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L2712-1
OM 960031W

Supporting Material for Crystal Structure of C_{2v}-(3a)$_2$

	C_{2v}-(3a)$_2$
formula	$C_{16}H_{28}B_2N_2$
fw	270.04
cryst system	monoclinic
space group	$P2_1/c$ (No. 14)
a, pm	837.0(6)
b, pm	1263.4(6)
c, pm	1533(1)
α, deg	
β, deg	97.04(6)
γ, deg	
V, nm^3	1.609(3)
d_{calcd}, gcm^{-3}	1.114
Z	4
$F(000)$	592.0
μ, cm^{-1}	0.59
cryst dimens, mm	0.7 x 0.6 x 0.6
radiation (λ, pm)	Mo K_α (71.07)
T, K	253
scan mode	ω
scan range, deg	$3 \leq \Theta \leq 27$
total data	3407
unique obsd data	2010 ($I > \sigma(I)$)
sec extinction coeff	-
no. of variables	292
R, R_w[a]	0.083, 0.078
max resid density e 10^{-6} pm^{-3}	0.31

[a] Refinement on F; $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $R_w = [\Sigma w(|F_o| - |F_c|)^2]^{\frac{1}{2}}/\Sigma w(F_o)^2$; $w = 1/\sigma^2(F_o)$

L2712-2

Table of Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
N1	B1	1.635(4)	C16	H16b	0.96(3)
N1	B2	1.634(4)	C17	H17a	1.04(3)
N1	C17	1.482(4)	C17	H17b	0.97(3)
N1	C18	1.479(4)	C17	H17c	1.01(3)
N2	B1	1.633(4)	C18	H18a	1.02(3)
N2	B2	1.628(4)	C18	H18b	0.97(3)
N2	C27	1.483(4)	C18	H18c	0.96(3)
N2	C28	1.484(4)	C21	C22	1.503(4)
B1	C11	1.603(4)	C21	H21a	1.02(3)
B1	C15	1.613(4)	C21	H21b	1.02(3)
B2	C21	1.606(4)	C22	C23	1.328(4)
B2	C25	1.604(4)	C22	H22a	1.00(3)
C11	C12	1.507(4)	C23	C24	1.450(4)
C11	H11a	1.03(3)	C23	H23a	0.98(3)
C11	H11b	0.97(3)	C24	C25	1.515(4)
C12	C13	1.328(4)	C24	C26	1.327(4)
C12	H12a	1.00(3)	C25	H25a	0.99(3)
C13	C14	1.446(4)	C25	H25b	0.99(3)
C13	H13a	1.01(3)	C26	H26a	1.01(3)
C14	C15	1.514(4)	C26	H26b	0.94(3)
C14	C16	1.323(5)	C27	H27a	1.00(3)
C15	H15a	1.01(3)	C27	H27b	1.01(3)
C15	H15b	0.99(3)	C27	H27c	0.99(4)
C16	H16a	1.03(4)	C28	H28a	1.00(3)
C28	H28b	0.98(3)	C28	H28c	1.02(3)

Numbers in parentheses are estimated standard deviations in the least significant digits.

L2712-3

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
B1	N1	B2	87.8(2)	B1	C11	C12	111.3(3)
B1	N1	C17	116.1(2)	B1	C11	H11a	117.(1)
B1	N1	C18	114.3(3)	B1	C11	H11b	112.(2)
B2	N1	C17	117.3(2)	C12	C11	H11a	108.(1)
B2	N1	C18	114.4(2)	C12	C11	H11b	107.(2)
C17	N1	C18	106.5(2)	H11a	C11	H11b	101.(2)
B1	N2	B2	88.1(2)	C11	C12	C13	124.3(3)
B1	N2	C27	117.4(2)	C11	C12	H12a	118.(2)
B1	N2	C28	114.6(2)	C13	C12	H12a	118.(2)
B2	N2	C27	115.8(2)	C12	C13	C14	124.5(3)
B2	N2	C28	114.5(2)	C12	C13	H13a	119.(2)
C27	N2	C28	106.1(3)	C14	C13	H13a	117.(2)
N1	B1	N2	90.5(1)	C13	C14	C15	116.5(3)
N1	B1	C11	113.8(2)	C13	C14	C16	121.2(3)
N1	B1	C15	114.9(2)	C15	C14	C16	122.4(3)
N2	B1	C11	113.6(2)	B1	C15	C14	112.2(3)
N2	B1	C15	115.3(2)	B1	C15	H15a	101.(2)
C11	B1	C15	108.2(3)	B1	C15	H15b	114.(2)
N1	B2	N2	90.7(1)	C14	C15	H15a	108.(2)
N1	B2	C21	113.2(3)	C14	C15	H15b	109.(2)
N1	B2	C25	115.7(3)	H15a	C15	H15b	112.(2)
N2	B2	C21	113.8(3)	C14	C16	H16a	121.(2)
N2	B2	C25	115.0(2)	C14	C16	H16b	120.(2)
C21	B2	C25	107.8(2)	H16a	C16	H16b	119.(3)

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Bond Angles (cont.)

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
N1	C17	H17a	106.(2)	C23	C24	C25	115.9(2)
N1	C17	H17b	108.(2)	C23	C24	C26	122.2(4)
N1	C17	H17c	110.(2)	C25	C24	C26	121.9(3)
H17a	C17	H17b	108.(2)	B2	C25	C24	112.8(3)
H17a	C17	H17c	113.(2)	B2	C25	H25a	105.(2)
H17b	C17	H17c	111.(2)	B2	C25	H25b	120.(2)
N1	C18	H18a	109.(2)	C24	C25	H25a	109.(2)
N1	C18	H18b	111.(2)	C24	C25	H25b	108.(2)
N1	C18	H18c	112.(2)	H25a	C25	H25b	101.(2)
H18a	C18	H18b	108.(2)	C24	C26	H26a	123.(2)
H18a	C18	H18c	106.(2)	C24	C26	H26b	117.(2)
H18b	C18	H18c	110.(2)	H26a	C26	H26b	120.(3)
B2	C21	C22	111.8(2)	N2	C27	H27a	112.(2)
B2	C21	H21a	114.(1)	N2	C27	H27b	109.(2)
B2	C21	H21b	106.(1)	N2	C27	H27c	108.(2)
C22	C21	H21a	111.(1)	H27a	C27	H27b	107.(2)
C22	C21	H21b	107.(1)	H27a	C27	H27c	111.(3)
H21a	C21	H21b	106.(2)	H27b	C27	H27c	109.(3)
C21	C22	C23	123.9(3)	N2	C28	H28a	111.(2)
C21	C22	H22a	117.(2)	N2	C28	H28b	109.(2)
C23	C22	H22a	119.(2)	N2	C28	H28c	110.(2)
C22	C23	C24	124.8(3)	H28a	C28	H28b	107.(3)
C22	C23	H23a	117.(2)	H28a	C28	H28c	106.(2)
C24	C23	H23a	118.(2)	H28b	C28	H28c	113.(2)

Numbers in parentheses are estimated standard deviations in the least significant digits.

L2712-5

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
N1	0.037(1)	0.034(1)	0.025(1)	-0.003(1)	-0.002(1)	-0.001(1)
N2	0.031(1)	0.037(1)	0.030(1)	0.003(1)	0.001(1)	-0.001(1)
B1	0.032(2)	0.035(2)	0.028(2)	0.002(2)	0.001(1)	0.001(2)
B2	0.032(2)	0.036(2)	0.025(2)	-0.003(2)	-0.002(1)	-0.002(1)
C11	0.051(2)	0.043(2)	0.037(2)	-0.001(2)	0.007(1)	-0.007(2)
C12	0.051(2)	0.058(2)	0.046(2)	0.012(2)	0.012(2)	-0.011(2)
C13	0.044(2)	0.077(2)	0.039(2)	0.007(2)	0.014(1)	-0.005(2)
C14	0.037(2)	0.064(2)	0.033(2)	-0.004(2)	0.003(1)	0.005(2)
C15	0.039(2)	0.046(2)	0.037(2)	-0.001(2)	0.007(1)	0.007(2)
C16	0.050(2)	0.081(3)	0.079(3)	-0.007(2)	0.018(2)	0.010(2)
C17	0.044(2)	0.052(2)	0.035(2)	-0.011(2)	-0.002(2)	-0.005(2)
C18	0.040(2)	0.045(2)	0.047(2)	0.005(2)	0.005(2)	0.011(2)
C21	0.044(2)	0.040(2)	0.031(2)	0.005(2)	0.002(1)	0.004(1)
C22	0.054(2)	0.040(2)	0.038(2)	-0.006(2)	-0.001(2)	0.012(1)
C23	0.039(2)	0.054(2)	0.038(2)	-0.006(2)	0.005(2)	0.005(2)
C24	0.041(2)	0.052(2)	0.025(2)	0.003(2)	0.004(1)	-0.004(1)
C25	0.036(2)	0.042(2)	0.036(2)	-0.006(1)	0.006(1)	-0.006(1)
C26	0.046(2)	0.059(2)	0.052(2)	-0.002(2)	0.014(2)	-0.008(2)
C27	0.034(2)	0.065(2)	0.044(2)	0.010(2)	-0.002(2)	0.005(2)
C28	0.042(2)	0.050(2)	0.047(2)	-0.011(2)	0.010(2)	-0.014(2)

The form of the anisotropic displacement parameter is:
exp[-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}] where a,b, and c are reciprocal lattice constants.

L2712-6

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(eq)
N1	0.5098(3)	0.2387(2)	0.7301(2)	2.56(5)
N2	0.2477(3)	0.2203(2)	0.6623(2)	2.61(5)
B1	0.3310(4)	0.2418(3)	0.7627(2)	2.53(7)
B2	0.4212(4)	0.2455(3)	0.6292(2)	2.48(7)
C11	0.2851(4)	0.3543(3)	0.8011(2)	3.44(7)
C12	0.1264(4)	0.3494(3)	0.8379(2)	4.03(8)
C13	0.0596(4)	0.2608(3)	0.8627(2)	4.15(8)
C14	0.1294(4)	0.1566(3)	0.8579(2)	3.50(7)
C15	0.2989(4)	0.1518(3)	0.8332(2)	3.20(7)
C16	0.0485(5)	0.0706(3)	0.8750(3)	5.5(1)
C17	0.6199(4)	0.3263(3)	0.7614(2)	3.48(7)
C18	0.5996(4)	0.1393(3)	0.7515(2)	3.47(7)
C21	0.4323(4)	0.3608(3)	0.5862(2)	3.05(7)
C22	0.5880(4)	0.3760(3)	0.5484(2)	3.52(8)
C23	0.6797(4)	0.2970(3)	0.5262(2)	3.45(7)
C24	0.6439(4)	0.1856(3)	0.5359(2)	3.11(7)
C25	0.4794(4)	0.1605(3)	0.5622(2)	2.99(7)
C26	0.7489(4)	0.1102(3)	0.5231(2)	4.05(8)
C27	0.1133(4)	0.2907(3)	0.6272(2)	3.78(8)
C28	0.1894(4)	0.1105(3)	0.6451(2)	3.63(7)
H11a	0.283(3)	0.418(2)	0.759(2)	0.3(6)*
H11b	0.365(4)	0.378(2)	0.849(2)	2.0(8)*
H12a	0.064(3)	0.417(2)	0.840(2)	0.4(6)*
H13a	-0.050(4)	0.264(2)	0.883(2)	2.3(8)*

L2712-7

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(eq)
H15a	0.375(4)	0.176(2)	0.886(2)	1.6(7)*
H15b	0.322(3)	0.079(2)	0.815(2)	1.0(fixed)*
H16a	0.097(4)	-0.004(3)	0.870(2)	5(1)*
H16b	-0.059(4)	0.077(3)	0.889(2)	3.6(9)*
H17a	0.724(4)	0.315(2)	0.732(2)	2.4(8)*
H17b	0.647(3)	0.319(2)	0.825(2)	0.1(6)*
H17c	0.566(3)	0.396(2)	0.746(2)	0.8(6)*
H18a	0.630(4)	0.134(3)	0.818(2)	2.5(8)*
H18b	0.699(4)	0.138(2)	0.724(2)	2.0(7)*
H18c	0.536(3)	0.078(2)	0.735(2)	0.4(6)*
H21a	0.413(3)	0.422(2)	0.627(2)	0.7(6)*
H21b	0.343(3)	0.364(2)	0.535(2)	0.3(6)*
H22a	0.625(3)	0.450(2)	0.542(2)	0.9(7)*
H23a	0.785(4)	0.316(2)	0.509(2)	1.6(7)*
H25a	0.398(3)	0.164(2)	0.510(2)	1.7(7)*
H25b	0.477(3)	0.084(2)	0.576(2)	0.6(6)*
H26a	0.725(3)	0.032(2)	0.528(2)	0.9(7)*
H26b	0.848(4)	0.132(3)	0.507(2)	2.7(8)*
H27a	0.138(4)	0.367(2)	0.640(2)	2.0(8)*
H27b	0.016(4)	0.272(2)	0.657(2)	2.5(8)*
H27c	0.090(4)	0.278(3)	0.563(2)	4(1)*
H28a	0.162(4)	0.097(2)	0.581(2)	2.1(8)*
H28b	0.091(4)	0.100(2)	0.673(2)	2.2(8)*
H28c	0.279(4)	0.058(2)	0.666(2)	1.4(7)*

Starred atoms were refined isotropically.
H15b was refined isotropically with fixed B(iso).
Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:
(4/3) * [a2*beta(1,1) + b2*beta(2,2) + c2*beta(3,3) + + ac(cos beta)*beta(1,3)]

