Supplementary Material

Steric Control of Coordination Number: Structure and Reactivity of a Series of Mo(VI) Dioxo Diaryloxide Complexes Bearing 4, 5 and 6-Coordinate Environments

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Table S1: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mo(1)	0	5611(1)	2500	32(1)
O(1)	106(1)	6492(1)	1711(1)	33(1)
O(2)	-815(1)	4745(2)	2185(1)	55(1)
C(1)	245(1)	7022(2)	1099(1)	30(1)
C(2)	-340(2)	6912(2)	372(1)	34(1)
C(3)	-172(2)	7485(2)	-220(2)	44(1)
C(4)	528(2)	8118(2)	-126(2)	43(1)
C(5)	1083(2)	8185(2)	598(2)	40(1)
C(6)	968(2)	7671(2)	1233(1)	33(1)
C(7)	-1123(2)	6197(2)	212(2)	39(1)
C(8)	-912(2)	4927(2)	382(2)	46(1)
C(9)	-1651(2)	6634(3)	668(2)	47(1)
C(10)	-1655(2)	6247(3)	-634(2)	59(1)
C(11)	692(2)	8721(3)	-794(2)	58(1)
C(12)	-77(5)	8768(9)	-1482(4)	223(5)
C(13)	1317(6)	8134(5)	-995(5)	228(5)
C(14)	853(4)	9951(4)	-614(3)	137(3)
C(15)	1610(2)	7829(2)	2019(2)	38(1)
C(17)	1228(2)	8367(2)	2574(2)	44(1)
C(16)	2022(2)	6682(3)	2315(2)	48(1)
C(18)	2302(2)	8641(3)	1998(2)	57(1)

Table S2: Bond lengths [Å] for compound **2**.

Mo(1)-O(2)	1.6820(19)
Mo(1)-O(2)#1	1.6820(19)
Mo(1)-O(1)#1	1.8502(16)
Mo(1)-O(1)	1.8502(16)
O(1)-C(1)	1.384(3)
C(1)-C(2)	1.407(3)
C(1)-C(6)	1.415(3)
C(2)-C(3)	1.397(4)
C(2)-C(7)	1.538(4)
C(3)-C(4)	1.382(4)
C(4)-C(5)	1.378(4)
C(4)-C(11)	1.532(4)
C(5)-C(6)	1.394(4)
C(6)-C(15)	1.533(4)
C(7)-C(9)	1.520(4)
C(7)-C(10)	1.541(4)
C(7)-C(8)	1.547(4)
C(11)-C(13)	1.429(6)
C(11)-C(14)	1.491(6)
C(11)-C(12)	1.515(8)
C(15)-C(17)	1.529(4)
C(15)-C(16)	1.541(4)
C(15)-C(18)	1.539(4)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Table S3: Bond angles [°] for compound **2**.

