

# ORGANOMETALLICS

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Supplementary Material for [PPN][AlCl(CMe<sub>2</sub>Et)<sub>3</sub>] (3)

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(A <sup>2</sup> )
----	-	-	-	-----
C1	1.2102(2)	0.08554(8)	0.26437(7)	6.11(3)
P1	0.8219(1)	0.42485(7)	0.33659(5)	3.22(2)
P2	0.7339(1)	0.37924(7)	0.17696(5)	2.96(2)
Al	1.1000(1)	-0.07423(8)	0.24738(6)	3.67(2)
N	0.7269(3)	0.3967(2)	0.2587(2)	3.80(7)
C11	1.2099(6)	-0.1132(4)	0.3312(3)	6.9(1)
C12	1.183(1)	-0.2294(5)	0.3154(4)	13.3(2)
C13	1.3821(7)	-0.0811(5)	0.3406(3)	10.0(2)
C14	1.159(1)	-0.0608(7)	0.4031(3)	14.9(3)
C15a	1.473(2)	-0.091(1)	0.3995(9)	15.9(7)
C15b	1.194(2)	0.033(1)	0.4397(7)	12.3(5)
C21	1.1414(5)	-0.1547(3)	0.1496(2)	4.6(1)
C22	1.0981(6)	-0.1045(4)	0.0916(3)	7.1(1)
C23	1.3110(5)	-0.1540(4)	0.1537(3)	7.0(1)
C24	1.0575(6)	-0.2642(4)	0.1261(3)	6.7(1)
C25	1.0912(7)	-0.3394(4)	0.0584(3)	8.2(2)
C31	0.8774(5)	-0.0711(4)	0.2508(3)	6.6(1)
C32	0.8085(6)	-0.1736(5)	0.2581(3)	9.7(2)
C33	0.8516(7)	0.0157(6)	0.3147(4)	12.6(2)

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

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Atom	x	y	z	B(A2)
----	-	-	-	-----
C34	0.7873(6)	-0.0644(5)	0.1837(4)	9.2(2)
C35	0.8222(8)	0.0363(5)	0.1672(5)	12.5(3)
C111	1.0225(4)	0.4390(3)	0.3406(2)	3.34(8)
C112	1.0847(4)	0.3535(3)	0.3097(2)	3.99(9)
C113	1.2370(4)	0.3628(3)	0.3084(2)	5.0(1)
C114	1.3258(4)	0.4551(3)	0.3378(2)	5.4(1)
C115	1.2651(5)	0.5399(3)	0.3699(3)	5.8(1)
C116	1.1124(4)	0.5324(3)	0.3710(2)	4.6(1)
C117	0.7738(4)	0.5409(3)	0.3919(2)	3.64(8)
C118	0.7719(5)	0.6235(3)	0.3669(2)	5.2(1)
C119	0.7290(6)	0.7116(3)	0.4071(3)	6.9(1)
C120	0.6867(6)	0.7164(4)	0.4719(3)	7.2(1)
C121	0.6890(6)	0.6357(4)	0.4970(2)	6.7(1)
C122	0.7327(5)	0.5477(3)	0.4578(2)	5.0(1)
C123	0.7716(4)	0.3290(3)	0.3771(2)	3.44(8)
C124	0.8733(5)	0.3068(3)	0.4267(2)	4.5(1)
C125	0.8261(5)	0.2361(3)	0.4587(2)	5.2(1)
C126	0.6798(5)	0.1882(3)	0.4415(2)	5.5(1)
C127	0.5793(5)	0.2102(3)	0.3930(2)	4.9(1)

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

Atom	x	y	z	B(A <sup>2</sup> )
----	-	-	-	-----
C128	0.6236(4)	0.2801(3)	0.3611(2)	4.11(9)
C211	0.6052(4)	0.2668(2)	0.1246(2)	3.05(7)
C212	0.5348(5)	0.2050(3)	0.1577(2)	4.5(1)
C213	0.4318(5)	0.1209(3)	0.1177(2)	5.5(1)
C214	0.3982(5)	0.0978(3)	0.0455(2)	5.3(1)
C215	0.4684(5)	0.1575(4)	0.0117(2)	5.9(1)
C216	0.5711(5)	0.2421(3)	0.0513(2)	4.9(1)
C217	0.9151(4)	0.3661(3)	0.1522(2)	3.52(8)
C218	1.0206(4)	0.4509(3)	0.1647(2)	4.8(1)
C219	1.1621(5)	0.4397(4)	0.1489(3)	7.0(1)
C220	1.1975(5)	0.3450(4)	0.1219(3)	7.5(1)
C221	1.0955(5)	0.2606(4)	0.1103(3)	6.7(1)
C222	0.9523(4)	0.2698(3)	0.1250(2)	4.8(1)
C223	0.6719(4)	0.4819(2)	0.1484(2)	3.25(8)
C224	0.7120(5)	0.5027(3)	0.0888(2)	4.40(9)
C225	0.6553(5)	0.5795(3)	0.0667(2)	5.4(1)
C226	0.5608(5)	0.6344(3)	0.1044(3)	6.2(1)
C227	0.5193(5)	0.6136(3)	0.1630(3)	5.9(1)
C228	0.5735(4)	0.5372(3)	0.1854(2)	4.42(9)

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 Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:  
 $(4/3) * [a^2*B(1,1) + b^2*B(2,2) + c^2*B(3,3) + ab(\cos \gamma)*B(1,2) + ac(\cos \beta)*B(1,3) + bc(\cos \alpha)*B(2,3)]$

## Table of Bond Distances in Angstroms

Atom 1 =====	Atom 2 =====	Distance =====	Atom 1 =====	Atom 2 =====	Distance =====
C1	Al	2.251(2)	C31	C33	1.538(8)
P1	N	1.581(3)	C31	C34	1.499(9)
P1	C111	1.807(4)	C34	C35	1.54(1)
P1	C117	1.803(4)	C111	C112	1.388(5)
P1	C123	1.797(4)	C111	C116	1.381(5)
P2	N	1.574(3)	C112	C113	1.385(6)
P2	C211	1.799(3)	C113	C114	1.365(5)
P2	C217	1.797(4)	C114	C115	1.379(6)
P2	C223	1.802(4)	C115	C116	1.388(6)
Al	C11	2.062(5)	C117	C118	1.381(6)
Al	C21	2.040(4)	C117	C122	1.383(6)
Al	C31	2.044(5)	C118	C119	1.382(6)
C11	C12	1.543(8)	C119	C120	1.371(8)
C11	C13	1.556(8)	C120	C121	1.357(8)
C11	C14	1.554(9)	C121	C122	1.377(6)
C13	C15a	1.39(2)	C123	C124	1.384(6)
C14	C15b	1.28(1)	C123	C128	1.395(5)
C21	C22	1.540(7)	C124	C125	1.380(7)
C21	C23	1.536(6)	C125	C126	1.376(6)
C21	C24	1.539(6)	C126	C127	1.362(6)
C24	C25	1.531(7)	C127	C128	1.362(6)
C31	C32	1.552(9)	C211	C212	1.379(6)

## Bond Distances (cont.)

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
=====	=====	=====	=====	=====	=====
C211	C216	1.373(5)	C220	C221	1.360(7)
C212	C213	1.380(5)	C221	C222	1.386(6)
C213	C214	1.353(6)	C223	C224	1.379(6)
C214	C215	1.369(7)	C223	C228	1.389(5)
C215	C216	1.381(5)	C224	C225	1.392(6)
C217	C218	1.380(5)	C225	C226	1.366(7)
C217	C222	1.390(5)	C226	C227	1.364(8)
C218	C219	1.382(6)	C227	C228	1.381(7)
C219	C220	1.363(8)			

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

## Table of Bond Angles in Degrees

Atom 1 =====	Atom 2 =====	Atom 3 =====	Angle =====	Atom 1 =====	Atom 2 =====	Atom 3 =====	Angle =====
N	P1	C111	115.0(2)	C12	C11	C13	106.4(5)
N	P1	C117	108.8(2)	C12	C11	C14	109.7(6)
N	P1	C123	110.0(2)	C13	C11	C14	108.2(4)
C111	P1	C117	109.2(2)	C11	C13	C15a	119(1)
C111	P1	C123	107.4(2)	C11	C14	C15b	126.(1)
C117	P1	C123	106.2(2)	Al	C21	C22	112.2(3)
N	P2	C211	108.6(2)	Al	C21	C23	109.1(3)
N	P2	C217	115.6(2)	Al	C21	C24	110.5(3)
N	P2	C223	111.1(2)	C22	C21	C23	104.4(4)
C211	P2	C217	108.3(1)	C22	C21	C24	109.7(3)
C211	P2	C223	106.1(2)	C23	C21	C24	110.8(4)
C217	P2	C223	106.6(2)	C21	C24	C25	117.6(5)
Cl	Al	C11	104.0(1)	Al	C31	C32	108.1(4)
Cl	Al	C21	104.2(1)	Al	C31	C33	112.2(3)
Cl	Al	C31	107.7(2)	Al	C31	C34	114.5(4)
C11	Al	C21	113.4(2)	C32	C31	C33	108.6(5)
C11	Al	C31	112.9(2)	C32	C31	C34	104.6(4)
C21	Al	C31	113.6(2)	C33	C31	C34	108.5(5)
P1	N	P2	145.3(2)	C31	C34	C35	115.6(5)
Al	C11	C12	110.4(3)	P1	C111	C112	118.1(2)
Al	C11	C13	110.5(4)	P1	C111	C116	121.6(3)
Al	C11	C14	111.5(5)	C112	C111	C116	120.2(3)

