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Table 3. Crystal data and structure refinement for 3e.

Empirical formula	C12 H16 B Mo N O3
Formula weight	329.01
Temperature	158(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 6.6918(19) A alpha = 90 deg. b = 9.452(3) A beta = 90.008(4) deg. c = 21.396(6) A gamma = 90 deg.
Volume	1353.3(7) A^3
Z, Calculated density	4, 1.615 Mg/m^3
Absorption coefficient	0.967 mm^-1
F(000)	664
Crystal size	0.03 x 0.04 x 0.30 mm
Theta range for data collection	2.36 to 23.36 deg.
Limiting indices	-7<=h<=7, -10<=k<=10, -23<=l<=23
Reflections collected / unique	10776 / 1952 [R(int) = 0.0849]
Completeness to theta = 23.36	99.1 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.962 and 0.715
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1952 / 0 / 170
Goodness-of-fit on F^2	1.213
Final R indices [I>2sigma(I)]	R1 = 0.0732, wR2 = 0.1848
R indices (all data)	R1 = 0.0798, wR2 = 0.1881
Extinction coefficient	0.038(4)
Largest diff. peak and hole	0.888 and -0.890 e.A^-3

The crystals form as pseudo-orthorhombic twins (twin law 1 0 0 0 -1 0 0 0 -1).

Structure Determination.

Gold needles of **5e** were crystallized from a hexane solution at -10 deg. C. A crystal of dimensions 0.30 x 0.04 x 0.03 mm was cut from a larger crystal and mounted on a standard Bruker SMART CCD-based X-ray diffractometer equipped with a LT-2 low temperature device and normal focus Mo-target X-ray tube (λ = 0.71073 A) operated at 2000 W power (50 kV, 40 mA). The X-ray intensities were measured at 158(2) K; the detector was placed at a distance 5.059 cm from the crystal. A total of 2474 frames were collected with a scan width of 0.3° in ω and phi with an exposure time of 60 s/frame. The frames were integrated with the Bruker SAINT software package with a narrow frame algorithm. The integration of the data yielded a total of 10776 reflections to a maximum 2θ value of 52.8° of which 1952 were independent and 1768 were greater that $2\sigma(I)$. The final cell constants (Table 1) were based on the xyz centroids of 8192 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection; the data were processed with SADABS and corrected for absorption. The structure was solved and refined with the Bruker SHELXTL (version 5.10) software package, using the space group P2(1)/c with Z = 4 for the formula $C_{12}H_{16}O_3BNMo$. The crystals form as pseudo-orthorhombic twins (twin law 1 0 0 0 -1 0 0 0 -1) with a ratio of 0.543(4)/0.457(4) for the twin domains. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms located on a difference Fourier map and allowed to refine independently. Full matrix least-squares refinement based on F^2 converged at R1 = 0.0732 and wR2 = 0.1848 [based on I > 2sigma(I)], R1 = 0.0798 and wR2 = 0.1881 for all data. Additional details are presented in Table 1 and are given as Supporting information as a CIF file.

Sheldrick, G.M. SHELXTL, v. 5.10; Bruker Analytical X-ray, Madison, WI, 1997.
Sheldrick, G.M. SADABS. Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen: Gottingen, Germany, 1996.
Saint Plus, v. 4.05, Bruker Analytical X-ray, Madison, WI, 1997.

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Table S-2 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 5e.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo	170(2)	802(1)	1173(1)	26(1)
C(1)	3200(20)	1621(17)	782(7)	31(4)
C(2)	3360(20)	120(19)	845(8)	41(4)
C(3)	2980(30)	-559(18)	1407(9)	46(4)
C(4)	2560(20)	223(14)	1935(7)	23(3)
C(5)	2460(20)	2680(20)	2560(7)	39(4)
C(6)	2670(20)	4045(15)	1151(8)	32(3)
C(7)	1030(30)	4796(17)	1524(9)	44(4)
C(8)	4670(20)	4614(12)	1409(6)	23(3)
C(9)	2520(30)	4402(17)	469(8)	40(4)
C(10)	-1440(20)	-903(17)	956(7)	29(3)
C(11)	-1910(30)	1353(17)	1814(8)	33(4)
C(12)	-1470(20)	1774(16)	547(7)	30(4)
O(1)	-2418(15)	-1833(10)	815(4)	25(2)
O(2)	-2861(15)	1767(11)	2191(5)	31(3)
O(3)	-2476(15)	2367(10)	180(4)	25(2)
B	2560(20)	1858(16)	1943(7)	16(3)
N	2704(14)	2460(12)	1289(5)	23(2)

Table S-3 Bond lengths [A] and angles [deg] for 5e.

