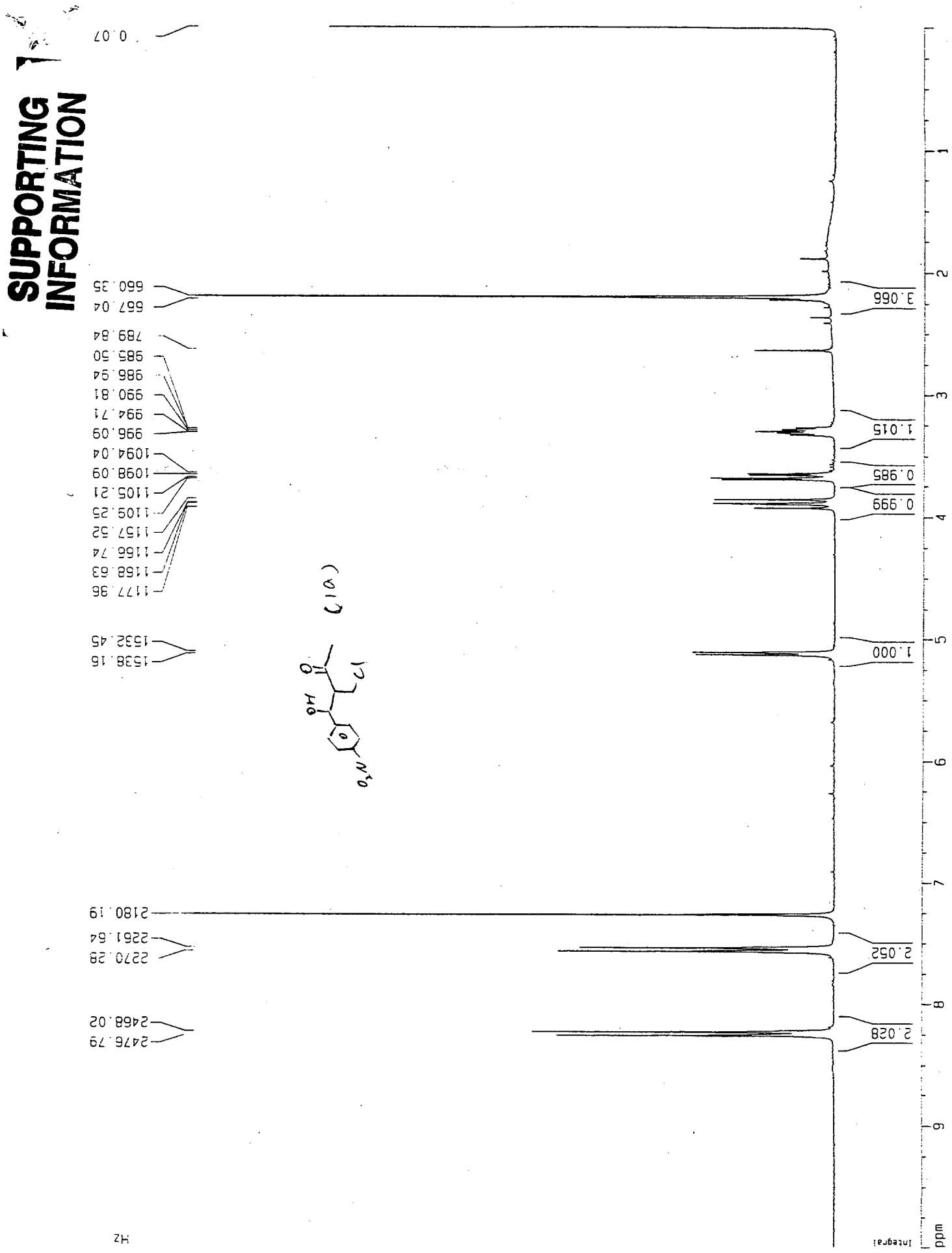
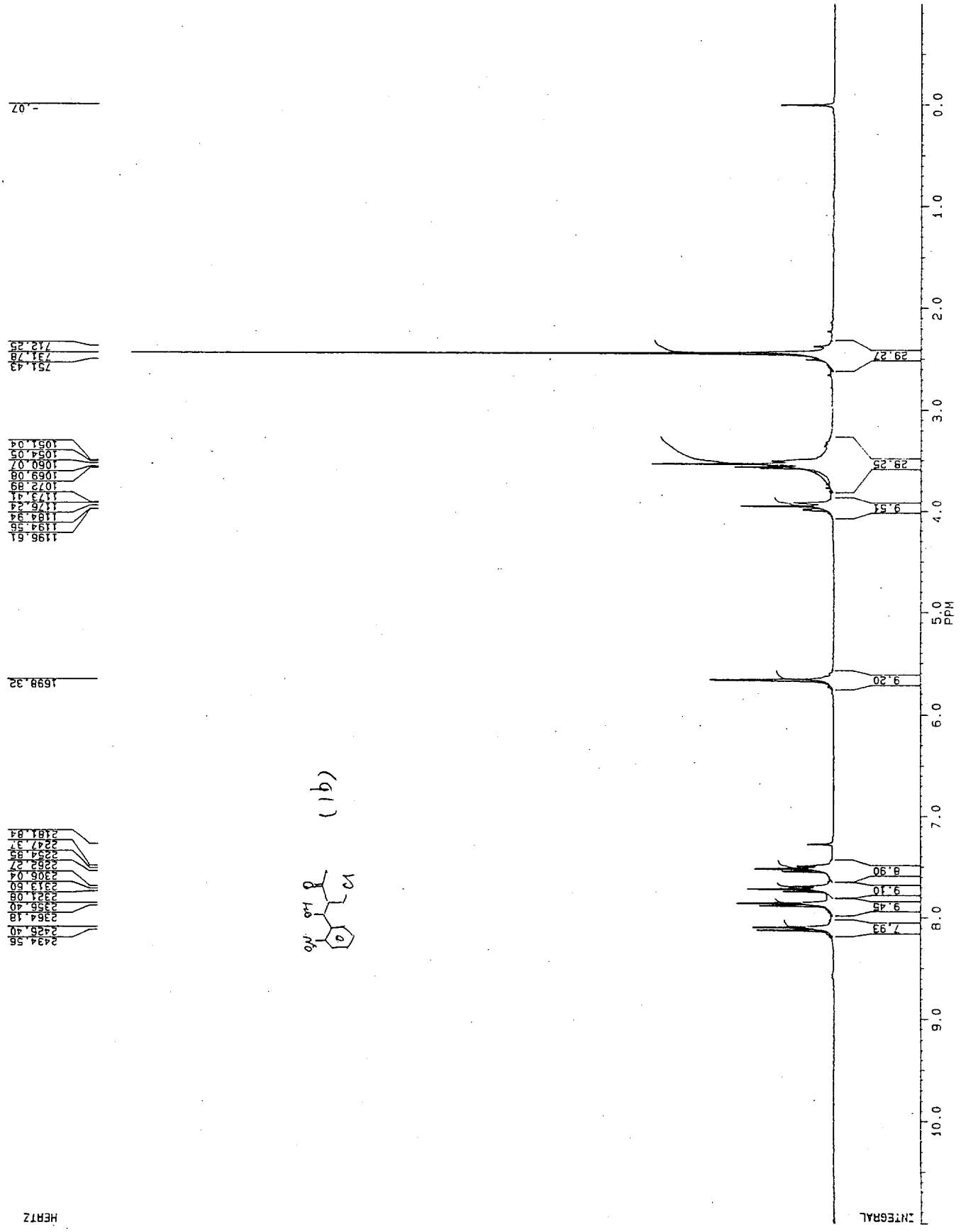
SUPPORTING INFORMATION




INTEGRAL
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PPM
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2.0
3.0
4.0
5.0
6.0
7.0
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29.27
29.25
9.51
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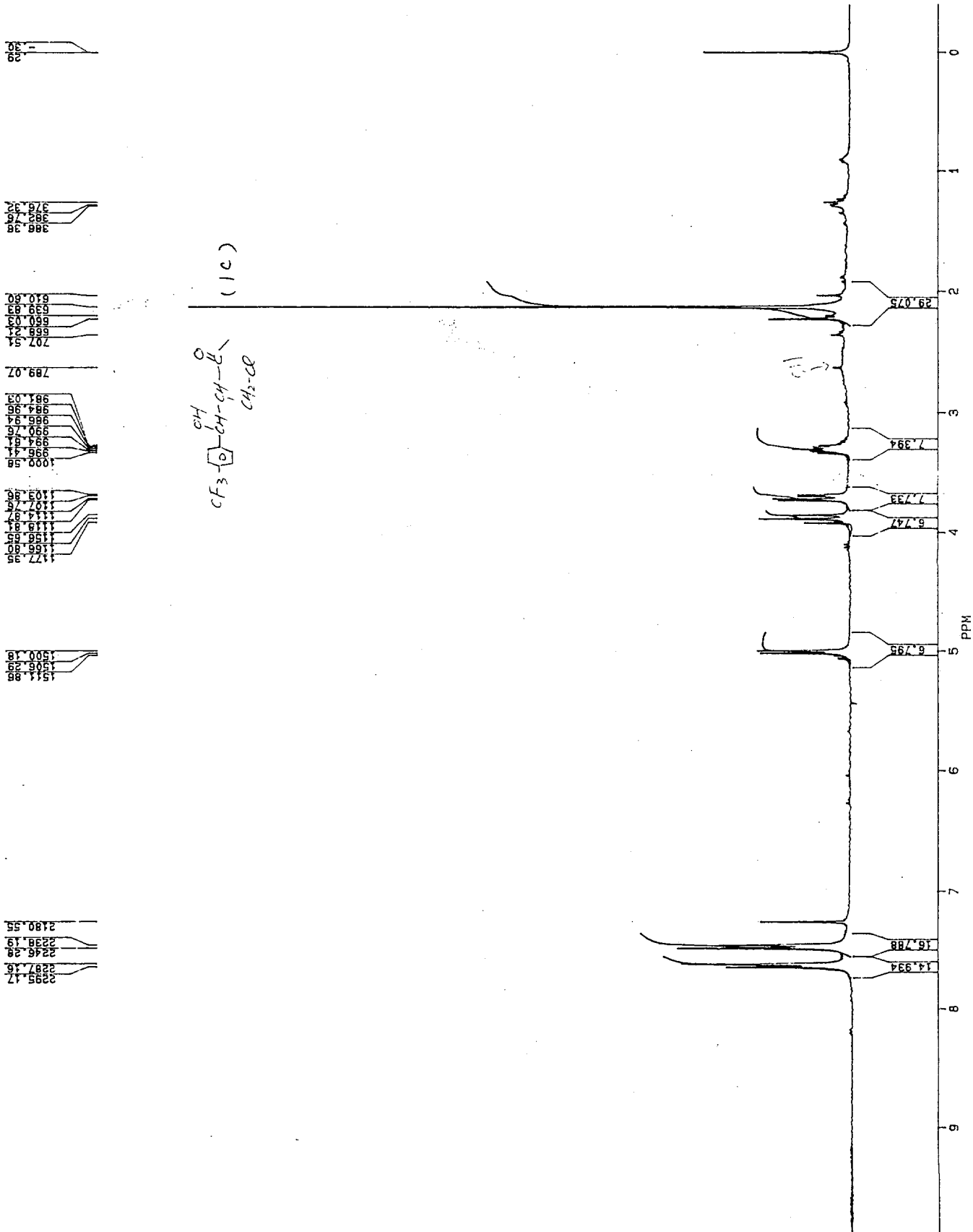
8.90
9.10
9.45
7.93
(1b)