## Bond Angles (cont.)

Atom 1 =====	Atom 2 =====	Atom 3 =====	Angle =====	Atom 1 =====	Atom 2 =====	Atom 3 =====	Angle =====
C111	C112	C113	119.6(3)	P2	C211	C216	121.0(3)
C112	C113	C114	120.3(4)	C212	C211	C216	118.5(3)
C113	C114	C115	120.3(4)	C211	C212	C213	120.4(4)
C114	C115	C116	120.2(4)	C212	C213	C214	120.5(4)
C111	C116	C115	119.3(4)	C213	C214	C215	119.8(4)
P1	C117	C118	119.4(3)	C214	C215	C216	120.1(4)
P1	C117	C122	121.4(3)	C211	C216	C215	120.7(4)
C118	C117	C122	119.1(4)	P2	C217	C218	120.3(3)
C117	C118	C119	120.3(4)	P2	C217	C222	119.7(3)
C118	C119	C120	119.6(5)	C218	C217	C222	119.9(3)
C119	C120	C121	120.4(5)	C217	C218	C219	119.8(4)
C120	C121	C122	120.6(5)	C218	C219	C220	120.0(4)
C117	C122	C121	119.9(4)	C219	C220	C221	121.0(4)
P1	C123	C124	121.8(3)	C220	C221	C222	120.2(5)
P1	C123	C128	118.8(3)	C217	C222	C221	119.2(4)
C124	C123	C128	119.3(4)	P2	C223	C224	122.0(3)
C123	C124	C125	119.1(4)	P2	C223	C228	118.5(3)
C124	C125	C126	120.5(4)	C224	C223	C228	119.4(4)
C125	C126	C127	120.6(4)	C223	C224	C225	120.0(4)
C126	C127	C128	119.9(4)	C224	C225	C226	119.8(4)
C123	C128	C127	120.7(4)	C225	C226	C227	120.6(5)
P2	C211	C212	120.5(2)	C226	C227	C228	120.3(4)
C223	C228	C227	119.8(4)				



Table of General Displacement Parameter Expressions - U's

<u>Name</u>	<u>U(1,1)</u>	<u>U(2,2)</u>	<u>U(3,3)</u>	<u>U(1,2)</u>	<u>U(1,3)</u>	<u>U(2,3)</u>
C1	0.0881(8)	0.0468(5)	0.0887(7)	-0.0057(5)	0.0006(7)	0.0201(5)
P1	0.0398(4)	0.0478(5)	0.0352(4)	0.0075(4)	0.0060(4)	0.0137(3)
P2	0.0345(4)	0.0435(4)	0.0373(4)	0.0106(3)	0.0071(3)	0.0148(3)
A1	0.0492(6)	0.0423(5)	0.0459(5)	0.0040(5)	0.0104(5)	0.0104(4)
N	0.036(1)	0.059(2)	0.050(2)	0.009(1)	0.009(1)	0.017(1)
C11	0.100(4)	0.083(3)	0.077(3)	-0.010(3)	-0.009(3)	0.043(2)
C12	0.201(7)	0.128(3)	0.187(4)	-0.020(4)	-0.051(5)	0.117(3)
C13	0.104(4)	0.140(4)	0.135(4)	0.007(3)	-0.041(3)	0.071(3)
C14	0.186(7)	0.330(9)	0.061(3)	0.035(7)	0.013(4)	0.082(4)
C15a	0.16(1)	0.27(2)	0.22(1)	0.04(1)	0.03(1)	0.15(1)
C15b	0.23(2)	0.099(8)	0.072(8)	-0.060(9)	0.001(9)	-0.030(7)
C21	0.064(2)	0.054(2)	0.057(2)	0.014(2)	0.023(2)	0.014(2)
C22	0.108(4)	0.097(3)	0.062(3)	0.007(3)	0.021(3)	0.022(2)
C23	0.075(3)	0.090(3)	0.108(3)	0.026(2)	0.047(2)	0.025(3)
C24	0.106(3)	0.060(3)	0.076(3)	0.001(3)	0.039(2)	-0.003(2)
C25	0.136(4)	0.076(3)	0.089(3)	0.015(3)	0.035(3)	0.004(3)
C31	0.057(2)	0.094(3)	0.082(3)	0.010(2)	0.022(2)	-0.006(3)
C32	0.087(3)	0.142(5)	0.124(4)	-0.031(3)	0.048(3)	0.020(4)
C33	0.097(4)	0.165(6)	0.160(5)	0.028(4)	0.056(3)	-0.051(5)

Table of General Anisotropic Displacement Parameter Expressions - U's (Conti

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C34	0.058(3)	0.118(4)	0.151(5)	0.027(3)	0.002(3)	0.014(4)
C35	0.139(5)	0.108(4)	0.213(7)	0.047(4)	-0.029(5)	0.043(4)
C111	0.038(2)	0.051(2)	0.038(2)	0.005(2)	0.002(1)	0.017(1)
C112	0.044(2)	0.050(2)	0.056(2)	0.008(2)	0.001(2)	0.016(2)
C113	0.050(2)	0.070(2)	0.078(2)	0.022(2)	0.010(2)	0.033(2)
C114	0.039(2)	0.083(2)	0.096(3)	0.012(2)	0.009(2)	0.046(2)
C115	0.049(2)	0.065(2)	0.101(3)	-0.009(2)	-0.006(2)	0.031(2)
C116	0.048(2)	0.056(2)	0.069(2)	0.004(2)	0.003(2)	0.019(2)
C117	0.044(2)	0.049(2)	0.042(2)	0.009(2)	0.004(2)	0.010(1)
C118	0.085(3)	0.056(2)	0.067(2)	0.020(2)	0.035(2)	0.021(2)
C119	0.124(4)	0.055(2)	0.097(3)	0.032(2)	0.050(3)	0.026(2)
C120	0.119(3)	0.075(3)	0.083(3)	0.037(3)	0.042(3)	0.009(3)
C121	0.110(3)	0.101(3)	0.048(2)	0.039(3)	0.032(2)	0.016(2)
C122	0.073(3)	0.074(2)	0.041(2)	0.021(2)	0.010(2)	0.014(2)
C123	0.048(2)	0.047(2)	0.036(2)	0.009(2)	0.009(1)	0.013(1)
C124	0.057(2)	0.064(2)	0.049(2)	0.007(2)	0.004(2)	0.022(2)
C125	0.084(3)	0.070(2)	0.050(2)	0.014(2)	0.005(2)	0.032(2)
C126	0.093(3)	0.061(2)	0.061(2)	0.002(2)	0.026(2)	0.028(2)
C127	0.061(2)	0.069(2)	0.057(2)	-0.001(2)	0.017(2)	0.021(2)

Table of General Anisotropic Displacement Parameter Expressions - U's (Conti

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C128	0.049(2)	0.064(2)	0.046(2)	0.008(2)	0.013(2)	0.019(2)
C211	0.034(2)	0.041(2)	0.043(2)	0.011(1)	0.011(1)	0.013(1)
C212	0.067(2)	0.052(2)	0.052(2)	0.003(2)	0.011(2)	0.018(2)
C213	0.076(3)	0.054(2)	0.080(3)	-0.008(2)	0.020(2)	0.026(2)
C214	0.057(2)	0.055(2)	0.076(3)	-0.005(2)	0.012(2)	0.002(2)
C215	0.082(3)	0.080(3)	0.047(2)	-0.013(3)	0.006(2)	0.005(2)
C216	0.068(2)	0.067(2)	0.047(2)	-0.009(2)	0.012(2)	0.015(2)
C217	0.037(2)	0.064(2)	0.041(2)	0.017(1)	0.010(1)	0.023(1)
C218	0.042(2)	0.075(2)	0.071(2)	0.008(2)	0.009(2)	0.033(2)
C219	0.041(2)	0.128(3)	0.113(3)	0.007(2)	0.017(2)	0.065(2)
C220	0.045(2)	0.165(4)	0.097(3)	0.038(2)	0.029(2)	0.057(3)
C221	0.062(2)	0.112(3)	0.081(3)	0.048(2)	0.018(2)	0.017(3)
C222	0.047(2)	0.074(2)	0.062(2)	0.023(2)	0.011(2)	0.017(2)
C223	0.040(2)	0.039(2)	0.043(2)	0.006(1)	-0.001(1)	0.014(1)
C224	0.064(2)	0.055(2)	0.049(2)	0.013(2)	0.001(2)	0.019(2)
C225	0.079(3)	0.067(2)	0.063(2)	0.007(2)	-0.004(2)	0.034(2)
C226	0.070(3)	0.057(2)	0.110(3)	0.012(2)	-0.012(2)	0.042(2)
C227	0.054(2)	0.058(2)	0.118(3)	0.023(2)	0.015(2)	0.028(2)
C228	0.048(2)	0.053(2)	0.071(2)	0.014(2)	0.014(2)	0.024(2)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2\{h^2a^2U(1,1) + k^2b^2U(2,2) + l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$  where a, b, and c are reciprocal lattice constants.

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(A <sup>2</sup> )
S1	0.4326(3)	0.0901(6)	0.7836(3)	7.9(2)
S2	0.4264(3)	0.3488(6)	0.6508(3)	7.9(2)
Al1	0.4407(3)	0.3313(7)	0.7792(3)	8.0(2)
Al2	0.4353(3)	0.1076(7)	0.6618(3)	7.8(2)
C11	0.371(1)	0.444(3)	0.811(1)	13.0(8)*
C12	0.415(2)	0.416(6)	0.918(3)	12.8(6)*
C13	0.274(2)	0.373(5)	0.748(3)	12.8*
C14	0.364(2)	0.600(5)	0.769(3)	12.8*
C12a	0.387(2)	0.371(5)	0.897(3)	12.8*
C13a	0.288(2)	0.450(5)	0.743(3)	12.8*
C14a	0.404(2)	0.557(6)	0.849(3)	12.8*
C15	0.424(2)	0.641(5)	0.815(2)	11(1)*
C21	0.362(1)	-0.016(3)	0.568(1)	11.3(7)*
C22	0.398(2)	-0.163(5)	0.582(2)	11.3(5)*
C23	0.275(2)	0.016(5)	0.562(2)	11.3*
C24	0.355(2)	0.056(5)	0.491(2)	11.3*
C22a	0.367(2)	-0.173(5)	0.614(2)	11.3*
C23a	0.278(2)	0.055(5)	0.530(2)	11.3*
C24a	0.398(2)	-0.031(5)	0.502(2)	11.3*
C25	0.403(2)	0.095(4)	0.479(2)	8(1)*

Starred atoms were refined isotropically.

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$$(4/3) * [a^2*B(1,1) + b^2*B(2,2) + c^2*B(3,3) + ab(\cos \gamma)*B(1,2) + ac(\cos \beta)*B(1,3) + bc(\cos \alpha)*B(2,3)]$$

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)
S1	0.101(3)	0.097(4)	0.107(3)	-0.007(3)	0.054(2)	0.001(3)
S2	0.099(3)	0.102(4)	0.091(3)	0.007(3)	0.039(2)	0.007(3)
Al1	0.104(3)	0.105(5)	0.101(3)	0.009(4)	0.055(2)	-0.001(4)
Al2	0.100(3)	0.093(5)	0.096(3)	-0.005(4)	0.042(2)	-0.008(4)

The form of the anisotropic displacement parameter is:  
 $\exp[-2\pi^2\{h^2a^2U(1,1) + k^2b^2U(2,2) + l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$  where a, b, and c are reciprocal lattice constants.

