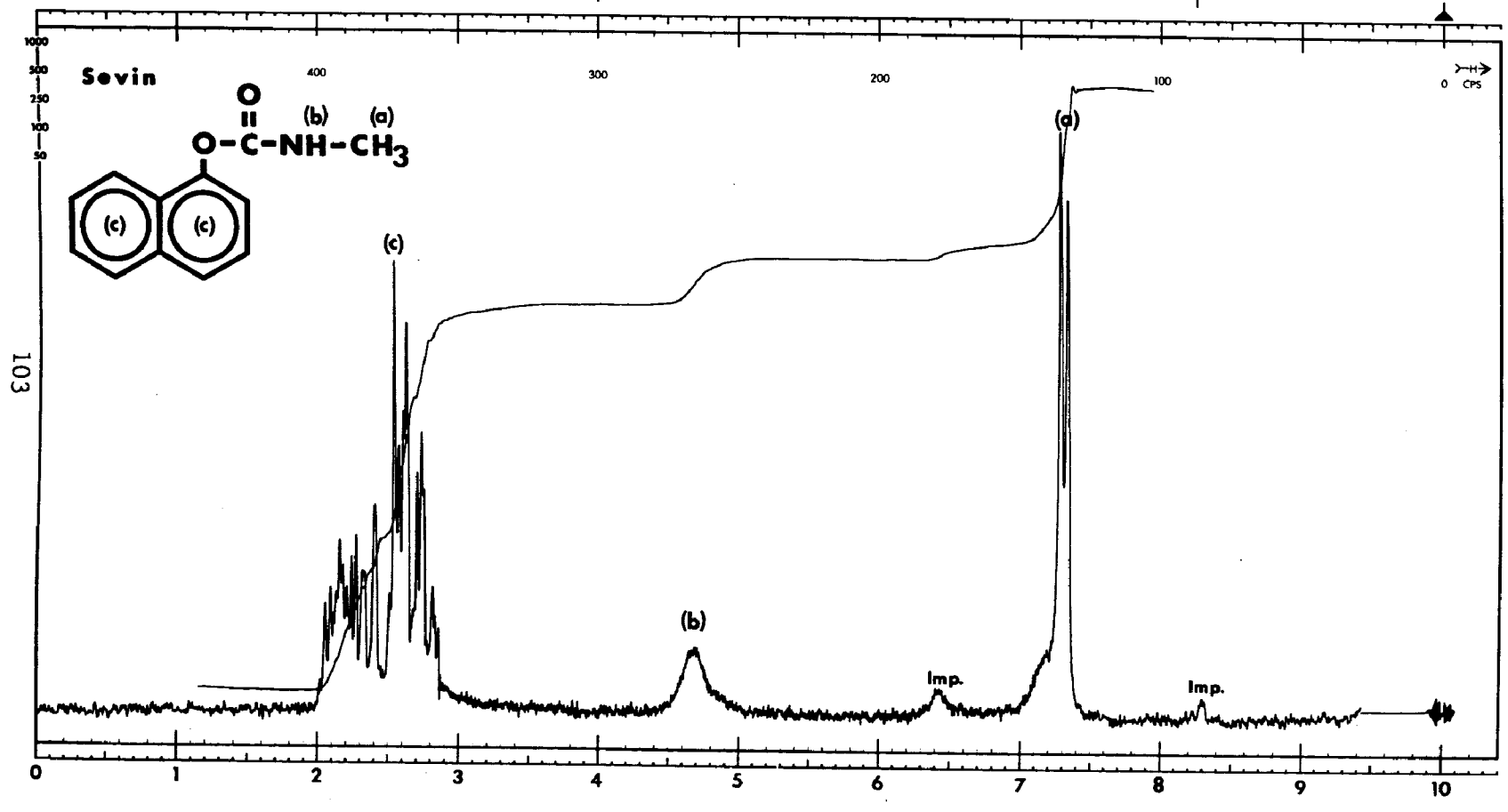

| | T | J |
|---|---|---|
| a | 9.02 | 7 |
| b | 8.2–8.7 | |
| c | 6.57 | $7(H_b-H_c)$ |
| d | 6.20 | $6(H_c-H_g)$ |
| e | 2.80 | |
| f | 1.66 | |
| g | - 0.14 | |
| h | - 1.4 | |

# C-8



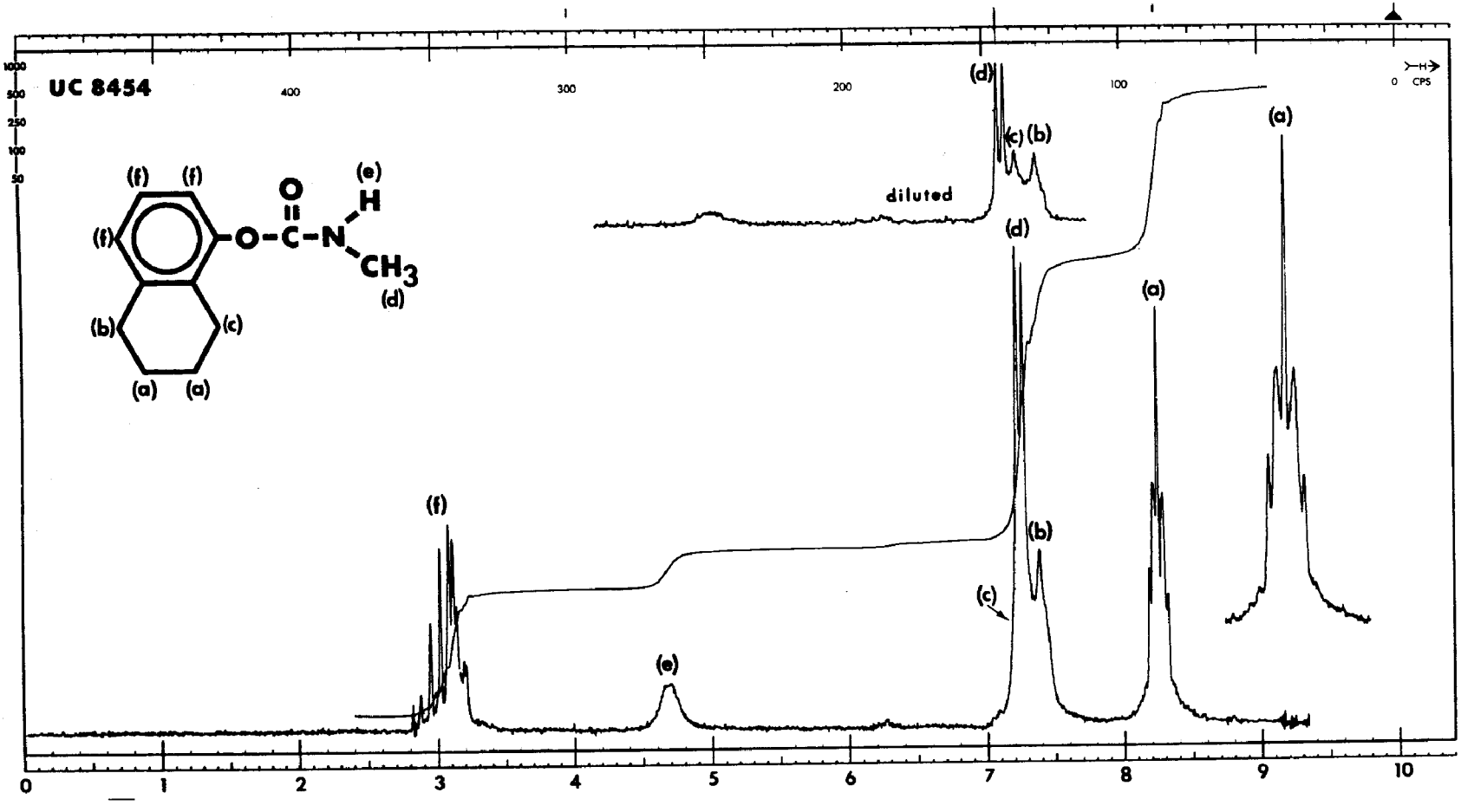

| | T | J |
|---|---|---|
| a | 6.30 | |
| b | 6.19 | |
| c | 3.40 | 8.5($H_c$-$H_e$)<br>2.5($H_c$-$H_d$) |
| d | 3.12 | 2.5($H_c$-$H_d$) |
| e | 2.76 | 4.5($H_c$-$H_e$) |

# C-9



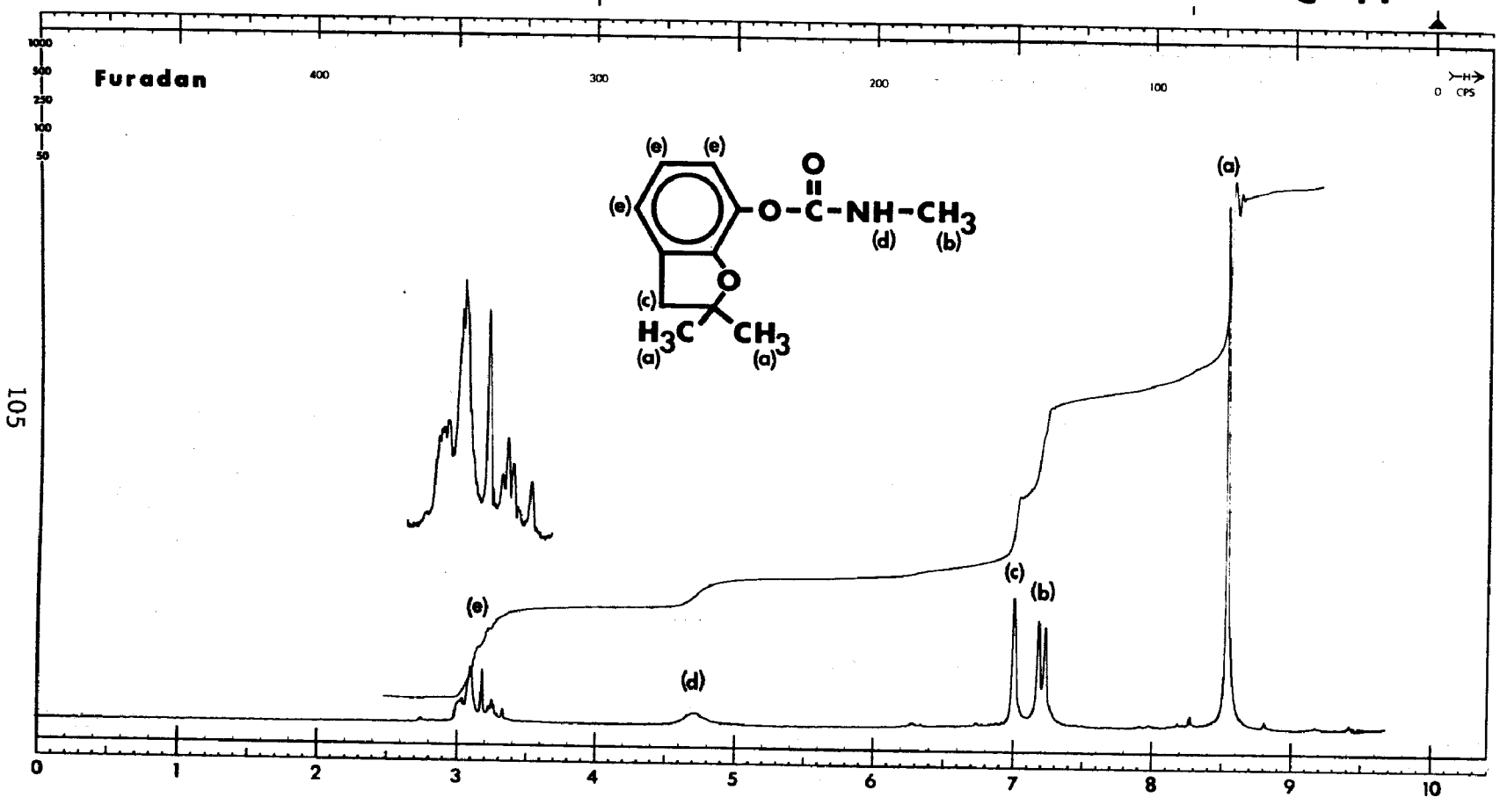

| | T | J |
|---|---|---|
| a | 7.29 | 5 |
| b | 4.7 | |
| c | 2.0-2.8 | |

# C-10



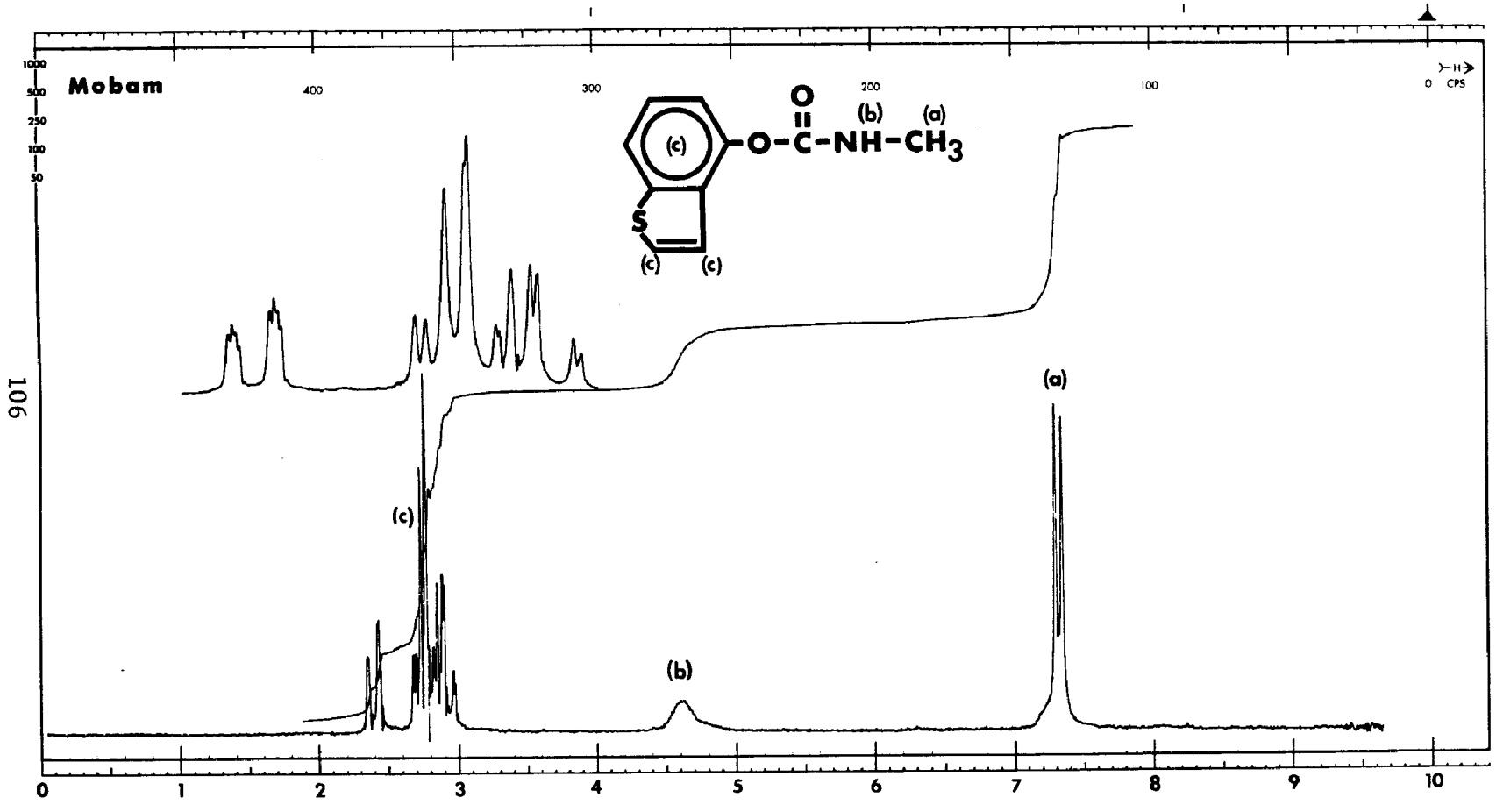

| | T | J |
|---|---|---|
| a | 8.24 | |
| b | 7.38 | |
| c | 7.2 | |
| d | 7.24 | 5 |
| e | 4.7 | |
| f | 2.9–3.2 | |

# C-11




| | T | J |
|---|---|---|
| a | 8.52 | |
| b | 7.20 | 5 |
| c | 7.00 | |
| d | 4.7 | |
| e | 3.0-3.3 | |