O(2)-Mo(1)-O(2)#1	105.42(17)	C(1)-C(6)-C(15)	123.9(2)
O(2)-Mo(1)-O(1)#1	109.18(8)	C(9)-C(7)-C(2)	110.8(2)
O(2)#1-Mo(1)-O(1)#1	110.47(9)	C(9)-C(7)-C(10)	106.7(2)
O(2)-Mo(1)-O(1)	110.47(9)	C(2)-C(7)-C(10)	111.9(2)
O(2)#1-Mo(1)-O(1)	109.18(8)	C(9)-C(7)-C(8)	110.9(2)
O(1)#1-Mo(1)-O(1)	111.92(10)	C(2)-C(7)-C(8)	110.76(19)
C(1)-O(1)-Mo(1)	171.89(15)	C(10)-C(7)-C(8)	105.6(2)
O(1)-C(1)-C(2)	119.0(2)	C(13)-C(11)-C(14)	115.1(5)
O(1)-C(1)-C(6)	118.5(2)	C(13)-C(11)-C(4)	110.0(3)
C(2)-C(1)-C(6)	122.4(2)	C(14)-C(11)-C(4)	109.7(3)
C(3)-C(2)-C(1)	116.3(2)	C(13)-C(11)-C(12)	109.1(6)
C(3)-C(2)-C(7)	120.3(2)	C(14)-C(11)-C(12)	101.7(5)
C(1)-C(2)-C(7)	123.3(2)	C(4)-C(11)-C(12)	111.0(4)
C(4)-C(3)-C(2)	123.8(2)	C(6)-C(15)-C(17)	110.8(2)
C(3)-C(4)-C(5)	117.2(2)	C(6)-C(15)-C(16)	110.0(2)
C(3)-C(4)-C(11)	122.0(3)	C(17)-C(15)-C(16)	111.8(2)
C(5)-C(4)-C(11)	120.8(3)	C(6)-C(15)-C(18)	112.3(2)
C(4)-C(5)-C(6)	123.8(3)	C(17)-C(15)-C(18)	105.5(2)
C(5)-C(6)-C(1)	116.4(2)	C(16)-C(15)-C(18)	106.3(2)
C(5)-C(6)-C(15)	119.7(2)		

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Table S4: Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **2**. The anisotropic displacement factor exponent takes the form: $-2\pi[h^2a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo(1)	35(1)	32(1)	34(1)	0	16(1)	0
O(1)	33(1)	38(1)	28(1)	0(1)	11(1)	-1(1)
O(2)	64(1)	51(1)	59(1)	-18(1)	34(1)	-25(1)
C(1)	34(1)	32(1)	27(1)	1(1)	13(1)	8(1)
C(2)	38(1)	32(1)	31(1)	-2(1)	11(1)	10(1)
C(3)	57(2)	42(2)	30(1)	2(1)	11(1)	19(1)
C(4)	63(2)	34(1)	39(2)	5(1)	26(1)	13(1)
C(5)	52(2)	34(1)	42(2)	3(1)	25(1)	3(1)
C(6)	39(1)	31(1)	34(1)	1(1)	17(1)	4(1)
C(7)	34(1)	46(2)	34(1)	-7(1)	6(1)	9(1)
C(8)	43(1)	44(2)	50(2)	-11(1)	14(1)	0(1)
C(9)	32(1)	60(2)	45(2)	-10(1)	7(1)	8(1)
C(10)	47(2)	80(2)	38(2)	-11(2)	-1(1)	11(2)
C(11)	92(2)	47(2)	44(2)	13(1)	37(2)	14(2)
C(12)	205(8)	353(12)	95(5)	136(7)	27(5)	-50(9)
C(13)	418(13)	150(5)	263(9)	138(6)	314(10)	174(7)
C(14)	267(8)	70(3)	121(5)	28(3)	130(5)	-4(4)
C(15)	35(1)	41(1)	39(1)	3(1)	12(1)	-5(1)
C(17)	50(2)	45(2)	36(1)	-5(1)	11(1)	-6(1)
C(16)	34(1)	55(2)	52(2)	8(1)	11(1)	5(1)
C(18)	51(2)	66(2)	57(2)	1(2)	19(1)	-20(2)

