

Supplementary Materials (SM)

Efficient Molybdenum Hydrazonato Epoxidation Catalysts Operating under Green Chemistry Conditions: Water vs. Decane Competition

Silvija Mrkonja, Edi Topić, Mirna Mandarić, Dominique Agustin and Jana Pisk

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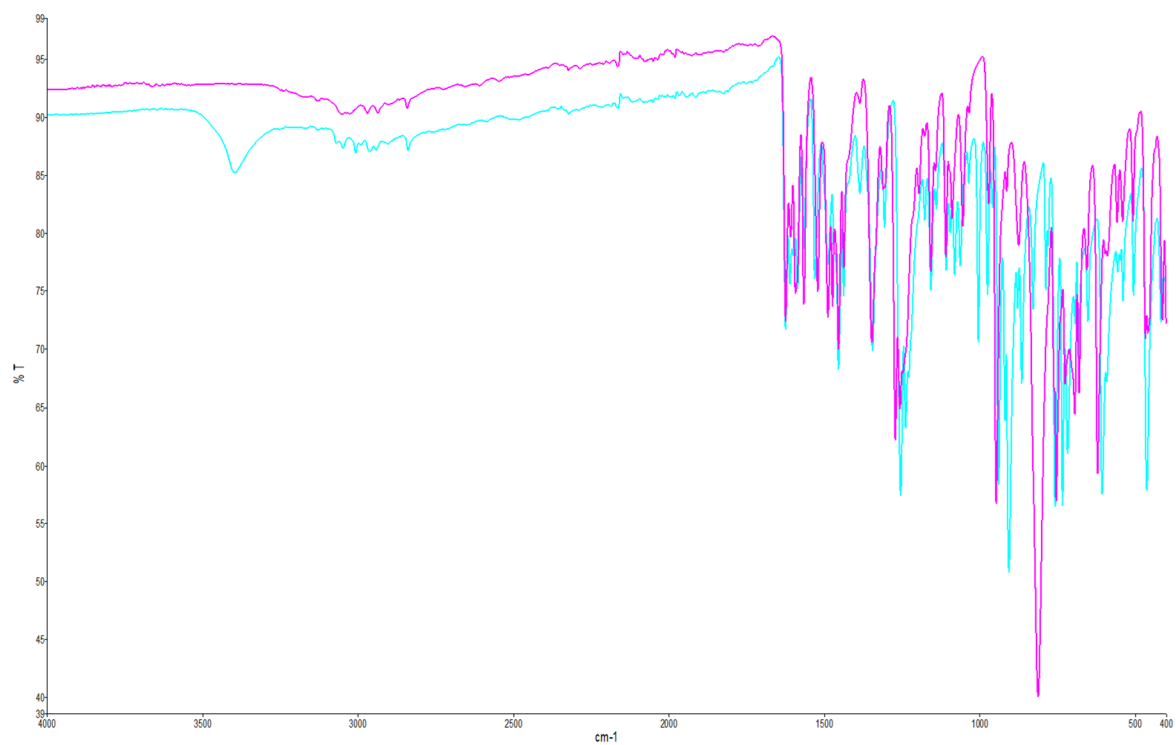


Figure S1. Comparison of IR-ATR spectra of the complex [MoO₂(L^{3OMe})(MeOH)] (pink) and [MoO₂(L^{3OMe})]_n (blue).

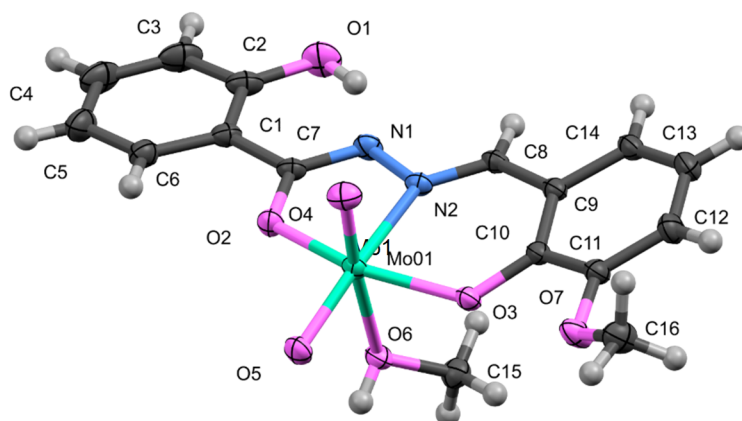


Figure S2. Enumeration of atoms in the crystal structure of $[\text{MoO}_2(\text{L}^{3\text{OMe}})(\text{MeOH})]$.

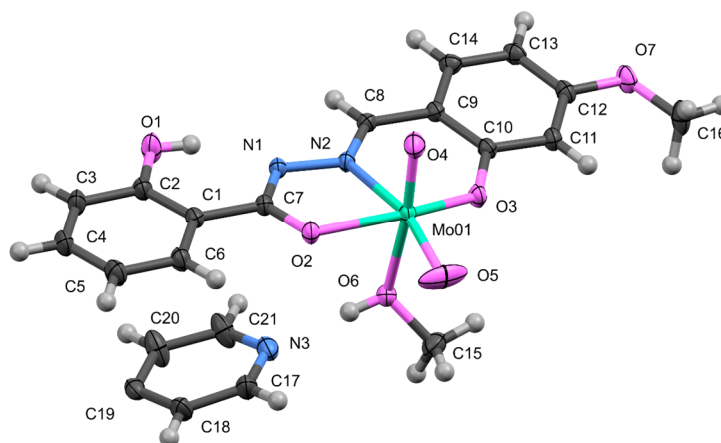


Figure S3. Enumeration of atoms in the crystal structure of $[\text{MoO}_2(\text{L}^{4\text{OMe}})(\text{MeOH})] \cdot 4,4\text{-bpy}$.

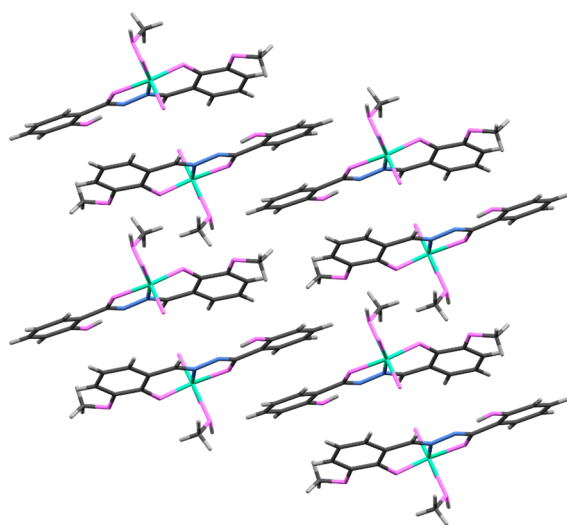


Figure S4. Crystal packing in the crystal structure of $[\text{MoO}_2(\text{L}^{3\text{OMe}})(\text{MeOH})]$ shown parallel to crystal a -axis.

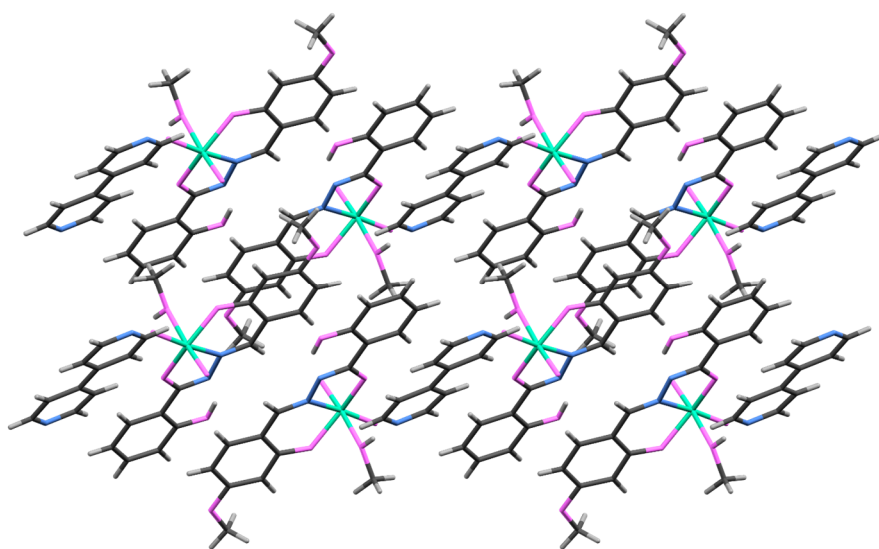


Figure S5. Crystal packing in the crystal structure of $[\text{MoO}_2(\text{L}^{4\text{OMe}})(\text{MeOH})] \cdot 4,4\text{-bpy}$ shown parallel to crystal b -axis.

