Supporting Information for

Novel Substitutions of 1-Alkoxy- and 1-Arylsulfonyloxy-η^3-Allylmolybdenum Complexes. A Case for η^1-Alkenyl Carbene Complexes as Intermediates

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Table of Contents

General Experimental Methods.

Unless otherwise indicated, all reactions were carried out under a positive pressure of argon in oven- or flame-dried glassware using solvents dried over 4 Å molecular sieves or dispensed and used directly from a Seca Solvent System purchased from Glass Contour. Analytical thin-layer chromatography (TLC) was performed using commercial Merck KGaA aluminum-supported silica gel plates with fluorescent indicator (F-254). Visualization was accomplished using UV light, 5 % phosphomolybdic acid in ethanol, or aqueous $KMnO_4$. Flash column chromatography was carried out using 32-63 μm silica gel, with compressed air as a source of positive pressure. All reagents were used as received, with the exception of amines, which were distilled and stored over 4 Å molecular sieves prior to use.

^1H and ^{13}C NMR spectra were recorded on Mercury 300 (300 MHz ^1H, 75 MHz ^{13}C), Varian INOVA 400 (400 MHz ^1H, 100 MHz ^{13}C), and Varian INOVA 600 (600 MHz ^1H, 150 MHz ^{13}C) instruments in $CDCl_3$, with $CHCl_3$ as internal reference (7.27 ppm for ^1H and 77.23 ppm for ^{13}C), and C_6D_6, with C_6H_6 as internal reference (7.16 ppm for ^1H and 128.39 ppm for ^{13}C). Infrared spectra were recorded on an ASI ReactIR® 1000 FT-IR spectrometer equipped with a silicon probe. Peaks are reported with the following relative intensities: s (strong, 67-100 %), m (medium, 40-67 %), w (weak, 20-40 %), and br (broad). *Since almost all of the Tp molybdenum complexes decompose over 180-200 ^oC, melting points are not significant and are not shown in the experimental section.* Optical rotations were measured with Perkin-Elmer 241MC or Perkin-Elmer Model 341 polarimeters. HPLC was performed using an Agilent 1100 Series with UV detector (254 nm or 210 nm) and Daicel® Chiralpak AS-RH, Chiralpak AD-RH, Chiralcel OJ-RH, Chiralcel OD-RH, or Agilent Eclipse XDB-C8 columns. Samples for HPLC

analysis were prepared by dissolving 1-2 mg of of the pure material in approximately 0.5 mL of acetonitrile. One microliter (1 μL) of the solution was injected for analysis.

Crystal Structure Analysis of (±)-4e.

Crystals of (±)-**4e** were generally poor and twinned, but a suitable crystal of (±)-**4e** was picked and coated with Paratone N oil, suspended in a small fiber loop and placed in a cooled nitrogen gas stream at 173 K on a Bruker D8 APEX II CCD sealed tube diffractometer with graphite monochromated CuK_α (1.54178 Å) radiation. Data were measured using a series of combinations of phi and omega scans with 10 -30 s frame exposures and 0.5^o frame widths. Data collection, indexing and initial cell refinements were all carried out using APEX II[1] software. Frame integration and final cell refinements were done using SAINT[2] software. The final cell parameters were determined from least-squares refinement on 6333 reflections.

The structure was solved using Direct methods and difference Fourier techniques (SHELXTL, V6.12).[3] Hydrogen atoms were placed their expected chemical positions using the HFIX command and were included in the final cycles of least squares with isotropic U_{ij} 's related to the atom's ridden upon. All non-hydrogen atoms were refined anisotropically. Scattering factors and anomalous dispersion corrections are taken from the *International Tables for X-ray Crystallography.*[4] Structure solution, refinement, graphics and generation of publication materials were performed by using SHELXTL, V6.12 software. Additional details of data collection and structure refinement are given in Table S-1.

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[1] APEX II, **2005**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[2] SAINT Version 6.45A, **2003**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[3] SHELXTL V6.12, **2002**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[4] A. J. C. Wilson (ed), *International Tables for X-ray Crystallography, Volume C.* Kynoch, Academic Publishers, Dordrecht, **1992**, Tables 6.1.1.4 (pp. 500-502) and 4.2.6.8 (pp. 219-222).

Table S-1. Crystal data and structure refinement for (±)-4e

Identification code	(±)-**4e**	
Empirical formula	C32 H41 B Mo N6 O5 S	
Formula weight	728.52	
Temperature	173(2) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.2747(5) Å	α= 117.430(2)°.
	b = 14.2031(7) Å	β= 91.938(2)°.
	c = 15.1516(7) Å	γ = 103.496(2)°.
Volume	1699.35(15) $Å^3$	
Z	2	
Density (calculated)	1.424 Mg/m^3	
Absorption coefficient	4.128 mm^{-1}	
F(000)	756	
Crystal size	0.29 x 0.19 x 0.08 mm^3	
Theta range for data collection	8.14 to 65.79°.	
Index ranges	-9<=h<=9, -16<=k<=14, 0<=l<=17	
Reflections collected	7555	
Independent reflections	7555 [R(int) = 0.0284]	
Completeness to theta = 65.79°	76.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7336 and 0.3807	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7555 / 0 / 422	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.0939, wR2 = 0.2227	
R indices (all data)	R1 = 0.0953, wR2 = 0.2246	
Extinction coefficient	0.0013(7)	
Largest diff. peak and hole	2.189 and -1.364 $e.Å^{-3}$	

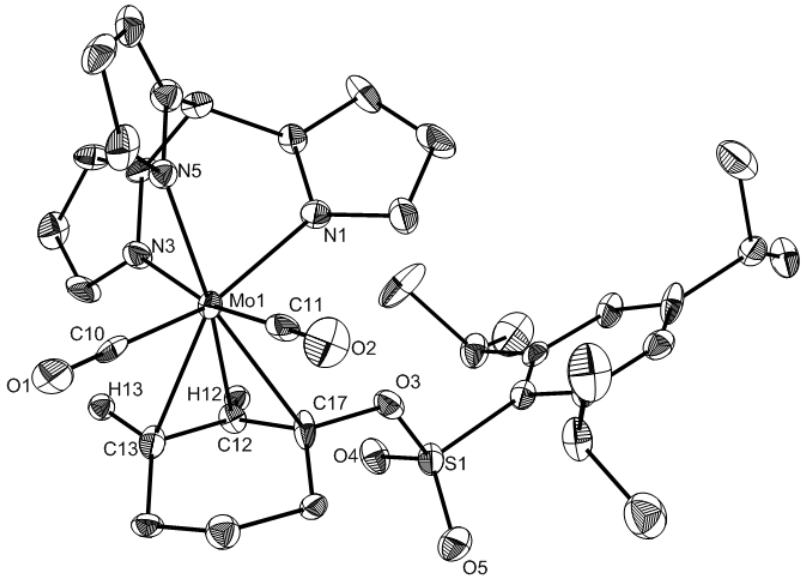


Figure S-1. ORTEP View of the Arylsulfonyloxy Substituted Cyclohexenyl Complex (±)-4e.

Table S-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 4e.**[*]

	x	y	z	U(eq)
B(1)	4104(7)	12334(5)	3712(5)	23(1)
C(1)	1593(7)	9855(5)	3541(4)	29(1)
C(2)	2921(7)	9777(5)	3915(4)	34(1)
C(3)	4026(7)	10638(5)	3967(4)	31(1)
C(4)	2652(6)	11988(5)	1302(4)	25(1)
C(5)	4159(6)	12399(5)	1306(4)	29(1)
C(6)	4881(6)	12572(4)	2189(4)	26(1)
C(7)	1431(7)	13831(5)	4887(5)	27(1)
C(8)	2661(7)	14584(5)	5589(5)	32(1)
C(9)	3833(6)	14121(5)	5268(4)	28(1)
C(10)	-703(6)	12508(4)	2865(4)	25(1)
C(11)	-1115(6)	11184(4)	3619(4)	25(1)
C(12)	-451(6)	10134(4)	1255(4)	20(1)
C(13)	-934(6)	11019(4)	1255(4)	21(1)
C(14)	-2607(6)	10880(5)	1073(5)	28(1)
C(15)	-3483(6)	10449(5)	1707(5)	28(1)
C(16)	-2995(6)	9493(4)	1707(4)	23(1)
C(17)	-1310(6)	9662(4)	1772(4)	20(1)
C(18)	-334(6)	7002(4)	1517(4)	19(1)
C(19)	977(6)	6654(4)	1272(4)	21(1)
C(20)	1431(6)	6135(4)	1763(4)	24(1)
C(21)	686(6)	5968(4)	2486(4)	22(1)
C(22)	-579(6)	6328(5)	2704(4)	25(1)

C(23)	-1130(6)	6855(4)	2241(4)	21(1)
C(24)	1947(6)	6848(5)	534(5)	26(1)
C(25)	2975(7)	8019(5)	1052(5)	41(2)
C(26)	2865(7)	6018(6)	76(5)	39(2)
C(27)	1254(6)	5451(5)	3064(4)	27(1)
C(28)	2349(7)	6330(6)	3994(5)	41(2)
C(29)	1914(7)	4512(5)	2424(5)	40(2)
C(30)	-2550(6)	7211(5)	2574(4)	29(1)
C(31)	-2354(8)	7931(5)	3714(5)	45(2)
C(32)	-3907(7)	6186(6)	2211(5)	41(2)
Mo(1)	376(1)	11476(1)	2825(1)	17(1)
N(1)	1875(5)	10720(4)	3351(3)	24(1)
N(2)	3404(5)	11203(4)	3630(3)	25(1)
N(3)	2440(5)	11911(4)	2136(3)	22(1)
N(4)	3852(5)	12276(4)	2683(3)	22(1)
N(5)	1787(5)	12957(4)	4173(3)	24(1)
N(6)	3304(5)	13152(4)	4425(3)	22(1)
O(1)	-1345(4)	13146(3)	2958(3)	34(1)
O(2)	-2006(5)	11023(3)	4086(3)	38(1)
O(3)	-864(4)	8811(3)	1876(3)	21(1)
O(4)	-233(4)	7781(3)	192(3)	30(1)
O(5)	-2679(4)	7073(3)	543(3)	32(1)
S(1)	-1107(1)	7619(1)	900(1)	22(1)

*U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S-3. Bond lengths [Å] and angles [°] for 4e.

B(1)-N(2)	1.530(7)	C(20)-C(21)	1.395(7)
B(1)-N(4)	1.529(7)	C(20)-H(20)	0.9500
B(1)-N(6)	1.539(7)	C(21)-C(22)	1.378(8)
B(1)-H(1)	1.0000	C(21)-C(27)	1.524(7)
C(1)-N(1)	1.358(6)	C(22)-C(23)	1.397(7)
C(1)-C(2)	1.386(8)	C(22)-H(22)	0.9500
C(1)-H(1)	0.9500	C(23)-C(30)	1.538(7)
C(2)-C(3)	1.368(8)	C(24)-C(25)	1.516(8)
C(2)-H(2)	0.9500	C(24)-C(26)	1.534(7)
C(3)-N(2)	1.345(7)	C(24)-H(24)	1.0000
C(3)-H(3)	0.9500	C(25)-H(25A)	0.9800
C(4)-N(3)	1.334(6)	C(25)-H(25B)	0.9800
C(4)-C(5)	1.382(8)	C(25)-H(25C)	0.9800
C(4)-H(4)	0.9500	C(26)-H(26A)	0.9800
C(5)-C(6)	1.363(8)	C(26)-H(26B)	0.9800
C(5)-H(5)	0.9500	C(26)-H(26C)	0.9800
C(6)-N(4)	1.342(7)	C(27)-C(28)	1.505(9)
C(6)-H(6)	0.9500	C(27)-C(29)	1.524(8)
C(7)-N(5)	1.341(7)	C(27)-H(27)	1.0000
C(7)-C(8)	1.370(9)	C(28)-H(28A)	0.9800
C(7)-H(7)	0.9500	C(28)-H(28B)	0.9800
C(8)-C(9)	1.387(8)	C(28)-H(28C)	0.9800
C(8)-H(8)	0.9500	C(29)-H(29A)	0.9800
C(9)-N(6)	1.338(7)	C(29)-H(29B)	0.9800
C(9)-H(9)	0.9500	C(29)-H(29C)	0.9800
C(10)-O(1)	1.156(6)	C(30)-C(31)	1.525(9)
C(10)-Mo(1)	1.939(5)	C(30)-C(32)	1.538(9)
C(11)-O(2)	1.156(7)	C(30)-H(30)	1.0000
C(11)-Mo(1)	1.957(6)	C(31)-H(31A)	0.9800
C(12)-C(17)	1.405(7)	C(31)-H(31B)	0.9800
C(12)-C(13)	1.429(7)	C(31)-H(31C)	0.9800
C(12)-Mo(1)	2.213(5)	C(32)-H(32A)	0.9800
C(12)-H(12)	0.9500	C(32)-H(32B)	0.9800
C(13)-C(14)	1.517(8)	C(32)-H(32C)	0.9800
C(13)-Mo(1)	2.361(5)	Mo(1)-N(5)	2.210(5)
C(13)-H(13)	0.9500	Mo(1)-N(1)	2.265(4)
C(14)-C(15)	1.524(7)	Mo(1)-N(3)	2.306(4)
C(14)-H(14A)	0.9900	N(1)-N(2)	1.378(6)
C(14)-H(14B)	0.9900	N(3)-N(4)	1.373(6)
C(15)-C(16)	1.528(7)	N(5)-N(6)	1.373(6)
C(15)-H(15A)	0.9900	O(3)-S(1)	1.611(4)
C(15)-H(15B)	0.9900	O(4)-S(1)	1.434(4)
C(16)-C(17)	1.517(7)	O(5)-S(1)	1.433(4)
C(16)-H(16A)	0.9900	N(2)-B(1)-N(4)	110.5(5)
C(16)-H(16B)	0.9900	N(2)-B(1)-N(6)	108.2(4)
C(17)-O(3)	1.436(5)	N(4)-B(1)-N(6)	107.6(4)
C(17)-Mo(1)	2.407(5)	N(2)-B(1)-H(1)	110.2
C(18)-C(23)	1.409(7)	N(4)-B(1)-H(1)	110.2
C(18)-C(19)	1.416(7)	N(6)-B(1)-H(1)	110.2
C(18)-S(1)	1.777(5)	N(1)-C(1)-C(2)	110.2(5)
C(19)-C(20)	1.380(7)	N(1)-C(1)-H(1)	124.9
C(19)-C(24)	1.540(7)	C(2)-C(1)-H(1)	124.9

C(3)-C(2)-C(1)	105.6(5)	C(12)-C(17)-O(3)	117.2(4)
C(3)-C(2)-H(2)	127.2	C(12)-C(17)-C(16)	122.2(4)
C(1)-C(2)-H(2)	127.2	O(3)-C(17)-C(16)	112.0(4)
N(2)-C(3)-C(2)	109.0(5)	C(12)-C(17)-Mo(1)	64.9(3)
N(2)-C(3)-H(3)	125.5	O(3)-C(17)-Mo(1)	113.0(3)
C(2)-C(3)-H(3)	125.5	C(16)-C(17)-Mo(1)	119.7(3)
N(3)-C(4)-C(5)	111.2(5)	C(23)-C(18)-C(19)	122.4(4)
N(3)-C(4)-H(4)	124.4	C(23)-C(18)-S(1)	115.9(4)
C(5)-C(4)-H(4)	124.4	C(19)-C(18)-S(1)	121.7(4)
C(6)-C(5)-C(4)	105.2(5)	C(20)-C(19)-C(18)	116.6(4)
C(6)-C(5)-H(5)	127.4	C(20)-C(19)-C(24)	118.4(4)
C(4)-C(5)-H(5)	127.4	C(18)-C(19)-C(24)	124.9(4)
N(4)-C(6)-C(5)	108.5(5)	C(19)-C(20)-C(21)	123.4(5)
N(4)-C(6)-H(6)	125.8	C(19)-C(20)-H(20)	118.3
C(5)-C(6)-H(6)	125.8	C(21)-C(20)-H(20)	118.3
N(5)-C(7)-C(8)	111.8(5)	C(22)-C(21)-C(20)	117.9(4)
N(5)-C(7)-H(7)	124.1	C(22)-C(21)-C(27)	119.5(5)
C(8)-C(7)-H(7)	124.1	C(20)-C(21)-C(27)	122.6(5)
C(7)-C(8)-C(9)	104.2(5)	C(21)-C(22)-C(23)	122.9(5)
C(7)-C(8)-H(8)	127.9	C(21)-C(22)-H(22)	118.6
C(9)-C(8)-H(8)	127.9	C(23)-C(22)-H(22)	118.6
N(6)-C(9)-C(8)	109.2(5)	C(22)-C(23)-C(18)	116.9(5)
N(6)-C(9)-H(9)	125.4	C(22)-C(23)-C(30)	116.3(4)
C(8)-C(9)-H(9)	125.4	C(18)-C(23)-C(30)	126.8(4)
O(1)-C(10)-Mo(1)	175.3(5)	C(25)-C(24)-C(26)	110.2(5)
O(2)-C(11)-Mo(1)	178.9(4)	C(25)-C(24)-C(19)	110.0(5)
C(17)-C(12)-C(13)	112.3(4)	C(26)-C(24)-C(19)	113.5(4)
C(17)-C(12)-Mo(1)	80.0(3)	C(25)-C(24)-H(24)	107.6
C(13)-C(12)-Mo(1)	77.5(3)	C(26)-C(24)-H(24)	107.6
C(17)-C(12)-H(12)	123.8	C(19)-C(24)-H(24)	107.6
C(13)-C(12)-H(12)	123.8	C(24)-C(25)-H(25A)	109.5
Mo(1)-C(12)-H(12)	110.5	C(24)-C(25)-H(25B)	109.5
C(12)-C(13)-C(14)	118.6(4)	H(25A)-C(25)-H(25B)	109.5
C(12)-C(13)-Mo(1)	66.3(3)	C(24)-C(25)-H(25C)	109.5
C(14)-C(13)-Mo(1)	122.9(3)	H(25A)-C(25)-H(25C)	109.5
C(12)-C(13)-H(13)	120.7	H(25B)-C(25)-H(25C)	109.5
C(14)-C(13)-H(13)	120.7	C(24)-C(26)-H(26A)	109.5
Mo(1)-C(13)-H(13)	82.1	C(24)-C(26)-H(26B)	109.5
C(13)-C(14)-C(15)	113.2(4)	H(26A)-C(26)-H(26B)	109.5
C(13)-C(14)-H(14A)	108.9	C(24)-C(26)-H(26C)	109.5
C(15)-C(14)-H(14A)	108.9	H(26A)-C(26)-H(26C)	109.5
C(13)-C(14)-H(14B)	108.9	H(26B)-C(26)-H(26C)	109.5
C(15)-C(14)-H(14B)	108.9	C(28)-C(27)-C(21)	110.2(5)
H(14A)-C(14)-H(14B)	107.8	C(28)-C(27)-C(29)	111.6(5)
C(14)-C(15)-C(16)	111.6(4)	C(21)-C(27)-C(29)	113.6(5)
C(14)-C(15)-H(15A)	109.3	C(28)-C(27)-H(27)	107.0
C(16)-C(15)-H(15A)	109.3	C(21)-C(27)-H(27)	107.0
C(14)-C(15)-H(15B)	109.3	C(29)-C(27)-H(27)	107.0
C(16)-C(15)-H(15B)	109.3	C(27)-C(28)-H(28A)	109.5
H(15A)-C(15)-H(15B)	108.0	C(27)-C(28)-H(28B)	109.5
C(17)-C(16)-C(15)	113.1(4)	H(28A)-C(28)-H(28B)	109.5
C(17)-C(16)-H(16A)	109.0	C(27)-C(28)-H(28C)	109.5
C(15)-C(16)-H(16A)	109.0	H(28A)-C(28)-H(28C)	109.5
C(17)-C(16)-H(16B)	109.0	H(28B)-C(28)-H(28C)	109.5
C(15)-C(16)-H(16B)	109.0	C(27)-C(29)-H(29A)	109.5
H(16A)-C(16)-H(16B)	107.8	C(27)-C(29)-H(29B)	109.5

H(29A)-C(29)-H(29B)	109.5
C(27)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(31)-C(30)-C(23)	111.9(5)
C(31)-C(30)-C(32)	110.3(5)
C(23)-C(30)-C(32)	110.0(4)
C(31)-C(30)-H(30)	108.2
C(23)-C(30)-H(30)	108.2
C(32)-C(30)-H(30)	108.2
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(10)-Mo(1)-C(11)	83.0(2)
C(10)-Mo(1)-N(5)	82.4(2)
C(11)-Mo(1)-N(5)	92.0(2)
C(10)-Mo(1)-C(12)	100.4(2)
C(11)-Mo(1)-C(12)	105.8(2)
N(5)-Mo(1)-C(12)	162.15(18)
C(10)-Mo(1)-N(1)	160.0(2)
C(11)-Mo(1)-N(1)	90.04(18)
N(5)-Mo(1)-N(1)	79.14(17)
C(12)-Mo(1)-N(1)	99.57(18)
C(10)-Mo(1)-N(3)	102.05(17)
C(11)-Mo(1)-N(3)	169.8(2)
N(5)-Mo(1)-N(3)	79.95(16)
C(12)-Mo(1)-N(3)	82.24(17)
N(1)-Mo(1)-N(3)	82.29(15)
C(10)-Mo(1)-C(13)	65.0(2)
C(11)-Mo(1)-C(13)	107.6(2)
N(5)-Mo(1)-C(13)	138.65(16)
C(12)-Mo(1)-C(13)	36.24(17)
N(1)-Mo(1)-C(13)	134.91(17)
N(3)-Mo(1)-C(13)	82.61(16)
C(10)-Mo(1)-C(17)	105.9(2)
C(11)-Mo(1)-C(17)	72.2(2)
N(5)-Mo(1)-C(17)	160.74(16)
C(12)-Mo(1)-C(17)	35.10(17)
N(1)-Mo(1)-C(17)	89.60(16)
N(3)-Mo(1)-C(17)	114.24(16)
C(13)-Mo(1)-C(17)	59.19(16)
C(1)-N(1)-N(2)	105.7(4)
C(1)-N(1)-Mo(1)	133.2(4)
N(2)-N(1)-Mo(1)	120.9(3)
C(3)-N(2)-N(1)	109.5(4)
C(3)-N(2)-B(1)	128.9(5)
N(1)-N(2)-B(1)	120.6(4)
C(4)-N(3)-N(4)	105.2(4)
C(4)-N(3)-Mo(1)	135.3(4)
N(4)-N(3)-Mo(1)	119.3(3)
C(6)-N(4)-N(3)	109.9(4)
C(6)-N(4)-B(1)	128.2(5)
N(3)-N(4)-B(1)	121.9(4)
C(7)-N(5)-N(6)	105.7(5)
C(7)-N(5)-Mo(1)	130.6(4)
N(6)-N(5)-Mo(1)	123.7(3)
C(9)-N(6)-N(5)	109.1(4)
C(9)-N(6)-B(1)	131.6(5)
N(5)-N(6)-B(1)	119.1(4)
C(17)-O(3)-S(1)	119.6(3)
O(5)-S(1)-O(4)	116.6(2)
O(5)-S(1)-O(3)	110.2(2)
O(4)-S(1)-O(3)	107.6(2)
O(5)-S(1)-C(18)	109.8(2)
O(4)-S(1)-C(18)	113.8(2)
O(3)-S(1)-C(18)	97.0(2)

Symmetry transformations used to generate equivalent atoms:

