JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1996, 118(34), 8077-8084, DOI:10.1021/ja953358h

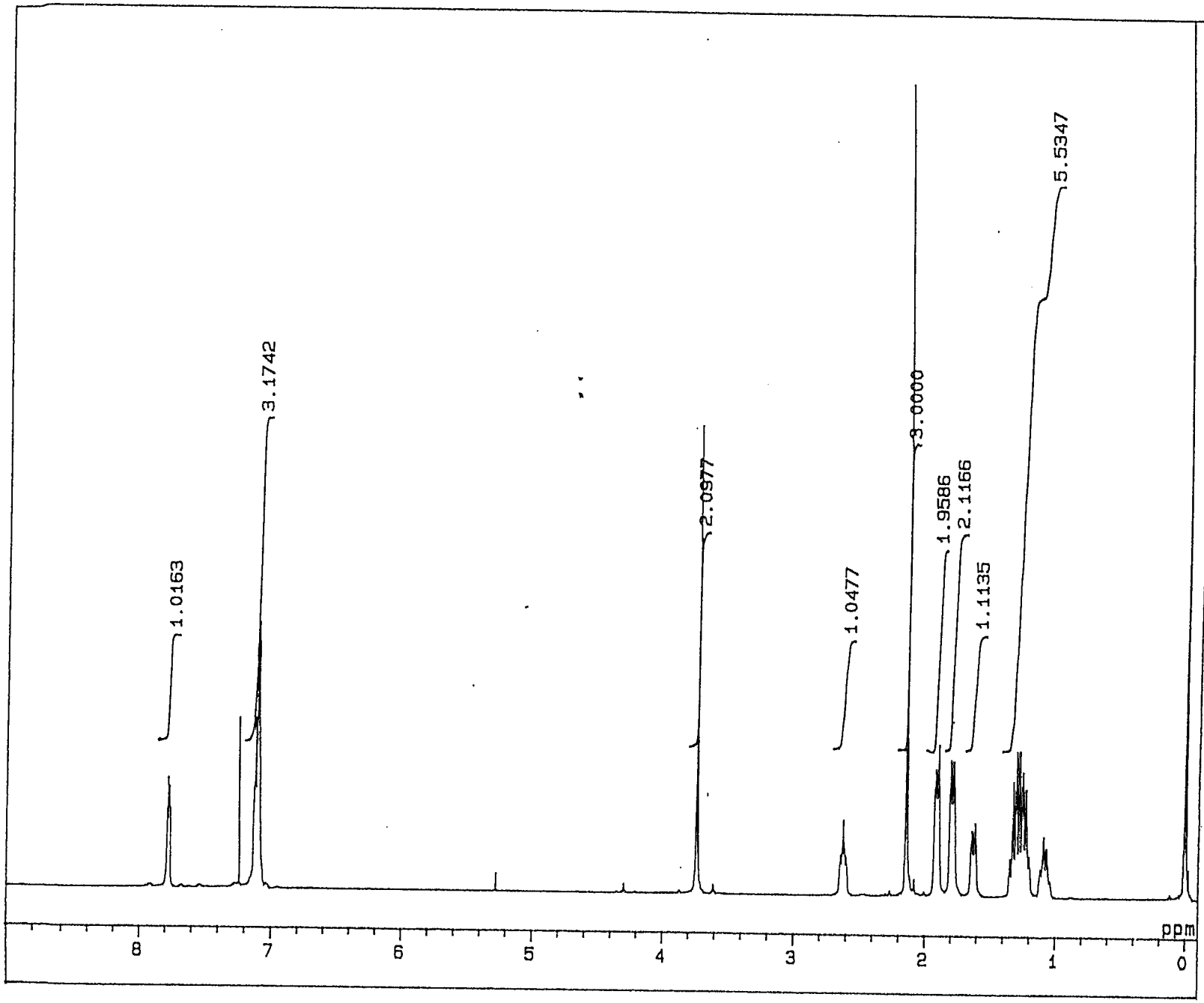
Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at http://pubs.acs.org/page/copyright/permissions.html

ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1996 American Chemical Society

^{1}H NMR Spectrum of **1** at 500 MHz.



22-APR-1995 13: 57: 17.52

DFILE : ALPHA
SFILE : TOMI_SEN_SE2_1H

COMNT : 1H
EXMOD : SINGL
IRMOD : NON
POINT : 32768
FREQU : 10000.00 Hz
SCANS : 4
DUMMY : 1
ACQTM : 3.2768 sec
PD : 2.7232 sec
RGAIN : 15

PW1 : 5.65 usec

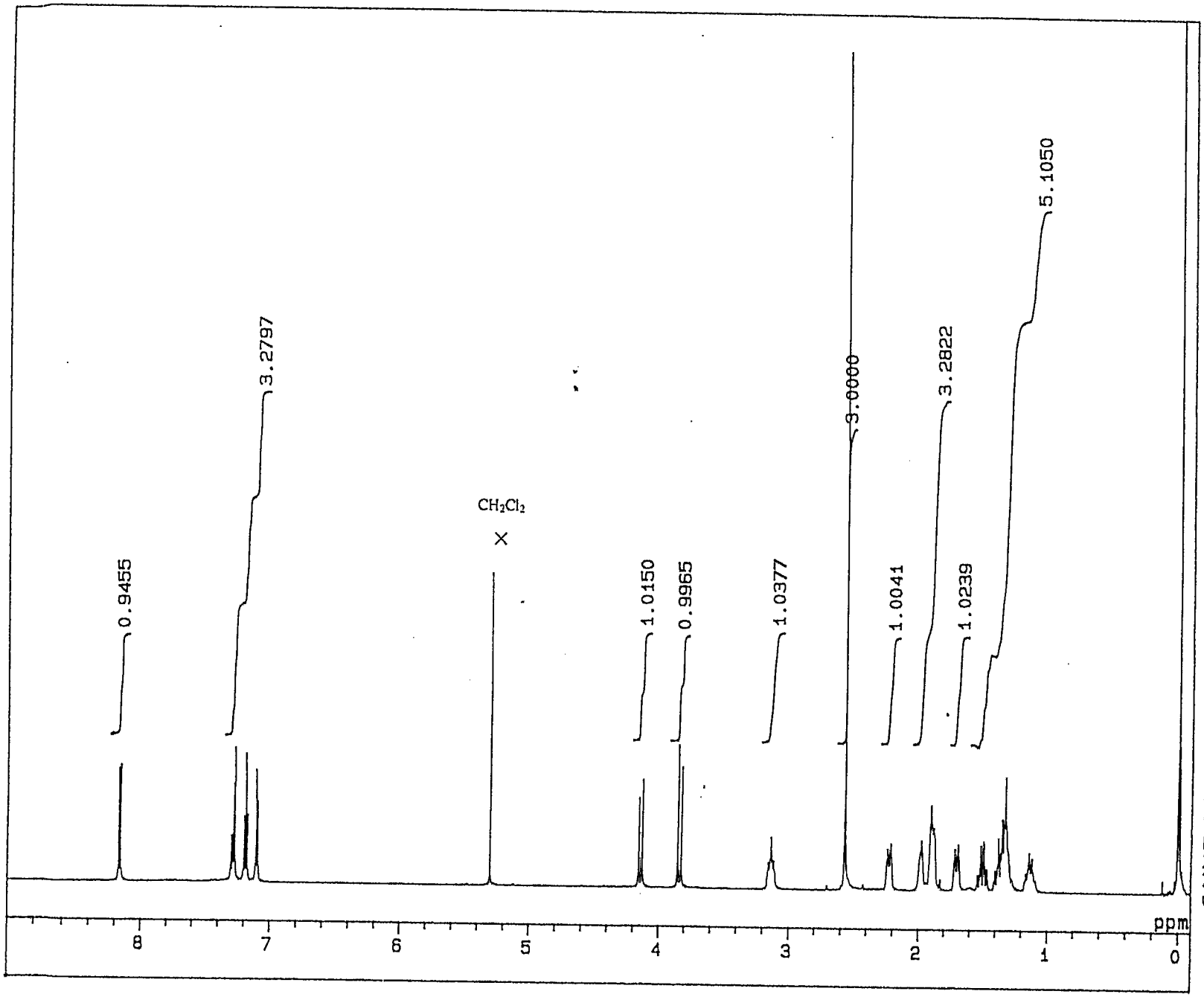
OBNUC : 1H
OBFRQ : 500.00 MHz
OBSET : 162410.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.5 c
CSPED : 11 Hz
SLVNT : CDCL3

RESOL : 0.31 Hz
BF : 0.15 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 4551.09 Hz
XS : 255.28 Hz
operator

^{1}H NMR Spectrum of **2** at 500 MHz.