Table of Bond Distances in Angstroms

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<u>Atom 1</u>	<u>Atom 2</u>	<u>Distance</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Distance</u>
S1	A11	2.316(9)	C11	C13a	1.53(4)
S1	A12	2.319(9)	C11	C14a	1.29(5)
S1	A12'	2.317(5)	C14	C15	1.16(5)
S2	A11	2.295(8)	C14a	C15	1.20(7)
S2	A12	2.315(8)	C21	C22	1.54(5)
S2	A11'	2.318(4)	C21	C23	1.70(5)
A11	C11	2.05(3)	C21	C24	1.54(5)
A12	C21	2.04(2)	C21	C22a	1.71(5)
C11	C12	1.79(5)	C21	C23a	1.62(5)
C11	C13	1.83(4)	C21	C24a	1.69(6)
C11	C14	1.66(6)	C24	C25	1.14(7)
C11	C12a	1.64(6)	C24a	C25	1.30(6)

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

Table of Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
Al1	S1	Al2	81.8(3)	Al1	C11	C14a	111.(3)
Al1	S1	Al2'	82.0(2)	C12	C11	C13	118.(3)
Al2	S1	Al2'	82.7(2)	C12	C11	C14	124.(3)
Al1	S2	Al2	82.4(3)	C13	C11	C14	101.(2)
Al1	S2	Al1'	82.3(2)	C12a	C11	C13a	117.(3)
Al1'	S2	Al2	82.0(2)	C12a	C11	C14a	91.(3)
S1	Al1	S2	97.7(3)	C13a	C11	C14a	119.(3)
S1	Al1	S2'	97.5(2)	C11	C14	C15	97.(4)
S1	Al1	C11	116.2(8)	C11	C14a	C15	119.(5)
S2	Al1	S2'	97.1(3)	Al2	C21	C22	108.(2)
S2	Al1	C11	120.5(7)	Al2	C21	C23	103.(2)
S2'	Al1	C11	122.6(6)	Al2	C21	C24	105.(2)
S1	Al2	S1'	96.7(2)	Al2	C21	C22a	103.(2)
S1	Al2	S2	97.1(3)	Al2	C21	C23a	107.(2)
S1	Al2	C21	117.8(8)	Al2	C21	C24a	108.(2)
S1'	Al2	S2	97.6(3)	C22	C21	C23	123.(3)
S1'	Al2	C21	121.6(8)	C22	C21	C24	114.(3)
S2	Al2	C21	120.6(7)	C23	C21	C24	103.(2)
Al1	C11	C12	102.(2)	C22a	C21	C23a	113.(3)
Al1	C11	C13	105.(2)	C22a	C21	C24a	110.(3)
Al1	C11	C14	104.(2)	C23a	C21	C24a	114.(2)
Al1	C11	C12a	103.(2)	C21	C24	C25	128.(3)
Al1	C11	C13a	112.(2)	C21	C24a	C25	107.(4)

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

Supplementary Material for [(Me<sub>2</sub>EtC)Al(μ<sub>3</sub>-Se)]<sub>4</sub> (8)Table 1. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement coefficients (Å<sup>2</sup> x 10<sup>3</sup>)

	x	y	z	U(eq)
Al(1)	7500	3762(5)	1394(7)	72(3)
Se(1)	6017(2)	2500	1183(3)	77(1)
C(1)	7500	5094(25)	574(37)	145(17)
C(2)	6486(20)	5745(16)	745(30)	210(17)
C(3)	7500	5301(33)	-865(39)	486(97)
C(4)	7500	4303(37)	-1665(41)	358(53)

\* Equivalent isotropic U defined as one third of the trace of the orthogonalized U<sub>ij</sub> tensor

Table 2. Bond lengths (Å)

Al(1)-Se(1)	2.444 (6)
Al(1)-C(1)	1.864 (33)
Al(1)-Se(1a)	2.444 (6)
Al(1)-Se(1b)	2.481 (9)
Se(1)-Al(1a)	2.444 (6)
Se(1)-Al(1b)	2.481 (9)
C(1)-C(2)	1.517 (30)
C(1)-C(3)	1.486 (54)
C(1)-C(2a)	1.517 (30)
C(3)-C(4)	1.490 (61)

Table 3. Bond angles (°)

Se(1)-Al(1)-C(1)	122.5(5)
Se(1)-Al(1)-Se(1a)	98.7(3)
Se(1)-Al(1)-Se(1b)	99.2(2)
C(1)-Al(1)-Se(1b)	110.2(11)
Al(1)-Se(1)-Al(1a)	80.4(3)
Al(1)-Se(1)-Al(1b)	80.1(3)
Al(1)-C(1)-C(2)	115.4(17)
Al(1)-C(1)-C(3)	126.6(26)
C(2)-C(1)-C(3)	91.1(21)
C(2)-C(1)-C(2a)	113.4(26)
C(1)-C(3)-C(4)	113.1(34)



Table 4. Anisotropic displacement coefficients ( $\text{\AA}^2 \times 10^3$ )

	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Al(1)	64(4)	56(4)	96(5)	0	0	4(4)
Se(1)	58(2)	69(2)	104(2)	0	-12(2)	0
C(1)	107(23)	105(23)	222(41)	0	0	89(28)
C(2)	160(22)	116(18)	354(44)	32(17)	-28(27)	121(24)
C(3)	916(260)	274(93)	268(94)	0	0	-3(89)
C(4)	466(104)	182(52)	428(108)	0	0	209(65)

Table 5. H-Atom coordinates ( $\times 10^4$ ) and isotropic displacement coefficients ( $\text{\AA}^2 \times 10^3$ )

	x	y	z	U
H(2A)	6551	6426	315	240
H(2B)	5922	5341	341	240
H(2C)	6324	5853	1657	240
H(3A)	6887	5719	-1107	480
H(4A)	7500	4554	-2556	500
H(4A)	6873	3877	-1514	500

Supplementary Material for [(Me<sub>2</sub>EtC)Ga(μ<sub>3</sub>-S)]<sub>4</sub> (10)

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(A <sup>2</sup> )
Ga1	0.4760(1)	-0.1429(3)	0.6607(1)	6.76(7)
Ga2	0.4096(1)	0.0868(3)	0.7199(1)	6.67(7)
S1	0.3972(3)	-0.1604(7)	0.7160(3)	7.1(2)
S2	0.4731(3)	0.1043(7)	0.6491(3)	7.1(2)
C11	0.438(2)	-0.258(4)	0.554(2)	13(1)*
C12	0.459(2)	-0.405(5)	0.586(2)	20(2)*
C13	0.350(2)	-0.200(5)	0.487(2)	18(1)*
C14	0.513(2)	-0.218(4)	0.547(2)	17(1)*
C21	0.305(2)	0.212(4)	0.684(2)	13(1)*
C22	0.334(2)	0.363(5)	0.686(2)	21(2)*
C23	0.243(2)	0.157(5)	0.596(2)	18(1)*
C24	0.286(2)	0.166(4)	0.749(2)	17(1)*

Starred atoms were refined isotropically.

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$$(4/3) * [a^2 * B(1,1) + b^2 * B(2,2) + c^2 * B(3,3) + ab(\cos \gamma) * B(1,2) + ac(\cos \beta) * B(1,3) + bc(\cos \alpha) * B(2,3)]$$

Table of Positional Parameters and Their Estimated Standard Deviations

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Atom	x	y	z	B(A <sup>2</sup> )
----	-	-	-	-----
H12a	0.4449	-0.4686	0.5427	25*
H12b	0.5153	-0.4118	0.6254	25*
H12c	0.4302	-0.4291	0.6097	25*
H13a	0.3299	-0.2480	0.4370	22*
H13b	0.3150	-0.2154	0.5046	22*
H13c	0.3529	-0.1019	0.4790	22*
H14a	0.5064	-0.2618	0.5000	21*
H14b	0.5152	-0.1185	0.5417	21*
H14c	0.5621	-0.2492	0.5935	21*
H22a	0.2906	0.4261	0.6712	26*
H22b	0.3777	0.3841	0.7396	26*
H22c	0.3500	0.3709	0.6496	26*
H23a	0.1935	0.2054	0.5735	23*
H23b	0.2639	0.1718	0.5633	23*
H23c	0.2345	0.0586	0.5979	23*
H24a	0.2403	0.2149	0.7392	21*
H24b	0.2760	0.0672	0.7442	21*
H24c	0.3312	0.1864	0.8017	21*

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Table of General Displacement Parameter Expressions - U's

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Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
-----	-----	-----	-----	-----	-----	-----
Ga1	0.092(1)	0.086(2)	0.083(1)	-0.004(1)	0.0511(7)	-0.010(1)
Ga2	0.078(1)	0.087(2)	0.089(1)	0.007(1)	0.0468(7)	0.003(1)
S1	0.084(3)	0.091(4)	0.097(3)	-0.009(3)	0.051(2)	-0.005(3)
S2	0.102(3)	0.086(4)	0.086(3)	-0.002(3)	0.053(2)	0.007(3)

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The form of the anisotropic displacement parameter is:

$\exp[-2\pi i \{h^2 a^2 U(1,1) + k^2 b^2 U(2,2) + l^2 c^2 U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$  where a, b, and c are reciprocal lattice constants.