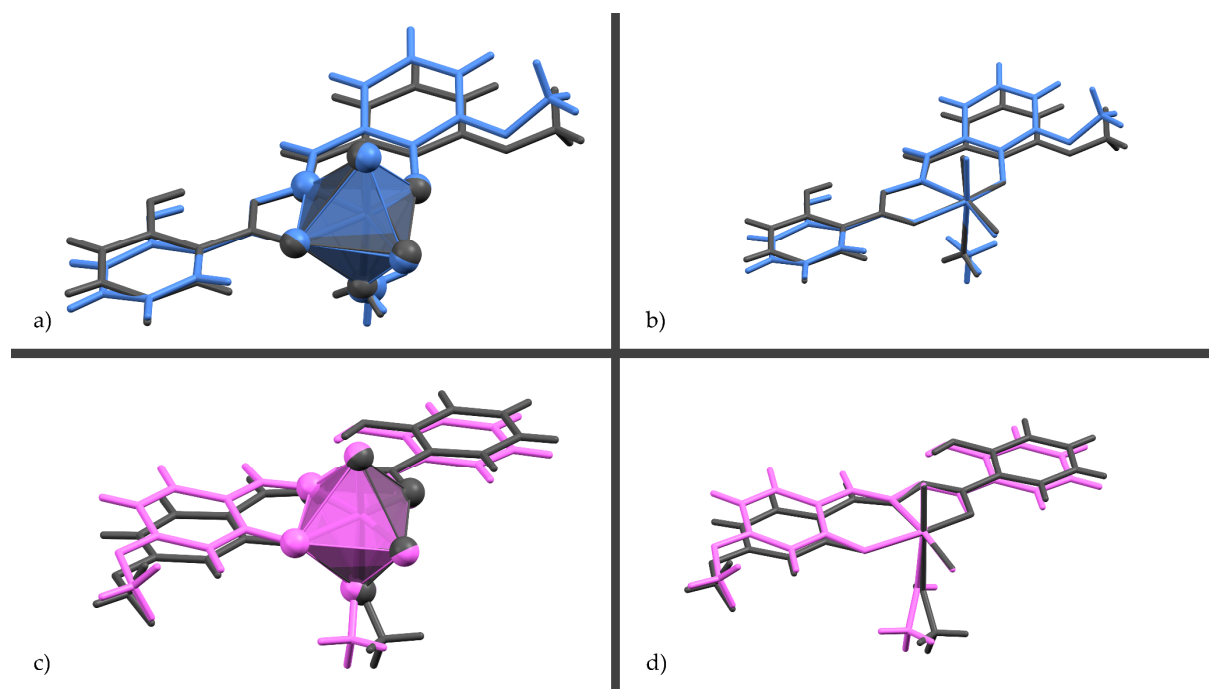


Figure S6. Comparison of molecular structures of: a) and b) $[\text{MoO}_2(\text{L}^{3\text{OMe}})(\text{MeOH})]$ (blue) and $[\text{MoO}_2(\text{L}^{3\text{OMe}})(\text{H}_2\text{O})]$ (gray); c) $[\text{MoO}_2(\text{L}^{4\text{OMe}})(\text{MeOH})]\cdot 4,4\text{-byp}$ (pink) and d) $[\text{MoO}_2(\text{L}^{4\text{OMe}})(\text{MeOH})]\cdot \text{MeOH}$ (gray). 4,4-bipyridine and methanol molecules are omitted for clarity. It can be seen that small variations in crystal composition have a significant effect on complex geometry.

Table S1. Geometrical parameters of the octahedral environment of molybdenum atom in the title complexes.

Bond length/Å	$[\text{MoO}_2(\text{L}^{\text{H}})(\text{MeOH})]$	$[\text{MoO}_2(\text{L}^{3\text{OMe}})(\text{H}_2\text{O})]$	$[\text{MoO}_2(\text{L}^{4\text{OMe}})(\text{MeOH})]\cdot \text{MeOH}$
Mo-hydrazone O	2.016	2.017	1.921
Mo-imine N	2.233	2.247	2.211
Mo-aryl O	1.927	1.920	2.000
Mo=O axial	1.705	1.683	1.692
Mo=O equatorial	1.692	1.688	1.713
Mo-solvent O	2.349	2.292	2.352
	$[\text{MoO}_2(\text{L}^{3\text{OMe}})(\text{MeOH})]$	$[\text{MoO}_2(\text{L}^{4\text{OMe}})(\text{MeOH})]\cdot 4,4\text{-byp}$	
Mo-hydrazone O	1.998	2.018	
Mo-imine N	2.238	2.216	
Mo-aryl O	1.939	1.949	
Mo=O axial	1.685	1.695	
Mo=O equatorial	1.701	1.732	
Mo-solvent O	2.368	2.293	

Table S2. Bond lengths (in Å) and angles (in °) for the prepared complexes. Atom enumeration is shown in Figures S1 and S2.