(1c)
29.075
7.394
7.733
6.747
6.795
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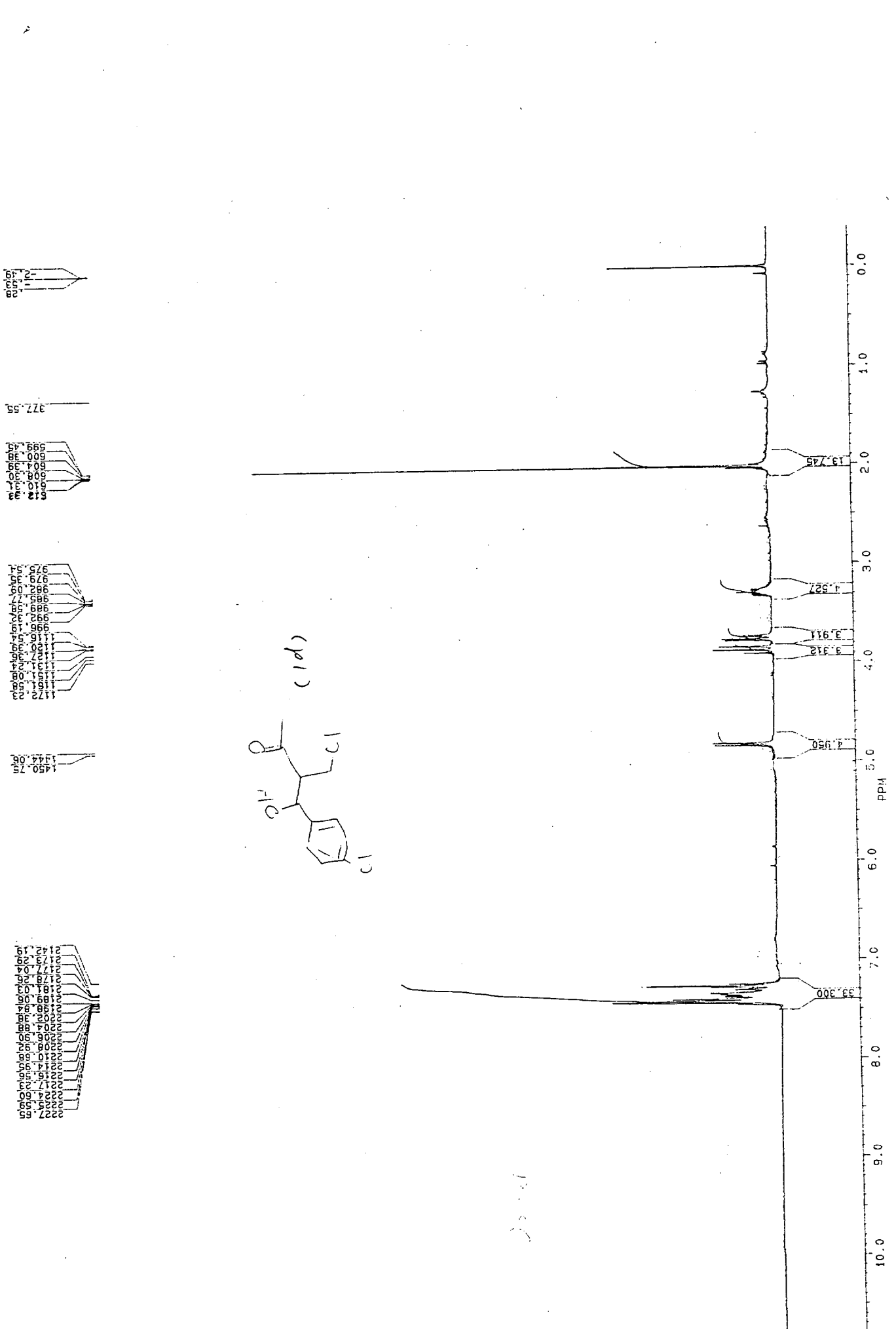
14.934
PPM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4.527
3.911
3.312
4.950
33.300
PPM
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1.0
2.0
3.0
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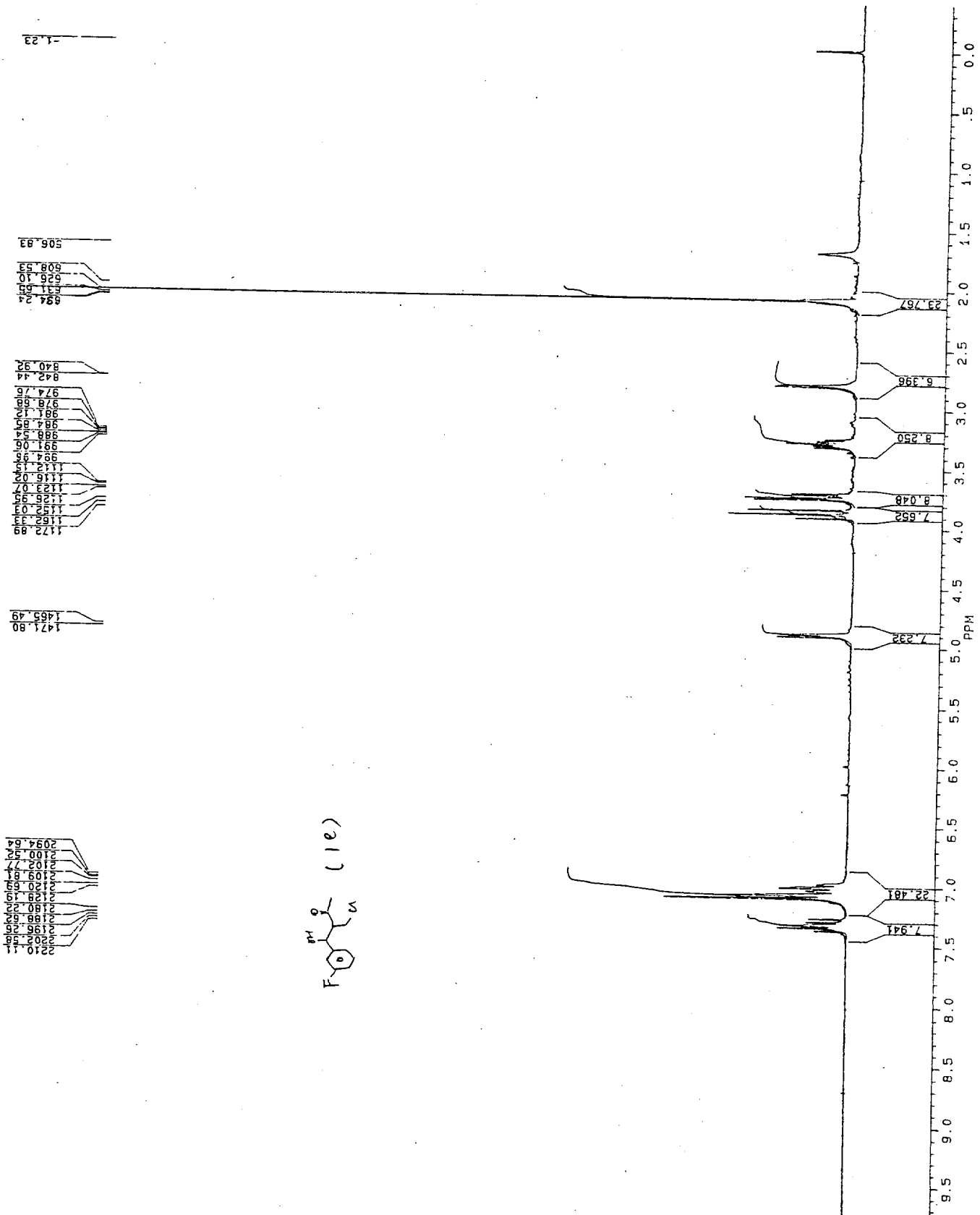
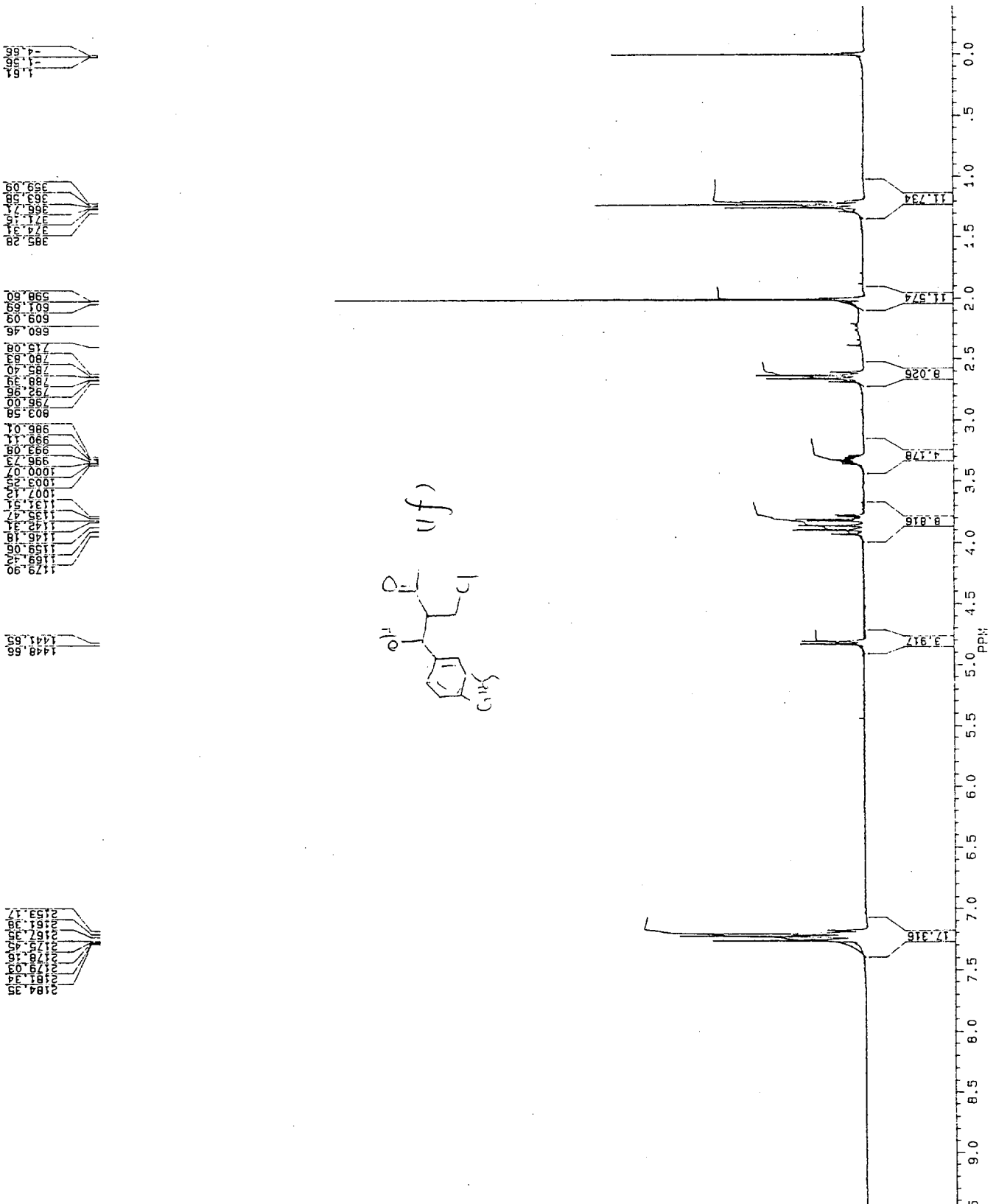
6.0
7.0
8.0
9.0
10.0