Mo-C(12)	1.959(16)
Mo-C(10)	1.994(16)
Mo-C(11)	2.024(19)
Mo-N	2.323(10)
Mo-C(1)	2.329(15)
Mo-C(3)	2.333(18)
Mo-C(2)	2.335(17)
Mo-C(4)	2.348(14)
Mo-B	2.504(16)
C(1)-N	1.386(19)
C(1)-C(2)	1.43(2)
C(2)-C(3)	1.39(3)
C(3)-C(4)	1.38(2)
C(4)-B	1.55(2)
C(5)-B	1.53(2)
C(6)-C(9)	1.50(2)
C(6)-C(7)	1.54(2)
C(6)-N	1.526(18)
C(6)-C(8)	1.540(19)
C(10)-O(1)	1.136(17)
C(11)-O(2)	1.098(19)
C(12)-O(3)	1.177(18)
B-N	1.512(19)
C(12)-Mo-C(10)	85.3(6)
C(12)-Mo-C(11)	87.6(6)
C(10)-Mo-C(11)	89.6(6)
C(12)-Mo-N	99.5(5)
C(10)-Mo-N	164.9(5)
C(11)-Mo-N	104.8(5)
C(12)-Mo-C(1)	94.9(6)
C(10)-Mo-C(1)	131.1(6)
C(11)-Mo-C(1)	139.3(6)
N-Mo-C(1)	34.7(5)
C(12)-Mo-C(3)	148.9(6)
C(10)-Mo-C(3)	92.4(6)
C(11)-Mo-C(3)	123.5(6)
N-Mo-C(3)	76.1(5)
C(1)-Mo-C(3)	63.7(6)
C(12)-Mo-C(2)	115.8(7)
C(10)-Mo-C(2)	101.6(6)
C(11)-Mo-C(2)	154.6(6)
N-Mo-C(2)	63.4(5)
C(1)-Mo-C(2)	35.7(6)
C(3)-Mo-C(2)	34.5(6)
C(12)-Mo-C(4)	164.7(5)
C(10)-Mo-C(4)	110.0(5)
C(11)-Mo-C(4)	93.4(5)
N-Mo-C(4)	65.5(4)
C(1)-Mo-C(4)	74.5(5)
C(3)-Mo-C(4)	34.2(6)
C(2)-Mo-C(4)	61.5(6)
C(12)-Mo-B	128.3(5)
C(10)-Mo-B	145.2(5)
C(11)-Mo-B	83.8(6)
N-Mo-B	36.3(4)
C(1)-Mo-B	63.0(5)
C(3)-Mo-B	64.1(6)
C(2)-Mo-B	74.0(5)
C(4)-Mo-B	37.0(5)
N-C(1)-C(2)	120.7(15)
N-C(1)-Mo	72.4(8)
C(2)-C(1)-Mo	72.4(9)
C(3)-C(2)-C(1)	122.0(15)
C(3)-C(2)-Mo	72.7(10)
C(1)-C(2)-Mo	71.9(9)
C(2)-C(3)-C(4)	120.0(15)
C(2)-C(3)-Mo	72.8(11)
C(4)-C(3)-Mo	73.5(9)
C(3)-C(4)-B	123.0(14)
C(3)-C(4)-Mo	72.3(10)
B-C(4)-Mo	77.0(8)

C(9)-C(6)-C(7)	110.6(13)
C(9)-C(6)-N	114.2(13)
C(7)-C(6)-N	111.3(12)
C(9)-C(6)-C(8)	109.2(13)
C(7)-C(6)-C(8)	105.9(13)
N-C(6)-C(8)	105.2(10)
O(1)-C(10)-Mo	176.6(13)
O(2)-C(11)-Mo	170.8(14)
O(3)-C(12)-Mo	178.7(14)
N-B-C(5)	127.4(13)
N-B-C(4)	111.5(12)
C(5)-B-C(4)	121.1(13)
N-B-Mo	65.3(7)
C(5)-B-Mo	137.8(11)
C(4)-B-Mo	66.0(8)
C(1)-N-B	121.6(12)
C(1)-N-C(6)	114.4(12)
B-N-C(6)	123.2(11)
C(1)-N-Mo	72.9(8)
B-N-Mo	78.4(8)
C(6)-N-Mo	129.2(8)

Symmetry transformations used to generate equivalent atoms:

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Table S-4 Anisotropic displacement parameters (A^2 x 10^3) for 5e.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mo	19(1)	30(1)	29(1)	-2(1)	-2(1)	-3(1)
C(1)	26(5)	36(5)	33(5)	0(4)	-1(4)	0(4)
C(2)	35(9)	47(10)	41(10)	-24(9)	11(8)	-7(8)
C(3)	46(8)	35(7)	57(8)	-7(7)	2(7)	-3(6)
C(4)	26(5)	18(5)	27(5)	4(4)	0(4)	0(4)
C(5)	20(8)	68(11)	30(8)	-10(8)	-2(7)	12(8)
C(6)	31(7)	28(8)	38(8)	11(7)	-3(9)	1(6)
C(7)	50(10)	23(8)	58(11)	-10(8)	-12(9)	-13(8)
C(8)	23(5)	17(4)	31(5)	-2(4)	-6(4)	-1(4)
C(9)	40(4)	40(4)	40(4)	1(2)	0(2)	0(2)
C(10)	29(5)	32(5)	27(5)	5(4)	1(4)	6(4)
C(11)	47(11)	24(8)	30(9)	-2(7)	-16(8)	8(7)
C(12)	28(5)	27(5)	34(5)	-2(4)	2(4)	-3(4)
O(1)	31(6)	22(5)	22(5)	0(4)	-2(4)	-13(5)
O(2)	32(4)	35(4)	27(4)	0(4)	10(4)	3(4)
O(3)	25(3)	24(3)	26(3)	1(2)	-1(2)	-1(2)
B	16(3)	16(3)	15(4)	0(2)	0(2)	-1(2)
N	29(4)	16(4)	25(4)	-2(4)	-2(4)	-1(4)