L2712-8

Supporting Material for Crystal Structure of 4c

	4c
formula	$C_{18}H_{37}BN_3Li$
fw	313.27
cryst system	triclinic
space group	$P\bar{1}$ (No. 2)
a, pm	884.86(9)
b, pm	1450.2(2)
c, pm	831.7(3)
α, deg	94.48(2)
β, deg	100.30(2)
γ, deg	87.87(1)
V, nm^3	1.0466(4)
d_{calcd}, gcm^{-3}	0.994
Z	2
$F(000)$	348.0
μ, cm^{-1}	3.98
cryst dimens, mm	0.5 x 0.5 x 0.5
radiation (λ, pm)	Cu K_α (154.18)
T, K	228
scan mode	ω/Θ
scan range, deg	$5 \leq \Theta \leq 70$
total data	2934
unique obsd data	2456 ($I > \sigma(I)$)
sec extinction coeff	$0.494 \cdot 10^{-5}$
no. of variables	233
R, R_w[a]	0.068, 0.083
max resid density e 10^{-6} pm^{-3}	0.33

[a] Refinement on F; $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $R_w = [\Sigma w(|F_o| - |F_c|)^2]^{\frac{1}{2}}/\Sigma w(F_o)^2$; $w = 1/\sigma^2(F_o)$

L2712-9

Bond distances (A)

N1	-	C11	1.445(2)	C6	-	Li	2.356(3)
N1	-	C12	1.447(2)	C6	-	H6	1.02(1)
N1	-	B	1.448(2)	C7	-	C71	1.542(3)
N2	-	C21	1.480(3)	C7	-	C72	1.535(2)
N2	-	C22	1.461(2)	C7	-	C73	1.533(3)
N2	-	C23	1.457(3)	C8	-	H8a	0.98(3)
N2	-	Li	2.139(3)	C8	-	H8b	1.02(2)
N3	-	C31	1.470(3)	C8	-	H8c	0.99(2)
N3	-	C32	1.475(2)	C11	-	H11	0.98
N3	-	C33	1.469(2)	C11	-	H11	0.98
N3	-	Li	2.134(3)	C11	-	H11	0.98
C2	-	C3	1.395(2)	C12	-	H12	0.98
C2	-	B	1.518(2)	C12	-	H12	0.98
C2	-	Li	2.389(3)	C12	-	H12	0.98
C2	-	H2	1.03(1)	C21	-	C31	1.408(3)
C3	-	C4	1.410(2)	C21	-	H21	0.98
C3	-	C7	1.546(2)	C21	-	H21	0.98
C4	-	C5	1.406(2)	C22	-	H22	0.98
C4	-	Li	2.387(3)	C22	-	H22	0.98
C4	-	H4	0.99(1)	C22	-	H22	0.98
C5	-	C6	1.389(2)	C23	-	H23	0.98
C5	-	C8	1.513(2)	C23	-	H23	0.98
C5	-	Li	2.370(3)	C23	-	H23	0.98
C6	-	B	1.520(2)	C31	-	H31	0.98

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Bond Distances (Cont.)

C31	-	H31	0.98	C71	-	H71	0.98
C32	-	H32	0.98	C72	-	H72	0.98
C32	-	H32	0.98	C72	-	H72	0.98
C32	-	H32	0.98	C72	-	H72	0.98
C33	-	H33	0.98	C73	-	H73	0.98
C33	-	H33	0.98	C73	-	H73	0.98
C33	-	H33	0.98	C73	-	H73	0.98
C71	-	H71	0.98	B	-	Li	2.451(4)
C71	-	H71	0.98				

Numbers in parentheses are estimated standard deviations in the least significant distances.

L2712-11

Bond Angles (deg.)

C11	-	N1	-	C12	112.7(1)	C3	-	C4	-	C5	121.9(1)
C11	-	N1	-	B	123.3(1)	C3	-	C4	-	Li	73.7(1)
C12	-	N1	-	B	122.6(1)	C3	-	C4	-	H4	122.5(8)
C21	-	N2	-	C22	109.0(2)	C5	-	C4	-	Li	72.2(1)
C21	-	N2	-	C23	112.9(2)	C5	-	C4	-	H4	115.6(8)
C21	-	N2	-	Li	104.7(1)	Li	-	C4	-	H4	130.1(9)
C22	-	N2	-	C23	108.3(2)	C4	-	C5	-	C6	121.5(1)
C22	-	N2	-	Li	113.8(2)	C4	-	C5	-	C8	118.1(1)
C23	-	N2	-	Li	108.2(1)	C4	-	C5	-	Li	73.5(1)
C31	-	N3	-	C32	108.1(2)	C6	-	C5	-	C8	120.3(1)
C31	-	N3	-	C33	111.0(2)	C6	-	C5	-	Li	72.3(1)
C31	-	N3	-	Li	105.7(1)	C8	-	C5	-	Li	129.5(2)
C32	-	N3	-	C33	107.7(1)	C5	-	C6	-	B	120.8(1)
C32	-	N3	-	Li	114.2(1)	C5	-	C6	-	Li	73.5(1)
C33	-	N3	-	Li	110.0(1)	C5	-	C6	-	H6	115.8(8)
C3	-	C2	-	B	122.2(1)	B	-	C6	-	Li	75.0(1)
C3	-	C2	-	Li	73.9(1)	B	-	C6	-	H6	123.1(8)
C3	-	C2	-	H2	115.7(8)	Li	-	C6	-	H6	128(1)
B	-	C2	-	Li	74.0(1)	C3	-	C7	-	C71	110.0(1)
B	-	C2	-	H2	122.0(8)	C3	-	C7	-	C72	113.0(1)
Li	-	C2	-	H2	128(1)	C3	-	C7	-	C73	108.5(1)
C2	-	C3	-	C4	119.9(1)	C71	-	C7	-	C72	107.5(2)
C2	-	C3	-	C7	119.6(1)	C71	-	C7	-	C73	109.3(2)
C4	-	C3	-	C7	120.4(1)	C72	-	C7	-	C73	108.4(2)

L2712-12

Bond angles (deg.)

C5	-	C8	-	H8a	113.(1)	N2	-	C22	-	H22	116.1(2)
C5	-	C8	-	H8b	111.(1)	N2	-	C22	-	H22	96.0(2)
C5	-	C8	-	H8c	115.(1)	N2	-	C22	-	H22	111.4(2)
H8a	-	C8	-	H8b	102.(2)	H22	-	C22	-	H22	100.1(2)
H8a	-	C8	-	H8c	105.(2)	H22	-	C22	-	H22	107.8(2)
H8b	-	C8	-	H8c	111.(2)	H22	-	C22	-	H22	125.3(2)
N1	-	C11	-	H11	112.7(1)	N2	-	C23	-	H23	120.3(2)
N1	-	C11	-	H11	108.5(2)	N2	-	C23	-	H23	106.4(2)
N1	-	C11	-	H11	108.2(2)	N2	-	C23	-	H23	106.4(2)
H11	-	C11	-	H11	99.9(2)	H23	-	C23	-	H23	107.0(2)
H11	-	C11	-	H11	112.7(2)	H23	-	C23	-	H23	107.0(3)
H11	-	C11	-	H11	114.6(2)	H23	-	C23	-	H23	109.5(2)
N1	-	C12	-	H12	102.8(2)	N3	-	C31	-	C21	116.2(2)
N1	-	C12	-	H12	104.8(1)	N3	-	C31	-	H31	109.4(2)
N1	-	C12	-	H12	115.3(2)	N3	-	C31	-	H31	106.6(3)
H12	-	C12	-	H12	106.1(2)	C21	-	C31	-	H31	111.9(3)
H12	-	C12	-	H12	114.6(2)	C21	-	C31	-	H31	102.8(3)
H12	-	C12	-	H12	112.2(2)	H31	-	C31	-	H31	109.5(3)
N2	-	C21	-	C31	115.8(2)	N3	-	C32	-	H32	91.7(2)
N2	-	C21	-	H21	110.5(2)	N3	-	C32	-	H32	99.6(2)
N2	-	C21	-	H21	105.2(3)	N3	-	C32	-	H32	129.6(2)
C31	-	C21	-	H21	112.4(3)	H32	-	C32	-	H32	120.9(3)
C31	-	C21	-	H21	102.8(2)	H32	-	C32	-	H32	111.2(2)
H21	-	C21	-	H21	109.5(3)	H32	-	C32	-	H32	105.0(2)

L2712-13

Bond Angles (deg.)

N3	-	C33	-	H33	109.2(2)	N1	-	B	-	C2	123.2(1)
N3	-	C33	-	H33	108.8(2)	N1	-	B	-	C6	123.2(1)
N3	-	C33	-	H33	109.7(2)	N1	-	B	-	Li	130.1(1)
H33	-	C33	-	H33	109.8(2)	C2	-	B	-	C6	113.5(1)
H33	-	C33	-	H33	109.8(2)	C2	-	B	-	Li	69.5(1)
H33	-	C33	-	H33	109.5(2)	C6	-	B	-	Li	68.2(1)
C7	-	C71	-	H71	100.6(2)	N2	-	Li	-	N3	84.6(1)
C7	-	C71	-	H71	111.3(2)	N2	-	Li	-	C2	106.8(1)
C7	-	C71	-	H71	111.3(2)	N2	-	Li	-	C4	167.5(1)
H71	-	C71	-	H71	112.0(2)	N2	-	Li	-	C5	149.7(1)
H71	-	C71	-	H71	112.0(2)	N2	-	Li	-	C6	117.3(1)
H71	-	C71	-	H71	109.5(2)	N2	-	Li	-	B	98.3(1)
C7	-	C72	-	H72	122.4(2)	N3	-	Li	-	C2	152.6(1)
C7	-	C72	-	H72	105.9(2)	N3	-	Li	-	C4	105.1(1)
C7	-	C72	-	H72	101.5(2)	N3	-	Li	-	C5	109.3(1)
H72	-	C72	-	H72	103.5(2)	N3	-	Li	-	C6	132.6(1)
H72	-	C72	-	H72	104.0(2)	N3	-	Li	-	B	168.7(1)
H72	-	C72	-	H72	121.0(2)	C2	-	Li	-	C4	61.10(9)
C7	-	C73	-	H73	109.7(2)	C2	-	Li	-	C5	73.5(1)
C7	-	C73	-	H73	108.8(2)	C2	-	Li	-	C6	64.7(1)
C7	-	C73	-	H73	109.4(2)	C2	-	Li	-	B	36.54(6)
H73	-	C73	-	H73	109.7(2)	C4	-	Li	-	C5	34.39(6)
H73	-	C73	-	H73	109.7(2)	C4	-	Li	-	C6	61.90(9)
H73	-	C73	-	H73	109.5(2)	C4	-	Li	-	B	73.8(1)
C5	-	Li	-	C6	34.18(6)	C6	-	Li	-	B	36.79(7)
C5	-	Li	-	B	63.3(1)						

Numbers in parentheses are estimated standard deviations in the least significant digit.

L2712-14

Table of General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
N1	0.0385(9)	0.0433(9)	0.046(2)	0.0010(8)	-0.000(1)	0.006(1)
N2	0.043(1)	0.101(2)	0.032(2)	-0.005(1)	0.012(1)	0.009(1)
N3	0.0421(9)	0.078(1)	0.033(2)	-0.005(1)	0.007(1)	0.003(1)
C2	0.040(1)	0.0327(9)	0.030(2)	-0.0047(8)	0.009(1)	-0.000(1)
C3	0.043(1)	0.0315(9)	0.032(2)	0.0021(8)	0.012(1)	0.001(1)
C4	0.0335(9)	0.039(1)	0.036(2)	0.0020(8)	0.011(1)	0.004(1)
C5	0.0378(9)	0.0354(9)	0.031(2)	-0.0062(8)	0.012(1)	0.002(1)
C6	0.041(1)	0.0298(9)	0.030(2)	0.0006(8)	0.010(1)	0.004(1)
C7	0.057(1)	0.033(1)	0.054(2)	0.0065(9)	0.018(1)	0.005(1)
C8	0.042(1)	0.044(1)	0.074(3)	-0.0120(9)	0.010(1)	0.006(1)
C11	0.039(1)	0.069(1)	0.052(2)	-0.008(1)	0.001(1)	0.004(1)
C12	0.048(1)	0.056(1)	0.075(3)	0.014(1)	0.010(1)	0.016(1)
C21	0.057(2)	0.255(5)	0.043(3)	-0.026(2)	0.013(2)	0.029(3)
C22	0.072(2)	0.120(2)	0.076(3)	-0.034(2)	0.027(2)	0.015(2)
C23	0.086(2)	0.105(3)	0.103(4)	0.013(2)	0.048(2)	-0.003(2)
C31	0.064(2)	0.223(5)	0.042(3)	-0.019(2)	0.019(2)	-0.010(3)
C32	0.082(2)	0.074(2)	0.081(3)	-0.018(2)	-0.010(2)	-0.008(2)
C33	0.089(2)	0.075(2)	0.072(3)	-0.001(2)	-0.016(2)	0.016(2)
C71	0.084(2)	0.043(1)	0.084(3)	0.007(1)	0.028(2)	0.023(1)
C72	0.064(1)	0.049(1)	0.107(3)	0.025(1)	0.021(2)	0.013(2)
C73	0.113(2)	0.040(1)	0.072(3)	0.009(1)	0.030(2)	-0.016(1)
B	0.038(1)	0.037(1)	0.019(2)	-0.0004(9)	0.009(1)	0.002(1)
Li	0.039(2)	0.040(2)	0.038(4)	-0.002(1)	0.008(2)	0.000(2)

The form of the anisotropic displacement parameter is:
exp[-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}] where a,b, and c are reciprocal lattice constants.