(1e)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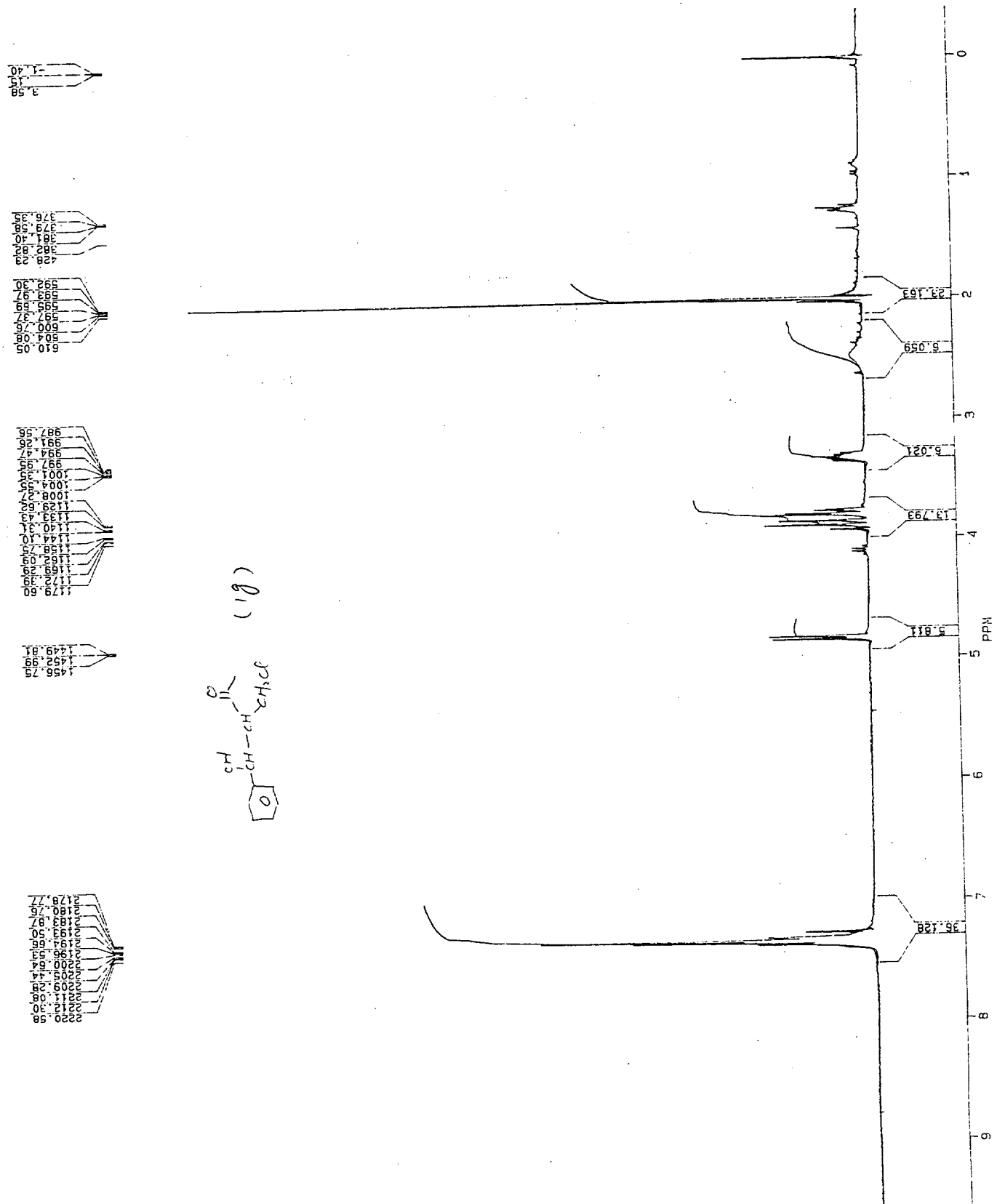
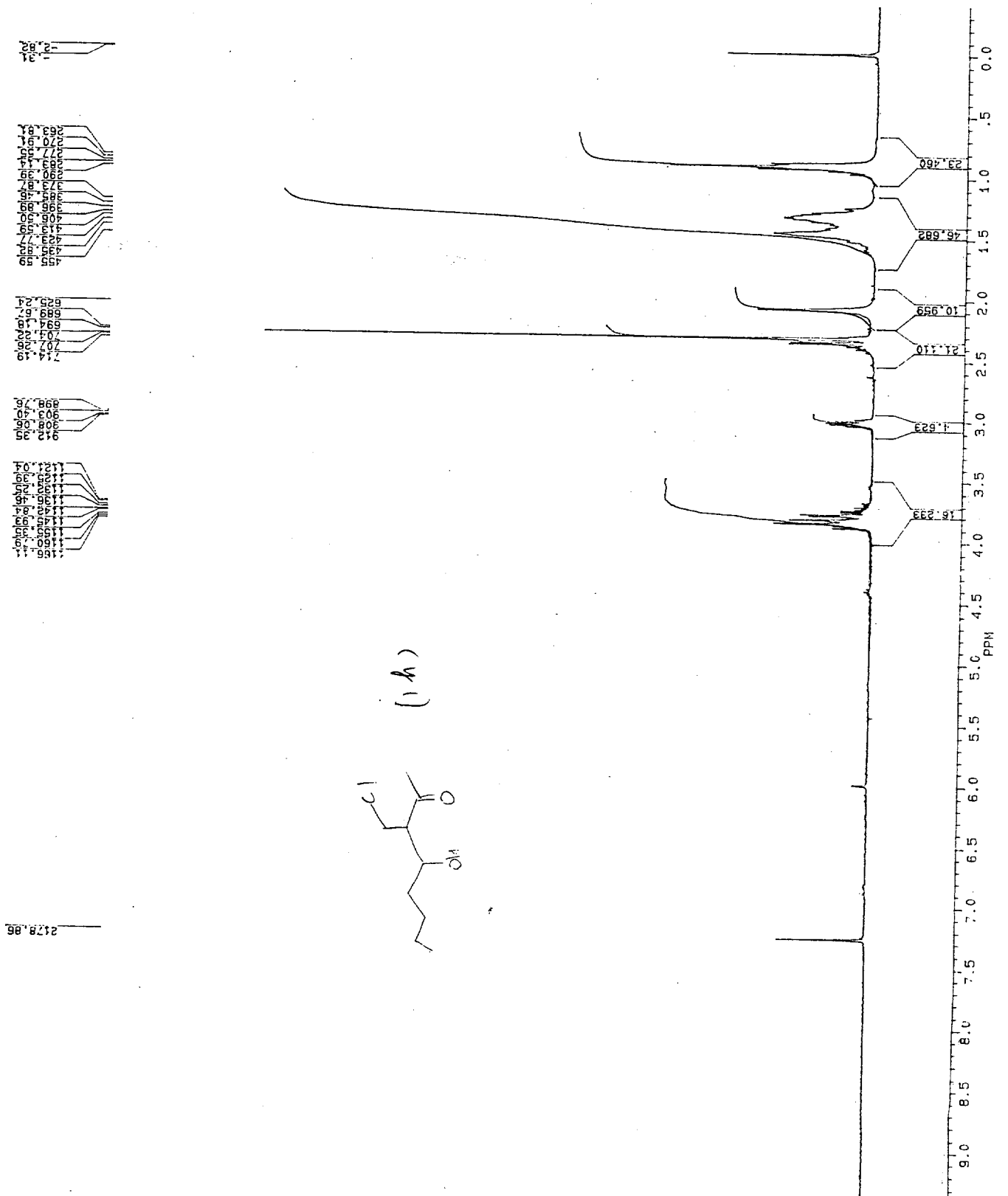
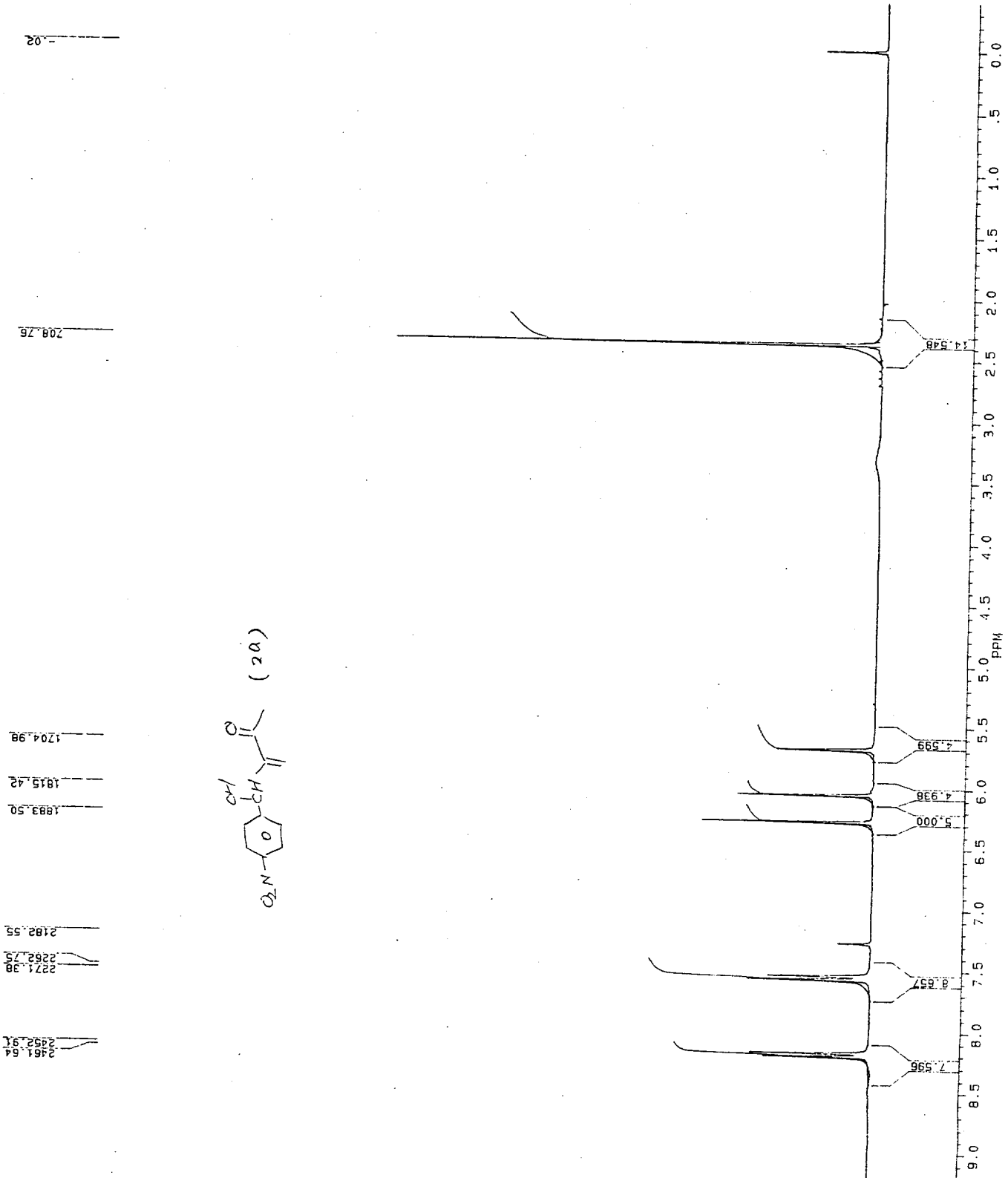
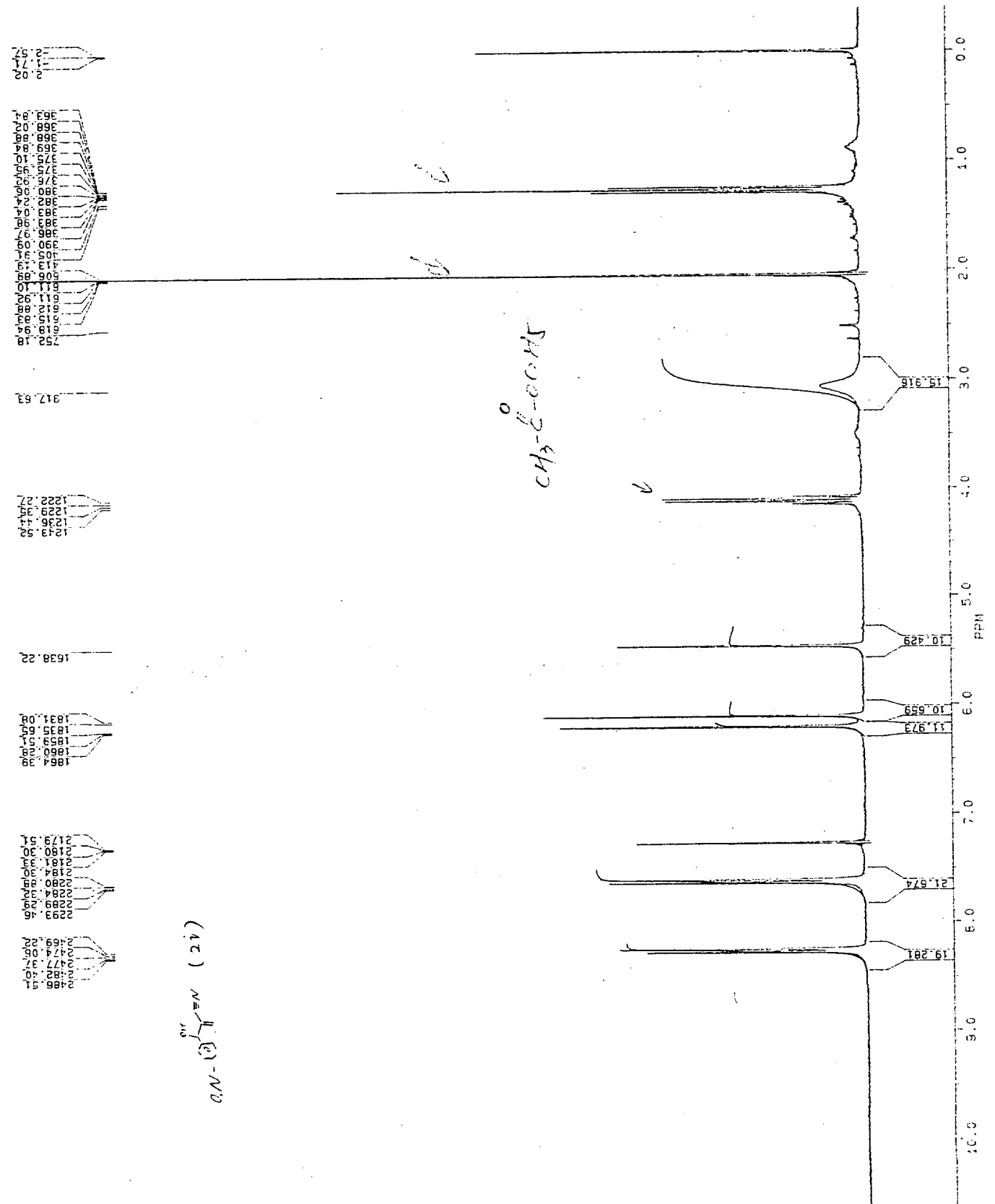
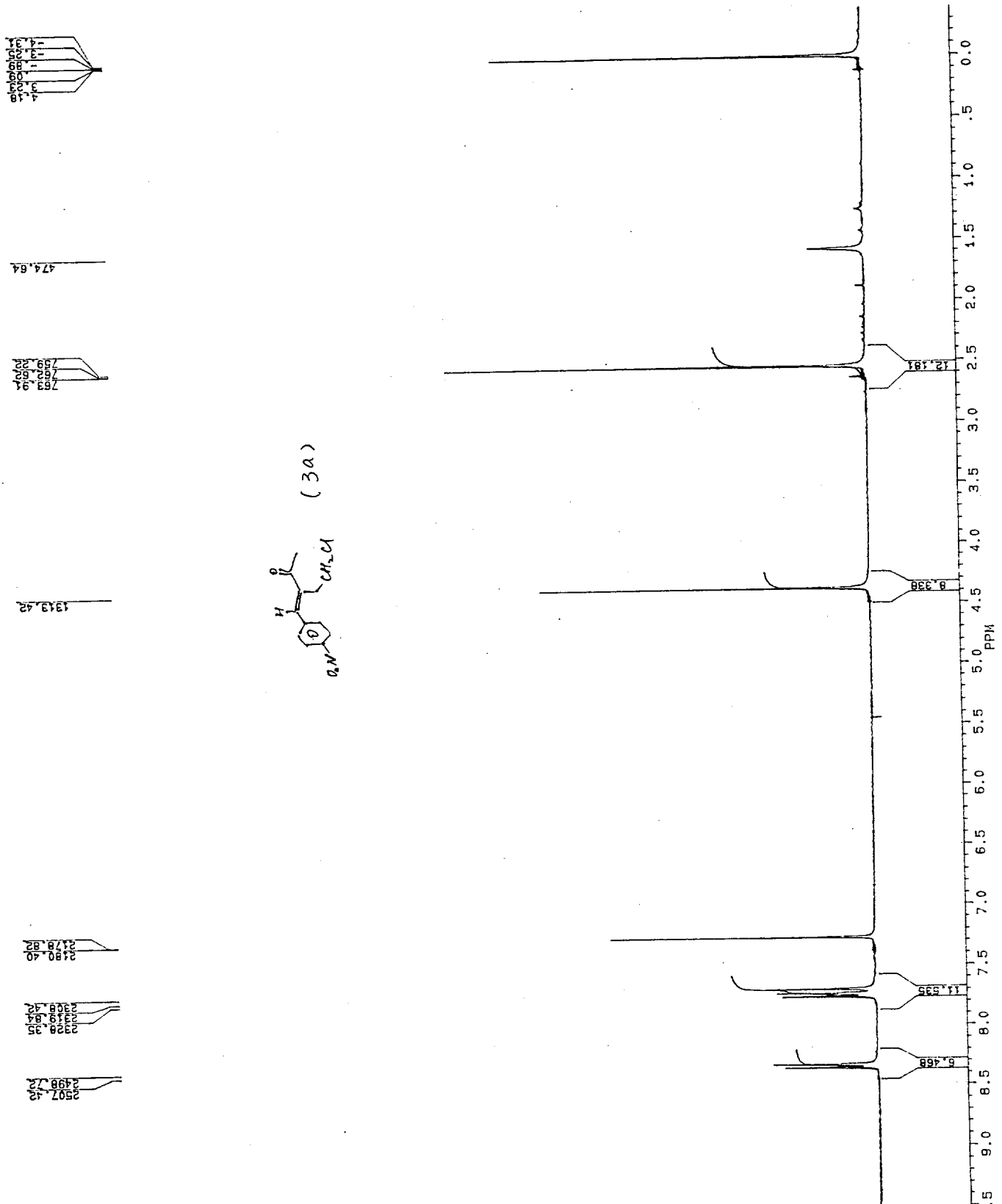
11.574
8.026
4.178
8.816
3.917
17.316
PPM