*Table S-4. Anisotropic displacement parameters (Å²x 10³)for 4e.**

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	21(3)	23(4)	19(4)	8(3)	-3(2)	-1(3)
C(1)	39(4)	22(3)	25(4)	14(3)	-2(3)	2(3)
C(2)	49(4)	27(3)	30(4)	16(3)	-3(3)	12(3)
C(3)	38(4)	33(4)	25(4)	14(3)	-2(3)	14(3)
C(4)	28(3)	30(3)	20(3)	14(3)	5(2)	7(3)
C(5)	25(3)	39(4)	28(4)	21(3)	9(2)	7(3)
C(6)	24(3)	24(3)	28(4)	13(3)	5(2)	4(2)
C(7)	30(3)	25(3)	27(4)	14(3)	9(3)	7(3)
C(8)	46(4)	20(3)	25(4)	9(3)	8(3)	5(3)
C(9)	27(3)	24(4)	25(4)	13(3)	-4(2)	-6(2)
C(10)	20(3)	20(3)	33(4)	15(3)	4(2)	0(2)
C(11)	28(3)	17(3)	27(4)	10(3)	-1(3)	3(2)
C(12)	26(3)	14(3)	13(3)	4(3)	0(2)	-1(2)
C(13)	26(3)	16(3)	19(3)	8(3)	-2(2)	0(2)
C(14)	27(3)	24(3)	36(4)	18(3)	-2(3)	5(2)
C(15)	19(3)	25(3)	38(4)	15(3)	-1(2)	2(2)
C(16)	23(3)	17(3)	25(3)	9(3)	1(2)	1(2)
C(17)	25(3)	11(3)	20(3)	7(3)	-1(2)	2(2)
C(18)	23(3)	13(3)	19(3)	11(3)	-3(2)	-2(2)
C(19)	24(3)	15(3)	18(3)	8(3)	-1(2)	-2(2)
C(20)	23(3)	23(3)	25(3)	14(3)	3(2)	3(2)
C(21)	26(3)	14(3)	22(3)	10(3)	-1(2)	-1(2)
C(22)	29(3)	23(3)	25(3)	16(3)	4(2)	2(2)
C(23)	26(3)	14(3)	17(3)	6(3)	0(2)	2(2)
C(24)	29(3)	24(3)	31(4)	17(3)	8(2)	7(3)
C(25)	36(4)	40(4)	47(4)	26(4)	11(3)	-3(3)
C(26)	40(4)	48(4)	42(4)	29(4)	19(3)	17(3)
C(27)	28(3)	31(3)	31(4)	21(3)	2(2)	7(3)
C(28)	49(4)	40(4)	33(4)	17(4)	-7(3)	12(3)
C(29)	52(4)	36(4)	46(4)	26(4)	8(3)	21(3)
C(30)	28(3)	34(3)	38(4)	25(3)	14(3)	13(3)
C(31)	53(4)	37(4)	48(5)	20(4)	26(3)	15(3)
C(32)	27(3)	52(4)	54(5)	32(4)	13(3)	13(3)
Mo(1)	19(1)	14(1)	19(1)	10(1)	3(1)	2(1)
N(1)	27(3)	21(3)	25(3)	14(2)	1(2)	4(2)
N(2)	25(3)	25(3)	23(3)	12(2)	0(2)	4(2)
N(3)	19(3)	23(3)	25(3)	14(2)	4(2)	5(2)
N(4)	19(2)	23(3)	23(3)	13(2)	2(2)	2(2)
N(5)	22(3)	24(3)	28(3)	15(3)	6(2)	3(2)
N(6)	24(3)	20(3)	18(3)	11(3)	0(2)	-3(2)
O(1)	29(2)	19(2)	52(3)	16(2)	4(2)	6(2)
O(2)	38(3)	39(3)	36(3)	21(2)	19(2)	3(2)
O(3)	27(2)	15(2)	23(2)	13(2)	1(2)	2(2)
O(4)	47(2)	30(2)	24(2)	18(2)	10(2)	18(2)
O(5)	31(2)	24(2)	33(3)	12(2)	-12(2)	1(2)

S(1)	29(1)	17(1)	19(1)	11(1)	1(1)	4(1)

* The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

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

	x	y	z	U(eq)
H(1)	5203	12592	3980	28
H(1)	626	9372	3434	35
H(2)	3039	9239	4096	41
H(3)	5064	10810	4204	38
H(4)	1868	11787	775	30
H(5)	4597	12532	802	35
H(6)	5936	12854	2416	31
H(7)	446	13917	4904	32
H(8)	2703	15266	6164	39
H(9)	4850	14441	5596	33
H(12)	359	9892	941	24
H(13)	-223	11680	1366	25
H(14A)	-3009	10361	351	34
H(14B)	-2765	11602	1226	34
H(15A)	-4570	10196	1437	33
H(15B)	-3322	11056	2408	33
H(16A)	-3319	9403	2286	28
H(16B)	-3509	8802	1083	28
H(20)	2296	5878	1602	28
H(22)	-1100	6214	3191	30
H(24)	1253	6767	-32	31
H(25A)	3694	8115	1597	62
H(25B)	2375	8542	1332	62
H(25C)	3522	8157	562	62
H(26A)	3720	6201	580	58
H(26B)	3234	6053	-510	58
H(26C)	2228	5271	-135	58
H(27)	368	5129	3296	33
H(28A)	3263	6636	3797	62
H(28B)	2606	6006	4405	62
H(28C)	1892	6921	4386	62
H(29A)	2803	4799	2195	60
H(29B)	1162	3944	1839	60
H(29C)	2201	4189	2828	60
H(30)	-2753	7651	2251	35
H(31A)	-3239	8203	3890	68
H(31B)	-1456	8560	3941	68
H(31C)	-2242	7494	4045	68
H(32A)	-3731	5742	2521	61
H(32B)	-4041	5743	1476	61
H(32C)	-4813	6420	2405	61

Table S-6. Torsion angles [°] for 4e.

N(1)-C(1)-C(2)-C(3)	1.2(7)
C(1)-C(2)-C(3)-N(2)	-0.8(7)
N(3)-C(4)-C(5)-C(6)	0.2(6)
C(4)-C(5)-C(6)-N(4)	0.1(6)
N(5)-C(7)-C(8)-C(9)	-0.1(6)
C(7)-C(8)-C(9)-N(6)	0.1(6)
C(17)-C(12)-C(13)-C(14)	-42.3(7)
Mo(1)-C(12)-C(13)-C(14)	-115.8(4)
C(17)-C(12)-C(13)-Mo(1)	73.5(4)
C(12)-C(13)-C(14)-C(15)	47.7(7)
Mo(1)-C(13)-C(14)-C(15)	-31.1(6)
C(13)-C(14)-C(15)-C(16)	-44.7(7)
C(14)-C(15)-C(16)-C(17)	40.0(7)
C(13)-C(12)-C(17)-O(3)	-176.1(4)
Mo(1)-C(12)-C(17)-O(3)	-104.2(4)
C(13)-C(12)-C(17)-C(16)	38.7(7)
Mo(1)-C(12)-C(17)-C(16)	110.6(5)
C(13)-C(12)-C(17)-Mo(1)	-71.9(4)
C(15)-C(16)-C(17)-C(12)	-39.2(7)
C(15)-C(16)-C(17)-O(3)	174.0(4)
C(15)-C(16)-C(17)-Mo(1)	38.2(6)
C(23)-C(18)-C(19)-C(20)	1.4(8)
S(1)-C(18)-C(19)-C(20)	-176.8(4)
C(23)-C(18)-C(19)-C(24)	-176.3(5)
S(1)-C(18)-C(19)-C(24)	5.5(7)
C(18)-C(19)-C(20)-C(21)	-1.3(8)
C(24)-C(19)-C(20)-C(21)	176.5(5)
C(19)-C(20)-C(21)-C(22)	0.9(8)
C(19)-C(20)-C(21)-C(27)	-176.5(5)
C(20)-C(21)-C(22)-C(23)	-0.5(8)
C(27)-C(21)-C(22)-C(23)	177.0(6)
C(21)-C(22)-C(23)-C(18)	0.5(8)
C(21)-C(22)-C(23)-C(30)	-179.7(5)
C(19)-C(18)-C(23)-C(22)	-1.0(8)
S(1)-C(18)-C(23)-C(22)	177.3(4)
C(19)-C(18)-C(23)-C(30)	179.3(5)
S(1)-C(18)-C(23)-C(30)	-2.4(7)
C(20)-C(19)-C(24)-C(25)	-97.9(6)
C(18)-C(19)-C(24)-C(25)	79.8(7)
C(20)-C(19)-C(24)-C(26)	26.1(8)
C(18)-C(19)-C(24)-C(26)	-156.2(6)
C(22)-C(21)-C(27)-C(28)	-89.7(6)
C(20)-C(21)-C(27)-C(28)	87.6(6)
C(22)-C(21)-C(27)-C(29)	144.2(5)
C(20)-C(21)-C(27)-C(29)	-38.4(8)
C(22)-C(23)-C(30)-C(31)	54.4(6)
C(18)-C(23)-C(30)-C(31)	-125.9(6)
C(22)-C(23)-C(30)-C(32)	-68.6(6)
C(18)-C(23)-C(30)-C(32)	111.1(6)
O(1)-C(10)-Mo(1)-C(11)	45(5)
O(1)-C(10)-Mo(1)-N(5)	-48(5)

O(1)-C(10)-Mo(1)-C(12)	149(5)
O(1)-C(10)-Mo(1)-N(1)	-26(6)
O(1)-C(10)-Mo(1)-N(3)	-126(5)
O(1)-C(10)-Mo(1)-C(13)	158(5)
O(1)-C(10)-Mo(1)-C(17)	114(5)
O(2)-C(11)-Mo(1)-C(10)	4(31)
O(2)-C(11)-Mo(1)-N(5)	86(31)
O(2)-C(11)-Mo(1)-C(12)	-95(31)
O(2)-C(11)-Mo(1)-N(1)	165(31)
O(2)-C(11)-Mo(1)-N(3)	124(30)
O(2)-C(11)-Mo(1)-C(13)	-57(31)
O(2)-C(11)-Mo(1)-C(17)	-105(31)
C(17)-C(12)-Mo(1)-C(10)	-102.9(3)
C(13)-C(12)-Mo(1)-C(10)	12.8(3)
C(17)-C(12)-Mo(1)-C(11)	-17.4(3)
C(13)-C(12)-Mo(1)-C(11)	98.4(3)
C(17)-C(12)-Mo(1)-N(5)	159.7(5)
C(13)-C(12)-Mo(1)-N(5)	-84.6(6)
C(17)-C(12)-Mo(1)-N(1)	75.4(3)
C(13)-C(12)-Mo(1)-N(1)	-168.9(3)
C(17)-C(12)-Mo(1)-N(3)	156.2(3)
C(13)-C(12)-Mo(1)-N(3)	-88.1(3)
C(17)-C(12)-Mo(1)-C(13)	-115.8(4)
C(13)-C(12)-Mo(1)-C(17)	115.8(4)
C(12)-C(13)-Mo(1)-C(10)	-166.1(3)
C(14)-C(13)-Mo(1)-C(10)	-56.3(4)
C(12)-C(13)-Mo(1)-C(11)	-92.9(3)
C(14)-C(13)-Mo(1)-C(11)	16.9(4)
C(12)-C(13)-Mo(1)-N(5)	152.5(3)
C(14)-C(13)-Mo(1)-N(5)	-97.7(4)
C(14)-C(13)-Mo(1)-C(12)	109.8(5)
C(12)-C(13)-Mo(1)-N(1)	15.6(4)
C(14)-C(13)-Mo(1)-N(1)	125.4(4)
C(12)-C(13)-Mo(1)-N(3)	86.9(3)
C(14)-C(13)-Mo(1)-N(3)	-163.3(4)
C(12)-C(13)-Mo(1)-C(17)	-37.1(3)
C(14)-C(13)-Mo(1)-C(17)	72.7(4)
C(12)-C(17)-Mo(1)-C(10)	85.4(3)
O(3)-C(17)-Mo(1)-C(10)	-164.1(3)
C(16)-C(17)-Mo(1)-C(10)	-28.8(4)
C(12)-C(17)-Mo(1)-C(11)	162.4(3)
O(3)-C(17)-Mo(1)-C(11)	-87.2(3)
C(16)-C(17)-Mo(1)-C(11)	48.2(4)
C(12)-C(17)-Mo(1)-N(5)	-161.2(4)
O(3)-C(17)-Mo(1)-N(5)	-50.7(7)
C(16)-C(17)-Mo(1)-N(5)	84.6(6)
O(3)-C(17)-Mo(1)-C(12)	110.4(5)
C(16)-C(17)-Mo(1)-C(12)	-114.2(5)
C(12)-C(17)-Mo(1)-N(1)	-107.4(3)
O(3)-C(17)-Mo(1)-N(1)	3.0(3)
C(16)-C(17)-Mo(1)-N(1)	138.4(4)
C(12)-C(17)-Mo(1)-N(3)	-26.0(3)
O(3)-C(17)-Mo(1)-N(3)	84.4(3)

C(16)-C(17)-Mo(1)-N(3)	-140.3(3)
C(12)-C(17)-Mo(1)-C(13)	38.3(3)
O(3)-C(17)-Mo(1)-C(13)	148.7(4)
C(16)-C(17)-Mo(1)-C(13)	-75.9(4)
C(2)-C(1)-N(1)-N(2)	-1.2(6)
C(2)-C(1)-N(1)-Mo(1)	-176.1(4)
C(10)-Mo(1)-N(1)-C(1)	105.6(7)
C(11)-Mo(1)-N(1)-C(1)	36.5(5)
N(5)-Mo(1)-N(1)-C(1)	128.6(5)
C(12)-Mo(1)-N(1)-C(1)	-69.5(5)
N(3)-Mo(1)-N(1)-C(1)	-150.3(5)
C(13)-Mo(1)-N(1)-C(1)	-78.8(6)
C(17)-Mo(1)-N(1)-C(1)	-35.7(5)
C(10)-Mo(1)-N(1)-N(2)	-68.7(6)
C(11)-Mo(1)-N(1)-N(2)	-137.8(4)
N(5)-Mo(1)-N(1)-N(2)	-45.7(4)
C(12)-Mo(1)-N(1)-N(2)	116.2(4)
N(3)-Mo(1)-N(1)-N(2)	35.5(4)
C(13)-Mo(1)-N(1)-N(2)	106.9(4)
C(17)-Mo(1)-N(1)-N(2)	150.0(4)
C(2)-C(3)-N(2)-N(1)	0.1(7)
C(2)-C(3)-N(2)-B(1)	168.0(5)
C(1)-N(1)-N(2)-C(3)	0.7(6)
Mo(1)-N(1)-N(2)-C(3)	176.4(4)
C(1)-N(1)-N(2)-B(1)	-168.4(5)
Mo(1)-N(1)-N(2)-B(1)	7.3(6)
N(4)-B(1)-N(2)-C(3)	130.2(6)
N(6)-B(1)-N(2)-C(3)	-112.3(6)
N(4)-B(1)-N(2)-N(1)	-63.0(6)
N(6)-B(1)-N(2)-N(1)	54.5(6)
C(5)-C(4)-N(3)-N(4)	-0.4(6)
C(5)-C(4)-N(3)-Mo(1)	173.7(4)
C(10)-Mo(1)-N(3)-C(4)	-54.3(5)
C(11)-Mo(1)-N(3)-C(4)	-172.9(9)
N(5)-Mo(1)-N(3)-C(4)	-134.2(5)
C(12)-Mo(1)-N(3)-C(4)	44.7(5)
N(1)-Mo(1)-N(3)-C(4)	145.5(5)
C(13)-Mo(1)-N(3)-C(4)	8.1(5)
C(17)-Mo(1)-N(3)-C(4)	59.4(5)
C(10)-Mo(1)-N(3)-N(4)	119.1(4)
C(11)-Mo(1)-N(3)-N(4)	0.6(11)
N(5)-Mo(1)-N(3)-N(4)	39.2(3)
C(12)-Mo(1)-N(3)-N(4)	-141.9(4)
N(1)-Mo(1)-N(3)-N(4)	-41.1(3)
C(13)-Mo(1)-N(3)-N(4)	-178.5(4)
C(17)-Mo(1)-N(3)-N(4)	-127.1(3)
C(5)-C(6)-N(4)-N(3)	-0.3(6)
C(5)-C(6)-N(4)-B(1)	-179.0(5)
C(4)-N(3)-N(4)-C(6)	0.4(6)
Mo(1)-N(3)-N(4)-C(6)	-174.8(3)
C(4)-N(3)-N(4)-B(1)	179.2(4)
Mo(1)-N(3)-N(4)-B(1)	4.0(6)
N(2)-B(1)-N(4)-C(6)	-125.6(5)

N(6)-B(1)-N(4)-C(6)	116.6(6)
N(2)-B(1)-N(4)-N(3)	55.9(6)
N(6)-B(1)-N(4)-N(3)	-61.9(6)
C(8)-C(7)-N(5)-N(6)	0.1(6)
C(8)-C(7)-N(5)-Mo(1)	-178.9(3)
C(10)-Mo(1)-N(5)-C(7)	31.7(4)
C(11)-Mo(1)-N(5)-C(7)	-50.9(5)
C(12)-Mo(1)-N(5)-C(7)	131.9(6)
N(1)-Mo(1)-N(5)-C(7)	-140.6(4)
N(3)-Mo(1)-N(5)-C(7)	135.4(4)
C(13)-Mo(1)-N(5)-C(7)	68.9(5)
C(17)-Mo(1)-N(5)-C(7)	-85.4(6)
C(10)-Mo(1)-N(5)-N(6)	-147.2(4)
C(11)-Mo(1)-N(5)-N(6)	130.2(4)
C(12)-Mo(1)-N(5)-N(6)	-46.9(7)
N(1)-Mo(1)-N(5)-N(6)	40.6(3)
N(3)-Mo(1)-N(5)-N(6)	-43.4(3)
C(13)-Mo(1)-N(5)-N(6)	-109.9(4)
C(17)-Mo(1)-N(5)-N(6)	95.8(6)
C(8)-C(9)-N(6)-N(5)	0.0(5)
C(8)-C(9)-N(6)-B(1)	175.2(5)
C(7)-N(5)-N(6)-C(9)	-0.1(5)
Mo(1)-N(5)-N(6)-C(9)	179.0(3)
C(7)-N(5)-N(6)-B(1)	-175.9(4)
Mo(1)-N(5)-N(6)-B(1)	3.1(5)
N(2)-B(1)-N(6)-C(9)	124.1(5)
N(4)-B(1)-N(6)-C(9)	-116.5(5)
N(2)-B(1)-N(6)-N(5)	-61.1(6)
N(4)-B(1)-N(6)-N(5)	58.2(5)
C(12)-C(17)-O(3)-S(1)	-70.5(5)
C(16)-C(17)-O(3)-S(1)	78.1(5)
Mo(1)-C(17)-O(3)-S(1)	-143.1(2)
C(17)-O(3)-S(1)-O(5)	-66.6(4)
C(17)-O(3)-S(1)-O(4)	61.5(4)
C(17)-O(3)-S(1)-C(18)	179.2(3)
C(23)-C(18)-S(1)-O(5)	-49.0(5)
C(19)-C(18)-S(1)-O(5)	129.3(4)
C(23)-C(18)-S(1)-O(4)	178.2(4)
C(19)-C(18)-S(1)-O(4)	-3.5(5)
C(23)-C(18)-S(1)-O(3)	65.5(4)
C(19)-C(18)-S(1)-O(3)	-116.2(4)

Symmetry transformations used to generate equivalent atoms:

Crystal Structure Analysis of (1*S*, *R*)-11.

A suitable crystal of (1*S*, *R*)-**11** was coated with Paratone N oil, suspended in a small fiber loop and placed in a cooled nitrogen gas stream at 173 K on a Bruker D8 SMART APEX CCD sealed tube diffractometer with graphite monochromated MoK_α (0.71073Å) radiation.

Data were measured using a series of combinations of phi and omega scans with 5 s frame exposures and 0.3° frame widths. Data collection, indexing and initial cell refinements were all carried out using SMART[5] software. Frame integration and final cell refinements were done using SAINT[6] software. The final cell parameters were determined from least-squares refinement on 8460 reflections. The SADABS[7] program was used to carry out absorption corrections.

The structure was solved using Direct methods and difference Fourier techniques (SHELXTL, V6.12).[8] Hydrogen atoms were placed their expected chemical positions using the HFIX command and were included in the final cycles of least squares with isotropic U_{ij} 's related to the atom's ridden upon. The C-H distances were fixed at 0.93 Å(aromatic and amide), 0.98 Å (methine), 0.97 Å (methylene), or 0.96 Å (methyl). All non-hydrogen atoms were refined anisotropically. Scattering factors and anomalous dispersion corrections are taken from the *International Tables for X-ray Crystallography.*[9] Structure solution, refinement, graphics and generation of publication materials were performed by using SHELXTL, V6.12 software. Additional details of data collection and structure refinement are given in Table S-7.

Table S-7. Crystal data and structure refinement for (1S, R)-11.

Identification code	(1*S*, *R*)-**11**
Empirical formula	C24 H27 B Mo N6 O7

[5] SMART Version 5.628, **2003**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[6] SAINT Version 6.45A, **2003**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[7] SADABS Version 2.10, **2003**, George Sheldrick, University of Göttingen.
[8] SHELXTL V6.12, **2002**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[9] A. J. C. Wilson (ed), *International Tables for X-ray Crystallography, Volume C.* Kynoch, Academic Publishers, Dordrecht, **1992**, Tables 6.1.1.4 (pp. 500-502) and 4.2.6.8 (pp. 219-222).