Table of Bond Distances in Angstroms

-----

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
=====	=====	=====	=====	=====	=====
Ga1	S1	2.357(8)	C11	C12	1.50(6)
Ga1	S2	2.357(7)	C11	C13	1.61(4)
Ga1	C11	2.12(3)	C11	C14	1.62(6)
Ga2	S1	2.358(7)	C21	C22	1.53(6)
Ga2	S2	2.350(8)	C21	C23	1.57(4)
Ga2	C21	2.15(3)	C21	C24	1.58(6)

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

Table of Bond Angles in Degrees

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle</u>	<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Angle</u>
S1	Ga1	S2	97.4(3)	Ga1	S2	Ga2	82.2(2)
S1	Ga1	C11	118(1)	Ga1	S2	Ga2'	82.3(2)
S1	Ga1	S1'	96.9(1)	Ga2	S2	Ga2'	82.5(2)
S2	Ga1	C11	116.1(9)	Ga1	C11	C12	101.(2)
S2	Ga1	S1'	97.2(1)	Ga1	C11	C13	106.(2)
C11	Ga1	S1'	125.8(8)	Ga1	C11	C14	97.(2)
S1	Ga2	S2	97.6(3)	C12	C11	C13	126.(3)
S1	Ga2	C21	118.6(9)	C12	C11	C14	102.(3)
S1	Ga2	S2'	97.4(1)	C13	C11	C14	119.(3)
S2	Ga2	C21	120(1)	Ga2	C21	C22	104.(2)
S2	Ga2	S2'	96.9(1)	Ga2	C21	C23	102.(2)
C21	Ga2	S2'	121.0(8)	Ga2	C21	C24	101.(2)
Ga1	S1	Ga2	82.0(2)	C22	C21	C23	113.(3)
Ga1	S1	Ga1'	82.6(2)	C22	C21	C24	119.(3)
Ga2	S1	Ga1'	82.1(2)	C23	C21	C24	114.(3)

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

Supplementary Material for [(Me<sub>2</sub>EtC)Ga(μ<sub>3</sub>-Se)]<sub>4</sub> (11)Table 1. Atomic coordinates (x 10<sup>4</sup>) and equivalent isotropic displacement coefficients (Å<sup>2</sup> x 10<sup>3</sup>)

	x	y	z	U(eq)
Ga(1)	4385(1)	1547(2)	7816(1)	69(1)
Ga(2)	4334(1)	3922(2)	6583(1)	69(1)
Se(1)	4221(1)	1336(2)	6428(1)	74(1)
Se(2)	4277(1)	4138(2)	7869(1)	74(1)
C(11)	3726(12)	408(28)	8114(15)	141(15)
C(12)	2890(14)	721(30)	7509(15)	241(24)
C(13)	3943(16)	840(34)	9024(16)	235(27)
C(14)	4058(23)	-1044(34)	8341(27)	285(38)
C(15)	3914(53)	-1697(54)	7635(48)	965(261)
C(21)	3626(9)	5106(23)	5641(10)	114(10)
C(22)	2848(12)	4677(29)	5418(14)	246(19)
C(23)	3894(14)	4694(34)	4909(11)	254(22)
C(24)	3805(17)	6642(25)	5917(21)	261(26)
C(25)	4269(58)	6732(80)	6831(34)	861(106)

\* Equivalent isotropic U defined as one third of the trace of the orthogonalized U<sub>ij</sub> tensor

Table 2. Bond lengths (Å).

Ga(1)-Se(1)	2.467(2)
Ga(1)-Se(2)	2.482(2)
Ga(1)-C(11)	1.97(3)
Ga(1)-Se(1A)	2.460(2)
Ga(2)-Se(1)	2.476(2)
Ga(2)-Se(2)	2.470(3)
Ga(2)-C(21)	2.00(1)
Ga(2)-Se(2A)	2.464(2)
Se(1)-Ga(1A)	2.460(2)
Se(2)-Ga(2A)	2.464(2)
C(11)-C(12)	1.53(3)
C(11)-C(13)	1.59(4)
C(11)-C(14)	1.50(4)
C(14)-C(15)	1.36(9)
C(21)-C(22)	1.46(3)
C(21)-C(23)	1.73(3)
C(21)-C(24)	1.53(3)
C(24)-C(25)	1.51(6)

Table 3. Bond angles (°)

Se(1)-Ga(1)-Se(2)	98.7(1)
Se(1)-Ga(1)-C(11)	118.5(7)
Se(2)-Ga(1)-C(11)	116.9(8)
Se(1)-Ga(1)-Se(1A)	98.8(1)
Se(2)-Ga(1)-Se(1A)	98.8(1)
C(11)-Ga(1)-Se(1A)	120.8(6)
Se(1)-Ga(2)-Se(2)	98.8(1)
Se(1)-Ga(2)-C(21)	117.9(6)
Se(2)-Ga(2)-C(21)	118.3(6)
Se(1)-Ga(2)-Se(2A)	98.8(1)
Se(2)-Ga(2)-Se(2A)	98.3(1)
C(21)-Ga(2)-Se(2A)	120.4(6)
Ga(1)-Se(1)-Ga(2)	80.6(1)
Ga(1)-Se(1)-Ga(1A)	80.4(1)
Ga(2)-Se(1)-Ga(1A)	80.6(1)
Ga(1)-Se(2)-Ga(2)	80.4(1)
Ga(1)-Se(2)-Ga(2A)	80.4(1)
Ga(2)-Se(2)-Ga(2A)	80.9(1)
Ga(1)-C(11)-C(12)	108.5(19)
Ga(1)-C(11)-C(13)	106.1(17)
C(12)-C(11)-C(13)	113.0(25)
Ga(1)-C(11)-C(14)	108.8(26)
C(12)-C(11)-C(14)	124.4(24)
C(13)-C(11)-C(14)	94.2(25)
C(11)-C(14)-C(15)	106.3(37)
Ga(2)-C(21)-C(22)	107.8(16)
Ga(2)-C(21)-C(23)	102.5(13)
C(22)-C(21)-C(23)	113.0(17)
Ga(2)-C(21)-C(24)	106.4(13)
C(22)-C(21)-C(24)	114.2(22)
C(23)-C(21)-C(24)	111.9(24)
C(21)-C(24)-C(25)	110.8(35)

Table 4. Anisotropic displacement coefficients ( $\text{\AA}^2 \times 10^3$ )

	U <sub>11</sub>	U <sub>22</sub>	U <sub>33</sub>	U <sub>12</sub>	U <sub>13</sub>	U <sub>23</sub>
Ga(1)	52(1)	82(1)	67(1)	-4(1)	23(1)	5(1)
Ga(2)	48(1)	80(1)	60(1)	5(1)	11(1)	8(1)
Se(1)	56(1)	85(1)	60(1)	-8(1)	11(1)	-8(1)
Se(2)	54(1)	89(1)	74(1)	7(1)	26(1)	-6(1)
C(11)	103(17)	194(24)	145(19)	-20(16)	74(15)	53(17)
C(12)	160(25)	415(49)	177(25)	-185(29)	101(23)	-46(30)
C(13)	234(34)	331(45)	190(29)	-78(29)	141(28)	61(27)
C(14)	332(54)	165(30)	328(51)	-103(33)	132(44)	86(34)
C(15)	1572(346)	398(94)	1638(380)	-256(126)	1345(340)	-503(148)
C(21)	65(12)	139(18)	81(11)	11(12)	-12(9)	36(12)
C(22)	98(18)	237(30)	236(27)	-4(19)	-60(17)	171(26)
C(23)	221(30)	397(47)	76(14)	2(30)	12(17)	150(21)
C(24)	193(30)	113(22)	302(43)	41(20)	-26(29)	115(24)



Table 5. H-Atom coordinates ( $\times 10^4$ ) and isotropic displacement coefficients ( $\text{\AA}^2 \times 10^3$ )

	x	y	z	U
H(12A)	2567	183	7659	250
H(12B)	2778	1702	7509	250
H(12C)	2800	447	6977	250
H(13A)	3643	347	9222	210
H(13B)	4471	613	9353	210
H(13C)	3871	1833	9046	210
H(14A)	3855	-1484	8660	390
H(14B)	4601	-947	8650	390
H(15A)	4104	-2642	7715	390
H(15B)	3368	-1712	7343	390
H(15C)	4108	-1178	7332	390
H(22A)	2485	5217	4969	220
H(22B)	2778	3696	5282	220
H(22C)	2774	4841	5883	220
H(23A)	3589	5204	4419	280
H(23B)	4421	4931	5105	280
H(23C)	3826	3703	4802	280
H(24A)	3349	7193	5719	220
H(24C)	4111	7004	5686	220
H(25D)	4398	7694	6991	990
H(25A)	3959	6374	7058	990
H(25B)	4726	6184	7025	990

Supplementary Material for [(Me<sub>2</sub>EtC)Ga( $\mu_3$ -Te)]<sub>4</sub> (12)

Table of Positional Parameters and Their Estimated Standard Deviations

Atom	x	y	z	B(A <sup>2</sup> )
----	-	-	-	-----
Te1	0.0766	0.0766	0.0766(2)	7.25(3)
Te2	0.4257(2)	0.3276(2)	0.0781(2)	7.48(7)
Ga1	0.0639(2)	0.0639	-0.0639	6.82(6)
Ga2	0.5663(3)	0.3136(3)	0.0623(3)	6.9(1)
C11	0.126(2)	0.126	-0.126	7(1)*
C12	0.209(3)	0.116(3)	-0.096(3)	9.3*
C13	0.2061	0.0660	-0.1324	12*
C21	0.634	0.388	0.134	18(1)*
C22	0.614	0.467	0.118	23.5*
C23	0.620	0.371	0.214	23.5*
C24	0.715	0.377	0.117	23.5*
C25b	0.383(6)	0.191(8)	0.236(7)	30.6*
C25a	0.265(5)	0.192(6)	0.071(6)	30.6*

Starred atoms were refined isotropically.

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as:

$$(4/3) * [a^2*B(1,1) + b^2*B(2,2) + c^2*B(3,3) + ab(\cos \gamma)*B(1,2) + ac(\cos \beta)*B(1,3) + bc(\cos \alpha)*B(2,3)]$$

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)
Te1	0.092(2)	U(1,1)	U(1,1)	-0.011(2)	U(1,2)	U(1,2)
Te2	0.092(2)	0.096(2)	0.096(2)	0.011(2)	0.008(2)	-0.013(2)
Ga1	0.086(3)	U(1,1)	U(1,1)	-0.006(3)	-U(1,2)	-U(1,2)
Ga2	0.080(3)	0.089(3)	0.094(3)	-0.007(3)	-0.009(4)	-0.012(3)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2\{h^2a^2U(1,1) + k^2b^2U(2,2) + l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$  where a, b, and c are reciprocal lattice constants.

Table of Bond Distances in Angstroms

Atom 1 =====	Atom 2 =====	Distance =====	Atom 1 =====	Atom 2 =====	Distance =====
Te1	Ga1	2.676(3)	C12	C13	1.17(6)
Te2	Ga2	2.685(6)	C21	C22	1.559(0)
Te2	Ga2'	2.670(4)	C21	C23	1.567(0)
Te2	Ga2''	2.686(3)	C21	C24	1.589(0)
Ga1	C11	2.04(3)	C23	C25a	1.6(1)
Ga2	C21	2.334(5)	C24	C25b	1.3(1)
C11	C12	1.67(7)			

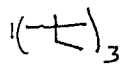
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 Numbers in parentheses are estimated standard deviations in the least significant digits.