22-APR-1995 13:37:03.72

DFILE : ALPHA
SFILE : TOMI_SEBR_1H_PURE

COMNT : 1H
EXMOD : SINGL
IRMOD : NON
POINT : 32768
FREQU : 10000.00 Hz
SCANS : 4
DUMMY : 1
ACQTM : 3.2768 sec
PD : 2.7232 sec
RGAIN : 16

PW1 : 5.65 usec

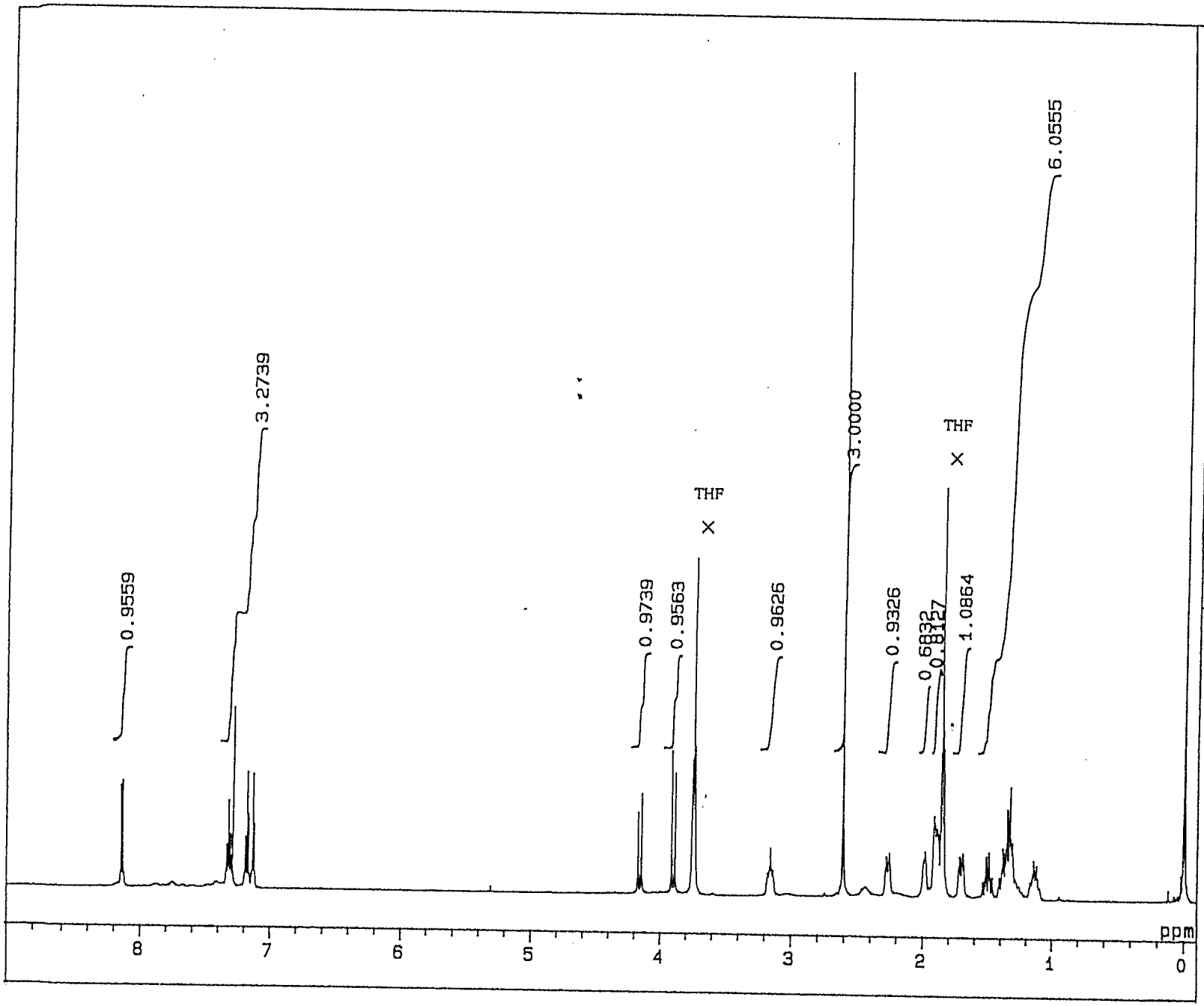
OBNUC : 1H
OBFRQ : 500.00 MHz
OBSET : 162410.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.8 c
CSPED : 13 Hz
SLVNT : CDCL3

RESOL : 0.31 Hz
BF : 0.15 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 4551.09 Hz
XS : 273.28 Hz
operator

^{1}H NMR Spectrum of **3** at 500 MHz.



22-APR-1995 13: 46: 20.91

DFILE : ALPHA
SFILE : TOMI_SECL_1H_PURE

COMNT : 1H
EXMOD : SINGL
IRMOD : NON
POINT : 32768
FREQU : 10000.00 Hz
SCANS : 4
DUMMY : 1
ACQTM : 3.2768 sec
PD : 2.7232 sec
RGAIN : 15

PW1 : 5.65 usec

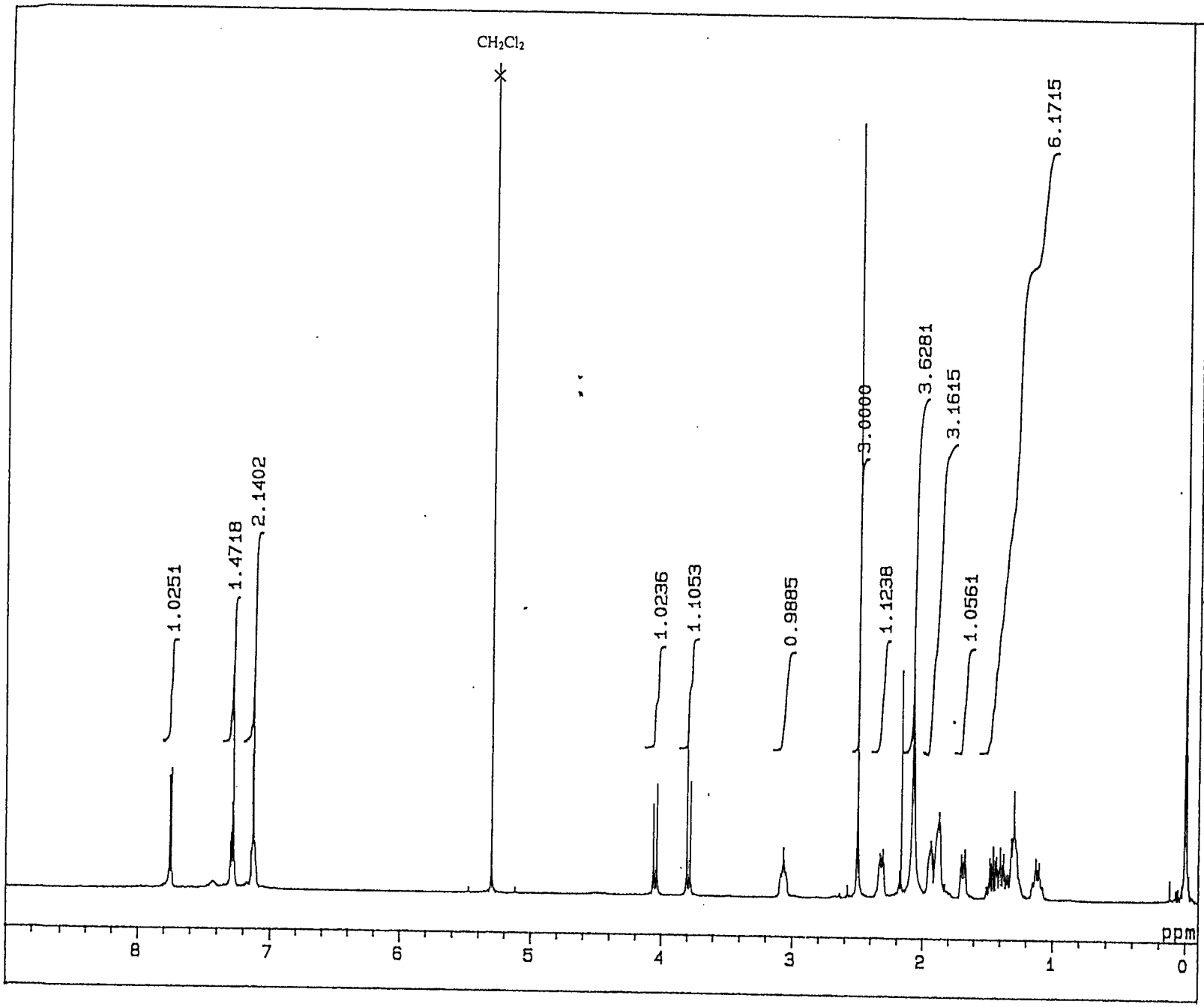
OBNUC : 1H
OBFRQ : 500.00 MHz
OBSET : 162410.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 22.8 c
CSPED : 11 Hz
SLVNT : CDCL3

RESOL : 0.31 Hz
BF : 0.15 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 4551.09 Hz
XS : 277.56 Hz
operator

^{1}H NMR Spectrum of **4** at 500 MHz.