Formula weight	618.27	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 7.9080(6) Å	α= 90°.
	b = 15.9173(12) Å	β= 90°.
	c = 21.9238(17) Å	γ = 90°.
Volume	2759.6(4) $Å^3$	
Z	4	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	0.528 mm^{-1}	
F(000)	1264	
Crystal size	0.45 x 0.43 x 0.28 mm^3	
Theta range for data collection	1.58 to 28.31°.	
Index ranges	-10<=h<=10, -21<=k<=21, -29<=l<=29	
Reflections collected	38329	
Independent reflections	6861 [R(int) = 0.0272]	
Completeness to theta = 28.31°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.000 and 0.855595	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6861 / 0 / 460	
Goodness-of-fit on F^2	1.053	
Final R indices [I>2sigma(I)]	R1 = 0.0186, wR2 = 0.0479	
R indices (all data)	R1 = 0.0191, wR2 = 0.0481	
Absolute structure parameter	0.001(15)	

Largest diff. peak and hole 0.235 and -0.312 e.Å^{-3}

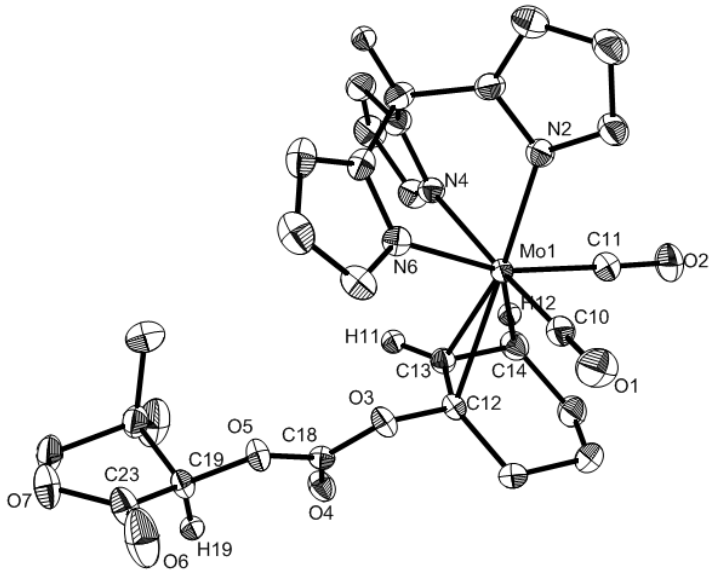


Figure S-2. ORTEP View of the Pantolactonecarbonyloxy Substituted Cyclohexenyl Complex (1S, R)-11

***Table S-8. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for (1S, R)-11.**

	x	y	z	U(eq)
B(1)	-1048(2)	5352(1)	8486(1)	24(1)
C(1)	-2607(2)	5022(1)	9516(1)	31(1)
C(2)	-2570(2)	4366(1)	9929(1)	35(1)
C(3)	-1285(2)	3843(1)	9725(1)	29(1)
C(4)	1466(2)	6389(1)	8400(1)	28(1)
C(5)	3197(2)	6328(1)	8375(1)	31(1)
C(6)	3519(2)	5472(1)	8444(1)	26(1)
C(7)	-2635(2)	4742(1)	7545(1)	30(1)
C(8)	-2680(2)	3984(1)	7247(1)	35(1)
C(9)	-1410(2)	3513(1)	7518(1)	29(1)
C(10)	524(2)	2495(1)	8733(1)	27(1)
C(11)	2522(2)	3395(1)	9415(1)	28(1)
C(12)	2737(2)	2766(1)	7861(1)	21(1)
C(13)	3617(2)	3509(1)	8000(1)	21(1)
C(14)	4411(2)	3481(1)	8587(1)	26(1)
C(15)	5319(2)	2679(1)	8771(1)	34(1)
C(16)	4286(3)	1887(1)	8648(1)	35(1)
C(17)	3403(3)	1906(1)	8025(1)	29(1)

C(18)	2640(2)	2891(1)	6786(1)	20(1)
C(19)	2111(2)	3202(1)	5756(1)	22(1)
C(20)	2324(2)	4151(1)	5651(1)	29(1)
C(21)	965(4)	4647(1)	5992(1)	48(1)
C(22)	4087(3)	4488(2)	5783(1)	48(1)
C(23)	774(2)	2945(1)	5292(1)	33(1)
C(24)	1988(2)	4167(1)	4959(1)	34(1)
Mo(1)	1445(1)	3630(1)	8631(1)	17(1)
N(1)	-1417(2)	4883(1)	9089(1)	25(1)
N(2)	-582(2)	4155(1)	9215(1)	24(1)
N(3)	816(2)	5612(1)	8476(1)	23(1)
N(4)	2093(2)	5033(1)	8507(1)	21(1)
N(5)	-1388(2)	4723(1)	7963(1)	24(1)
N(6)	-603(2)	3957(1)	7948(1)	23(1)
O(1)	-23(2)	1828(1)	8793(1)	44(1)
O(2)	3073(2)	3242(1)	9892(1)	43(1)
O(3)	1793(1)	2747(1)	7306(1)	23(1)
O(4)	4142(1)	2938(1)	6721(1)	26(1)
O(5)	1471(1)	2969(1)	6348(1)	23(1)
O(6)	-126(2)	2342(1)	5302(1)	55(1)
O(7)	715(2)	3523(1)	4846(1)	38(1)

*U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S-9. Bond lengths [Å] and angles [°] for(1S, R)-11.

B(1)-N(3)	1.531(2)	C(10)-O(1)	1.154(2)
B(1)-N(5)	1.544(2)	C(10)-Mo(1)	1.9609(16)
B(1)-N(1)	1.547(2)	C(11)-O(2)	1.159(2)
B(1)-H(1)	1.12(2)	C(11)-Mo(1)	1.9530(17)
C(1)-N(1)	1.345(2)	C(12)-C(13)	1.405(2)
C(1)-C(2)	1.382(3)	C(12)-O(3)	1.4290(17)
C(1)-H(2)	0.91(2)	C(12)-C(17)	1.510(2)
C(2)-C(3)	1.388(2)	C(12)-Mo(1)	2.4055(14)
C(2)-H(3)	0.95(2)	C(13)-C(14)	1.435(2)
C(3)-N(2)	1.3434(19)	C(13)-Mo(1)	2.2144(14)
C(3)-H(4)	0.98(2)	C(13)-H(11)	0.951(18)
C(4)-N(3)	1.3493(19)	C(14)-C(15)	1.519(2)
C(4)-C(5)	1.374(2)	C(14)-Mo(1)	2.3595(15)
C(4)-H(5)	0.96(2)	C(14)-H(12)	0.99(2)
C(5)-C(6)	1.395(2)	C(15)-C(16)	1.527(3)
C(5)-H(6)	0.87(2)	C(15)-H(13)	0.90(2)
C(6)-N(4)	1.334(2)	C(15)-H(14)	0.98(2)
C(6)-H(7)	0.88(2)	C(16)-C(17)	1.533(3)
C(7)-N(5)	1.348(2)	C(16)-H(15)	0.94(2)
C(7)-C(8)	1.371(3)	C(16)-H(16)	0.94(3)
C(7)-H(8)	0.92(2)	C(17)-H(17)	0.95(2)
C(8)-C(9)	1.388(3)	C(17)-H(18)	0.95(2)
C(8)-H(9)	0.89(2)	C(18)-O(4)	1.1984(18)
C(9)-N(6)	1.341(2)	C(18)-O(5)	1.3398(18)
C(9)-H(10)	0.91(2)	C(18)-O(3)	1.3404(18)

C(19)-O(5)	1.4400(17)	C(9)-C(8)-H(9)	127.6(15)
C(19)-C(23)	1.523(2)	N(6)-C(9)-C(8)	111.10(15)
C(19)-C(20)	1.537(2)	N(6)-C(9)-H(10)	122.2(14)
C(19)-H(19)	0.905(19)	C(8)-C(9)-H(10)	126.6(14)
C(20)-C(22)	1.522(3)	O(1)-C(10)-Mo(1)	179.77(17)
C(20)-C(21)	1.529(3)	O(2)-C(11)-Mo(1)	176.16(17)
C(20)-C(24)	1.540(2)	C(13)-C(12)-O(3)	117.38(12)
C(21)-H(20)	0.96(3)	C(13)-C(12)-C(17)	122.61(14)
C(21)-H(21)	0.98(3)	O(3)-C(12)-C(17)	111.53(12)
C(21)-H(22)	0.99(2)	C(13)-C(12)-Mo(1)	64.99(8)
C(22)-H(23)	0.92(3)	O(3)-C(12)-Mo(1)	112.82(9)
C(22)-H(24)	0.92(3)	C(17)-C(12)-Mo(1)	119.92(9)
C(22)-H(25)	1.03(3)	C(12)-C(13)-C(14)	112.61(13)
C(23)-O(6)	1.196(2)	C(12)-C(13)-Mo(1)	79.90(9)
C(23)-O(7)	1.344(2)	C(14)-C(13)-Mo(1)	77.32(8)
C(24)-O(7)	1.458(2)	C(12)-C(13)-H(11)	122.0(11)
C(24)-H(26)	1.01(2)	C(14)-C(13)-H(11)	125.3(11)
C(24)-H(27)	0.99(2)	Mo(1)-C(13)-H(11)	108.9(11)
Mo(1)-N(2)	2.2143(13)	C(13)-C(14)-C(15)	118.15(14)
Mo(1)-N(6)	2.2663(13)	C(13)-C(14)-Mo(1)	66.29(8)
Mo(1)-N(4)	2.3075(12)	C(15)-C(14)-Mo(1)	122.93(11)
N(1)-N(2)	1.3625(18)	C(13)-C(14)-H(12)	116.0(13)
N(3)-N(4)	1.3696(18)	C(15)-C(14)-H(12)	112.8(12)
N(5)-N(6)	1.3694(18)	Mo(1)-C(14)-H(12)	113.3(12)
N(3)-B(1)-N(5)	109.43(13)	C(14)-C(15)-C(16)	113.22(14)
N(3)-B(1)-N(1)	108.94(13)	C(14)-C(15)-H(13)	105.3(13)
N(5)-B(1)-N(1)	106.80(12)	C(16)-C(15)-H(13)	107.6(13)
N(3)-B(1)-H(1)	109.3(11)	C(14)-C(15)-H(14)	111.4(13)
N(5)-B(1)-H(1)	109.8(11)	C(16)-C(15)-H(14)	111.2(13)
N(1)-B(1)-H(1)	112.5(11)	H(13)-C(15)-H(14)	107.9(19)
N(1)-C(1)-C(2)	108.49(15)	C(15)-C(16)-C(17)	112.66(15)
N(1)-C(1)-H(2)	117.5(14)	C(15)-C(16)-H(15)	111.4(13)
C(2)-C(1)-H(2)	134.0(14)	C(17)-C(16)-H(15)	108.3(13)
C(1)-C(2)-C(3)	104.89(15)	C(15)-C(16)-H(16)	110.7(14)
C(1)-C(2)-H(3)	130.3(14)	C(17)-C(16)-H(16)	108.4(15)
C(3)-C(2)-H(3)	124.6(14)	H(15)-C(16)-H(16)	105.0(19)
N(2)-C(3)-C(2)	110.48(15)	C(12)-C(17)-C(16)	112.91(13)
N(2)-C(3)-H(4)	115.2(14)	C(12)-C(17)-H(17)	104.8(13)
C(2)-C(3)-H(4)	134.2(14)	C(16)-C(17)-H(17)	112.2(14)
N(3)-C(4)-C(5)	108.64(15)	C(12)-C(17)-H(18)	110.5(12)
N(3)-C(4)-H(5)	119.7(13)	C(16)-C(17)-H(18)	112.4(12)
C(5)-C(4)-H(5)	131.6(13)	H(17)-C(17)-H(18)	103.2(18)
C(4)-C(5)-C(6)	104.31(15)	O(4)-C(18)-O(5)	126.32(14)
C(4)-C(5)-H(6)	127.3(14)	O(4)-C(18)-O(3)	127.37(14)
C(6)-C(5)-H(6)	128.4(14)	O(5)-C(18)-O(3)	106.31(12)
N(4)-C(6)-C(5)	111.60(16)	O(5)-C(19)-C(23)	106.75(12)
N(4)-C(6)-H(7)	123.3(14)	O(5)-C(19)-C(20)	115.25(12)
C(5)-C(6)-H(7)	125.0(14)	C(23)-C(19)-C(20)	103.81(13)
N(5)-C(7)-C(8)	108.84(16)	O(5)-C(19)-H(19)	110.4(11)
N(5)-C(7)-H(8)	119.3(13)	C(23)-C(19)-H(19)	109.9(11)
C(8)-C(7)-H(8)	131.8(13)	C(20)-C(19)-H(19)	110.3(11)
C(7)-C(8)-C(9)	104.73(15)	C(22)-C(20)-C(21)	111.63(18)
C(7)-C(8)-H(9)	127.6(14)	C(22)-C(20)-C(19)	114.70(16)

C(21)-C(20)-C(19)	110.94(15)	N(2)-Mo(1)-N(4)	82.17(5)
C(22)-C(20)-C(24)	109.83(16)	C(13)-Mo(1)-N(4)	80.69(5)
C(21)-C(20)-C(24)	110.62(16)	N(6)-Mo(1)-N(4)	81.87(5)
C(19)-C(20)-C(24)	98.38(13)	C(11)-Mo(1)-C(14)	65.36(6)
C(20)-C(21)-H(20)	110.9(15)	C(10)-Mo(1)-C(14)	106.34(6)
C(20)-C(21)-H(21)	111.3(17)	N(2)-Mo(1)-C(14)	141.35(5)
H(20)-C(21)-H(21)	112(2)	C(13)-Mo(1)-C(14)	36.39(5)
C(20)-C(21)-H(22)	111.4(13)	N(6)-Mo(1)-C(14)	134.98(5)
H(20)-C(21)-H(22)	110(2)	N(4)-Mo(1)-C(14)	82.64(5)
H(21)-C(21)-H(22)	102(2)	C(11)-Mo(1)-C(12)	108.82(6)
C(20)-C(22)-H(23)	111.3(16)	C(10)-Mo(1)-C(12)	73.20(6)
C(20)-C(22)-H(24)	110.1(16)	N(2)-Mo(1)-C(12)	158.22(5)
H(23)-C(22)-H(24)	109(2)	C(13)-Mo(1)-C(12)	35.11(5)
C(20)-C(22)-H(25)	108.1(16)	N(6)-Mo(1)-C(12)	88.36(5)
H(23)-C(22)-H(25)	106(2)	N(4)-Mo(1)-C(12)	112.11(5)
H(24)-C(22)-H(25)	113(2)	C(14)-Mo(1)-C(12)	59.45(5)
O(6)-C(23)-O(7)	122.83(17)	C(1)-N(1)-N(2)	109.78(13)
O(6)-C(23)-C(19)	128.05(16)	C(1)-N(1)-B(1)	130.35(14)
O(7)-C(23)-C(19)	109.11(14)	N(2)-N(1)-B(1)	119.47(12)
O(7)-C(24)-C(20)	106.01(13)	C(3)-N(2)-N(1)	106.36(13)
O(7)-C(24)-H(26)	107.3(13)	C(3)-N(2)-Mo(1)	129.88(11)
C(20)-C(24)-H(26)	113.0(12)	N(1)-N(2)-Mo(1)	123.72(9)
O(7)-C(24)-H(27)	106.6(14)	C(4)-N(3)-N(4)	110.03(13)
C(20)-C(24)-H(27)	115.4(14)	C(4)-N(3)-B(1)	128.08(13)
H(26)-C(24)-H(27)	108.0(18)	N(4)-N(3)-B(1)	121.76(12)
C(11)-Mo(1)-C(10)	83.41(7)	C(6)-N(4)-N(3)	105.42(12)
C(11)-Mo(1)-N(2)	83.10(6)	C(6)-N(4)-Mo(1)	134.95(11)
C(10)-Mo(1)-N(2)	90.73(6)	N(3)-N(4)-Mo(1)	119.62(9)
C(11)-Mo(1)-C(13)	101.26(6)	C(7)-N(5)-N(6)	109.59(13)
C(10)-Mo(1)-C(13)	106.22(6)	C(7)-N(5)-B(1)	128.18(14)
N(2)-Mo(1)-C(13)	162.82(5)	N(6)-N(5)-B(1)	121.06(12)
C(11)-Mo(1)-N(6)	159.46(6)	C(9)-N(6)-N(5)	105.72(13)
C(10)-Mo(1)-N(6)	91.23(6)	C(9)-N(6)-Mo(1)	133.16(11)
N(2)-Mo(1)-N(6)	77.15(5)	N(5)-N(6)-Mo(1)	120.85(10)
C(13)-Mo(1)-N(6)	99.27(5)	C(18)-O(3)-C(12)	117.33(11)
C(11)-Mo(1)-N(4)	101.08(6)	C(18)-O(5)-C(19)	115.33(12)
C(10)-Mo(1)-N(4)	171.02(6)	C(23)-O(7)-C(24)	109.41(13)

Symmetry transformations used to generate equivalent atoms:

Table S-10. Anisotropic displacement parameters (Å^{2}x 10^3) for (1S, R)-11.*

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	23(1)	20(1)	30(1)	2(1)	2(1)	2(1)
C(1)	26(1)	34(1)	33(1)	-6(1)	7(1)	3(1)
C(2)	34(1)	41(1)	29(1)	0(1)	12(1)	1(1)
C(3)	35(1)	30(1)	22(1)	2(1)	8(1)	0(1)
C(4)	36(1)	19(1)	30(1)	1(1)	4(1)	-1(1)
C(5)	36(1)	24(1)	33(1)	-1(1)	6(1)	-11(1)
C(6)	25(1)	26(1)	27(1)	-2(1)	3(1)	-4(1)

C(7)	21(1)	39(1)	31(1)	10(1)	-2(1)	-1(1)
C(8)	24(1)	53(1)	30(1)	-2(1)	-5(1)	-7(1)
C(9)	24(1)	36(1)	27(1)	-6(1)	2(1)	-5(1)
C(10)	34(1)	24(1)	22(1)	3(1)	6(1)	1(1)
C(11)	36(1)	28(1)	20(1)	0(1)	0(1)	5(1)
C(12)	26(1)	23(1)	14(1)	0(1)	2(1)	2(1)
C(13)	21(1)	23(1)	18(1)	0(1)	0(1)	2(1)
C(14)	24(1)	31(1)	22(1)	-3(1)	-2(1)	3(1)
C(15)	32(1)	44(1)	26(1)	2(1)	-5(1)	14(1)
C(16)	47(1)	30(1)	28(1)	5(1)	0(1)	16(1)
C(17)	41(1)	21(1)	24(1)	-1(1)	4(1)	8(1)
C(18)	25(1)	16(1)	18(1)	-2(1)	0(1)	1(1)
C(19)	25(1)	25(1)	16(1)	1(1)	1(1)	-1(1)
C(20)	36(1)	25(1)	24(1)	3(1)	-3(1)	-2(1)
C(21)	70(2)	33(1)	42(1)	-2(1)	3(1)	17(1)
C(22)	53(1)	43(1)	47(1)	13(1)	-13(1)	-21(1)
C(23)	38(1)	41(1)	21(1)	-1(1)	-4(1)	-7(1)
C(24)	39(1)	38(1)	26(1)	10(1)	-3(1)	-1(1)
Mo(1)	22(1)	16(1)	14(1)	0(1)	1(1)	0(1)
N(1)	24(1)	22(1)	28(1)	-1(1)	4(1)	3(1)
N(2)	29(1)	20(1)	22(1)	1(1)	4(1)	-1(1)
N(3)	26(1)	17(1)	26(1)	2(1)	1(1)	0(1)
N(4)	23(1)	20(1)	22(1)	-1(1)	1(1)	0(1)
N(5)	23(1)	24(1)	26(1)	5(1)	-1(1)	0(1)
N(6)	23(1)	23(1)	23(1)	0(1)	-1(1)	-1(1)
O(1)	58(1)	23(1)	53(1)	3(1)	17(1)	-9(1)
O(2)	56(1)	51(1)	21(1)	4(1)	-7(1)	12(1)
O(3)	26(1)	28(1)	15(1)	-2(1)	1(1)	-3(1)
O(4)	21(1)	37(1)	20(1)	0(1)	1(1)	3(1)
O(5)	22(1)	31(1)	16(1)	2(1)	0(1)	-2(1)
O(6)	70(1)	63(1)	33(1)	3(1)	-16(1)	-36(1)
O(7)	41(1)	49(1)	23(1)	7(1)	-9(1)	-6(1)

*The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table S-11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for (1S, R)-11.

	x	y	z	U(eq)
H(1)	-1860(30)	5921(13)	8426(9)	34(5)
H(2)	-3250(30)	5493(13)	9478(10)	34(5)
H(3)	-3300(30)	4244(14)	10263(10)	43(6)
H(4)	-850(30)	3293(14)	9854(10)	40(6)
H(5)	730(30)	6866(13)	8396(9)	31(5)
H(6)	3920(30)	6736(13)	8321(9)	32(5)
H(7)	4540(30)	5244(13)	8470(9)	33(5)
H(8)	-3300(30)	5218(13)	7510(9)	34(5)
H(9)	-3340(30)	3837(14)	6940(11)	43(6)
H(10)	-1160(30)	2962(13)	7442(9)	32(5)
H(11)	3620(20)	3978(11)	7731(8)	19(4)
H(12)	5030(30)	3993(14)	8712(10)	40(6)
H(13)	6250(30)	2658(13)	8534(9)	31(5)
H(14)	5690(30)	2702(13)	9197(10)	39(6)

H(15)	4960(30)	1404(14)	8666(9)	39(5)
H(16)	3460(30)	1810(14)	8950(11)	43(6)
H(17)	4150(30)	1762(13)	7702(11)	40(6)
H(18)	2530(30)	1498(13)	7994(9)	29(5)
H(19)	3090(20)	2930(11)	5678(8)	20(4)
H(20)	1000(30)	5228(16)	5882(11)	53(7)
H(21)	-170(40)	4405(18)	5926(13)	66(9)
H(22)	1090(30)	4589(14)	6440(11)	43(6)
H(23)	4900(30)	4163(16)	5603(12)	48(7)
H(24)	4270(30)	4501(15)	6196(12)	51(7)
H(25)	4190(40)	5070(17)	5583(13)	65(8)
H(26)	1510(30)	4718(13)	4814(10)	39(5)
H(27)	2970(30)	4026(15)	4698(11)	46(6)

Table S-12. Torsion angles [°] for (1S, R)-11.