 L2712-15

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(eq)
N1	0.1477(2)	0.6803(1)	0.4130(3)	3.43(5)
N2	0.0456(2)	0.7210(2)	-0.0441(3)	4.55(6)
N3	-0.2790(2)	0.7125(2)	-0.1671(3)	4.03(6)
C2	-0.0746(2)	0.8015(1)	0.3399(3)	2.68(6)
C3	-0.2308(2)	0.8218(1)	0.2923(3)	2.76(6)
C4	-0.3357(2)	0.7494(1)	0.2503(3)	2.79(6)
C5	-0.2878(2)	0.6559(1)	0.2544(3)	2.67(6)
C6	-0.1340(2)	0.6304(1)	0.2988(3)	2.61(6)
C7	-0.2885(3)	0.9238(2)	0.2946(4)	3.73(7)
C8	-0.4095(3)	0.5831(2)	0.2163(4)	4.18(7)
C11	0.2614(3)	0.7490(2)	0.4768(4)	4.25(7)
C12	0.2020(3)	0.5873(2)	0.4472(4)	4.68(8)
C21	-0.0197(4)	0.7350(4)	-0.2174(5)	9.2(1)
C22	0.1543(4)	0.7942(3)	0.0193(5)	6.8(1)
C23	0.1259(4)	0.6320(3)	-0.0229(6)	7.5(1)
C31	-0.1655(4)	0.6977(4)	-0.2763(5)	8.6(1)
C32	-0.3855(4)	0.6346(2)	-0.2006(5)	6.5(1)
C33	-0.3697(4)	0.7980(2)	-0.1994(5)	6.5(1)
C71	-0.2021(4)	0.9788(2)	0.1894(4)	5.35(9)
C72	-0.4609(3)	0.9344(2)	0.2275(5)	5.77(9)
C73	-0.2574(4)	0.9656(2)	0.4721(5)	5.89(9)
B	-0.0125(3)	0.7030(2)	0.3547(4)	2.44(7)
Li	-0.1494(4)	0.7230(3)	0.0758(6)	3.1(1)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:
(4/3) * [a2*beta(1,1) + b2*beta(2,2) + c2*beta(3,3) + ab(cos gamma) *beta(1,2)+ ac(cos beta)*beta(1,3) + bc(cos alpha)*beta(2,3)]

L2712-16

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(eq)
H2	-0.005(2)	0.858(1)	0.372(3)	1.0(5)*
H4	-0.448(2)	0.761(1)	0.223(3)	0.3(4)*
H6	-0.111(2)	0.561(1)	0.301(3)	0.9(5)*
H8a	-0.429(3)	0.556(2)	0.315(4)	4.4(8)*
H8b	-0.373(3)	0.527(2)	0.152(4)	3.9(7)*
H8c	-0.511(3)	0.606(2)	0.161(4)	2.5(6)*
H11a	0.237	0.809	0.430	5.5
H11b	0.356	0.732	0.434	5.5
H11c	0.274	0.754	0.597	5.5
H12a	0.200	0.586	0.564	5.9
H12b	0.311	0.586	0.437	5.9
H12c	0.145	0.538	0.378	6.1
H21a	0.055	0.716	-0.288	11.7
H21b	-0.040	0.802	-0.221	11.7
H22a	0.118	0.858	-0.001	8.5
H22b	0.218	0.783	-0.065	8.5
H22c	0.191	0.792	0.137	8.7
H23a	0.156	0.610	0.087	9.7
H23b	0.220	0.636	-0.069	9.7

L2712-17

Table of Positional Parameters and Their Estimated Standard Deviations (cont.)

Atom	x	y	z	B(eq)
H23c	0.059	0.586	-0.088	9.7
H31a	-0.210	0.718	-0.385	11.1
H31b	-0.143	0.631	-0.285	11.1
H32a	-0.448	0.662	-0.122	8.5
H32b	-0.313	0.583	-0.172	8.5
H32c	-0.451	0.613	-0.304	8.5
H33a	-0.442	0.807	-0.123	7.8
H33b	-0.426	0.793	-0.312	7.8
H33c	-0.301	0.851	-0.185	7.8
H71a	-0.236	1.042	0.218	6.5
H71b	-0.233	0.961	0.072	6.5
H71c	-0.091	0.970	0.221	6.5
H72a	-0.514	0.995	0.221	7.6
H72b	-0.475	0.909	0.113	7.6
H72c	-0.506	0.904	0.309	7.5
H73a	-0.276	1.033	0.474	8.0
H73b	-0.150	0.952	0.520	8.0
H73c	-0.325	0.938	0.535	8.0

Starred atoms were refined isotropically.
Other hydrogen atoms were not refined but included isotropically in structure factor calculations.

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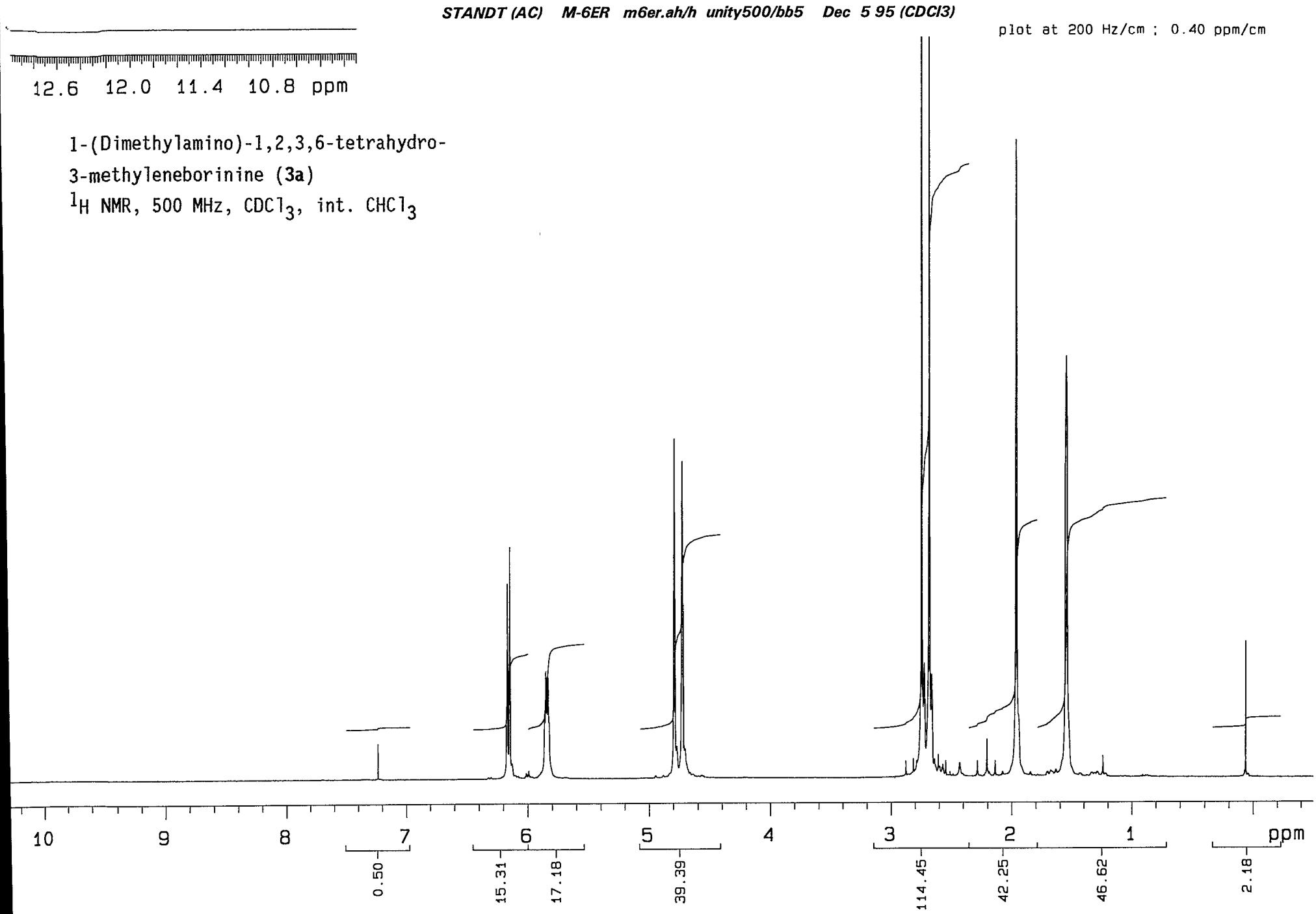

L2718-18

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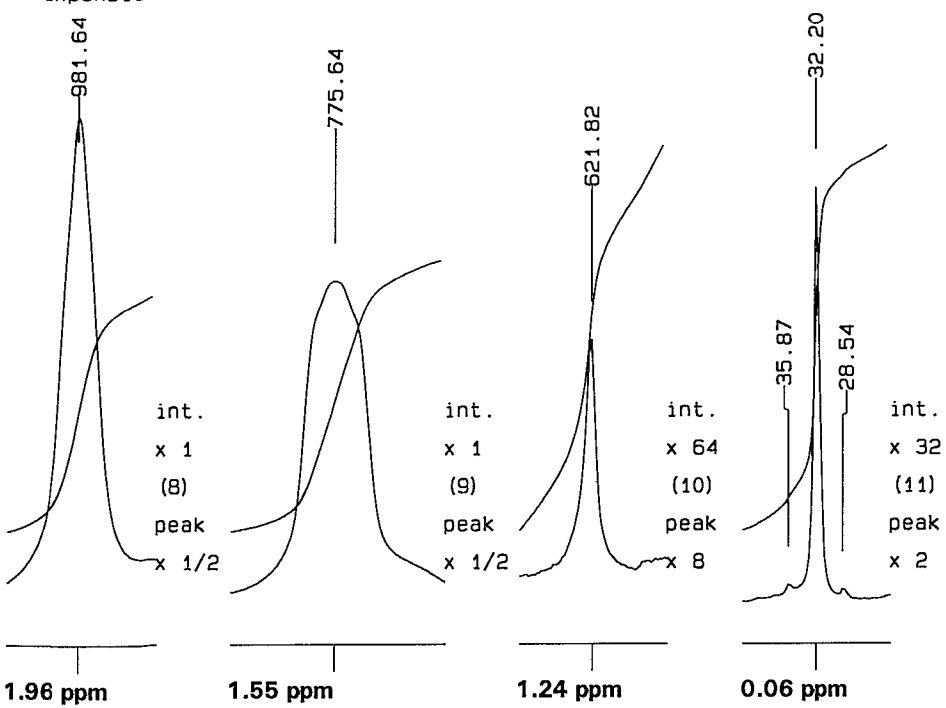
L2712-20

Expansions at 10 Hz/cm 0.020 ppm/cm (p.2) ***STANDT (AC) M-6ER m6er.ah/h unity500/bb5 Dec 5 95 (CDCl3)***



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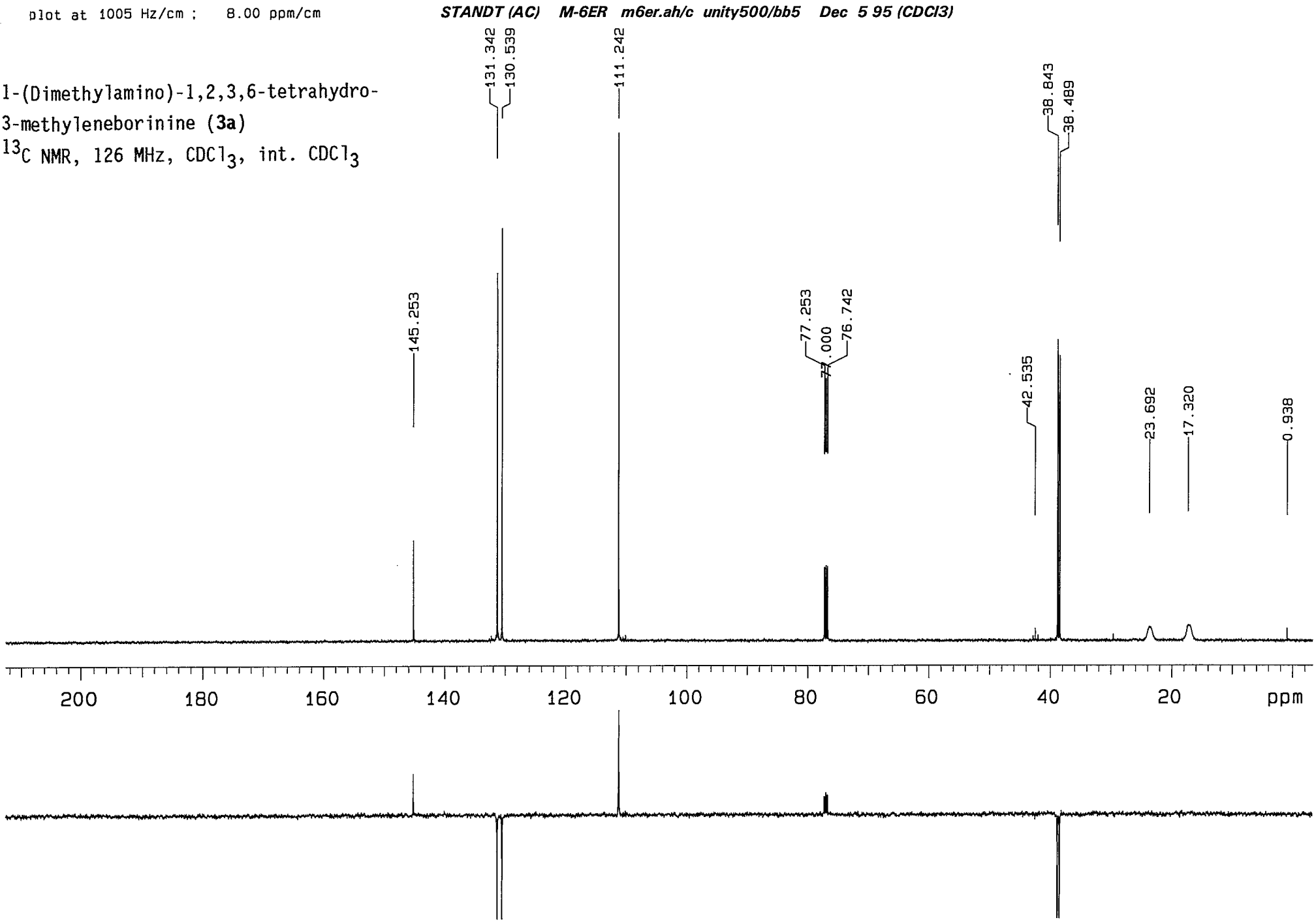
1-(Dimethylamino)-1,2,3,6-tetrahydro-3-methyleneborinine (**3a**)