Table S-5 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 5e.

	x	y	z	U(eq)
H(1)	3449	2048	387	53(13)
H(2)	3727	-429	492	53(13)
H(3)	3014	-1562	1428	53(13)
H(4)	2254	-266	2311	53(13)
H(5A)	3004	3635	2497	53(13)
H(5B)	3255	2188	2878	53(13)
H(5C)	1072	2747	2698	53(13)
H(7A)	-284	4536	1354	53(13)
H(7B)	1206	5823	1492	53(13)
H(7C)	1101	4511	1963	53(13)
H(8A)	4776	4377	1854	53(13)
H(8B)	4709	5644	1358	53(13)
H(8C)	5779	4184	1180	53(13)
H(9A)	3645	3975	244	53(13)
H(9B)	2560	5432	416	53(13)
H(9C)	1262	4034	302	53(13)

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Table S-6 Crystal data and structure refinement for 6c.

Empirical formula	C14 H12 B Cr N O3
Formula weight	305.06
Temperature	158(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 13.0008(18) A alpha = 90 deg. b = 13.9518(19) A beta = 90 deg. c = 15.406(2) A gamma = 90 deg.
Volume	2794.4(7) A^3
Z, Calculated density	8, 1.450 Mg/m^3
Absorption coefficient	0.822 mm^-1
F(000)	1248
Crystal size	0.02 x 0.04 x 0.22 mm
Theta range for data collection	2.52 to 26.46 deg.
Limiting indices	-16<=h<=16, -17<=k<=17, -19<=l<=19
Reflections collected / unique	22382 / 2877 [R(int) = 0.1474]
Completeness to theta = 26.46	99.8 %
Absorption correction	Sadabs
Max. and min. transmission	0.956 and 0.739
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2877 / 0 / 184
Goodness-of-fit on F^2	0.873
Final R indices [I>2sigma(I)]	R1 = 0.0476, wR2 = 0.1049
R indices (all data)	R1 = 0.1177, wR2 = 0.1384
Extinction coefficient	0.0011(4)
Largest diff. peak and hole	0.342 and -0.382 e.A^-3

C(6)-Cr(1)-B(1)	78.76(16)
C(5)-Cr(1)-B(1)	67.27(16)
C(4)-Cr(1)-B(1)	38.07(15)
O(1)-C(1)-Cr(1)	177.9(4)
O(2)-C(2)-Cr(1)	179.6(5)
O(3)-C(3)-Cr(1)	179.2(4)
C(5)-C(4)-B(1)	122.0(4)
C(5)-C(4)-Cr(1)	70.3(2)
B(1)-C(4)-Cr(1)	75.0(2)
C(4)-C(5)-C(6)	120.0(4)
C(4)-C(5)-Cr(1)	73.3(2)
C(6)-C(5)-Cr(1)	70.8(2)
C(7)-C(6)-C(5)	120.7(4)
C(7)-C(6)-Cr(1)	69.8(2)
C(5)-C(6)-Cr(1)	72.0(2)
C(6)-C(7)-N(1)	121.7(4)
C(6)-C(7)-Cr(1)	73.4(2)
N(1)-C(7)-Cr(1)	73.0(2)
C(14)-C(9)-C(10)	116.7(4)
C(14)-C(9)-B(1)	119.2(3)
C(10)-C(9)-B(1)	124.0(4)
C(11)-C(10)-C(9)	121.0(4)
C(12)-C(11)-C(10)	120.6(4)
C(11)-C(12)-C(13)	119.5(4)
C(14)-C(13)-C(12)	119.8(4)
C(13)-C(14)-C(9)	122.4(4)

Symmetry transformations used to generate equivalent atoms:

Table S-7 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 6c.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
B(1)	8498(4)	1170(4)	3337(3)	27(1)
N(1)	7475(3)	1364(2)	2976(2)	28(1)
Cr(1)	7237(1)	1597(1)	4374(1)	26(1)
O(3)	7640(3)	-325(2)	5175(2)	45(1)
O(2)	7096(3)	2422(2)	6163(2)	59(1)
O(1)	4984(3)	1172(3)	4515(2)	64(1)
C(1)	5849(4)	1323(3)	4447(3)	40(1)
C(2)	7146(4)	2106(3)	5474(3)	39(1)
C(3)	7490(3)	416(3)	4862(3)	32(1)
C(4)	8859(3)	1937(3)	3958(3)	30(1)
C(5)	8313(3)	2786(3)	4081(3)	33(1)
C(6)	7382(4)	2939(3)	3634(3)	34(1)
C(7)	6965(3)	2234(3)	3120(3)	32(1)
C(8)	6900(3)	673(3)	2434(3)	32(1)
C(9)	9124(3)	237(3)	3111(2)	24(1)
C(10)	9185(3)	-161(3)	2277(3)	29(1)
C(11)	9796(3)	-958(3)	2114(3)	34(1)
C(12)	10347(3)	-1384(3)	2774(3)	35(1)
C(13)	10302(3)	-1003(3)	3604(3)	37(1)
C(14)	9707(3)	-205(3)	3761(3)	32(1)