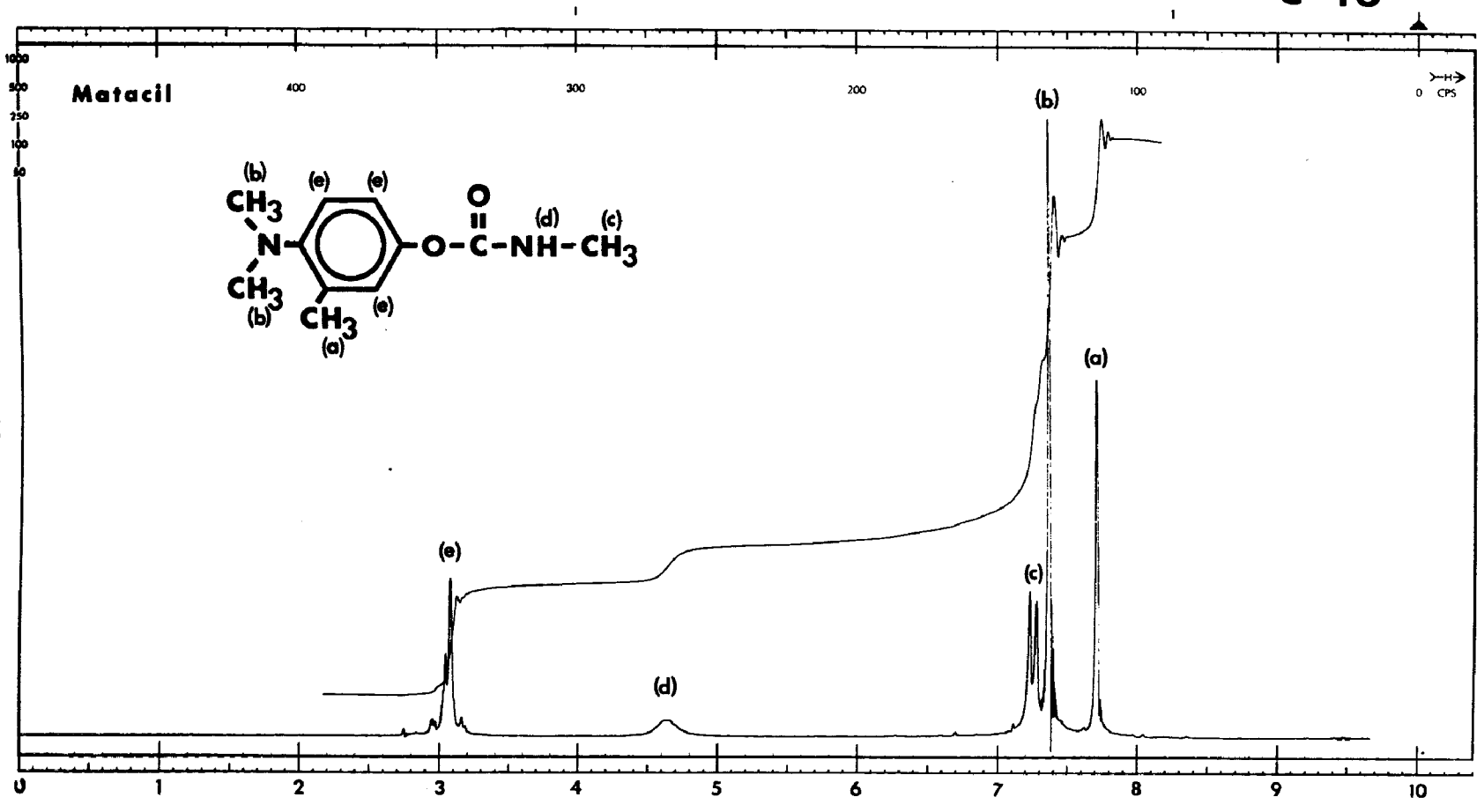
# C-12




106

| | T | J |
|---|---|---|
| a | 7.32 | 5 |
| b | 4.59 | |
| c | 2.3-3.0 | |

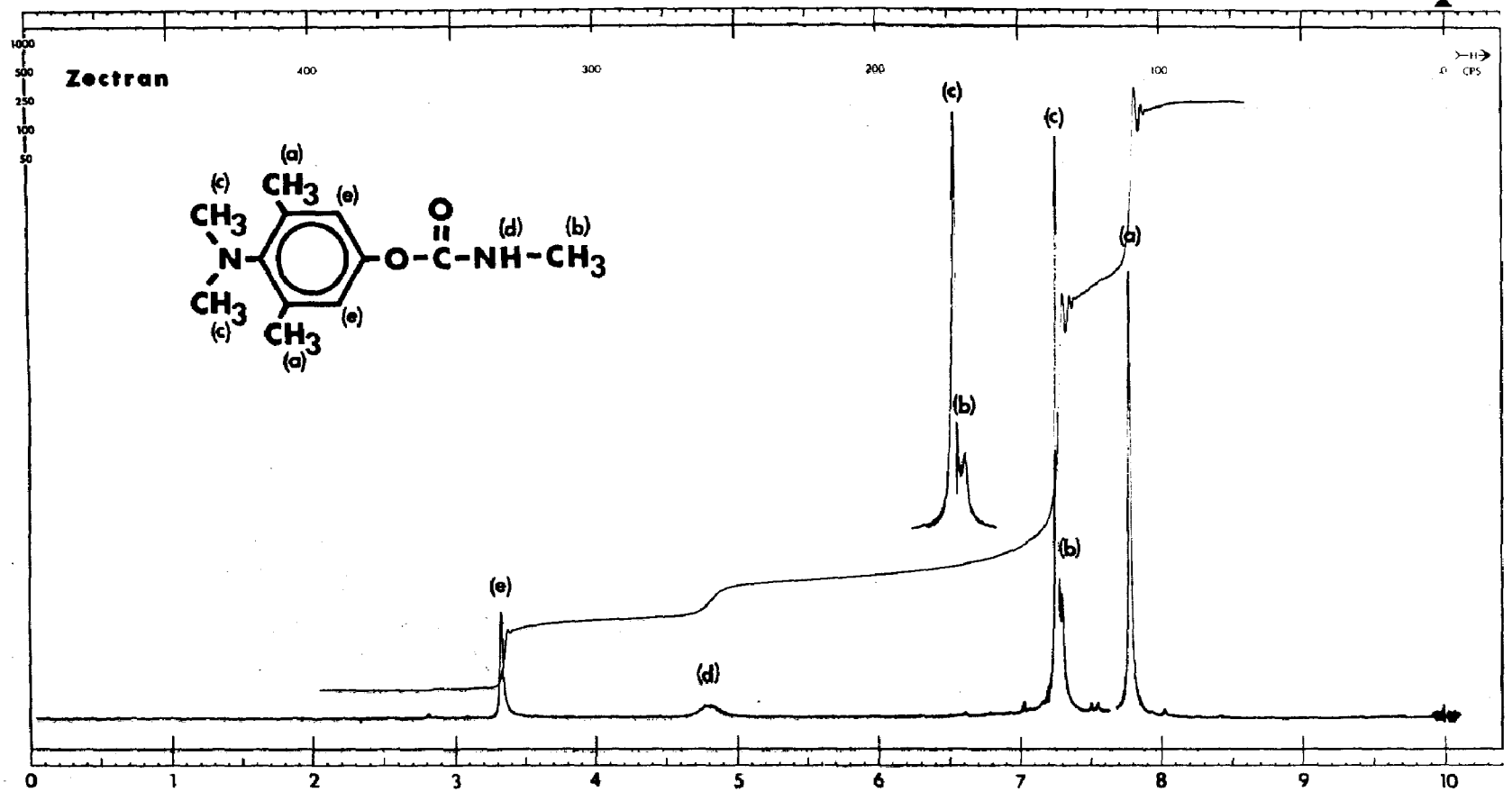
# C-13




107

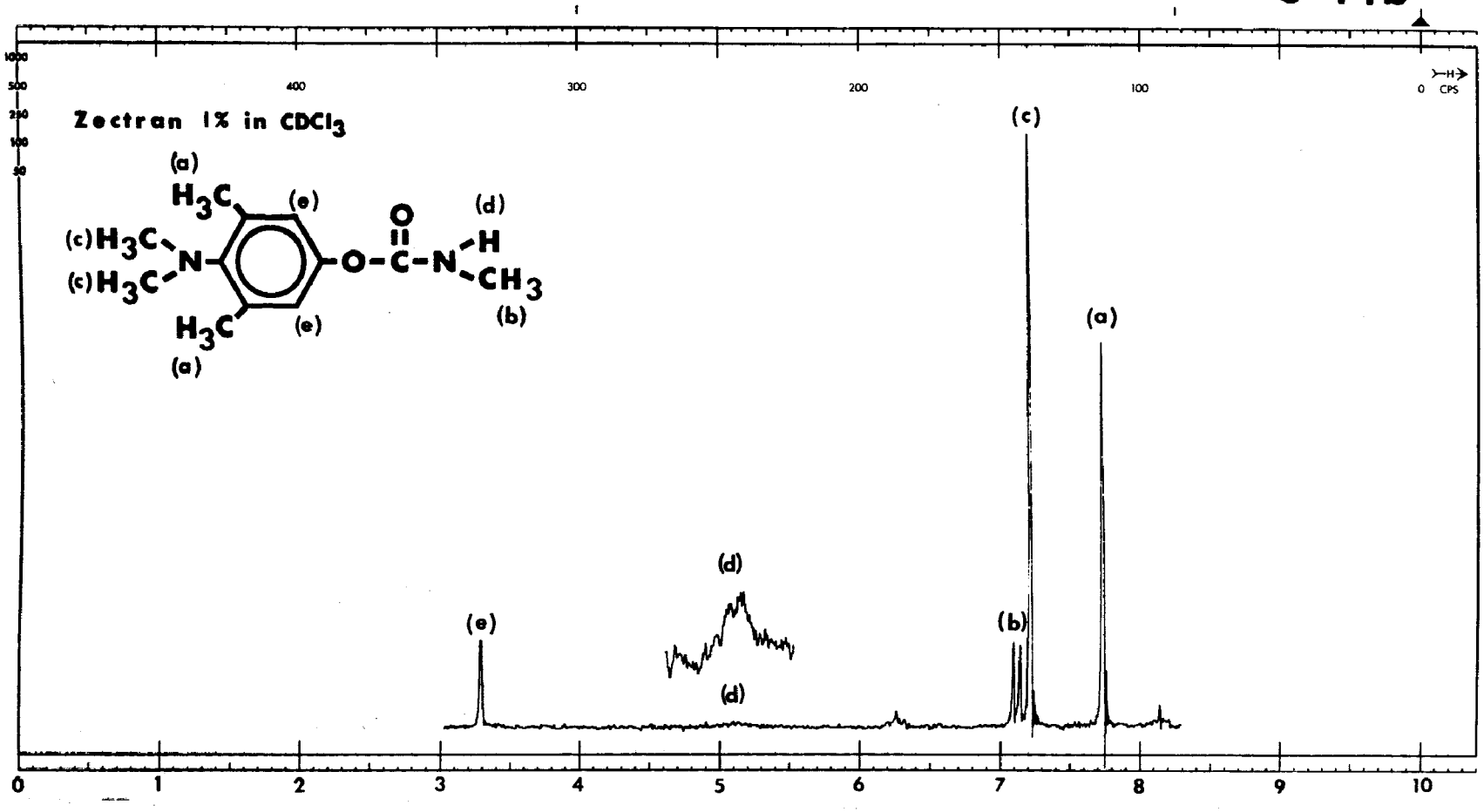
| | T | J |
|---|---|---|
| a | 7.71 | |
| b | 7.37 | |
| c | 7.26 | 5 |
| d | 4.6 | |
| e | 3.1 | |

# C-14a




| | T | J |
|---|---|---|
| a | 7.88 | |
| b | 7.28 | 5 |
| c | 7.26 | |
| d | 4.80 | |
| e | 3.33 | |

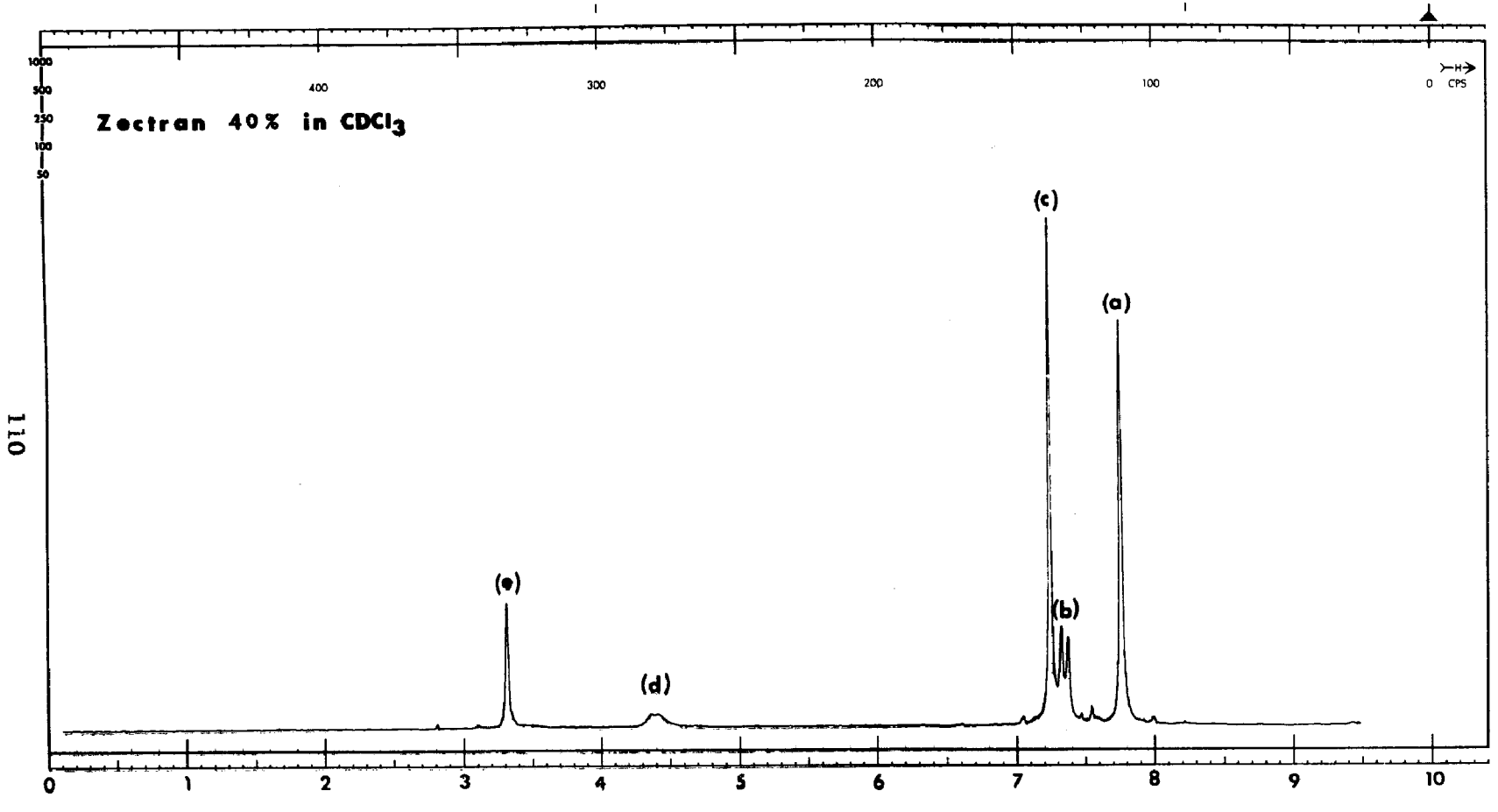
# C-14b




| | T | J |
|---|---|---|
| a | 7.75 | |
| b | 7.1–7.15 | 5 |
| c | 7.22 | |
| d | 5.14 | |
| e | 3.28 | |

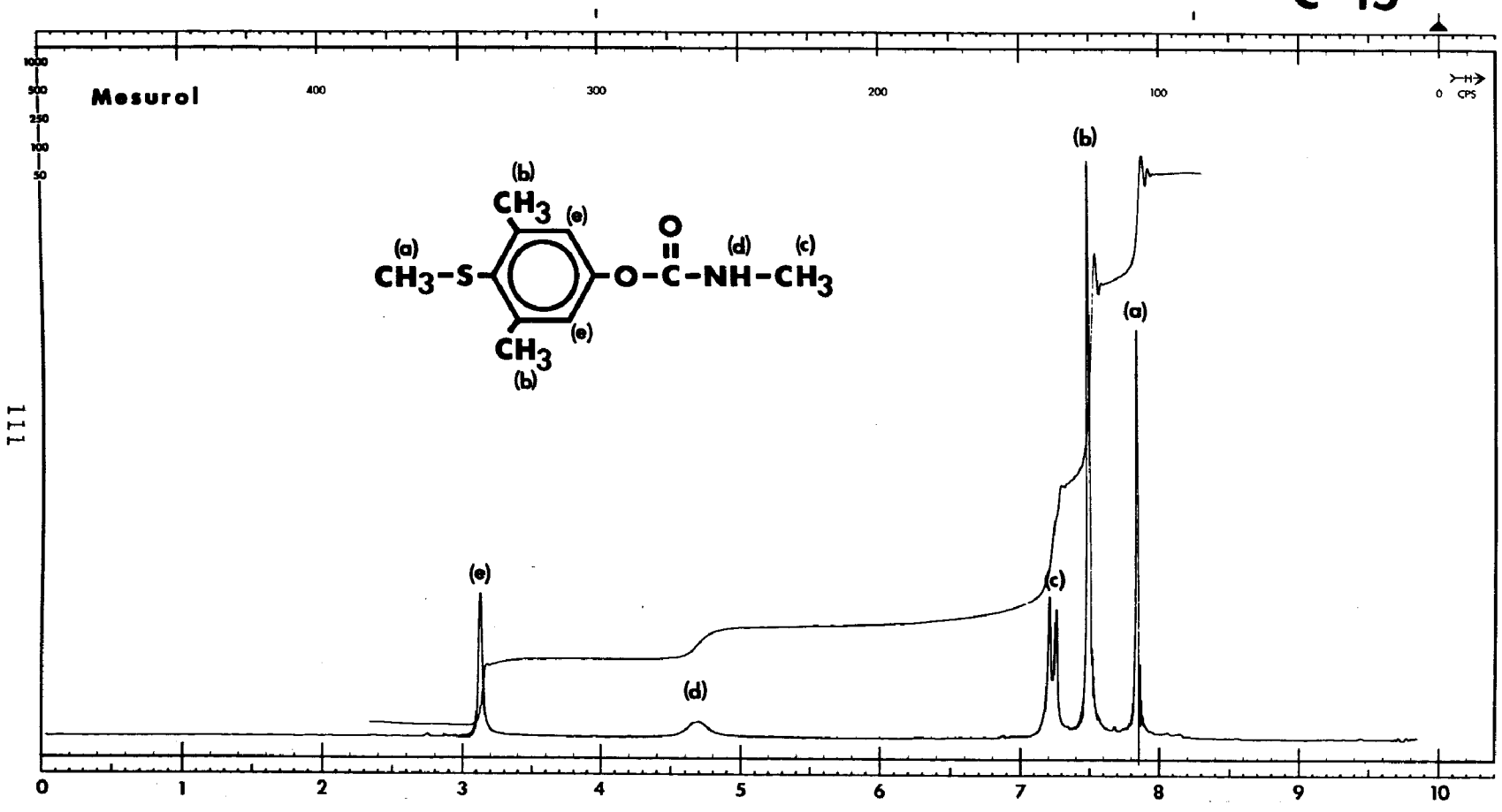
601

# C-14c




| | T | J |
|---|---|---|
| a | 7.78 | |
| b | 7.33–7.38 | 5 |
| c | 7.25 | |
| d | 4.39 | |
| e | 3.31 | |

