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Electronic Supplementary Information (ESI)

Oxidoperoxidomolybdenum(VI) complexes with acylpyrazolonate ligands: synthesis, structure and catalytic properties

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Table S1. Crystal data and structure refinement for compounds **1**, **2**, **9**, **10** and **12**.

Table S2. Selected structural parameters of $[Mo(O_2)_2(Q^{C6})_2]$, **12**.

Figure S1. Comparison of the relative orientations of the hexyl groups in the two polymorphs of $[Mo(O)_2(Q^{C6})_2]$, **12**.

Figure S2. Optimized structures of the isomers **A** and **B**, respectively, of the anion of complex $Ph_4P[Mo(O)(O_2)_2(Q^{nPe})]$, **1**.

Figure S3. Optimized structures of the isomers **A** and **B**, respectively, of the anion of complex $Ph_4P[Mo(O)(O_2)_2(Q^{C2F5})]$, **2**.

Table S3. Comparison between selected experimental and theoretical structural parameters of the anions of compounds $Ph_4P[Mo(O)(O_2)_2(Q^{nPe})]$, **1**, and $Ph_4P[Mo(O)(O_2)_2(Q^{C2F5})]$, **2**.

Table S4. Comparison between selected experimental and theoretical structural parameters of compounds $[MoO(O_2)(Q^{nPe})_2]$, **9**, and $[MoO(O_2)(Q^{C6})_2]$, **10**.

Figure S4 Optimised structures of the four isomers of complex $[MoO(O_2)(Q^{nPe})_2]$, **9**.

Figure S5 Optimised structures of the four isomers of complex $[MoO(O_2)(Q^{C6})_2]$, **10**.

Figure S6 Isomerisation of complex $[MoO(O_2)(Q^{C6})_2]$, **10**, followed by ^1H NMR ($CDCl_3$): blue line, room temperature (isomer **C**); red line, after heating at 50 ºC for 24h (mixture of isomers **C** and **D**).

Table S5. Coordinates of the calculated compounds.

Table S1. Crystal data and structure refinement for compounds **1**, **2**, **9**, **10** and **12**.

	1	**2**	**9**	**10**	**12**
Formula	$C_{40}H_{39}MoN_2O_7P$	$C_{37}H_{28}F_5MoN_2O_7P$	$C_{32}H_{38}MoN_4O_7$	$C_{34}H_{42}MoN_4O_7$	$C_{34}H_{42}MoN_4O_6$
M	786.64	834.52	686.60	714.65	698.66
T [K]	193(2) K	193(2)	213(2)	193(2)	193(2)
Wavelength [Å]	0.71073 Å	0.71073 Å	0.71073	0.71073	0.71073
Crystal system	Triclinic	Triclinic	Triclinic	Orthorhombic	Orthorhombic
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	Aba2	Aba2
a [Å]	10.5112(6)	10.1318(4)	9.0124(4)	9.7458(2)	9.5954(8)
b [Å]	13.1936(7)	13.3189(6)	13.5773(7)	20.3853(4)	20.5989(14)
c [Å]	13.8181(8)	13.8696(6)	13.8352(7)	17.2757(3)	17.1471(14)
α [°]	89.653(2)	88.5380(10)	78.094(2)	90	90
β [°]	87.507(2)	84.4170(10)	73.696(2)	90	90
γ [°]	71.931(2)	71.8310(10)	82.144(2)	90	90
V [Å^3]	1820.02(18)	1769.85(13)	1584.30(13)	3432.18(11)	3389.2(5)
Z	2	2	2	4	4
$D_{calcd.}$ [Mg·m^{-3}]	1.435	1.566	1.439	1.383	1.369
μ [mm^{-1}]	0.457	0.495	0.467	0.434	0.436
F(000)	812	844	712	1488	1456
Crystal size [mm^3]	0.50 x 0.40 x 0.30	0.50 x 0.40 x 0.20	0.50 x 0.50 x 0.40	0.40 x 0.30 x 0.20	0.40 x 0.30 x 0.20
Theta range for data collection [°]	1.48 to 25.25	1.61 to 25.25	2.36 to 25.25	2.36 to 25.25	2.38 to 25.25