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Table S-8 Bond lengths [A] and angles [deg] for 6c

B(1)-N(1)	1.466(6)
B(1)-C(4)	1.510(6)
B(1)-C(9)	1.574(6)
B(1)-Cr(1)	2.366(5)
N(1)-C(7)	1.400(5)
N(1)-C(8)	1.479(5)
N(1)-Cr(1)	2.200(3)
Cr(1)-C(2)	1.840(4)
Cr(1)-C(3)	1.842(5)
Cr(1)-C(1)	1.848(5)
Cr(1)-C(7)	2.156(4)
Cr(1)-C(6)	2.201(4)
Cr(1)-C(5)	2.216(4)
Cr(1)-C(4)	2.254(4)
O(3)-C(3)	1.157(5)
O(2)-C(2)	1.151(5)
O(1)-C(1)	1.149(5)
C(4)-C(5)	1.394(6)
C(5)-C(6)	1.410(6)
C(6)-C(7)	1.375(6)
C(9)-C(14)	1.399(5)
C(9)-C(10)	1.402(5)
C(10)-C(11)	1.389(5)
C(11)-C(12)	1.379(6)
C(12)-C(13)	1.386(6)
C(13)-C(14)	1.377(6)

N(1)-B(1)-C(4)	113.0(4)
N(1)-B(1)-C(9)	122.6(4)
C(4)-B(1)-C(9)	124.4(4)
N(1)-B(1)-Cr(1)	65.2(2)
C(4)-B(1)-Cr(1)	67.0(2)
C(9)-B(1)-Cr(1)	135.7(3)
C(7)-N(1)-B(1)	122.0(4)
C(7)-N(1)-C(8)	114.5(3)
B(1)-N(1)-C(8)	123.5(3)
C(7)-N(1)-Cr(1)	69.6(2)
B(1)-N(1)-Cr(1)	77.5(2)
C(8)-N(1)-Cr(1)	125.3(3)
C(2)-Cr(1)-C(3)	88.92(18)
C(2)-Cr(1)-C(1)	87.8(2)
C(3)-Cr(1)-C(1)	88.0(2)
C(2)-Cr(1)-C(7)	130.99(18)
C(3)-Cr(1)-C(7)	139.78(17)
C(1)-Cr(1)-C(7)	88.83(18)
C(2)-Cr(1)-N(1)	165.27(16)
C(3)-Cr(1)-N(1)	104.00(15)
C(1)-Cr(1)-N(1)	99.56(16)
C(7)-Cr(1)-N(1)	37.46(14)
C(2)-Cr(1)-C(6)	98.90(17)
C(3)-Cr(1)-C(6)	163.36(18)
C(1)-Cr(1)-C(6)	106.90(19)
C(7)-Cr(1)-C(6)	36.76(15)
N(1)-Cr(1)-C(6)	66.81(14)
C(2)-Cr(1)-C(5)	86.54(17)
C(3)-Cr(1)-C(5)	129.84(18)
C(1)-Cr(1)-C(5)	141.58(19)
C(7)-Cr(1)-C(5)	67.20(16)
N(1)-Cr(1)-C(5)	79.77(14)
C(6)-Cr(1)-C(5)	37.22(16)
C(2)-Cr(1)-C(4)	103.95(18)
C(3)-Cr(1)-C(4)	97.90(17)
C(1)-Cr(1)-C(4)	166.92(17)
C(7)-Cr(1)-C(4)	79.14(16)
N(1)-Cr(1)-C(4)	67.73(14)
C(6)-Cr(1)-C(4)	66.03(16)
C(5)-Cr(1)-C(4)	36.32(14)
C(2)-Cr(1)-B(1)	139.79(19)
C(3)-Cr(1)-B(1)	85.77(17)
C(1)-Cr(1)-B(1)	131.71(18)
C(7)-Cr(1)-B(1)	67.14(16)
N(1)-Cr(1)-B(1)	37.24(14)

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Table S-9 Anisotropic displacement parameters (A^2 x 10^3) for 6c
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
B(1)	24(3)	37(3)	21(2)	6(2)	2(2)	-2(2)
N(1)	30(2)	32(2)	21(2)	-1(1)	0(2)	-1(1)
Cr(1)	26(1)	29(1)	24(1)	-1(1)	3(1)	-1(1)
O(3)	66(2)	32(2)	38(2)	5(2)	3(2)	-4(2)
O(2)	90(3)	54(2)	33(2)	-14(2)	17(2)	-14(2)
O(1)	28(2)	99(3)	64(2)	-16(2)	13(2)	-13(2)
C(1)	35(3)	53(3)	33(2)	-9(2)	6(2)	1(2)
C(2)	47(3)	34(2)	36(3)	-2(2)	9(2)	-6(2)
C(3)	32(3)	37(3)	25(2)	-1(2)	4(2)	-6(2)
C(4)	27(2)	33(2)	30(2)	1(2)	5(2)	-2(2)
C(5)	35(3)	32(3)	31(2)	-1(2)	9(2)	-7(2)
C(6)	40(3)	27(2)	35(2)	2(2)	3(2)	1(2)
C(7)	30(2)	36(3)	30(2)	9(2)	0(2)	8(2)
C(8)	26(2)	35(2)	34(2)	-5(2)	-1(2)	-1(2)
C(9)	18(2)	27(2)	28(2)	0(2)	-1(2)	-4(2)
C(10)	22(2)	39(2)	27(2)	2(2)	3(2)	-2(2)
C(11)	28(3)	41(3)	34(2)	-11(2)	8(2)	0(2)
C(12)	25(2)	33(2)	47(3)	-1(2)	7(2)	3(2)
C(13)	30(3)	44(3)	37(3)	9(2)	-1(2)	5(2)
C(14)	27(2)	39(3)	30(2)	0(2)	2(2)	1(2)