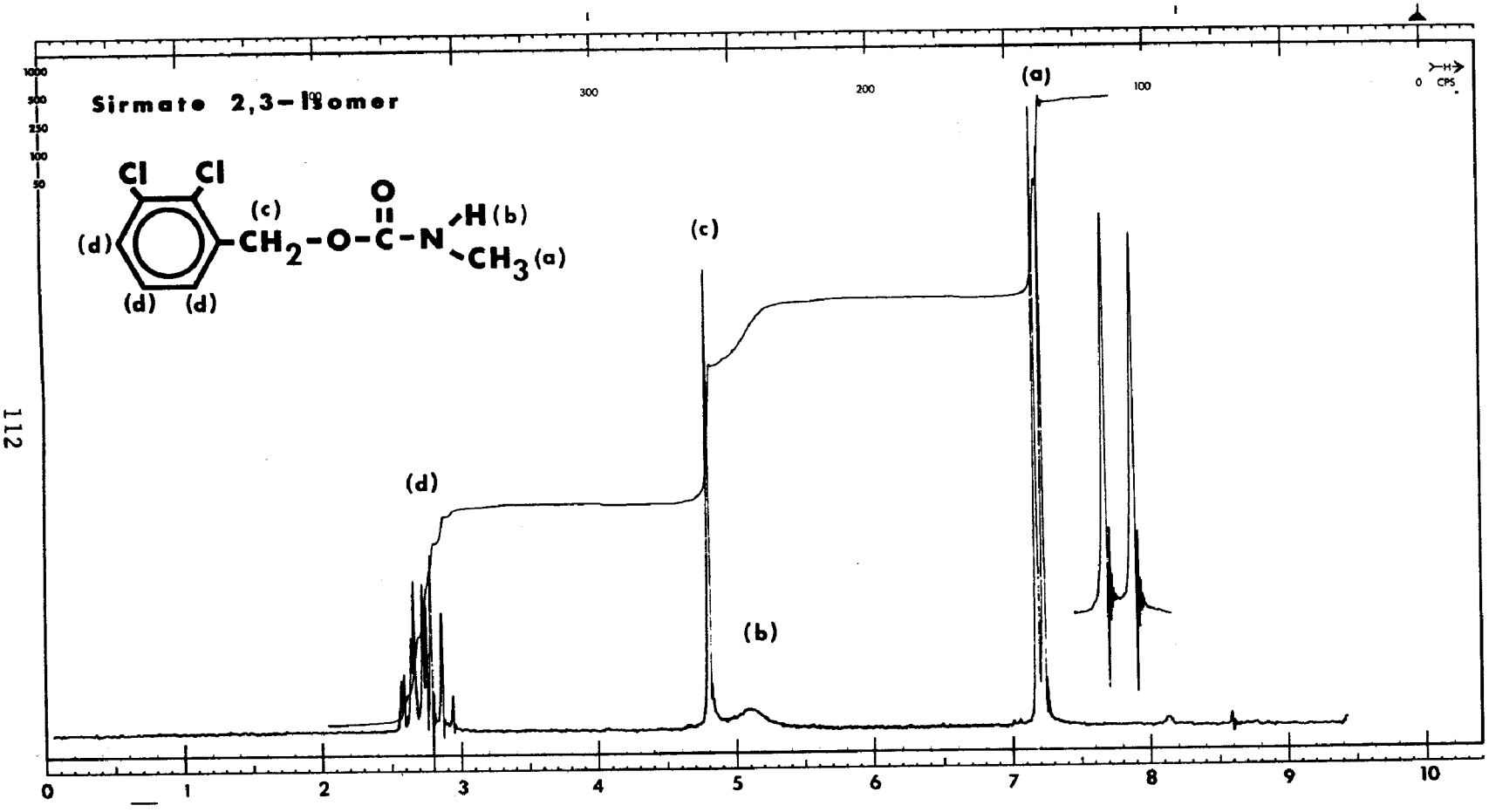
# C-15



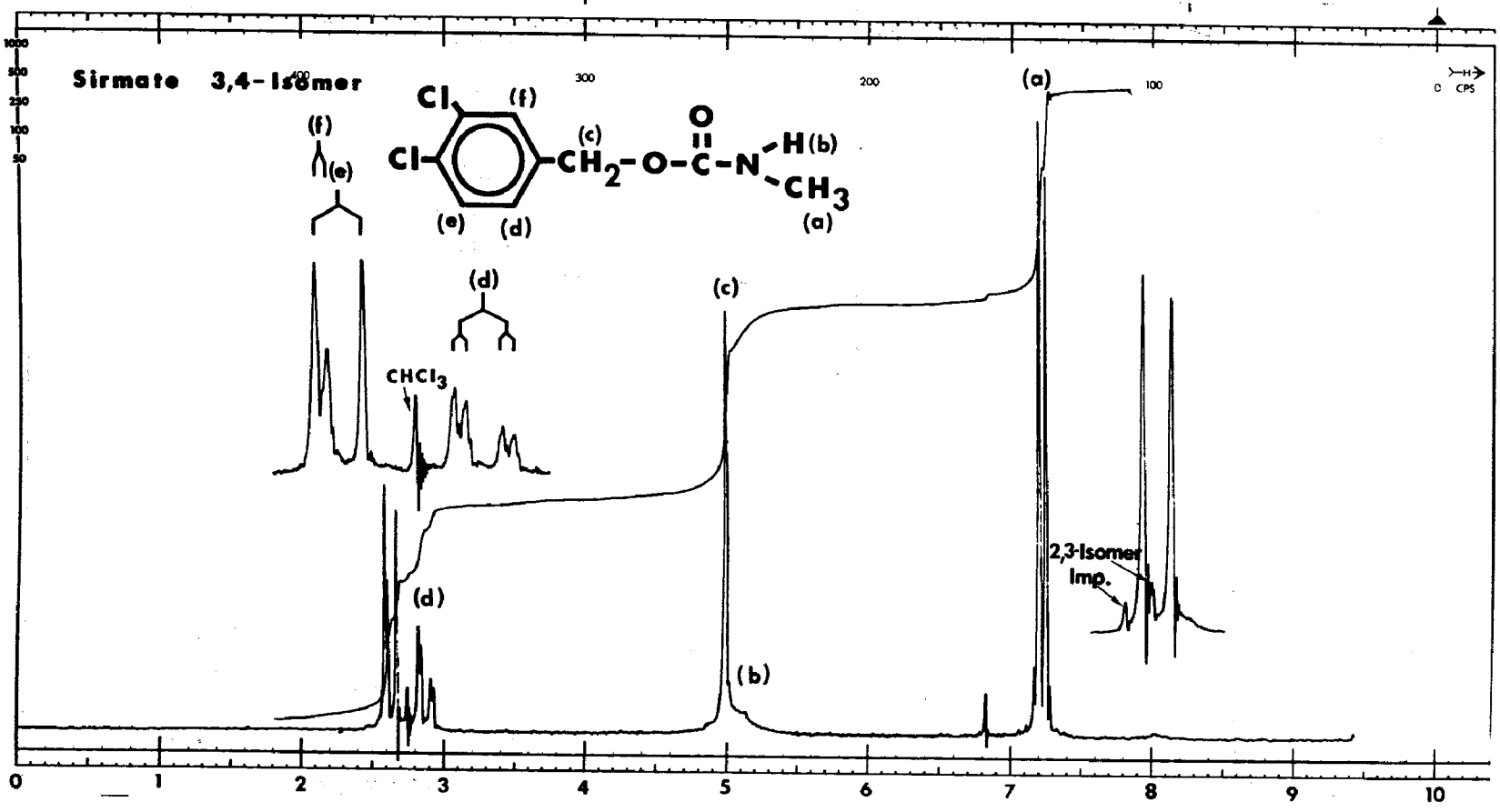

111

| | T | J |
|---|---|---|
| a | 7.93 | |
| b | 7.48 | |
| c | 7.24 | 5 |
| d | 4.7 | |
| e | 3.13 | |

# C-16

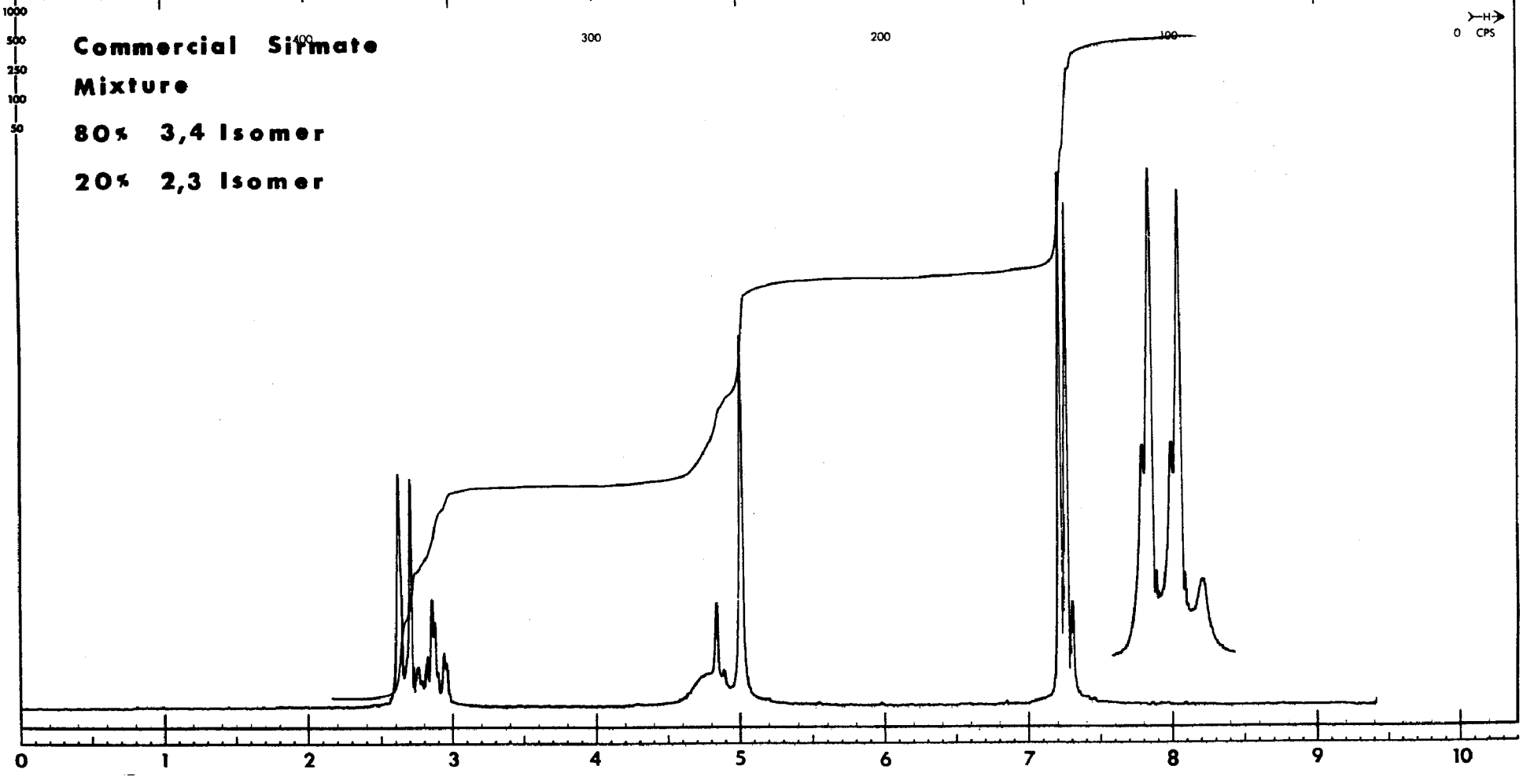



| | T | J |
|---|---|---|
| a | 7.18 | 5 |
| b | 5.10 | |
| c | 4.78 | |
| d | 2.55 - 2.92 | |

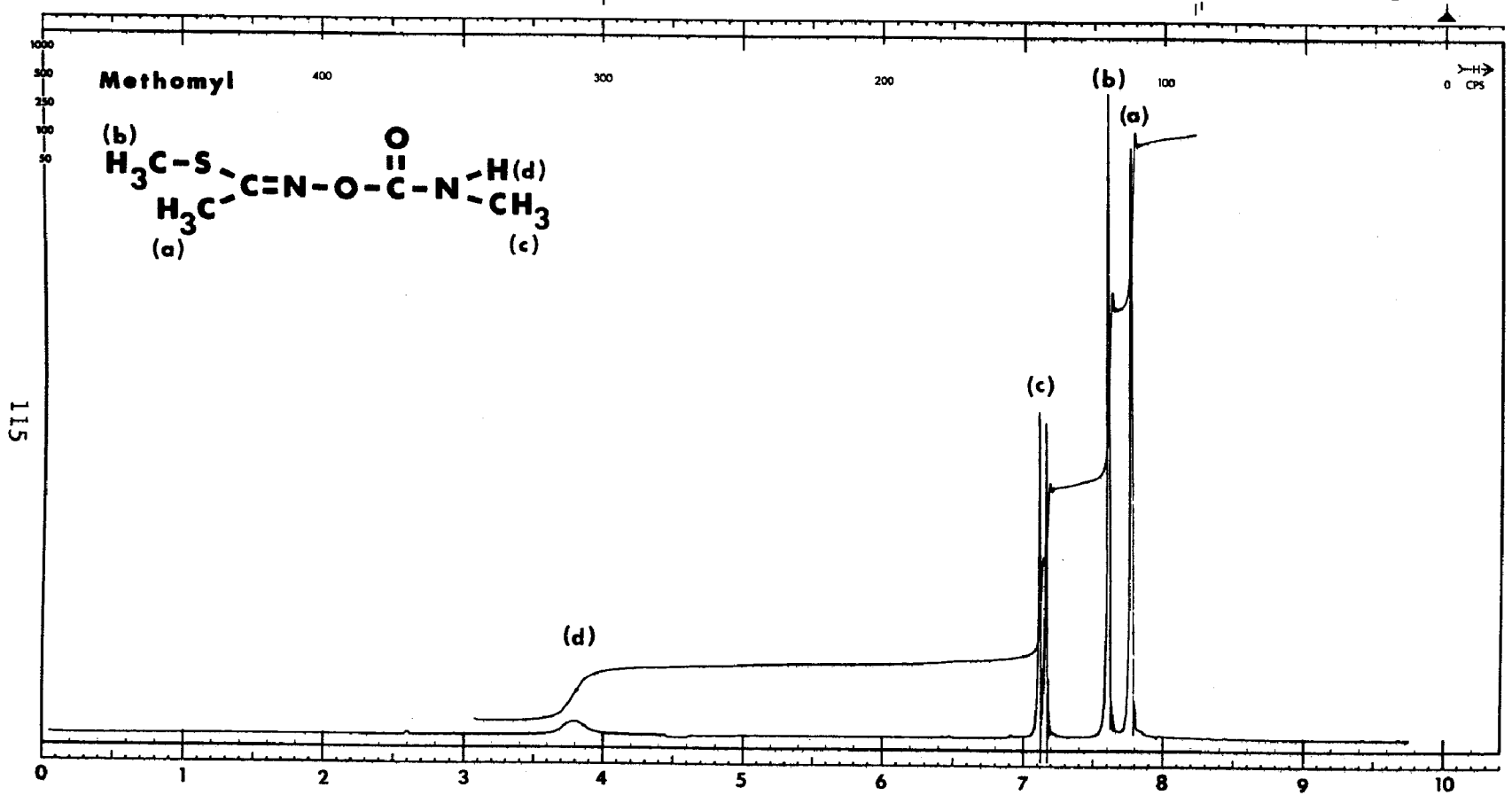



| | T | J |
|---|---|---|
| a | 7.20 | 5 |
| b | 5.0 | |
| c | 4.97 | |
| d | 2.86 | 8.5($H_d-H_e$) |
| | | 2.0($H_d-H_f$) |
| e | 2.61 | 8.5($H_d-H_e$) |
| f | 2.58 | 2.0($H_d-H_f$) |

C-17b

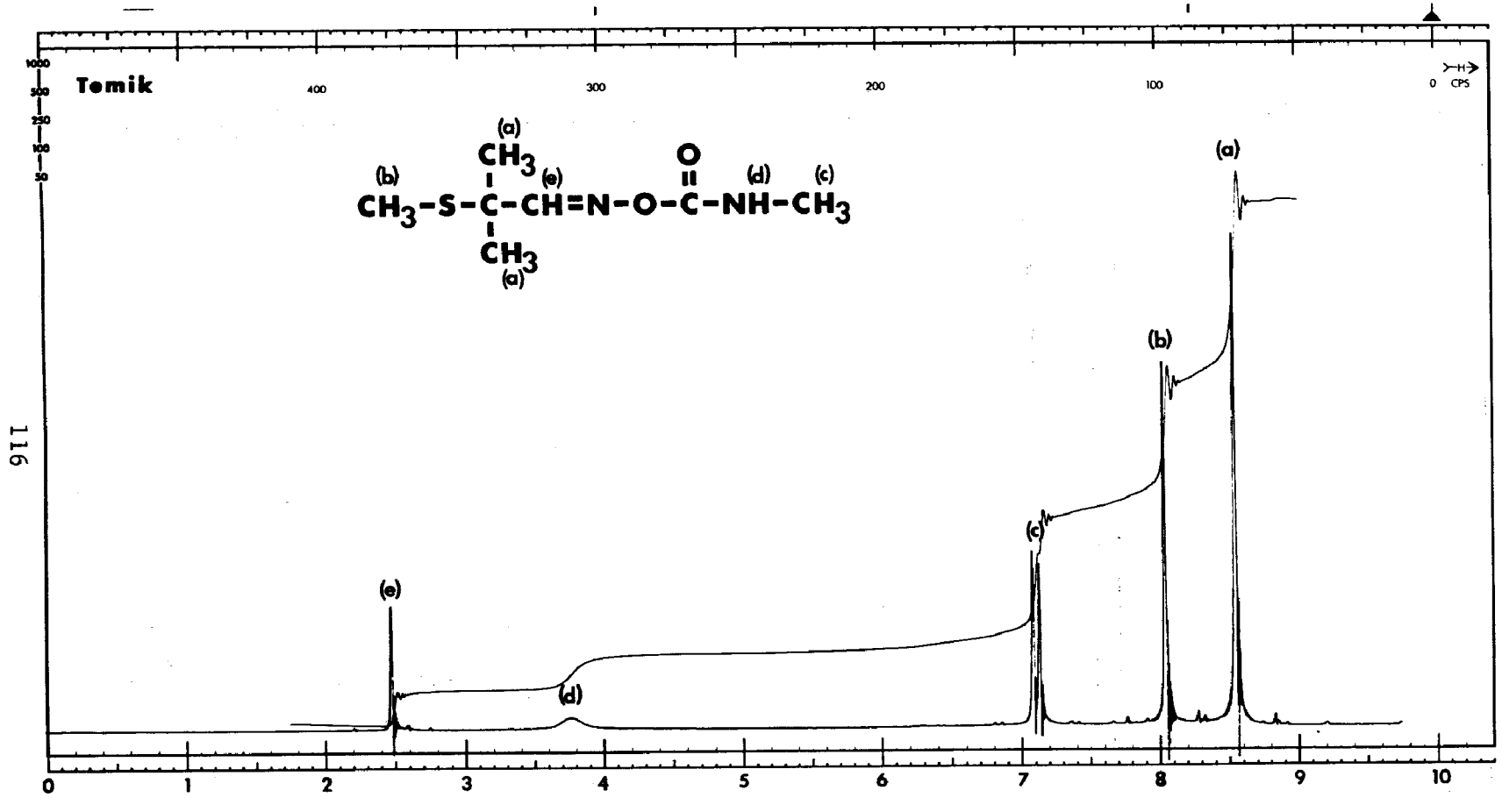

Commercial Sirmate
Mixture
80% 3,4 Isomer
20% 2,3 Isomer
1000
500
250
100
50
400
300
200
100
0 CPS
0
1
2
3
4
5
6
7
8
9
10

# C-18




| | T | J |
|---|---|---|
| a | 7.77 | |
| b | 7.61 | |
| c | 7.13 | 5 |
| d | 3.80 | |