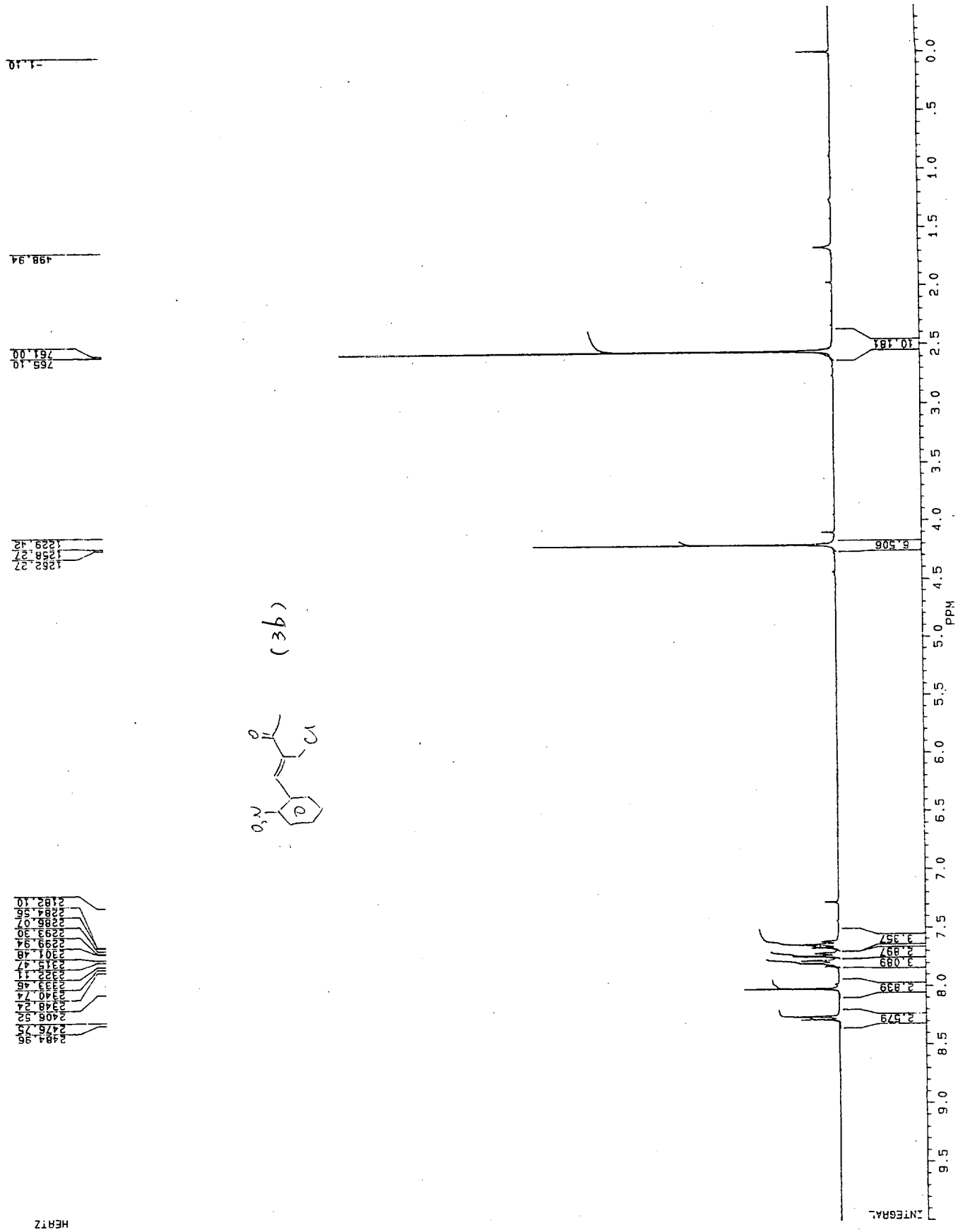


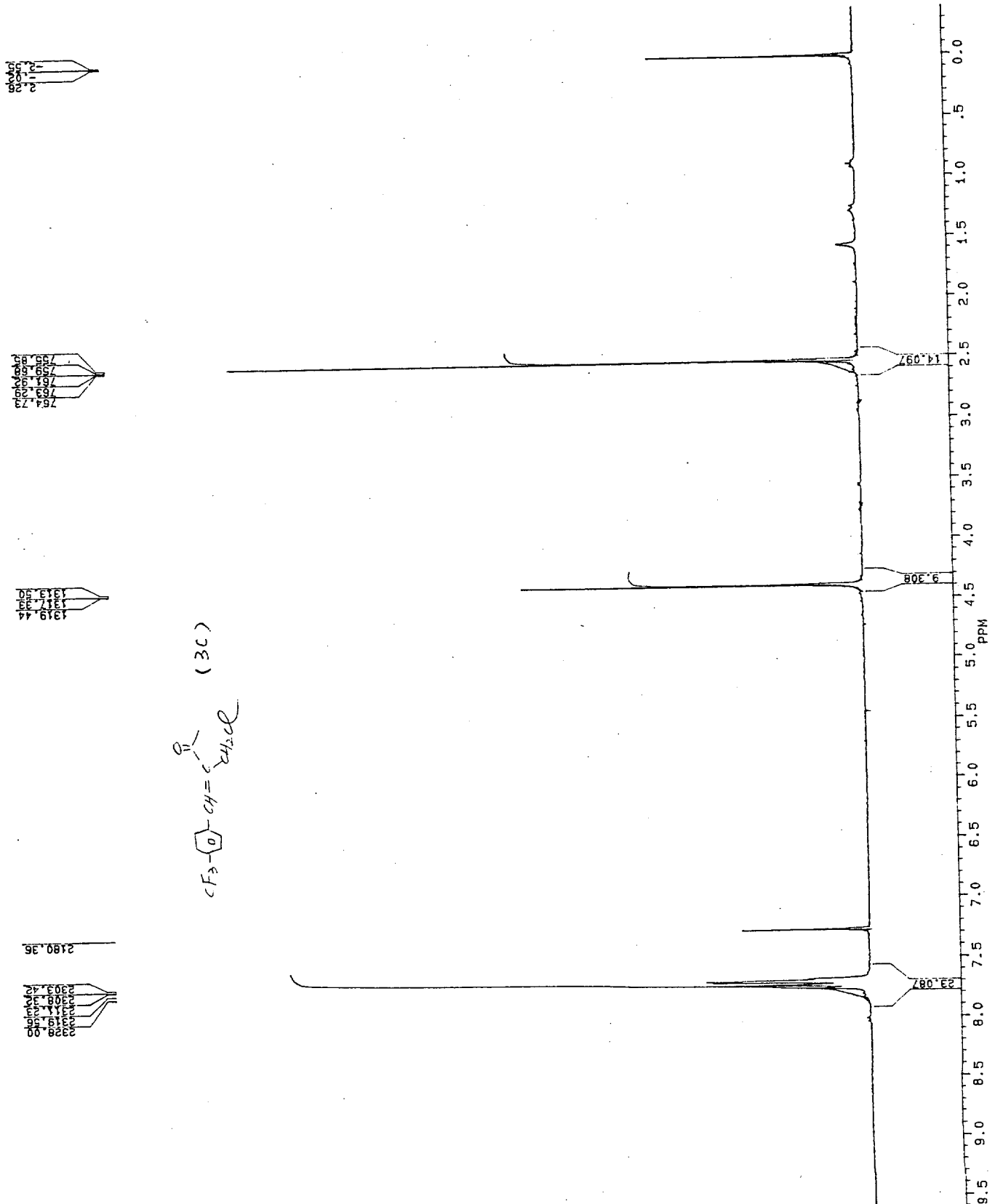








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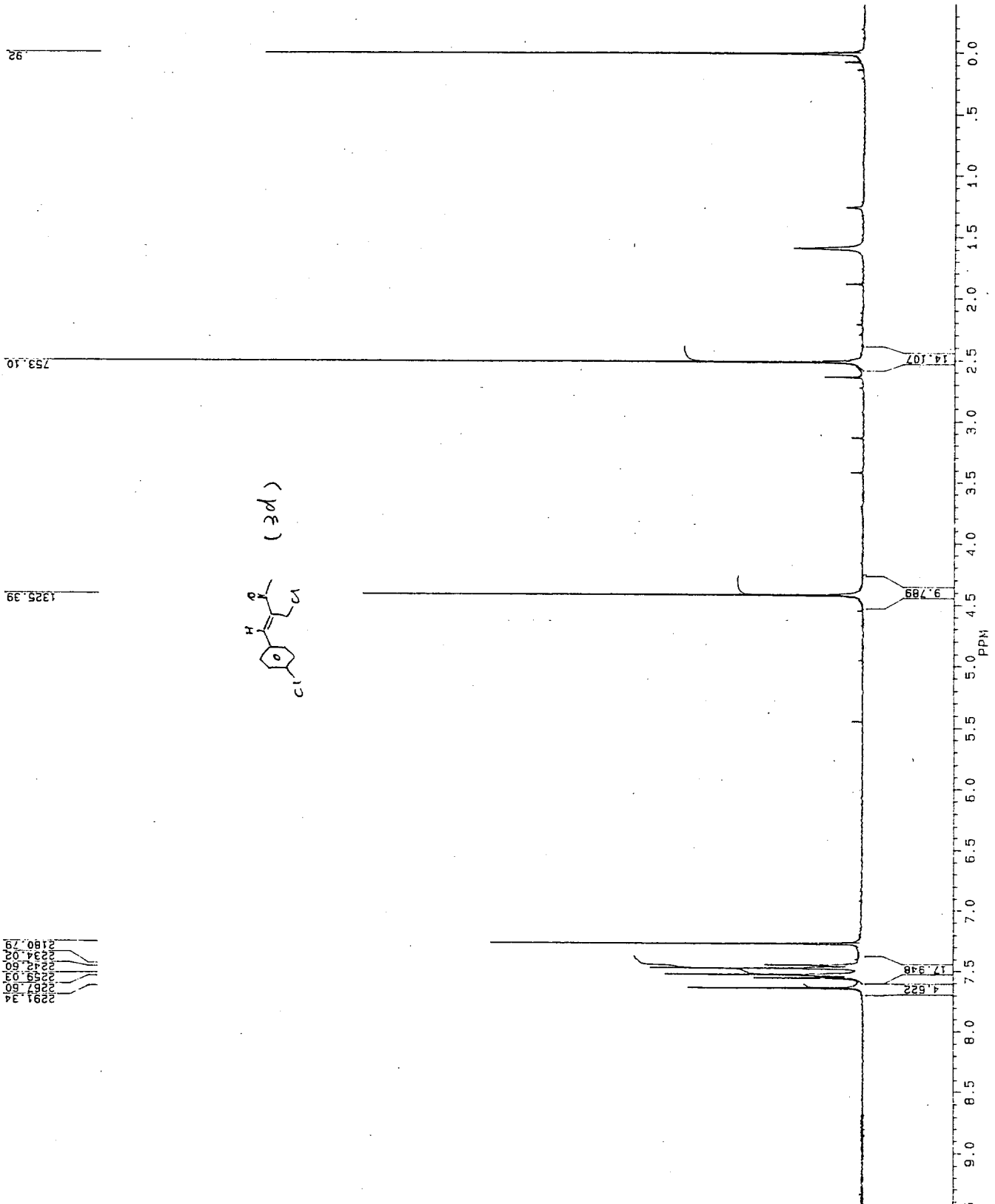
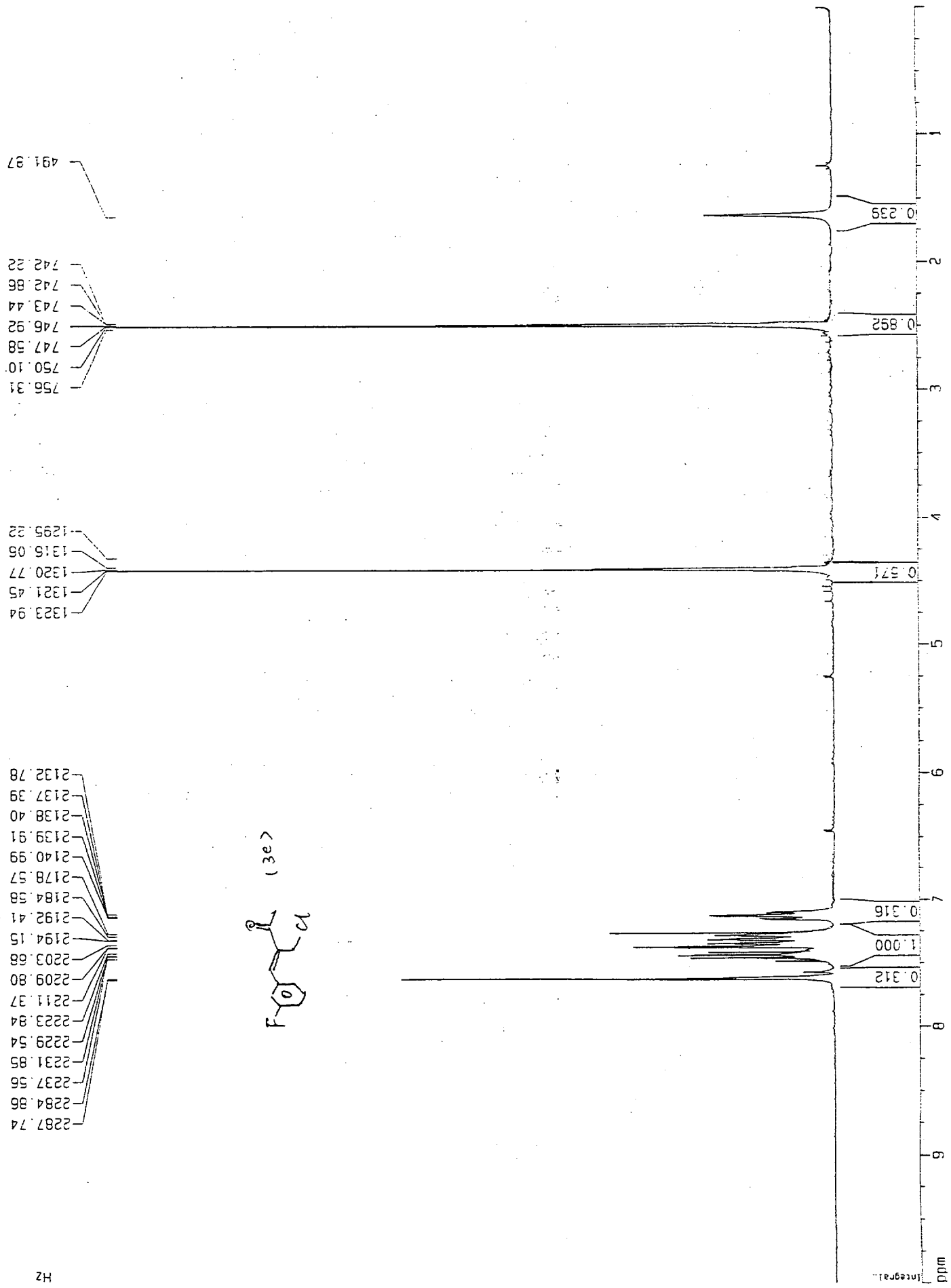
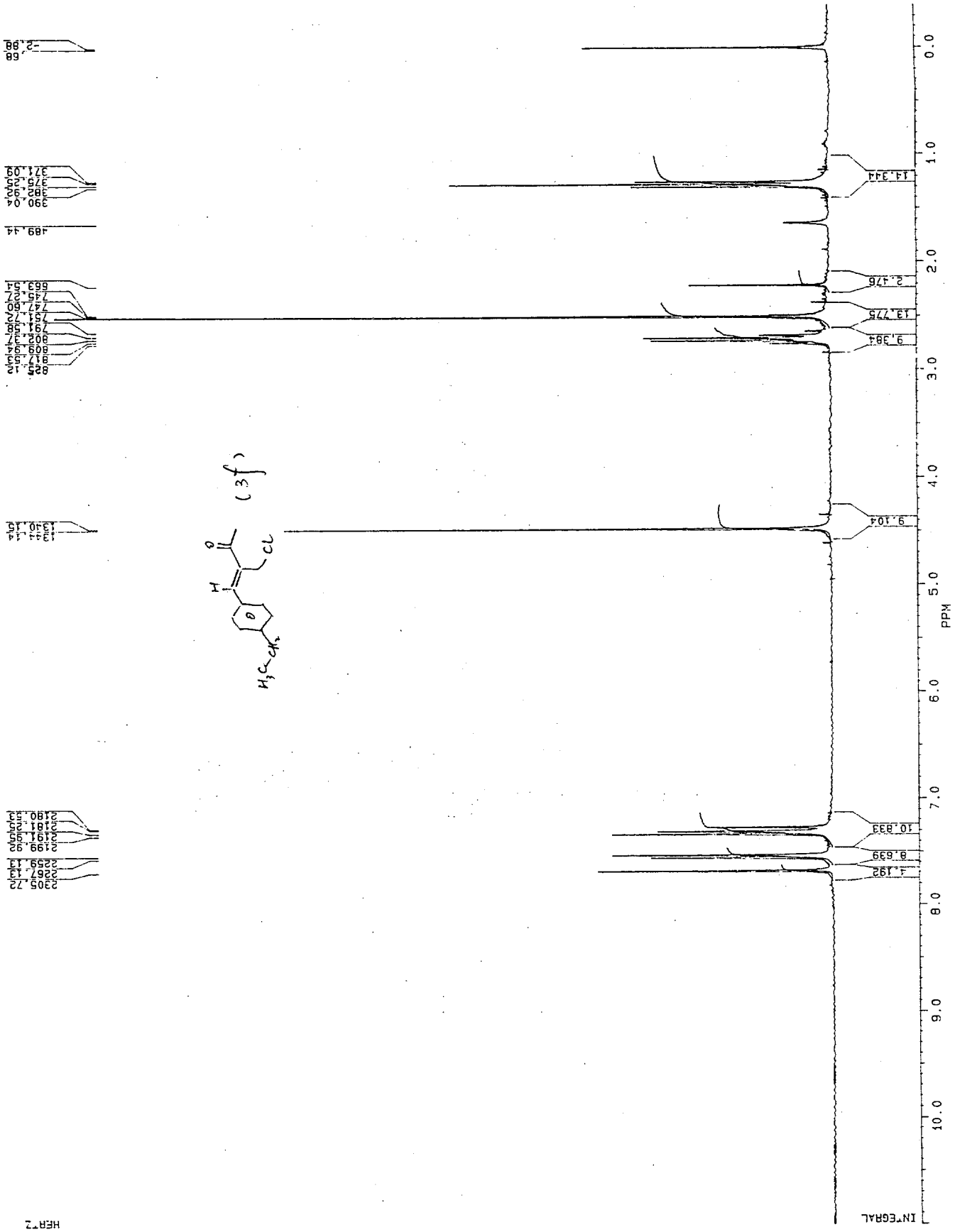
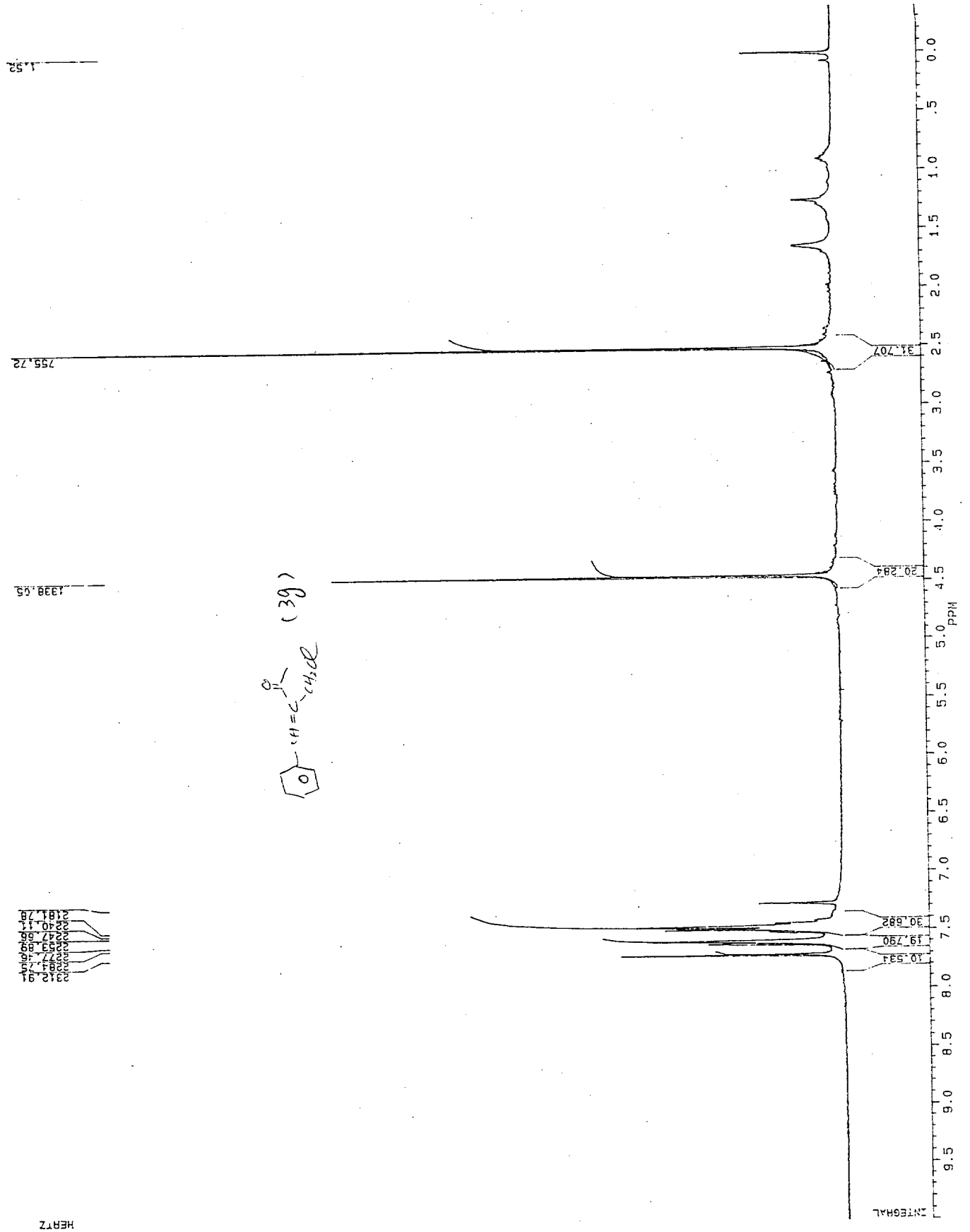
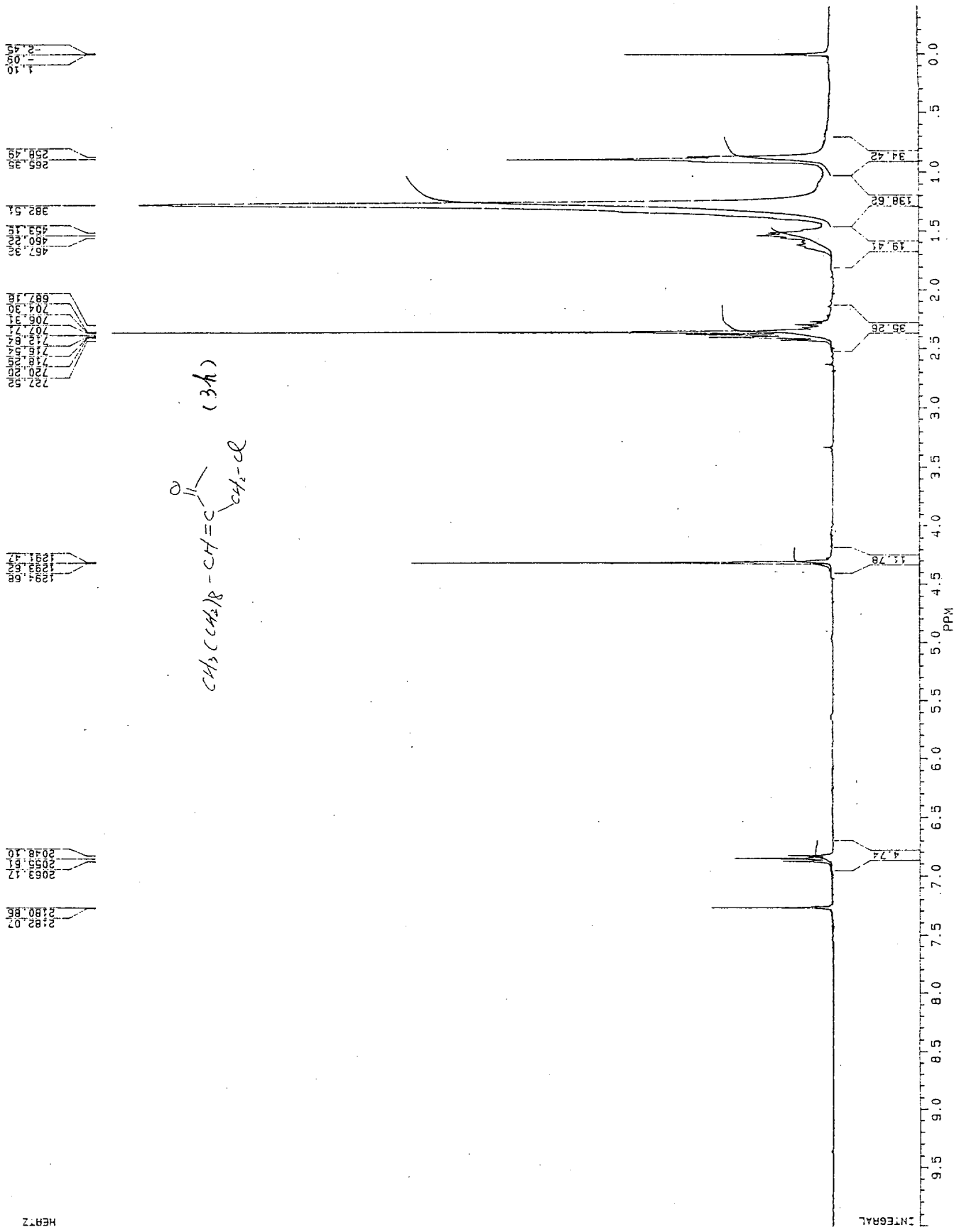
23.082
PPM

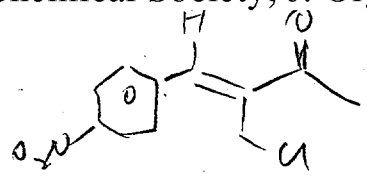












3a

Experimental

Data Collection

A colorless prismatic crystal of $C_{22}H_{20}N_2O_6Cl_2$ having approximate dimensions of 0.20 x 0.20 x 0.30 mm was mounted on a glass fiber. All measurements were made on a Rigaku AFC7R diffractometer with graphite monochromated Mo-Kα radiation and a 12kW rotating anode generator.