Table S-10 Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 6c.

	x	y	z	U(eq)
H(4)	9477	1838	4274	32(4)
H(5)	8569	3261	4467	32(4)
H(6)	7038	3537	3688	32(4)
H(7)	6315	2339	2855	32(4)
H(8A)	6163	725	2561	48
H(8B)	7135	21	2562	48
H(8C)	7019	816	1819	48
H(10)	8803	119	1817	32(4)
H(11)	9833	-1212	1543	32(4)
H(12)	10755	-1935	2661	32(4)
H(13)	10680	-1291	4063	32(4)
H(14)	9692	54	4331	32(4)

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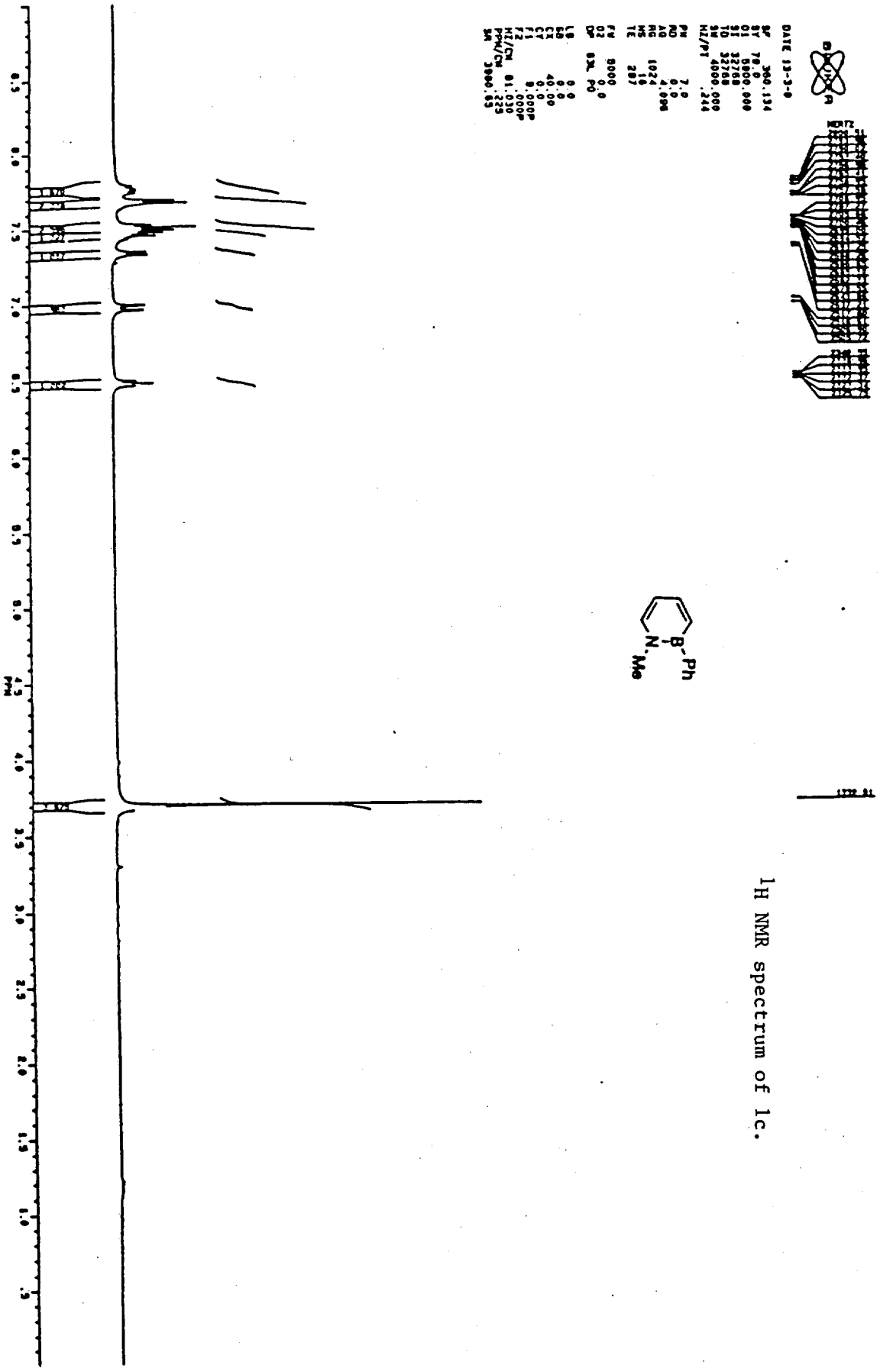

^{1}H NMR spectrum of 1c.