Bond	[MoO ₂ (L ^{3OMe})(MeOH)]	[MoO ₂ (L ^{4OMe})(MeOH)] ·4,4-byp	Angle	[MoO ₂ (L ^{3OMe})(MeOH)]	[MoO ₂ (L ^{4OMe})(MeOH)] ·4,4-byp
C1–C2	1.415(3)	1.405(5)	C2–C1–C7	121.4(2)	121.3(3)
C1–C6	1.394(3)	1.401(5)	C6–C1–C7	119.90(19)	119.6(3)
C2–C3	1.386(4)	1.399(5)	C6–C1–C2	118.7(2)	119.1(3)
C3–C4	1.371(5)	1.378(6)	O1–C2–C1	123.4(2)	123.1(3)
C5–C4	1.379(4)	1.389(6)	O1–C2–C3	118.0(2)	117.7(3)
C6–C5	1.369(3)	1.385(5)	C3–C2–C1	118.6(3)	119.3(3)
C7–C1	1.464(3)	1.468(4)	C4–C3–C2	121.1(3)	120.5(3)
C8–C9	1.439(3)	1.432(4)	C3–C4–C5	120.8(3)	120.8(3)
C9–C14	1.405(3)	1.409(4)	C6–C5–C4	119.2(3)	119.2(4)
C10–C9	1.403(3)	1.409(4)	C5–C6–C1	121.6(2)	121.1(3)
C10–C11	1.394(3)	1.399(4)	O2–C7–C1	118.20(19)	117.5(3)
C11–C12	1.389(3)	1.390(5)	N1–C7–O2	122.14(19)	122.6(3)
C12–C13	1.387(3)	1.400(5)	N1–C7–C1	119.66(18)	119.9(3)
C13–C14	1.364(3)	1.369(5)	N2–C8–C9	123.31(18)	124.4(3)
C18–C17		1.386(6)	C10–C9–C8	122.70(18)	122.9(3)
C19–C19'		1.489(7)	C10–C9–C14	119.8(2)	118.7(3)
C19–C18		1.389(6)	C14–C9–C8	117.48(18)	118.3(3)
C19–C20		1.387(6)	O3–C10–C9	122.82(19)	123.1(3)
C21–C20		1.385(6)	O3–C10–C11	118.12(18)	116.6(3)
Mo1–O2	1.9978(15)	2.019(2)	C11–C10–C9	119.05(18)	120.3(3)
Mo1–O3	1.9392(15)	1.949(2)	C12–C11–C10	120.0(2)	119.2(3)
Mo1–O6	2.3680(16)	2.293(2)	O7–C12–C11		124.1(3)
Mo1–O4	1.6855(16)	1.695(3)	O7–C12–C13		114.6(3)
Mo1–N2	2.2385(16)	2.216(2)	C11–C12–C13		121.3(3)
Mo1–O5	1.7012(14)	1.732(3)	C11–O7–C16	117.73(18)	
N1–C7	1.304(3)	1.298(4)	O7–C11–C10	116.03(18)	
N2–N1	1.384(2)	1.396(3)	O7–C11–C12	123.9(2)	
N2–C8	1.287(3)	1.293(4)	C14–C13–C12	120.1(2)	119.2(3)
N3–C21		1.323(6)	C13–C14–C9	120.4(2)	121.4(3)
N3–C17		1.328(6)	N3–C17–C18		123.5(4)
O1–C2	1.345(3)	1.346(4)	C17–C18–C19		119.3(4)
O2–C7	1.317(2)	1.325(4)	C18–C19–C19'		121.5(4)
O3–C10	1.349(2)	1.341(4)	C20–C19–C19'		121.4(5)
O6–C15	1.429(3)	1.423(4)	C20–C19–C18		117.1(3)
O7–C12		1.354(4)	C21–C20–C19		119.2(4)
O7–C11	1.371(3)		N3–C21–C20		123.8(4)
O7–C16	1.412(3)	1.428(5)	O2–Mo1–O6	80.68(6)	79.46(9)
			O2–Mo1–N2	71.52(6)	72.14(9)
			O3–Mo1–O2	149.56(6)	149.79(10)
			O3–Mo1–O6	80.57(6)	79.94(10)
			O3–Mo1–N2	81.14(6)	82.01(9)
			O4–Mo1–O2	98.39(7)	97.71(11)
			O4–Mo1–O3	97.62(7)	98.89(12)
			O4–Mo1–O6	173.66(7)	170.28(11)
			O4–Mo1–N2	96.26(7)	92.71(12)
			O4–Mo1–O5	105.53(8)	105.39(15)
			N2–Mo1–O6	77.48(6)	77.57(9)
			O5–Mo1–O2	96.20(7)	98.9(2)
			O5–Mo1–O3	104.20(7)	100.7(2)
			O5–Mo1–O6	80.80(7)	84.27(13)
			O5–Mo1–N2	156.46(7)	160.90(14)
			C7–N1–N2	109.87(16)	110.1(3)
			N1–N2–Mo1	115.51(12)	115.72(18)
			C8–N2–Mo1	128.16(14)	127.7(2)
			C8–N2–N1	116.08(16)	116.4(3)
			C21–N3–C17		117.1(3)
			C7–O2–Mo1	120.84(13)	119.40(19)
			C10–O3–Mo1	131.10(13)	133.9(2)
			C15–O6–Mo1	127.28(14)	122.7(2)
			C12–O7–C16		118.2(3)

Table S3. Summary of general and crystallographic data for the prepared complexes.

Identification code	[MoO ₂ (L ^{3OMe})(MeOH)]	[MoO ₂ (L ^{4OMe})(MeOH)]·4,4-byp
Empirical formula	C ₁₆ H ₁₆ MoN ₂ O ₇	C ₂₁ H ₂₀ MoN ₃ O ₇
Formula weight	444.25	522.34
Temperature/K	293(2)	170.15
Crystal system	triclinic	triclinic
Space group	<i>P</i> -1	<i>P</i> -1
<i>a</i> /Å	6.8456(3)	8.0480(3)
<i>b</i> /Å	10.7610(4)	9.8129(4)
<i>c</i> /Å	12.7677(6)	14.0421(5)
α /°	102.702(4)	90.980(3)
β /°	102.098(4)	94.142(3)
γ /°	107.076(4)	104.614(3)
Volume/Å ³	838.31(7)	1069.57(7)
<i>Z</i>	2	2
ρ_{calc} /cm ³	1.76	1.622
μ /mm ⁻¹	0.826	5.45
<i>F</i> (000)	448	530
Crystal size/mm ³	0.5 × 0.1 × 0.1	0.86 × 0.47 × 0.05
Radiation	MoK α (λ = 0.71073)	CuK α (λ = 1.54184)
2 θ range for data collection/°	8.542 to 65.674	6.316 to 160.6
Index ranges	-10 ≤ <i>h</i> ≤ 10, -15 ≤ <i>k</i> ≤ 16, -18 ≤ <i>l</i> ≤ 18	-10 ≤ <i>h</i> ≤ 9, -12 ≤ <i>k</i> ≤ 12, -17 ≤ <i>l</i> ≤ 17
Reflections collected	19202	14113
Independent reflections	5680 [<i>R</i> _{int} = 0.0373, <i>R</i> _{sigma} = 0.0411]	4543 [<i>R</i> _{int} = 0.0326, <i>R</i> _{sigma} = 0.0295]
Data/restraints/parameters	5680/2/245	4543/2/297
Goodness-of-fit on <i>F</i> ²	1.087	1.094
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0342, <i>wR</i> ₂ = 0.0691	<i>R</i> ₁ = 0.0399, <i>wR</i> ₂ = 0.1102
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0499, <i>wR</i> ₂ = 0.0769	<i>R</i> ₁ = 0.0407, <i>wR</i> ₂ = 0.1107
Largest diff. peak/hole / e Å ⁻³	1.34/-0.50	1.73/-1.00

Table S4. Simplified images of all the calculated Mo-containing species.

The non-relevant H on the ligand an tBu group have been omitted for clarity.

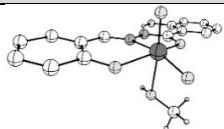
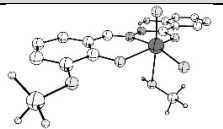
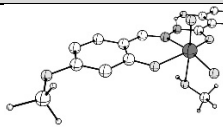
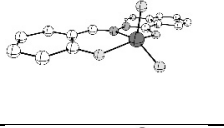
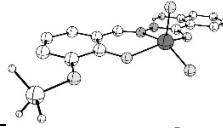
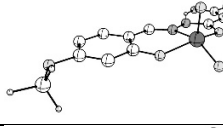


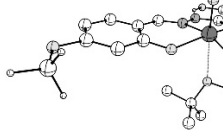
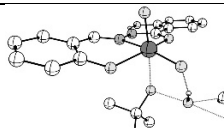

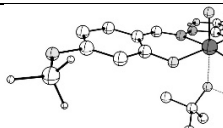
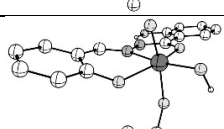
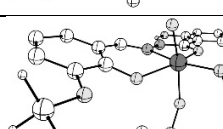
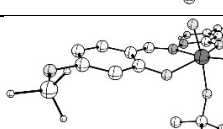
	L ^H	L ^{3OMe}	L ^{4OMe}
TBHP as oxidant			
Gas phase			
[MoO ₂ (L)(MeOH)]			
[MoO ₂ (L)]			
[MoO ₂ (L)(TBHP)]			
TS			
[MoO(OH)(L)(OtBu)]			

Table S5. Imaginary frequency (cm⁻¹) of the calculated transition states shown in Table S1

	L ^H	L ^{3OMe}	L ^{4OMe}
TS	469i	471i	471i

Table S6. DFT Coordinates of all optimized species

A - Organic molecules

C ₂ H ₄							
6	0.000000000	0.665616000	0.000000000	6	0.663277000	-0.487998000	0.000000000
1	0.923789000	1.239603000	0.000000000	1	-0.044284000	1.406100000	0.920513000
1	-0.923751000	1.239647000	0.000000000	1	1.105429000	-0.869573000	0.920803000
6	0.000000000	-0.665616000	0.000000000	8	-0.762744000	-0.385408000	0.000000000
1	-0.923789000	-1.239603000	0.000000000	1	-0.044284000	1.406100000	-0.920513000
1	0.923751000	-1.239647000	0.000000000	1	1.105429000	-0.869573000	-0.920803000
C ₂ H ₄ O				TBHP			
6	0.000000000	0.823033000	0.000000000	6	0.386063000	0.000211000	0.035516000
				8	-0.724877000	-0.051131000	-0.892876000
				8	-1.972121000	0.107335000	-0.155683000
				6	1.585594000	-0.148364000	-0.908710000