# C-19

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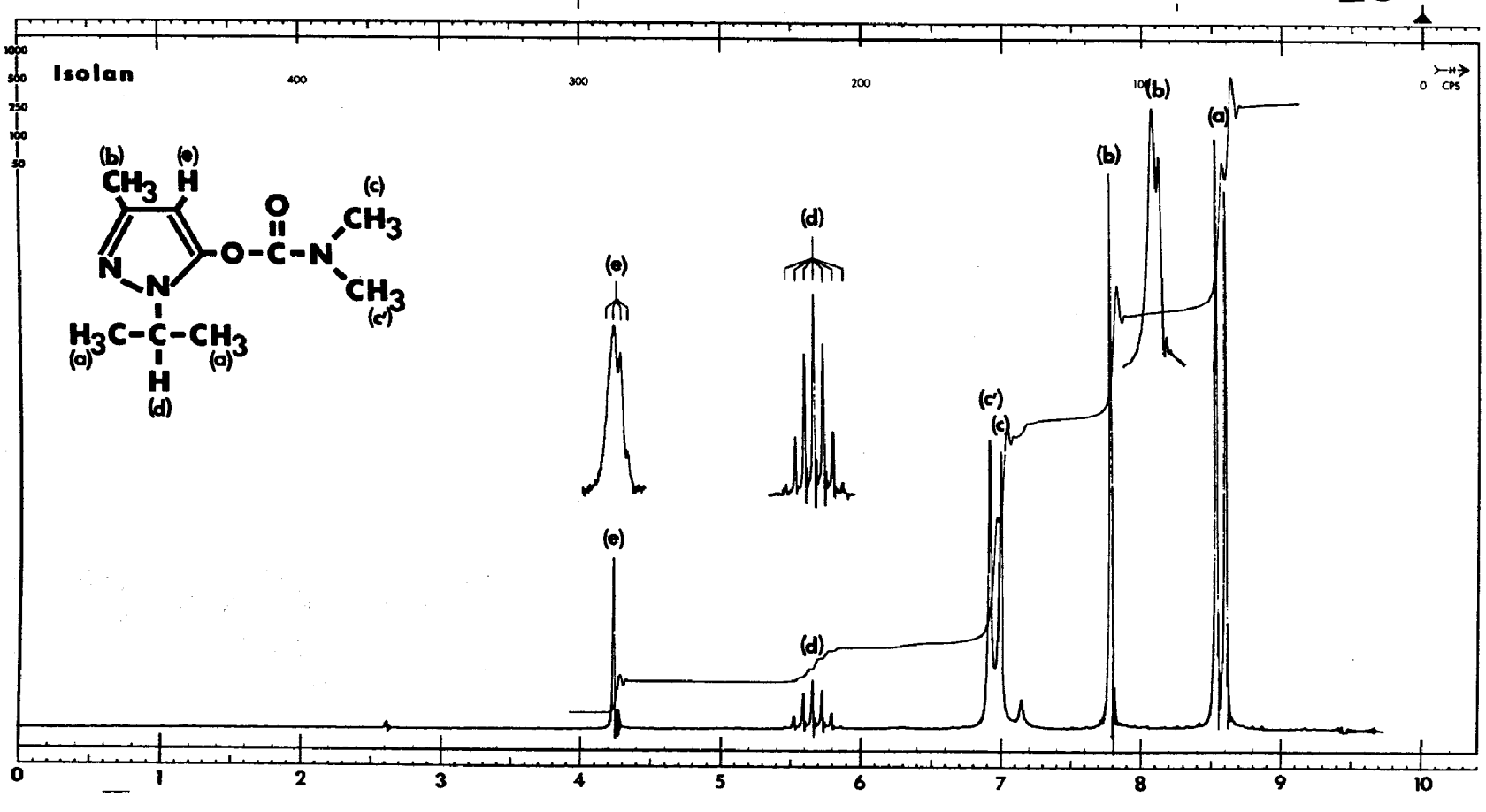
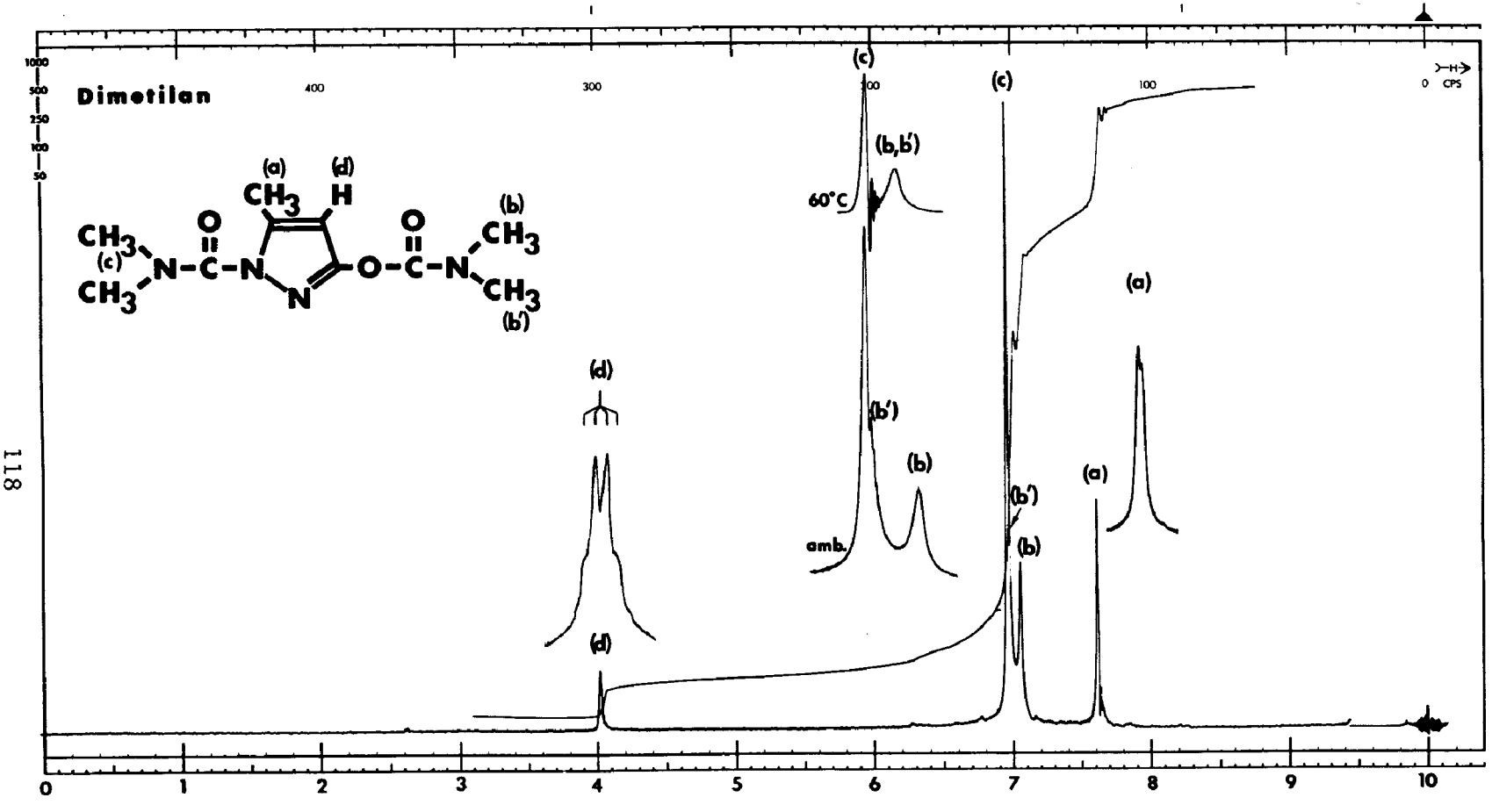
| | T | J |
|---|---|---|
| a | 8.54 | |
| b | 8.03 | |
| c | 7.10 | 5 |
| d | 3.75 | |
| e | 2.46 | |

# C-20



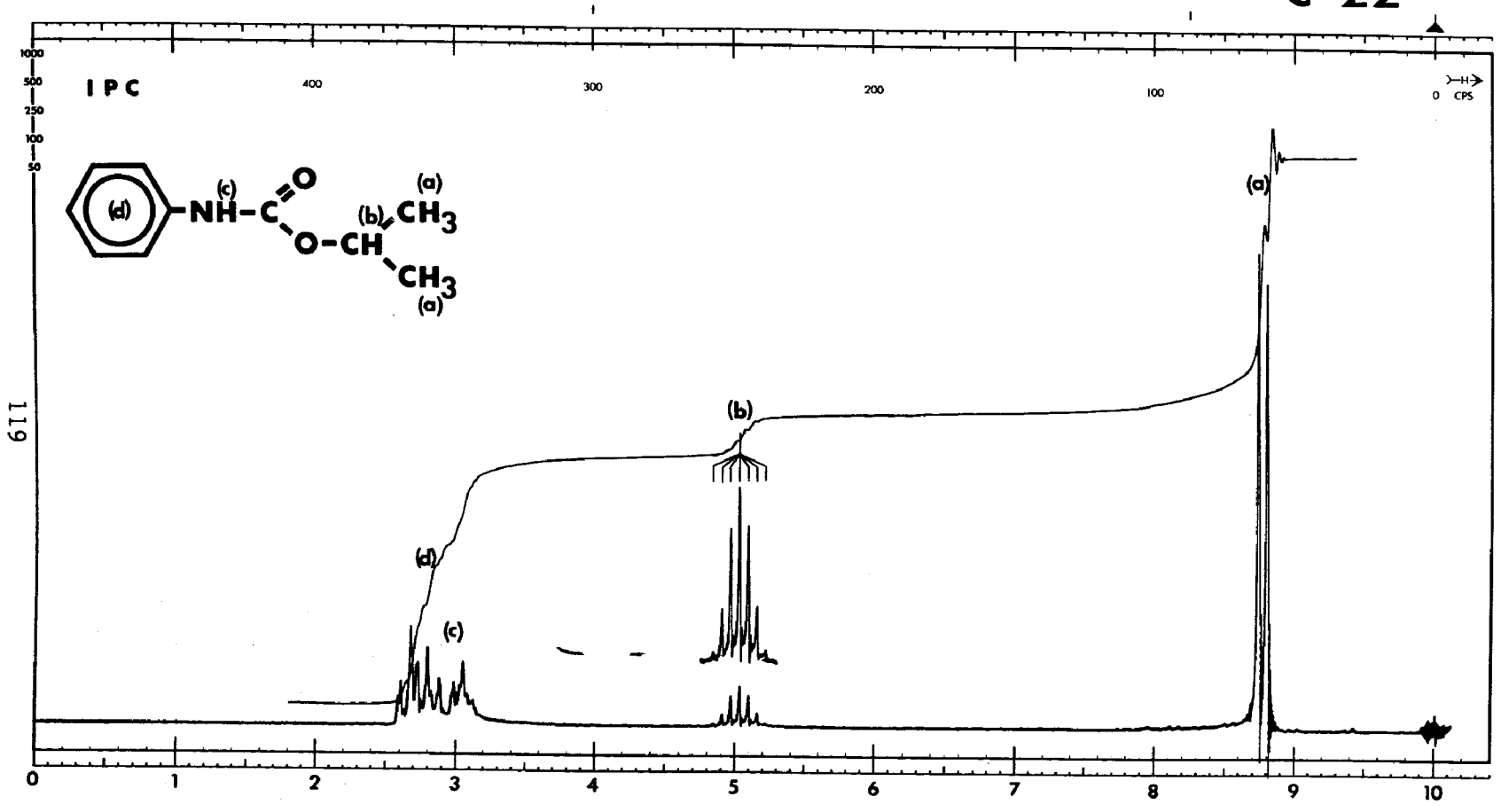

| | T | J |
|---|---|---|
| a | 8.57 | 7 |
| b | 7.78 | 0.5 |
| c | 6.99 | |
| c' | 6.91 | |
| d | 5.66 | 7 |
| e | 4.23 | 0.5 |

# C-21



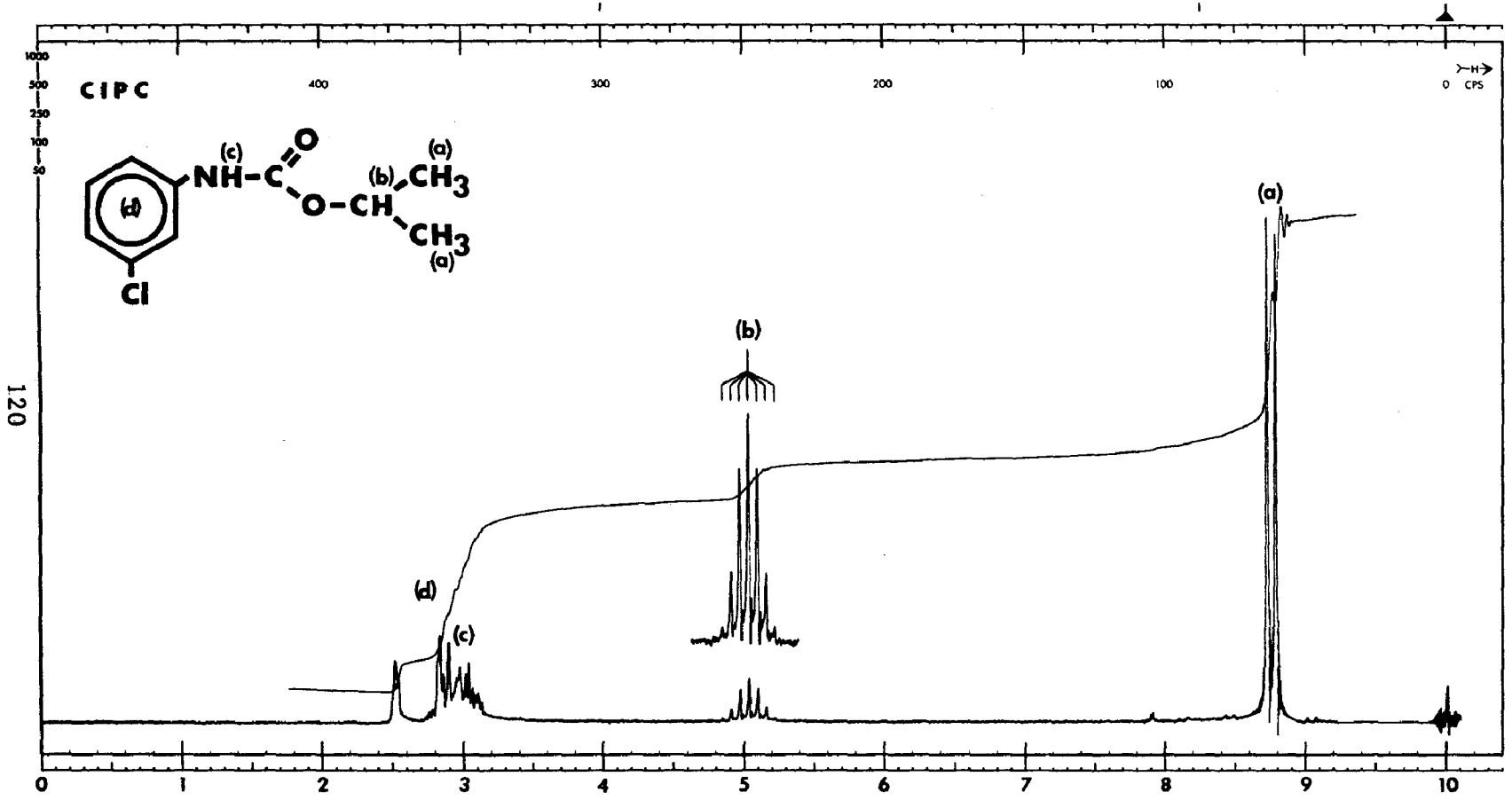

| | T | J |
|---|---|---|
| a | 7.60 | 0.8 |
| b | 7.03 | |
| b' | 6.95 | |
| c | 6.94 | |
| d | 3.99 | 0.8 |

# C-22



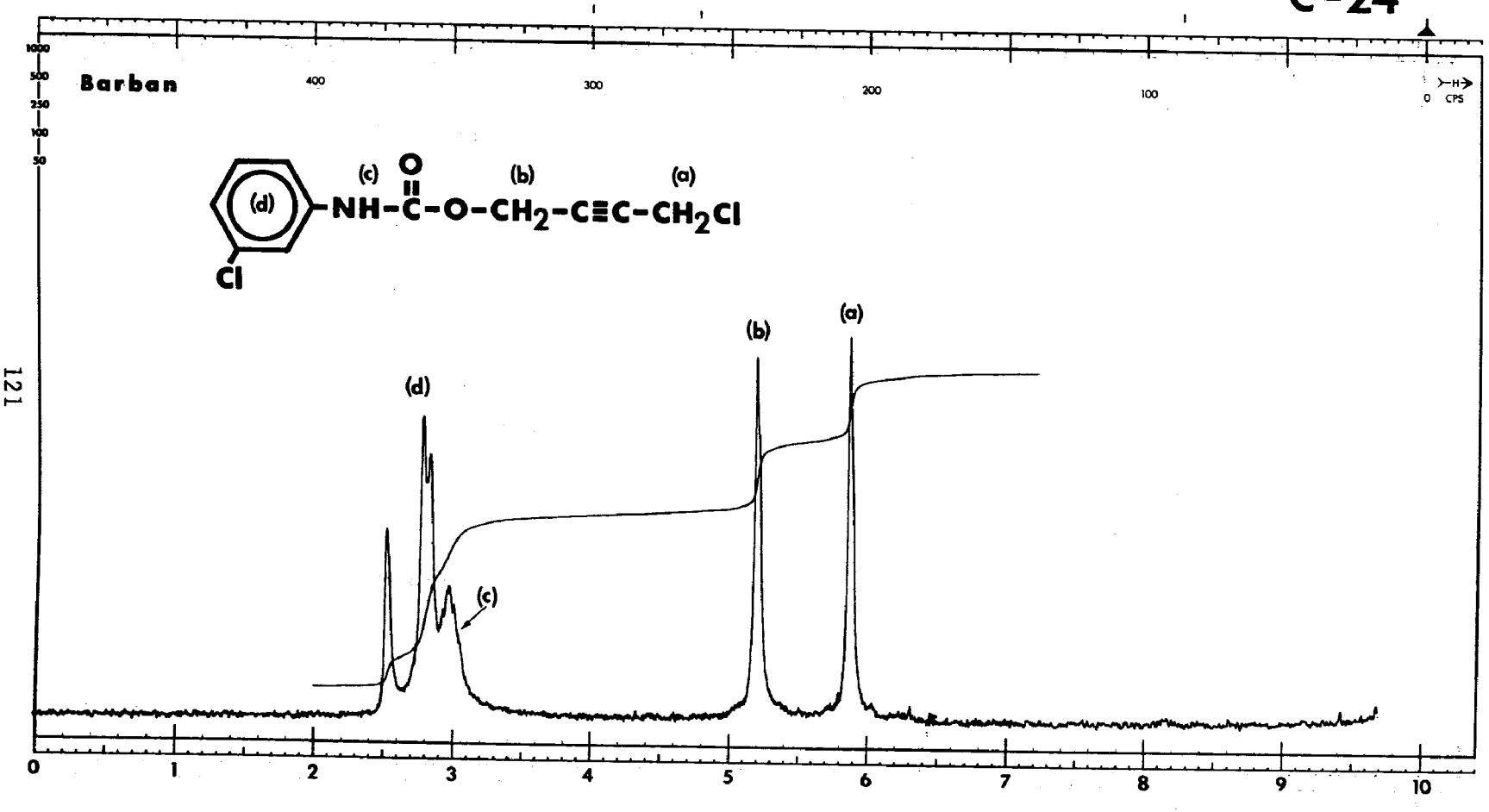

| | T | J |
|---|---|---|
| a | 8.76 | 6 |
| b | 5.00 | 6 |
| c | 3.0 | |
| d | 2.6-3.1 | |