Table of Bond Angles in Degrees

Atom 1 =====	Atom 2 =====	Atom 3 =====	Angle =====	Atom 1 =====	Atom 2 =====	Atom 3 =====	Angle =====
Ga1	Te1	Ga1'	79.2(1)	Ga1	C11	C12	106.(2)
Ga2	Te2	Ga2'	79.8(2)	C12	C11	C12'	113.(2)
Ga2	Te2	Ga2''	79.0(1)	C11	C12	C13	81.(3)
Ga2'	Te2	Ga2''	79.28(9)	Ga2	C21	C22	109.9(1)
Te1	Ga1	C11	118.0(5)	Ga2	C21	C23	109.8(1)
Te1	Ga1	Te1'	99.8(1)	Ga2	C21	C24	109.5(1)
Te2	Ga2	C21	114.6(2)	C22	C21	C23	110.(0)
Te2	Ga2	Te2'	99.0(2)	C22	C21	C24	108.(0)
Te2	Ga2	Te2''	99.8(2)	C23	C21	C24	108.(0)
C21	Ga2	Te2'	119.0(2)	C21	C23	C25a	120.(4)
C21	Ga2	Te2''	120.4(2)	C21	C24	C25b	115.(5)
Te2'	Ga2	Te2''	100.2(2)				