6	0.308477000	-1.169459000	1.023961000
6	0.408392000	1.352799000	0.755437000
1	-2.332288000	-0.792908000	-0.245178000
1	1.280879000	1.423828000	1.414956000
1	1.184972000	-1.179544000	1.681110000
1	2.518340000	-0.109351000	-0.336278000
1	-0.583795000	-1.085739000	1.651566000
1	0.273436000	-2.124477000	0.486863000
1	1.545636000	-1.103632000	-1.442442000
1	1.596327000	0.660559000	-1.645981000
1	0.455220000	2.169404000	0.027401000

tBuOH

6	-0.005589000	-0.000026000	0.014420000
8	0.015118000	-0.000431000	1.451985000
1	0.945639000	0.001902000	1.728630000
6	-1.490947000	-0.005338000	-0.356041000
6	0.694937000	-1.262772000	-0.510972000
6	0.685524000	1.268259000	-0.510112000
1	0.646742000	1.325318000	-1.604317000
1	0.656167000	-1.319650000	-1.605180000
1	-1.623187000	-0.004815000	-1.443350000
1	1.752964000	-1.271531000	-0.216357000

1	0.219546000	-2.158915000	-0.098630000
1	-1.981082000	-0.894002000	0.055230000
1	-1.987701000	0.878867000	0.056897000
1	0.203120000	2.160551000	-0.097564000
1	1.743307000	1.284985000	-0.215007000

MeOH

8	-0.748606000	-0.122482000	0.000001000
6	0.661940000	0.019648000	0.000035000
1	1.036807000	0.543842000	0.893075000
1	1.036822000	0.543722000	-0.893232000
1	1.079608000	-0.990888000	-0.000013000
1	-1.136031000	0.765290000	-0.000051000

B1 - With Ligand L^H

MoO₂(L^H)(MeOH)

6	-0.395539000	-2.252625000	2.632740000
1	-1.454536000	-2.140510000	2.376096000
1	-0.257951000	-2.183615000	3.717179000
1	-0.037342000	-3.215677000	2.272591000
1	-2.084603000	2.588829000	0.291398000
1	0.120217000	-0.376413000	2.257296000
42	0.713423000	-1.333027000	-0.508264000
7	-0.933001000	1.268524000	0.089882000
8	-1.276627000	-0.971094000	-0.319007000
8	0.652495000	-3.005449000	-0.197298000
8	0.406699000	-1.257719000	1.970510000
7	0.386967000	0.878399000	0.012313000
6	-3.766694000	1.725267000	0.099066000
6	-1.739431000	0.245374000	-0.125911000
6	4.662532000	0.103721000	0.012781000
1	5.064039000	-0.903789000	-0.016941000
6	3.267399000	0.257983000	0.034326000
6	4.958039000	2.513795000	0.081650000
1	5.613098000	3.379011000	0.097378000
6	1.291654000	1.804838000	0.121097000
1	0.948060000	2.833737000	0.243418000
8	0.844747000	-1.127600000	-2.184927000
8	2.512618000	-0.844444000	0.055488000
6	-5.164702000	1.856462000	0.089351000
1	-5.583005000	2.842246000	0.265331000
6	-3.188667000	0.445623000	-0.128410000
6	-4.036374000	-0.656951000	-0.362947000
1	-3.578257000	-1.623673000	-0.541677000
6	2.710771000	1.565959000	0.079987000
6	5.493579000	1.217566000	0.032251000
6	3.582754000	2.677032000	0.109467000
1	3.151366000	3.674494000	0.147688000
6	-5.414417000	-0.513160000	-0.371467000
1	-6.052446000	-1.371683000	-0.556148000
6	-5.974313000	0.753299000	-0.142185000
1	-7.054125000	0.877251000	-0.147014000
1	6.570916000	1.077832000	0.011659000
8	-3.043242000	2.835746000	0.330570000

MoO₂(L^H)

42	-0.699122000	-1.512301000	0.075624000
8	1.250418000	-1.116757000	-0.172756000
8	-0.651250000	-2.942585000	-0.835295000
7	0.924962000	1.146894000	-0.053115000
6	3.769206000	1.584277000	-0.001089000
7	-0.388752000	0.734988000	-0.046214000
6	1.735295000	0.111298000	-0.091703000
8	-2.478789000	-0.918227000	-0.439945000
6	5.167969000	1.700025000	0.022359000
1	5.594048000	2.696483000	0.077984000
6	-3.257153000	0.149494000	-0.231413000
8	-0.820982000	-1.871395000	1.727261000

6	3.182033000	0.290341000	-0.072552000
6	-3.587633000	2.540699000	0.123639000
1	-3.163373000	3.530795000	0.270921000
6	-4.960600000	2.364591000	0.096541000
1	-5.624193000	3.213839000	0.223506000
6	-1.294606000	1.672037000	-0.013822000
1	-0.938556000	2.701750000	0.034192000
6	4.020788000	-0.843296000	-0.121477000
1	3.556537000	-1.821826000	-0.177187000
6	-4.648983000	-0.019705000	-0.264527000
1	-5.042677000	-1.017633000	-0.426019000
6	-2.710202000	1.443468000	-0.030870000
6	5.399339000	-0.713811000	-0.098038000
1	6.031546000	-1.595218000	-0.135206000
6	5.968508000	0.567578000	-0.025241000
1	7.049401000	0.679409000	-0.006081000
6	-5.486620000	1.076879000	-0.098076000
1	-6.563020000	0.931906000	-0.123276000
8	3.054487000	2.722998000	0.045568000
1	2.094807000	2.488423000	0.019211000

MoO₂(L^H)(TBHP)

42	-0.545548000	0.088465000	-1.542207000
8	1.401598000	0.078615000	-1.109905000
8	-0.549483000	1.630458000	-2.290094000
7	1.117670000	-1.345728000	0.663991000
6	3.962735000	-1.466678000	1.060313000
7	-0.196757000	-1.196702000	0.294117000
6	1.905778000	-0.655499000	-0.133476000
8	-2.333843000	0.059569000	-0.784941000
6	5.361162000	-1.460588000	1.182364000
1	5.805164000	-2.068593000	1.963885000
6	-3.080062000	-0.851663000	-0.142165000
8	-0.644630000	-1.097323000	-2.742576000
6	3.352336000	-0.680275000	0.043699000
6	-3.352079000	-2.695871000	1.427987000
1	-2.906424000	-3.421426000	2.103954000
6	-4.725719000	-2.658803000	1.249313000
1	-5.365575000	-3.355133000	1.781783000
6	-1.083839000	-1.871072000	0.965191000
1	-0.718148000	-2.531778000	1.752065000
6	4.168013000	0.089788000	-0.811950000
1	3.685275000	0.688596000	-1.576229000
6	-4.471018000	-0.813686000	-0.310906000
1	-4.887902000	-0.070484000	-0.982496000
6	-2.502184000	-1.806194000	0.734756000
6	5.546505000	0.086756000	-0.679219000
1	6.160742000	0.685158000	-1.344511000
6	6.138927000	-0.695556000	0.324737000
1	7.219992000	-0.704431000	0.436827000
6	-5.281190000	-1.712183000	0.374984000
1	-6.357365000	-1.674794000	0.231071000
1	2.307536000	-2.125590000	1.727100000
6	-0.911674000	2.845569000	1.508109000