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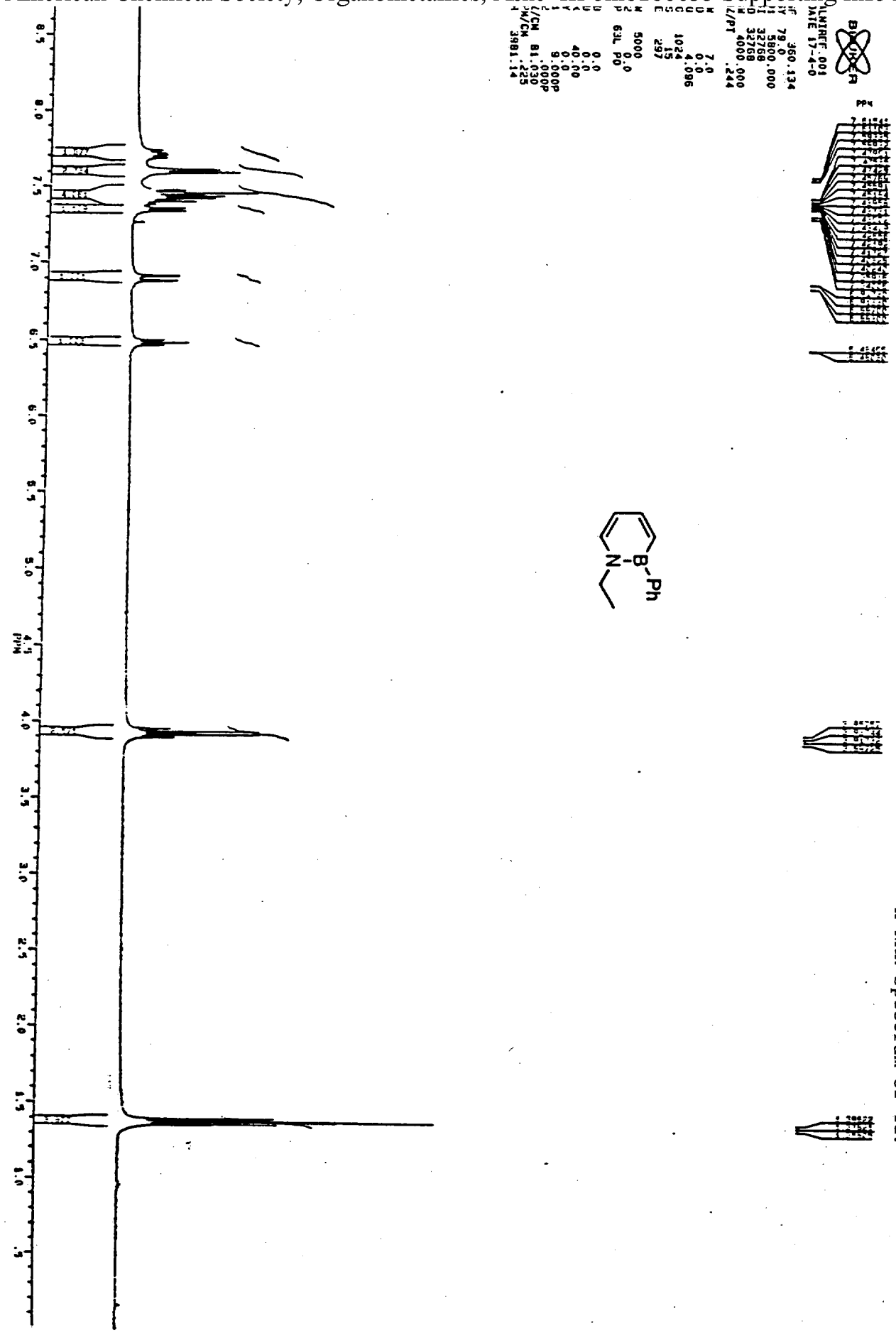

^{1}H NMR spectrum of 1d.