# C-23



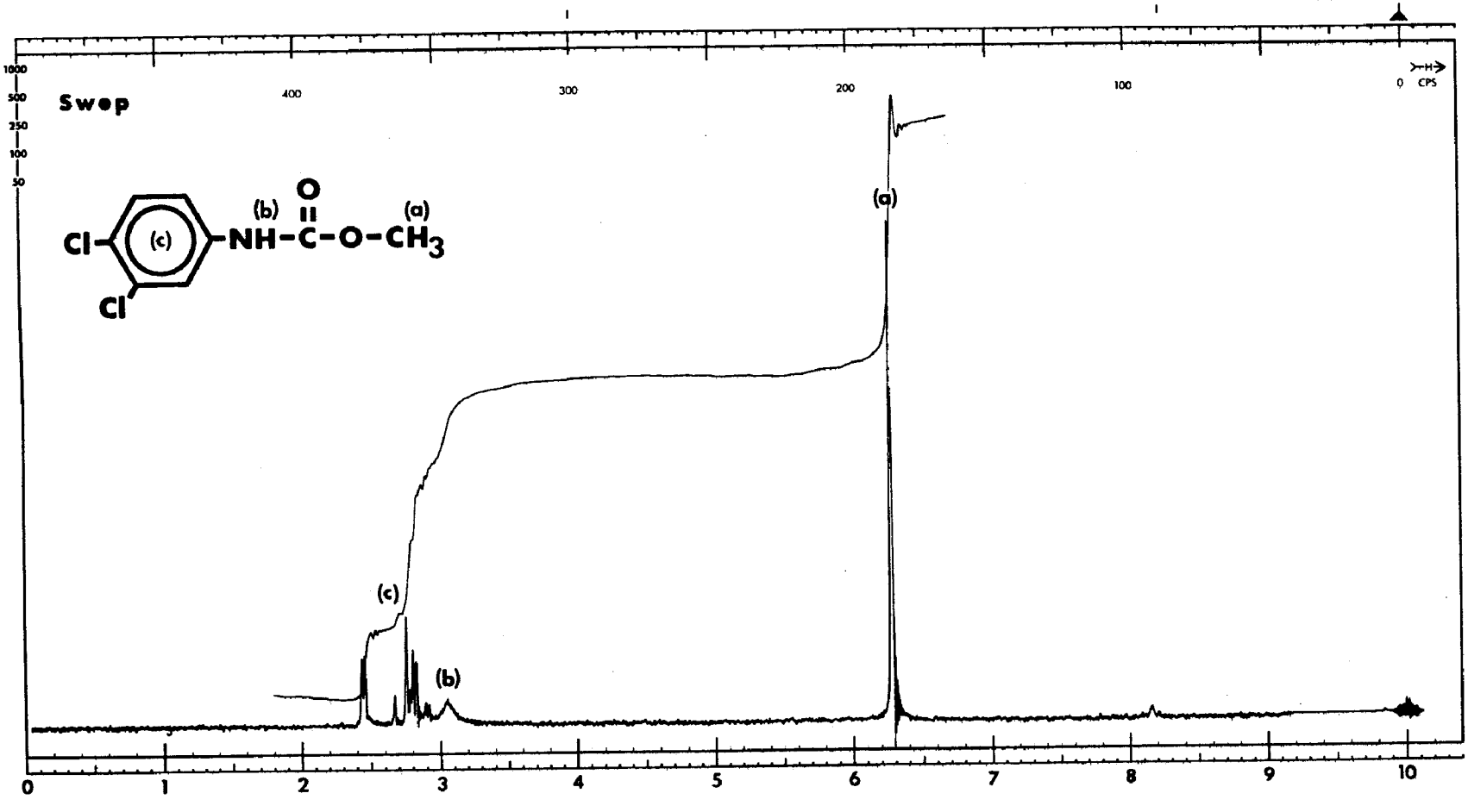

| | T | J |
|---|---|---|
| a | 8.75 | 6 |
| b | 5.03 | 6 |
| c | 3.0 | |
| d | 2.5-3.1 | |

# C-24




| | T |
|---|---|
| a | 5.86 |
| b | 5.20 |
| c | 2.9 |
| d | 2.5-3.0 |

# C-25

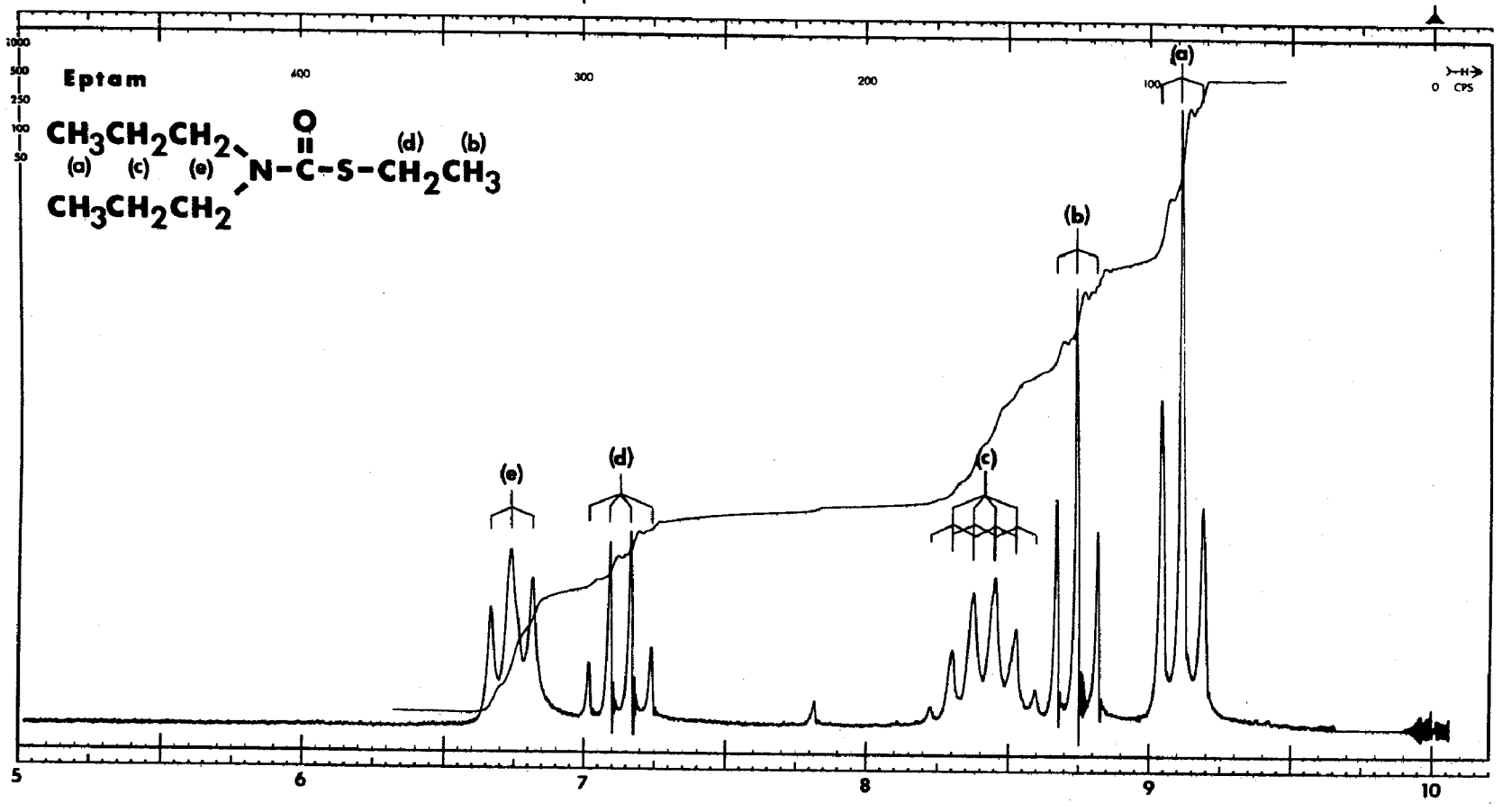




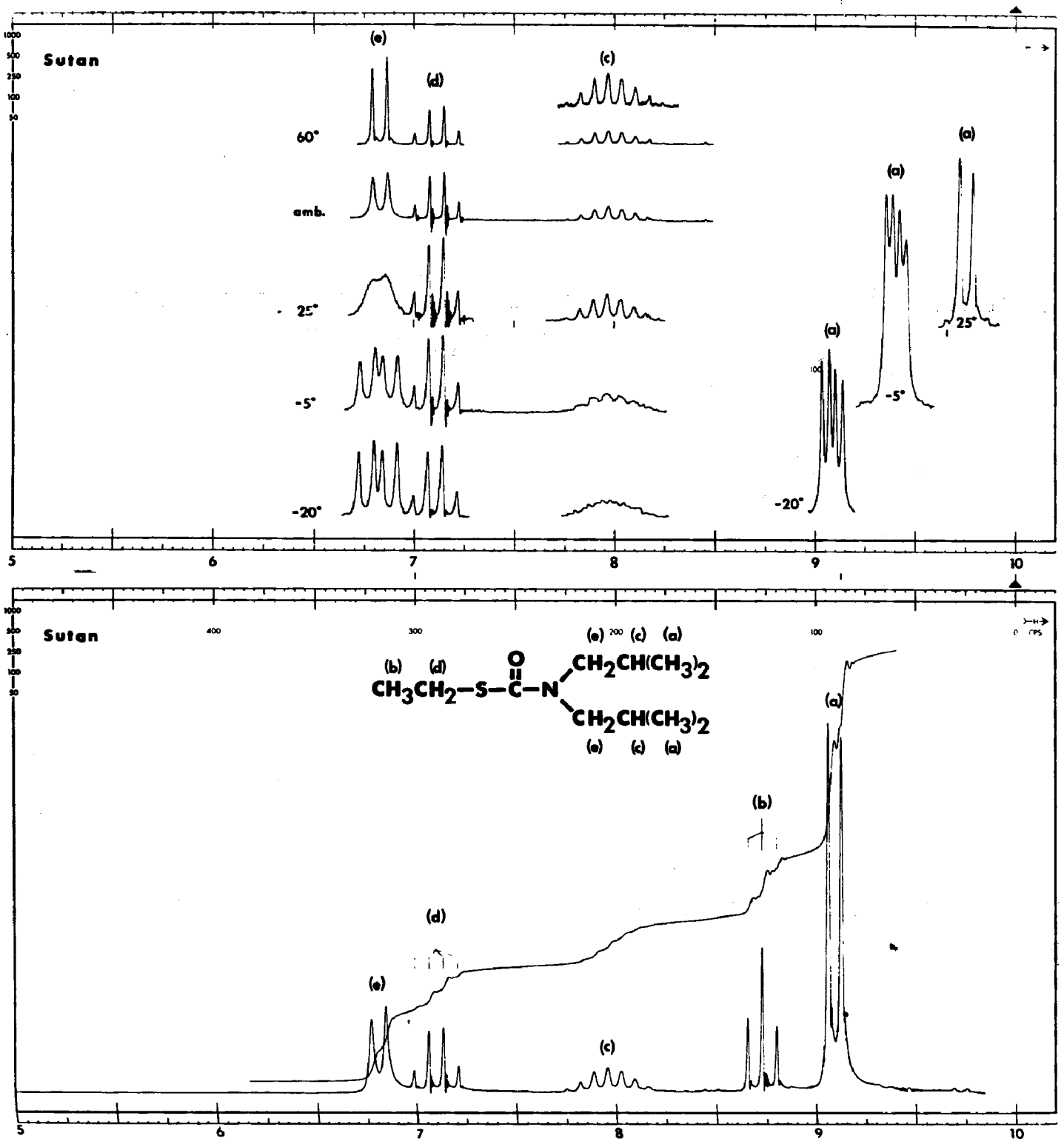


| | T |
|---|---|
| a | 6.25 |
| b | 3.05 |
| c | 2.4-2.9 |

# C-26

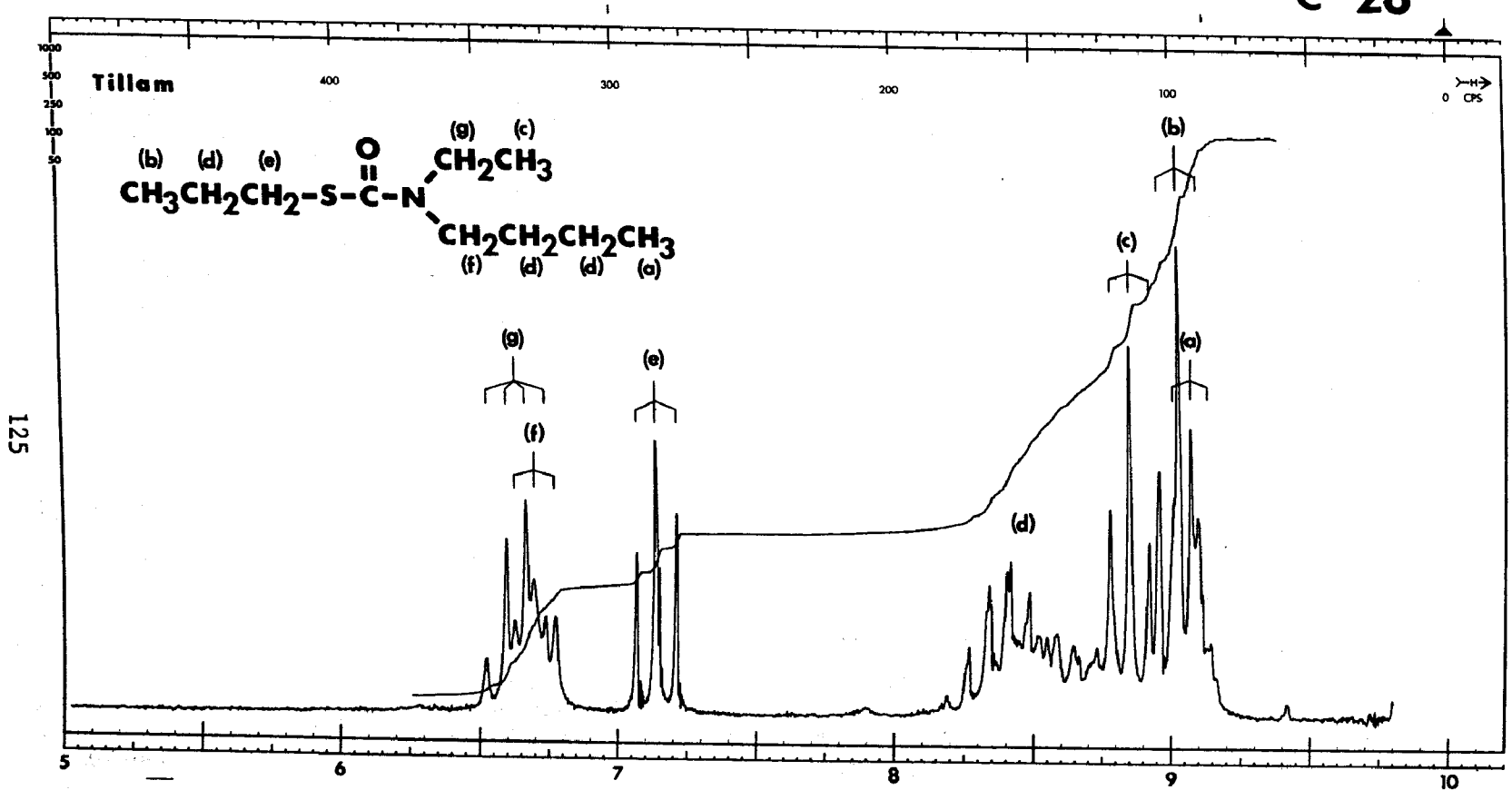



| | T | J |
|---|---|---|
| a | 9.10 | 7 |
| b | 8.73 | 7.5 |
| c | 8.40 | 7-7.5 |
| d | 7.11 | 7.5 |
| e | 6.72 | 7.5 |



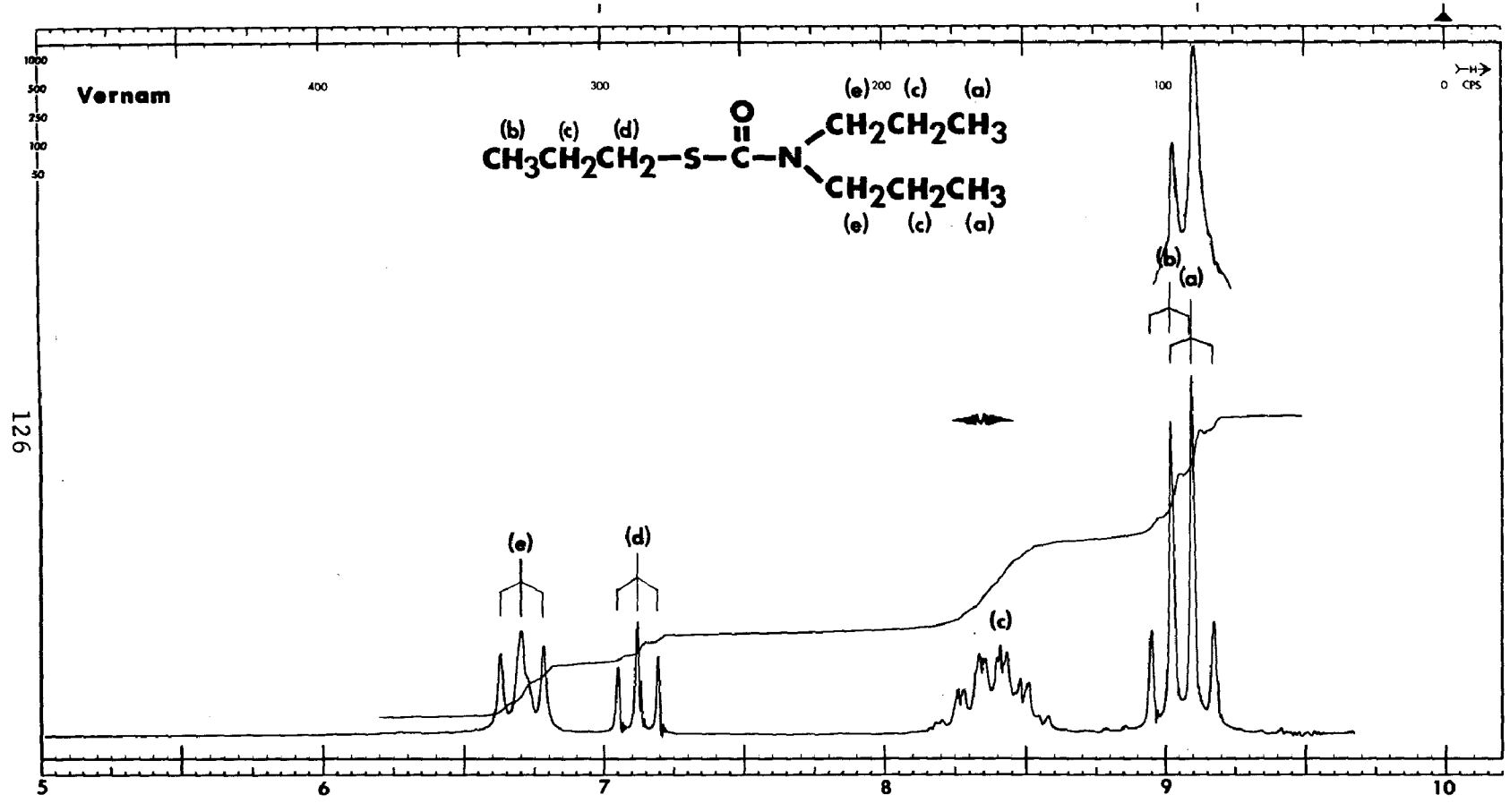

| | T | J |
|---|---|---|
| a | 9.09 | 6.5 |
| b | 8.73 | 7 |
| c | 7.96 | |
| d | 7.10 | 7 |
| e | 6.81 | 7.5 |