8	-0.061583000	2.131156000	0.558952000
8	0.622518000	3.108639000	-0.277052000
6	-1.458319000	1.721663000	2.393443000
6	-2.034174000	3.572158000	0.761590000
6	-0.049020000	3.810526000	2.328449000
1	0.211824000	2.888131000	-1.142997000
1	-0.660232000	4.302768000	3.093331000
1	-2.693628000	4.086245000	1.469967000
1	-2.077263000	2.151147000	3.188365000
1	-1.619420000	4.319121000	0.079231000
1	-2.633878000	2.861907000	0.182500000
1	-2.077148000	1.028422000	1.817574000
1	-0.638290000	1.164574000	2.858420000
1	0.761561000	3.268521000	2.826762000
1	0.390808000	4.577310000	1.687081000
8	3.270663000	-2.228433000	1.926733000

TS

42	0.346056000	0.546289000	1.229159000
8	-1.604977000	0.363144000	0.732386000
8	0.188039000	2.020588000	2.125012000
7	-1.132034000	-1.186425000	-0.903143000
6	-3.910419000	-1.363071000	-1.580342000
7	0.146219000	-0.984956000	-0.445361000
6	-1.992282000	-0.452219000	-0.224775000
8	2.207483000	0.440037000	0.667646000
6	-5.291142000	-1.398999000	-1.836130000
1	-5.640540000	-2.035078000	-2.643058000
6	2.979845000	-0.581789000	0.268150000
8	0.416070000	-0.684235000	2.388807000
6	-3.420778000	-0.536489000	-0.531438000
6	3.366441000	-2.656340000	-0.950400000
1	2.975835000	-3.474208000	-1.551127000
6	4.713074000	-2.615099000	-0.622611000
1	5.383215000	-3.398424000	-0.962366000
6	1.084063000	-1.756151000	-0.898243000
1	0.803303000	-2.535235000	-1.608848000
6	-4.337671000	0.217921000	0.227749000
1	-3.946616000	0.835375000	1.029010000
6	4.345183000	-0.543178000	0.586769000
1	4.709102000	0.291590000	1.176849000
6	2.471755000	-1.657304000	-0.511044000
6	-5.698291000	0.170233000	-0.031374000
1	-6.390672000	0.754862000	0.566551000
6	-6.170068000	-0.644052000	-1.072548000
1	-7.234967000	-0.688865000	-1.285913000
6	5.198412000	-1.551254000	0.150866000
1	6.251991000	-1.507607000	0.412898000
1	-2.183208000	-2.000017000	-2.049177000
6	0.879292000	2.576224000	-1.717601000
8	0.142026000	2.042282000	-0.617178000
8	-0.734189000	3.526757000	0.170004000
6	1.451158000	1.387514000	-2.517435000
6	2.018849000	3.476101000	-1.213706000
6	-0.080566000	3.358147000	-2.632398000
1	-0.347804000	3.137474000	1.003887000

1	0.438779000	3.695420000	-3.537177000
1	2.600205000	3.881813000	-2.050504000
1	1.964899000	1.762990000	-3.410269000
1	1.611025000	4.313784000	-0.639646000
1	2.693240000	2.907270000	-0.565580000
1	2.171697000	0.818732000	-1.927157000
1	0.646157000	0.719469000	-2.839186000
1	-0.919004000	2.719943000	-2.931062000
1	-0.479401000	4.234893000	-2.116265000
6	-2.221443000	4.307529000	0.910435000
1	-2.815156000	4.437022000	0.012495000
1	-2.572484000	3.551852000	1.605703000
6	-1.325286000	5.276018000	1.310595000
1	-0.822174000	5.214313000	2.270361000
1	-1.065056000	6.103180000	0.659920000
8	-3.118160000	-2.122113000	-2.357414000

MoO(OR)(OH)(L^H)

42	-0.566502000	0.674285000	-1.071543000
8	1.415670000	0.439959000	-0.944399000
8	-0.439004000	2.190475000	-2.221206000
7	1.199947000	-1.327646000	0.495956000
6	4.058252000	-1.522470000	0.733992000
7	-0.129132000	-1.110056000	0.217432000
6	1.955979000	-0.482852000	-0.171315000
8	-2.370146000	0.326018000	-0.354051000
6	5.461045000	-1.544132000	0.788321000
1	5.933031000	-2.293952000	1.414968000
6	-3.041558000	-0.807556000	-0.148395000
8	-0.924414000	-0.385490000	-2.348711000
6	3.411653000	-0.550448000	-0.078293000
6	-3.176914000	-3.101530000	0.674790000
1	-2.679408000	-3.981113000	1.076217000
6	-4.545092000	-3.112833000	0.457686000
1	-5.129157000	-3.998497000	0.686409000
6	-0.979491000	-2.009196000	0.613290000
1	-0.576812000	-2.872868000	1.143254000
6	4.196376000	0.364368000	-0.810112000
1	3.686609000	1.095912000	-1.427675000
6	-4.429836000	-0.825614000	-0.356497000
1	-4.902815000	0.068866000	-0.748347000
6	-2.396890000	-1.964454000	0.369635000
6	5.580133000	0.330700000	-0.748494000
1	6.170201000	1.040893000	-1.319166000
6	6.208523000	-0.631175000	0.057625000
1	7.293450000	-0.666221000	0.113082000
6	-5.166680000	-1.966862000	-0.062597000
1	-6.238967000	-1.966619000	-0.238567000
1	2.426362000	-2.301990000	1.323833000
6	-0.983189000	2.586430000	1.580219000
8	-0.507725000	1.899878000	0.430203000
6	-1.312978000	1.555416000	2.672244000
6	-2.234219000	3.391774000	1.190568000
6	0.143323000	3.523412000	2.047186000
1	-0.208612000	2.985077000	-1.707418000
1	-0.159293000	4.081971000	2.940422000

1	-2.624744000	3.941047000	2.054978000
1	-1.648019000	2.057935000	3.587033000
1	-1.993598000	4.118603000	0.406167000
1	-3.015633000	2.724447000	0.816113000
1	-2.105846000	0.880248000	2.337826000

B2 - With Ligand L^{3OMe}

MoO₂(L^{3OMe})(MeOH)

6	-0.712029000	-2.215418000	2.625165000
1	-1.773566000	-2.147753000	2.363348000
1	-0.583809000	-2.153000000	3.711227000
1	-0.309025000	-3.157331000	2.256458000
1	-2.675321000	2.514479000	0.296625000
1	-0.276718000	-0.314152000	2.273529000
42	0.374856000	-1.215843000	-0.497159000
7	-1.442596000	1.272976000	0.099449000
8	-1.639026000	-0.983450000	-0.316383000
8	0.417329000	-2.890733000	-0.197124000
8	0.048948000	-1.179098000	1.978960000
7	-0.099985000	0.970104000	0.025728000
6	-4.298301000	1.547811000	0.090804000
6	-2.179390000	0.199766000	-0.123658000
6	4.221001000	0.469666000	0.021076000
6	2.801876000	0.544715000	0.051446000
6	4.344697000	2.898879000	0.084963000
1	4.951962000	3.798589000	0.094997000
6	0.742039000	1.953229000	0.137602000
1	0.331923000	2.957159000	0.261201000
8	0.498046000	-0.991539000	-2.172431000
8	2.123970000	-0.602243000	0.083956000
6	-5.701746000	1.590610000	0.070540000
1	-6.182580000	2.547687000	0.245405000
6	-3.638995000	0.307830000	-0.134988000
6	-4.413763000	-0.845157000	-0.378166000
1	-3.894120000	-1.780472000	-0.555796000
6	2.175377000	1.812158000	0.094934000
6	4.973195000	1.642930000	0.035392000
6	2.967011000	2.985509000	0.118720000
1	2.472964000	3.952516000	0.154622000
6	-5.798191000	-0.788622000	-0.397097000
1	-6.379296000	-1.685269000	-0.588537000
6	-6.438591000	0.439339000	-0.169697000
1	-7.524025000	0.495096000	-0.182741000
1	6.055741000	1.593026000	0.009887000
8	-3.648121000	2.701106000	0.330129000
8	4.728934000	-0.787195000	-0.017688000
6	6.138663000	-0.940612000	-0.063985000
1	6.564984000	-0.473052000	-0.961378000
1	6.619165000	-0.518133000	0.828622000
1	6.318073000	-2.016122000	-0.096702000