N(1)-C(1)-C(2)-C(3)	0.6(2)
C(1)-C(2)-C(3)-N(2)	-0.4(2)
N(3)-C(4)-C(5)-C(6)	-0.24(18)
C(4)-C(5)-C(6)-N(4)	-0.07(19)
N(5)-C(7)-C(8)-C(9)	0.8(2)
C(7)-C(8)-C(9)-N(6)	-1.2(2)
O(3)-C(12)-C(13)-C(14)	175.51(12)
C(17)-C(12)-C(13)-C(14)	-39.20(19)
Mo(1)-C(12)-C(13)-C(14)	71.59(11)
O(3)-C(12)-C(13)-Mo(1)	103.91(11)
C(17)-C(12)-C(13)-Mo(1)	-110.80(13)
C(12)-C(13)-C(14)-C(15)	42.8(2)
Mo(1)-C(13)-C(14)-C(15)	116.00(14)
C(12)-C(13)-C(14)-Mo(1)	-73.23(11)
C(13)-C(14)-C(15)-C(16)	-46.9(2)
Mo(1)-C(14)-C(15)-C(16)	31.78(19)
C(14)-C(15)-C(16)-C(17)	43.0(2)
C(13)-C(12)-C(17)-C(16)	38.1(2)
O(3)-C(12)-C(17)-C(16)	-174.83(14)
Mo(1)-C(12)-C(17)-C(16)	-39.7(2)
C(15)-C(16)-C(17)-C(12)	-38.0(2)
O(5)-C(19)-C(20)-C(22)	94.44(19)
C(23)-C(19)-C(20)-C(22)	-149.19(17)
O(5)-C(19)-C(20)-C(21)	-33.2(2)
C(23)-C(19)-C(20)-C(21)	83.19(17)
O(5)-C(19)-C(20)-C(24)	-149.13(13)
C(23)-C(19)-C(20)-C(24)	-32.76(16)
O(5)-C(19)-C(23)-O(6)	-36.0(3)
C(20)-C(19)-C(23)-O(6)	-158.2(2)
O(5)-C(19)-C(23)-O(7)	143.28(14)
C(20)-C(19)-C(23)-O(7)	21.09(18)
C(22)-C(20)-C(24)-O(7)	154.98(16)
C(21)-C(20)-C(24)-O(7)	-81.35(19)
C(19)-C(20)-C(24)-O(7)	34.84(17)
O(2)-C(11)-Mo(1)-C(10)	-51(2)
O(2)-C(11)-Mo(1)-N(2)	41(2)

O(2)-C(11)-Mo(1)-C(13)	-156(2)
O(2)-C(11)-Mo(1)-N(6)	25(2)
O(2)-C(11)-Mo(1)-N(4)	121(2)
O(2)-C(11)-Mo(1)-C(14)	-162(2)
O(2)-C(11)-Mo(1)-C(12)	-120(2)
O(1)-C(10)-Mo(1)-C(11)	120(24)
O(1)-C(10)-Mo(1)-N(2)	37(24)
O(1)-C(10)-Mo(1)-C(13)	-141(100)
O(1)-C(10)-Mo(1)-N(6)	-41(24)
O(1)-C(10)-Mo(1)-N(4)	-1(25)
O(1)-C(10)-Mo(1)-C(14)	-179(100)
O(1)-C(10)-Mo(1)-C(12)	-128(84)
C(12)-C(13)-Mo(1)-C(11)	106.77(9)
C(14)-C(13)-Mo(1)-C(11)	-9.35(10)
C(12)-C(13)-Mo(1)-C(10)	20.44(10)
C(14)-C(13)-Mo(1)-C(10)	-95.68(9)
C(12)-C(13)-Mo(1)-N(2)	-149.98(16)
C(14)-C(13)-Mo(1)-N(2)	93.90(18)
C(12)-C(13)-Mo(1)-N(6)	-73.58(9)
C(14)-C(13)-Mo(1)-N(6)	170.30(8)
C(12)-C(13)-Mo(1)-N(4)	-153.67(9)
C(14)-C(13)-Mo(1)-N(4)	90.20(9)
C(12)-C(13)-Mo(1)-C(14)	116.12(12)
C(14)-C(13)-Mo(1)-C(12)	-116.12(12)
C(13)-C(14)-Mo(1)-C(11)	169.90(11)
C(15)-C(14)-Mo(1)-C(11)	60.67(13)
C(13)-C(14)-Mo(1)-C(10)	95.33(9)
C(15)-C(14)-Mo(1)-C(10)	-13.90(14)
C(13)-C(14)-Mo(1)-N(2)	-151.85(8)
C(15)-C(14)-Mo(1)-N(2)	98.92(14)
C(15)-C(14)-Mo(1)-C(13)	-109.23(16)
C(13)-C(14)-Mo(1)-N(6)	-13.60(12)
C(15)-C(14)-Mo(1)-N(6)	-122.83(12)
C(13)-C(14)-Mo(1)-N(4)	-84.28(8)
C(15)-C(14)-Mo(1)-N(4)	166.48(13)
C(13)-C(14)-Mo(1)-C(12)	36.84(8)
C(15)-C(14)-Mo(1)-C(12)	-72.39(13)
C(13)-C(12)-Mo(1)-C(11)	-82.76(10)
O(3)-C(12)-Mo(1)-C(11)	166.49(10)
C(17)-C(12)-Mo(1)-C(11)	31.92(14)
C(13)-C(12)-Mo(1)-C(10)	-159.50(10)
O(3)-C(12)-Mo(1)-C(10)	89.75(10)
C(17)-C(12)-Mo(1)-C(10)	-44.81(13)
C(13)-C(12)-Mo(1)-N(2)	156.53(12)
O(3)-C(12)-Mo(1)-N(2)	45.78(18)
C(17)-C(12)-Mo(1)-N(2)	-88.78(17)
O(3)-C(12)-Mo(1)-C(13)	-110.75(13)
C(17)-C(12)-Mo(1)-C(13)	114.69(16)
C(13)-C(12)-Mo(1)-N(6)	108.73(9)
O(3)-C(12)-Mo(1)-N(6)	-2.02(10)
C(17)-C(12)-Mo(1)-N(6)	-136.58(13)
C(13)-C(12)-Mo(1)-N(4)	28.19(9)
O(3)-C(12)-Mo(1)-N(4)	-82.56(10)
C(17)-C(12)-Mo(1)-N(4)	142.88(12)
C(13)-C(12)-Mo(1)-C(14)	-38.21(8)
O(3)-C(12)-Mo(1)-C(14)	-148.96(12)

C(17)-C(12)-Mo(1)-C(14)	76.48(13)
C(2)-C(1)-N(1)-N(2)	-0.6(2)
C(2)-C(1)-N(1)-B(1)	171.95(16)
N(3)-B(1)-N(1)-C(1)	126.52(17)
N(5)-B(1)-N(1)-C(1)	-115.39(18)
N(3)-B(1)-N(1)-N(2)	-61.52(17)
N(5)-B(1)-N(1)-N(2)	56.57(17)
C(2)-C(3)-N(2)-N(1)	0.03(19)
C(2)-C(3)-N(2)-Mo(1)	-177.49(12)
C(1)-N(1)-N(2)-C(3)	0.36(18)
B(1)-N(1)-N(2)-C(3)	-173.13(14)
C(1)-N(1)-N(2)-Mo(1)	178.07(11)
B(1)-N(1)-N(2)-Mo(1)	4.58(19)
C(11)-Mo(1)-N(2)-C(3)	-44.34(15)
C(10)-Mo(1)-N(2)-C(3)	38.93(15)
C(13)-Mo(1)-N(2)-C(3)	-150.27(17)
N(6)-Mo(1)-N(2)-C(3)	130.02(15)
N(4)-Mo(1)-N(2)-C(3)	-146.58(15)
C(14)-Mo(1)-N(2)-C(3)	-78.87(17)
C(12)-Mo(1)-N(2)-C(3)	80.6(2)
C(11)-Mo(1)-N(2)-N(1)	138.52(13)
C(10)-Mo(1)-N(2)-N(1)	-138.21(12)
C(13)-Mo(1)-N(2)-N(1)	32.6(2)
N(6)-Mo(1)-N(2)-N(1)	-47.12(11)
N(4)-Mo(1)-N(2)-N(1)	36.28(12)
C(14)-Mo(1)-N(2)-N(1)	103.99(13)
C(12)-Mo(1)-N(2)-N(1)	-96.54(16)
C(5)-C(4)-N(3)-N(4)	0.46(17)
C(5)-C(4)-N(3)-B(1)	-175.50(15)
N(5)-B(1)-N(3)-C(4)	119.28(16)
N(1)-B(1)-N(3)-C(4)	-124.29(15)
N(5)-B(1)-N(3)-N(4)	-56.24(17)
N(1)-B(1)-N(3)-N(4)	60.18(17)
C(5)-C(6)-N(4)-N(3)	0.34(17)
C(5)-C(6)-N(4)-Mo(1)	179.29(10)
C(4)-N(3)-N(4)-C(6)	-0.49(16)
B(1)-N(3)-N(4)-C(6)	175.77(13)
C(4)-N(3)-N(4)-Mo(1)	-179.64(10)
B(1)-N(3)-N(4)-Mo(1)	-3.38(17)
C(11)-Mo(1)-N(4)-C(6)	63.21(15)
C(10)-Mo(1)-N(4)-C(6)	-177.4(3)
N(2)-Mo(1)-N(4)-C(6)	144.55(15)
C(13)-Mo(1)-N(4)-C(6)	-36.55(14)
N(6)-Mo(1)-N(4)-C(6)	-137.41(15)
C(14)-Mo(1)-N(4)-C(6)	0.19(14)
C(12)-Mo(1)-N(4)-C(6)	-52.53(15)
C(11)-Mo(1)-N(4)-N(3)	-117.95(11)
C(10)-Mo(1)-N(4)-N(3)	1.4(4)
N(2)-Mo(1)-N(4)-N(3)	-36.61(10)
C(13)-Mo(1)-N(4)-N(3)	142.29(11)
N(6)-Mo(1)-N(4)-N(3)	41.43(10)
C(14)-Mo(1)-N(4)-N(3)	179.03(11)
C(12)-Mo(1)-N(4)-N(3)	126.31(10)
C(8)-C(7)-N(5)-N(6)	-0.15(19)
C(8)-C(7)-N(5)-B(1)	-167.75(15)
N(3)-B(1)-N(5)-C(7)	-130.64(16)

N(1)-B(1)-N(5)-C(7)	111.58(17)
N(3)-B(1)-N(5)-N(6)	63.01(17)
N(1)-B(1)-N(5)-N(6)	-54.76(17)
C(8)-C(9)-N(6)-N(5)	1.11(18)
C(8)-C(9)-N(6)-Mo(1)	175.02(12)
C(7)-N(5)-N(6)-C(9)	-0.59(17)
B(1)-N(5)-N(6)-C(9)	168.05(14)
C(7)-N(5)-N(6)-Mo(1)	-175.42(10)
B(1)-N(5)-N(6)-Mo(1)	-6.78(18)
C(11)-Mo(1)-N(6)-C(9)	-109.4(2)
C(10)-Mo(1)-N(6)-C(9)	-35.05(15)
N(2)-Mo(1)-N(6)-C(9)	-125.52(15)
C(13)-Mo(1)-N(6)-C(9)	71.60(15)
N(4)-Mo(1)-N(6)-C(9)	150.72(15)
C(14)-Mo(1)-N(6)-C(9)	79.73(16)
C(12)-Mo(1)-N(6)-C(9)	38.11(15)
C(11)-Mo(1)-N(6)-N(5)	63.8(2)
C(10)-Mo(1)-N(6)-N(5)	138.12(11)
N(2)-Mo(1)-N(6)-N(5)	47.65(11)
C(13)-Mo(1)-N(6)-N(5)	-115.23(11)
N(4)-Mo(1)-N(6)-N(5)	-36.11(11)
C(14)-Mo(1)-N(6)-N(5)	-107.10(12)
C(12)-Mo(1)-N(6)-N(5)	-148.72(11)
O(4)-C(18)-O(3)-C(12)	9.4(2)
O(5)-C(18)-O(3)-C(12)	-170.75(11)
C(13)-C(12)-O(3)-C(18)	57.98(17)
C(17)-C(12)-O(3)-C(18)	-90.98(15)
Mo(1)-C(12)-O(3)-C(18)	130.62(10)
O(4)-C(18)-O(5)-C(19)	-5.5(2)
O(3)-C(18)-O(5)-C(19)	174.70(11)
C(23)-C(19)-O(5)-C(18)	159.36(13)
C(20)-C(19)-O(5)-C(18)	-85.95(17)
O(6)-C(23)-O(7)-C(24)	-178.9(2)
C(19)-C(23)-O(7)-C(24)	1.82(19)
C(20)-C(24)-O(7)-C(23)	-24.25(19)

Symmetry transformations used to generate equivalent atoms:

Crystal Structure Analysis of (1*R*, *R*)-12.

A suitable crystal of (1*R, R*)-**12** grown from EtOAc/hexanes was coated with Paratone N oil, suspended in a small fiber loop and placed in a cooled nitrogen gas stream at 173 K on a Bruker D8 APEX II CCD sealed tube diffractometer with graphite monochromated MoK_α (0.71073 Å) radiation. Data were measured using a series of combinations of phi and omega scans with 10 s frame exposures and 0.5^o frame widths. Data collection, indexing and initial cell

refinements were all carried out using APEX II[10] software. Frame integration and final cell refinements were done using SAINT[11] software. The final cell parameters were determined from least-squares refinement on 5662 reflections.

The structure was solved using Direct methods and difference Fourier techniques (SHELXTL, V6.12).[12] The complex crystallized with 1 EtOAc solvent molecule per molecule of complex. Hydrogen atoms were placed their expected chemical positions using the HFIX command and were included in the final cycles of least squares with isotropic U_{ij} 's related to the atom's ridden upon except for the hydrogen attached to boron that was located in a difference map and refined with an AFIX 2 command. All non-hydrogen atoms were refined anisotropically except for those in the ethyl acetate solvent molecule. Scattering factors and anomalous dispersion corrections are taken from the *International Tables for X-ray Crystallography*.[13] Structure solution, refinement, graphics and generation of publication materials were performed by using SHELXTL, V6.12 software. Additional details of data collection and structure refinement are given in Table S-13.

Table S-13. Crystal data and structure refinement for (1R, R)-12.

Identification code	(1*R*, *R*)-**12**
Empirical formula	C26 H33 B Mo N6 O9
Formula weight	680.33
Temperature	173(2) K
Wavelength	0.71073 Å

[10] APEX II, **2005**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[11] SAINT Version 6.45A, **2003**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[12] "A short history of SHEL*X*". Sheldrick, G.M. (2008). *Acta Cryst*. A64, 112-122. SHELXTL V6.12, **2002**, Bruker AXS, Inc., Analytical X-ray Systems, 5465 East Cheryl Parkway, Madison WI 53711-5373.
[13] A. J. C. Wilson (ed), *International Tables for X-ray Crystallography, Volume C.* Kynoch, Academic Publishers, Dordrecht, **1992**, Tables 6.1.1.4 (pp. 500-502) and 4.2.6.8 (pp. 219-222).

Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 10.3216(16) Å	α= 90°.
	b = 16.393(3) Å	β= 90°.
	c = 17.924(3) Å	γ = 90°.
Volume	3032.8(8) $Å^3$	
Z	4	
Density (calculated)	1.490 Mg/m^3	
Absorption coefficient	0.493 mm^{-1}	
F(000)	1400	
Crystal size	0.48 x 0.15 x 0.11 mm^3	
Theta range for data collection	2.27 to 30.53°.	
Index ranges	-14<=h<=14, -23<=k<=23, -25<=l<=25	
Reflections collected	61127	
Independent reflections	9282 [R(int) = 0.1031]	
Completeness to theta = 30.53°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9496 and 0.7978	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9282 / 0 / 361	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0490, wR2 = 0.1125	
R indices (all data)	R1 = 0.0827, wR2 = 0.1272	
Absolute structure parameter	-0.02(4)	
Largest diff. peak and hole	1.233 and -0.648 $e.Å^{-3}$	

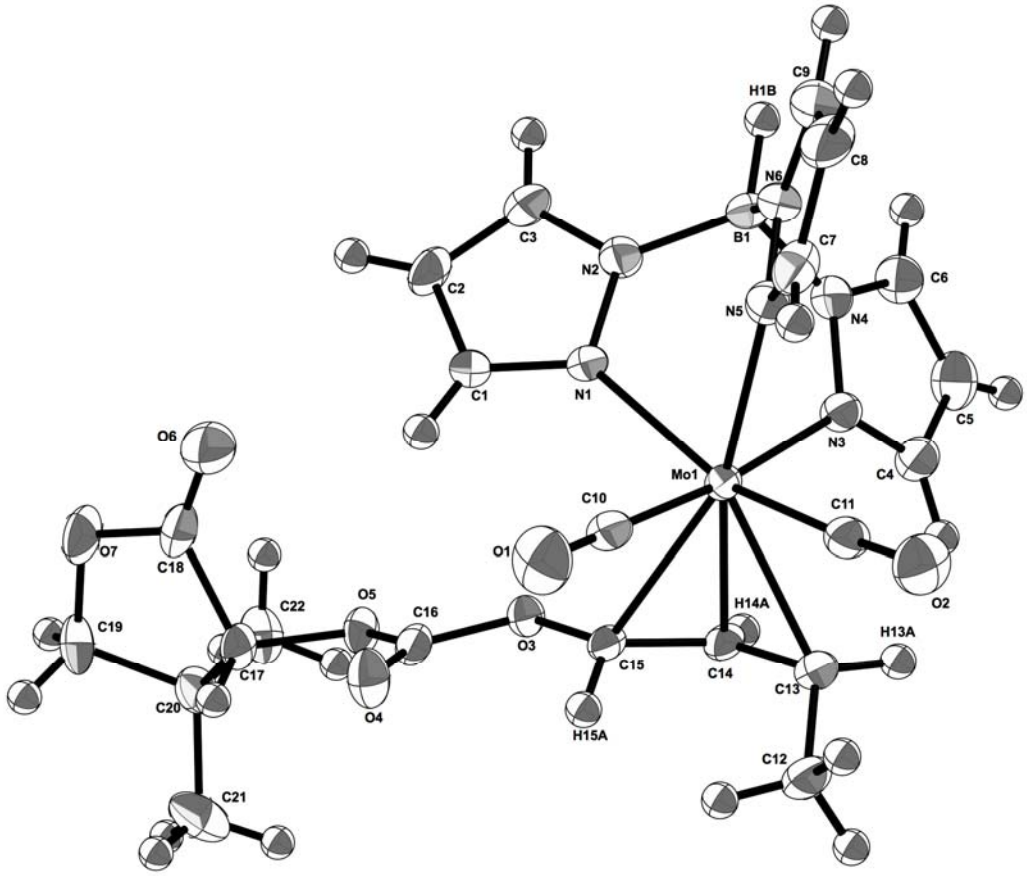


Figure S-3. ORTEP View of Pantolactonecarbonyloxy Substituted 2-Butenyl Complex (1R, R)-12 (EtOAc solvate molecule not shown).

***Table S-14. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (1R, R)-12.**

	x	y	z	U(eq)
B(1)	-1697(5)	8271(3)	2780(2)	28(1)
C(1)	406(4)	6806(3)	1886(2)	25(1)
C(2)	52(5)	7226(3)	1249(2)	31(1)
C(3)	-714(4)	7851(3)	1502(2)	31(1)
C(4)	482(4)	8773(3)	4292(2)	30(1)
C(5)	126(6)	9554(3)	4115(2)	35(1)
C(6)	-739(5)	9473(3)	3534(2)	32(1)
C(7)	-3110(4)	6539(3)	3745(2)	31(1)
C(8)	-4257(4)	6907(4)	3534(2)	42(1)
C(9)	-3909(4)	7601(3)	3162(3)	39(1)
C(10)	-24(5)	5679(2)	3506(2)	27(1)
C(11)	-638(4)	6475(3)	4678(2)	25(1)

C(12)	1851(5)	6095(3)	5117(2)	33(1)
C(13)	1486(4)	6866(3)	4712(2)	27(1)
C(14)	2063(4)	7080(2)	4024(2)	23(1)
C(15)	2206(3)	6477(3)	3484(2)	21(1)
C(16)	3274(4)	6166(3)	2371(2)	24(1)
C(17)	4488(4)	6031(3)	1267(2)	26(1)
C(18)	3570(5)	6055(3)	605(2)	34(1)
C(19)	5668(5)	5951(4)	179(3)	39(1)
C(20)	5772(4)	6324(3)	953(2)	31(1)
C(21)	6940(5)	6021(3)	1377(3)	49(1)
C(22)	5777(5)	7257(3)	895(3)	37(1)
Mo(1)	-6(1)	6843(1)	3711(1)	19(1)
N(1)	-81(4)	7153(2)	2494(2)	23(1)
N(2)	-804(3)	7802(2)	2241(2)	26(1)
N(3)	-111(4)	8227(2)	3853(2)	23(1)
N(4)	-872(3)	8675(2)	3387(2)	26(1)
N(5)	-2101(3)	6993(2)	3517(2)	25(1)
N(6)	-2607(3)	7648(2)	3153(2)	27(1)
O(1)	-73(4)	4979(2)	3404(2)	44(1)
O(2)	-1098(3)	6242(2)	5228(2)	38(1)
O(3)	2817(3)	6748(2)	2822(1)	24(1)
O(4)	3091(3)	5446(2)	2424(2)	35(1)
O(5)	3992(3)	6542(2)	1854(1)	26(1)
O(6)	2430(3)	6121(2)	606(2)	51(1)
O(7)	4291(4)	5982(2)	-23(2)	41(1)
O(1S)	4080(3)	9009(2)	1680(2)	43(1)
O(2S)	3701(5)	9130(3)	477(3)	79(1)
C(1S)	5740(5)	9550(4)	944(3)	45(1)
C(2S)	4404(5)	9243(3)	1003(3)	40(1)
C(3S)	2799(5)	8678(3)	1796(3)	42(1)
C(4S)	2424(6)	8850(4)	2572(3)	56(2)

*U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

Table S-15. Bond lengths [Å] and angles [°] for (1R, R)-12.

B(1)-N(4)	1.531(6)	C(6)-H(6A)	0.9500
B(1)-N(6)	1.540(6)	C(7)-N(5)	1.343(5)
B(1)-N(2)	1.542(6)	C(7)-C(8)	1.381(6)
B(1)-H(1B)	1.12(5)	C(7)-H(7A)	0.9500
C(1)-N(1)	1.329(5)	C(8)-C(9)	1.366(7)
C(1)-C(2)	1.381(5)	C(8)-H(8A)	0.9500
C(1)-H(1A)	0.9500	C(9)-N(6)	1.347(5)
C(2)-C(3)	1.372(6)	C(9)-H(9A)	0.9500
C(2)-H(2A)	0.9500	C(10)-O(1)	1.164(5)
C(3)-N(2)	1.329(5)	C(10)-Mo(1)	1.943(4)
C(3)-H(3A)	0.9500	C(11)-O(2)	1.159(5)
C(4)-N(3)	1.340(5)	C(11)-Mo(1)	1.947(4)
C(4)-C(5)	1.370(6)	C(12)-C(13)	1.507(6)
C(4)-H(4A)	0.9500	C(12)-H(12A)	0.9800
C(5)-C(6)	1.379(6)	C(12)-H(12B)	0.9800
C(5)-H(5A)	0.9500	C(12)-H(12C)	0.9800
C(6)-N(4)	1.341(5)	C(13)-C(14)	1.415(5)

C(13)-Mo(1)	2.364(4)	N(1)-C(1)-H(1A)	124.3
C(13)-H(13A)	1.0000	C(2)-C(1)-H(1A)	124.3
C(14)-C(15)	1.390(5)	C(3)-C(2)-C(1)	104.5(3)
C(14)-Mo(1)	2.241(4)	C(3)-C(2)-H(2A)	127.7
C(14)-H(14A)	1.0000	C(1)-C(2)-H(2A)	127.7
C(15)-O(3)	1.416(4)	N(2)-C(3)-C(2)	108.9(4)
C(15)-Mo(1)	2.395(4)	N(2)-C(3)-H(3A)	125.5
C(15)-H(15A)	1.0000	C(2)-C(3)-H(3A)	125.5
C(16)-O(4)	1.199(5)	N(3)-C(4)-C(5)	111.5(4)
C(16)-O(3)	1.337(5)	N(3)-C(4)-H(4A)	124.3
C(16)-O(5)	1.338(5)	C(5)-C(4)-H(4A)	124.3
C(17)-O(5)	1.438(5)	C(4)-C(5)-C(6)	105.0(4)
C(17)-C(20)	1.518(6)	C(4)-C(5)-H(5A)	127.5
C(17)-C(18)	1.519(6)	C(6)-C(5)-H(5A)	127.5
C(17)-H(17A)	1.0000	N(4)-C(6)-C(5)	108.0(4)
C(18)-O(6)	1.182(6)	N(4)-C(6)-H(6A)	126.0
C(18)-O(7)	1.355(5)	C(5)-C(6)-H(6A)	126.0
C(19)-O(7)	1.468(6)	N(5)-C(7)-C(8)	109.8(4)
C(19)-C(20)	1.519(6)	N(5)-C(7)-H(7A)	125.1
C(19)-H(19A)	0.9900	C(8)-C(7)-H(7A)	125.1
C(19)-H(19B)	0.9900	C(9)-C(8)-C(7)	105.8(4)
C(20)-C(21)	1.509(7)	C(9)-C(8)-H(8A)	127.1
C(20)-C(22)	1.534(6)	C(7)-C(8)-H(8A)	127.1
C(21)-H(21A)	0.9800	N(6)-C(9)-C(8)	108.4(4)
C(21)-H(21B)	0.9800	N(6)-C(9)-H(9A)	125.8
C(21)-H(21C)	0.9800	C(8)-C(9)-H(9A)	125.8
C(22)-H(22A)	0.9800	O(1)-C(10)-Mo(1)	177.3(4)
C(22)-H(22B)	0.9800	O(2)-C(11)-Mo(1)	175.0(4)
C(22)-H(22C)	0.9800	C(13)-C(12)-H(12A)	109.5
Mo(1)-N(5)	2.204(3)	C(13)-C(12)-H(12B)	109.5
Mo(1)-N(1)	2.242(3)	H(12A)-C(12)-H(12B)	109.5
Mo(1)-N(3)	2.285(3)	C(13)-C(12)-H(12C)	109.5
N(1)-N(2)	1.376(5)	H(12A)-C(12)-H(12C)	109.5
N(3)-N(4)	1.362(4)	H(12B)-C(12)-H(12C)	109.5
N(5)-N(6)	1.361(5)	C(14)-C(13)-C(12)	121.6(4)
O(1S)-C(2S)	1.317(6)	C(14)-C(13)-Mo(1)	67.4(2)
O(1S)-C(3S)	1.444(6)	C(12)-C(13)-Mo(1)	121.0(3)
O(2S)-C(2S)	1.203(6)	C(14)-C(13)-H(13A)	113.2
C(1S)-C(2S)	1.471(7)	C(12)-C(13)-H(13A)	113.2
C(1S)-H(1SA)	0.9800	Mo(1)-C(13)-H(13A)	113.2
C(1S)-H(1SB)	0.9800	C(15)-C(14)-C(13)	118.4(4)
C(1S)-H(1SC)	0.9800	C(15)-C(14)-Mo(1)	78.7(2)
C(3S)-C(4S)	1.471(7)	C(13)-C(14)-Mo(1)	76.9(2)
C(3S)-H(3SA)	0.9900	C(15)-C(14)-H(14A)	120.6
C(3S)-H(3SB)	0.9900	C(13)-C(14)-H(14A)	120.6
C(4S)-H(4SA)	0.9800	Mo(1)-C(14)-H(14A)	120.6
C(4S)-H(4SB)	0.9800	C(14)-C(15)-O(3)	114.1(3)
C(4S)-H(4SC)	0.9800	C(14)-C(15)-Mo(1)	66.6(2)
		O(3)-C(15)-Mo(1)	119.2(2)
N(4)-B(1)-N(6)	108.6(3)	C(14)-C(15)-H(15A)	115.9
N(4)-B(1)-N(2)	109.2(3)	O(3)-C(15)-H(15A)	115.9
N(6)-B(1)-N(2)	107.8(4)	Mo(1)-C(15)-H(15A)	115.9
N(4)-B(1)-H(1B)	112(2)	O(4)-C(16)-O(3)	126.8(4)
N(6)-B(1)-H(1B)	104(2)	O(4)-C(16)-O(5)	126.6(4)
N(2)-B(1)-H(1B)	115(2)	O(3)-C(16)-O(5)	106.6(3)
N(1)-C(1)-C(2)	111.4(4)	O(5)-C(17)-C(20)	113.5(3)