22-APR-1995 13:51:07.05

DFILE : ALPHA
SFILE : TOMI_SEOAC_1H_PURE

COMNT : 1H
EXMOD : SINGL
IRMOD : NON
POINT : 32768
FREQU : 10000.00 Hz
SCANS : 4
DUMMY : 1
ACQTM : 3.2768 sec
PD : 2.7232 sec
RGAIN : 16

PW1 : 5.65 usec

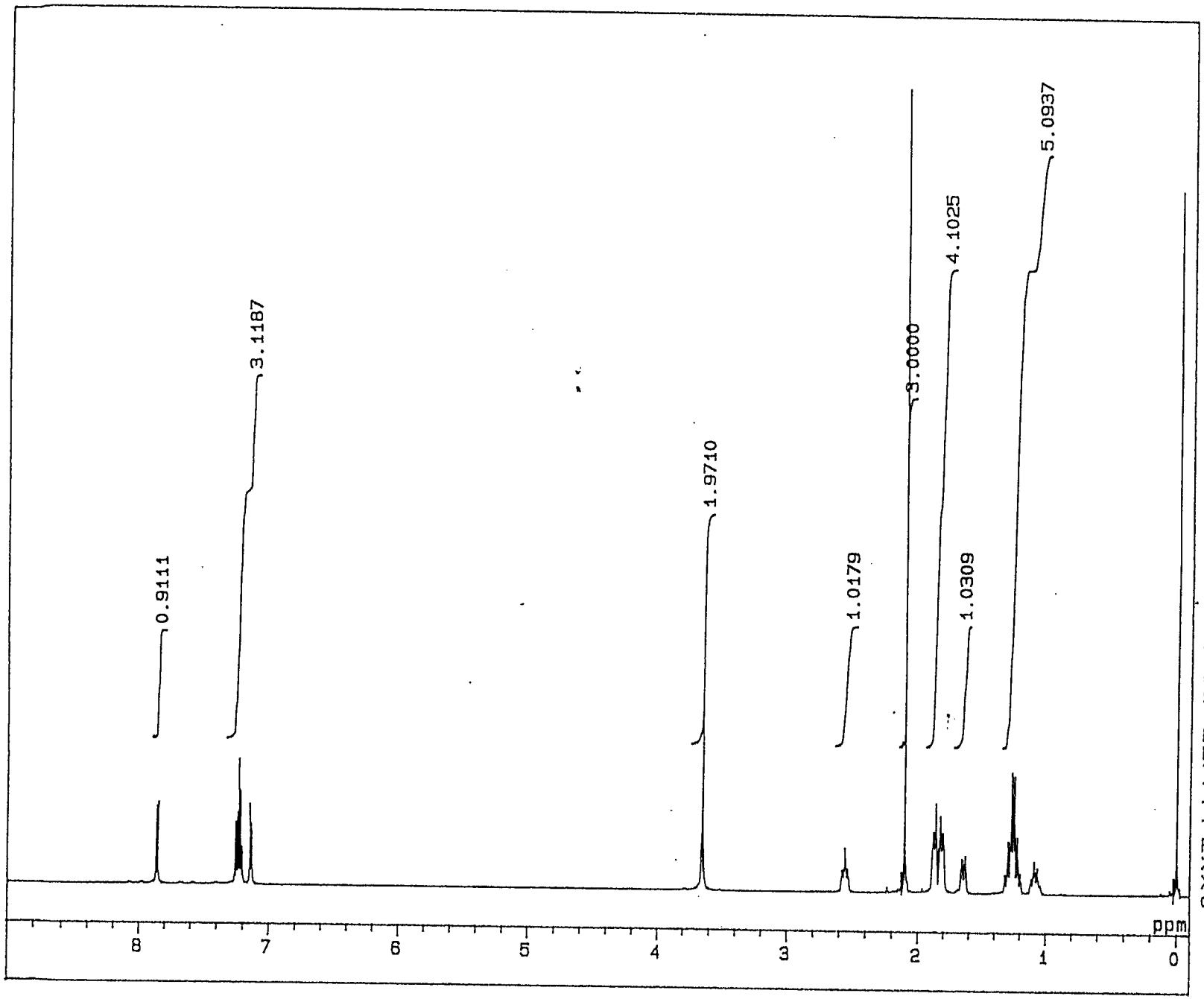
OBNUC : 1H
OBFRQ : 500.00 MHz
OBSET : 162410.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRAPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 22.8 c
CSPED : 14 Hz
SLVNT : CDCL3

RESOL : 0.31 Hz
BF : 0.15 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 4551.09 Hz
XS : 271.76 Hz
operator

^{1}H NMR Spectrum of **5** at 500 MHz.



22-APR-1995 13: 59: 56.52

DFILE : ALPHA
SFILE : TOMI_SEN_SECN_1H

COMNT : 1H
EXMOD : SINGL
IRMOD : NON
POINT : 32768
FREQU : 10000.00 Hz
SCANS : 4
DUMMY : 1
ACQTM : 3.2768 sec
PD : 2.7232 sec
RGAIN : 13

PW1 : 5.65 usec

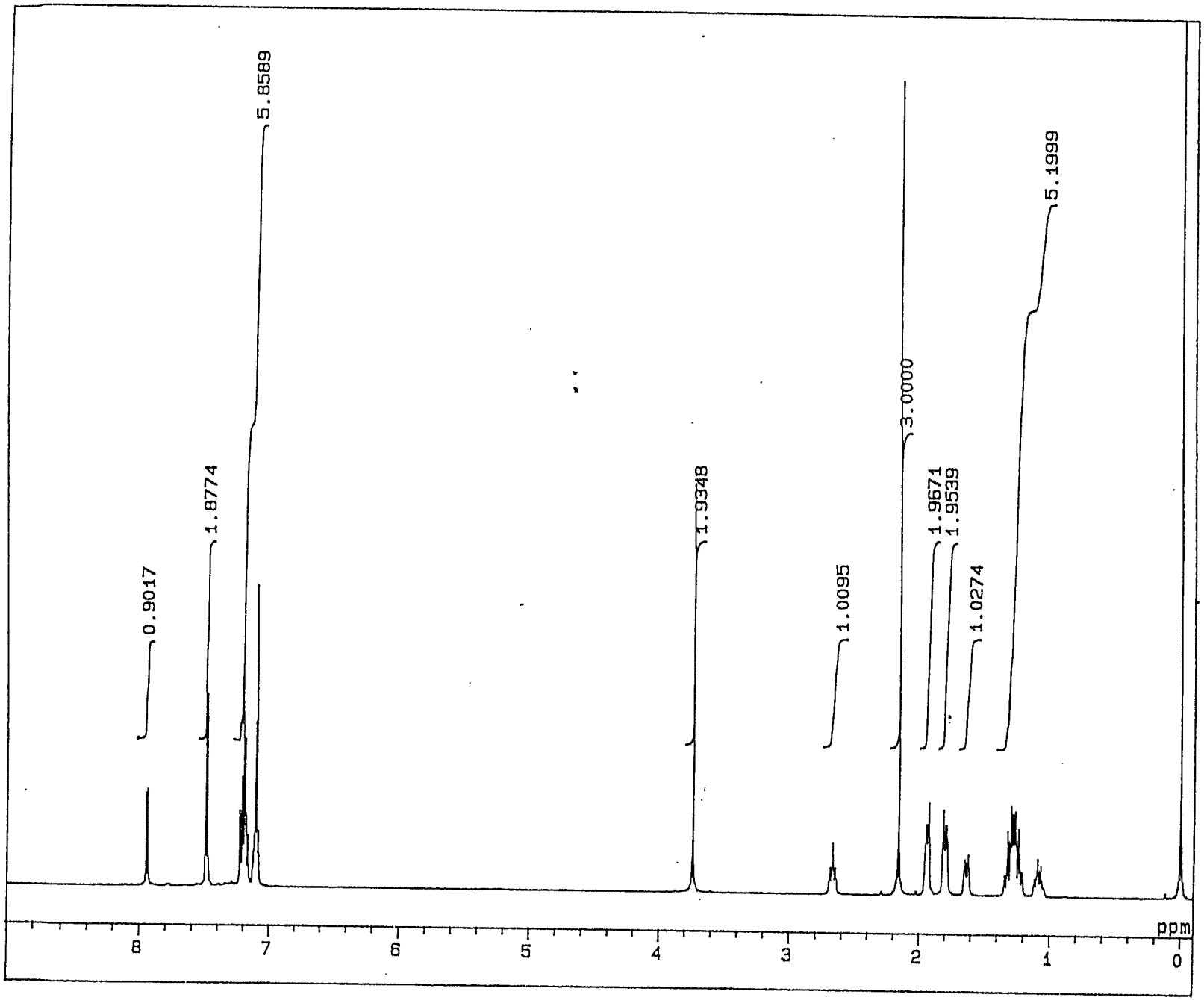
OBNUC : 1H
OBFRQ : 500.00 MHz
OBSET : 162410.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.0 c
CSPED : 12 Hz
SLVNT : CDCL3

RESOL : 0.31 Hz
BF : 0.15 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 4551.09 Hz
XS : 267.18 Hz
operator

^{1}H NMR Spectrum of **6** at 500 MHz.