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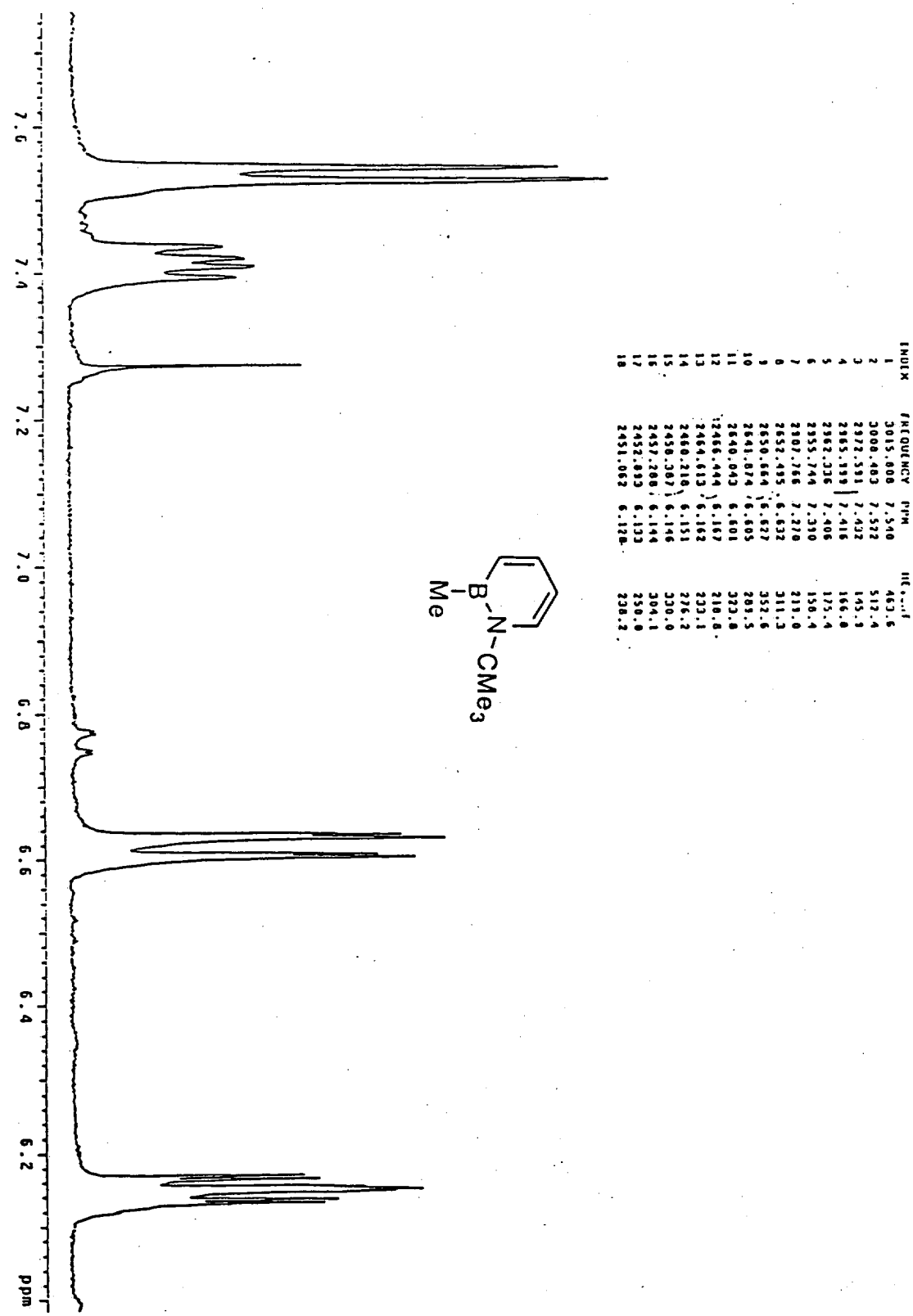

^{1}H NMR spectrum of 1e.

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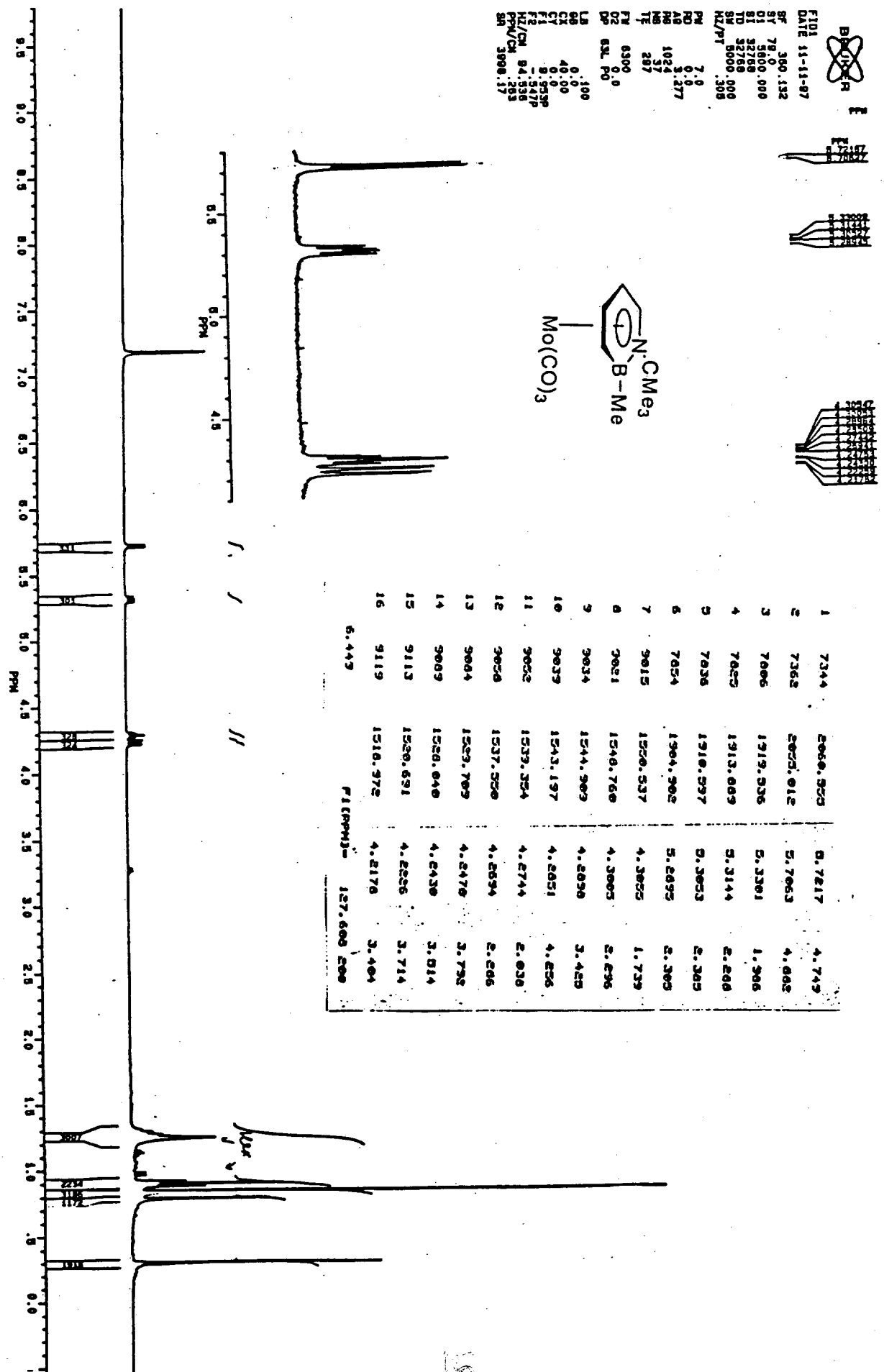