Table S5: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for compound **3**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	5905(1)	8296(1)	3033(1)	19(1)
O(1)	5915(4)	6920(4)	2704(2)	32(1)
O(2)	5990(4)	9421(4)	2542(2)	30(1)
O(3)	7336(3)	8248(4)	3546(2)	30(1)
O(4)	5288(3)	8572(4)	3688(2)	23(1)
N(1)	4112(4)	8252(5)	2536(2)	23(1)
C(1)	3601(6)	7210(6)	2321(3)	30(2)
C(2)	2519(6)	7202(7)	2043(3)	38(2)
C(3)	1929(6)	8262(7)	1971(3)	45(2)
C(4)	2442(6)	9325(7)	2179(3)	35(2)
C(5)	3542(5)	9290(6)	2459(3)	24(1)
C(6)	8175(5)	7465(6)	3621(3)	24(1)
C(7)	8307(5)	6531(6)	4058(3)	26(1)
C(8)	9186(5)	5777(6)	4139(3)	29(2)
C(9)	9931(5)	5907(6)	3803(3)	31(2)
C(10)	9781(5)	6811(6)	3375(3)	32(2)
C(11)	8913(5)	7588(6)	3268(3)	23(1)
C(12)	7477(6)	6398(7)	4420(3)	37(2)
C(13)	7772(11)	7166(17)	4969(6)	152(8)
C(14)	7365(12)	5120(11)	4595(8)	137(7)
C(15)	8760(5)	8550(6)	2783(3)	33(2)
C(16)	9665(7)	9468(8)	2907(4)	56(2)
C(17)	8644(8)	7972(8)	2166(4)	57(2)
C(18)	4352(5)	8939(6)	3812(3)	21(1)
C(19)	3594(5)	8055(6)	3858(3)	28(2)
C(20)	2620(5)	8472(7)	3951(3)	39(2)
C(21)	2438(6)	9688(8)	4009(3)	42(2)
C(22)	3217(5)	10533(7)	3984(3)	36(2)
C(23)	4194(5)	10187(6)	3886(3)	26(1)
C(24)	3855(6)	6726(7)	3834(3)	36(2)
C(25)	2872(6)	5904(7)	3611(4)	49(2)
C(26)	4513(7)	6322(7)	4455(4)	51(2)
C(27)	5090(5)	11069(6)	3879(3)	31(2)
C(28)	4710(7)	12388(7)	3805(3)	45(2)
C(29)	6034(6)	10935(8)	4438(3)	47(2)

Table S6: Bond lengths [Å] for compound **3**.

Mo(1)-O(1)	1.701(4)	C(10)-C(11)	1.380(9)
Mo(1)-O(2)	1.705(4)	C(11)-C(15)	1.519(9)
Mo(1)-O(4)	1.909(4)	C(12)-C(13)	1.490(13)
Mo(1)-O(3)	1.912(4)	C(12)-C(14)	1.486(13)
Mo(1)-N(1)	2.292(5)	C(15)-C(16)	1.514(10)
O(3)-C(6)	1.358(7)	C(15)-C(17)	1.531(11)
O(4)-C(18)	1.369(7)	C(18)-C(23)	1.411(9)
N(1)-C(5)	1.348(8)	C(18)-C(19)	1.405(9)
N(1)-C(1)	1.354(8)	C(19)-C(20)	1.403(9)
C(1)-C(2)	1.372(10)	C(19)-C(24)	1.512(10)
C(2)-C(3)	1.381(11)	C(20)-C(21)	1.376(11)
C(3)-C(4)	1.372(10)	C(21)-C(22)	1.383(11)
C(4)-C(5)	1.394(9)	C(22)-C(23)	1.387(9)
C(6)-C(11)	1.410(8)	C(23)-C(27)	1.514(9)
C(6)-C(7)	1.422(9)	C(24)-C(26)	1.527(10)
C(7)-C(8)	1.376(9)	C(24)-C(25)	1.533(10)
C(7)-C(12)	1.525(9)	C(27)-C(28)	1.533(10)
C(8)-C(9)	1.390(9)	C(27)-C(29)	1.530(10)
C(9)-C(10)	1.382(10)		

Table S7: Bond angles [°] for compound **3**.