MoO₂(L^{3OMe})

42	-0.338408000	-1.372968000	0.142471000
8	1.632208000	-1.120022000	-0.151581000
8	-0.399309000	-2.833334000	-0.718616000

1	-0.425562000	0.959995000	2.912564000
1	1.043836000	2.947966000	2.285714000
1	0.394423000	4.243079000	1.260144000
8	3.396533000	-2.435676000	1.467466000

7	1.468645000	1.163477000	-0.067768000
6	4.336238000	1.399623000	-0.064096000
7	0.130112000	0.846200000	-0.030772000
6	2.202435000	0.071452000	-0.099540000
8	-2.064285000	-0.657671000	-0.381173000
6	5.739968000	1.416972000	-0.064366000
1	6.235764000	2.381743000	-0.033018000
6	-2.761001000	0.459554000	-0.161928000
8	-0.458993000	-1.666171000	1.807625000
6	3.658860000	0.149304000	-0.103958000
6	-2.931346000	2.877071000	0.170278000
1	-2.441086000	3.838066000	0.296807000
6	-4.308340000	2.778722000	0.176042000
1	-4.920615000	3.665391000	0.306847000
6	-0.708549000	1.843537000	-0.004526000
1	-0.282988000	2.847343000	0.015916000
6	4.415226000	-1.040945000	-0.144819000
1	3.882272000	-1.984933000	-0.176031000
6	-4.178214000	0.369871000	-0.157592000
6	-2.138386000	1.714974000	0.009676000
6	5.799841000	-1.008664000	-0.144273000
1	6.367935000	-1.932964000	-0.175072000
6	6.458518000	0.230405000	-0.103506000
1	7.544792000	0.266249000	-0.102730000
6	-4.932887000	1.529422000	0.013858000
1	-6.015423000	1.474474000	0.020688000
8	3.703879000	2.586505000	-0.026783000
1	2.729464000	2.418805000	-0.034453000
8	-4.677914000	-0.877093000	-0.328848000
6	-6.088404000	-1.043198000	-0.326467000
1	-6.526736000	-0.732159000	0.630785000
1	-6.560085000	-0.481327000	-1.143280000
1	-6.259902000	-2.110106000	-0.474131000

MoO₂(L^{3OMe})(TBHP)

42	-0.248178000	0.102538000	-1.437587000
8	1.719724000	0.141424000	-1.098404000
8	-0.321515000	1.655467000	-2.159091000
7	1.566377000	-1.354593000	0.633061000
6	4.431276000	-1.424201000	0.863888000
7	0.230717000	-1.225906000	0.340845000
6	2.292640000	-0.616308000	-0.180508000
8	-1.979547000	0.011906000	-0.575979000
6	5.833943000	-1.388720000	0.908705000
1	6.334539000	-2.017185000	1.638127000
6	-2.666165000	-0.931939000	0.078544000
8	-0.376068000	-1.066149000	-2.652473000
6	3.747464000	-0.612334000	-0.083517000
6	-2.823320000	-2.828834000	1.610627000
1	-2.329312000	-3.565187000	2.238067000

6	-4.200364000	-2.803397000	1.501201000
1	-4.806194000	-3.522781000	2.043150000
6	-0.604054000	-1.936097000	1.040913000
1	-0.182696000	-2.609483000	1.788059000
6	4.496489000	0.212442000	-0.948838000
1	3.958506000	0.829862000	-1.659609000
6	-4.081474000	-0.907878000	-0.019919000
6	-2.035843000	-1.897900000	0.892966000
6	5.880057000	0.238659000	-0.892053000
1	6.442265000	0.879502000	-1.563839000
6	6.545260000	-0.569635000	0.043230000
1	7.630842000	-0.556202000	0.095327000
6	-4.831171000	-1.846194000	0.688874000
1	-5.912798000	-1.840482000	0.618679000
1	2.830639000	-2.147809000	1.593249000
6	-0.618540000	2.791615000	1.653124000
8	0.250074000	2.128669000	0.683217000
8	0.859907000	3.144557000	-0.164368000
6	-1.062867000	1.639956000	2.560059000
6	-1.807903000	3.437566000	0.935930000
6	0.200588000	3.816855000	2.444610000
1	0.431549000	2.913564000	-1.019157000
1	-0.420958000	4.271739000	3.224170000
1	-2.475218000	3.917521000	1.660922000
1	-1.686686000	2.032988000	3.369883000
1	-1.461889000	4.203071000	0.235597000
1	-2.379966000	2.686588000	0.381125000
1	-1.649119000	0.902320000	2.006225000
1	-0.194410000	1.142606000	3.004296000
1	1.059030000	3.333246000	2.922579000
1	0.571000000	4.607058000	1.788145000
8	3.805677000	-2.237145000	1.734352000
8	-4.587731000	0.063414000	-0.818659000
6	-5.997130000	0.134484000	-0.979313000
1	-6.397279000	-0.788532000	-1.418558000
1	-6.500727000	0.331552000	-0.023795000
1	-6.174811000	0.966959000	-1.661243000

TS

42	0.887463000	0.031384000	2.585039000
8	-0.714635000	1.200364000	2.184471000
8	0.877144000	0.255784000	4.303203000
7	-0.221477000	1.258013000	-0.064038000
6	-2.526693000	2.884323000	-0.558989000
7	0.818373000	0.461812000	0.345652000
6	-0.986960000	1.589513000	0.957904000
8	2.693511000	-0.481353000	2.091763000
6	-3.679233000	3.672375000	-0.712952000
1	-3.924259000	4.022082000	-1.710701000
6	3.203607000	-1.108921000	1.026532000
8	0.163798000	-1.476258000	2.324431000
6	-2.177515000	2.411928000	0.736499000
6	3.338692000	-1.577220000	-1.367402000
1	2.946625000	-1.431906000	-2.370148000
6	4.436477000	-2.388753000	-1.151844000
1	4.918843000	-2.891137000	-1.984576000

6	1.567862000	-0.077745000	-0.563240000
1	1.321849000	0.117856000	-1.608104000
6	-3.002219000	2.745108000	1.829629000
1	-2.724029000	2.370164000	2.808466000
6	4.339210000	-1.935256000	1.233891000
6	2.700363000	-0.931153000	-0.283416000
6	-4.138120000	3.521818000	1.664358000
1	-4.763557000	3.766019000	2.517545000
6	-4.471573000	3.985384000	0.382432000
1	-5.359973000	4.595451000	0.240439000
6	4.939234000	-2.569089000	0.146785000
1	-1.037167000	2.054078000	-1.395765000
6	3.045666000	2.920072000	2.353132000
8	1.835848000	2.221910000	2.650607000
8	1.300344000	2.847126000	4.356786000
6	3.407825000	2.617858000	0.884390000
6	4.175621000	2.459446000	3.288208000
6	2.798856000	4.433849000	2.487677000
1	1.196179000	1.868533000	4.527760000
1	3.681839000	4.997539000	2.163976000
1	5.110760000	2.987783000	3.065295000
1	4.290651000	3.201877000	0.598315000
1	3.906516000	2.662262000	4.329575000
1	4.347658000	1.384159000	3.177923000
1	3.640622000	1.561647000	0.739795000
1	2.581756000	2.894970000	0.221913000
1	1.948524000	4.733477000	1.865829000
1	2.580521000	4.700512000	3.524667000
6	0.010005000	3.452965000	5.508037000
1	-0.129655000	4.449872000	5.105220000
1	-0.807659000	2.757951000	5.346125000
6	0.966448000	3.207660000	6.470726000
1	1.027359000	2.245873000	6.969954000
1	1.712733000	3.952428000	6.723060000
8	-1.806871000	2.620316000	-1.663428000
1	5.803065000	-3.206131000	0.298398000
8	4.753483000	-2.029612000	2.523718000
6	5.870017000	-2.856921000	2.809367000
1	5.679211000	-3.900979000	2.527957000
1	6.775338000	-2.503195000	2.298030000
1	6.016562000	-2.794508000	3.888652000