^{13}C NMR, 126 MHz, $CDCl_3$, int. $CDCl_3$



LG7148-21

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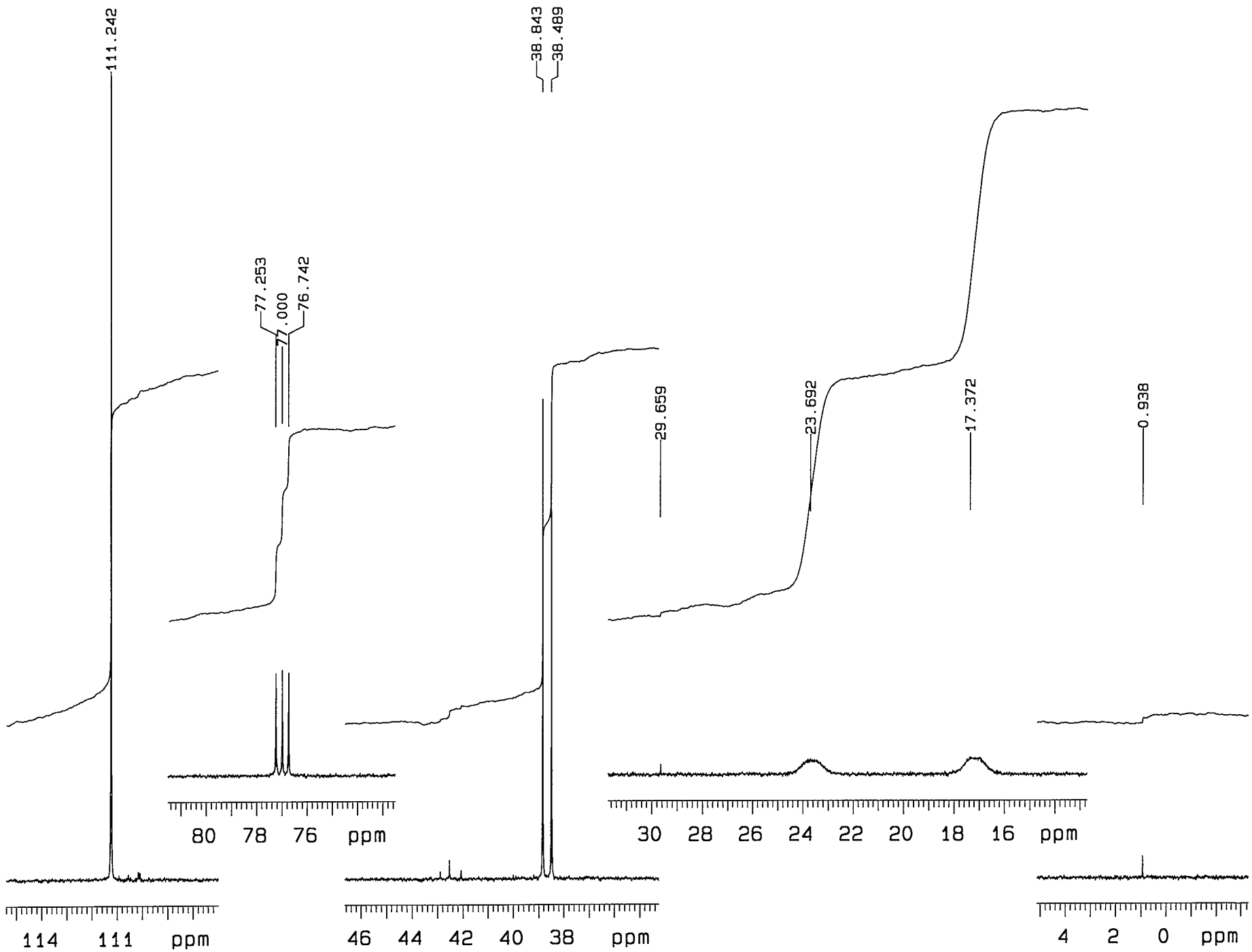
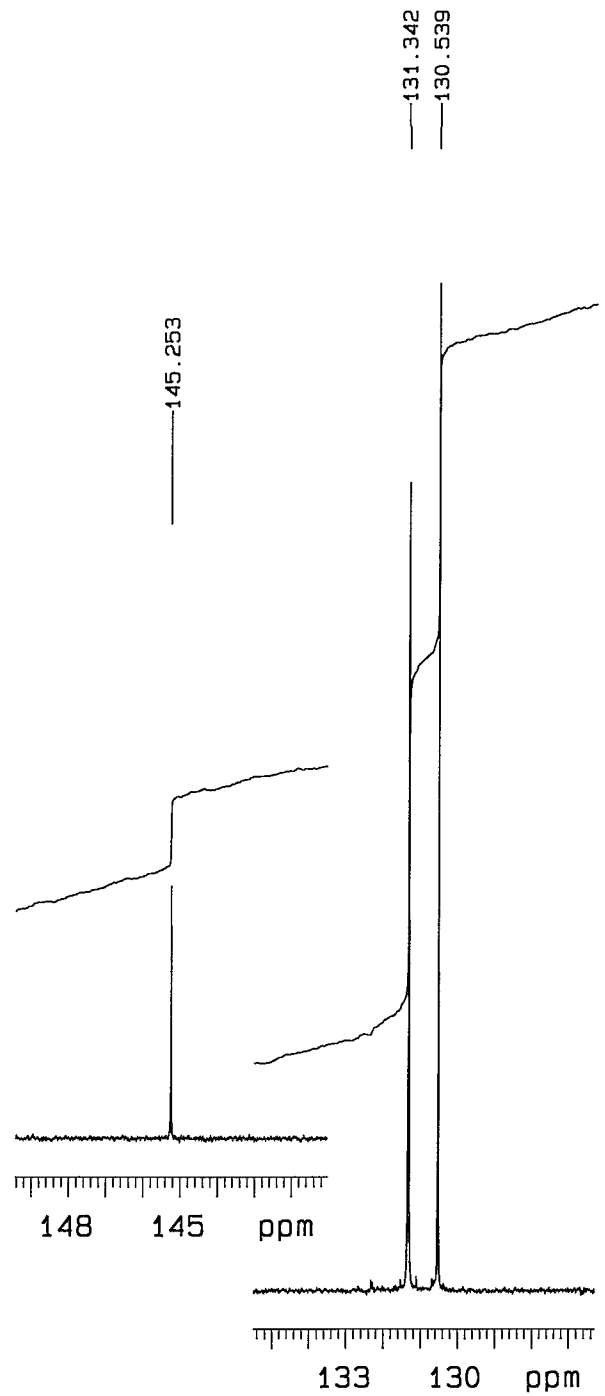
EXPANSIONS at 251.3 Hz/cm 2.00 ppm/cm (p.1) ***STANDT (AC) M-6ER m6er.ah/c unity500/bb5 Dec 5 95 (CDCl3)***



L27B-22

EXPANSIONS at 251.3 Hz/cm 2.00 ppm/cm (p.2) ***STANDT (AC) M-6ER m6er.ah/c unity500/bb5 Dec 5 95 (CDCl3)***



L2918-23

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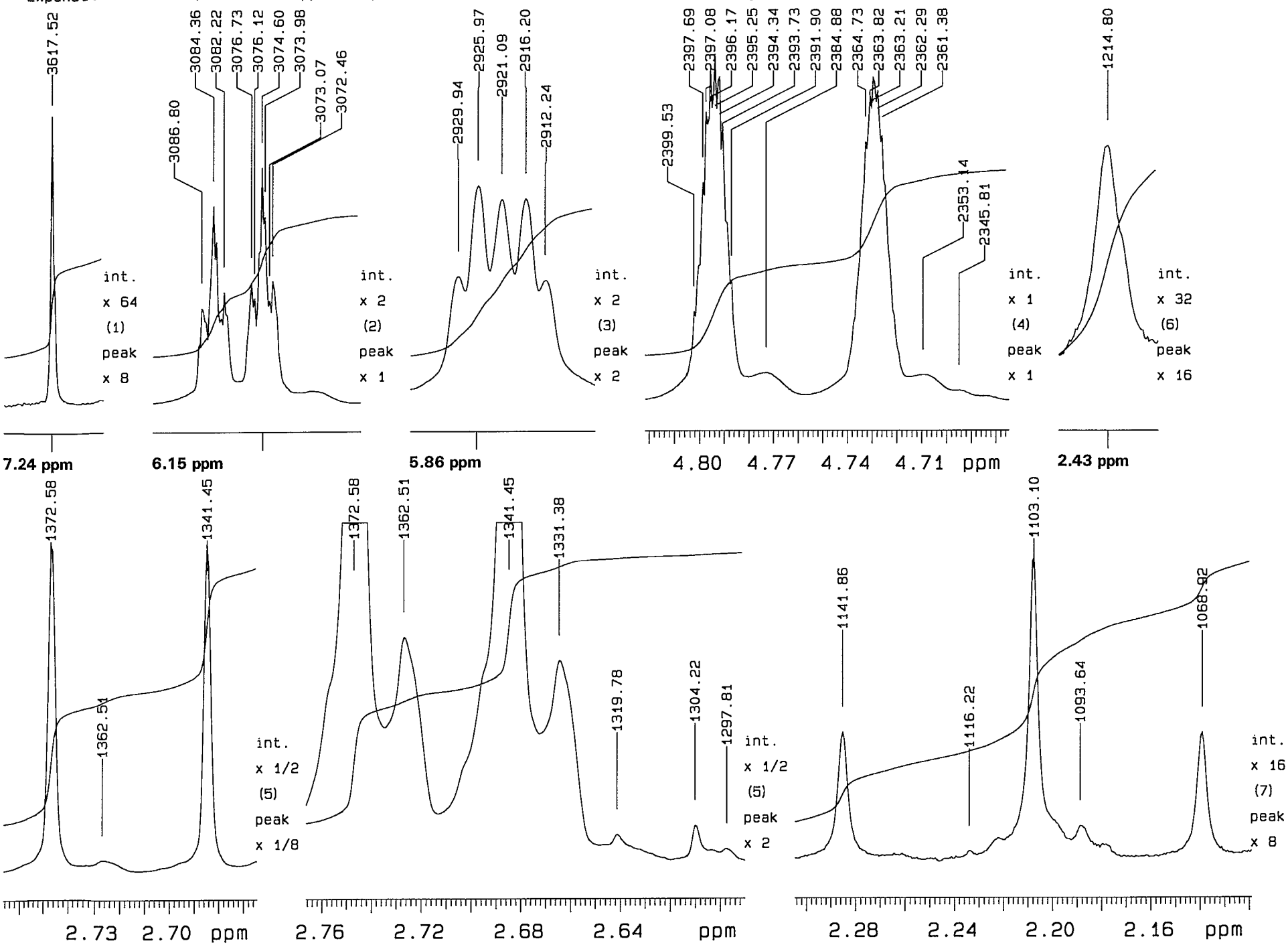
L2718-19

Expansions at 10 Hz/cm 0.020 ppm/cm (p.1) **STANDT (AC) M-6ER m6er.ah/h unity500/bb5 Dec 5 95 (CDCl3)**



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L2712-24

THRESHOLD : 2.0

STANDT (AC) M-6ER m6er.ah/c unity500/bb5 Dec 5 95 (CDCl3)

Pulse sequence s2pulrd
OBSERVE C13
 Frequency 125.639 MHz
 Spectral width 35938.9 Hz
 Acquisition time 1.824 sec
 Relaxation delay 0.100 sec
 Pulse width 45.0 degrees
 Ambient temperature
 No. repetitions 640
DECOUPLE H1
 High power 45
 Decoupler continuously on
 WALTZ-16 modulated
Double precision acquisition
DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
Total acquisition time 21 minutes
End acquisition time 08:30

INDEX	FREQ. (Hz)	PPM	HEIGHT
1	18249.4	145.253	33.3
2	16501.7	131.342	106.8
3	16400.8	130.539	133.0
4	13976.3	111.242	155.8
5	9706.0	77.253	19.8
6	9674.2	77.000	20.4
7	9641.8	76.742	19.9
8	5344.1	42.535	3.7
9	4880.2	38.843	93.0
10	4835.7	38.489	86.0
11	3726.3	29.659	2.0
12	2976.7	23.692	3.0
13	2182.6	17.372	3.4
14	117.9	0.938	4.3