# C-28



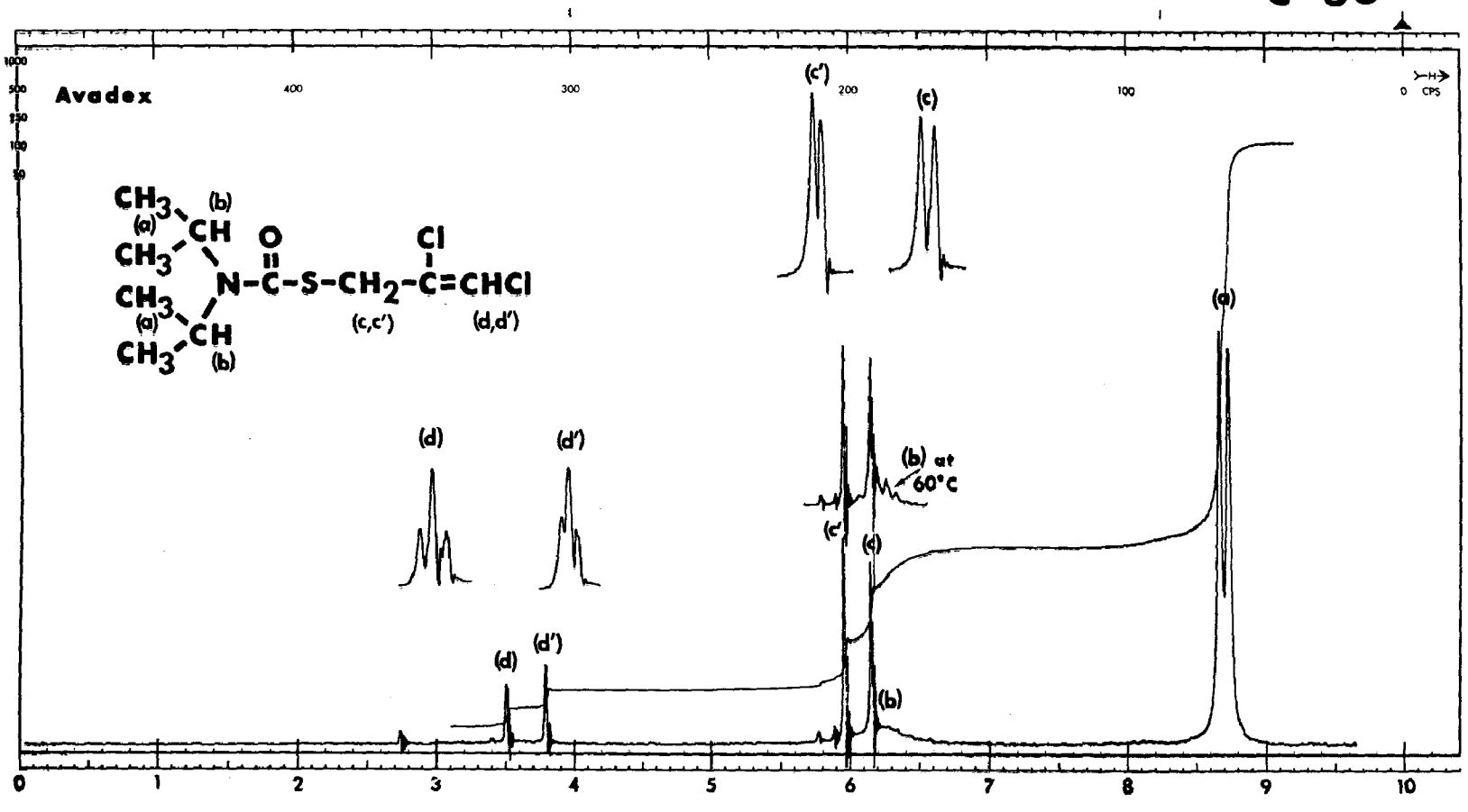

| | T | J |
|---|---|---|
| a | 9.08 | 6.5 |
| b | 9.03 | 7 |
| c | 8.86 | 7 |
| d | 8.2–8.7 | |
| e | 7.15 | 7 |
| f | 6.70 | 7 |
| g | 6.64 | 7 |

# C-29



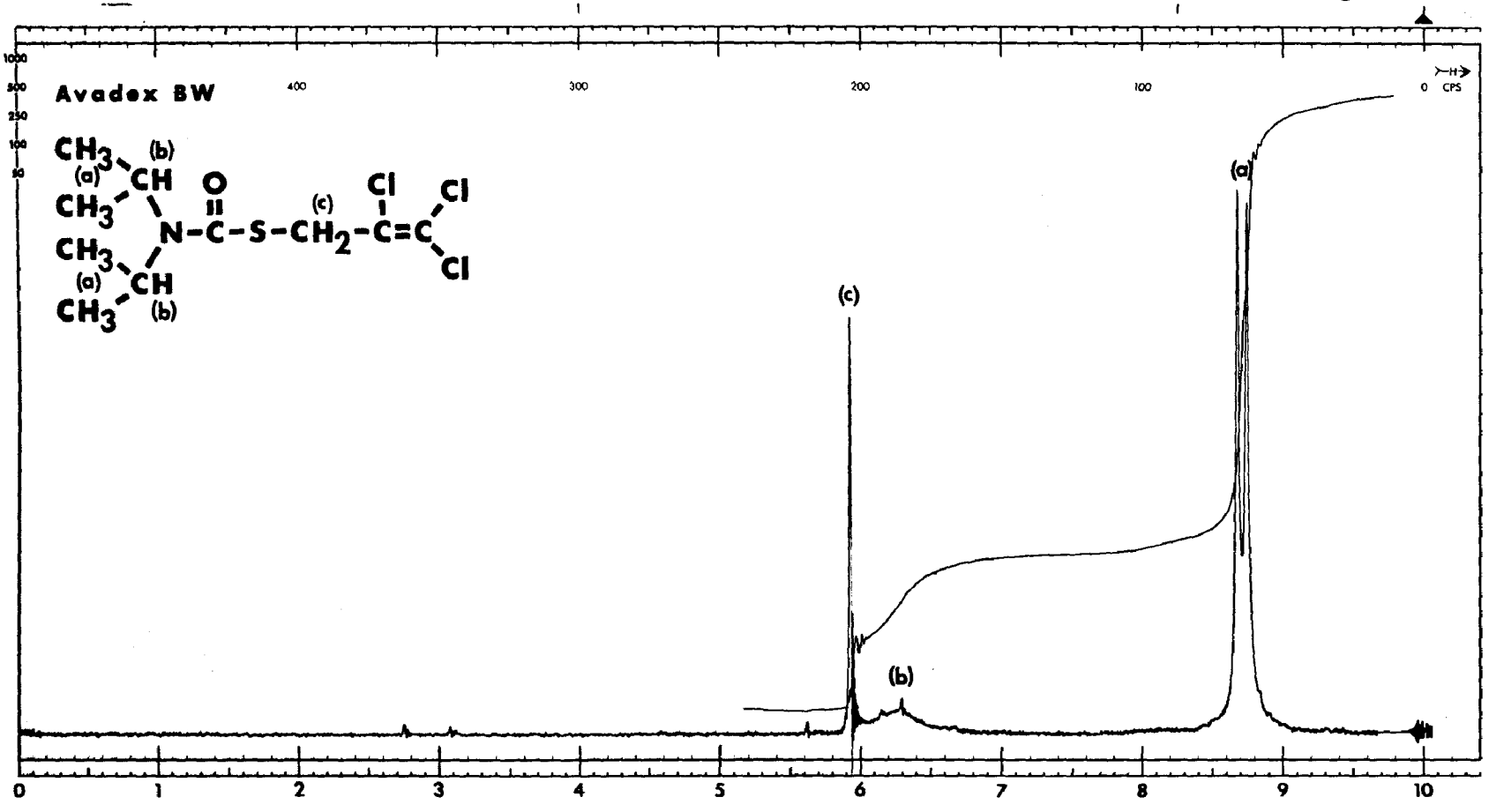

| | T | J |
|---|---|---|
| a | 9.10 | 7.5 |
| b | 9.02 | 7 |
| c | 8.2–8.6 | |
| d | 7.12 | 7 |
| e | 6.71 | 7.5 |

# C-30



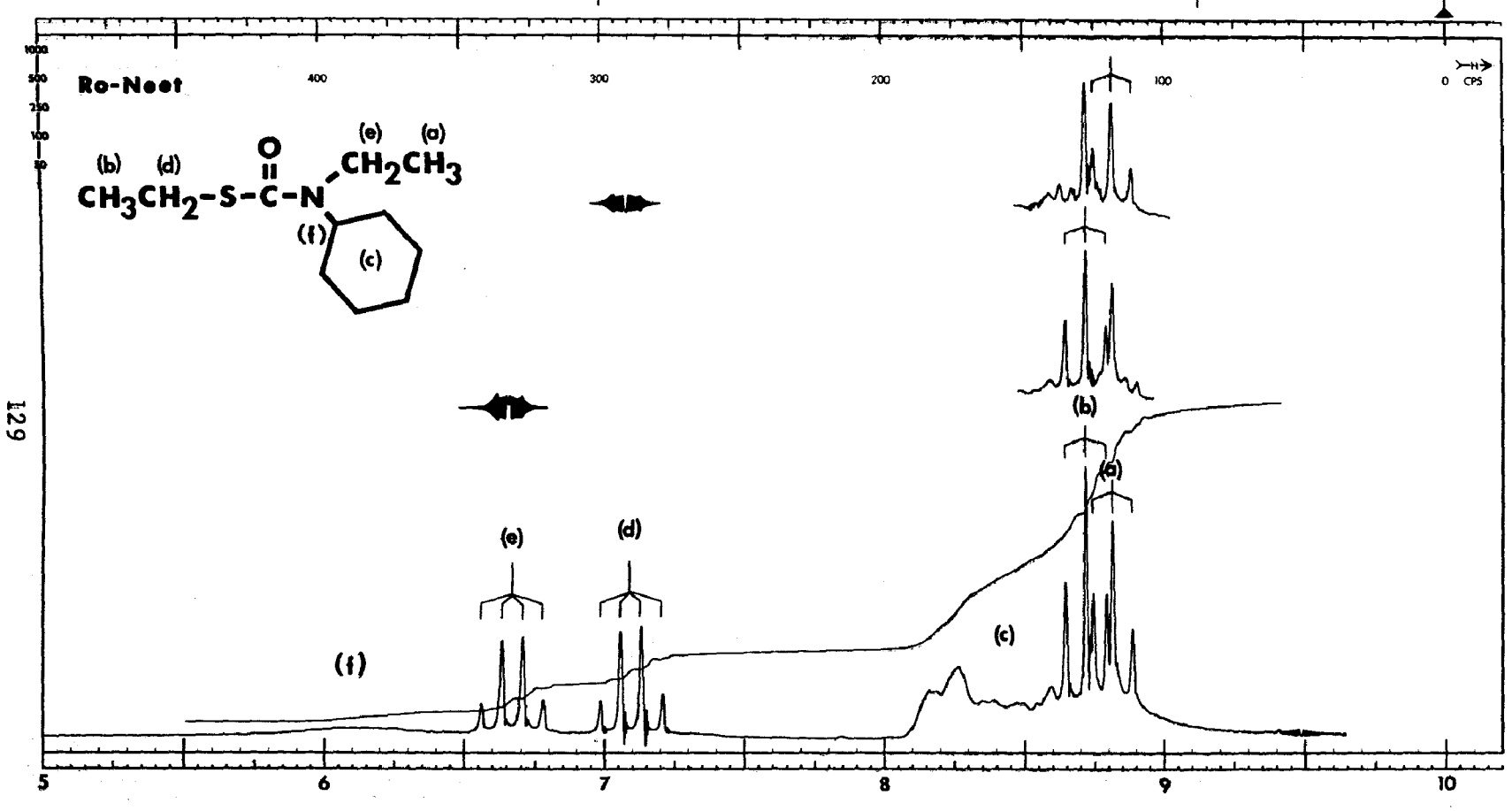

| | T | J |
|---|---|---|
| a | 8.70 | 7 |
| b | 6.2 | |
| c | 6.15 | 1.0 |
| c' | 5.96 | 0.6 |
| d | 3.78 | 0.6 |
| d' | 3.49 | 1.0 |

# C-31



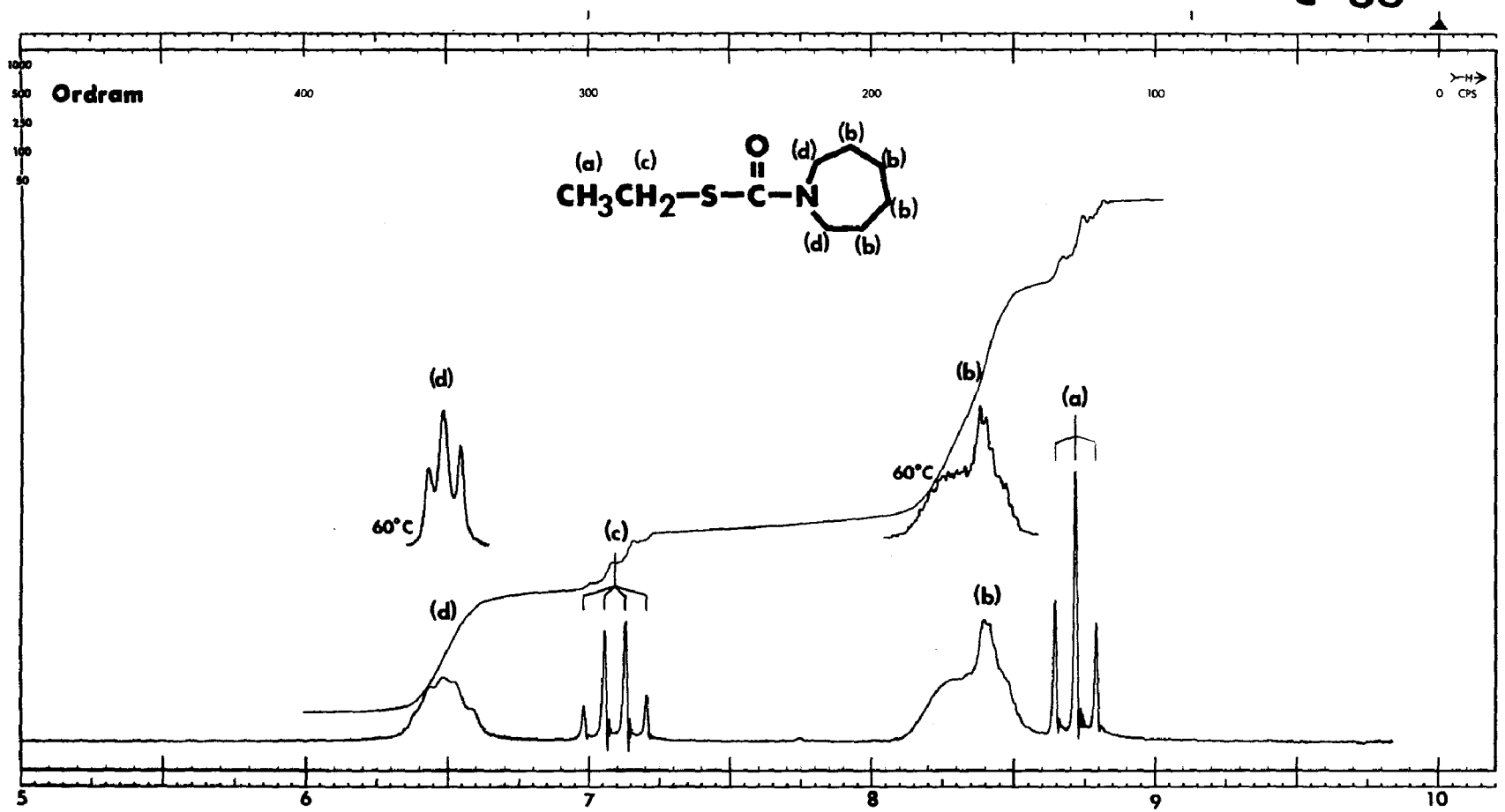

| | T | J |
|---|---|---|
| a | 8.71 | 7 |
| b | 6.3 | |
| c | 5.90 | |

# C-32



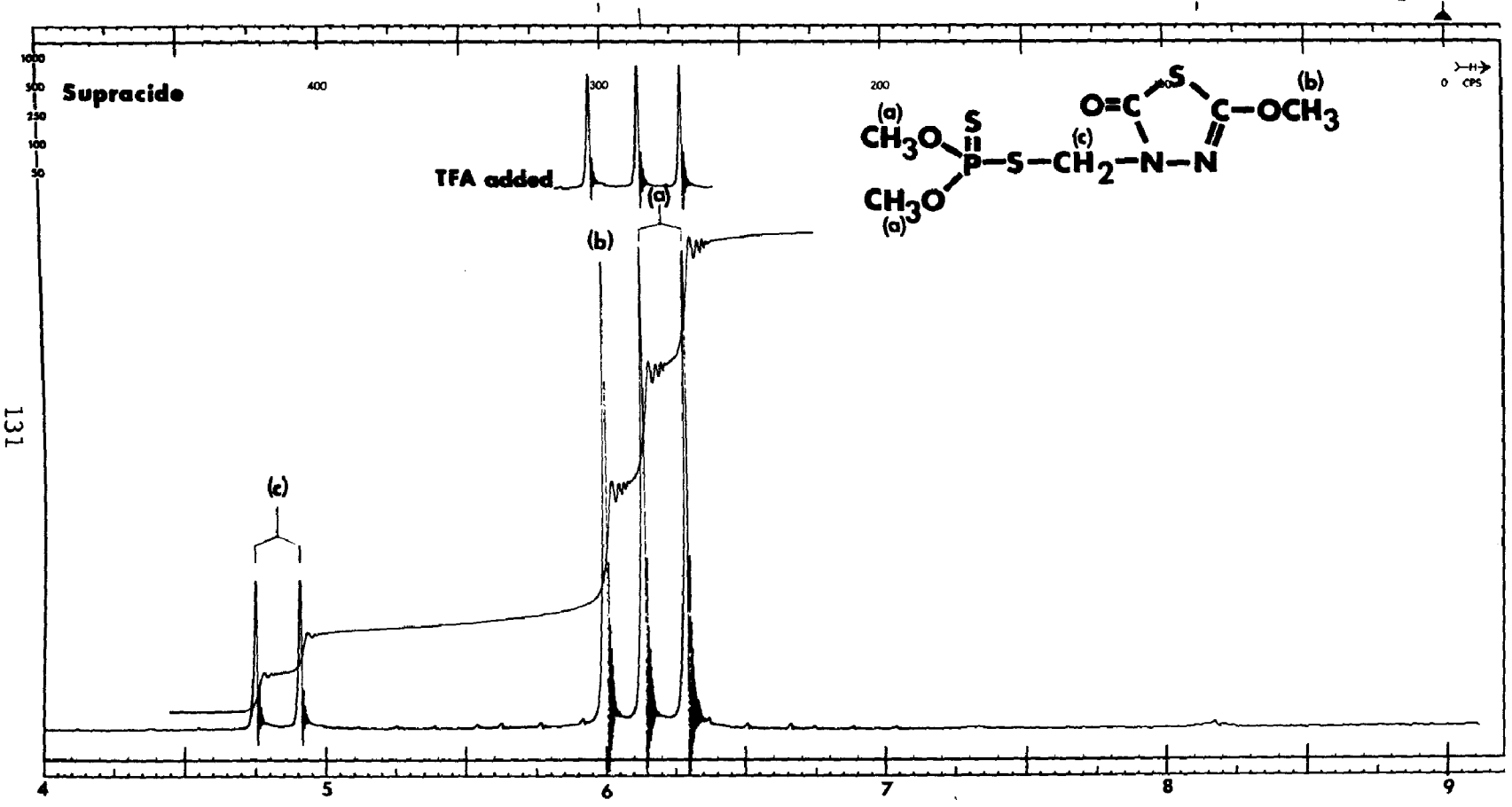

| | T | J |
|---|---|---|
| a | 8.82 | 7 |
| b | 8.72 | 7 |
| c | 8.1-8.9 | |
| d | 7.10 | 7 |
| e | 6.68 | 7 |
| f | 6.2 | |