O(5)-C(17)-C(18)	109.5(3)
C(20)-C(17)-C(18)	104.2(3)
O(5)-C(17)-H(17A)	109.8
C(20)-C(17)-H(17A)	109.8
C(18)-C(17)-H(17A)	109.8
O(6)-C(18)-O(7)	123.8(4)
O(6)-C(18)-C(17)	128.5(4)
O(7)-C(18)-C(17)	107.7(4)
O(7)-C(19)-C(20)	106.2(4)
O(7)-C(19)-H(19A)	110.5
C(20)-C(19)-H(19A)	110.5
O(7)-C(19)-H(19B)	110.5
C(20)-C(19)-H(19B)	110.5
H(19A)-C(19)-H(19B)	108.7
C(21)-C(20)-C(17)	113.9(4)
C(21)-C(20)-C(19)	112.6(4)
C(17)-C(20)-C(19)	98.7(4)
C(21)-C(20)-C(22)	111.0(4)
C(17)-C(20)-C(22)	110.1(4)
C(19)-C(20)-C(22)	109.9(4)
C(20)-C(21)-H(21A)	109.5
C(20)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(20)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(20)-C(22)-H(22A)	109.5
C(20)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(20)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(10)-Mo(1)-C(11)	82.03(17)
C(10)-Mo(1)-N(5)	94.01(19)
C(11)-Mo(1)-N(5)	81.17(15)
C(10)-Mo(1)-C(14)	103.12(19)
C(11)-Mo(1)-C(14)	98.68(15)
N(5)-Mo(1)-C(14)	162.71(14)
C(10)-Mo(1)-N(1)	92.15(12)
C(11)-Mo(1)-N(1)	157.61(17)
N(5)-Mo(1)-N(1)	77.68(14)
C(14)-Mo(1)-N(1)	103.70(15)
C(10)-Mo(1)-N(3)	174.40(14)
C(11)-Mo(1)-N(3)	101.10(14)
N(5)-Mo(1)-N(3)	81.97(13)
C(14)-Mo(1)-N(3)	81.10(14)
N(1)-Mo(1)-N(3)	83.21(10)
C(10)-Mo(1)-C(13)	99.57(17)
C(11)-Mo(1)-C(13)	63.14(15)
N(5)-Mo(1)-C(13)	139.21(13)
C(14)-Mo(1)-C(13)	35.65(13)
N(1)-Mo(1)-C(13)	139.25(15)
N(3)-Mo(1)-C(13)	86.01(14)
C(10)-Mo(1)-C(15)	74.41(19)
C(11)-Mo(1)-C(15)	113.15(15)
N(5)-Mo(1)-C(15)	159.41(12)
C(14)-Mo(1)-C(15)	34.70(13)
N(1)-Mo(1)-C(15)	85.68(14)
N(3)-Mo(1)-C(15)	108.23(14)
C(13)-Mo(1)-C(15)	60.81(13)
C(1)-N(1)-N(2)	105.3(3)
C(1)-N(1)-Mo(1)	133.5(3)
N(2)-N(1)-Mo(1)	121.0(2)
C(3)-N(2)-N(1)	109.8(3)
C(3)-N(2)-B(1)	129.5(4)
N(1)-N(2)-B(1)	120.2(3)
C(4)-N(3)-N(4)	105.3(3)
C(4)-N(3)-Mo(1)	135.0(3)
N(4)-N(3)-Mo(1)	119.6(2)
C(6)-N(4)-N(3)	110.3(3)
C(6)-N(4)-B(1)	128.1(4)
N(3)-N(4)-B(1)	121.6(3)
C(7)-N(5)-N(6)	106.6(3)
C(7)-N(5)-Mo(1)	130.6(3)
N(6)-N(5)-Mo(1)	122.7(2)
C(9)-N(6)-N(5)	109.4(4)
C(9)-N(6)-B(1)	130.7(4)
N(5)-N(6)-B(1)	119.8(3)
C(16)-O(3)-C(15)	116.1(3)
C(16)-O(5)-C(17)	115.8(3)
C(18)-O(7)-C(19)	109.3(4)
C(2S)-O(1S)-C(3S)	118.3(4)
C(2S)-C(1S)-H(1SA)	109.5
C(2S)-C(1S)-H(1SB)	109.5
H(1SA)-C(1S)-H(1SB)	109.5
C(2S)-C(1S)-H(1SC)	109.5
H(1SA)-C(1S)-H(1SC)	109.5
H(1SB)-C(1S)-H(1SC)	109.5
O(2S)-C(2S)-O(1S)	121.6(5)
O(2S)-C(2S)-C(1S)	124.2(5)
O(1S)-C(2S)-C(1S)	113.8(5)
O(1S)-C(3S)-C(4S)	107.7(4)
O(1S)-C(3S)-H(3SA)	110.2
C(4S)-C(3S)-H(3SA)	110.2
O(1S)-C(3S)-H(3SB)	110.2
C(4S)-C(3S)-H(3SB)	110.2
H(3SA)-C(3S)-H(3SB)	108.5
C(3S)-C(4S)-H(4SA)	109.5
C(3S)-C(4S)-H(4SB)	109.5
H(4SA)-C(4S)-H(4SB)	109.5
C(3S)-C(4S)-H(4SC)	109.5
H(4SA)-C(4S)-H(4SC)	109.5
H(4SB)-C(4S)-H(4SC)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S-16. Anisotropic displacement parameters (Å²x 10³)for (1R, R)-12.*

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
B(1)	27(2)	33(3)	22(2)	0(2)	-8(2)	8(2)
C(1)	20(2)	32(2)	24(2)	-4(2)	-4(1)	4(2)
C(2)	31(2)	48(2)	16(1)	2(2)	3(3)	-2(3)
C(3)	34(2)	37(2)	20(2)	3(2)	-5(2)	2(2)
C(4)	26(2)	41(3)	24(2)	-2(2)	-1(2)	2(2)
C(5)	43(3)	29(2)	34(2)	-5(2)	7(2)	-7(3)
C(6)	38(2)	26(2)	32(2)	3(2)	1(2)	3(2)
C(7)	23(2)	47(2)	23(2)	-5(2)	3(2)	-8(2)
C(8)	19(2)	75(4)	31(2)	-12(2)	-3(2)	-7(2)
C(9)	20(2)	61(3)	36(2)	-13(2)	-6(2)	6(2)
C(10)	26(2)	36(2)	20(1)	2(1)	-3(2)	6(3)
C(11)	21(2)	30(2)	23(2)	3(2)	1(2)	2(2)
C(12)	32(2)	48(3)	20(2)	6(2)	-3(2)	4(2)
C(13)	25(2)	35(2)	21(2)	1(2)	-2(1)	4(2)
C(14)	16(2)	32(2)	20(2)	-3(2)	-3(1)	-3(2)
C(15)	15(2)	33(2)	14(2)	2(2)	1(1)	2(2)
C(16)	22(2)	34(2)	18(2)	-5(2)	0(1)	0(2)
C(17)	29(2)	31(2)	18(2)	1(2)	7(2)	0(2)
C(18)	43(3)	39(3)	21(2)	-7(2)	2(2)	-1(2)
C(19)	43(3)	45(3)	30(3)	-9(2)	15(2)	2(2)
C(20)	28(2)	34(3)	30(2)	0(2)	6(2)	1(2)
C(21)	33(3)	52(3)	62(3)	7(3)	9(2)	11(2)
C(22)	38(3)	35(3)	39(3)	-2(2)	15(2)	-6(2)
Mo(1)	16(1)	24(1)	16(1)	0(1)	0(1)	0(1)
N(1)	22(2)	27(1)	19(1)	1(1)	-4(2)	4(2)
N(2)	25(2)	29(2)	23(2)	5(1)	1(1)	4(2)
N(3)	23(2)	26(2)	21(1)	2(1)	-1(1)	0(2)
N(4)	26(2)	30(2)	23(2)	0(1)	2(1)	3(2)
N(5)	19(2)	32(2)	24(2)	-3(1)	0(1)	-1(1)
N(6)	21(2)	36(2)	26(2)	-4(2)	-4(1)	8(2)
O(1)	56(2)	27(2)	50(2)	-5(1)	-1(2)	-5(2)
O(2)	35(2)	48(2)	31(2)	8(2)	8(1)	0(2)
O(3)	21(1)	32(2)	19(1)	-1(1)	4(1)	2(1)
O(4)	45(2)	28(2)	30(2)	-2(1)	11(1)	-1(2)
O(5)	28(2)	29(2)	20(1)	-3(1)	7(1)	-2(1)
O(6)	32(2)	79(3)	43(2)	-14(2)	-7(2)	1(2)
O(7)	49(2)	52(2)	22(2)	-6(2)	9(2)	-1(2)

*The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

Table 17. Hydrogen coordinates (x 10⁴) and isotropic displacement parameters (Å²x 10³) for (1R, R)-12.

	x	y	z	U(eq)

H(1B)	-2360(50)	8720(30)	2510(20)	33
H(1A)	931	6330	1888	30
H(2A)	287	7108	748	37
H(3A)	-1115	8254	1199	37
H(4A)	1075	8635	4678	36
H(5A)	412	10045	4343	42
H(6A)	-1166	9906	3282	38
H(7A)	-3044	6040	4013	37
H(8A)	-5111	6716	3627	50
H(9A)	-4488	7985	2947	47
H(12A)	2470	6223	5515	50
H(12B)	2247	5711	4766	50
H(12C)	1073	5848	5335	50
H(13A)	1362	7343	5053	32
H(14A)	2455	7632	3950	27
H(15A)	2479	5929	3671	25
H(17A)	4577	5458	1451	31
H(19A)	6194	6265	-183	47
H(19B)	5980	5379	184	47
H(21A)	6915	5425	1405	74
H(21B)	6931	6250	1882	74
H(21C)	7731	6194	1119	74
H(22A)	5847	7494	1395	56
H(22B)	4970	7441	660	56
H(22C)	6516	7433	591	56
H(1SA)	5915	9712	428	67
H(1SB)	6346	9119	1092	67
H(1SC)	5848	10022	1274	67
H(3SA)	2801	8082	1706	50
H(3SB)	2176	8934	1447	50
H(4SA)	1555	8631	2666	84
H(4SB)	2421	9441	2654	84
H(4SC)	3044	8593	2912	84

Table S-18. Torsion angles [°] for (1R, R)-12.

N(1)-C(1)-C(2)-C(3)	-1.2(5)
C(1)-C(2)-C(3)-N(2)	0.0(5)
N(3)-C(4)-C(5)-C(6)	0.1(5)
C(4)-C(5)-C(6)-N(4)	0.1(5)
N(5)-C(7)-C(8)-C(9)	0.4(5)
C(7)-C(8)-C(9)-N(6)	-0.1(5)
C(12)-C(13)-C(14)-C(15)	44.2(5)
Mo(1)-C(13)-C(14)-C(15)	-69.3(3)
C(12)-C(13)-C(14)-Mo(1)	113.5(4)
C(13)-C(14)-C(15)-O(3)	-178.8(3)
Mo(1)-C(14)-C(15)-O(3)	112.9(3)
C(13)-C(14)-C(15)-Mo(1)	68.3(3)
O(5)-C(17)-C(18)-O(6)	-33.4(7)
C(20)-C(17)-C(18)-O(6)	-155.1(5)
O(5)-C(17)-C(18)-O(7)	146.9(4)
C(20)-C(17)-C(18)-O(7)	25.2(5)

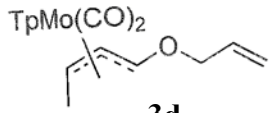
O(5)-C(17)-C(20)-C(21)	86.3(5)
C(18)-C(17)-C(20)-C(21)	-154.7(4)
O(5)-C(17)-C(20)-C(19)	-154.2(4)
C(18)-C(17)-C(20)-C(19)	-35.2(4)
O(5)-C(17)-C(20)-C(22)	-39.2(5)
C(18)-C(17)-C(20)-C(22)	79.8(4)
O(7)-C(19)-C(20)-C(21)	154.8(4)
O(7)-C(19)-C(20)-C(17)	34.3(5)
O(7)-C(19)-C(20)-C(22)	-80.8(5)
O(1)-C(10)-Mo(1)-C(11)	25(9)
O(1)-C(10)-Mo(1)-N(5)	-55(9)
O(1)-C(10)-Mo(1)-C(14)	122(9)
O(1)-C(10)-Mo(1)-N(1)	-133(9)
O(1)-C(10)-Mo(1)-N(3)	-99(8)
O(1)-C(10)-Mo(1)-C(13)	86(9)
O(1)-C(10)-Mo(1)-C(15)	142(9)
O(2)-C(11)-Mo(1)-C(10)	-71(4)
O(2)-C(11)-Mo(1)-N(5)	24(4)
O(2)-C(11)-Mo(1)-C(14)	-173(4)
O(2)-C(11)-Mo(1)-N(1)	5(5)
O(2)-C(11)-Mo(1)-N(3)	104(4)
O(2)-C(11)-Mo(1)-C(13)	-176(4)
O(2)-C(11)-Mo(1)-C(15)	-140(4)
C(15)-C(14)-Mo(1)-C(10)	34.8(3)
C(13)-C(14)-Mo(1)-C(10)	-88.2(3)
C(15)-C(14)-Mo(1)-C(11)	118.6(2)
C(13)-C(14)-Mo(1)-C(11)	-4.4(3)
C(15)-C(14)-Mo(1)-N(5)	-153.3(4)
C(13)-C(14)-Mo(1)-N(5)	83.8(5)
C(15)-C(14)-Mo(1)-N(1)	-60.8(2)
C(13)-C(14)-Mo(1)-N(1)	176.3(3)
C(15)-C(14)-Mo(1)-N(3)	-141.5(2)
C(13)-C(14)-Mo(1)-N(3)	95.6(3)
C(15)-C(14)-Mo(1)-C(13)	122.9(4)
C(13)-C(14)-Mo(1)-C(15)	-122.9(4)
C(14)-C(13)-Mo(1)-C(10)	99.2(3)
C(12)-C(13)-Mo(1)-C(10)	-15.1(4)
C(14)-C(13)-Mo(1)-C(11)	175.1(3)
C(12)-C(13)-Mo(1)-C(11)	60.8(3)
C(14)-C(13)-Mo(1)-N(5)	-153.1(2)
C(12)-C(13)-Mo(1)-N(5)	92.6(4)
C(12)-C(13)-Mo(1)-C(14)	-114.3(4)
C(14)-C(13)-Mo(1)-N(1)	-5.5(4)
C(12)-C(13)-Mo(1)-N(1)	-119.8(3)
C(14)-C(13)-Mo(1)-N(3)	-80.3(3)
C(12)-C(13)-Mo(1)-N(3)	165.4(3)
C(14)-C(13)-Mo(1)-C(15)	33.2(2)
C(12)-C(13)-Mo(1)-C(15)	-81.1(3)
C(14)-C(15)-Mo(1)-C(10)	-144.8(3)
O(3)-C(15)-Mo(1)-C(10)	109.8(3)
C(14)-C(15)-Mo(1)-C(11)	-70.8(3)
O(3)-C(15)-Mo(1)-C(11)	-176.3(3)
C(14)-C(15)-Mo(1)-N(5)	157.7(4)
O(3)-C(15)-Mo(1)-N(5)	52.2(5)
O(3)-C(15)-Mo(1)-C(14)	-105.5(4)
C(14)-C(15)-Mo(1)-N(1)	121.8(2)

O(3)-C(15)-Mo(1)-N(1)	16.3(3)
C(14)-C(15)-Mo(1)-N(3)	40.4(2)
O(3)-C(15)-Mo(1)-N(3)	-65.1(3)
C(14)-C(15)-Mo(1)-C(13)	-34.1(2)
O(3)-C(15)-Mo(1)-C(13)	-139.5(3)
C(2)-C(1)-N(1)-N(2)	1.8(5)
C(2)-C(1)-N(1)-Mo(1)	178.3(4)
C(10)-Mo(1)-N(1)-C(1)	-34.4(5)
C(11)-Mo(1)-N(1)-C(1)	-108.6(6)
N(5)-Mo(1)-N(1)-C(1)	-128.0(4)
C(14)-Mo(1)-N(1)-C(1)	69.7(4)
N(3)-Mo(1)-N(1)-C(1)	148.7(4)
C(13)-Mo(1)-N(1)-C(1)	73.0(5)
C(15)-Mo(1)-N(1)-C(1)	39.8(4)
C(10)-Mo(1)-N(1)-N(2)	141.6(3)
C(11)-Mo(1)-N(1)-N(2)	67.5(5)
N(5)-Mo(1)-N(1)-N(2)	48.0(3)
C(14)-Mo(1)-N(1)-N(2)	-114.3(3)
N(3)-Mo(1)-N(1)-N(2)	-35.2(3)
C(13)-Mo(1)-N(1)-N(2)	-111.0(4)
C(15)-Mo(1)-N(1)-N(2)	-144.2(3)
C(2)-C(3)-N(2)-N(1)	1.1(5)
C(2)-C(3)-N(2)-B(1)	-170.0(4)
C(1)-N(1)-N(2)-C(3)	-1.8(5)
Mo(1)-N(1)-N(2)-C(3)	-178.8(3)
C(1)-N(1)-N(2)-B(1)	170.3(4)
Mo(1)-N(1)-N(2)-B(1)	-6.7(5)
N(4)-B(1)-N(2)-C(3)	-126.4(5)
N(6)-B(1)-N(2)-C(3)	115.8(5)
N(4)-B(1)-N(2)-N(1)	63.3(5)
N(6)-B(1)-N(2)-N(1)	-54.5(5)
C(5)-C(4)-N(3)-N(4)	-0.3(5)
C(5)-C(4)-N(3)-Mo(1)	175.7(3)
C(10)-Mo(1)-N(3)-C(4)	-171.9(16)
C(11)-Mo(1)-N(3)-C(4)	64.5(4)
N(5)-Mo(1)-N(3)-C(4)	143.8(4)
C(14)-Mo(1)-N(3)-C(4)	-32.6(4)
N(1)-Mo(1)-N(3)-C(4)	-137.7(4)
C(13)-Mo(1)-N(3)-C(4)	2.9(4)
C(15)-Mo(1)-N(3)-C(4)	-54.6(4)
C(10)-Mo(1)-N(3)-N(4)	3.7(19)
C(11)-Mo(1)-N(3)-N(4)	-119.9(3)
N(5)-Mo(1)-N(3)-N(4)	-40.6(3)
C(14)-Mo(1)-N(3)-N(4)	142.9(3)
N(1)-Mo(1)-N(3)-N(4)	37.9(3)
C(13)-Mo(1)-N(3)-N(4)	178.5(3)
C(15)-Mo(1)-N(3)-N(4)	121.0(3)
C(5)-C(6)-N(4)-N(3)	-0.3(5)
C(5)-C(6)-N(4)-B(1)	-178.4(4)
C(4)-N(3)-N(4)-C(6)	0.4(4)
Mo(1)-N(3)-N(4)-C(6)	-176.3(3)
C(4)-N(3)-N(4)-B(1)	178.7(4)
Mo(1)-N(3)-N(4)-B(1)	1.9(5)
N(6)-B(1)-N(4)-C(6)	-125.0(4)
N(2)-B(1)-N(4)-C(6)	117.7(5)
N(6)-B(1)-N(4)-N(3)	57.1(5)

N(2)-B(1)-N(4)-N(3)	-60.1(5)
C(8)-C(7)-N(5)-N(6)	-0.5(4)
C(8)-C(7)-N(5)-Mo(1)	175.4(3)
C(10)-Mo(1)-N(5)-C(7)	44.7(4)
C(11)-Mo(1)-N(5)-C(7)	-36.6(4)
C(14)-Mo(1)-N(5)-C(7)	-127.4(5)
N(1)-Mo(1)-N(5)-C(7)	136.0(4)
N(3)-Mo(1)-N(5)-C(7)	-139.2(4)
C(13)-Mo(1)-N(5)-C(7)	-64.9(4)
C(15)-Mo(1)-N(5)-C(7)	99.3(5)
C(10)-Mo(1)-N(5)-N(6)	-139.9(3)
C(11)-Mo(1)-N(5)-N(6)	138.8(3)
C(14)-Mo(1)-N(5)-N(6)	48.0(6)
N(1)-Mo(1)-N(5)-N(6)	-48.6(3)
N(3)-Mo(1)-N(5)-N(6)	36.2(3)
C(13)-Mo(1)-N(5)-N(6)	110.4(3)
C(15)-Mo(1)-N(5)-N(6)	-85.3(5)
C(8)-C(9)-N(6)-N(5)	-0.3(5)
C(8)-C(9)-N(6)-B(1)	176.5(4)
C(7)-N(5)-N(6)-C(9)	0.5(4)
Mo(1)-N(5)-N(6)-C(9)	-175.9(3)
C(7)-N(5)-N(6)-B(1)	-176.7(3)
Mo(1)-N(5)-N(6)-B(1)	6.9(4)
N(4)-B(1)-N(6)-C(9)	120.3(5)
N(2)-B(1)-N(6)-C(9)	-121.5(5)
N(4)-B(1)-N(6)-N(5)	-63.2(5)
N(2)-B(1)-N(6)-N(5)	55.0(4)
O(4)-C(16)-O(3)-C(15)	9.4(6)
O(5)-C(16)-O(3)-C(15)	-169.8(3)
C(14)-C(15)-O(3)-C(16)	163.4(3)
Mo(1)-C(15)-O(3)-C(16)	-121.0(3)
O(4)-C(16)-O(5)-C(17)	6.1(6)
O(3)-C(16)-O(5)-C(17)	-174.7(3)
C(20)-C(17)-O(5)-C(16)	-149.8(4)
C(18)-C(17)-O(5)-C(16)	94.3(4)
O(6)-C(18)-O(7)-C(19)	177.5(5)
C(17)-C(18)-O(7)-C(19)	-2.8(5)
C(20)-C(19)-O(7)-C(18)	-20.8(6)
C(3S)-O(1S)-C(2S)-O(2S)	-5.8(8)
C(3S)-O(1S)-C(2S)-C(1S)	-178.4(4)
C(2S)-O(1S)-C(3S)-C(4S)	-151.7(5)