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

PPM



distilled 145°C 10<sup>-2</sup> torr

C<sub>6</sub>D<sub>6</sub>  
AM250

<sup>1</sup>H NMR

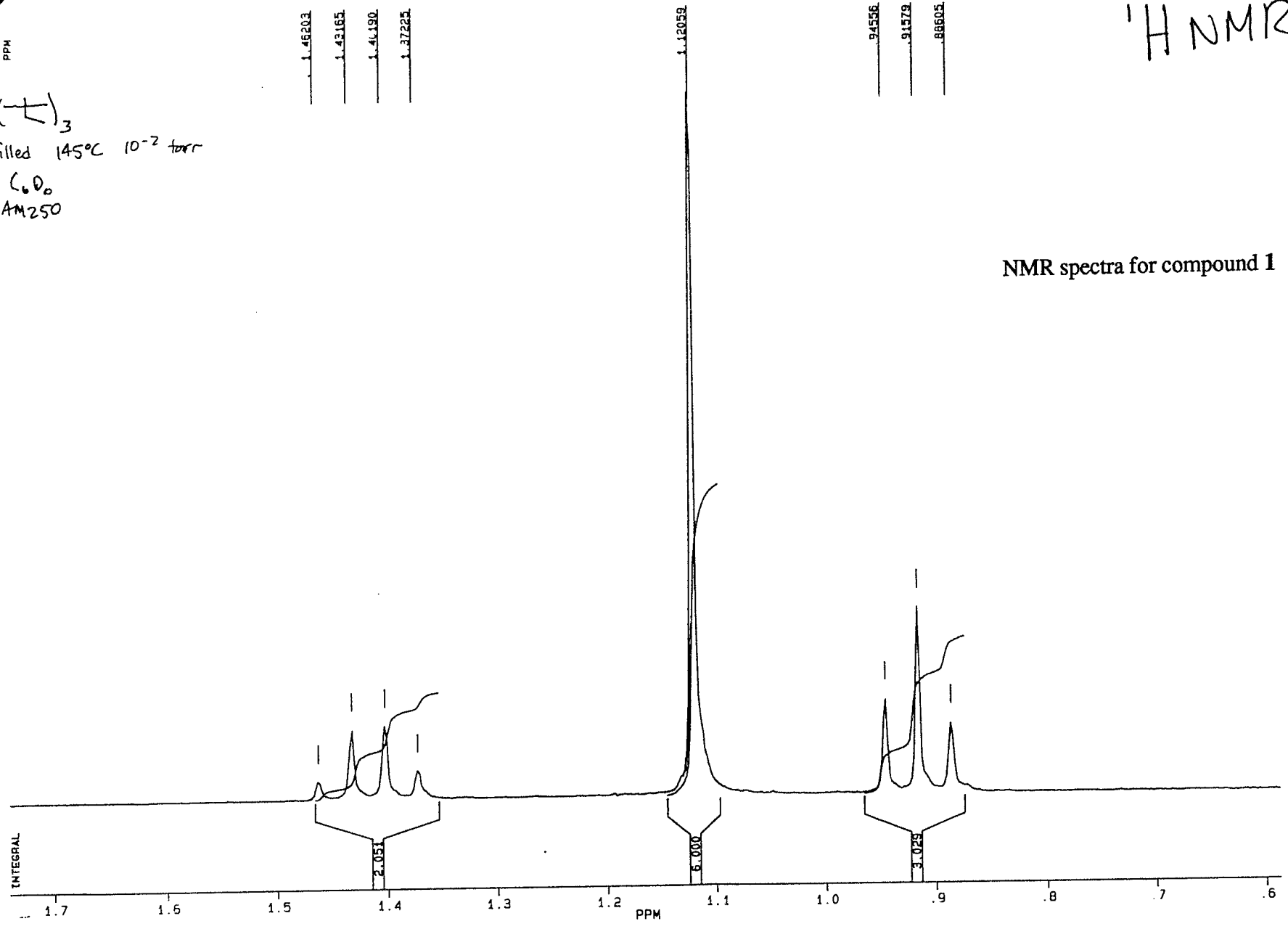
1

1.46203  
1.43165  
1.41190  
1.37225

94556  
91579  
88605

1.12059

NMR spectra for compound 1



<sup>13</sup>C NMR

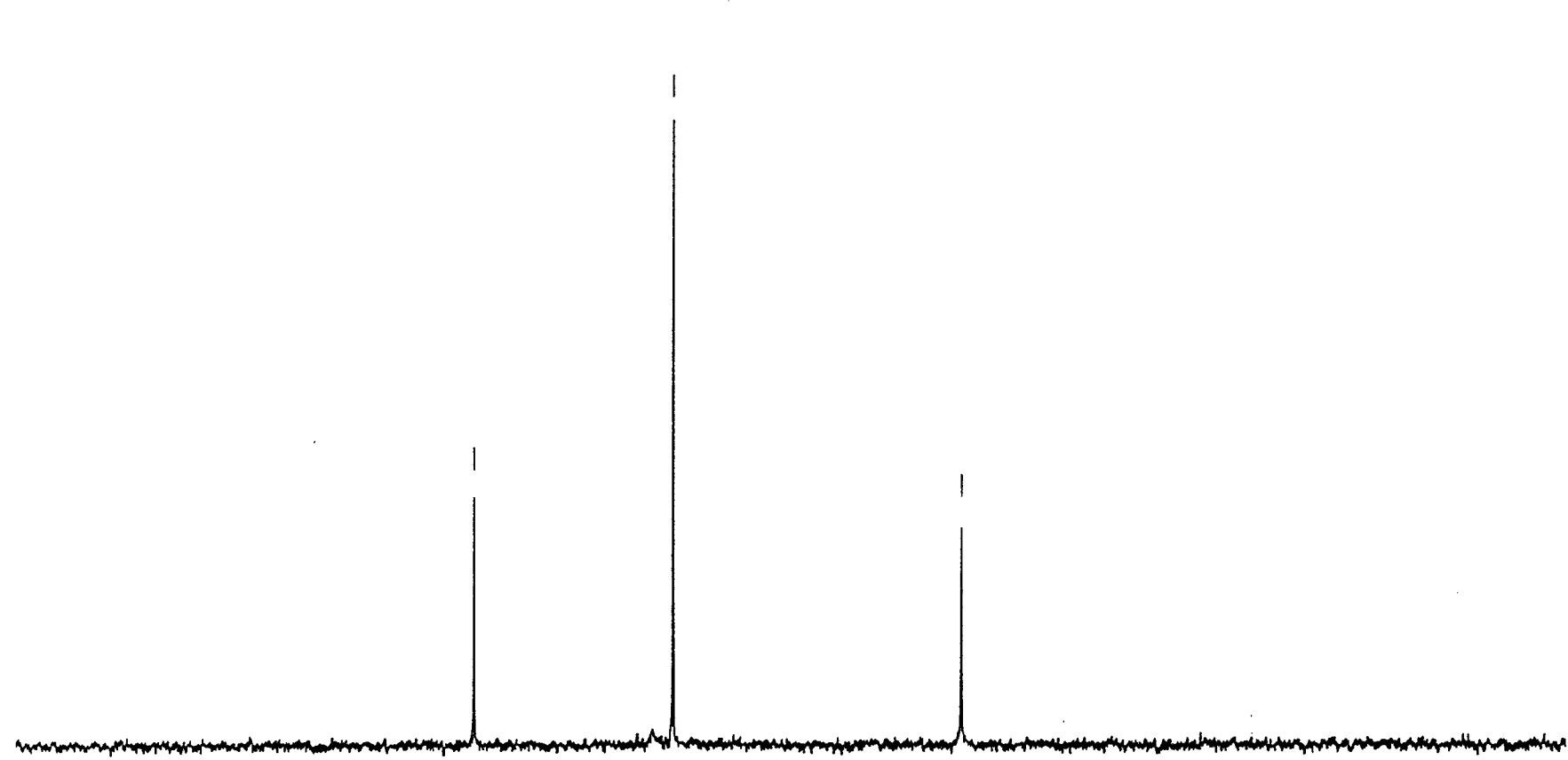
PPM

1(-C-)<sub>3</sub>  
C<sub>60</sub>  
AM400N

52.1914

28.1458

14.9512



50

40

30

PPM

20

10

0

-10



$\text{CH}_3\text{Al}(\text{MeCN})$

PPM

1.79896  
1.7694E  
1.7400E

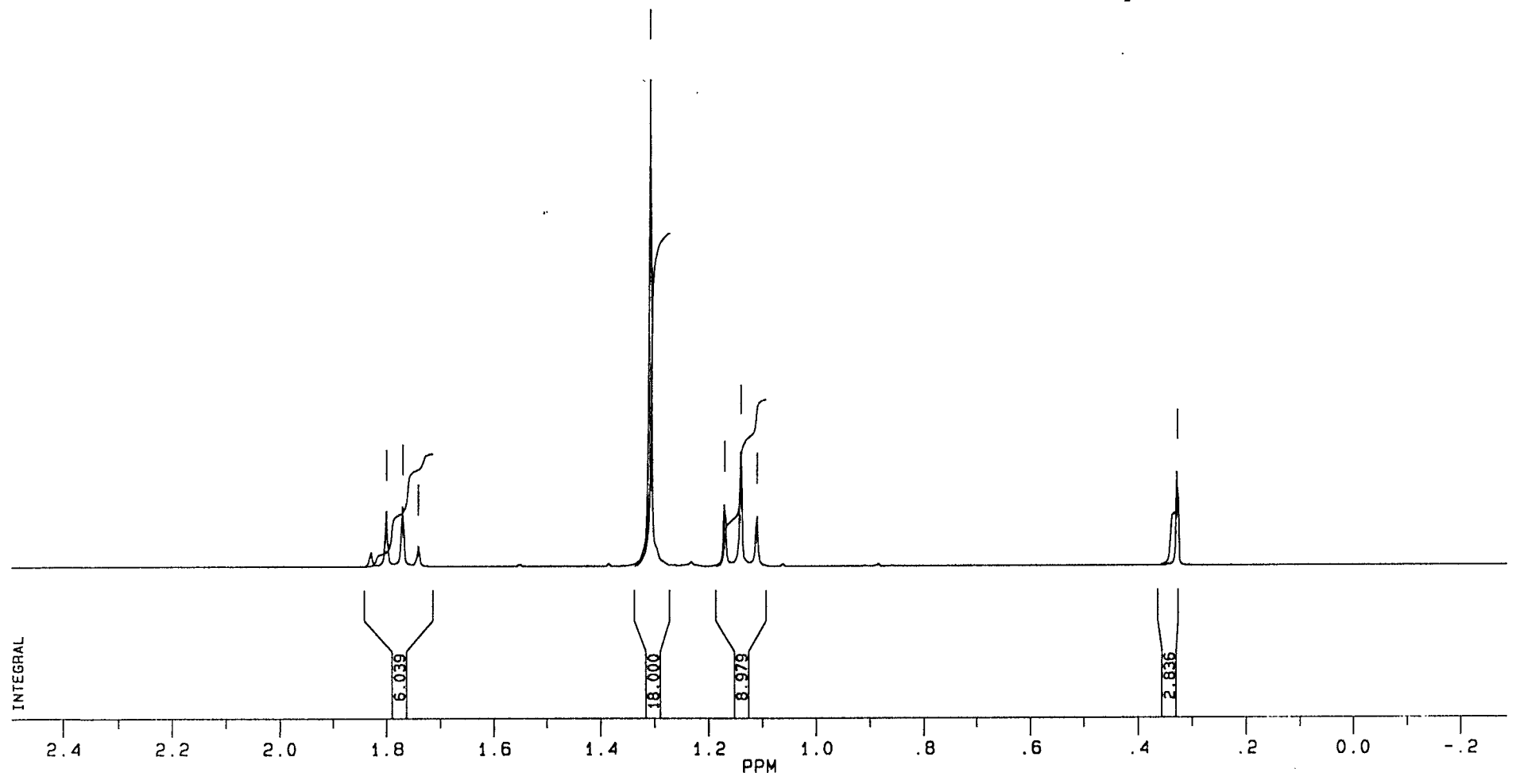
1.30790

1.16866  
1.13911  
1.10899

0.32694

$^1\text{H NMR } 2$

NMR spectra for compound 2