# C-33




| | T | J |
|---|---|---|
| a | 8.72 | 7.5 |
| b | 8.2-8.5 | |
| c | 7.09 | 7.5 |
| d | 6.5 | |

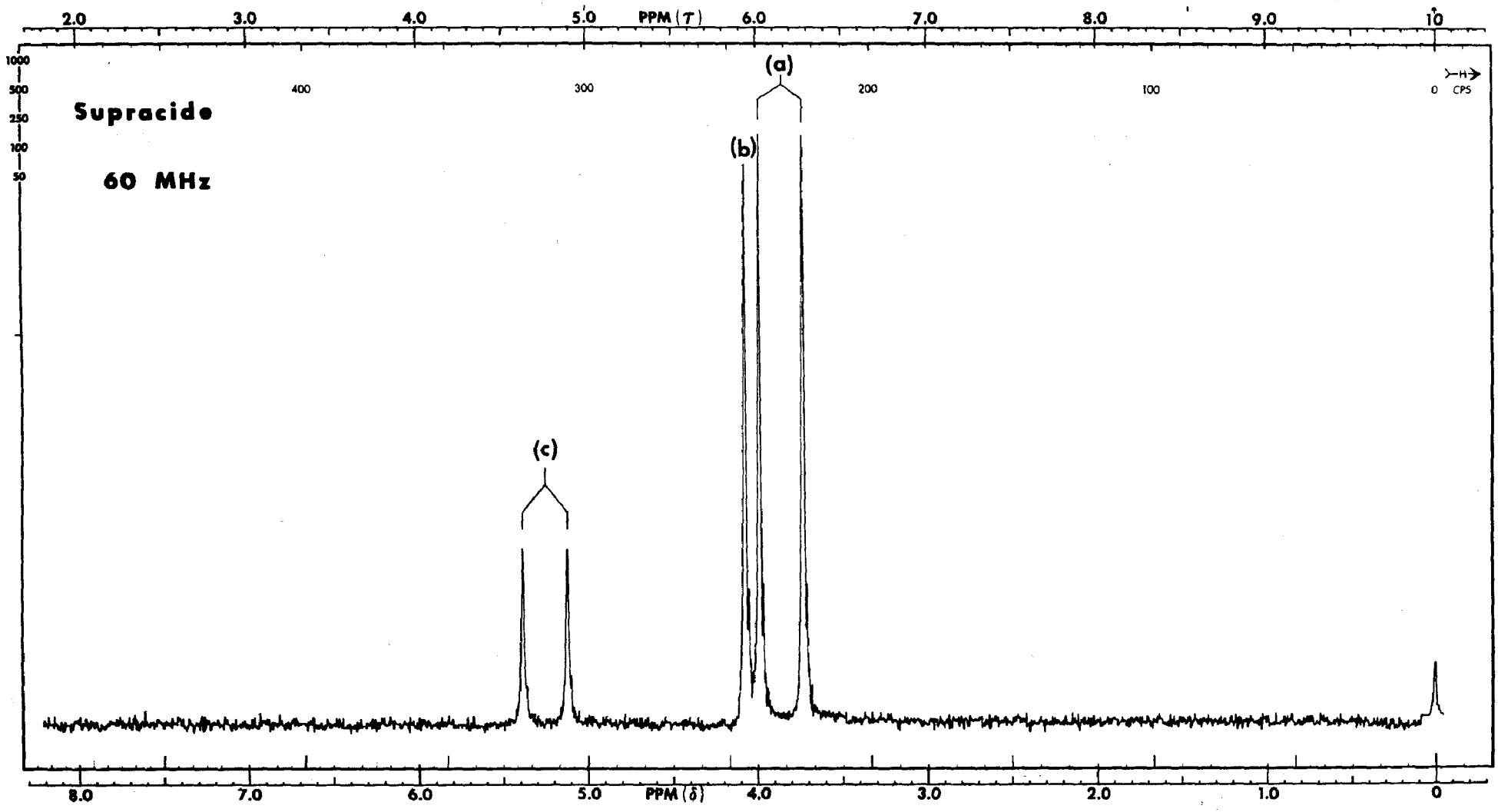
# C-34a



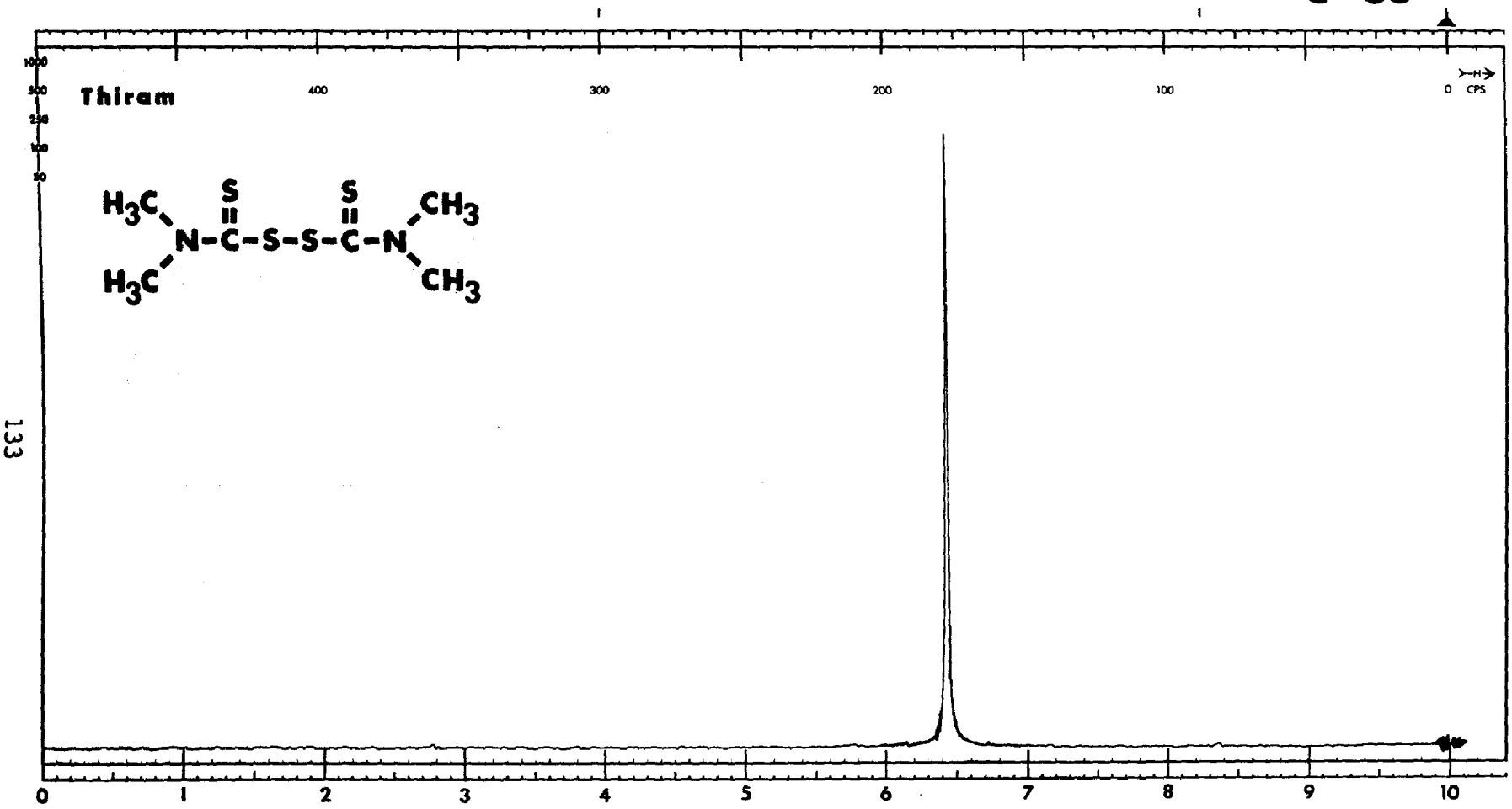




| | T | J |
|---|---|---|
| a | 6.29 | 15 |
| b | 5.99 | |
| c | 4.82 | 16 |


2.0
3.0
4.0
5.0
PPM (τ)
6.0
7.0
8.0
9.0
10
1000
500
250
100
50
400
300
200
100
0 CPS
(a)
(b)
(c)
Supracide
60 MHz
8.0
7.0
6.0
5.0
PPM (δ)
4.0
3.0
2.0
1.0
0

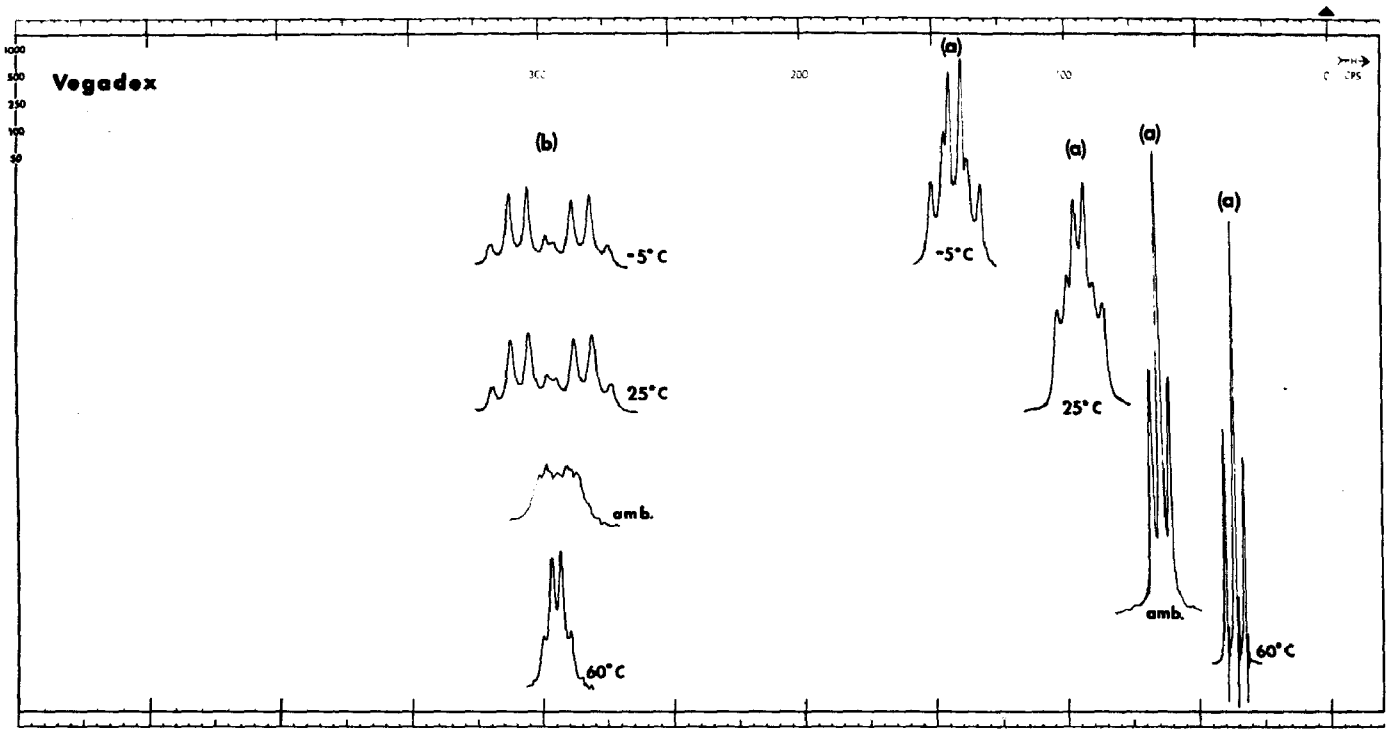
C-35

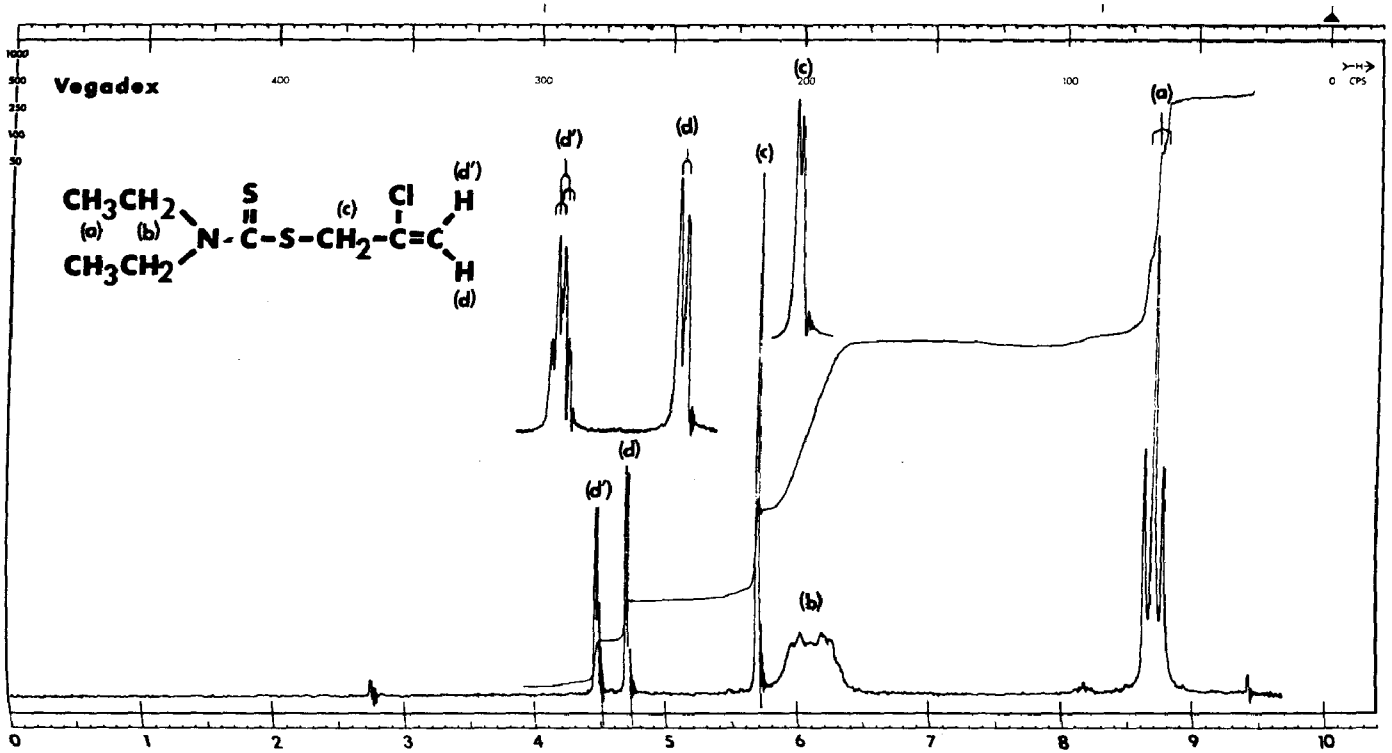



T

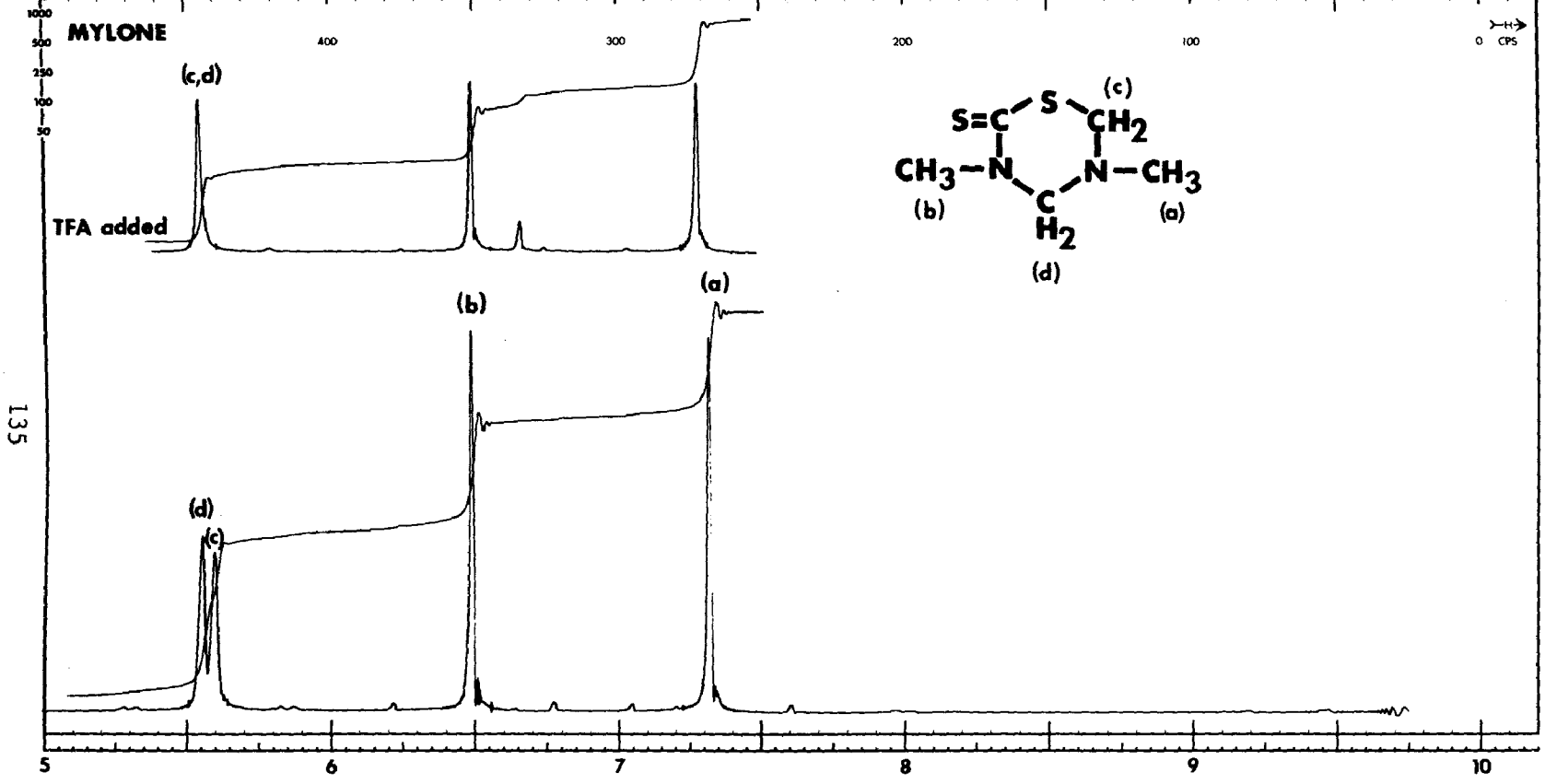
6.40

133




| | T | J |
|---|---|---|
| a | 8.72 | 7 |
| b | 6.12 | 7 |
| c | 5.72 | 1.0($H_c$-$H_{d'}$) |
| d | 4.73 | 1.5($H_d$-$H_{d'}$) |
| d' | 4.48 | 1.0($H_{d'}$-$H_c$)<br>1.5($H_{d'}$-$H_d$) |




| | T |
|---|---|
| a | 7.28 |
| b | 6.49 |
| c | 5.59 |
| d | 5.55 |

## SECTION IV

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Carbofuran - see Furadan®

Carbophenothion - see Trithion®

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Propham - see IPC

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## SECTION V

## ACKNOWLEDGMENTS

Ann L. Alford and Lawrence H. Keith performed the experimental work, interpreted the spectra, and prepared the spectral catalog. Arthur W. Garrison's advice and assistance with the organophosphorus and DDT pesticide spectra are gratefully acknowledged.