MoO(OR)(OH)(L^{3OMe})

42	-0.226918000	0.639872000	-0.965170000
8	1.767972000	0.482625000	-0.899942000
8	-0.152497000	2.156746000	-2.123490000
7	1.665560000	-1.335596000	0.488511000
6	4.535387000	-1.436329000	0.620696000
7	0.321218000	-1.156331000	0.261492000
6	2.367373000	-0.444004000	-0.176636000
8	-1.975697000	0.215754000	-0.156680000
6	5.939146000	-1.410410000	0.625050000
1	6.458761000	-2.162417000	1.210016000
6	-2.596627000	-0.944327000	0.027824000
8	-0.635501000	-0.400804000	-2.242040000
6	3.827173000	-0.462946000	-0.136583000

6	-2.636107000	-3.282235000	0.750599000
1	-2.097780000	-4.164066000	1.086549000
6	-4.006604000	-3.312548000	0.587974000
1	-4.564179000	-4.220712000	0.794290000
6	-0.483144000	-2.099832000	0.652867000
1	-0.030610000	-2.965999000	1.136104000
6	4.553179000	0.501236000	-0.865356000
1	3.996384000	1.233429000	-1.440018000
6	-4.009053000	-0.984253000	-0.118853000
6	-1.909574000	-2.101352000	0.463606000
6	5.938718000	0.514252000	-0.853630000
1	6.483232000	1.262266000	-1.421297000
6	6.628243000	-0.449463000	-0.101645000
1	7.715052000	-0.448071000	-0.085476000
6	-4.694711000	-2.165018000	0.153413000
1	-5.771163000	-2.207520000	0.032531000
1	2.953223000	-2.290241000	1.241993000
6	-0.769992000	2.601152000	1.607163000
8	-0.195841000	1.889281000	0.516791000
6	-1.028747000	1.613311000	2.756798000

6	-2.080709000	3.257721000	1.141192000
6	0.252665000	3.667142000	2.035218000
1	0.081734000	2.951789000	-1.612343000
1	-0.124466000	4.250339000	2.883239000
1	-2.539635000	3.821677000	1.961727000
1	-1.417548000	2.139752000	3.636260000
1	-1.889221000	3.954697000	0.317012000
1	-2.787113000	2.498298000	0.795185000
1	-1.757132000	0.855561000	2.455801000
1	-0.097559000	1.110781000	3.040067000
1	1.195910000	3.195371000	2.330061000
1	0.458385000	4.356646000	1.208747000
8	3.931957000	-2.394936000	1.346644000
8	-4.576150000	0.183205000	-0.522487000
6	-5.981206000	0.209604000	-0.719953000
1	-6.291123000	-0.505809000	-1.492933000
1	-6.523036000	-0.004686000	0.211055000
1	-6.215420000	1.222605000	-1.050289000

B3 - With Ligand L^{4OMe}

MoO₂(L^{4OMe})(MeOH)

6	-0.947235000	-2.227545000	2.654052000
1	-2.003728000	-2.108570000	2.389994000
1	-0.815419000	-2.144259000	3.738385000
1	-0.597951000	-3.199789000	2.310105000
1	-2.560296000	2.604083000	0.277549000
1	-0.418855000	-0.362936000	2.242957000
42	0.168715000	-1.360898000	-0.505153000
7	-1.431032000	1.263853000	0.079698000
8	-1.811517000	-0.969773000	-0.320562000
8	0.083080000	-3.027838000	-0.166041000
8	-0.131185000	-1.251780000	1.981588000
7	-0.116521000	0.846639000	0.002886000
6	-4.257909000	1.769729000	0.089970000
6	-2.255080000	0.257403000	-0.131421000
6	4.144254000	-0.005468000	0.016812000
1	4.508909000	-1.024233000	-0.011035000
6	2.755053000	0.184647000	0.033996000
6	4.481321000	2.408327000	0.091557000
1	5.172215000	3.243690000	0.110714000
6	0.806793000	1.759392000	0.111035000
1	0.477735000	2.793709000	0.227927000
8	0.311677000	-1.186054000	-2.184593000
8	1.985374000	-0.904431000	0.052013000
6	-5.653311000	1.924538000	0.081505000
1	-6.054704000	2.917924000	0.254368000
6	-3.701679000	0.480161000	-0.133533000
6	-4.567619000	-0.608603000	-0.362618000
1	-4.125945000	-1.583584000	-0.538020000
6	2.214472000	1.499932000	0.077577000
6	5.002495000	1.095767000	0.040026000
6	3.116936000	2.591260000	0.113143000
1	2.710866000	3.599090000	0.150726000
6	-5.943552000	-0.441861000	-0.370001000
1	-6.595896000	-1.290515000	-0.550552000
6	-6.482014000	0.834209000	-0.144889000
1	-7.559625000	0.976279000	-0.148787000
8	-3.514354000	2.868475000	0.316688000
8	6.352344000	1.009149000	0.021077000
6	6.956374000	-0.278947000	-0.041432000
1	6.698596000	-0.882537000	0.837375000
1	6.659445000	-0.813568000	-0.951742000
1	8.032326000	-0.100121000	-0.057647000

MoO₂(L^{4OMe})

42	-0.115923000	-1.531022000	0.086230000
8	1.828993000	-1.121135000	-0.156796000
8	-0.069272000	-2.927175000	-0.877930000
7	1.475662000	1.136410000	-0.051244000
6	4.315018000	1.613960000	-0.022369000
7	0.164990000	0.703380000	-0.032946000
6	2.299344000	0.115014000	-0.088688000
8	-1.925766000	-0.959612000	-0.373371000
6	5.712023000	1.749216000	-0.011165000
1	6.124674000	2.751845000	0.034536000

6	-2.705963000	0.104181000	-0.172721000
8	-0.214691000	-1.947800000	1.726622000
6	3.745075000	0.312329000	-0.081099000
6	-3.053401000	2.492544000	0.147541000
1	-2.642381000	3.490649000	0.275486000
6	-4.416980000	2.311243000	0.137474000
1	-5.106086000	3.139985000	0.254859000
6	-0.752534000	1.634825000	0.005147000
1	-0.400004000	2.665919000	0.048204000
6	4.598287000	-0.809608000	-0.129311000
1	4.146986000	-1.794730000	-0.175233000
6	-4.093139000	-0.086784000	-0.188589000
1	-4.462433000	-1.094110000	-0.331553000
6	-2.158766000	1.402407000	0.002552000
6	5.975710000	-0.661406000	-0.117576000
1	6.619314000	-1.534637000	-0.154189000
6	6.528101000	0.627449000	-0.057727000
1	7.607528000	0.754075000	-0.048000000
6	-4.945202000	1.009127000	-0.030179000
8	3.583915000	2.743147000	0.022725000
1	2.627487000	2.493808000	0.005512000
8	-6.293046000	0.929035000	-0.027413000
6	-6.907786000	-0.346822000	-0.188216000
1	-6.646694000	-0.793606000	-1.154951000
1	-6.621854000	-1.029291000	0.620936000
1	-7.982106000	-0.163232000	-0.149046000

MoO₂(L^{4OMe})(TBHP)