O(1)-Mo(1)-O(2)	110.3(2)	C(9)-C(10)-C(11)	122.2(6)
O(1)-Mo(1)-O(4)	123.3(2)	C(10)-C(11)-C(6)	118.2(6)
O(2)-Mo(1)-O(4)	121.46(19)	C(10)-C(11)-C(15)	120.8(6)
O(1)-Mo(1)-O(3)	97.7(2)	C(6)-C(11)-C(15)	121.1(6)
O(2)-Mo(1)-O(3)	102.3(2)	C(13)-C(12)-C(14)	109.4(11)
O(4)-Mo(1)-O(3)	92.60(18)	C(13)-C(12)-C(7)	110.7(7)
O(1)-Mo(1)-N(1)	83.2(2)	C(14)-C(12)-C(7)	111.8(7)
O(2)-Mo(1)-N(1)	85.1(2)	C(16)-C(15)-C(11)	112.6(6)
O(4)-Mo(1)-N(1)	79.98(17)	C(16)-C(15)-C(17)	109.8(7)
O(3)-Mo(1)-N(1)	171.56(18)	C(11)-C(15)-C(17)	110.8(6)
C(6)-O(3)-Mo(1)	134.4(4)	O(4)-C(18)-C(23)	118.6(5)
C(18)-O(4)-Mo(1)	141.6(4)	O(4)-C(18)-C(19)	118.4(5)
C(5)-N(1)-C(1)	118.7(6)	C(23)-C(18)-C(19)	123.1(6)
C(5)-N(1)-Mo(1)	119.3(4)	C(20)-C(19)-C(18)	116.6(6)
C(1)-N(1)-Mo(1)	122.0(4)	C(20)-C(19)-C(24)	122.8(6)
N(1)-C(1)-C(2)	120.8(6)	C(18)-C(19)-C(24)	120.5(6)
C(1)-C(2)-C(3)	120.6(7)	C(21)-C(20)-C(19)	121.2(7)
C(4)-C(3)-C(2)	119.0(7)	C(20)-C(21)-C(22)	120.8(7)
C(3)-C(4)-C(5)	118.4(7)	C(23)-C(22)-C(21)	121.2(7)
N(1)-C(5)-C(4)	122.4(6)	C(22)-C(23)-C(18)	117.1(6)
O(3)-C(6)-C(11)	119.8(6)	C(22)-C(23)-C(27)	123.3(6)
O(3)-C(6)-C(7)	119.8(5)	C(18)-C(23)-C(27)	119.6(6)
C(11)-C(6)-C(7)	120.4(6)	C(19)-C(24)-C(26)	108.9(6)
C(8)-C(7)-C(6)	118.6(6)	C(19)-C(24)-C(25)	114.6(6)
C(8)-C(7)-C(12)	122.3(6)	C(26)-C(24)-C(25)	110.3(6)
C(6)-C(7)-C(12)	119.1(6)	C(23)-C(27)-C(28)	113.1(6)
C(7)-C(8)-C(9)	121.5(6)	C(23)-C(27)-C(29)	111.5(6)
C(10)-C(9)-C(8)	119.1(6)	C(28)-C(27)-C(29)	110.2(6)