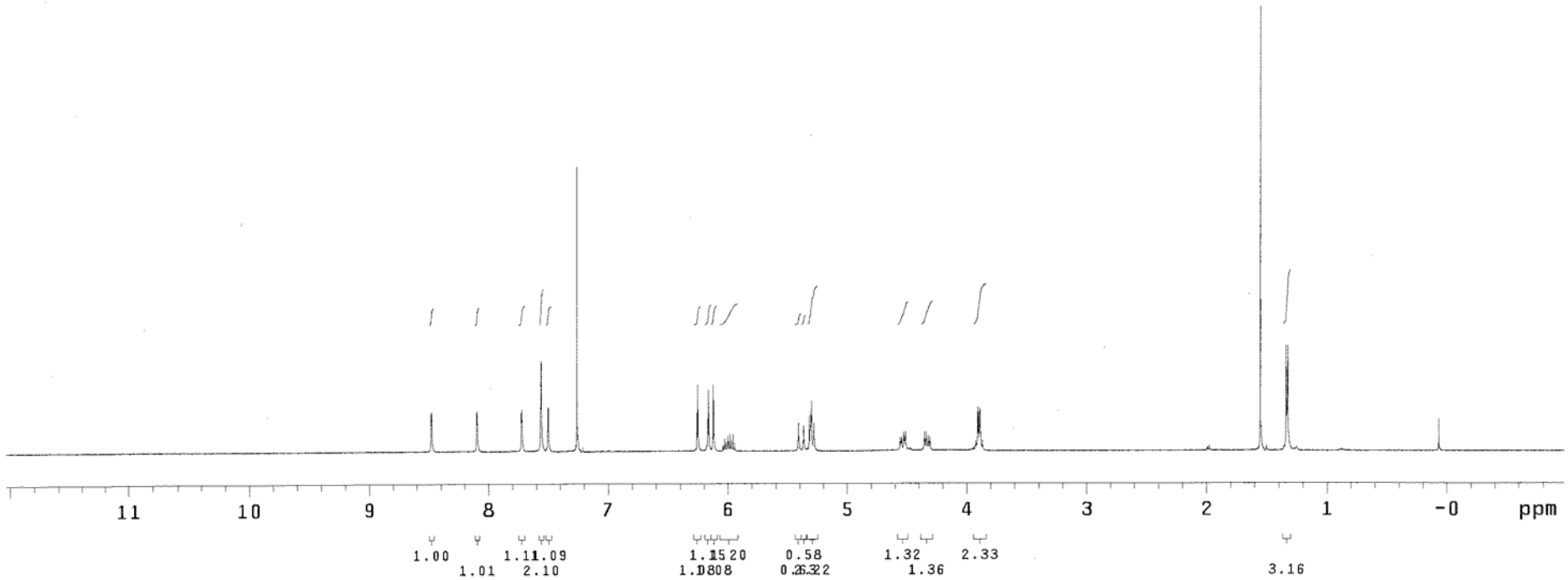
Symmetry transformations used to generate equivalent atoms:

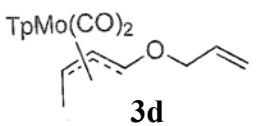
Scans of ^{1}H and ^{13}C NMR Data for All New Compounds



3d

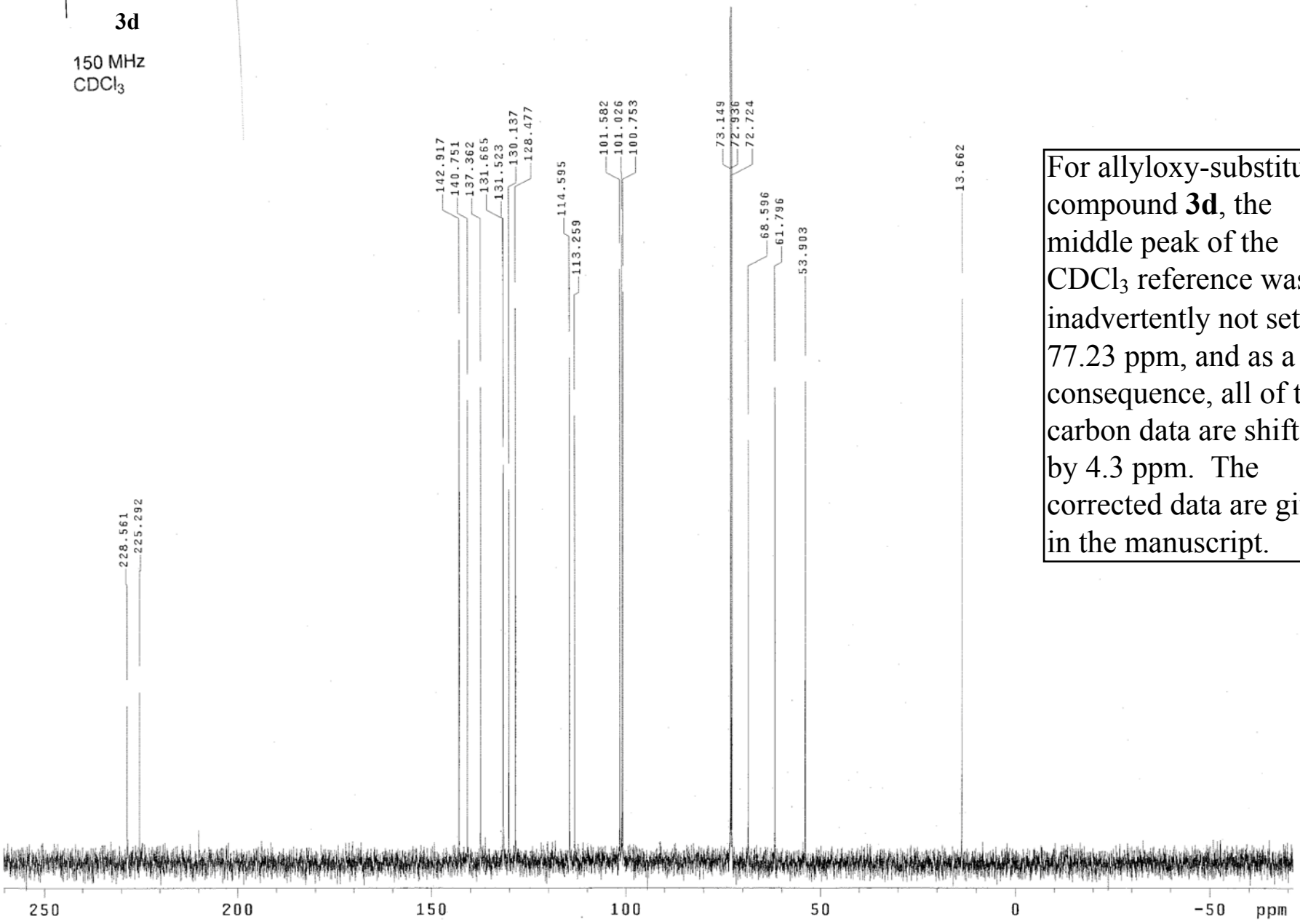
400 MHz
$CDCl_3$



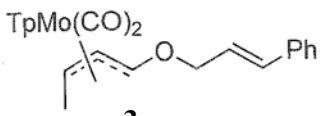


3d

150 MHz
$CDCl_3$

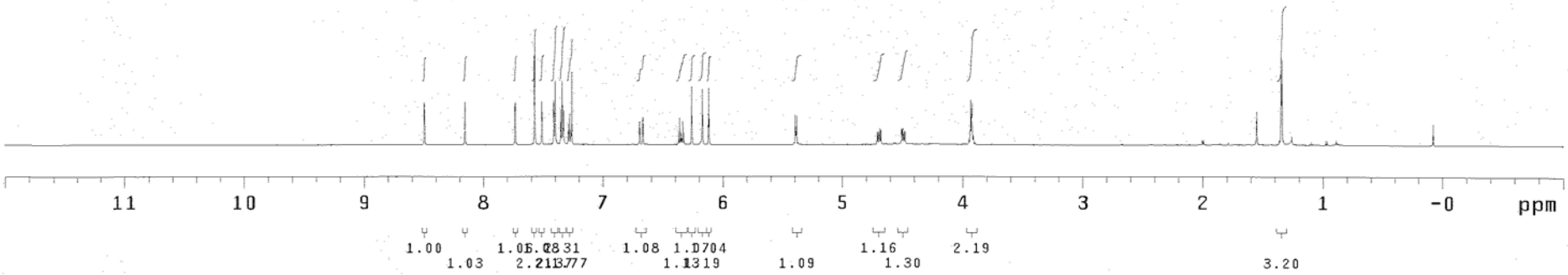


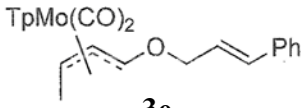
For allyloxy-substituted compound **3d**, the middle peak of the $CDCl_3$ reference was inadvertently not set to 77.23 ppm, and as a consequence, all of the carbon data are shifted by 4.3 ppm. The corrected data are given in the manuscript.



3e

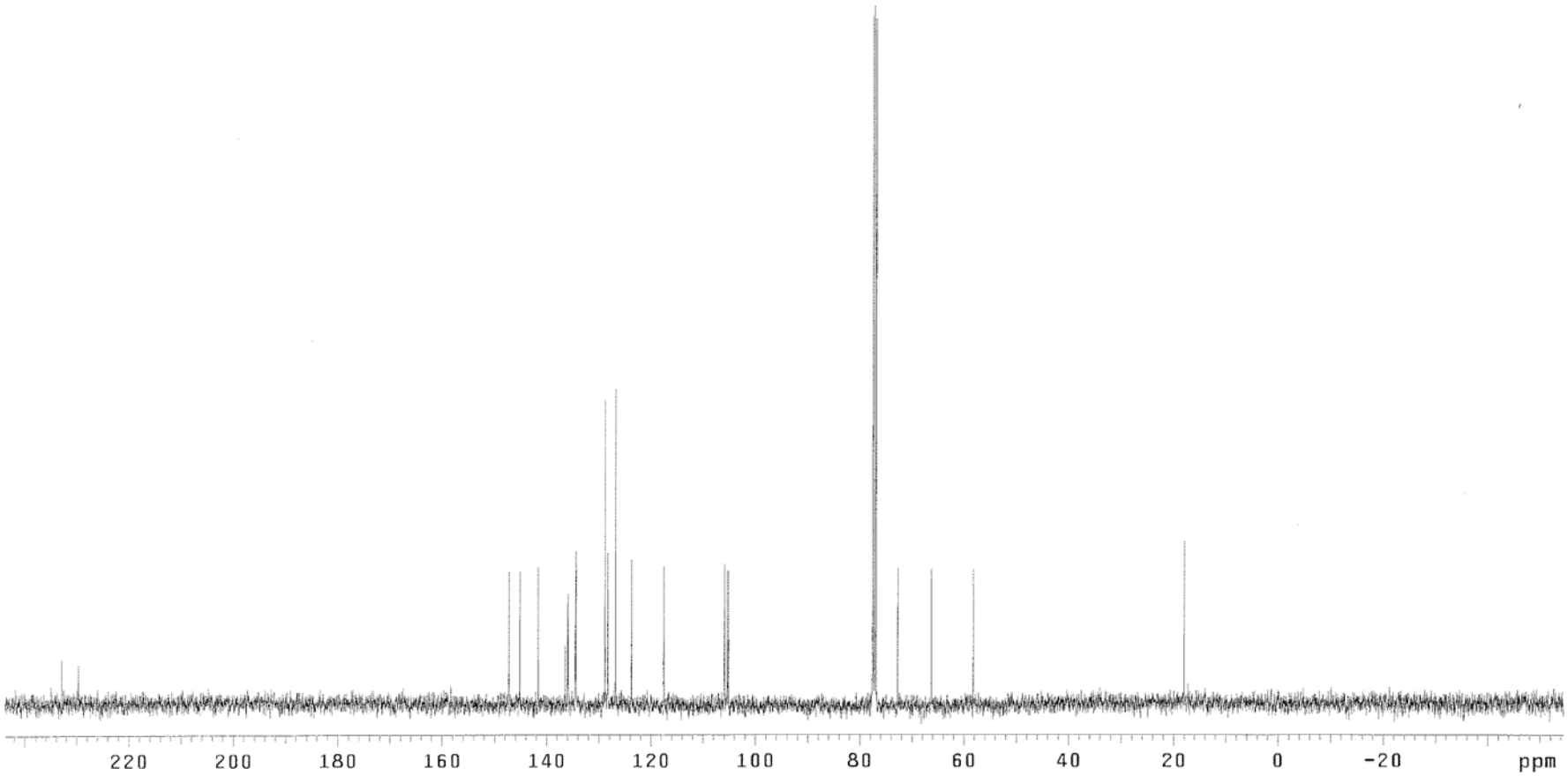
600 MHz
$CDCl_3$

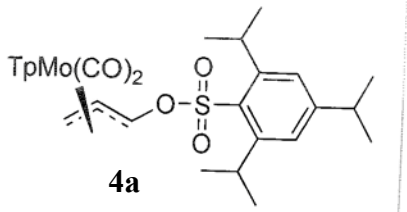




3e

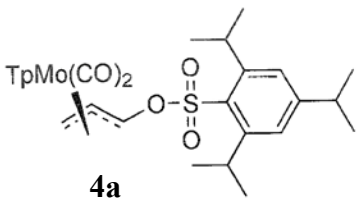
100 MHz
$CDCl_3$





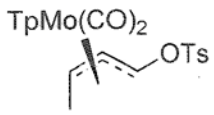
4a

400 MHz
$CDCl_3$



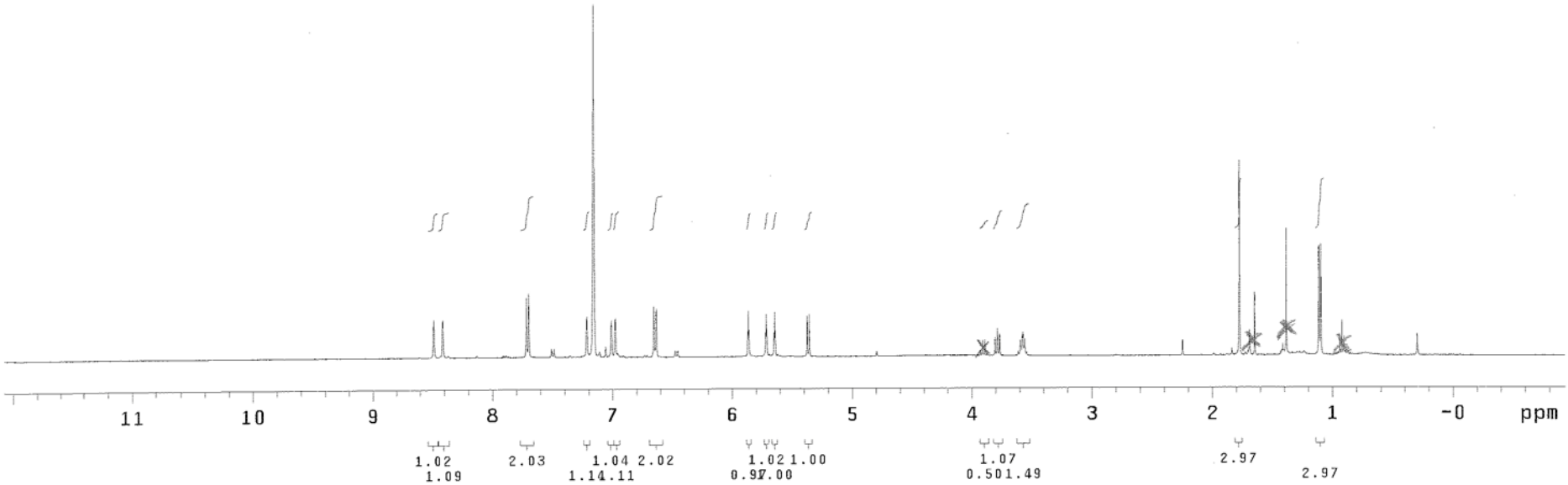
4a

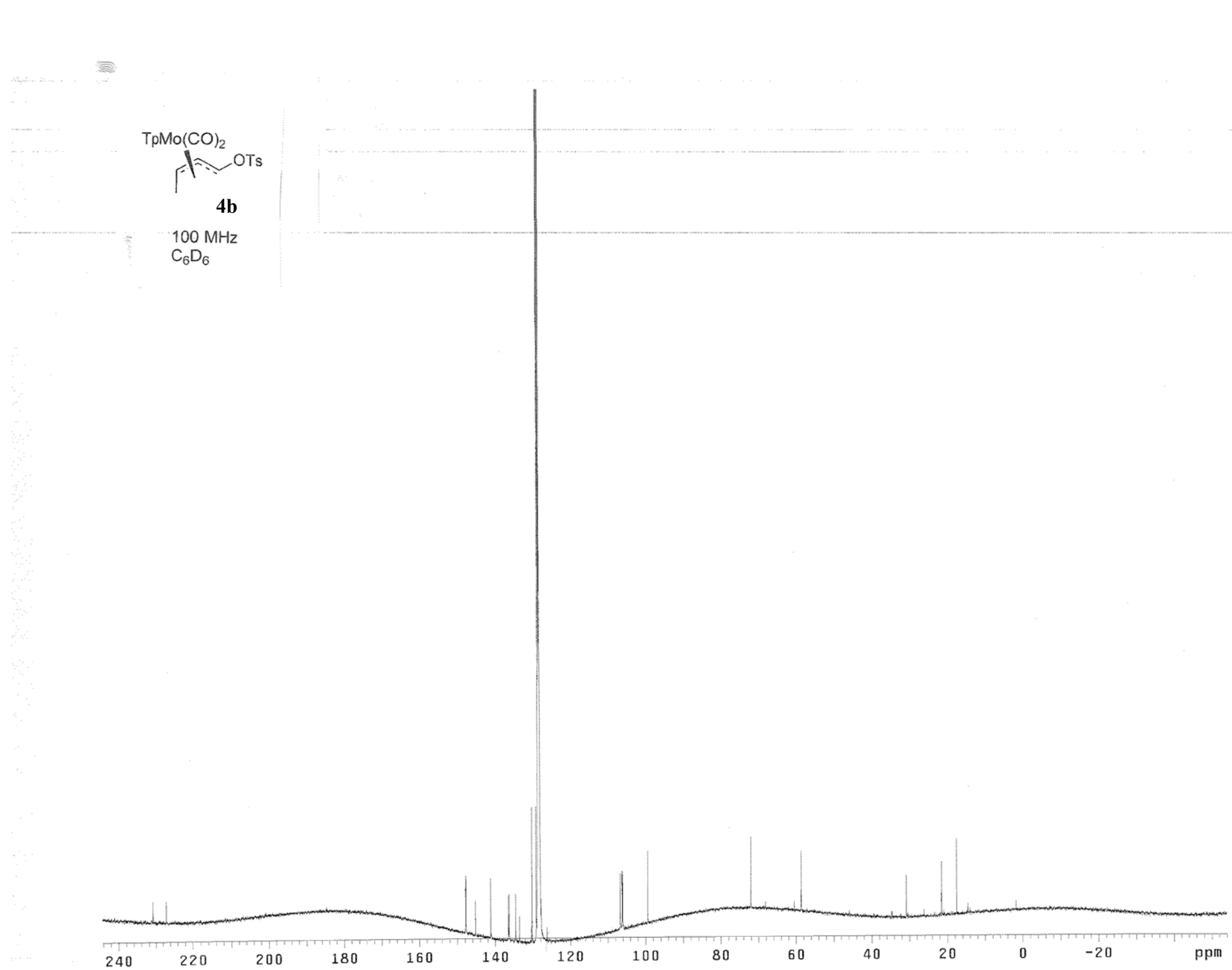
100 MHz
$CDCl_3$

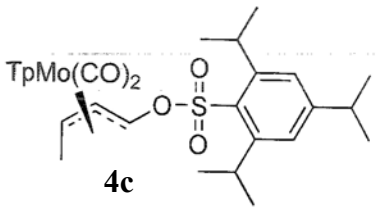


4b

400 MHz
C_6D_6

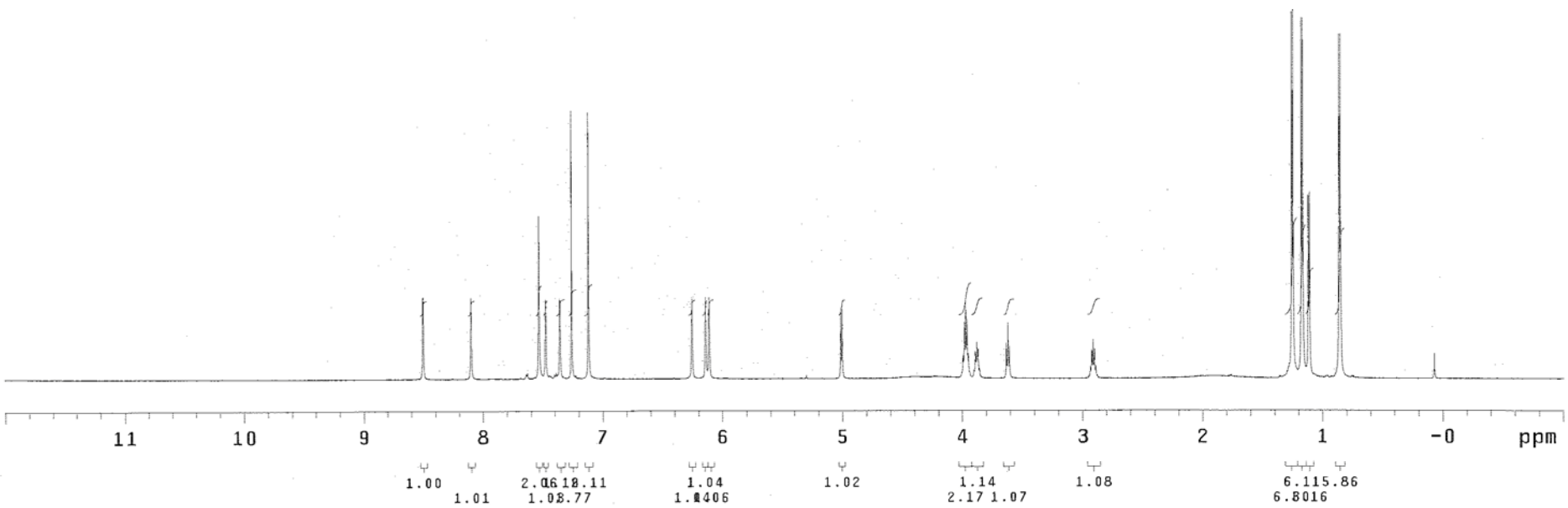


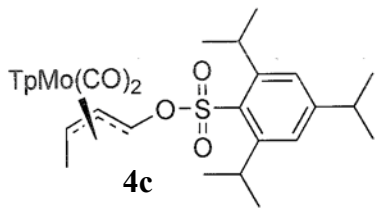

TpMo(CO)2
OTs
4b
100 MHz
C6D6
240
220
200
180
160
140
120
100
80
60
40
20
0
-20
ppm