22-APR-1995 14:02:24.47

DFILE : ALPHA
SFILE : TOMI_SEN_SESPH_1H

COMNT : 1H
EXMOD : SINGL
IRMOD : NON
POINT : 32768
FREQU : 10000.00 Hz
SCANS : 4
DUMMY : 1
ACQTM : 3.2768 sec
PD : 2.7232 sec
RGAIN : 16

PW1 : 5.65 usec

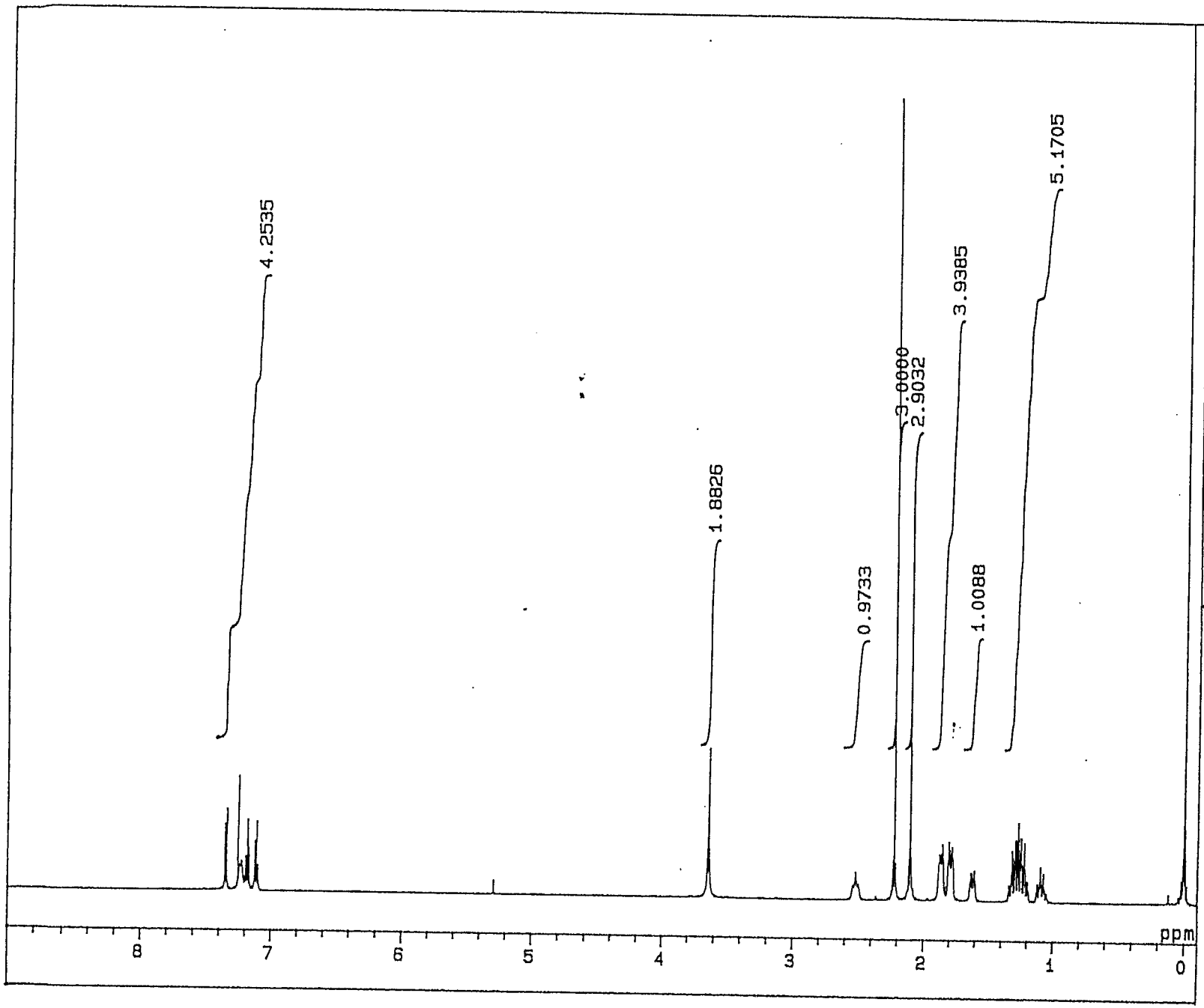
OBNUC : 1H
OBFRQ : 500.00 MHz
OBSET : 162410.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.6 c
CSPED : 11 Hz
SLVNT : CDCL3

RESOL : 0.31 Hz
BF : 0.15 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 4551.09 Hz
XS : 250.09 Hz
operator

^{1}H NMR Spectrum of 7 at 500 MHz.



22-APR-1995 13:54:32.95

DFILE : ALPHA
SFILE : TOMI_SEN_SEME_1H

COMNT : 1H
EXMOD : SINGL
IRMOD : NON
POINT : 32768
FREQU : 10000.00 Hz
SCANS : 4
DUMMY : 1
ACQTM : 3.2768 sec
PD : 2.7232 sec
RGAIN : 17

PW1 : 5.65 usec

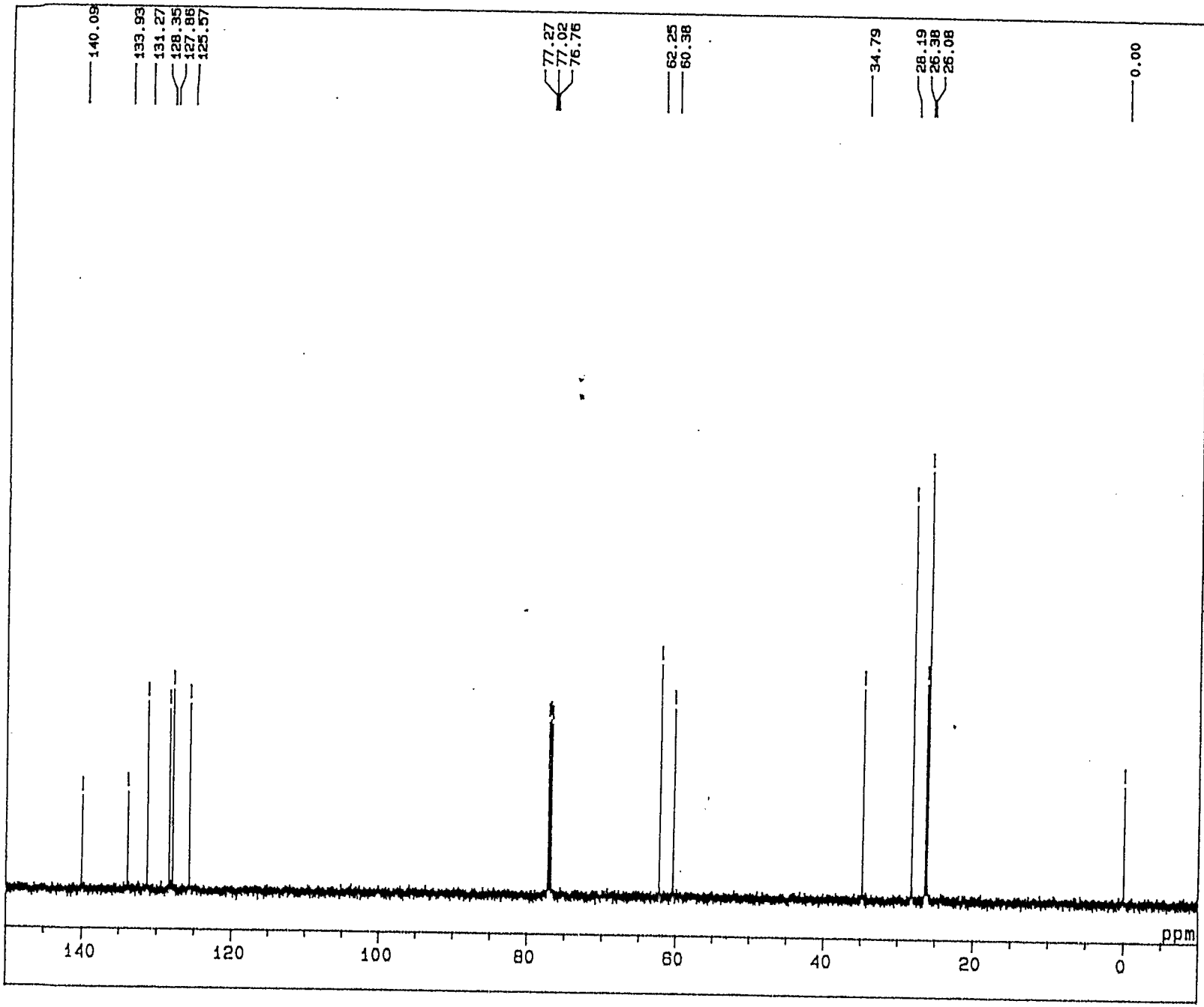
OBNUC : 1H
OBFRQ : 500.00 MHz
OBSET : 162410.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.8 c
CSPED : 10 Hz
SLVNT : CDCL3