Table S8: Anisotropic displacement parameters ($Å^2$x 10^3) for compound **3**. The anisotropic displacement factor exponent takes the form: $-2\pi[h^2a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo(1)	22(1)	14(1)	24(1)	1(1)	12(1)	1(1)
O(1)	43(3)	20(2)	36(3)	2(2)	15(2)	3(2)
O(2)	30(3)	28(3)	39(3)	5(2)	21(2)	-1(2)
O(3)	23(2)	32(2)	38(3)	-2(2)	15(2)	3(2)
O(4)	21(2)	28(2)	24(2)	-2(2)	12(2)	-1(2)
N(1)	26(3)	21(3)	24(3)	2(2)	11(2)	1(2)
C(1)	43(4)	24(3)	25(4)	-5(3)	13(3)	-3(3)
C(2)	38(4)	32(4)	43(5)	-6(3)	8(4)	-13(3)
C(3)	35(4)	47(5)	48(5)	8(4)	3(3)	-4(4)
C(4)	34(4)	34(4)	34(4)	8(3)	5(3)	6(3)
C(5)	35(4)	19(3)	21(3)	11(3)	12(3)	0(3)
C(6)	24(3)	24(3)	24(3)	-3(3)	5(3)	-4(3)
C(7)	24(3)	27(4)	28(3)	-3(3)	7(3)	-6(3)
C(8)	28(4)	28(4)	29(4)	3(3)	3(3)	-1(3)
C(9)	15(3)	34(4)	39(4)	-1(3)	-2(3)	3(3)
C(10)	23(3)	36(4)	38(4)	-4(3)	10(3)	2(3)
C(11)	16(3)	28(3)	24(3)	1(3)	4(3)	-2(3)
C(12)	31(4)	42(4)	39(4)	7(3)	13(3)	3(3)
C(13)	97(10)	290(20)	94(10)	-105(12)	72(8)	-66(12)
C(14)	153(13)	89(9)	232(18)	58(11)	160(14)	12(9)
C(15)	24(3)	32(4)	45(4)	12(3)	12(3)	3(3)
C(16)	56(5)	45(5)	64(6)	20(4)	12(5)	-8(4)
C(17)	64(6)	62(6)	43(5)	7(4)	13(4)	7(5)
C(18)	18(3)	25(3)	18(3)	1(3)	4(2)	5(3)
C(19)	23(3)	40(4)	19(3)	-1(3)	5(3)	-1(3)
C(20)	25(4)	61(5)	32(4)	1(4)	10(3)	-7(4)
C(21)	23(4)	68(6)	37(4)	-5(4)	11(3)	10(4)
C(22)	31(4)	48(5)	29(4)	-5(3)	6(3)	14(3)
C(23)	31(4)	33(4)	11(3)	-2(3)	3(3)	2(3)
C(24)	35(4)	39(4)	35(4)	11(4)	11(3)	5(4)
C(25)	45(5)	47(5)	58(5)	-1(4)	15(4)	-18(4)
C(26)	58(5)	42(5)	51(5)	14(4)	10(4)	-2(4)
C(27)	37(4)	35(4)	21(3)	-4(3)	10(3)	-3(3)
C(28)	62(5)	40(4)	29(4)	-4(3)	6(4)	7(4)
C(29)	44(5)	53(5)	37(4)	-3(4)	0(4)	-13(4)

Table S9: Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for compound **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Mo(1)	5000	7796(1)	2500	31(1)
O(1)	3500(6)	8426(3)	2702(2)	42(2)
O(2)	4051(5)	7531(2)	1460(2)	26(1)
N(1)	3438(6)	6615(3)	2749(3)	28(2)
C(1)	2976(8)	6078(4)	2206(4)	32(2)
C(2)	2322(9)	5346(5)	2344(4)	39(2)
C(3)	2092(9)	5155(5)	3069(4)	45(2)
C(4)	2501(8)	5692(5)	3630(4)	41(2)
C(5)	3181(8)	6413(4)	3456(4)	34(2)
C(6)	3242(8)	8077(4)	954(4)	29(2)
C(7)	1551(9)	8181(4)	925(4)	32(2)
C(8)	777(9)	8719(4)	409(4)	36(2)
C(9)	1614(9)	9144(4)	-70(4)	38(2)
C(10)	3276(8)	9039(4)	-43(4)	30(2)
C(11)	4129(8)	8504(4)	463(3)	24(2)
C(12)	602(8)	7697(5)	1440(3)	45(2)
C(13)	5914(8)	8380(4)	468(4)	37(2)

Table S10: Bond lengths [Å] for compound **4**.