4c

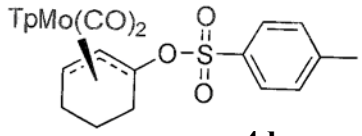
600 MHz
$CDCl_3$





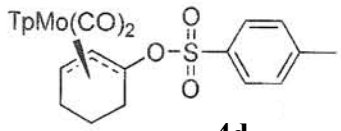
4c

150 MHz
$CDCl_3$



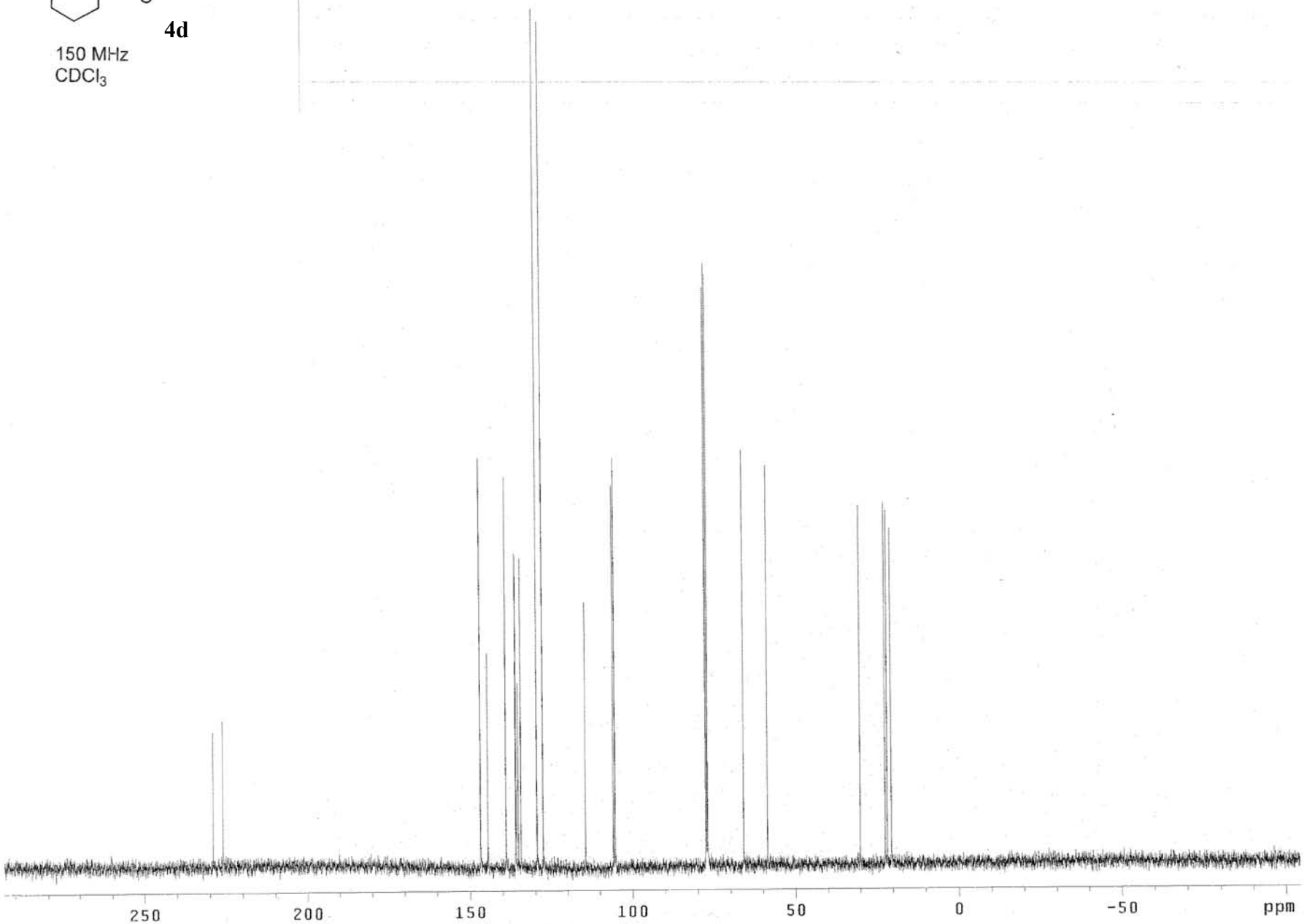
4d

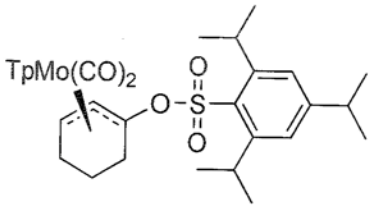
600 MHz
$CDCl_3$



4d

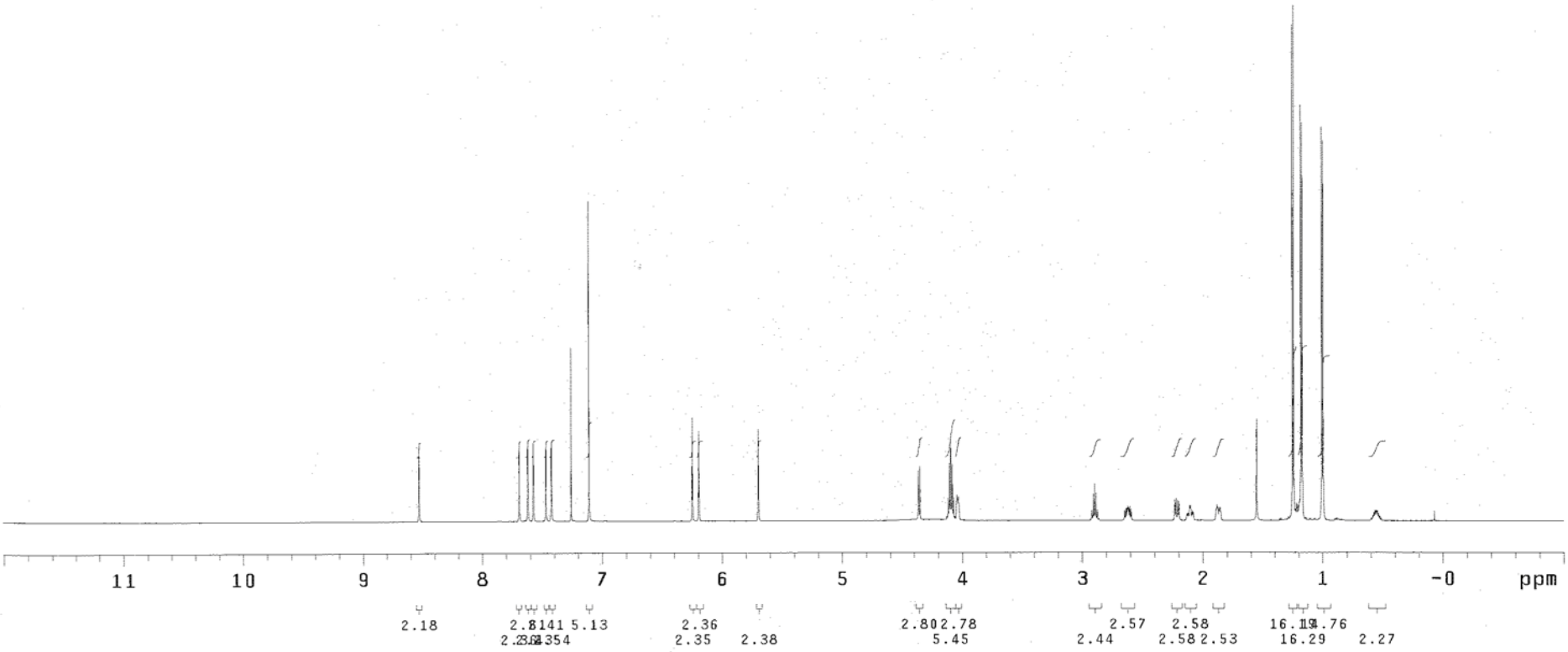
150 MHz
$CDCl_3$

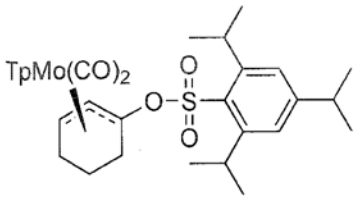




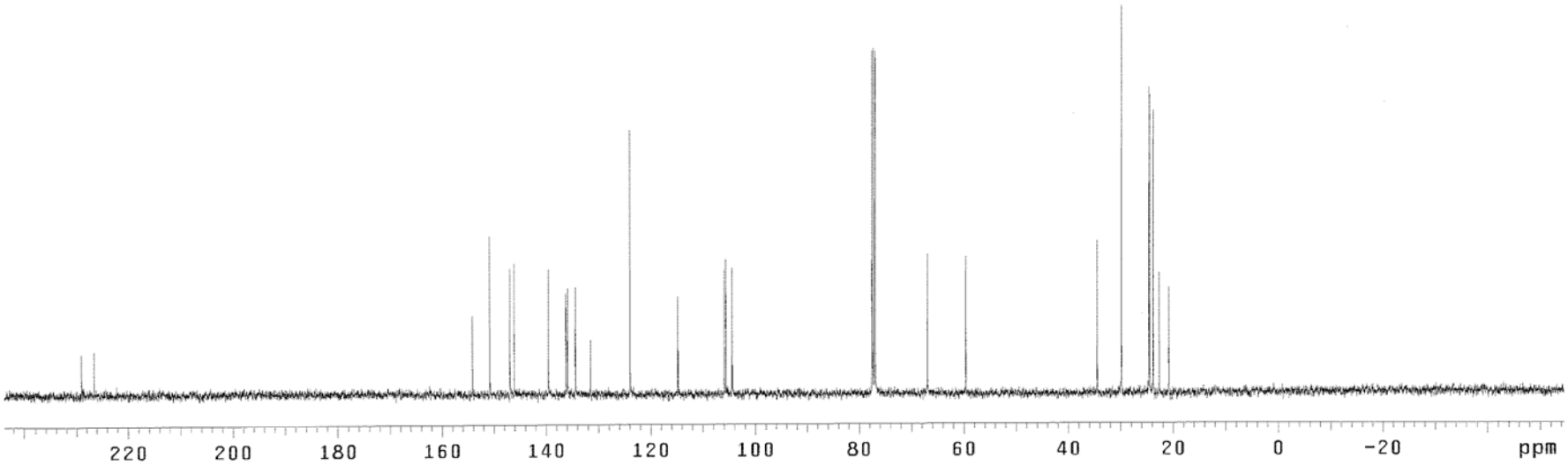
600 MHz
$CDCl_3$

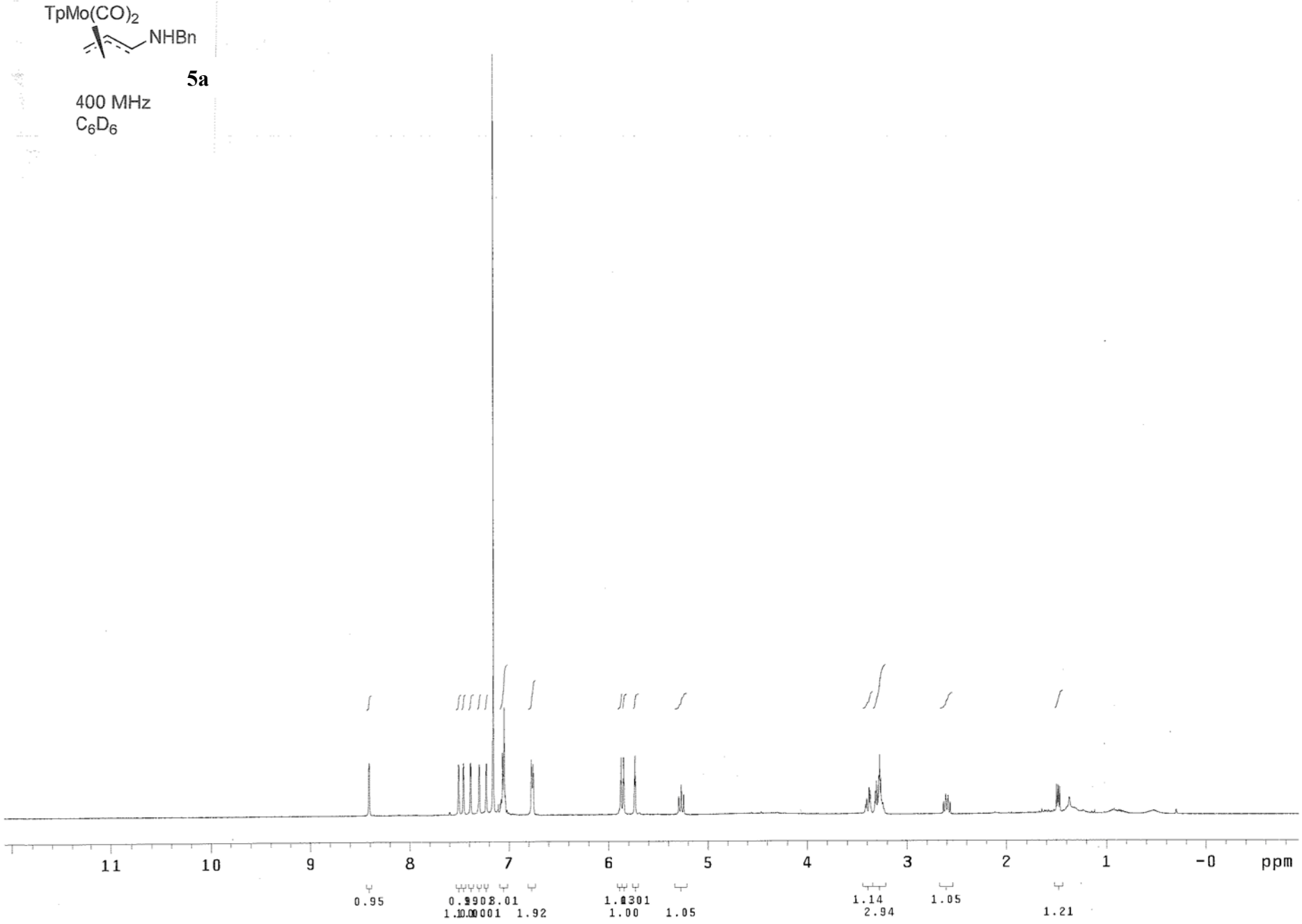
4e

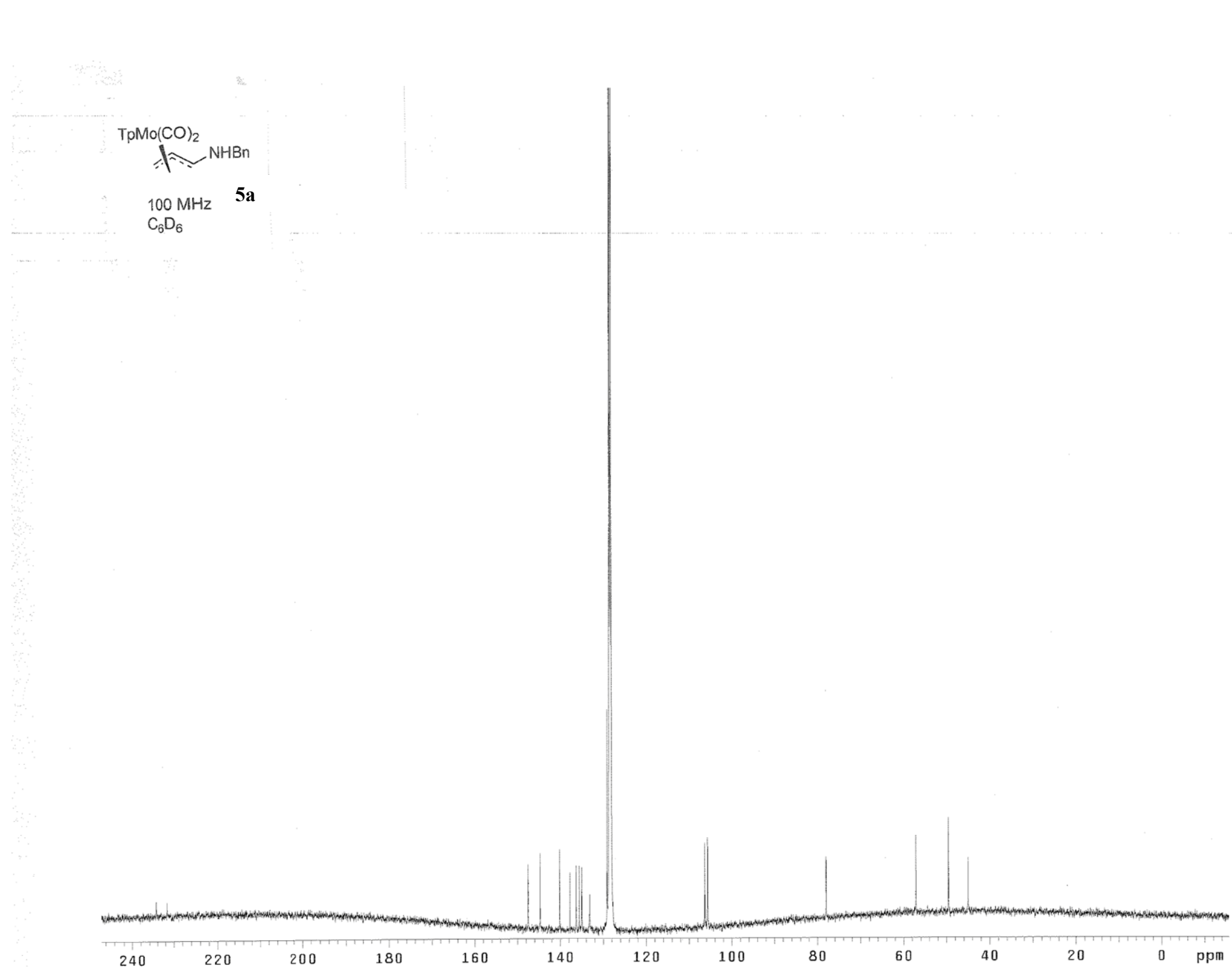


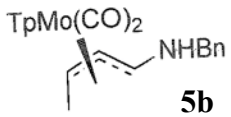


4e 100 MHz
$CDCl_3$



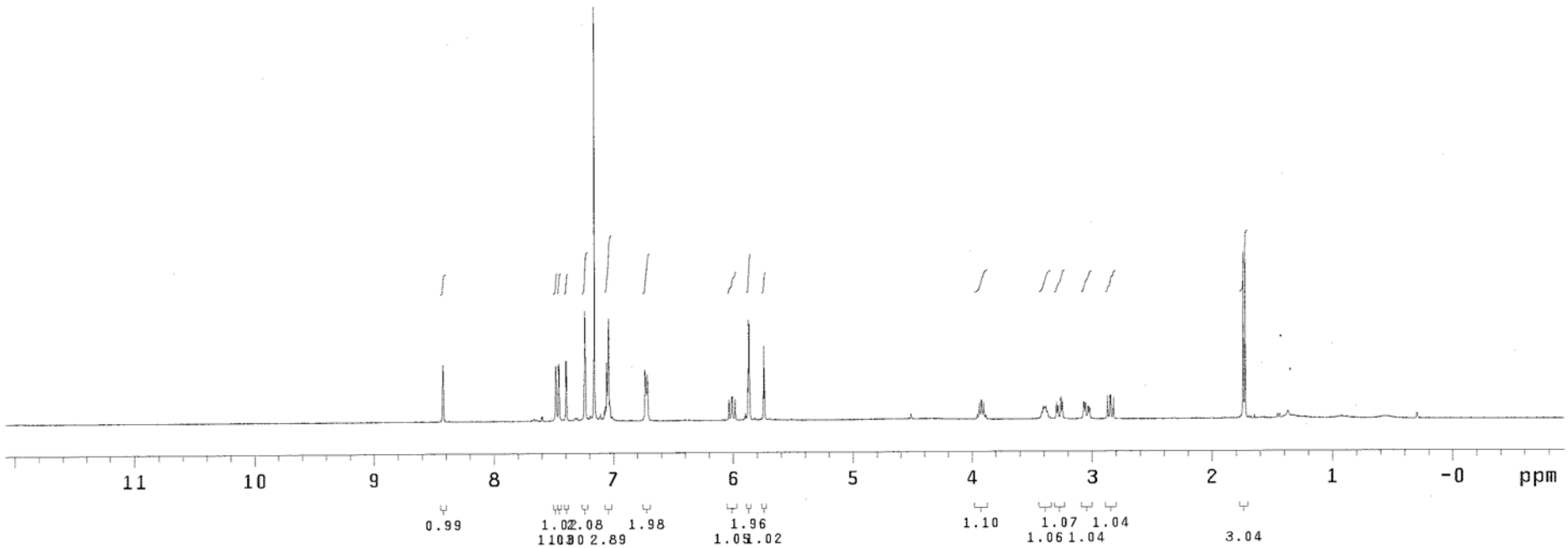

TpMo(CO)2
NHBn
5a
400 MHz
C6D6
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
0.95
1.92
1.00
1.05
2.94
1.05
1.21