RESOL : 0.31 Hz
BF : 0.15 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 4551.09 Hz
XS : 261.38 Hz
operator

^{13}C NMR Spectrum of **1** at 125.65 MHz.



22-APR-1995 14:24:04.79

DFILE : ALPHA
SFILE : TOMI_SEN_SE2_13C

COMNT : 13C
EXMOD : SINGL
IRMOD : BCM
POINT : 32768
FREQU : 33898.31 Hz
SCANS : 116
DUMMY : 1
ACQTM : 0.9667 sec
PD : 1.0333 sec
RGAIN : 23

PW1 : 4.70 usec

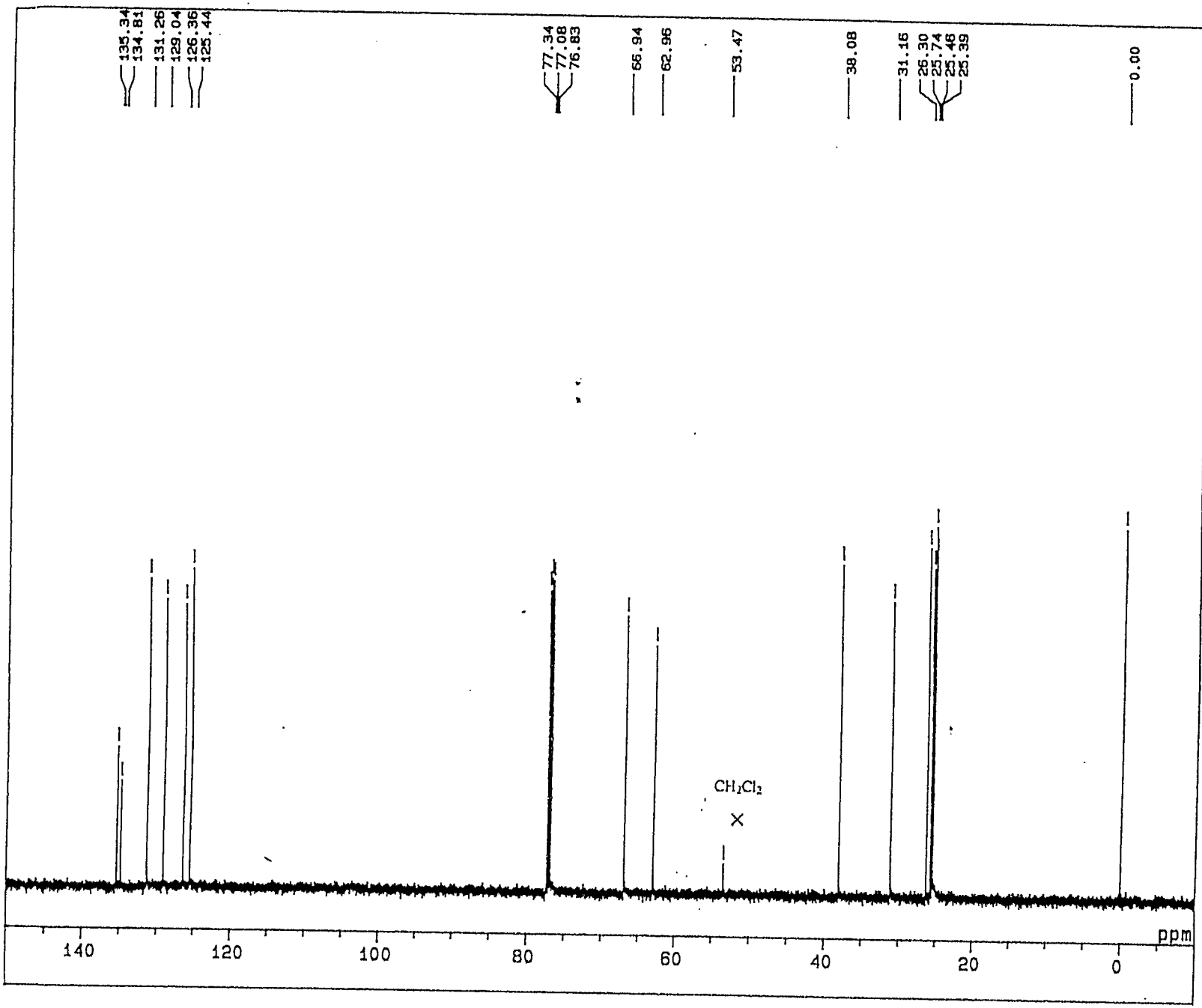
OBNUC : 13C
OBFRQ : 125.65 MHz
OBSET : 127958.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.7 c
CSPED : 11 Hz
SLVNT : CDCL3

RESOL : 1.03 Hz
BF : 1.50 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 20120.91 Hz
XS : 3841.08 Hz
operator

^{13}C NMR Spectrum of **2** at 125.65 MHz.



22-APR-1995 14: 47: 03.72

DFILE : ALPHA
SFILE : TOMI_SEBR_13C_PURE

COMNT : 13C
EXMOD : SINGL
IRMOD : BCM
POINT : 32768
FREQU : 33898.31 Hz
SCANS : 256
DUMMY : 1
ACQTM : 0.9667 sec
PD : 1.0333 sec
RGAIN : 23