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## SECTION VI

## REFERENCES


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## SECTION VII

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## SECTION VIII

## APPENDIX: CHEMICAL NAMES AND SOURCES OF THE PESTICIDES

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| A-1 | Malathion | O,O-Dimethyl S-(1,2-dicarboethoxyethyl) phosphorodithioate | American Cyanamid |
| A-2 | Malaoxon | O,O-Dimethyl S-(1,2-dicarboethoxyethyl) phosphorothioate | American Cyanamid |
| A-3 | Cygon® | O,O-Dimethyl S-(N-methylcarbamoylmethyl) phosphorodithioate | American Cyanamid |
| A-4 | Dimethoxon | O,O-Dimethyl S-(N-methylcarbamoylmethyl) phosphorothioate | American Cyanamid |
| A-5 | Meta-Systox-R® | O,O-Dimethyl S-[2-(ethylsulfinyl) ethyl] phosphorothioate | Chemagro Corp |
| A-6 | Dibrom® | O,O-Dimethyl O-1,2-dibromo-2,2-dichloroethyl phosphate | Chevron Chem Co |
| A-7 | Neguvon® | O,O-Dimethyl (1-hydroxy-2,2,2-trichloroethyl) phosphonate | Chemagro Corp |
| A-8 | DDVP | O,O-Dimethyl O-2,2-dichlorovinyl phosphate | Shell Development Corp |
| A-9 | Ciodrin® | α-Methylbenzyl 3-(dimethoxyphosphinyloxy)-cis-crotonate | Shell Development Corp |
| A-10 | Azodrin® | 3-(Dimethoxyphosphinyloxy)-N-methyl-cis-crotonamide | Shell Development Corp |
| A-11 | Bidrin® | 3-(Dimethoxylphosphinyloxy)-N,N-dimethyl-cis-crotonamide | Shell Development Corp |

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| A-12 | Phosdrin® | 0,0-Dimethyl 0-(2-carbomethoxy-1-methylvinyl) phosphate | FDA |
| A-13 | Phosphamidon | 0,0-Dimethyl 0-[2-chloro-2-(N,N-diethyl carbamoyl)-1-methylvinyl] phosphate | Chevron Chem Co |
| A-14 | Methyl Trithion® | 0,0-Dimethyl S-(p-chlorophenylthio)methyl phosphorodithioate | Stauffer Chem Co |
| A-15 | Guthion® | 0,0-Dimethyl S-[4-oxo-1,2,3-benzotriazin-3(4H)-yl methyl] phosphorodithioate | Chemagro Corp |
| A-16 | Guthion oxygen analog | 0,0-Dimethyl S-[4-oxo-1,2,3-benzotriazin-3(4H)-yl methyl] phosphorothioate | Chemagro Corp |
| A-17 | Imidan® | 0,0-Dimethyl S-phthalimidomethyl phosphorodithioate | Stauffer Chem Co |
| A-18 | Tiguvon® | 0,0-Dimethyl 0-[4-(methylthio-m-tolyl] phosphorothioate | Chemagro Corp |
| A-19 | Abate® | 0,0,0',0'-Tetramethyl 0,0'-thiodi-p-phenylene phosphorothioate | American Cyanamid |
| A-20 | Ronnel | 0,0-Dimethyl 0-(2,4,5-trichlorophenyl) phosphorothioate | Dow Chem Co |
| A-21 | Gardona® | vinyl dimethyl ester 2-chloro-1-(2,4,5-trichlorophenyl) phosphoric acid | Shell Development Corp |
| A-22 | Methyl parathion | 0,0-Dimethyl 0-(4-nitrophenyl) phosphorothioate | Monsanto Chem Co |
| A-23 | Sumithion® | 0,0-dimethyl 0-(4-nitro-m-tolyl) phosphorothioate | Chemagro Corp |

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| A-24 | Dicapthon | O,O-Dimethyl O-(2-chloro-4-nitrophenyl) phosphorothioate | American Cyanamid |
| A-25 | Ruelene® | 4-t-Butyl-2-chlorophenyl methyl methylphosphoramidate | Dow Chemical Co |
| A-26 | Zytron® | 2,4-Dichlorophenyl methyl isopropyl-phosphoramidothioate | Dow Chemical Co |
| A-27 | Thimet® | O,O-Diethyl S-(ethylthio) methyl phosphorodithioate | American Cyanamid |
| A-28 | Di-Syston® | O,O-Diethyl S-2-(ethylthio) ethyl phosphorodithioate | Chemagro Corporation |
| A-29 | Systox® | O,O-Diethyl O-2-(ethylthio) ethyl phosphorothioate | Chemagro Corporation |
| A-30 | Iso-Systox® | O,O-Diethyl S-2-(ethylthio) ethyl phosphorothioate | Chemagro Corporation |
| A-31 | Delnav® | 2,3-p-Dioxanedithiol S,S'-bis(O,O-diethyl phosphorodithioate) | Hercules Powder Company |
| A-32 | Trithion® | O,O-Diethyl S-(4-chlorophenylthiomethyl) phosphorodithioate | Stauffer Chemical Co |
| A-33 | Ethion | O,O,O',O'-Tetraethyl S,S'-methylene bis-phosphorodithioate | Niagara Chem Div, FMC Corp |
| A-34 | Phenacapton | O,O-Diethyl S-(2,5-dichlorophenylthio) methyl phosphorodithioate | Geigy Chemical Corporation |
| A-35 | Dursban® | O,O-Diethyl O-(3,5,6-trichloro-2-pyridyl) phosphorothioate | Dow Chemical Co |

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| A-36 | Zinophos® | O,O-Diethyl O-2-pyrazinyl phosphorothioate | American Cyanamid |
| A-37 | Diazinon | O,O-Diethyl O-(2-isopropyl-4-methyl-6-pyrimidyl) phosphorothioate | Geigy Chemical Corp |
| A-38 | Diazoxon | O,O-Diethyl O-(2-isopropyl-4-methyl-6-pyrimidyl) phosphate | Geigy Chemical Corp |
| A-39 | Ethyl Guthion® | O,O-Diethyl S- [4-oxo-1,2,3-benzotriazin-3-(4H)yl methyl] phosphorodithioate | Chemagro Corporation |
| A-40 | Co-Ral® | O,O-Diethyl O-(3-chloro-4-methyl-2-oxo-2H-1-benzopyran-7-yl) phosphorothioate | Chemagro Corporation |
| A-41 | Ethyl parathion | O,O-Diethyl O-4-nitrophenyl phosphorothioate | Monsanto Chemical Co |
| A-42 | Paraoxon | O,O-Diethyl O-4-nitrophenyl phosphate | American Cyanamid |
| A-43 | Supona® | O,O-Diethyl-1-(2,4-dichlorophenyl)-2-chlorovinyl phosphate | Shell Development Corp |
| A-44 | EPN | O-Ethyl O-4-nitrophenyl phenylphosphonothioate | E. I. Dupont de Nemours and Co |
| A-45 | Sulfotepp | O,O,O',O'-Tetraethyl dithiopyrophosphate | Chemagro Corporation |
| A-46 | Aspon | O,O,O',O'-Tetrapropyl dithiopyrophosphate | Stauffer Chemical Co |
| A-47 | Falone | Tris-(2,4-dichlorophenoxyethyl) phosphite | U S Rubber |
| A-48 | Merphos | Tributyl phosphorotrithioite | V-C Chemical Co |

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| A-49 | DEF[R] | S,S,S-Tributyl phosphorotrithioate | Chemagro Corporation |
| A-50 | Wepsyn[R] | 5-Amino-1-bis(diethylamido)phosphoryl-3-phenyl-1,2,4-triazole | Thompson-Hayward |
| B-1 | p,p'-DDT | 1,1,1-Trichloro-2,2-bis(p-chlorophenyl)-ethane | FDA |
| B-2 | o,p'-DDT | 1,1,1-Trichloro-2-p-chlorophenyl-2-o-chlorophenylethane | FDA |
| B-3 | Tech DDT | Mixture of o,p'-DDT and p,p'-DDT | Allied Chemical Corp |
| B-4 | o-MDT | 1,1,1-Trichloro-2-o-chlorophenyl-2-phenylethane | CDC, PHS |
| B-5 | Methoxychlor | 1,1,1-Trichloro-2,2-bis (p-methoxyphenyl)-ethane | Geigy Chemical Corp |
| B-6 | Kelthane[R] | 1,1-bis(p-Chlorophenyl)-2,2,2-trichloro-ethanol | Rohm & Haas Co |
| B-7 | p,p'-DDD | 1,1-Dichloro-2,2-bis(p-chlorophenyl) ethane | FDA |
| B-8 | o,p'-DDD | 1,1-Dichloro-2-p-chlorophenyl-2-o-chlorophenylethane | FDA |
| B-9 | DDMS | 1-Chloro-2,2-bis(p-chlorophenyl) ethane | CDC, PHS |
| B-10 | Perthane[R] | 1,1-Dichloro-2,2-bis(p-ethylphenyl)-ethane | Rohm & Haas Co |

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| B-11 | DDE | 1,1-Dichloro-2,2-bis(p-chlorophenyl)-ethylene | FDA |
| B-12 | p,p'-DDMU | 1-Chloro-2,2-bis(p-chlorophenyl)ethylene | CDC, PHS |
| B-13 | o,p'-DDMU | 1-Chloro-2-p-chlorophenyl-2-o-chlorophenyl-ethylene | FDA |
| B-14 | DDNU | 1,1-bis(p-Chlorophenyl)ethylene | CDC, PHS |
| B-15 | DBP | p,p'-Dichlorobenzophenone | Eastman Org Chem |
| B-16 | DDA | bis(p-Chlorophenyl)acetic acid | CDC, PHS |
| B-17 | DDA methyl ester | Methyl bis(p-chlorophenyl)acetate | CDC, PHS |
| B-18 | Diphenamid | N,N-Dimethyl-2,2-diphenylacetamide | Upjohn Co |
| B-19 | Chlorobenzilate | Ethyl-p,p'-dichlorobenzilate | Geigy Chemical Corp |
| B-20 | Chloropropylate® | Isopropyl-p,p'-dichlorobenzilate | Geigy Chemical Corp |
| B-21 | Prolan® | 2-Nitro-1,1-bis(p-chlorophenyl)propane | Commercial Solvents Corp |
| B-22 | Bulan® | 2-Nitro-1,1-bis(p-chlorophenyl)butane | Commercial Solvents Corp |
| B-23 | Dilan® | Mixture of Prolan and Bulan | Commercial Solvents Corp |
| B-24 | DDOH | 2,2-bis(p-Chlorophenyl)ethanol | CDC, PHS |
| B-25 | Preventol® GD | bis(o-Hydroxy-p-chlorophenyl)methane | General Aniline & Film Corp |
| B-26 | DDT acetal | 2-bis(p-Chlorophenyl)methyl-1,3-dioxolane | CDC, PHS |

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| B-27 | Isobutyl triphenyl-methylamine | | Imperial Chem Industries LTD |
| C-1 | SD 8530 | 3,4,5-Trimethylphenyl-N-methylcarbamate | Shell Development Corp |
| C-2 | UC 10854 | 3-Isopropylphenyl-N-methylcarbamate | Union Carbide Corp |
| C-3 | Azak® | 2,6-Di-tert-butyl-4-methylphenyl-N-methylcarbamate | Hercules Powder Co |
| C-4 | RE 5305 | 3-sec-Butylphenyl-N-methylcarbamate | Chevron Chemical Co |
| C-5 | Baygon® | 2-Isopropoxyphenyl-N-methylcarbamate | Chemagro Corporation |
| C-6 | Carbanolate | 3,4-Xylyl-6-chloro-N-methylcarbamate | Upjohn Company |
| C-7 | Benomyl | Methyl 1-(butylcarbamoyl)-2-benzimidazole carbamate | E. I. DuPont de Nemours & Co |
| C-8 | Benomyl metabolite | Methyl 5-hydroxy-2-benzimidazole carbamate | E. I. DuPont de Nemours & Co |
| C-9 | Sevin® | 1-Naphthyl-N-methylcarbamate | Union Carbide Corporation |
| C-10 | UC 8454 | 1-(5,6,7,8-Tetrahydro)-naphthyl-N-methylcarbamate | Union Carbide Corporation |
| C-11 | Furadan® | 7-(2,3-Dihydro-2,2-dimethyl)-benzofuranyl-N-methylcarbamate | Niagara Chemical Div, FMC Corp |
| C-12 | Mobam® | 4-Benzothienyl-N-methylcarbamate | Mobil Chemical Co |
| C-13 | Matacil® | 4-Dimethylamino-3-methylphenyl-N-methylcarbamate | Chemagro Corporation |

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| C-14 | Zectran® | 4-Dimethylamino-3,5-dimethylphenyl-N-methylcarbamate | Dow Chemical Co |
| C-15 | Mesurol® | 4-Methylthio-3,5-dimethylphenyl-N-methylcarbamate | Chemagro Corporation |
| C-16 | Sirmate, 2,3-isomer | 2,3-Dichlorobenzyl-N-methylcarbamate | FDA |
| C-17 | Sirmate, 3,4-isomer | 3,4-Dichlorobenzyl-N-methylcarbamate | FDA |
| C-18 | Methomyl | S-Methyl N-[(methylcarbamoyl)oxy] thioacetimidate | E. I. DuPont de Nemours & Co |
| C-19 | Temik® | 2-Methyl-2-methylthiopropionaldehyde-O-methylcarbamoyl oxime | Union Carbide Corp |
| C-20 | Isolan | 5-(1-Isopropyl-3-methyl)-pyrazolyl-N,N-dimethylcarbamate | Geigy Chemical Corp |
| C-21 | Dimetilan® | 3-(1-N,N-Dimethylcarbamoyl-5-methyl)-pyrazolyl-N,N-dimethylcarbamate | Geigy Chemical Corp |
| C-22 | IPC | Isopropyl-N-phenylcarbamate | Pittsburgh Plate Glass Co |
| C-23 | CIPC | Isopropyl-N-(3-chlorophenyl)carbamate | Pittsburgh Plate Glass Co |
| C-24 | Barban | 4-Chloro-2-butynyl-N-(3-chlorophenyl)-carbamate | Gulf Res & Dev Co |
| C-25 | Swep | Methyl-N-(3,4-dichlorophenyl)carbamate | Niagara Chem Div, FMC Corp |
| C-26 | Eptam® | S-Ethyl-N,N-dipropylthiolcarbamate | Stauffer Chemical Co |
| C-27 | Sutan | S-Ethyl-N,N-diisobutylthiolcarbamate | Stauffer Chemical Co |

| Spectrum No. | Common or Trade Name | Chemical Name | Source |
|---|---|---|---|
| C-28 | Tillam® | S-Propyl-N-butyl-N-ethylthiolcarbamate | Stauffer Chemical Co |
| C-29 | Vernam® | S-Propyl-N,N-dipropylthiolcarbamate | Stauffer Chemical Co |
| C-30 | Avadex® | S-(2,3-Dichloroallyl)-N,N-diisopropyl thiolcarbamate | Monsanto Chemical Co |
| C-31 | Avadex BW® | S-(2,3,3-Trichloroallyl)-N,N-diisopropyl thiolcarbamate | Monsanto Chemical Co |
| C-32 | Ro-Neet | S-Ethyl-N-ethyl-N-cyclohexylthiolcarbamate | Stauffer Chemical Co |
| C-33 | Ordram® | S-Ethyl-hexahydroazepine-1-carbothioate | Stauffer Chemical Co |
| C-34 | Supracide® | O,O-Dimethyl-S-[2-methoxy-1,3,4-thiadiazol-5(4H)-onyl-4-methyl]-dithiophosphate | Geigy Chemical Corp |
| C-35 | Thiram | bis(Dimethylthiocarbamoyl)disulfide | E. I. DuPont de Nemours & Co |
| C-36 | Vegadex® | 2-Chloroallyl-N,N-diethyl dithiocarbamate | Monsanto Chemical Co |
| C-37 | Mylone® | 3,5-Dimethyl-1,3,5-tetrahydrothiadiazine-2-thione | Union Carbide Corp |

| 1 Accession Number | 2 Subject Field & Group | SELECTED WATER RESOURCES ABSTRACTS<br>INPUT TRANSACTION FORM |
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5 Organization

Water Quality Office, Environmental Protection Agency, Southeast Water Laboratory, Athens, Georgia

6 Title

CATALOG OF PESTICIDE NMR SPECTRA


10 Author(s)

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16 Project Designation

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*Chemical shifts, *Coupling constants, spin decoupling

27 Abstract


This catalog contains the 100 MHz nuclear magnetic resonance spectra of 114 organophosphorus, DDT, and carbamate pesticides and a brief discussion of their most important features. Chemical shifts and coupling constants are shown on each spectrum. (Alford - Southeast Water Laboratory)


| Abstractor | Institution |
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