42	-0.102878000	0.140188000	-1.531619000
8	1.842398000	0.024478000	-1.122729000
8	-0.026600000	1.680981000	-2.280615000
7	1.493900000	-1.355430000	0.672020000
6	4.332190000	-1.641356000	1.044503000
7	0.185459000	-1.129380000	0.309649000
6	2.313864000	-0.728085000	-0.140361000
8	-1.890684000	0.229969000	-0.761506000
6	5.729461000	-1.720076000	1.151310000
1	6.144240000	-2.339428000	1.940006000
6	-2.679176000	-0.620142000	-0.091544000
8	-0.290193000	-1.039922000	-2.727849000
6	3.759339000	-0.838340000	0.019785000
6	-3.049164000	-2.404487000	1.518474000
1	-2.648528000	-3.145042000	2.205902000
6	-4.411853000	-2.286177000	1.361051000
1	-5.107613000	-2.914737000	1.905437000
6	-0.735895000	-1.738258000	1.003646000
1	-0.397749000	-2.409671000	1.793786000
6	4.610285000	-0.137676000	-0.859825000
1	4.156426000	0.474864000	-1.630958000
6	-4.063965000	-0.489077000	-0.251354000
1	-4.423188000	0.268910000	-0.935395000
6	-2.143272000	-1.589805000	0.795751000
6	5.988006000	-0.224406000	-0.742782000
1	6.629673000	0.321385000	-1.427242000
6	6.543180000	-1.022042000	0.269789000

1	7.622921000	-1.096311000	0.370018000
6	-4.927588000	-1.321512000	0.465667000
1	2.646692000	-2.184696000	1.740261000
6	-0.303661000	2.960723000	1.509073000
8	0.508602000	2.197512000	0.567295000
8	1.222716000	3.131877000	-0.292747000
6	-0.886185000	1.874020000	2.418058000
6	-1.403888000	3.717552000	0.758943000
6	0.601681000	3.906018000	2.306301000
1	0.799818000	2.906180000	-1.151587000
1	0.017139000	4.432348000	3.069482000
1	-2.037435000	4.268503000	1.463316000
1	-1.484185000	2.339463000	3.208925000
1	-0.965730000	4.435549000	0.060388000
1	-2.034344000	3.020409000	0.196717000
1	-1.532995000	1.193174000	1.858085000
1	-0.084310000	1.294980000	2.887727000
1	1.396867000	3.341898000	2.804839000
1	1.063094000	4.646258000	1.649010000
8	3.603752000	-2.341966000	1.933390000
8	-6.275146000	-1.277543000	0.375488000
6	-6.875176000	-0.340773000	-0.514868000
1	-6.630603000	0.690022000	-0.231293000
1	-6.561756000	-0.520579000	-1.550172000
1	-7.950914000	-0.497378000	-0.426427000

TS

42	0.363401000	0.571591000	1.217078000
8	-1.586777000	0.383229000	0.738819000
8	0.204494000	2.059206000	2.092340000
7	-1.121151000	-1.169078000	-0.893965000
6	-3.905703000	-1.364086000	-1.547141000
7	0.160593000	-0.956417000	-0.444313000
6	-1.979768000	-0.440086000	-0.213144000
8	2.228645000	0.474331000	0.645897000
6	-5.288304000	-1.409549000	-1.789779000
1	-5.641198000	-2.049383000	-2.592251000
6	2.999617000	-0.543825000	0.242142000
8	0.456481000	-0.640233000	2.394643000
6	-3.411358000	-0.532641000	-0.504724000
6	3.394614000	-2.608187000	-0.978624000
1	3.012522000	-3.430657000	-1.578139000
6	4.735868000	-2.561744000	-0.664856000
1	5.428688000	-3.326103000	-0.998639000
6	1.101534000	-1.725636000	-0.902624000
1	0.815736000	-2.509235000	-1.606336000
6	-4.325495000	0.216869000	0.261767000
1	-3.930994000	0.838082000	1.058483000
6	4.364025000	-0.487603000	0.557557000
1	4.708208000	0.354259000	1.144669000
6	2.485788000	-1.619451000	-0.532737000
6	-5.688665000	0.159772000	0.015969000
1	-6.378873000	0.740915000	0.619862000
6	-6.165209000	-0.659093000	-1.018967000
1	-7.231812000	-0.711404000	-1.221965000
6	5.227188000	-1.492746000	0.114960000

1	-2.178099000	-1.990230000	-2.030267000
6	0.876896000	2.596007000	-1.752278000
8	0.145486000	2.060768000	-0.650150000
8	-0.745910000	3.538362000	0.131326000
6	1.455642000	1.407754000	-2.548106000
6	2.010895000	3.505790000	-1.252989000
6	-0.088408000	3.368559000	-2.669631000
1	-0.351188000	3.160150000	0.966645000
1	0.427638000	3.704423000	-3.576888000
1	2.587661000	3.914504000	-2.091599000
1	1.969734000	1.782722000	-3.441056000
1	1.597590000	4.341291000	-0.679551000
1	2.690493000	2.943093000	-0.604801000
1	2.176438000	0.842765000	-1.954551000
1	0.653957000	0.735415000	-2.869043000
1	-0.923646000	2.724148000	-2.963831000
1	-0.491332000	4.245459000	-2.156878000
6	-2.247044000	4.281540000	0.854168000
1	-2.834908000	4.401158000	-0.049081000
1	-2.590095000	3.515533000	1.542154000
6	-1.388918000	5.276894000	1.274217000
1	-0.897664000	5.224419000	2.240619000
1	-1.142429000	6.113626000	0.630437000
8	-3.114879000	-2.119437000	-2.330026000
8	6.555165000	-1.526805000	0.378441000
6	7.122461000	-0.489617000	1.170726000
1	8.183345000	-0.729124000	1.256331000
1	7.006350000	0.489134000	0.689059000
1	6.671520000	-0.460092000	2.170154000

MoO(OR)(OH)(L^{4OMe})

42	-0.075436000	0.748277000	-1.023679000
8	1.886267000	0.384524000	-0.943209000
8	0.164862000	2.233829000	-2.201642000
7	1.584491000	-1.357118000	0.509545000
6	4.428524000	-1.752160000	0.681300000
7	0.267331000	-1.042988000	0.259090000
6	2.382097000	-0.572271000	-0.176925000
8	-1.890910000	0.538573000	-0.249325000
6	5.827037000	-1.871445000	0.703436000
1	6.260116000	-2.651553000	1.321205000
6	-2.629004000	-0.545472000	-0.027771000
8	-0.578273000	-0.267768000	-2.286988000
6	3.832160000	-0.739136000	-0.118556000
6	-2.906688000	-2.818449000	0.804965000
1	-2.468988000	-3.733268000	1.196524000
6	-4.269333000	-2.737016000	0.628828000
1	-4.929323000	-3.562917000	0.869151000
6	-0.637375000	-1.884566000	0.674636000
1	-0.278574000	-2.775376000	1.191031000
6	4.660924000	0.118234000	-0.870065000
1	4.188861000	0.882830000	-1.477508000
6	-4.018062000	-0.456187000	-0.201780000
1	-4.419155000	0.473943000	-0.583320000
6	-2.045861000	-1.743364000	0.472977000
6	6.040572000	-0.011178000	-0.840188000

1	6.664895000	0.656125000	-1.426077000
6	6.619386000	-1.013233000	-0.046661000
1	7.700289000	-1.123394000	-0.015903000
6	-4.831400000	-1.546053000	0.113999000
1	2.759914000	-2.414503000	1.311319000
6	-0.367426000	2.769966000	1.554937000
8	0.083273000	2.003030000	0.446485000
6	-0.752409000	1.811660000	2.694192000
6	-1.574175000	3.617503000	1.117902000
6	0.801843000	3.672550000	1.983759000
1	0.486575000	3.005459000	-1.702352000
1	0.521619000	4.291245000	2.844163000
1	-1.938721000	4.228655000	1.951640000

1	-1.065790000	2.373896000	3.581604000
1	-1.294261000	4.291237000	0.299805000
1	-2.387264000	2.973118000	0.772305000
1	-1.575337000	1.159950000	2.387572000
1	0.103832000	1.185597000	2.967317000
1	1.670584000	3.065983000	2.259868000
1	1.094274000	4.337285000	1.163295000
8	3.721229000	-2.616222000	1.432618000
8	-6.176097000	-1.560258000	-0.034519000
6	-6.820465000	-0.407424000	-0.566208000
1	-6.673292000	0.465755000	0.081265000
1	-6.457491000	-0.179466000	-1.575643000
1	-7.882096000	-0.654899000	-0.607190000