Index ranges	-12≤h≤12, -15≤k≤15, -16≤l≤16	-12≤h≤11, -15≤k≤15, -14≤l≤16	-9≤h≤10, -12≤k≤16, -16≤l≤16	-11≤h≤11, -23≤k≤24, -20≤l≤9	-11≤h≤11, -24≤k≤24, -20≤l≤20
Reflections collected	30917	29875	29597	11966	16514
Independent reflections	6498 [R(int) = 0.0300]	6358 [R(int) = 0.0308]	5709 [R(int) = 0.0254]	2157 [R(int) = 0.0240]	3066 [R(int) = 0.0910]
Completeness to theta = 25.25° %	98.7	99.2	99.3	99.8 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.8750 and 0.8036	0.9075 and 0.7900	0.8352 and 0.8001	0.9182 and 0.8456	0.9179 and 0.8450
Refinement method	Full-matrix least-squares on F^2	Full-matrix-block least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2	Full-matrix least-squares on F^2
Data / restraints / parameters	6498 / 0 / 464	6358 / 62 / 479	5709 / 106 / 433	2157 / 54 / 224	3066 / 1 / 206
Goodness-of-fit on F^2	1.055	1.044	1.058	1.168	1.084
Final *R* indices [$I>2\sigma(I)$]	R1 = 0.0265, wR2 = 0.0730	R1 = 0.0292, wR2 = 0.0787	R1 = 0.0288, wR2 = 0.0731	R1 = 0.0231, wR2 = 0.0510	R1 = 0.0448, wR2 = 0.1012
R indices (all data)	R1 = 0.0285, wR2 = 0.0743	R1 = 0.0310, wR2 = 0.0801	R1 = 0.0331, wR2 = 0.0749	R1 = 0.0239, wR2 = 0.0512	R1 = 0.0500, wR2 = 0.1050
Largest diff. peak and hole [e·Å^{-3}]	0.813 and -0.831	0.935 and -0.716	0.614 and -0.598	0.242 and -0.293	1.081 and -0.816

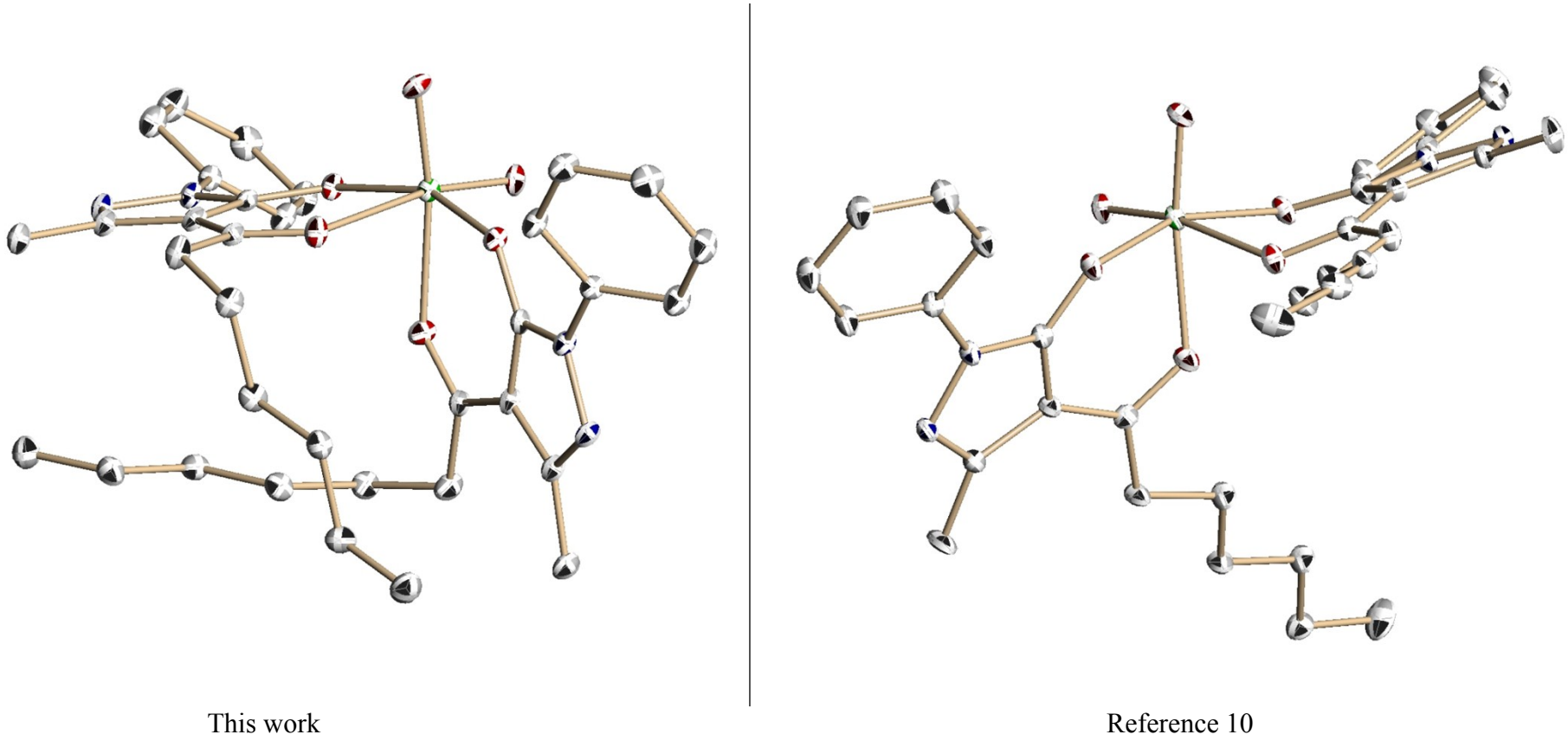
Table S2. Selected structural parameters of $[Mo(O)_2(Q^{C6})_2]$, **12**.