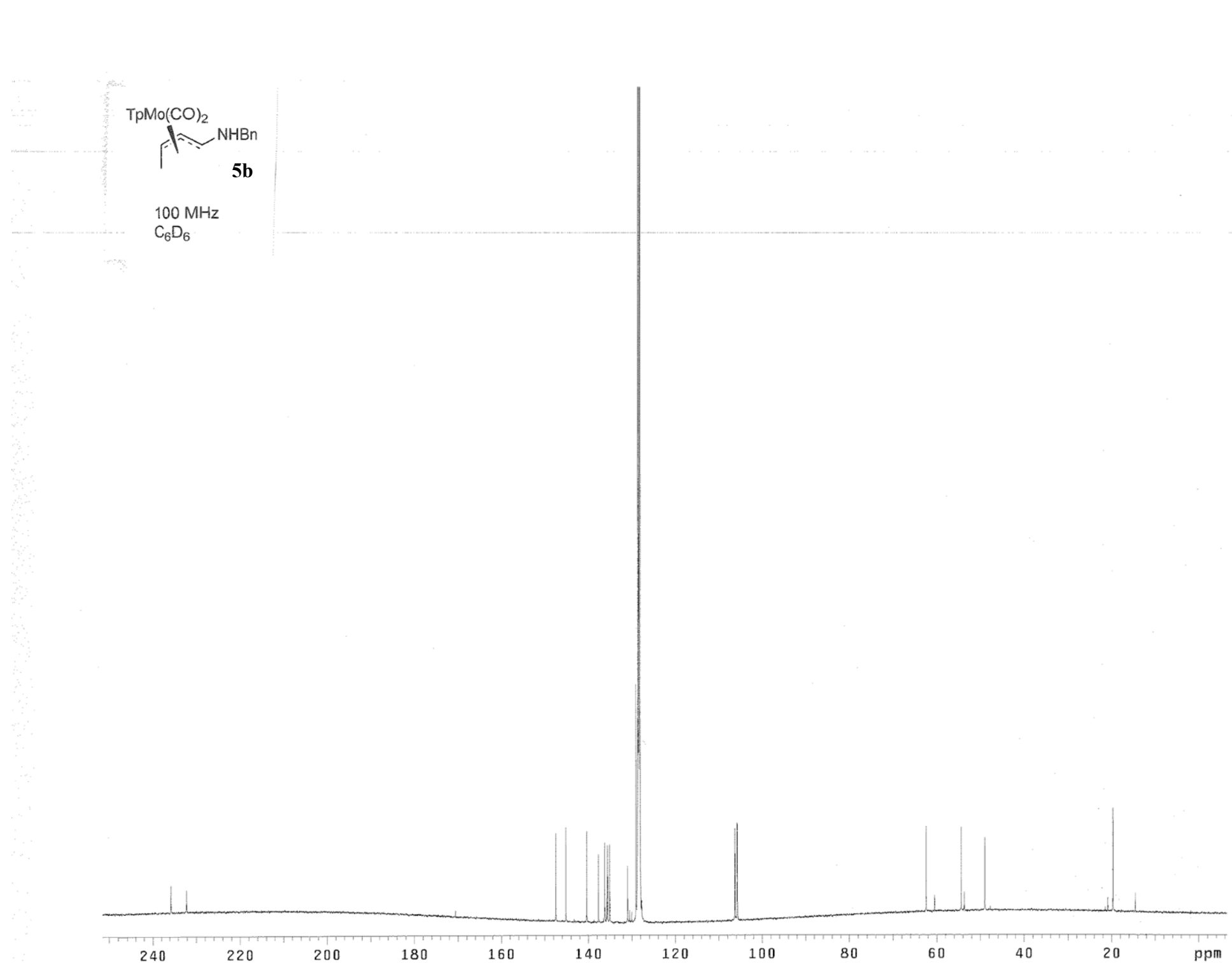

TpMo(CO)2
NHBn
5a
100 MHz
C6D6
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm

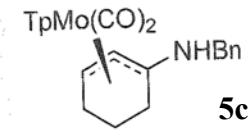


5b

400 MHz
C_6D_6

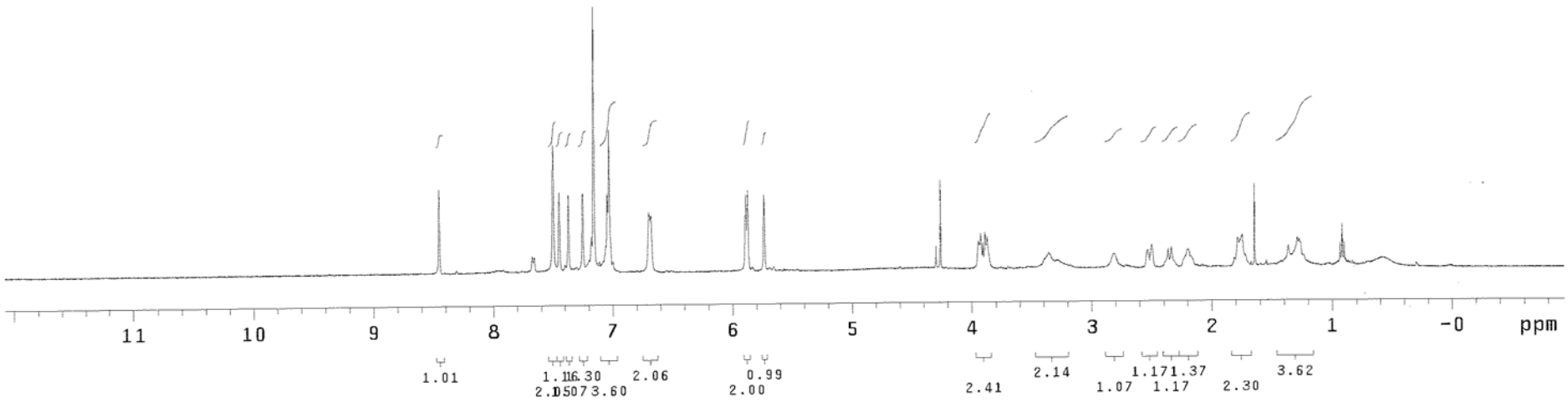


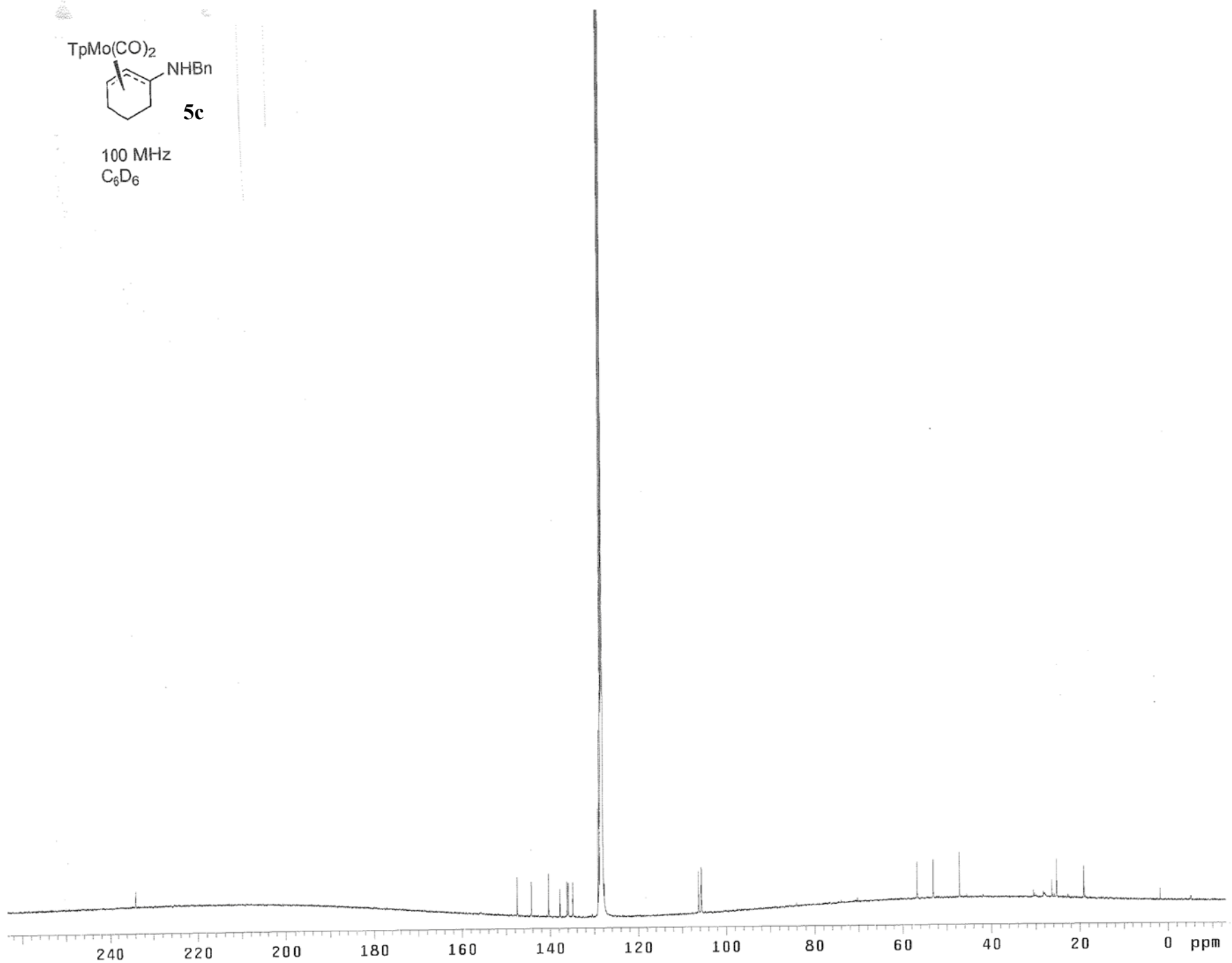

TpMo(CO)2
NHBn
5b
100 MHz
C6D6
240
220
200
180
160
140
120
100
80
60
40
20
ppm



5c

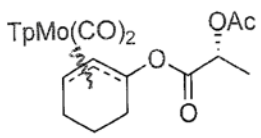
400 MHz
C_6D_6




TpMo(CO)2
NHBn
5c
100 MHz
C6D6
240
220
200
180
160
140
120
100
80
60
40
20
0
ppm

s-(-)-2-acetoxypropionate-cyclohexenyl molybdenum//400MHz//11-1-04

Pulse Sequence: s2pul

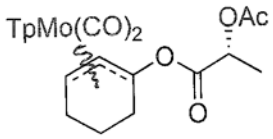


8

400 MHz
$CDCl_3$

s-(-)-acetoxypropionatecyclohexenylmolybdenum//400MHz//10-31-04

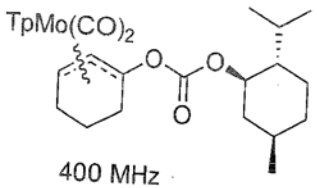
Pulse Sequence: s2pul



100 MHz **8**
$CDCl_3$

(-)-menthylcarbonate-cyclohexenylmolybdenum//400MHz//11-1-04

Pulse Sequence: s2pul

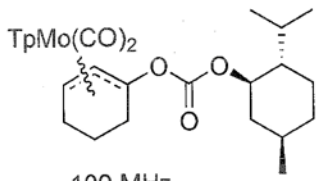


400 MHz
$CDCl_3$

10

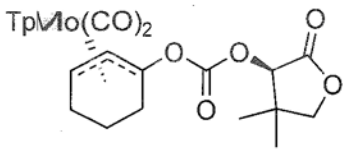
(-)-menthylcarbonatecyclohexenylmolybdenum//400MHz//10-31-04

Pulse Sequence: s2pul



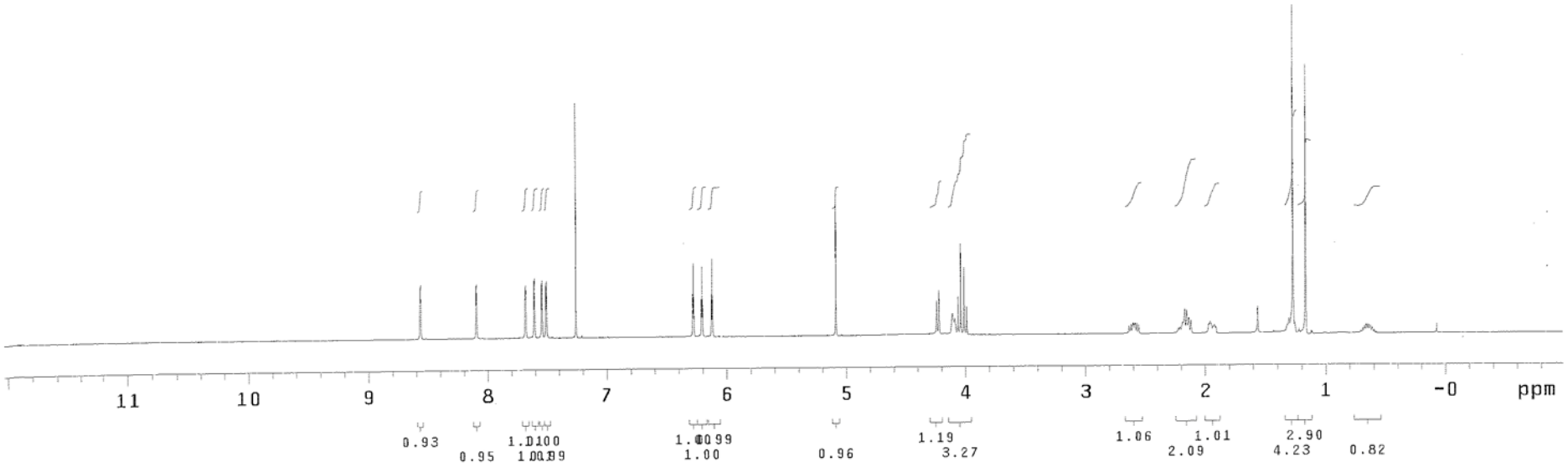
100 MHz
$CDCl_3$

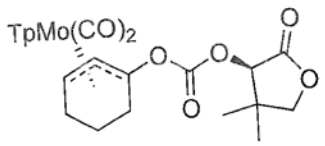
10



400 MHz
$CDCl_3$

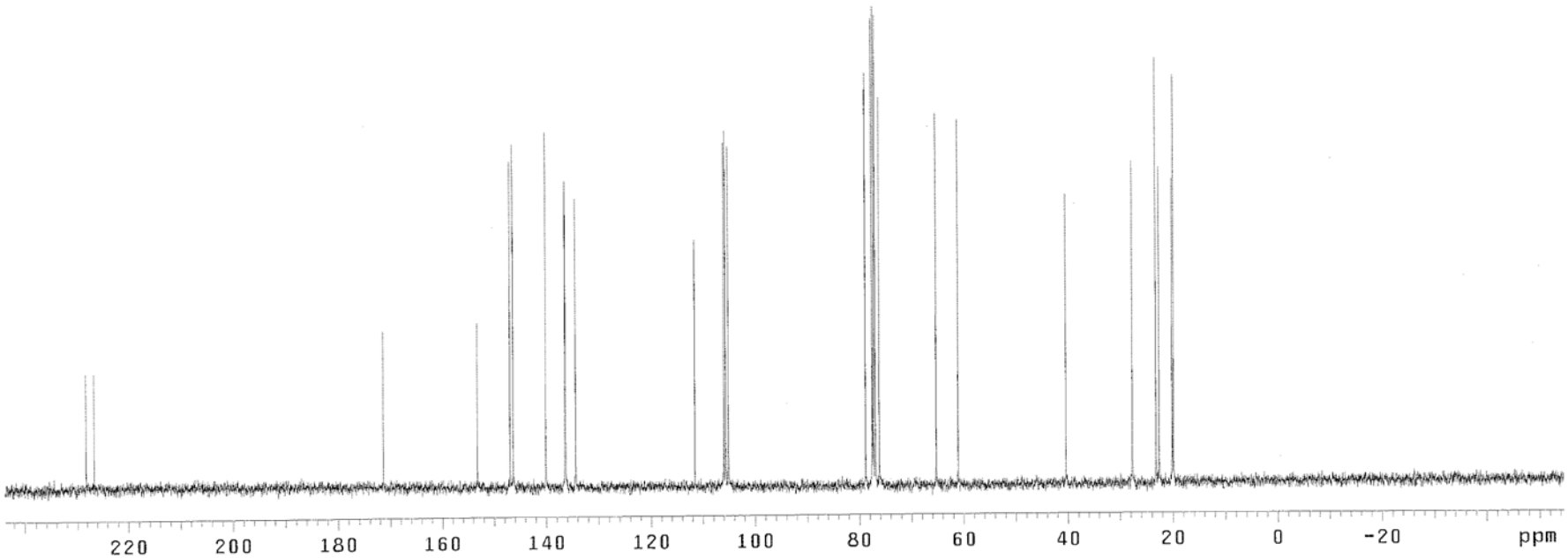
(1*R*, *R*)-**11**

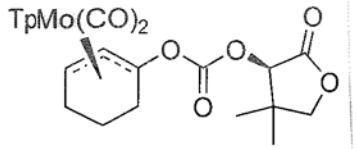




100 MHz
$CDCl_3$

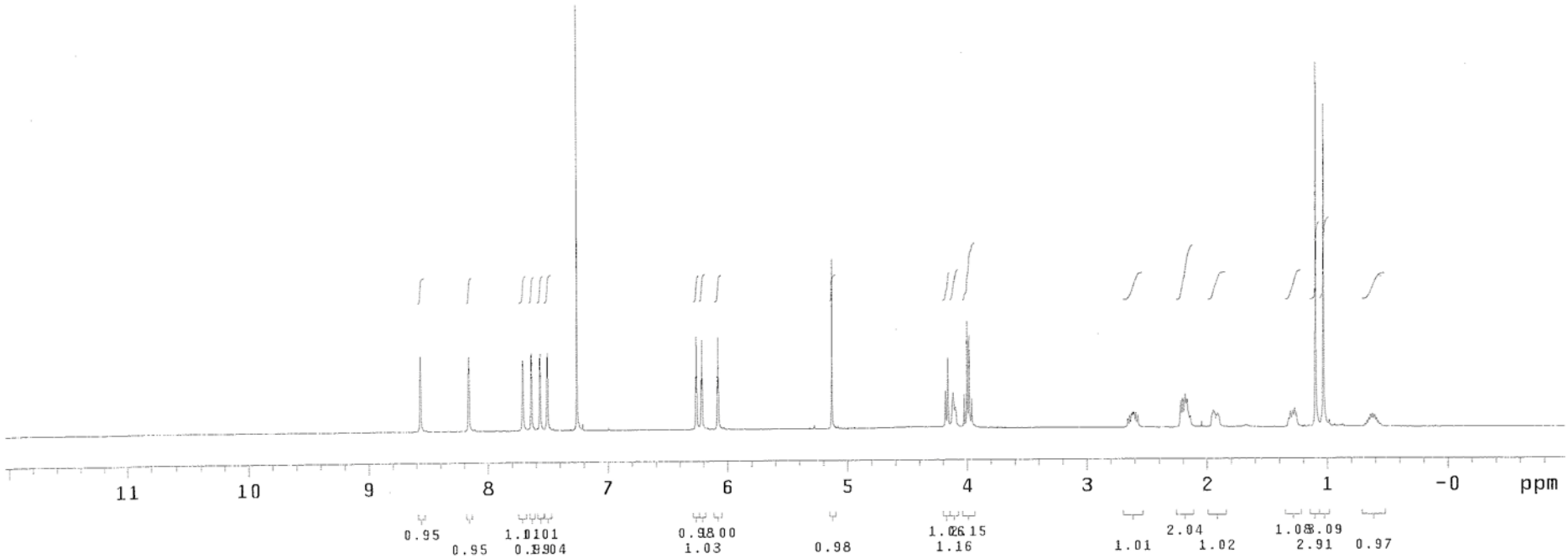
(1*R*, *R*)-**11**

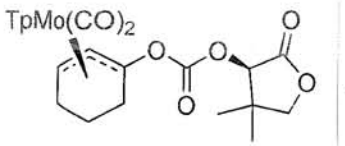




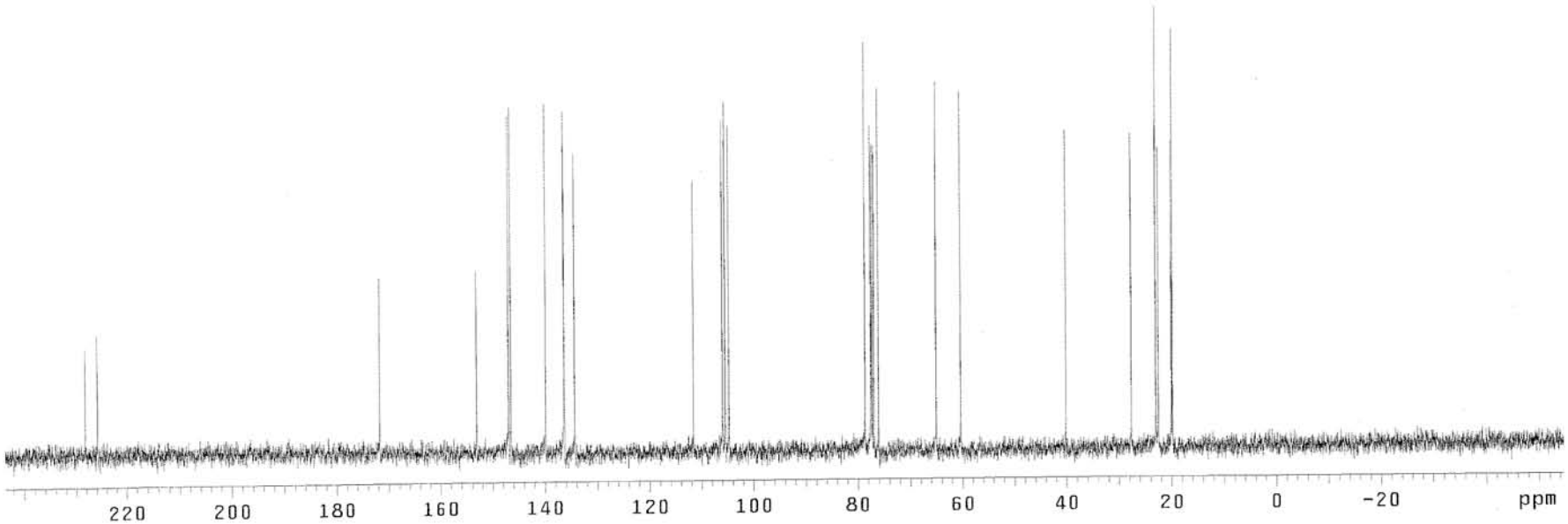
400 MHz
$CDCl_3$

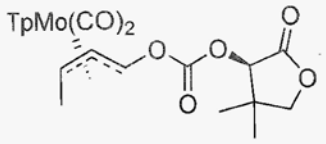
(1*S*, *R*)-**11**





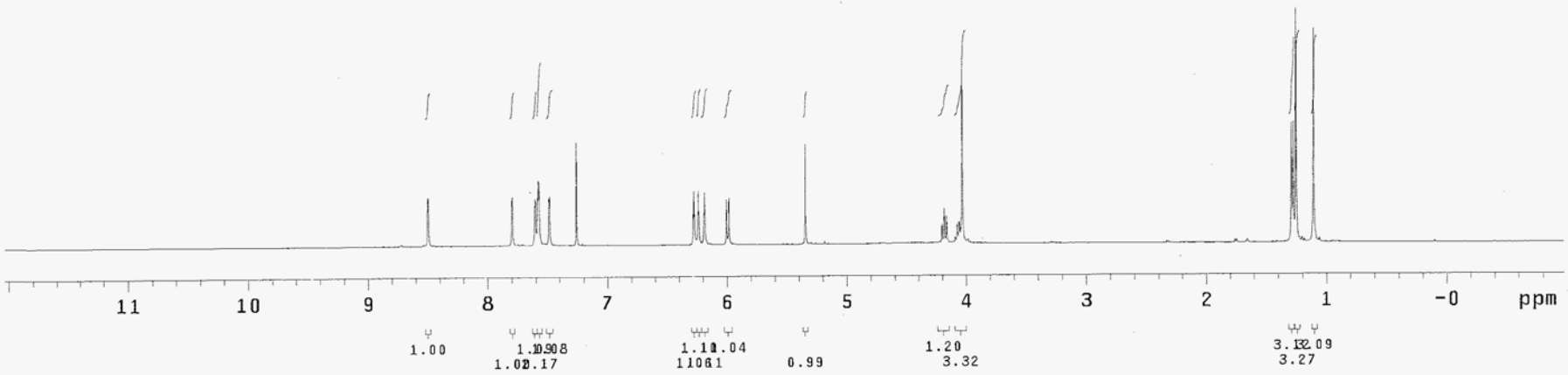
100 MHz
$CDCl_3$ (1*S*, *R*)-**11**

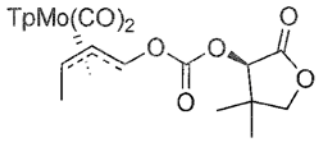




400 MHz
$CDCl_3$

(1*R*, *R*)-**12**





100 MHz
$CDCl_3$ (1*R*, *R*)-**12**