Cell constants and an orientation matrix for data collection, obtained from a least-squares refinement using the setting angles of 18 carefully centered reflections in the range $13.96 < 2\theta < 19.70°$ corresponded to a primitive monoclinic cell with dimensions:

a = 7.524(2) Å
b = 17.541(3) Å $\beta = 98.64(4)°$
c = 17.07(1) Å
V = 2227(1) $Å^3$

For Z = 4 and F.W. = 479.32, the calculated density is 1.43 g/cm^3. The systematic absences of:

h0l: h+l $\neq$ 2n
0k0: k $\neq$ 2n

uniquely determine the space group to be:

$P2_1/n$ (#14)

The data were collected at a temperature of 20 $\pm$ 1°C using the ω-2θ scan technique to a maximum 2θ value of 44.9°. Omega scans of several intense reflections, made prior to data collection, had an average width at half-height of 0.36° with a take-off angle of 6.0°. Scans of $(1.37 + 0.30 \tan\theta)°$ were made at a speed of 16.0°/min (in omega). The weak reflections ($I < 13.0\sigma(I)$) were rescanned (maximum of 3 scans) and the counts were accumulated to ensure good counting statistics. Stationary background counts were recorded on each side of the reflection. The ratio of peak counting time to background counting time was 2:1. The diameter of the incident beam collimator was 1.0 mm, the crystal to detector distance was 235 mm, and the computer controlled detector aperture was set to 9.0 x 13.0 mm (horizontal x vertical).

Data Reduction

Of the 2515 reflections which were collected, 2248 were unique (R_{int} = 0.126). The intensities of three representative reflection were measured after every 200 reflections. Over the course of data collection, the standards decreased by -2.1%. A linear correction factor was applied to the data to account for this phenomenon.

The linear absorption coefficient, μ, for Mo-Kα radiation is 3.3 cm^{-1}. Azimuthal scans of several reflections indicated no need for an absorption correction. The data were corrected for Lorentz and polarization effects. A correction for secondary extinction was applied (coefficient = 1.30272e-07).

Structure Solution and Refinement

The structure was solved by direct methods[1] and expanded using Fourier techniques[2]. Some non-hydrogen atoms were refined anisotropically, while the rest were refined isotropically. Hydrogen atoms were included but not refined. The final cycle of full-matrix least-squares refinement[3] was based on 1110 observed reflections ($I > 1.50\sigma(I)$) and 220 variable parameters and converged (largest parameter was 0.04 times its esd) with unweighted and weighted agreement factors of:

$$R = \Sigma||Fo| - |Fc||/\Sigma|Fo| = 0.066$$

$$R_w = \sqrt{(\Sigma w(|Fo| - |Fc|)^2/\Sigma wFo^2)} = 0.061$$

The standard deviation of an observation of unit weight[4] was 1.50. The weighting scheme was based on counting statistics and included a factor (p = 0.030) to downweight the intense reflections. Plots of $\Sigma w(|Fo| - |Fc|)^2$ versus $|Fo|$, reflection order in data collection, $\sin\theta/\lambda$ and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.29 and -0.30 $e^-/\AA^3$, respectively.

Neutral atom scattering factors were taken from Cromer and Waber[5] . Anomalous dispersion effects were included in Fcalc[6]; the values for Δf' and Δf" were those of Creagh and McAuley[7]. The values for the mass attenuation coefficients are those of Creagh and Hubbel[8]. All calculations were performed using the teXsan[9] crystallographic software package of Molecular Structure Corporation.

References

(1) SHELXS86: Sheldrick, G.M. (1985). In: "Crystallographic Computing 3" (Eds G.M. Sheldrick, C. Kruger and R. Goddard) Oxford University Press, pp. 175-189.

(2) DIRDIF92: Beurskens, P.T., Admiraal, G., Beurskens, G., Bosman, W.P., Garcia-Granda, S., Gould, R.O., Smits, J.M.M. and Smykalla, C. (1992). The DIRDIF program system, Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.

(3) Least-Squares:

Function minimized: $\Sigma w(|Fo| - |Fc|)^2$

where w = $\frac{1}{\sigma^2(Fo)} = \frac{4Fo^2}{\sigma^2(Fo^2)}$

$\sigma^2(Fo^2) = \frac{S^2(C+R^2B)+(pFo^2)^2}{Lp^2}$

S = Scan rate

C = Total Integrated Peak Count

R = Ratio of Scan Time to background counting time

B = Total Background Count

Lp = Lorentz-polarization factor

p = p-factor

(4) Standard deviation of an observation of unit weight:

$$\sqrt{\Sigma w(|Fo| - |Fc|)^2/(No - Nv)}$$

where: No = number of observations

Nv = number of variables

(5) Cromer, D. T. & Waber, J. T.; "International Tables for X-ray Crystallography", Vol. IV, The Kynoch Press, Birmingham, England, Table 2.2 A (1974).

(6) Ibers, J. A. & Hamilton, W. C.; Acta Crystallogr., 17, 781 (1964).

(7) Creagh, D. C. & McAuley, W.J .; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.6.8, pages 219-222 (1992).

(8) Creagh, D. C. & Hubbell, J.H..; "International Tables for Crystallography", Vol C, (A.J.C. Wilson, ed.), Kluwer Academic Publishers, Boston, Table 4.2.4.3, pages 200-206 (1992).

(9) teXsan: Crystal Structure Analysis Package, Molecular Structure Corporation (1985 & 1992).

EXPERIMENTAL DETAILS

A. Crystal Data

Empirical Formula	$C_{22}H_{20}N_2O_6Cl_2$
Formula Weight	479.32
Crystal Color, Habit	colorless, prismatic
Crystal Dimensions	0.20 X 0.20 X 0.30 mm
Crystal System	monoclinic
Lattice Type	Primitive
No. of Reflections Used for Unit Cell Determination (2θ range)	18 (14.0 - 19.7°)
Omega Scan Peak Width at Half-height	0.36°
Lattice Parameters	a = 7.524(2) Å b = 17.541(3) Å c = 17.07(1) Å β = 98.64(4)°
	V = 2227(1) Å^3
Space Group	$P2_1/n$ (#14)
Z value	4
D_{calc}	1.429 g/cm^3
F_{000}	992.00
μ(MoKα)	3.33 cm^{-1}

B. Intensity Measurements

Diffractometer	Rigaku AFC7R
Radiation	MoKα (λ = 0.71069 Å) graphite monochromated

Attenuator	Zr foil (factors = 1.00, 8.46, 8.46, 8.46)
Take-off Angle	6.0°
Detector Aperture	9.0 mm horizontal 13.0 mm vertical
Crystal to Detector Distance	235 mm
Temperature	20.0°C
Scan Type	ω-2θ
Scan Rate	16.0°/min (in ω) – up to 3 scans
Scan Width	$(1.37 + 0.30 \tan \theta)°$
$2\theta_{max}$	44.9°
No. of Reflections Measured	Total: 2515 Unique: 2248 (R_{int} = 0.126)
Corrections	Lorentz-polarization Decay (-2.10% decline) Secondary Extinction (coefficient: 1.30272e-07)

C. Structure Solution and Refinement

Structure Solution	Direct Methods (SHELXS86)
Refinement	Full-matrix least-squares
Function Minimized	$\Sigma w(\|Fo\| - \|Fc\|)^2$
Least Squares Weights	$\frac{1}{\sigma^2(Fo)} = \frac{4Fo^2}{\sigma^2(Fo^2)}$
p-factor	0.03
Anomalous Dispersion	All non-hydrogen atoms
No. Observations (I>1.50σ(I))	1110
No. Variables	220
Reflection/Parameter Ratio	5.05
Residuals: R; Rw	0.066 ; 0.061
Goodness of Fit Indicator	1.50

Max Shift/Error in Final Cycle	0.04
Maximum peak in Final Diff. Map	0.29 $e^-/\AA^3$
Minimum peak in Final Diff. Map	-0.30 $e^-/\AA^3$

Table 1. Atomic coordinates and B_{iso}/B_{eq}

atom	x	y	z	B_{eq}
Cl(1)	0.6596(5)	0.2792(2)	0.7133(2)	5.93(9)
Cl(2)	0.2282(4)	0.0229(2)	0.2990(2)	4.74(9)
O(1)	0.392(1)	0.1791(5)	0.5738(5)	5.1(2)
O(2)	0.977(1)	0.6578(5)	0.6087(5)	6.9(3)
O(3)	0.894(1)	0.6761(5)	0.4853(6)	6.1(3)
O(4)	0.061(1)	-0.1373(4)	0.1926(4)	5.2(2)
O(5)	0.270(1)	-0.0862(5)	0.7684(5)	7.2(3)
O(6)	0.326(1)	0.0279(5)	0.7298(4)	5.4(3)
N(1)	0.908(1)	0.6365(6)	0.5445(7)	4.5(3)
N(2)	0.277(1)	-0.0378(7)	0.7178(5)	4.3(3)
C(1)	0.692(1)	0.4603(6)	0.4532(5)	2.8(2)
C(2)	0.763(1)	0.5336(6)	0.4629(6)	2.9(2)
C(3)	0.833(1)	0.5589(6)	0.5367(6)	3.1(2)
C(4)	0.845(1)	0.5124(6)	0.6021(6)	4.0(3)
C(5)	0.777(1)	0.4404(6)	0.5935(6)	3.3(2)
C(6)	0.697(1)	0.4128(6)	0.5195(6)	3.0(2)
C(7)	0.612(1)	0.3378(6)	0.5064(6)	3.5(3)
C(8)	0.527(2)	0.2950(6)	0.5550(6)	3.6(3)
C(9)	0.445(1)	0.2201(7)	0.5260(6)	3.7(3)
C(10)	0.500(1)	0.3181(6)	0.6375(6)	3.8(3)
C(11)	0.429(2)	0.1980(6)	0.4408(7)	4.7(3)
C(12)	0.206(1)	-0.0371(6)	0.4968(6)	3.5(2)
C(13)	0.260(1)	-0.0148(6)	0.5754(6)	3.0(2)
C(14)	0.225(1)	-0.0609(6)	0.6349(6)	2.8(2)

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
C(15)	0.131(1)	-0.1286(6)	0.6185(6)	3.3(2)
C(16)	0.076(1)	-0.1499(6)	0.5413(6)	3.0(2)
C(17)	0.116(1)	-0.1049(6)	0.4797(6)	2.7(2)
C(18)	0.047(1)	-0.1314(5)	0.3981(6)	3.2(3)
C(19)	0.106(1)	-0.1190(6)	0.3286(6)	3.0(3)
C(20)	0.006(1)	-0.1509(6)	0.2532(6)	3.2(3)
C(21)	0.271(2)	-0.0763(6)	0.3220(6)	3.3(3)
C(22)	-0.152(2)	-0.2021(7)	0.2551(7)	5.4(3)
H(1)	0.6402	0.4430	0.4023	5.0363
H(2)	0.7626	0.5662	0.4185	5.0363
H(3)	0.9006	0.5303	0.6525	5.0363
H(4)	0.7837	0.4086	0.6388	5.0363
H(5)	0.6190	0.3161	0.4559	3.7777
H(6)	0.5074	0.3721	0.6407	5.0363
H(7)	0.3842	0.3019	0.6455	3.6190
H(8)	0.3055	0.1917	0.4191	4.7021
H(9)	0.4907	0.1514	0.4361	4.7021
H(10)	0.4799	0.2367	0.4121	4.7021
H(11)	0.2328	-0.0056	0.4546	5.0363
H(12)	0.3190	0.0326	0.5866	5.0363
H(13)	0.1050	-0.1601	0.6608	5.0363
H(14)	0.0103	-0.1958	0.5301	5.0363
H(15)	-0.0558	-0.1628	0.3944	5.9691
H(16)	0.3490	-0.0804	0.3717	5.0363

Table 1. Atomic coordinates and B_{iso}/B_{eq} (continued)

atom	x	y	z	B_{eq}
H(17)	0.3283	-0.0994	0.2821	5.0363
H(18)	-0.2317	-0.1980	0.2067	5.0363
H(19)	-0.1114	-0.2534	0.2623	5.0363
H(20)	-0.2131	-0.1881	0.2978	5.9991