^{1}H NMR spectrum of 5e.

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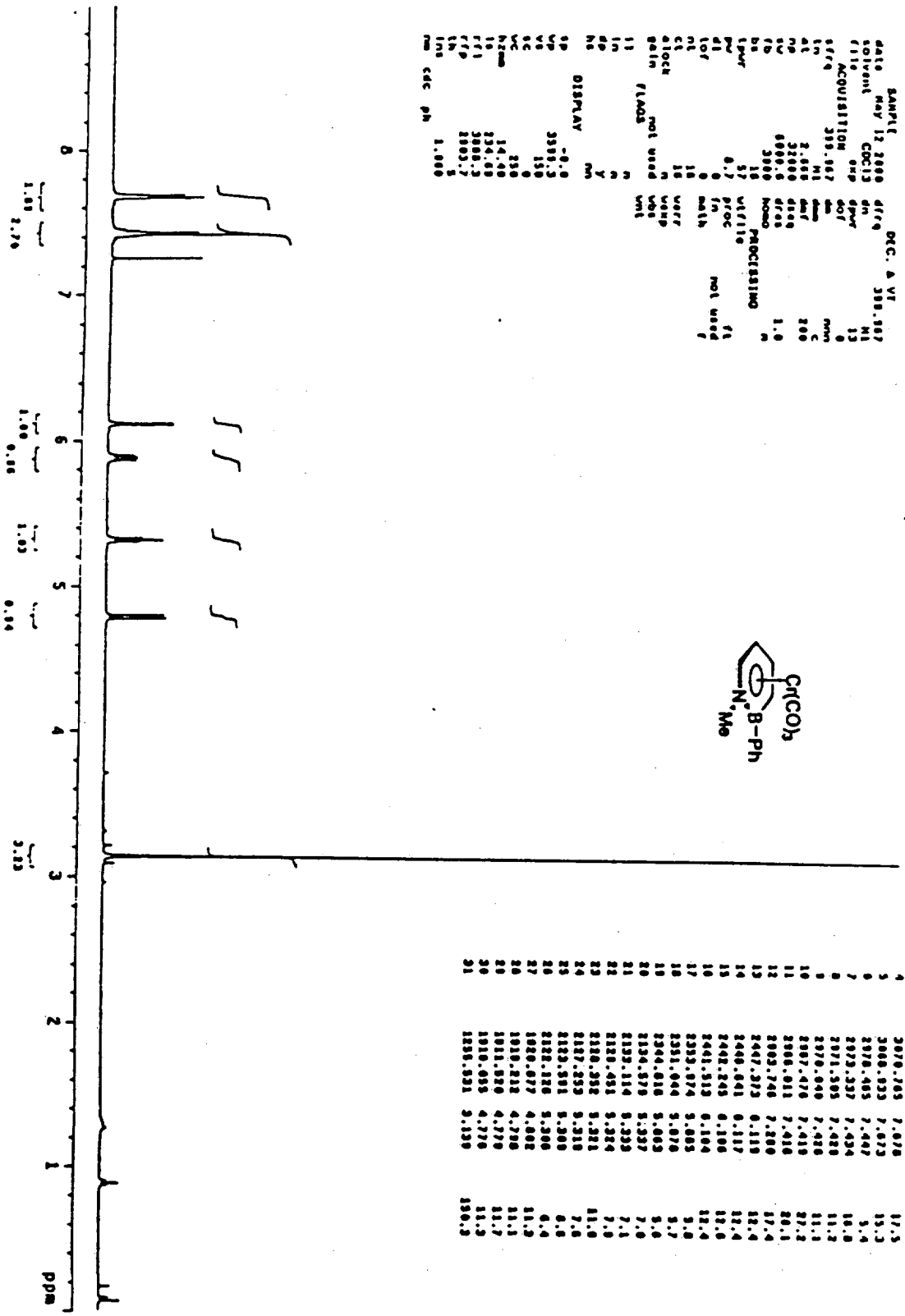

^{1}H NMR spectrum of 6c.