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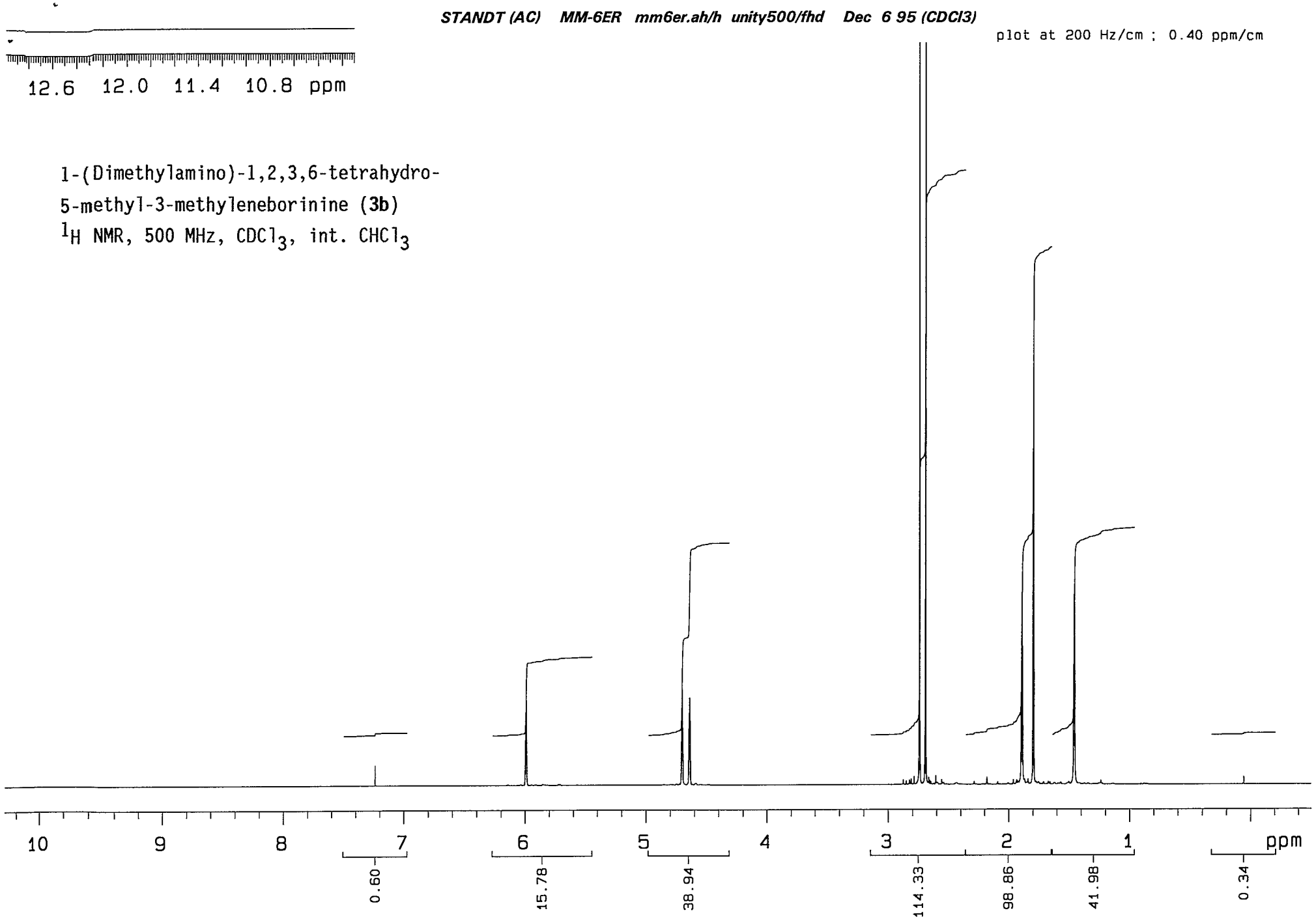
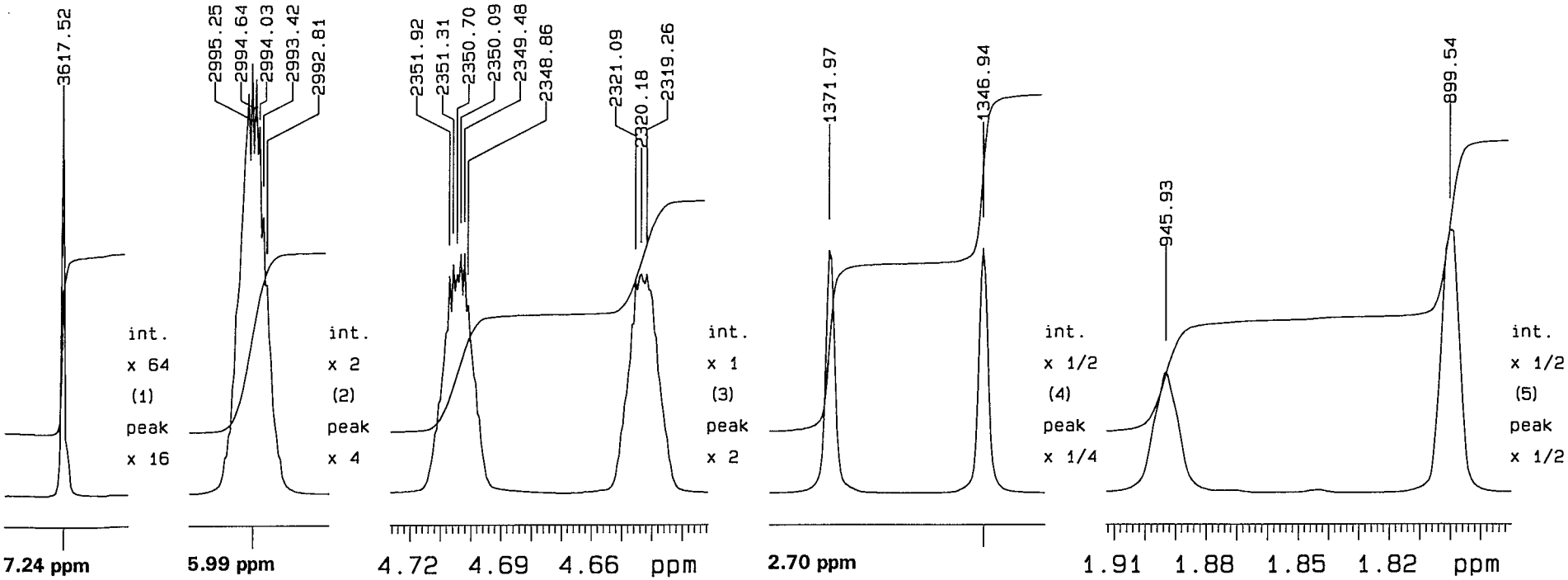
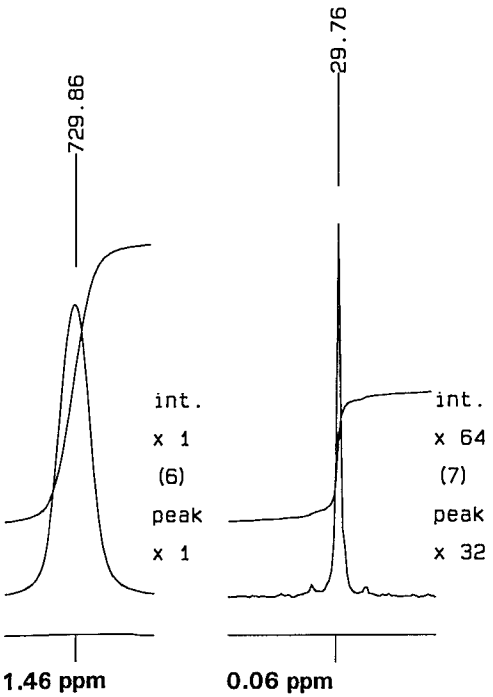


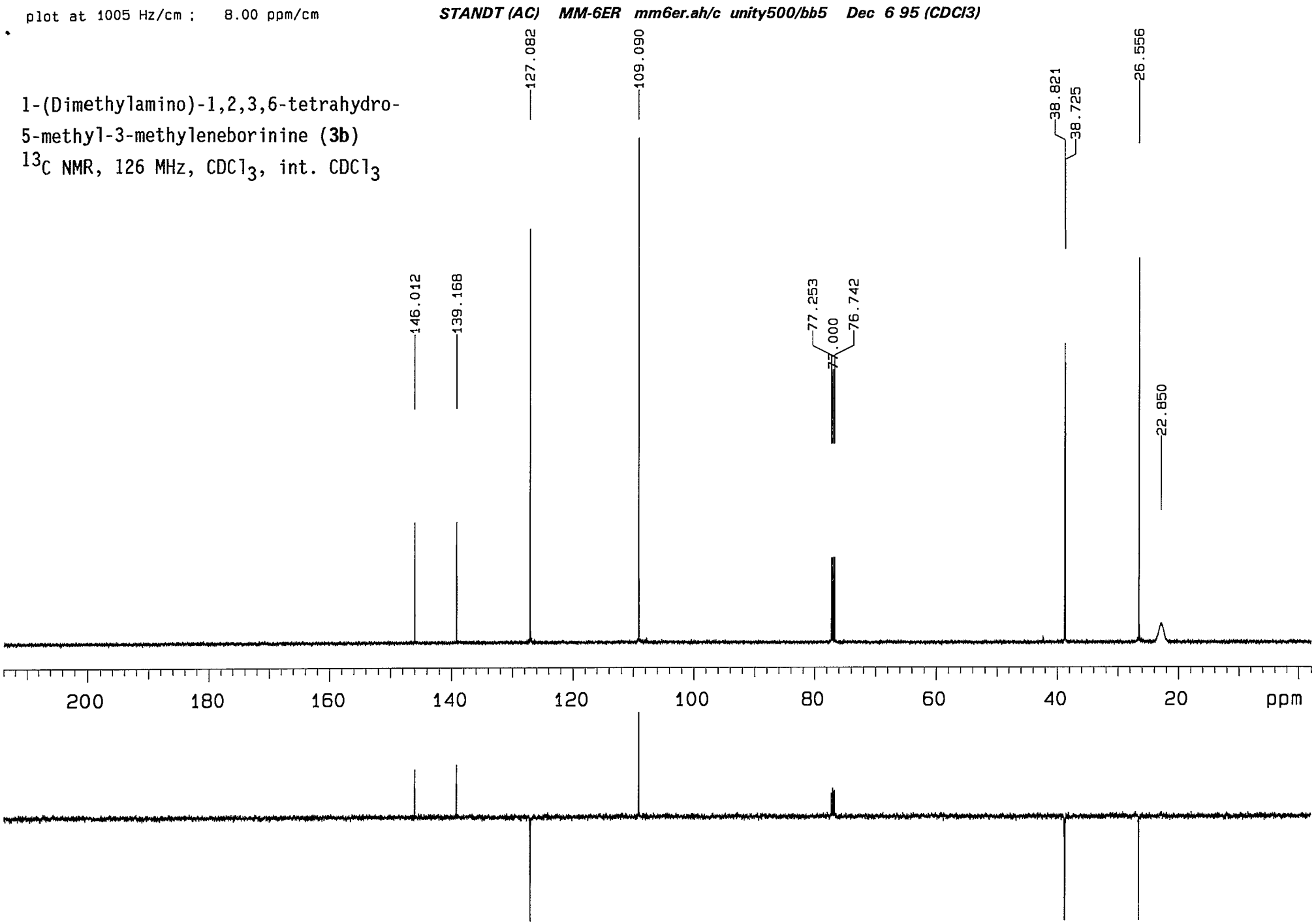
L2718-25

Expansions at 10 Hz/cm 0.020 ppm/cm (p.1) ***STANDT (AC) MM-6ER mm6er.ah/h unity500/fhd Dec 6 95 (CDCl3)***



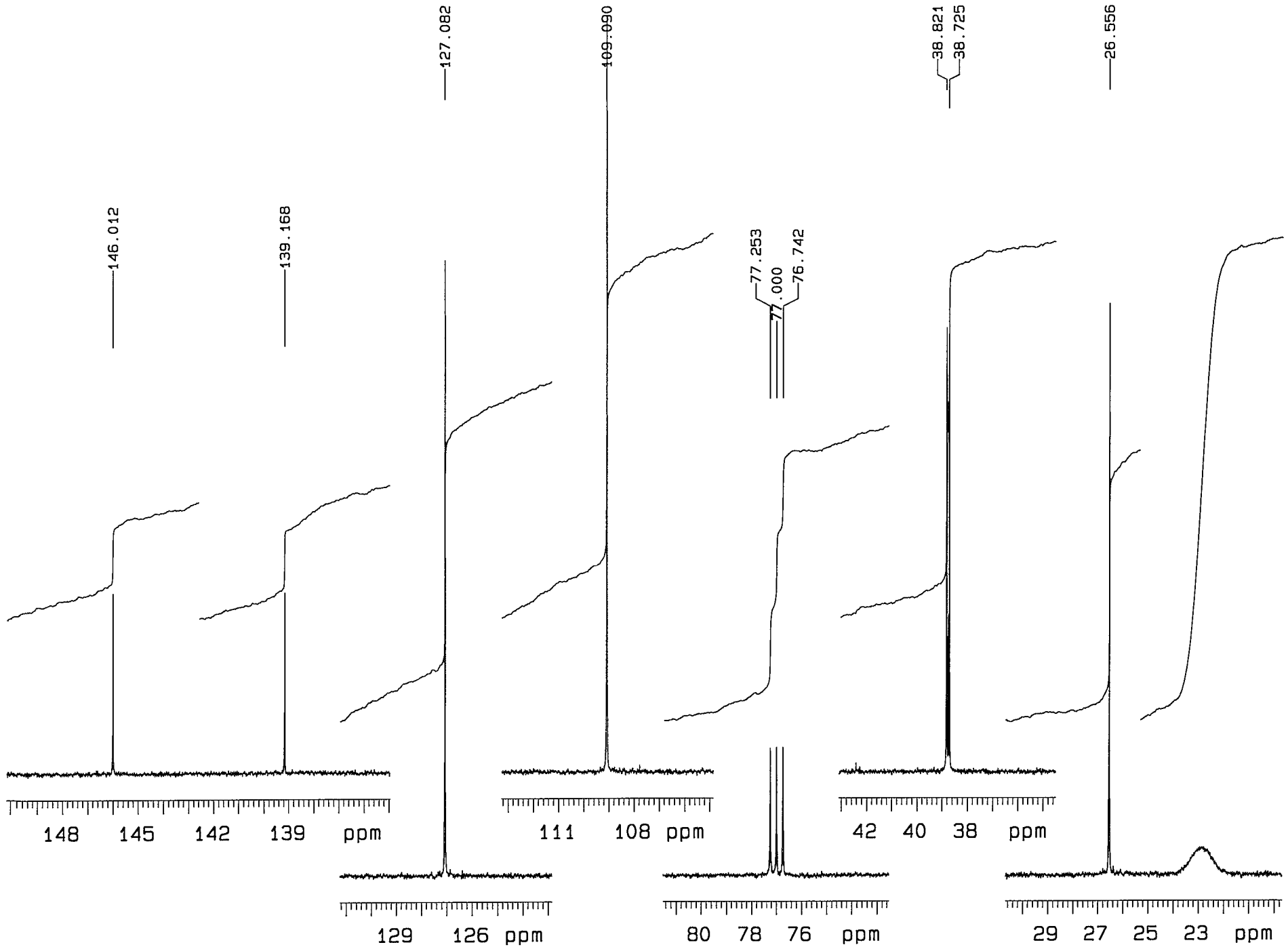


L3713-36


plot at 1005 Hz/cm ; 8.00 ppm/cm
STANDT (AC) MM-6ER mm6er.ah/c unity500/bb5 Dec 6 95 (CDCl3)
1-(Dimethylamino)-1,2,3,6-tetrahydro-
5-methyl-3-methyleneborinine (3b)
13C NMR, 126 MHz, CDCl3, int. CDCl3
146.012
139.168
127.082
109.090
77.253
77.000
76.742
38.821
38.725
26.556
22.850
200
180
160
140
120
100
80
60
40
20
ppm