Mo(1)-O(3)	1.686(3)	C(3)-C(11)	1.496(6)
Mo(1)-O(1)	2.012(2)	C(4)-C(5)	1.505(6)
Mo(1)-O(2)	2.192(3)	C(5)-C(6)	1.522(6)
O(1)-C(1)	1.305(5)	C(6)-C(7)	1.520(6)
O(2)-C(4)	1.260(5)	C(7)-C(8)	1.522(6)
N(1)-C(1)	1.337(5)	C(8)-C(9)	1.513(6)
N(1)-N(2)	1.399(4)	C(12)-C(13)	1.382(6)
N(1)-C(12)	1.428(6)	C(12)-C(17)	1.388(6)
N(2)-C(3)	1.322(5)	C(13)-C(14)	1.398(6)
C(1)-C(2)	1.396(6)	C(14)-C(15)	1.379(6)
C(2)-C(3)	1.421(6)	C(15)-C(16)	1.373(7)
C(2)-C(4)	1.425(6)	C(16)-C(17)	1.389(6)

O(3)-Mo(1)-O(3)#1	103.7(2)	C(1)-C(2)-C(4)	121.8(4)
O(3)-Mo(1)-O(1)#1	95.37(12)	C(3)-C(2)-C(4)	132.7(4)
O(3)-Mo(1)-O(1)	99.36(13)	N(2)-C(3)-C(2)	110.9(4)
O(3)#1-Mo(1)-O(1)	95.37(12)	N(2)-C(3)-C(11)	118.5(4)
O(1)#1-Mo(1)-O(1)	156.07(15)	C(2)-C(3)-C(11)	130.6(4)
O(3)-Mo(1)-O(2)#1	168.27(14)	O(2)-C(4)-C(2)	119.6(4)
O(1)-Mo(1)-O(2)#1	79.68(11)	O(2)-C(4)-C(5)	117.2(4)
O(3)-Mo(1)-O(2)	88.04(14)	C(2)-C(4)-C(5)	123.2(4)
O(3)#1-Mo(1)-O(2)	168.27(14)	C(4)-C(5)-C(6)	113.2(3)
O(1)#1-Mo(1)-O(2)	79.68(11)	C(7)-C(6)-C(5)	112.3(4)
O(1)-Mo(1)-O(2)	82.08(10)	C(6)-C(7)-C(8)	114.4(3)
O(2)#1-Mo(1)-O(2)	80.23(17)	C(9)-C(8)-C(7)	112.9(4)
C(1)-O(1)-Mo(1)	129.0(2)	C(8)-C(9)-C(10)	113.6(4)
C(4)-O(2)-Mo(1)	135.0(3)	C(13)-C(12)-C(17)	121.4(4)
C(1)-N(1)-N(2)	111.8(3)	C(13)-C(12)-N(1)	120.0(4)
C(1)-N(1)-C(12)	129.5(3)	C(17)-C(12)-N(1)	118.6(4)
N(2)-N(1)-C(12)	118.7(3)	C(12)-C(13)-C(14)	119.6(4)
C(3)-N(2)-N(1)	105.1(3)	C(15)-C(14)-C(13)	119.1(4)
O(1)-C(1)-N(1)	121.6(4)	C(16)-C(15)-C(14)	120.8(4)
O(1)-C(1)-C(2)	131.6(4)	C(15)-C(16)-C(17)	121.0(4)
N(1)-C(1)-C(2)	106.8(3)	C(12)-C(17)-C(16)	118.1(5)
C(1)-C(2)-C(3)	105.4(4)		

Symmetry transformations used to generate equivalent atoms: #1 -x, -y, z.

Figure S1. Comparison of the relative orientations of the hexyl groups in the two polymorphs of $[Mo(O)_2(Q^{C6})_2]$, **12**. ORTEP diagrams drawing with ellipsoid probability at 30% label. Hydrogen atoms omitted and without label for clarity.



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Reference 10

Figure S2. Optimized structures of the isomers **A** and **B**, respectively, of the anion of complex $Ph_4P[Mo(O)(O_2)_2(Q^{nPe})]$, **1**.