PW1 : 4.70 usec

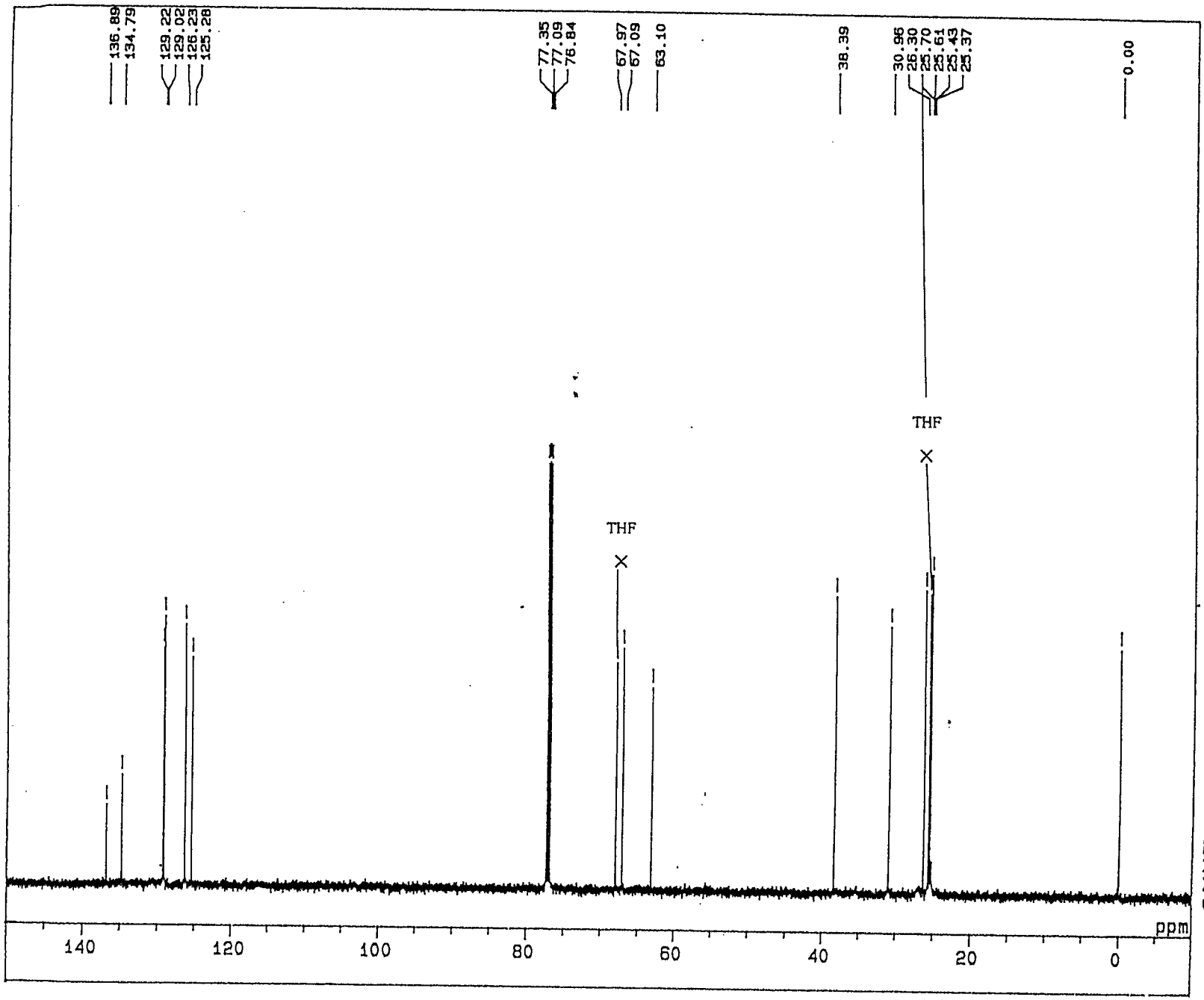
OBNUC : 13C
OBFRQ : 125.65 MHz
OBSET : 127958.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 24.9 c
CSPED : 12 Hz
SLVNT : CDCL3

RESOL : 1.03 Hz
BF : 1.50 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 20120.91 Hz
XS : 3846.25 Hz
operator

^{13}C NMR Spectrum of **3** at 125.65 MHz.



22-APR-1995 14: 26: 41.97

DFILE : ALPHA
SFILE : TOMI_SECL_13C_PURE

COMNT : 13C
EXMOD : SINGL
IRMOD : BCM
POINT : 32768
FREQU : 33898.31 Hz
SCANS : 413
DUMMY : 1
ACQTM : 0.9667 sec
PD : 1.0333 sec
RGAIN : 23

PW1 : 4.70 usec

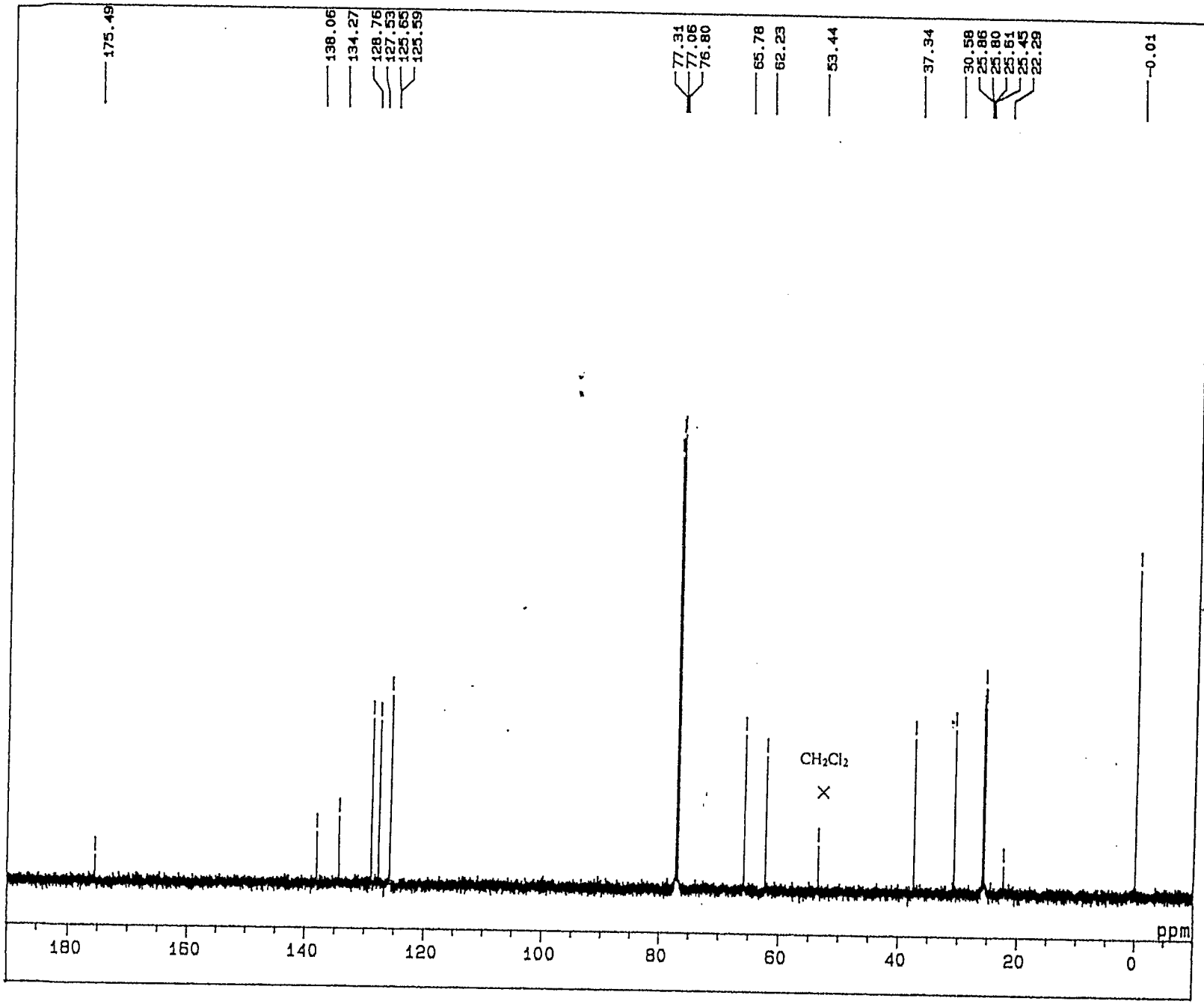
OBNUC : 13C
OBFRQ : 125.65 MHz
OBSET : 127958.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 24.0 c
CSPED : 12 Hz
SLVNT : CDCL3

RESOL : 1.03 Hz
BF : 1.50 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 20120.91 Hz
XS : 3847.28 Hz
operator

^{13}C NMR Spectrum of **4** at 125.65 MHz.



22-APR-1995 14:36:24.28

DFILE : ALPHA
SFILE : TOMI_SEOAC_13C_PURE

COMNT : 13C
EXMOD : SINGL
IRMOD : BCM
POINT : 32768
FREQU : 33898.31 Hz
SCANS : 256
DUMMY : 1
ACQTM : 0.9667 sec
PD : 1.0333 sec
RGAIN : 23