L8714-31

EXPANSIONS at 251.3 Hz/cm 2.00 ppm/cm (p.1) ***STANDT (AC) MM-6ER mm6er.ah/c unity500/bb5 Dec 6 95 (CDCl3)***



LATB-28

THRESHOLD : 2.0

STANDT (AC) MM-6ER mm6er.ah/c unity500/bb5 Dec 6 95 (CDCl3)

Pulse sequence s2pulrd
OBSERVE C13
 Frequency 125.639 MHz
 Spectral width 35938.9 Hz
 Acquisition time 1.824 sec
 Relaxation delay 0.100 sec
 Pulse width 45.0 degrees
 Ambient temperature
 No. repetitions 544
DECOUPLE H1
 High power 45
 Decoupler continuously on
 WALTZ-16 modulated
Double precision acquisition
DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
Total acquisition time 18 minutes
End acquisition time 08:41

INDEX	FREQ. (Hz)	PPM	HEIGHT
1	18344.8	146.012	34.9
2	17485.0	139.168	35.0
3	15966.5	127.082	119.7
4	13706.0	109.090	145.6
5	9706.0	77.253	24.7
6	9674.2	77.000	24.8
7	9641.8	76.742	24.8
8	4877.4	38.821	86.5
9	4865.3	38.725	80.9
10	3336.4	26.556	111.2
11	2870.8	22.850	5.5

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L2713-29

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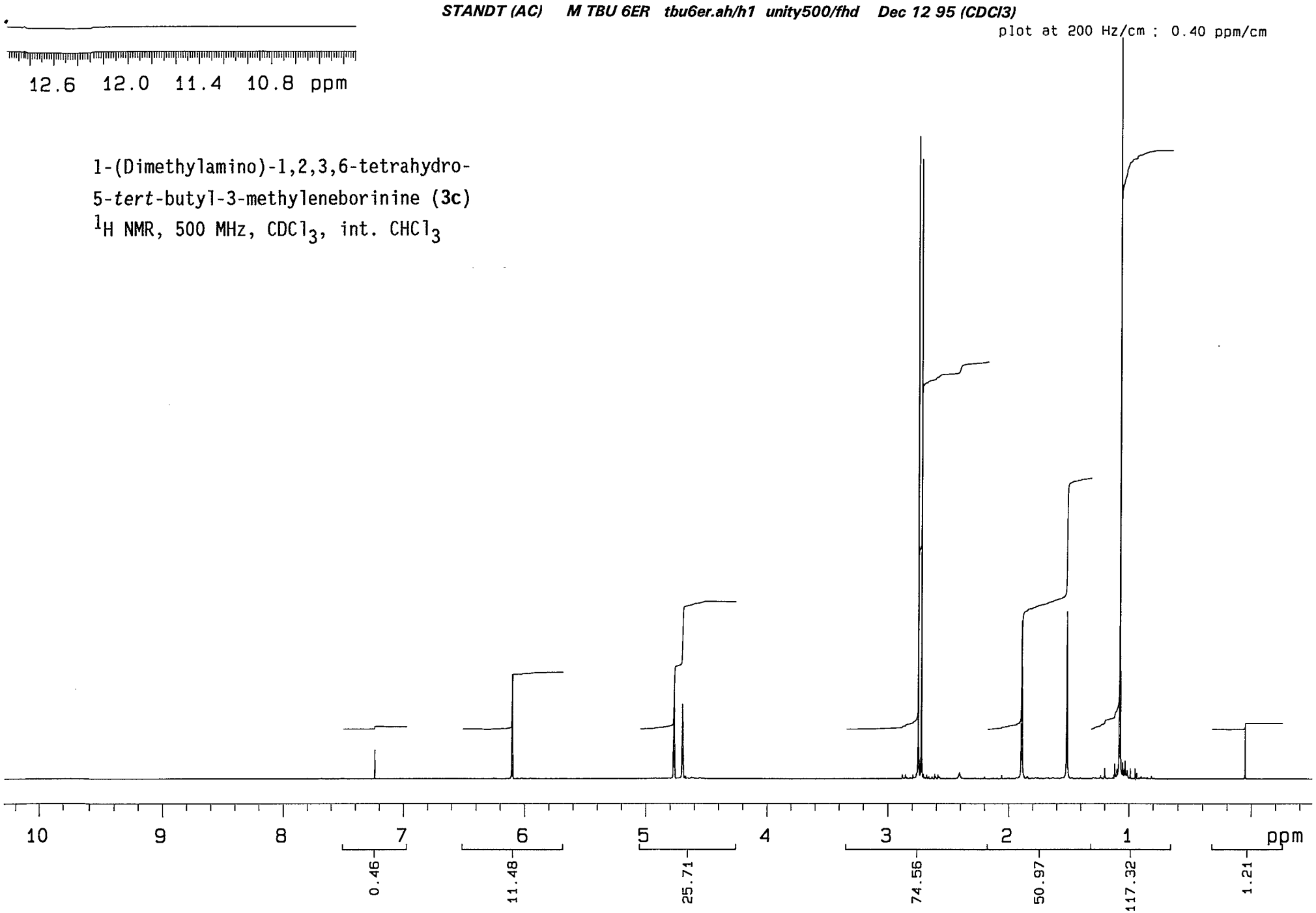
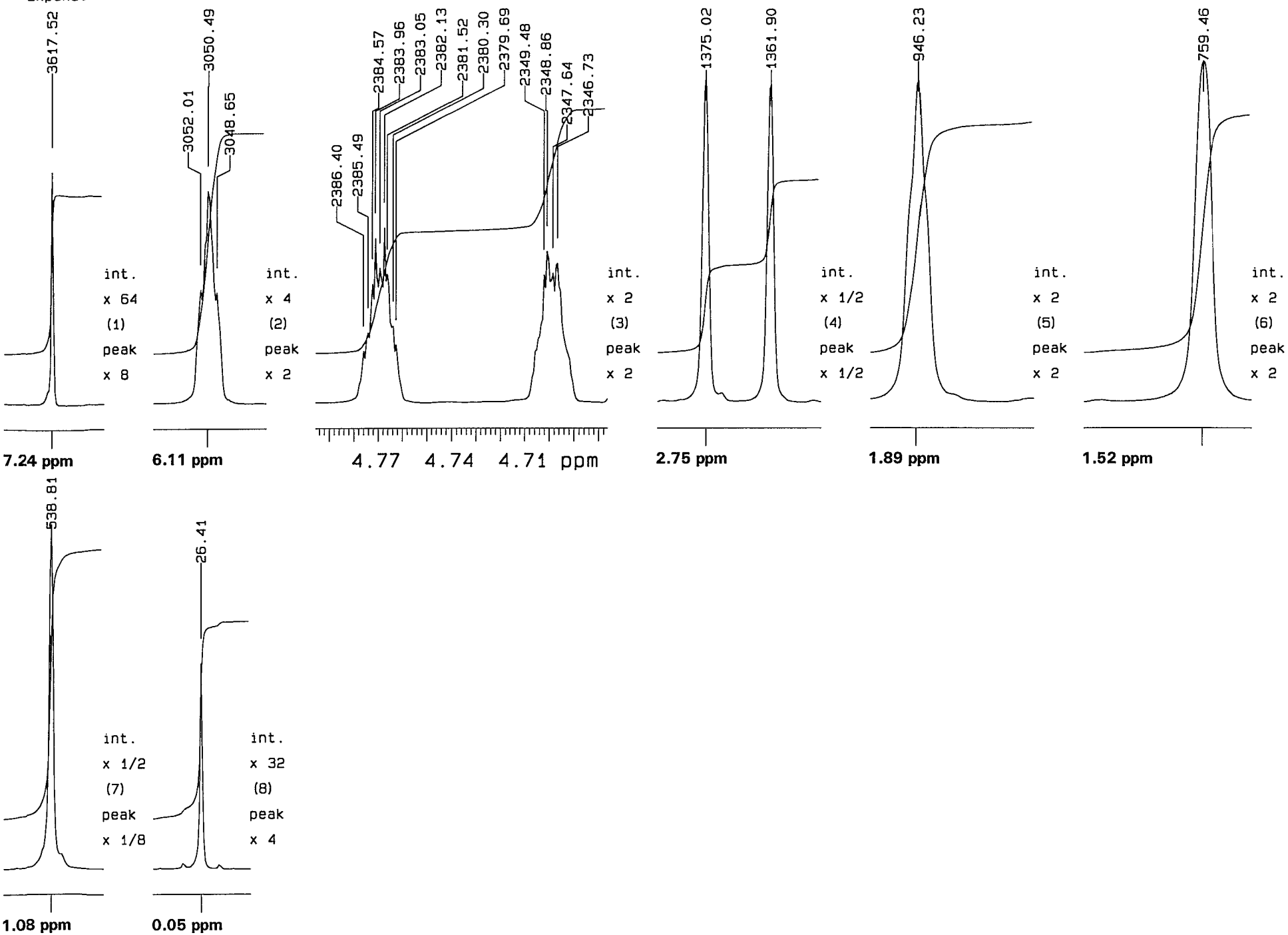
L2712-30



Expansions at 10 Hz/cm 0.020 ppm/cm (p.1) ***STANDT (AC) M TBU 6ER tbu6er.ah/h1 unity500/fhd Dec 12 95 (CDCl3)***



KdIIId-31

THRESHOLD : 2.0

STANDT (AC) M TBU 6ER tbu6er.ah/h1 unity500/fhd Dec 12 95 (CDCl3)

Pulse sequence s2pulrd
OBSERVE H1
Frequency 499.657 MHz
Spectral width 10000.0 Hz
Acquisition time 3.277 sec
Relaxation delay 0.100 sec
Pulse width 30.0 degrees
Ambient temperature
No. repetitions 32
Double precision acquisition
DATA PROCESSING
FT size 65536
Total acquisition time 2 minutes
End acquisition time 12:04

INDEX	FREQ. (Hz)	PPM	HEIGHT
1	3617.5	7.240	5.8
2	3052.0	6.108	11.3
3	3050.5	6.105	21.0
4	3048.7	6.101	11.0
5	2386.4	4.776	5.2
6	2385.5	4.774	7.0
7	2384.6	4.772	11.8
8	2384.0	4.771	16.3
9	2383.0	4.769	13.4
10	2382.1	4.768	17.4
11	2381.5	4.766	12.8
12	2380.3	4.764	7.6
13	2379.7	4.763	5.8
14	2349.5	4.702	12.7
15	2348.9	4.701	15.0
16	2347.6	4.699	12.9
17	2346.7	4.697	13.9
18	1375.0	2.752	130.0
19	1372.0	2.746	3.9
20	1361.9	2.726	125.5
21	946.2	1.894	31.8
22	759.5	1.520	33.7
23	600.8	1.202	2.1
24	560.5	1.122	3.0
25	545.8	1.092	2.3
26	538.8	1.078	546.1
27	527.5	1.056	3.3
28	517.1	1.035	3.7
29	495.8	0.992	2.0
30	475.3	0.951	2.0
31	26.4	0.053	10.1