Mo(1)-O(1)#1	1.697(5)
Mo(1)-O(1)	1.697(5)
Mo(1)-O(2)#1	1.964(4)
Mo(1)-O(2)	1.964(4)
Mo(1)-N(1)	2.421(5)
Mo(1)-N(1)#1	2.421(5)
O(2)-C(6)	1.387(7)
N(1)-C(1)	1.333(7)
N(1)-C(5)	1.345(7)
C(1)-C(2)	1.365(9)
C(2)-C(3)	1.364(9)
C(3)-C(4)	1.348(9)
C(4)-C(5)	1.374(9)
C(6)-C(11)	1.403(8)
C(6)-C(7)	1.406(8)
C(7)-C(8)	1.378(8)
C(7)-C(12)	1.512(8)
C(8)-C(9)	1.362(8)
C(9)-C(10)	1.383(8)
C(10)-C(11)	1.390(8)
C(11)-C(13)	1.492(8)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Table S11: Bond angles [°] for compound **4**.

O(1)#1-Mo(1)-O(1)	103.9(3)	C(5)-N(1)-Mo(1)	121.7(5)
O(1)#1-Mo(1)-O(2)#1	96.98(19)	N(1)-C(1)-C(2)	123.2(7)
O(1)-Mo(1)-O(2)#1	98.87(18)	C(3)-C(2)-C(1)	119.0(7)
O(1)#1-Mo(1)-O(2)	98.87(18)	C(4)-C(3)-C(2)	119.5(8)
O(1)-Mo(1)-O(2)	96.97(19)	C(3)-C(4)-C(5)	118.8(8)
O(2)#1-Mo(1)-O(2)	154.2(2)	N(1)-C(5)-C(4)	123.1(7)
O(1)#1-Mo(1)-N(1)	163.9(2)	O(2)-C(6)-C(11)	119.0(6)
O(1)-Mo(1)-N(1)	92.1(2)	O(2)-C(6)-C(7)	120.0(6)
O(2)#1-Mo(1)-N(1)	78.82(17)	C(11)-C(6)-C(7)	120.9(7)
O(2)-Mo(1)-N(1)	80.31(17)	C(8)-C(7)-C(6)	118.7(7)
O(1)#1-Mo(1)-N(1)#1	92.1(2)	C(8)-C(7)-C(12)	120.9(7)
O(1)-Mo(1)-N(1)#1	163.9(2)	C(6)-C(7)-C(12)	120.4(6)
O(2)#1-Mo(1)-N(1)#1	80.31(17)	C(9)-C(8)-C(7)	121.4(7)
O(2)-Mo(1)-N(1)#1	78.82(17)	C(8)-C(9)-C(10)	119.8(7)
N(1)-Mo(1)-N(1)#1	71.8(3)	C(9)-C(10)-C(11)	121.7(7)
C(6)-O(2)-Mo(1)	124.5(4)	C(10)-C(11)-C(6)	117.5(7)
C(1)-N(1)-C(5)	116.5(6)	C(10)-C(11)-C(13)	120.9(6)
C(1)-N(1)-Mo(1)	121.3(5)	C(6)-C(11)-C(13)	121.6(6)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Table S12: Anisotropic displacement parameters ($Å^2$ x 10^3) for compound **4**. The anisotropic displacement factor exponent takes the form: $-2\pi[h^2a^{*2}U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mo(1)	42(1)	26(1)	24(1)	0	0(1)	0

Pulse Sequence: s2pul

INDEX	FREQUENCY	PPM	HEIGHT
1	3361.118	8.403	50.1
2	2861.091	7.153	116.3
3	2859.901	7.150	118.7
4	2858.710	7.147	110.9
5	2735.466	6.839	40.8
6	2728.233	6.821	47.3
7	2679.155	6.698	36.3
8	2671.463	6.679	30.5
9	2553.347	6.384	42.3
10	2547.395	6.369	58.1
11	2541.535	6.354	36.0
12	965.456	2.414	202.5