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cl(1)	0.108(3)	0.069(2)	0.048(2)	0.020(2)	0.008(2)	0.007(2)
Cl(2)	0.087(3)	0.046(2)	0.052(2)	-0.004(2)	0.025(2)	0.008(2)
O(1)	0.072(7)	0.060(6)	0.064(6)	-0.016(5)	0.022(5)	0.016(5)
O(2)	0.109(9)	0.068(7)	0.079(7)	-0.028(6)	-0.009(6)	-0.019(6)
O(3)	0.087(8)	0.040(6)	0.097(7)	-0.007(5)	-0.007(6)	0.025(5)
O(4)	0.088(7)	0.083(7)	0.030(5)	0.014(5)	0.015(5)	0.008(5)
O(5)	0.143(10)	0.094(7)	0.035(5)	-0.039(7)	0.012(6)	0.004(5)
O(6)	0.075(7)	0.074(7)	0.054(6)	-0.008(6)	-0.001(5)	-0.026(5)
N(1)	0.047(8)	0.042(8)	0.080(9)	0.004(6)	0.007(7)	-0.007(7)
N(2)	0.044(7)	0.081(10)	0.037(7)	-0.017(7)	0.001(6)	-0.011(7)
C(7)	0.052(9)	0.044(8)	0.039(7)	0.004(7)	0.014(6)	0.000(6)
C(8)	0.057(9)	0.035(8)	0.045(8)	0.003(7)	0.013(7)	0.000(6)
C(9)	0.043(9)	0.055(9)	0.045(8)	0.014(8)	0.012(6)	0.010(7)
C(10)	0.055(9)	0.052(8)	0.045(8)	-0.003(7)	0.032(7)	0.000(6)
C(18)	0.044(9)	0.029(7)	0.047(7)	-0.007(6)	0.005(6)	0.004(6)
C(19)	0.034(8)	0.042(8)	0.040(7)	0.006(6)	0.010(6)	0.007(6)
C(20)	0.040(9)	0.052(8)	0.026(7)	0.001(7)	-0.004(7)	-0.008(6)
C(21)	0.055(9)	0.036(7)	0.035(7)	-0.002(7)	0.005(6)	0.004(6)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
Cl(1)	C(10)	1.76(1)	Cl(2)	C(21)	1.801(10)
O(1)	C(9)	1.20(1)	O(2)	N(1)	1.20(1)
O(3)	N(1)	1.22(1)	O(4)	C(20)	1.20(1)
O(5)	N(2)	1.22(1)	O(6)	N(2)	1.22(1)
N(1)	C(3)	1.47(1)	N(2)	C(14)	1.47(1)
C(1)	C(2)	1.39(1)	C(1)	C(6)	1.40(1)
C(2)	C(3)	1.37(1)	C(3)	C(4)	1.37(1)
C(4)	C(5)	1.36(1)	C(5)	C(6)	1.40(1)
C(6)	C(7)	1.46(1)	C(7)	C(8)	1.35(1)
C(8)	C(9)	1.50(1)	C(8)	C(10)	1.51(1)
C(9)	C(11)	1.49(1)	C(12)	C(13)	1.40(1)
C(12)	C(17)	1.38(1)	C(13)	C(14)	1.35(1)
C(14)	C(15)	1.39(1)	C(15)	C(16)	1.37(1)
C(16)	C(17)	1.38(1)	C(17)	C(18)	1.49(1)
C(18)	C(19)	1.34(1)	C(19)	C(20)	1.50(1)
C(19)	C(21)	1.47(1)	C(20)	C(22)	1.50(1)

Table 4. Bond Lengths($\AA$)

atom	atom	distance	atom	atom	distance
C(1)	H(1)	0.95	C(2)	H(2)	0.95
C(4)	H(3)	0.95	C(5)	H(4)	0.95
C(7)	H(5)	0.95	C(10)	H(6)	0.95
C(10)	H(7)	0.95	C(11)	H(8)	0.95
C(11)	H(9)	0.95	C(11)	H(10)	0.95
C(12)	H(11)	0.95	C(13)	H(12)	0.95
C(15)	H(13)	0.95	C(16)	H(14)	0.95
C(18)	H(15)	0.95	C(21)	H(16)	0.96
C(21)	H(17)	0.95	C(22)	H(18)	0.95
C(22)	H(19)	0.95	C(22)	H(20)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
O(2)	N(1)	O(3)	123(1)	O(2)	N(1)	C(3)	118(1)
O(3)	N(1)	C(3)	117(1)	O(5)	N(2)	O(6)	125(1)
O(5)	N(2)	C(14)	117(1)	O(6)	N(2)	C(14)	116(1)
C(2)	C(1)	C(6)	119.2(9)	C(1)	C(2)	C(3)	119.9(10)
N(1)	C(3)	C(2)	118.3(10)	N(1)	C(3)	C(4)	119(1)
C(2)	C(3)	C(4)	121(1)	C(3)	C(4)	C(5)	119(1)
C(4)	C(5)	C(6)	121.4(10)	C(1)	C(6)	C(5)	118.6(10)
C(1)	C(6)	C(7)	116.8(9)	C(5)	C(6)	C(7)	124.6(9)
C(6)	C(7)	C(8)	130.0(10)	C(7)	C(8)	C(9)	119.6(10)
C(7)	C(8)	C(10)	124(1)	C(9)	C(8)	C(10)	115.9(9)
O(1)	C(9)	C(8)	117(1)	O(1)	C(9)	C(11)	121(1)
C(8)	C(9)	C(11)	121(1)	Cl(1)	C(10)	C(8)	114.3(8)
C(13)	C(12)	C(17)	120.5(10)	C(12)	C(13)	C(14)	119(1)
N(2)	C(14)	C(13)	120(1)	N(2)	C(14)	C(15)	118.9(9)
C(13)	C(14)	C(15)	120.6(10)	C(14)	C(15)	C(16)	119.8(10)
C(15)	C(16)	C(17)	120.4(10)	C(12)	C(17)	C(16)	119.2(9)
C(12)	C(17)	C(18)	124.0(9)	C(16)	C(17)	C(18)	116.8(9)
C(17)	C(18)	C(19)	131.7(10)	C(18)	C(19)	C(20)	120(1)
C(18)	C(19)	C(21)	122.9(10)	C(20)	C(19)	C(21)	116.5(9)
O(4)	C(20)	C(19)	118(1)	O(4)	C(20)	C(22)	121(1)
C(19)	C(20)	C(22)	120.3(10)	Cl(2)	C(21)	C(19)	112.5(8)

Table 6. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
C(2)	C(1)	H(1)	120.0	C(6)	C(1)	H(1)	120.7
C(1)	C(2)	H(2)	120.4	C(3)	C(2)	H(2)	119.7
C(3)	C(4)	H(3)	120.2	C(5)	C(4)	H(3)	120.8
C(4)	C(5)	H(4)	119.0	C(6)	C(5)	H(4)	119.5
C(6)	C(7)	H(5)	114.7	C(8)	C(7)	H(5)	115.4
Cl(1)	C(10)	H(6)	108.6	Cl(1)	C(10)	H(7)	108.5
C(8)	C(10)	H(6)	108.0	C(8)	C(10)	H(7)	107.9
H(6)	C(10)	H(7)	109.6	C(9)	C(11)	H(8)	109.6
C(9)	C(11)	H(9)	109.8	C(9)	C(11)	H(10)	109.7
H(8)	C(11)	H(9)	109.2	H(8)	C(11)	H(10)	109.0
H(9)	C(11)	H(10)	109.6	C(13)	C(12)	H(11)	120.0
C(17)	C(12)	H(11)	119.5	C(12)	C(13)	H(12)	119.9
C(14)	C(13)	H(12)	120.6	C(14)	C(15)	H(13)	120.0
C(16)	C(15)	H(13)	120.2	C(15)	C(16)	H(14)	119.8
C(17)	C(16)	H(14)	119.8	C(17)	C(18)	H(15)	114.2
C(19)	C(18)	H(15)	114.1	Cl(2)	C(21)	H(16)	109.4
Cl(2)	C(21)	H(17)	110.0	C(19)	C(21)	H(16)	107.8
C(19)	C(21)	H(17)	108.4	H(16)	C(21)	H(17)	108.8
C(20)	C(22)	H(18)	109.6	C(20)	C(22)	H(19)	109.1
C(20)	C(22)	H(20)	109.7	H(18)	C(22)	H(19)	109.5
H(18)	C(22)	H(20)	109.7	H(19)	C(22)	H(20)	109.2

Table 7. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Cl(1)	C(10)	C(8)	C(7)	-97(1)	Cl(1)	C(10)	C(8)	C(9)	84(1)
Cl(2)	C(21)	C(19)	C(18)	-95(1)	Cl(2)	C(21)	C(19)	C(20)	86.7(10)
O(1)	C(9)	C(8)	C(7)	170(1)	O(1)	C(9)	C(8)	C(10)	-11(1)
O(2)	N(1)	C(3)	C(2)	-176(1)	O(2)	N(1)	C(3)	C(4)	0(1)
O(3)	N(1)	C(3)	C(2)	4(1)	O(3)	N(1)	C(3)	C(4)	-179(1)
O(4)	C(20)	C(19)	C(18)	178(1)	O(4)	C(20)	C(19)	C(21)	-3(1)
O(5)	N(2)	C(14)	C(13)	-167(1)	O(5)	N(2)	C(14)	C(15)	15(1)
O(6)	N(2)	C(14)	C(13)	10(1)	O(6)	N(2)	C(14)	C(15)	-165(1)
N(1)	C(3)	C(2)	C(1)	179.5(9)	N(1)	C(3)	C(4)	C(5)	-178.9(10)
N(2)	C(14)	C(13)	C(12)	-178.6(9)	N(2)	C(14)	C(15)	C(16)	177.6(10)
C(1)	C(2)	C(3)	C(4)	3(1)	C(1)	C(6)	C(5)	C(4)	1(1)
C(1)	C(6)	C(7)	C(8)	-147(1)	C(2)	C(1)	C(6)	C(5)	-1(1)
C(2)	C(1)	C(6)	C(7)	177.0(9)	C(2)	C(3)	C(4)	C(5)	-3(1)
C(3)	C(2)	C(1)	C(6)	-1(1)	C(3)	C(4)	C(5)	C(6)	0(1)
C(4)	C(5)	C(6)	C(7)	-176(1)	C(5)	C(6)	C(7)	C(8)	30(1)
C(6)	C(7)	C(8)	C(9)	177(1)	C(6)	C(7)	C(8)	C(10)	0(1)
C(7)	C(8)	C(9)	C(11)	-9(1)	C(10)	C(8)	C(9)	C(11)	167.7(9)
C(12)	C(13)	C(14)	C(15)	-2(1)	C(12)	C(17)	C(16)	C(15)	-2(1)
C(12)	C(17)	C(18)	C(19)	29(1)	C(13)	C(12)	C(17)	C(16)	1(1)
C(13)	C(12)	C(17)	C(18)	177.4(10)	C(13)	C(14)	C(15)	C(16)	1(1)
C(14)	C(13)	C(12)	C(17)	1(1)	C(14)	C(15)	C(16)	C(17)	1(1)
C(15)	C(16)	C(17)	C(18)	-178.8(10)	C(16)	C(17)	C(18)	C(19)	-154(1)
C(17)	C(18)	C(19)	C(20)	-177(1)	C(17)	C(18)	C(19)	C(21)	4(1)
C(18)	C(19)	C(20)	C(22)	-4(1)	C(21)	C(19)	C(20)	C(22)	173.4(10)

Table 7. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle

Table 8. Non-bonded Contacts out to 3.60 Å

atom	atom	distance	ADC	atom	atom	distance	ADC
Cl(1)	C(20)	3.36(1)	65603	Cl(1)	C(19)	3.45(1)	65603
Cl(1)	O(4)	3.489(8)	65603	Cl(2)	O(6)	3.577(9)	65603
O(1)	O(3)	3.38(1)	66603	O(1)	C(21)	3.39(1)	65603
O(1)	C(18)	3.51(1)	55603	O(1)	C(13)	3.54(1)	1
O(2)	C(1)	3.52(1)	76603	O(2)	C(22)	3.54(1)	65504
O(3)	C(9)	3.12(1)	66603	O(3)	C(8)	3.18(1)	66603
O(3)	C(10)	3.37(1)	66603	O(3)	C(16)	3.42(1)	66501
O(3)	C(6)	3.46(1)	76603	O(4)	C(1)	3.36(1)	54502
O(4)	C(7)	3.48(1)	54502	O(4)	C(4)	3.57(1)	45404
O(5)	C(10)	3.24(1)	54602	O(5)	C(2)	3.46(1)	45504
O(6)	C(20)	3.34(1)	55603	O(6)	C(22)	3.35(1)	55603
O(6)	C(21)	3.39(1)	65603	O(6)	C(4)	3.51(1)	64602
N(1)	C(6)	3.43(1)	76603	N(1)	C(1)	3.45(1)	76603
C(1)	C(3)	3.57(1)	76603	C(2)	C(4)	3.40(1)	76603
C(2)	C(3)	3.45(1)	76603	C(2)	C(10)	3.55(1)	66603
C(12)	C(12)	3.38(2)	55603	C(12)	C(17)	3.54(1)	55603
C(13)	C(18)	3.53(1)	55603	C(13)	C(17)	3.53(1)	55603

The ADC (atom designator code) specifies the position of an atom in a crystal. The 5-digit number shown in the table is a composite of three one-digit numbers and one two-digit number: TA (first digit) + TB (second digit) + TC (third digit) + SN (last two digits). TA, TB and TC are the crystal lattice translation digits along cell edges a, b and c. A translation digit of 5 indicates the origin unit cell. If TA = 4, this indicates a translation of one unit cell length along the a-axis in the negative direction. Each translation digit can range in value from 1 to 9 and thus ±4 lattice translations from the origin (TA=5, TB=5, TC=5) can be represented.