PW1 : 4.70 usec

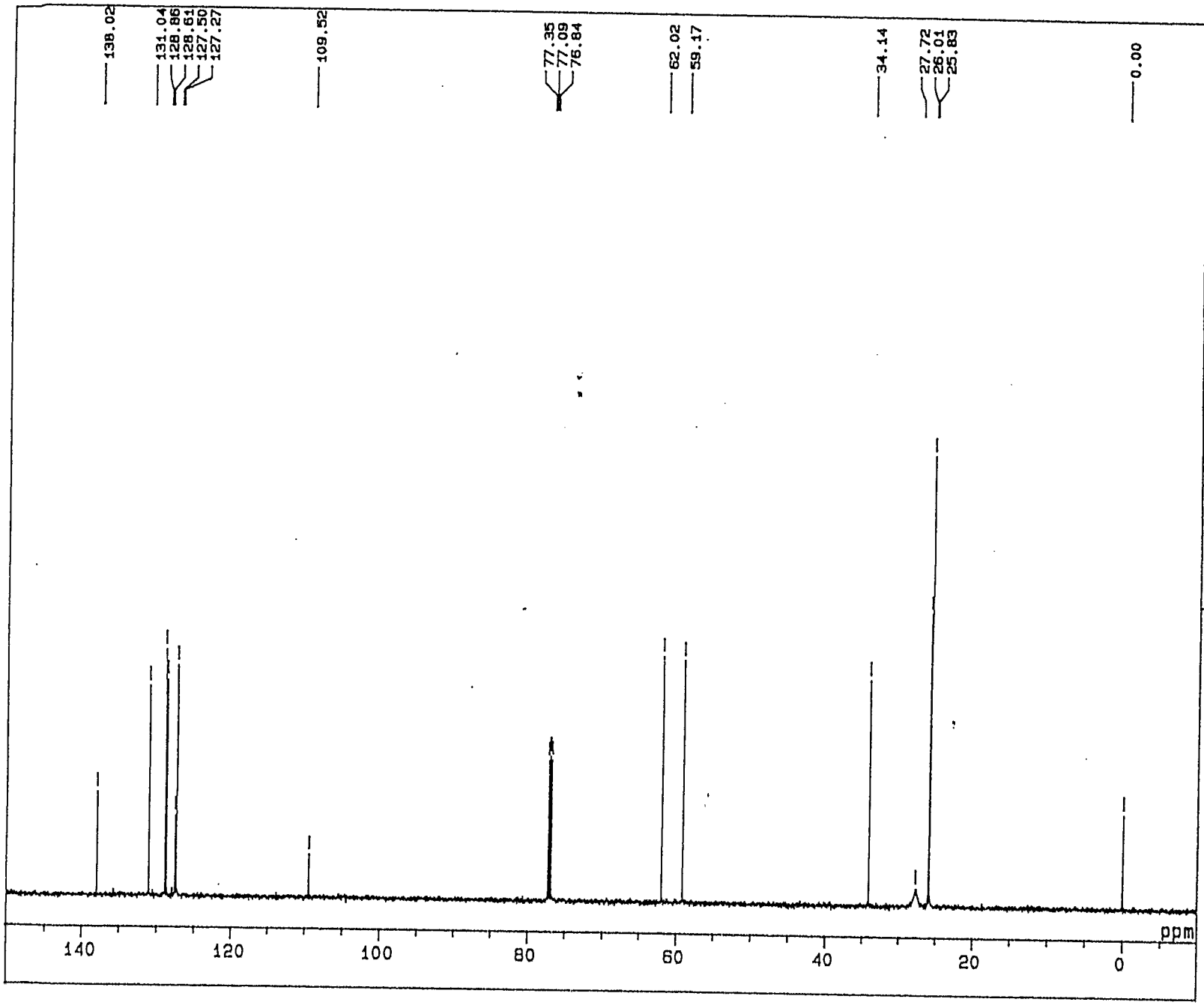
OBNUC : 13C
OBFRQ : 125.65 MHz
OBSET : 127958.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.9 c
CSPED : 12 Hz
SLVNT : CDCL3

RESOL : 1.03 Hz
BF : 2.00 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 25151.66 Hz
XS : 1330.88 Hz
operator

^{13}C NMR Spectrum of **5** at 125.65 MHz.



22-APR-1995 14: 22: 34.16

DFILE : ALPHA
SFILE : TOMI_SEN_SECN_13C

COMNT : 13C
EXMOD : SINGL
IRMOD : BCM
POINT : 32768
FREQU : 33898.31 Hz
SCANS : 198
DUMMY : 1
ACQTM : 0.9667 sec
PD : 1.0333 sec
RGAIN : 23

PW1 : 4.70 usec

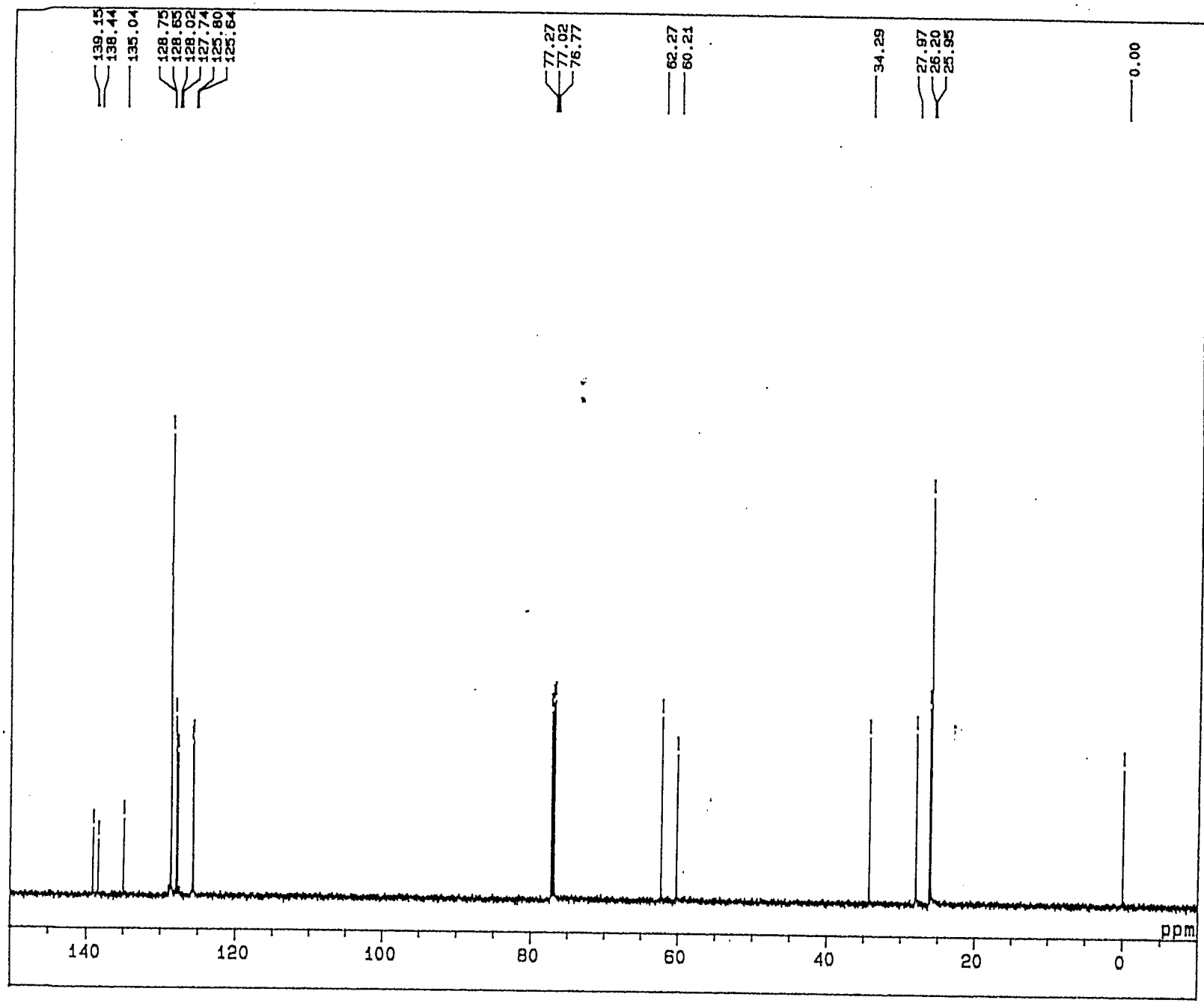
OBNUC : 13C
OBFRQ : 125.65 MHz
OBSET : 127958.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.9 c
CSPED : 14 Hz
SLVNT : CDCL3

RESOL : 1.03 Hz
BF : 1.50 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 20120.91 Hz
XS : 3842.11 Hz
operator

^{13}C NMR Spectrum of **6** at 125.65 MHz.