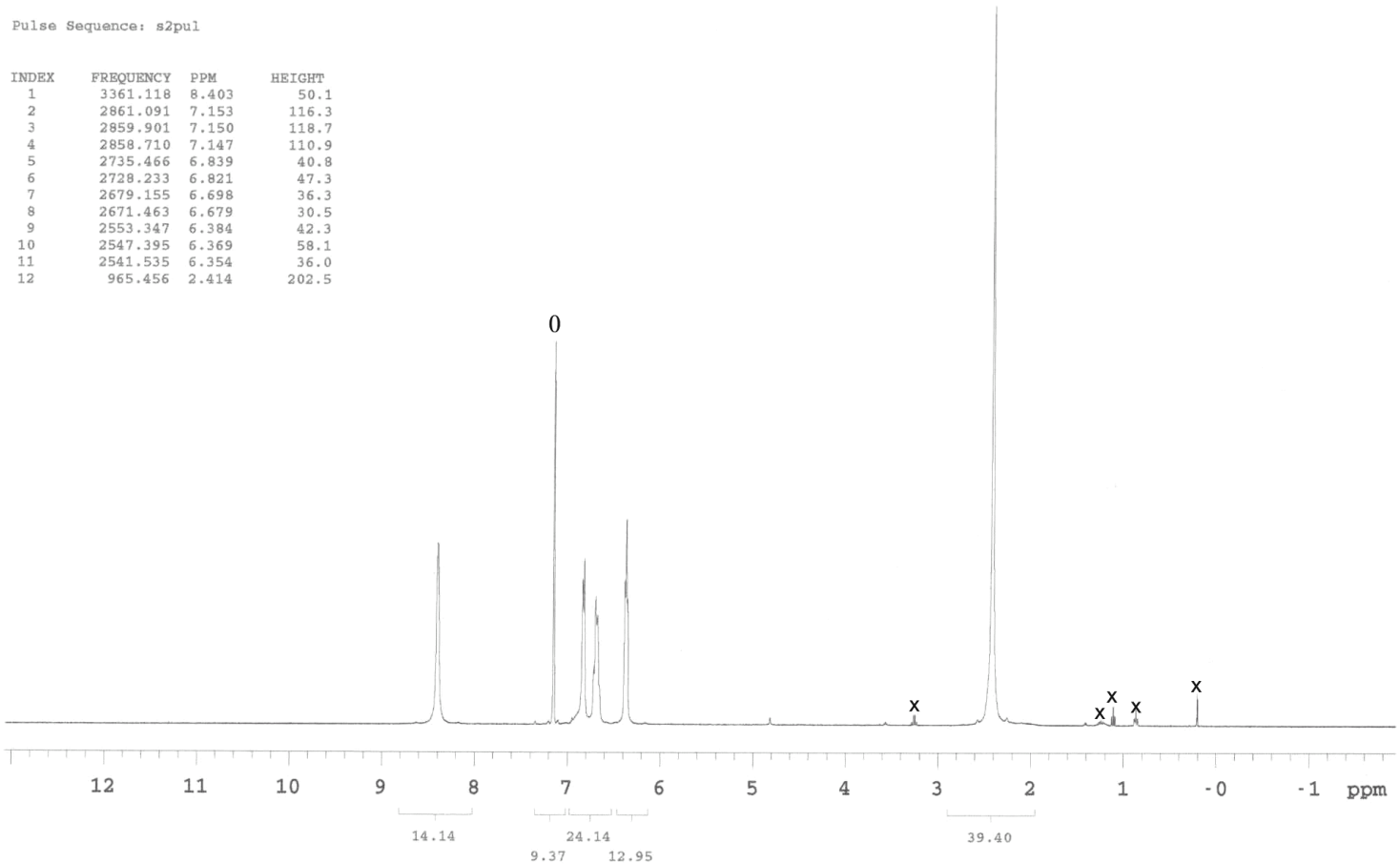

Figure S1: ^{1}H NMR spectrum of compound **4**. The small peaks marked with (x) are due to presence of grease and crystallizing solvents, ether and pentane. The peak marked with (o) is due to C_6H_6 in the NMR solvent.