PPM

35.5787

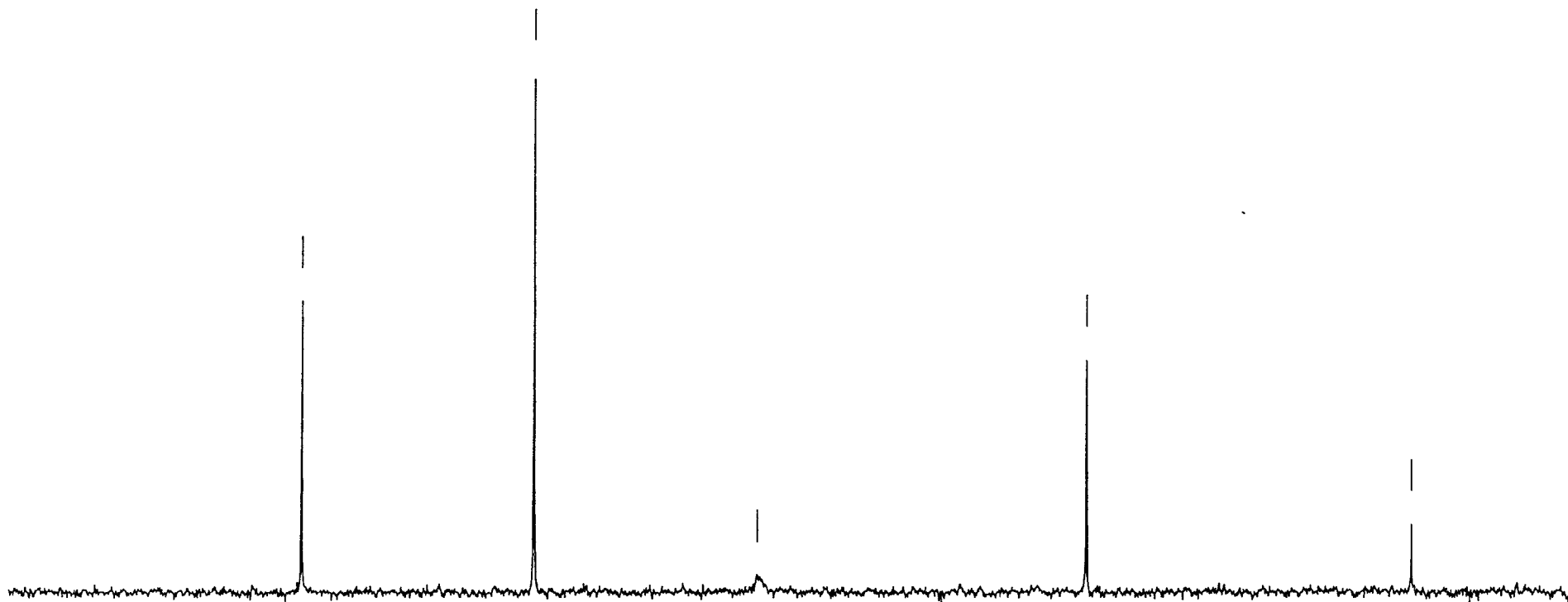
28.7176

21.1802

10.0303

-1.0015

<sup>13</sup>C NMR  
2

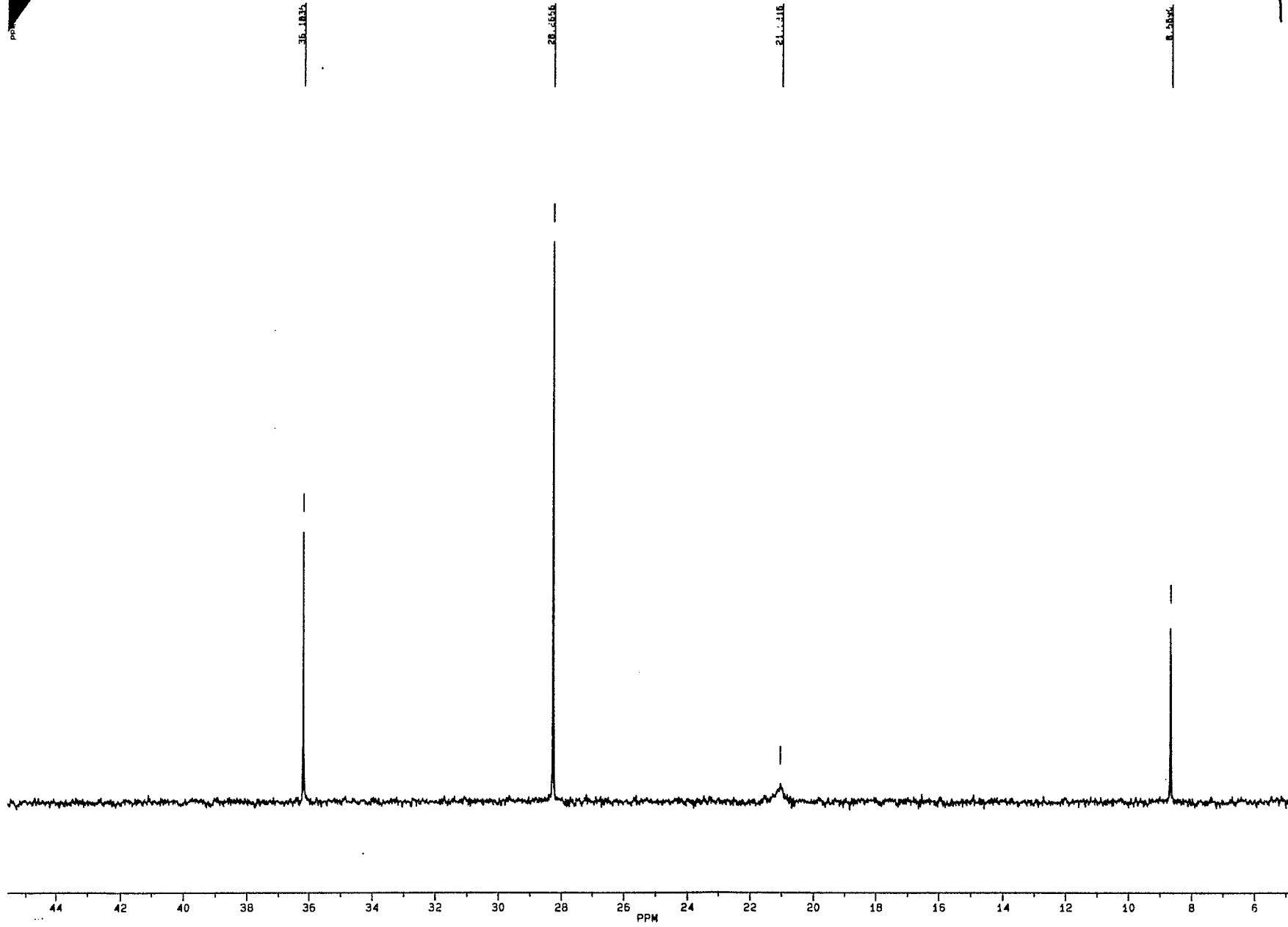


45.0 40.0 35.0 30.0 25.0 20.0 15.0 10.0 5.0 -0.0 -5.0

PPM

750 MHz 13C NMR (CDCl3) of 1,2-dichloroethane





$^{13}\text{C}$  3



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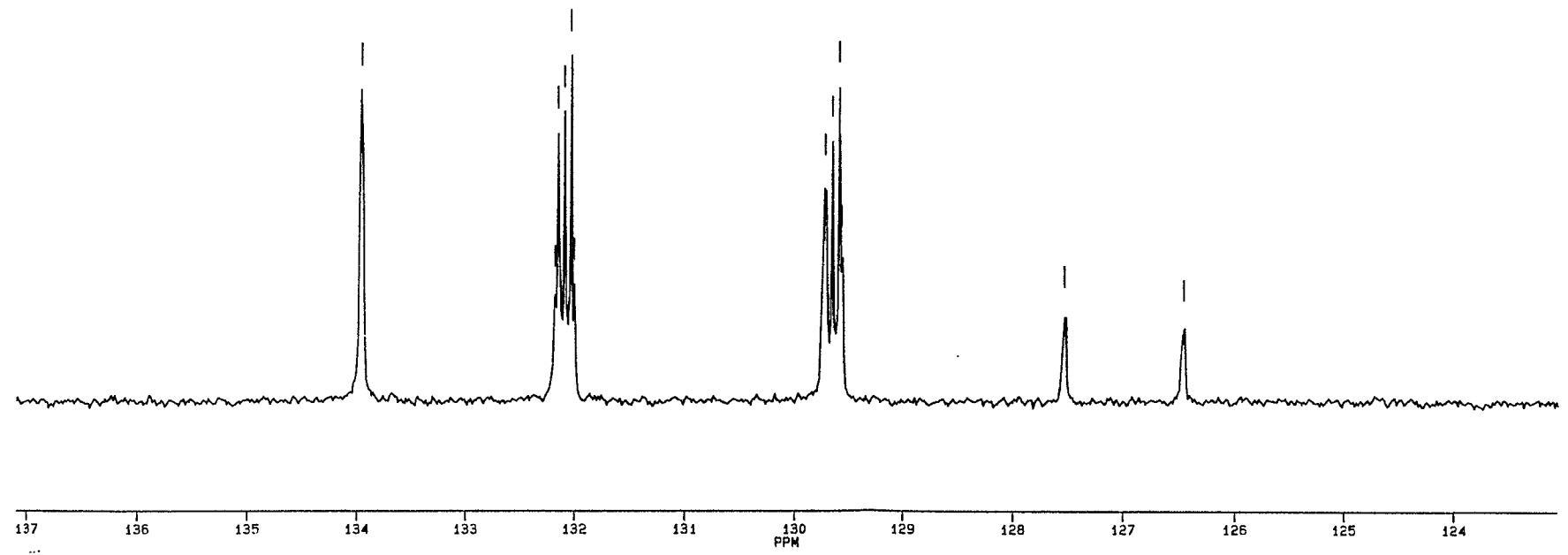
133.956

132.777  
132.601  
132.501

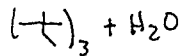
129.749  
129.649  
129.549

127.534

126.456



PPM



-tals from hexane

$\text{C}_6\text{D}_6$

An 250

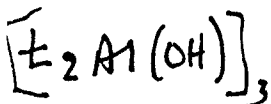
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6:2:3:1