22-APR-1995 14: 19: 48.01

DFILE : ALPHA
SFILE : TOMI_SEN_SESPH_13C

COMNT : 13C
EXMOD : SINGL
IRMOD : BCM
POINT : 32768
FREQU : 33898.31 Hz
SCANS : 270
DUMMY : 1
ACQTM : 0.9667 sec
PD : 1.0333 sec
RGAIN : 23

PW1 : 4.70 usec

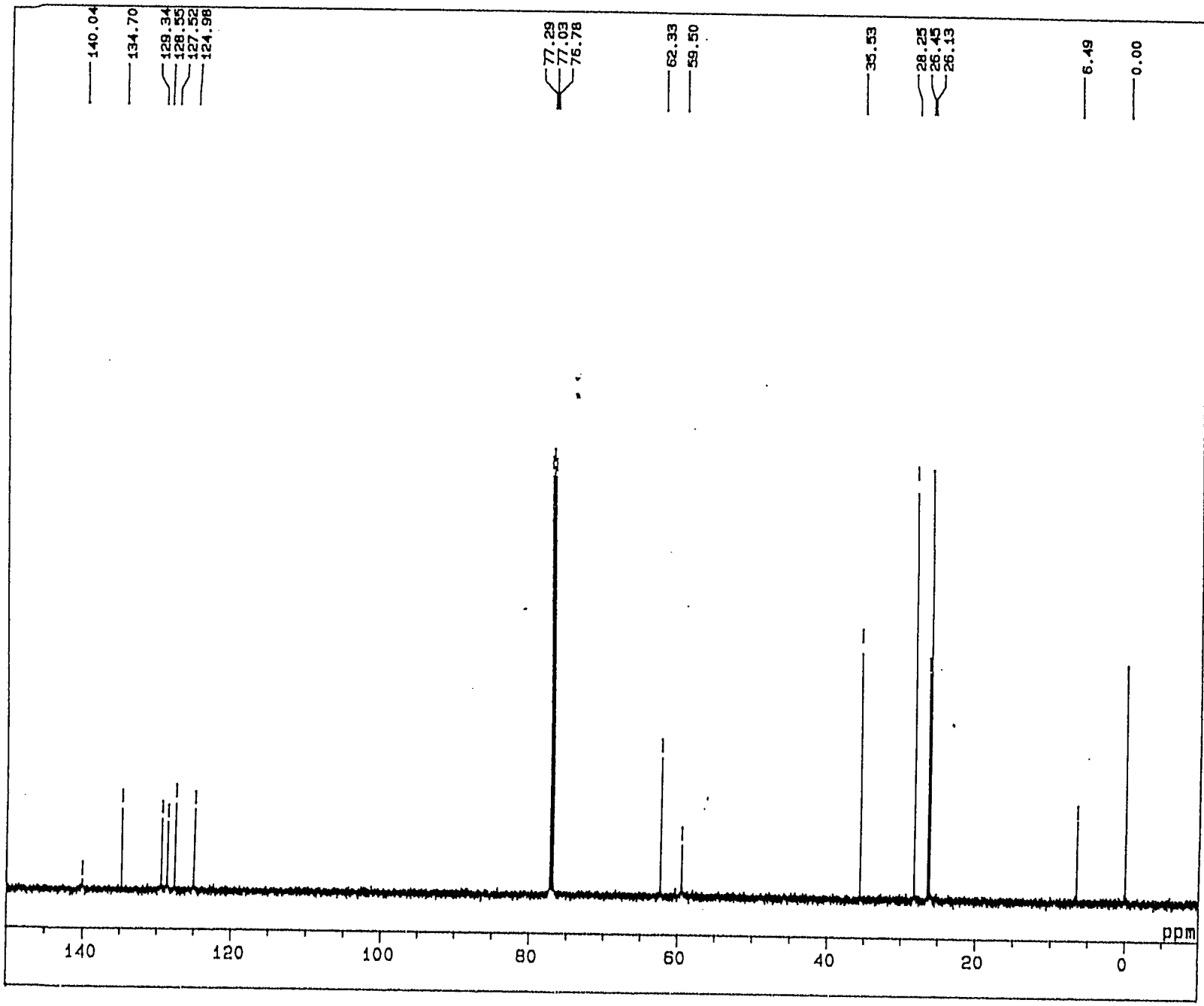
OBNUC : 13C
OBFRQ : 125.65 MHz
OBSET : 127958.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.9 c
CSPED : 11 Hz
SLVNT : CDCL3

RESOL : 1.03 Hz
BF : 1.50 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 20120.91 Hz
XS : 3839.01 Hz
operator

^{13}C NMR Spectrum of 7 at 125.65 MHz.



22-APR-1995 14: 15: 40.12

DFILE : ALPHA
SFILE : TOMI_SEN_SEME_13C

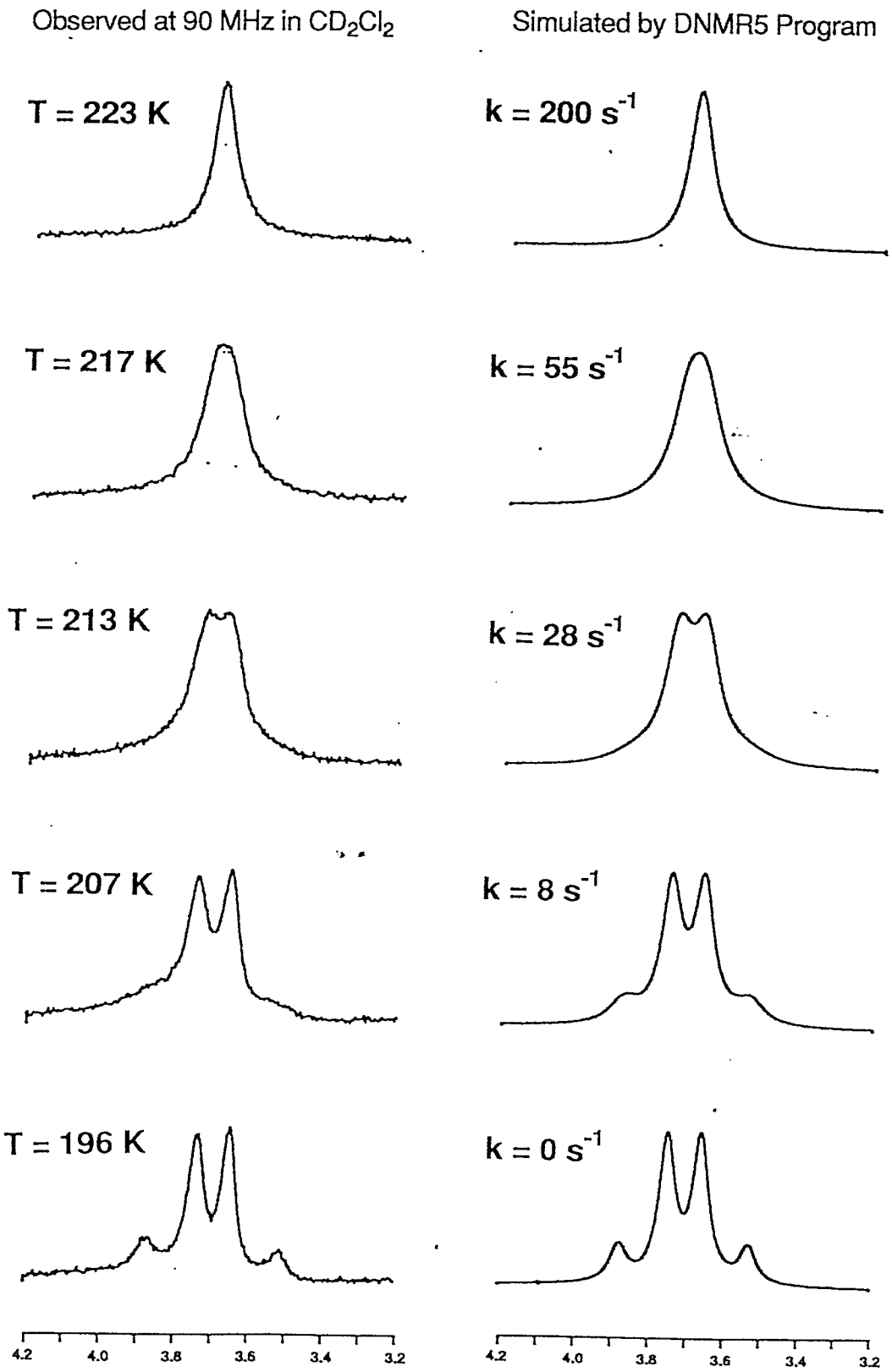
COMNT : 13C
EXMOD : SINGL
IRMOD : BCM
POINT : 32768
FREQU : 33898.31 Hz
SCANS : 512
DUMMY : 1
ACQTM : 0.9667 sec
PD : 1.0333 sec
RGAIN : 23

PW1 : 4.70 usec

OBNUC : 13C
OBFRQ : 125.65 MHz
OBSET : 127958.00 Hz

IRNUC : 1H
IRFRQ : 500.00 MHz
IRSET : 162160.00 Hz
IRATN : 511
IRRPW : 48.0 usec
IRBP1 : 20
IRBP2 : 6
IRRNS : 0

ADBIT : 16
CTEMP : 23.9 c
CSPED : 11 Hz
SLVNT : CDCL3

RESOL : 1.03 Hz
BF : 1.50 Hz
T1 : 0.00 %
T2 : 0.00 %
T3 : 90.00 %
T4 : 100.00 %
REFVL : 0.00 ppm
XE : 20120.91 Hz
XS : 3845.21 Hz
operator

90 MHz ^{1}H NMR spectra of benzylic protons for **6** (X = SPh) at various temperatires with simulated ones.