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L2712-32

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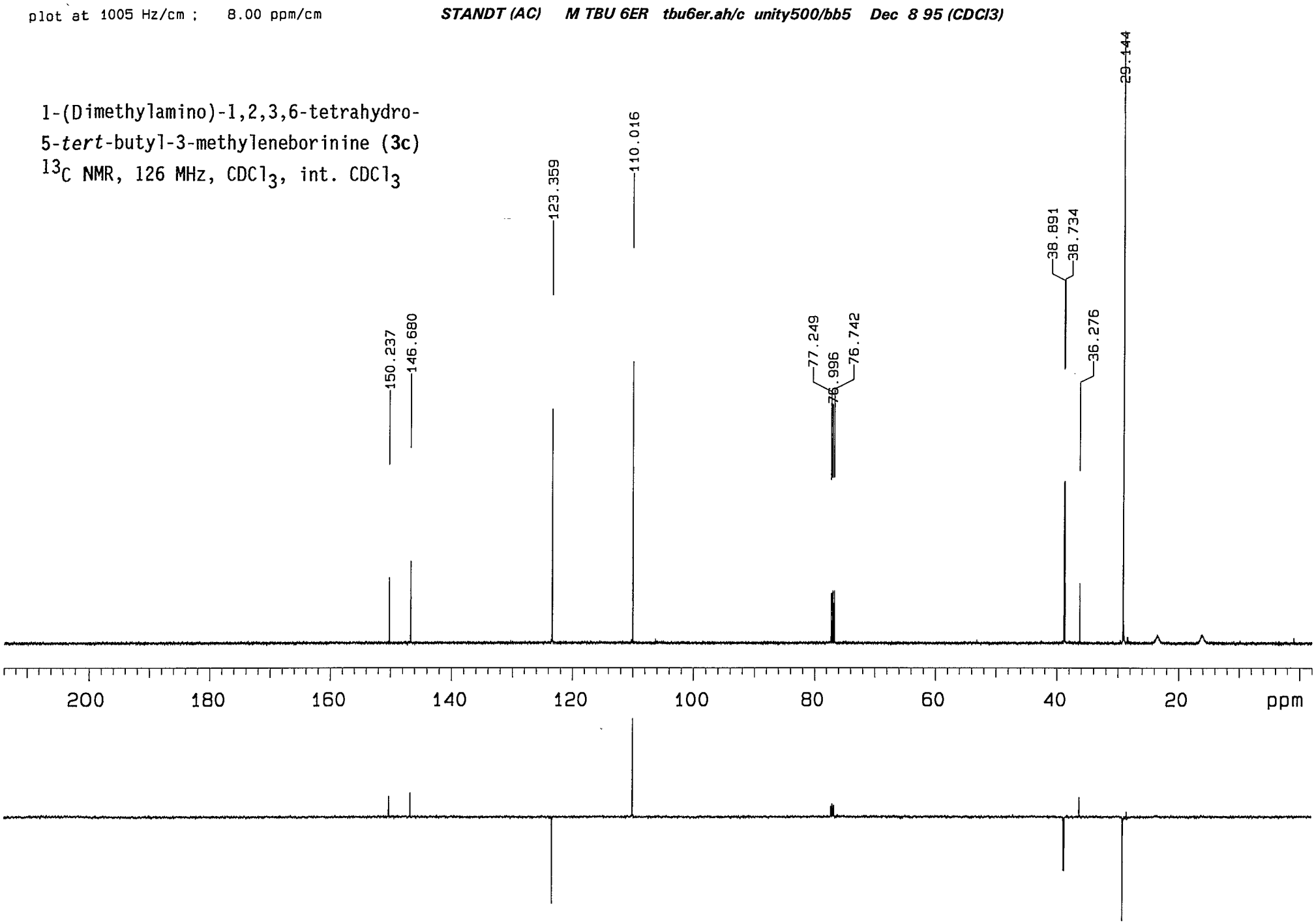

Lid'Ha-33

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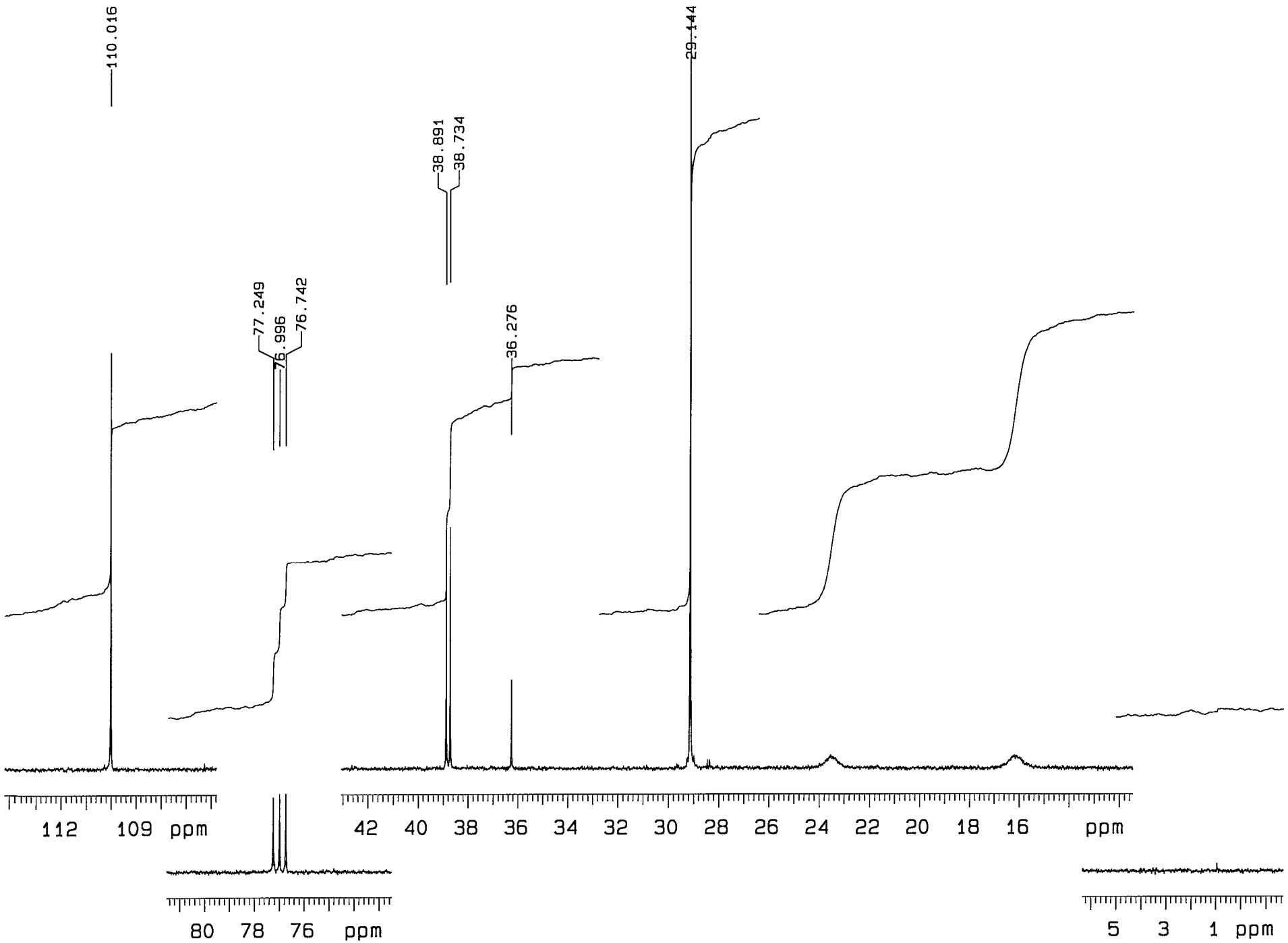
EXPANSIONS at 251.3 Hz/cm 2.00 ppm/cm (p.1) ***STANDT (AC) M TBU 6ER tbu6er.ah/c unity500/bb5 Dec 8 95 (CDCl3)***



LX 116-37

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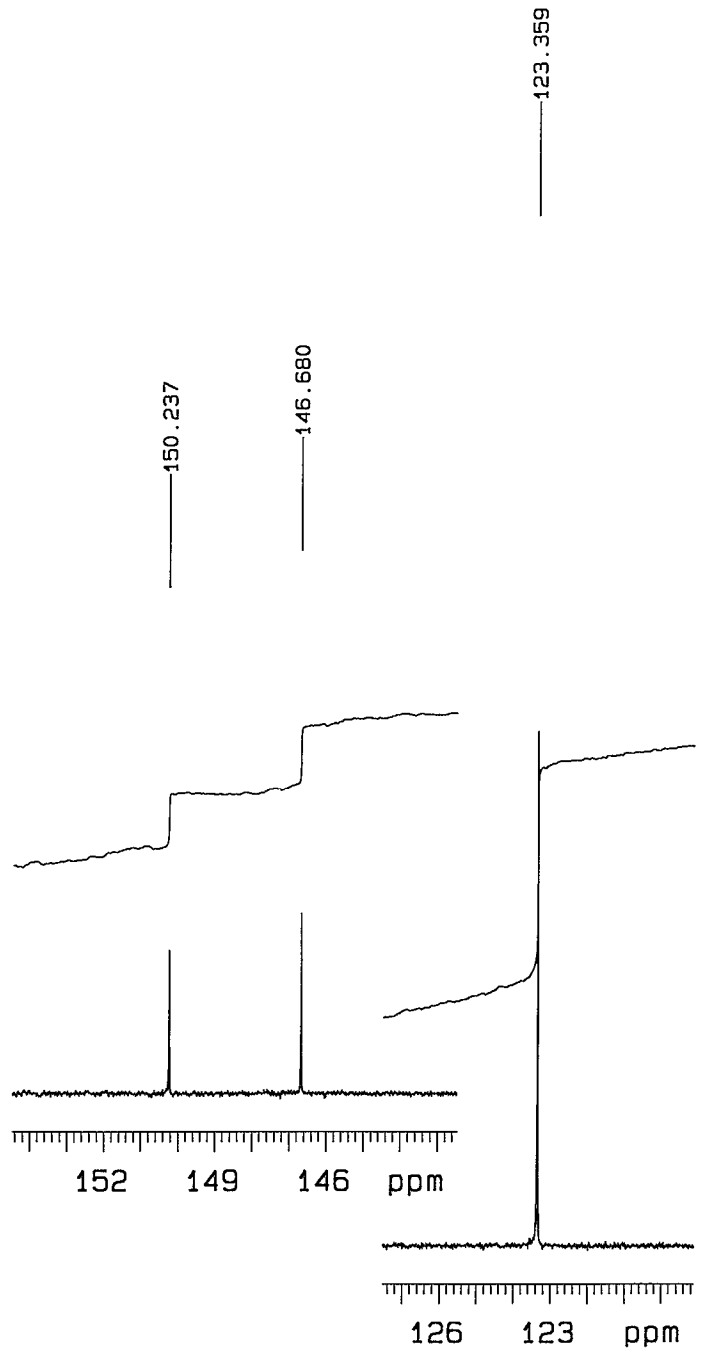
EXPANSIONS at 251.3 Hz/cm 2.00 ppm/cm (p.2) ***STANDT (AC) M TBU 6ER tbu6er.ah/c unity500/bb5 Dec 8 95 (CDCl3)***



C-1/19-C

THRESHOLD : 2.0

STANDT (AC) M TBU 6ER tbu6er.ah/c unity500/bb5 Dec 8 95 (CDCl3)

Pulse sequence s2pulrd
OBSERVE C13
 Frequency 125.639 MHz
 Spectral width 35938.9 Hz
 Acquisition time 1.824 sec
 Relaxation delay 0.100 sec
 Pulse width 45.0 degrees
 Ambient temperature
 No. repetitions 352
DECOUPLE H1
 High power 45
 Decoupler continuously on
 WALTZ-16 modulated
Double precision acquisition
DATA PROCESSING
 Line broadening 1.0 Hz
 FT size 131072
Total acquisition time 11 minutes
End acquisition time 08:41

INDEX	FREQ. (Hz)	PPM	HEIGHT
1	18875.7	150.237	18.9
2	18428.7	146.680	23.7
3	15498.7	123.359	67.8
4	13822.2	110.016	81.5
5	9705.5	77.249	14.4
6	9673.6	76.996	15.1
7	9641.8	76.742	15.2
8	4886.2	38.891	46.7
9	4866.4	38.734	47.1
10	4557.7	36.276	17.3
11	3661.6	29.144	285.7
12	3643.0	28.996	2.4
13	2958.6	23.548	2.6
14	2035.6	16.202	2.5