The SN, or symmetry operator number, refers to the number of the symmetry operator used to generate the coordinates of the target atom. A list of symmetry operators relevant to this structure are given below.

For a given intermolecular contact, the first atom (origin atom) is located in the origin unit cell and its position can be generated using the identity operator (SN=1). Thus, the ADC for an origin atom is always 55501. The position of the second atom (target atom) can be generated using the ADC and the coordinates of the atom in the parameter table. For example, an ADC of 47502 refers to the target atom moved through symmetry operator two, then translated -1 cell translations along the a axis, +2 cell translations along the b axis, and 0 cell translations along the c axis.

An ADC of 1 indicates an intermolecular contact between two fragments (eg. cation and anion) that reside in the same asymmetric unit.

Symmetry Operators:

(1)	X,	Y,	Z	(2)	1/2-X,	1/2+Y,	1/2-Z
(3)	-X,	-Y,	-Z	(4)	1/2+X,	1/2-Y,	1/2+Z

Table 9. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
C(1)	0.002(10)
C(2)	0.013(9)
C(3)	-0.02(1)
C(4)	0.01(1)
C(5)	0.01(1)
C(6)	-0.014(10)

Plane number 2

Atoms defining plane	Distance
C(12)	0.00(1)
C(13)	-0.012(10)
C(14)	0.013(10)
C(15)	0.00(1)
C(16)	-0.012(10)
C(17)	0.011(9)

Summary

plane	mean deviation	χ^2
1	0.0116	9.1
2	0.0083	5.8

Dihedral angles between planes (°)

plane	1
2	12.48

10|F|o vs 10|F|c

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
^^^^^^^ h =		0	^^^^^^^		4	8	384	387	14	9	6	460	493	15
					4	9	187	227	16	9	7	341	352	14
0	2	409	413	9	4	10	214	211	15	9	8	140	133	23
0	4	1510	1550	24	4	12	286	280	14	9	11	147	199	27
0	6	388	417	15	4	13	109	162	32	9	12	117	108	33
0	8	101	110	23	4	14	367	370	14	9	14	154	146	30
0	10	386	391	14	4	16	172	166	27	10	0	201	173	14
0	12	435	446	15	4	17	123	158	39	10	1	247	269	13
0	18	159	33	29	5	1	113	89	19	10	3	278	275	12
1	2	404	408	9	5	3	238	231	11	10	4	104	93	28
1	3	1103	1111	18	5	5	178	173	13	10	8	123	58	27
1	4	406	399	13	5	6	246	247	11	10	9	451	499	17
1	5	507	517	14	5	7	576	624	16	10	11	137	132	30
1	6	520	520	14	5	13	134	118	27	10	13	289	307	17
1	7	314	343	11	5	15	130	78	29	11	5	123	53	25
1	8	200	185	13	6	0	1071	1070	19	11	7	426	465	16
1	9	139	135	19	6	1	1100	1094	19	11	8	219	245	19
1	10	320	322	12	6	2	433	423	15	11	9	283	278	15
1	11	109	141	27	6	3	129	134	17	11	10	196	202	22
1	13	171	133	20	6	6	306	274	12	12	0	351	338	14
1	14	345	364	14	6	7	298	311	11	12	1	133	110	24
1	15	240	251	18	6	8	121	94	23	12	7	242	251	18
2	0	682	683	12	6	9	483	493	19	12	8	187	171	22
2	1	206	205	8	6	10	116	109	26	12	12	187	220	27
2	2	232	231	9	6	11	303	285	13	13	3	177	178	21
2	9	253	262	12	6	13	276	268	16	13	4	224	254	18
2	10	176	207	18	7	2	427	426	16	13	8	408	427	15
2	11	178	163	17	7	3	148	196	17	13	9	328	342	15
2	13	337	374	14	7	4	410	423	16	14	1	174	195	23
2	16	153	39	24	7	5	227	235	12	14	2	171	155	22
3	1	206	204	8	7	6	455	441	17	14	3	197	208	21
3	2	433	452	12	7	7	629	617	17	14	4	153	106	24
3	3	738	774	14	7	8	165	148	17	14	5	159	179	24
3	4	219	224	11	7	9	232	252	15	14	6	175	171	23
3	5	1377	1422	23	8	0	329	300	13	14	7	271	294	17
3	6	445	466	15	8	1	302	323	12	14	9	132	128	30
3	7	184	216	14	8	2	468	466	16	14	11	158	164	31
3	8	160	180	16	8	3	111	35	21	15	2	168	155	23
3	9	593	641	17	8	4	146	141	18	15	7	137	141	31
3	10	250	239	13	8	5	302	295	11	15	8	133	54	34
3	12	131	122	25	8	7	495	500	18	15	9	146	18	32
3	14	437	421	17	8	8	137	147	23	16	0	237	207	19
3	15	427	414	17	8	10	246	247	15	16	2	125	111	32
3	16	160	159	28	8	11	125	144	30	16	4	398	402	16
4	1	408	415	13	8	12	122	94	31	17	2	119	96	39
4	2	643	662	14	8	14	128	121	31	17	5	154	133	32
4	3	251	271	10	9	1	517	488	17	17	6	226	219	24
4	4	503	548	14	9	2	746	761	17	18	0	143	103	32
4	6	404	378	16	9	3	448	428	17					
4	7	642	623	16	9	4	157	191	18	^^^^^^^ h =		1	^^^^^^^	

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
					2	-6	139	128	16	4	-3	239	241	10
0	-15	430	413	17	2	-5	610	593	14	4	-2	691	674	14
0	-13	245	252	15	2	-4	176	165	12	4	-1	1026	1036	18
0	-11	476	474	18	2	-3	318	298	10	4	0	998	1006	17
0	-9	929	914	19	2	-2	496	508	12	4	1	551	560	14
0	-7	204	201	11	2	-1	928	911	16	4	2	186	193	13
0	-5	98	104	20	2	0	653	669	12	4	3	473	488	14
0	-3	325	321	13	2	1	515	525	12	4	4	162	165	14
0	-1	160	161	7	2	2	384	391	13	4	5	111	126	21
0	1	539	532	11	2	3	193	198	12	4	6	274	272	11
0	3	146	109	13	2	4	346	365	12	4	8	197	228	15
0	5	1032	1006	18	2	5	318	321	12	4	9	362	389	13
0	7	1219	1209	21	2	6	534	502	15	4	11	468	481	16
0	9	445	454	17	2	9	219	209	13	4	12	187	208	20
0	11	670	663	19	2	10	242	261	14	4	13	154	180	26
1	-16	129	122	27	2	13	311	296	14	4	15	214	200	19
1	-14	158	153	22	2	14	238	269	18	5	-14	408	421	15
1	-13	283	279	13	3	-14	399	395	14	5	-12	400	410	16
1	-12	166	190	18	3	-11	404	409	14	5	-10	201	172	14
1	-11	204	215	14	3	-9	308	325	12	5	-9	118	129	22
1	-10	221	224	13	3	-8	273	253	11	5	-8	505	465	16
1	-8	230	223	11	3	-7	966	896	18	5	-5	186	196	13
1	-7	100	33	19	3	-6	759	753	16	5	-3	710	705	15
1	-6	157	141	14	3	-5	437	429	15	5	-2	345	326	12
1	-5	242	242	10	3	-4	241	232	10	5	0	359	351	12
1	-4	832	789	15	3	-3	169	153	12	5	1	624	655	15
1	-3	1187	1165	19	3	-2	654	639	13	5	2	700	709	15
1	-2	130	132	10	3	-1	1052	1070	18	5	3	648	692	15
1	0	450	433	10	3	0	810	839	15	5	4	313	326	11
1	1	368	378	10	3	1	343	352	14	5	8	386	377	14
1	2	619	594	13	3	2	1071	1074	18	5	10	152	166	22
1	3	343	312	14	3	3	418	437	14	5	11	115	122	29
1	4	478	495	14	3	4	387	400	12	5	13	199	235	19
1	5	338	345	12	3	5	496	510	15	5	14	159	123	24
1	6	867	841	17	3	6	585	560	15	5	15	151	128	27
1	7	191	185	14	3	7	551	522	16	6	-14	190	201	19
1	8	314	297	12	3	11	176	187	20	6	-10	171	194	17
1	9	339	336	12	3	12	140	144	25	6	-9	298	282	11
1	11	202	187	16	3	14	184	188	23	6	-8	223	227	12
1	12	140	145	24	3	15	147	93	26	6	-7	249	229	12
1	13	242	262	17	4	-15	173	155	19	6	-6	458	471	16
1	14	201	175	19	4	-14	242	252	17	6	-5	291	272	11
1	17	161	132	29	4	-13	339	323	14	6	-4	477	481	15
2	-17	192	241	24	4	-12	259	250	14	6	-3	406	375	16
2	-15	237	244	16	4	-10	267	246	12	6	-2	797	764	16
2	-13	375	327	13	4	-9	268	252	12	6	-1	200	204	12
2	-11	221	225	14	4	-8	474	415	16	6	0	966	1007	18
2	-9	149	142	16	4	-7	370	322	13	6	2	662	682	15
2	-8	227	216	11	4	-5	359	337	12	6	3	285	297	10
2	-7	491	500	15	4	-4	556	538	14	6	5	281	253	11

10|F|o vs 10|F|c

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
6	6	141	169	19	9	-3	301	314	11	13	-3	413	426	17
6	7	252	261	13	9	0	356	359	14	13	-1	197	208	19
6	8	440	457	14	9	1	109	83	25	13	2	195	230	20
6	9	133	125	23	9	3	376	364	14	13	3	348	341	13
6	12	329	342	14	9	5	154	232	21	13	5	180	206	23
6	13	261	253	16	9	6	159	179	19	13	6	239	222	17
6	14	165	179	26	9	9	107	95	33	13	9	382	368	16
7	-13	141	171	25	9	13	139	148	29	14	-8	146	128	24
7	-10	217	194	15	10	-12	224	227	17	14	-6	333	345	14
7	-7	229	235	13	10	-10	188	197	21	14	-5	440	440	17
7	-6	88	76	27	10	-5	219	207	14	14	-4	263	213	16
7	-5	149	174	17	10	-4	202	217	16	14	0	242	212	16
7	-4	327	329	13	10	-2	821	811	18	14	1	125	146	30
7	-1	646	658	16	10	-1	428	414	14	14	2	208	177	19
7	0	142	146	17	10	0	273	272	12	15	0	112	50	33
7	2	90	80	26	10	1	194	179	15	15	3	206	196	19
7	3	463	460	16	10	2	595	585	17	15	4	173	221	24
7	4	242	248	12	10	4	352	376	13	16	-1	170	166	23
7	5	444	451	17	10	5	186	215	18	16	1	132	25	27
7	6	391	409	14	10	6	160	171	21	16	3	142	136	29
7	8	154	128	20	10	7	230	218	15	16	4	332	337	15
7	10	226	261	17	10	8	202	194	18					
7	12	146	133	26	10	9	140	149	26	^^^^^^^ h = 2 ^^^^^^^				
7	13	207	223	19	10	11	262	287	17					
8	-11	185	181	18	10	12	264	252	17	0	-16	241	249	17
8	-8	136	142	21	11	-10	384	388	15	0	-14	399	398	16
8	-7	138	113	19	11	-8	270	262	15	0	-10	180	176	14
8	-6	519	533	17	11	-7	152	155	22	0	-8	124	101	18
8	-5	374	369	14	11	-5	210	167	15	0	-6	152	117	14
8	-4	188	201	14	11	-4	300	321	13	0	-4	1455	1408	24
8	-3	141	153	17	11	-3	424	433	15	0	-2	584	576	14
8	-2	327	334	13	11	-1	110	120	27	0	0	1096	1095	19
8	-1	124	82	20	11	0	334	312	13	0	2	1103	1103	19
8	0	200	217	14	11	2	268	280	13	0	8	249	235	12
8	1	809	789	17	11	3	137	61	21	0	10	480	465	19
8	2	517	506	16	11	4	299	297	13	0	12	214	222	18
8	3	230	254	13	11	6	343	325	13	1	-15	676	636	21
8	5	238	271	13	11	8	149	88	23	1	-14	201	185	18
8	6	479	454	18	12	-11	175	168	21	1	-12	100	78	28
8	7	105	12	26	12	-9	127	143	28	1	-11	233	247	13
8	8	108	132	29	12	-8	347	342	13	1	-6	344	340	12
8	9	165	107	19	12	-7	151	146	24	1	-5	828	758	16
8	12	144	165	28	12	-4	119	40	26	1	-4	600	632	14
8	13	129	109	29	12	-2	213	221	17	1	-3	1757	1757	28
9	-13	279	278	14	12	0	158	163	21	1	-2	331	308	11
9	-11	103	118	31	12	2	163	189	21	1	-1	382	356	14
9	-10	226	189	16	12	8	122	72	30	1	0	238	274	10
9	-8	241	224	14	12	9	136	143	29	1	1	233	237	11
9	-7	105	127	29	13	-7	403	407	15	1	2	413	404	15
9	-5	508	474	18	13	-4	316	316	14	1	3	169	169	13