12:4:6:1

36 12 18 3



2.05813

5.1736  
4.4699  
4.738  
4.2855

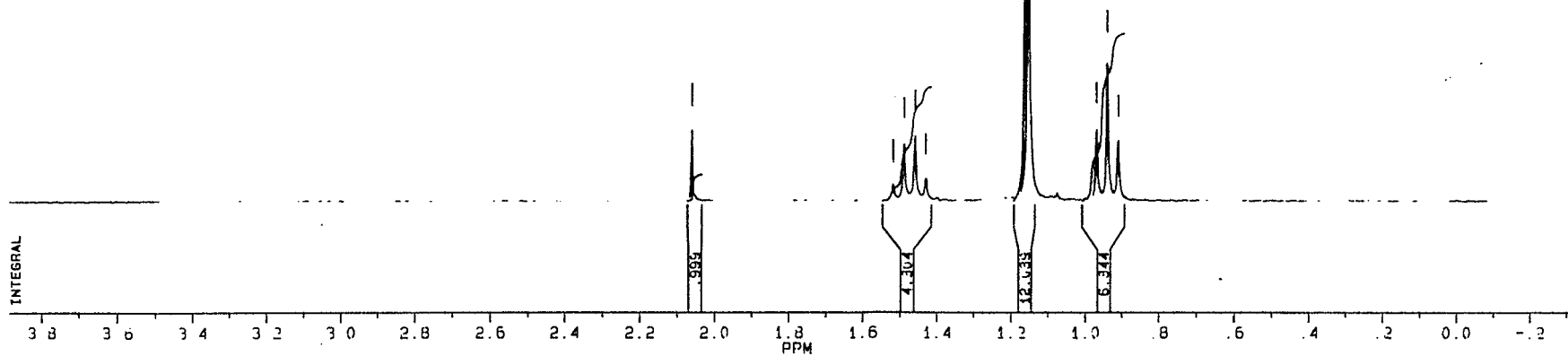
1.15233

0.5722  
0.4776  
0.4823

4

$^1\text{H}$  NMR

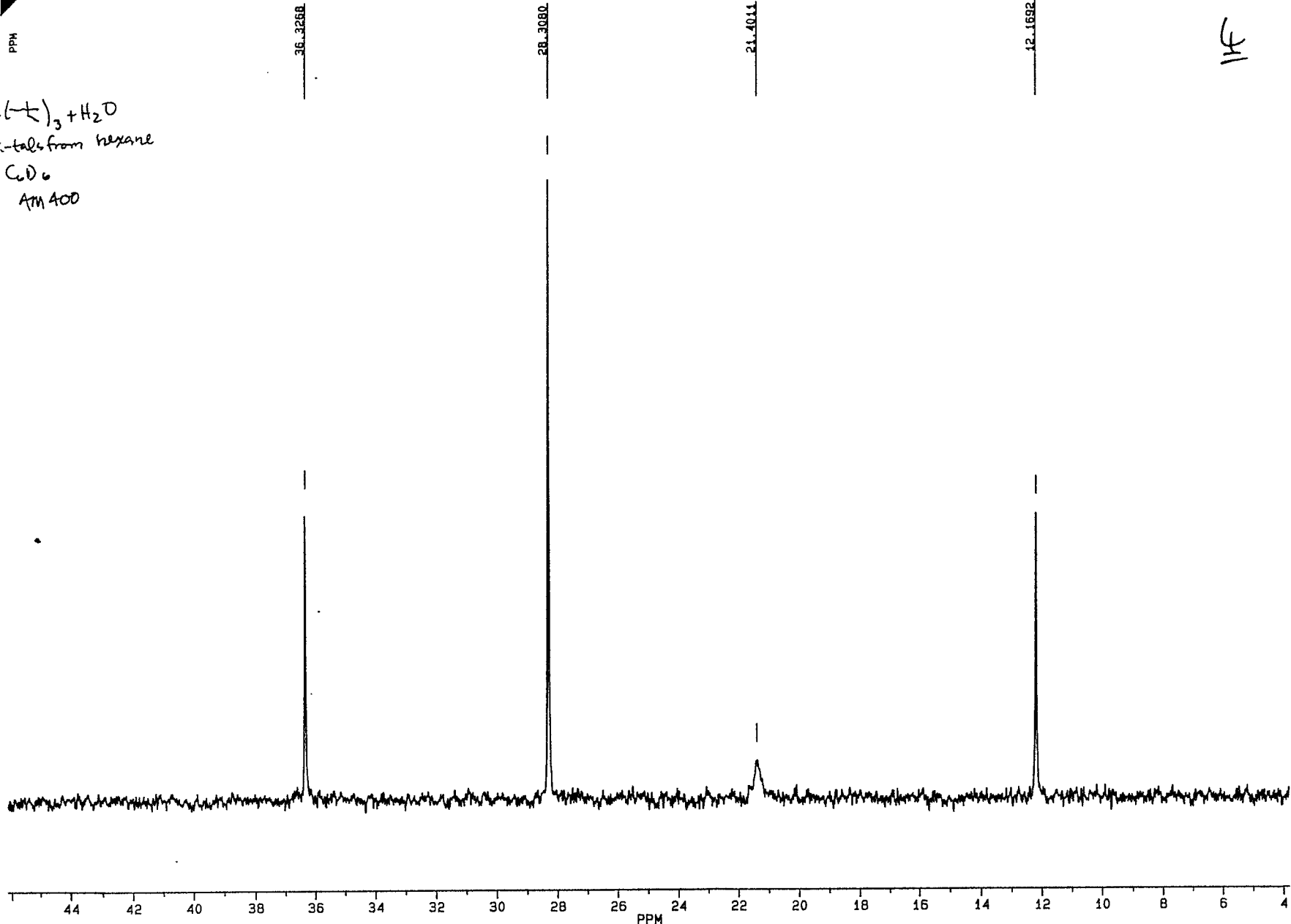
NMR spectra for compound 4



PPM

$(-t)_3 + H_2O$   
-tals from hexane  
 $C_6D_6$   
PM 400

1H  $^{13}C$  NMR



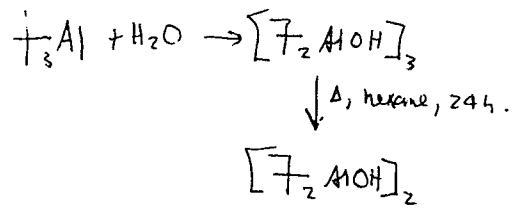
PPM

1.55245  
 1.50166  
 1.47141  
 1.44142  
 1.41249

1.07532

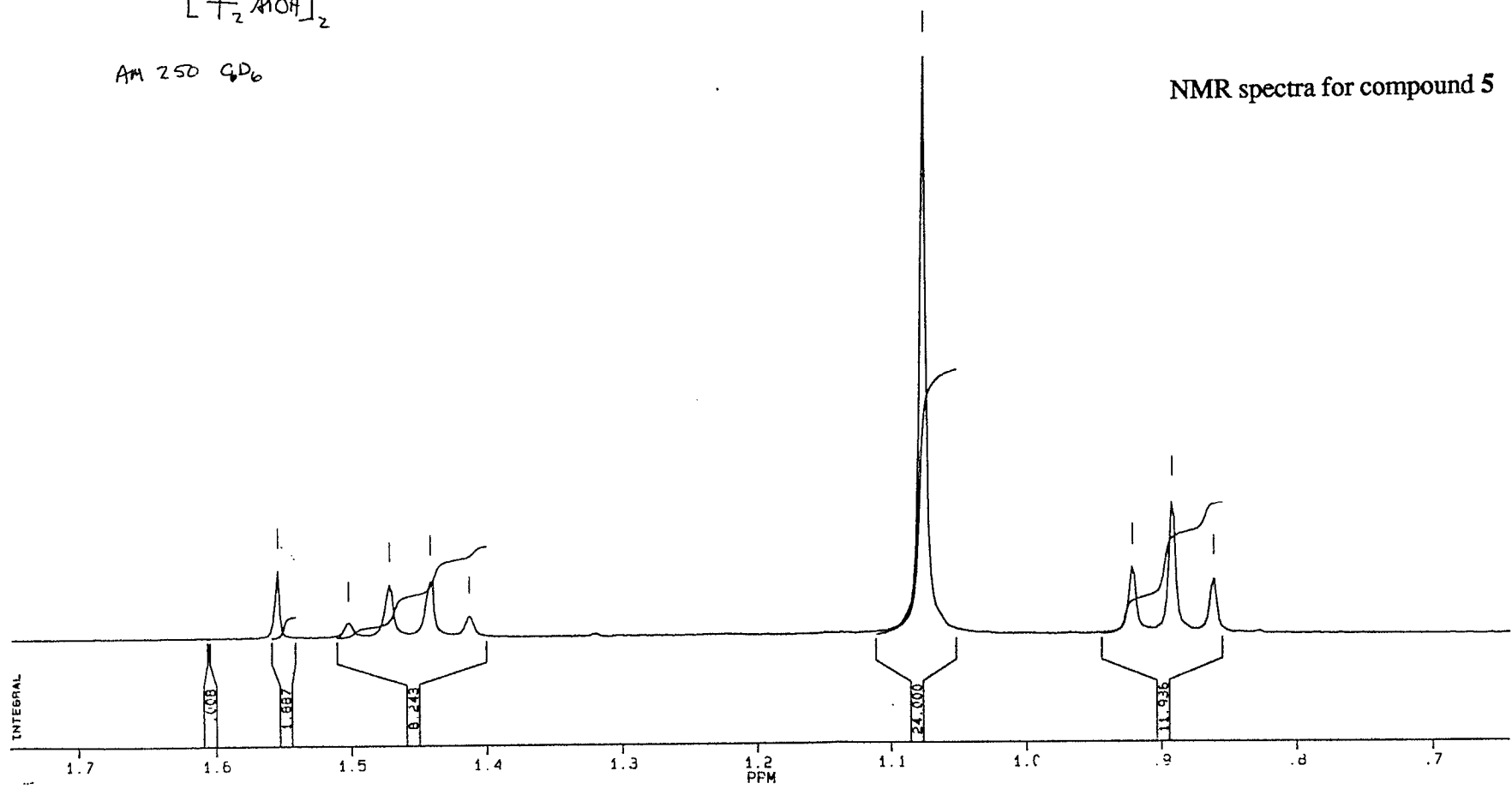
0.92425  
 0.91119  
 0.9066

<sup>1</sup>H NMR 5



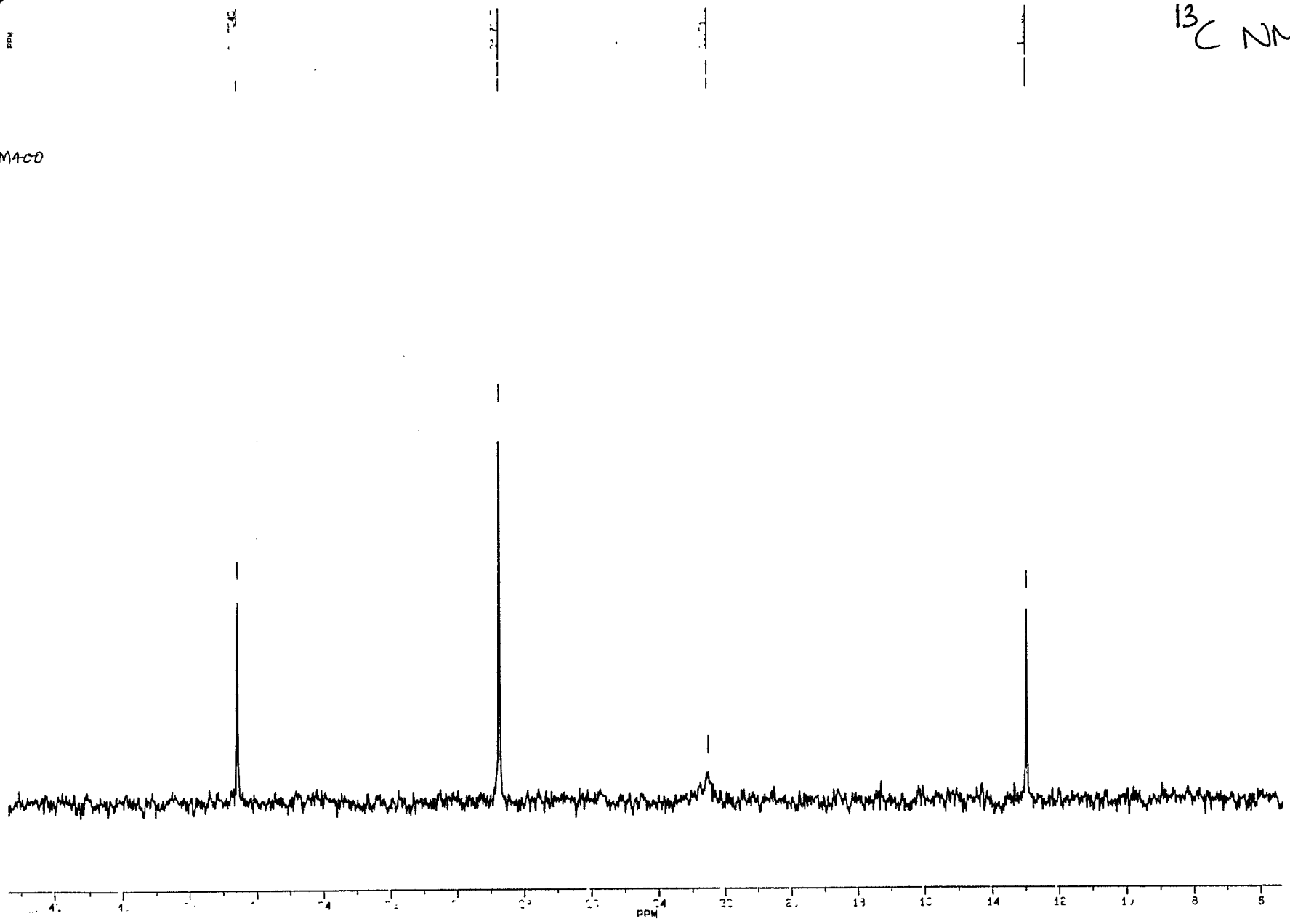
AM 250 CD6

NMR spectra for compound 5



$^{13}\text{C}$  NMR  $\text{Si}$

TM400





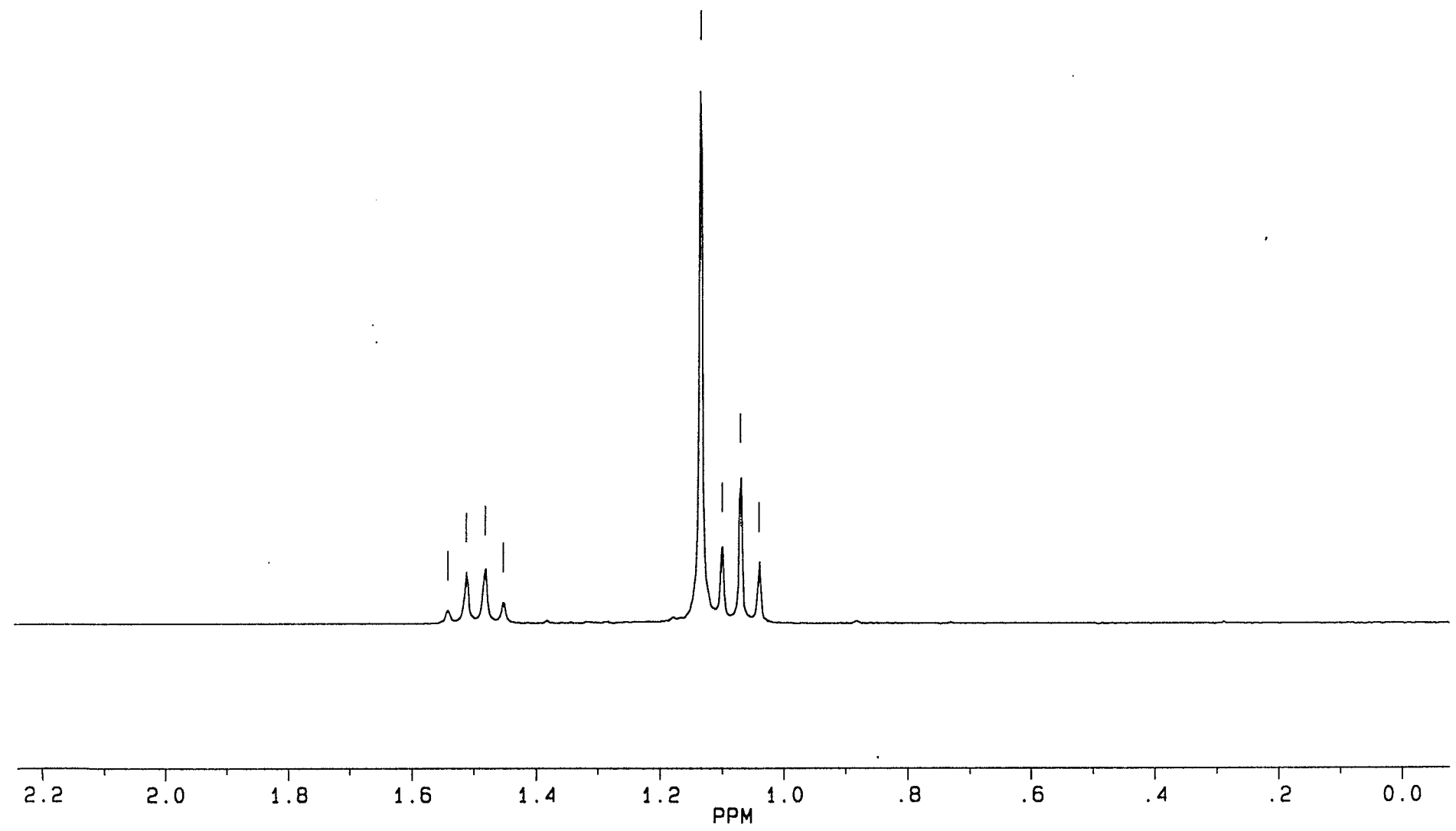
-MS]4

PPM

<sup>1</sup>H NMR 6

1.54120	1.13432
1.51066	1.09968
1.48024	1.07001
1.45136	1.03997

NMR spectra for compound 6



0123456789101112131415161718192021222324252627282930313233343536373839404142434445464748495051525354555657585960616263646566676869707172737475767778798081828384858687888990919293949596979899100