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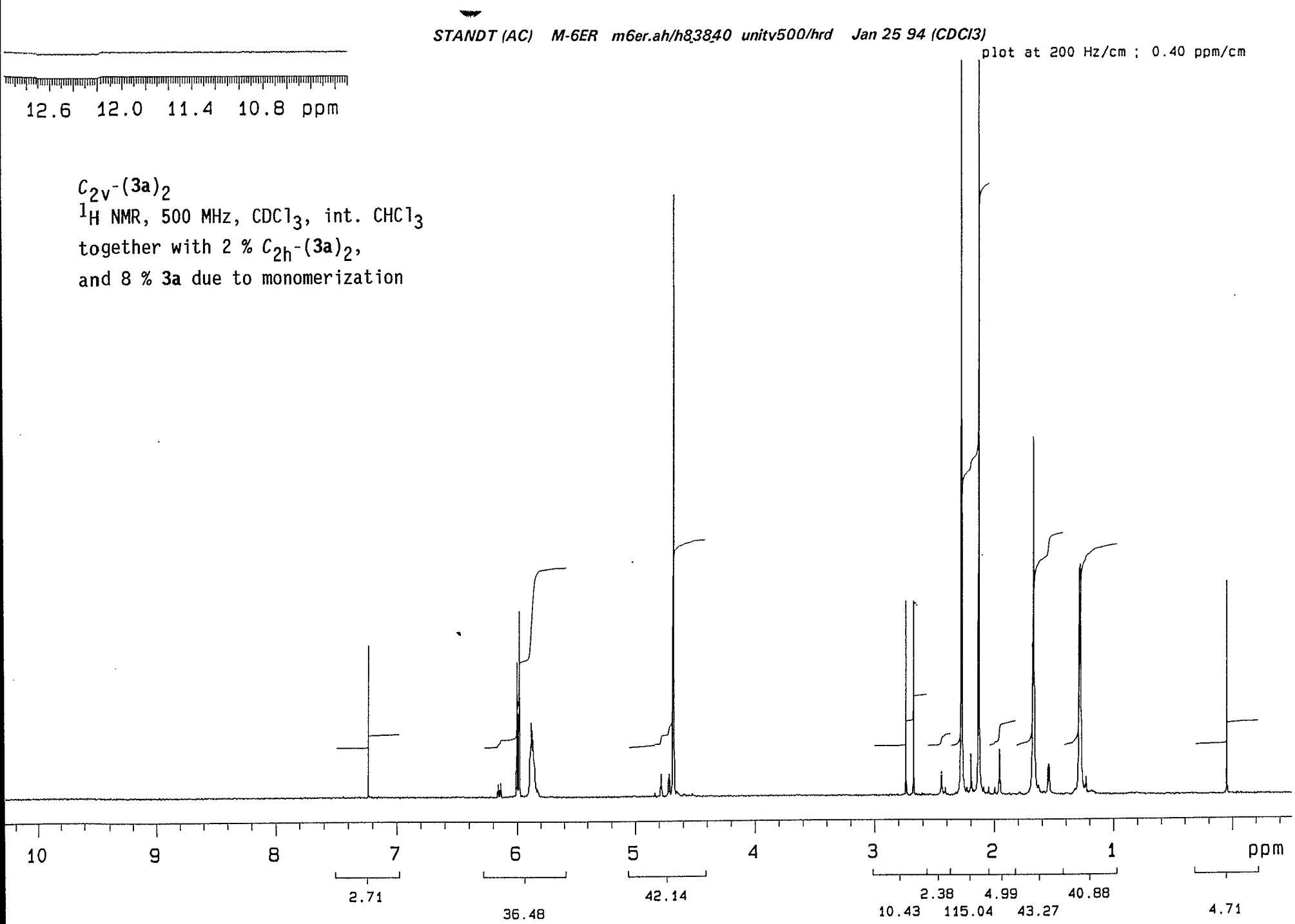
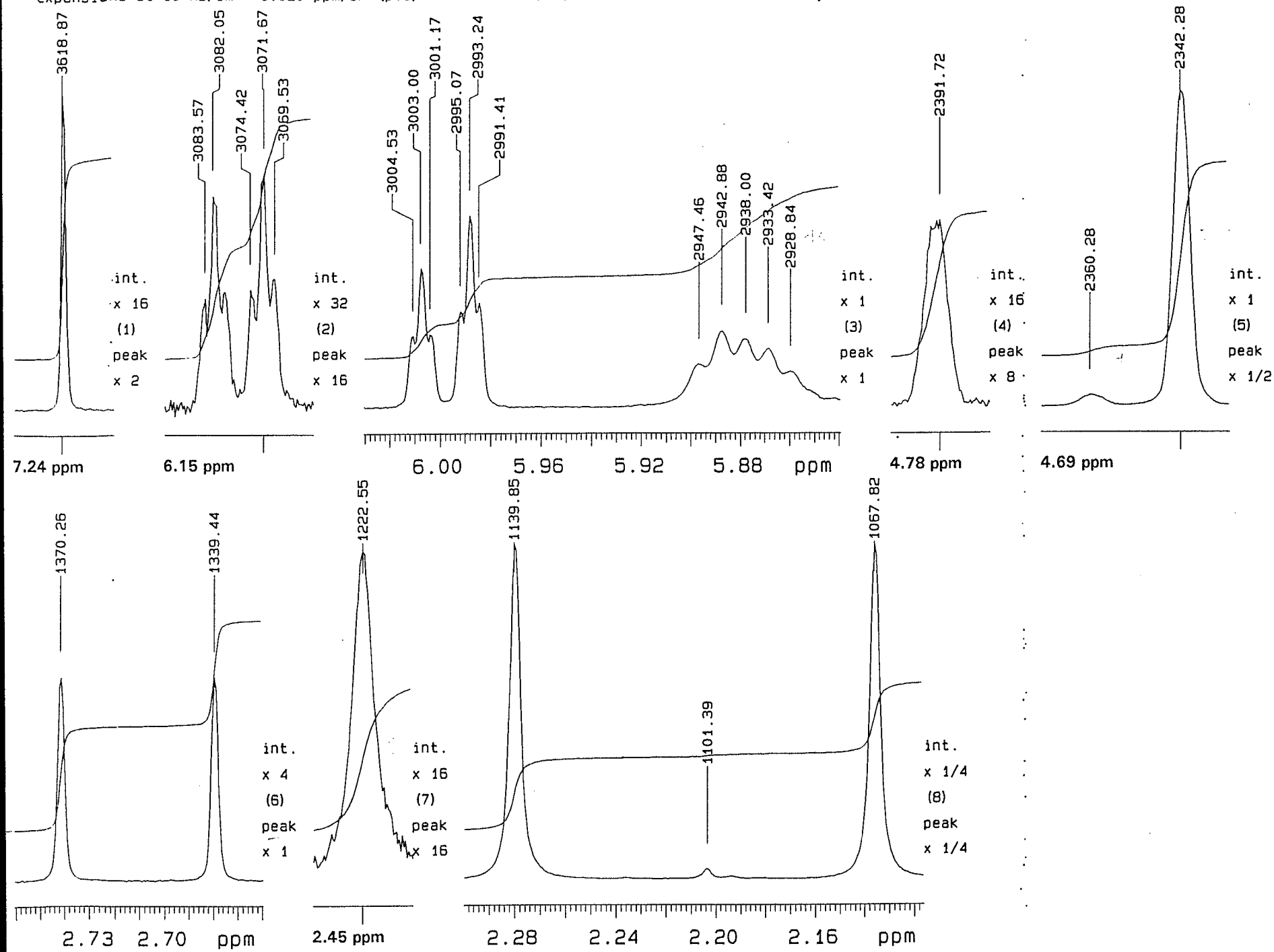
L2712-36


STANDT (AC) M-6ER m6er.ah/h838840 unitv500/hrd Jan 25 94 (CDCl3)
plot at 200 Hz/cm ; 0.40 ppm/cm
12.6 12.0 11.4 10.8 ppm
C_{2v}-(3a)$_2$
^{1}H NMR, 500 MHz, $CDCl_3$, int. $CHCl_3$
together with 2 % C_{2h}-(3a)$_2$,
and 8 % 3a due to monomerization
10 9 8 7 6 5 4 3 2 1 ppm
2.71
36.48
42.14
10.43
2.38
115.04
4.99
43.27
40.88
4.71

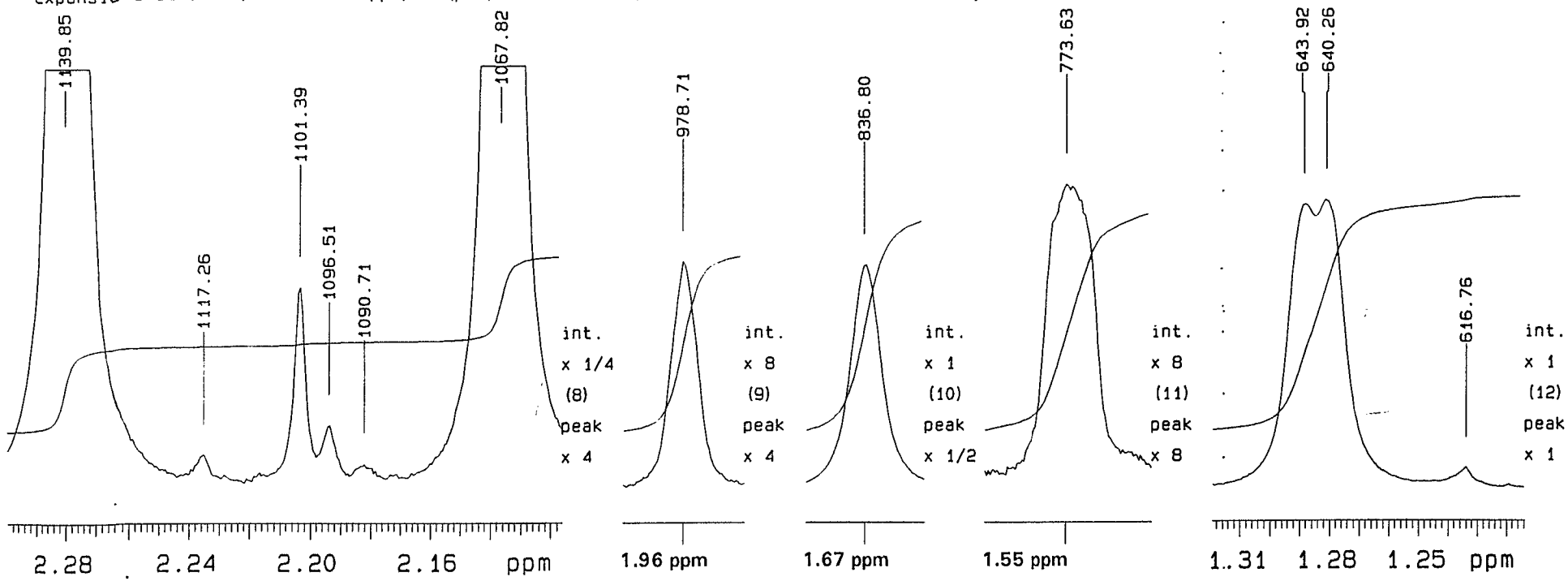
L278-31

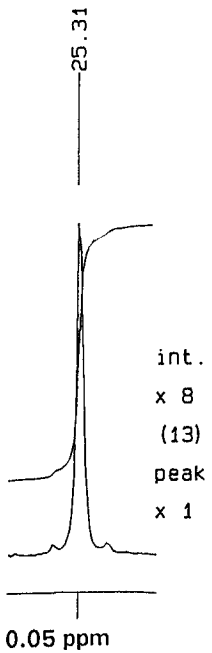
Expansions at 10 Hz/cm 0.020 ppm/cm (p.1) *STANDT (AC) M-6ER m6er.ah/h83840 unity500/hrd Jan 25 94 (CDCl3)*



L3713-38

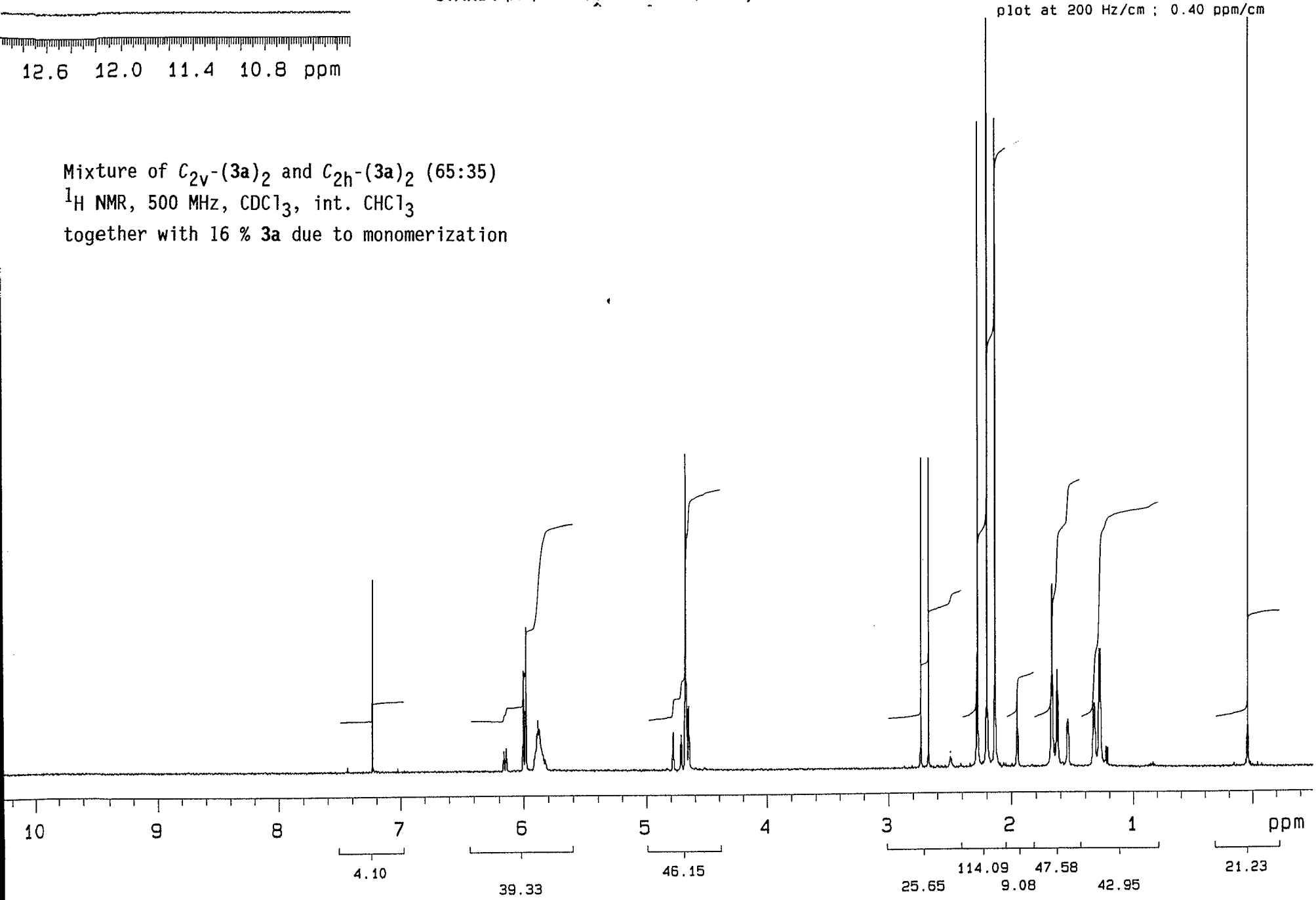
Expansions at 10 Hz/cm 0.020 ppm/cm (p.2) *STANDT (AC) M-6ER m6er.ah/h83840 unity500/hrd Jan 25 94 (CDCl3)*





L3716-39

STANDT (AC) RS C5.4 rsc54.ah/h unity500/hrd Feb 16 94 (CDCl3)

plot at 200 Hz/cm ; 0.40 ppm/cm

Mixture of C_{2v}-(**3a**)$_2$ and C_{2h}-(**3a**)$_2$ (65:35)
^{1}H NMR, 500 MHz, $CDCl_3$, int. $CHCl_3$
together with 16 % **3a** due to monomerization