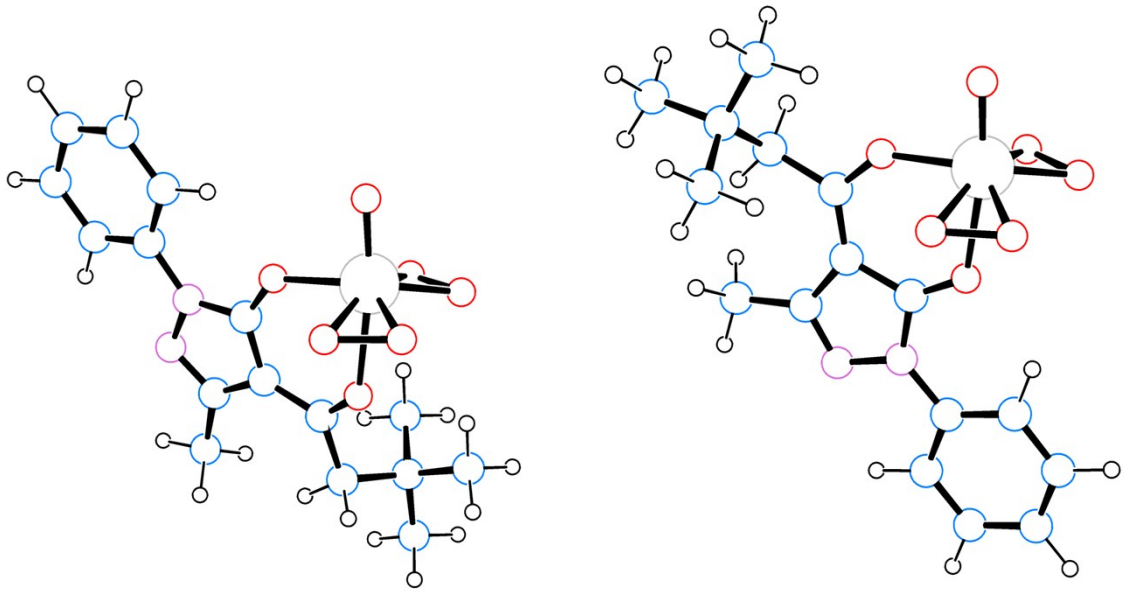


Figure S3. Optimized structures of the isomers **A** and **B**, respectively, of the anion of complex $Ph_4P[Mo(O)(O_2)_2(Q^{C2F5})]$, **2**.

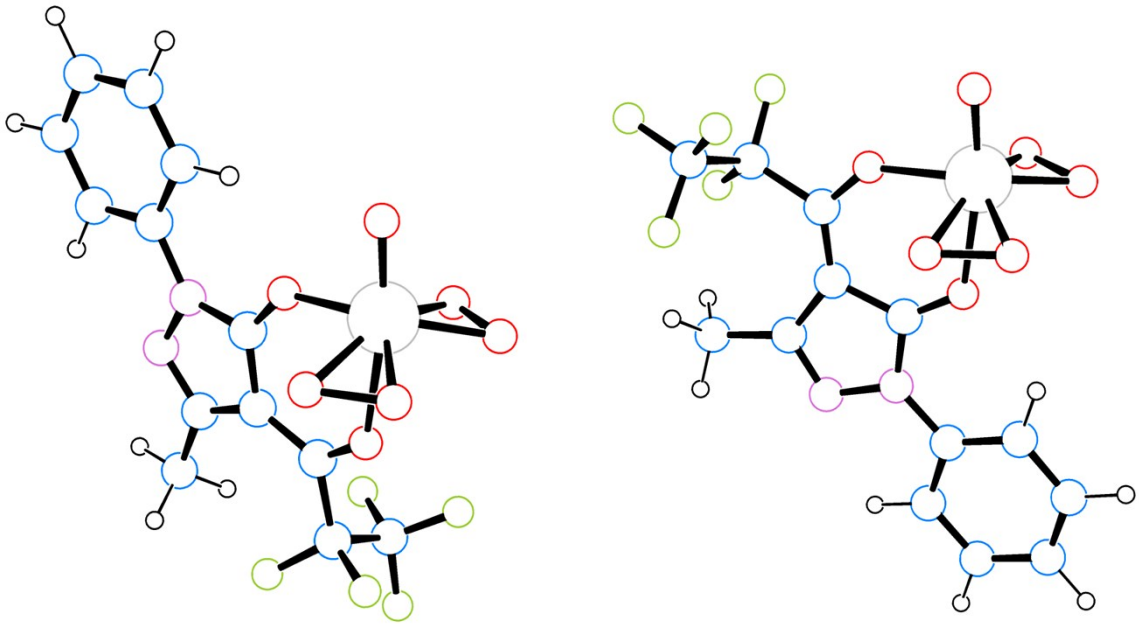


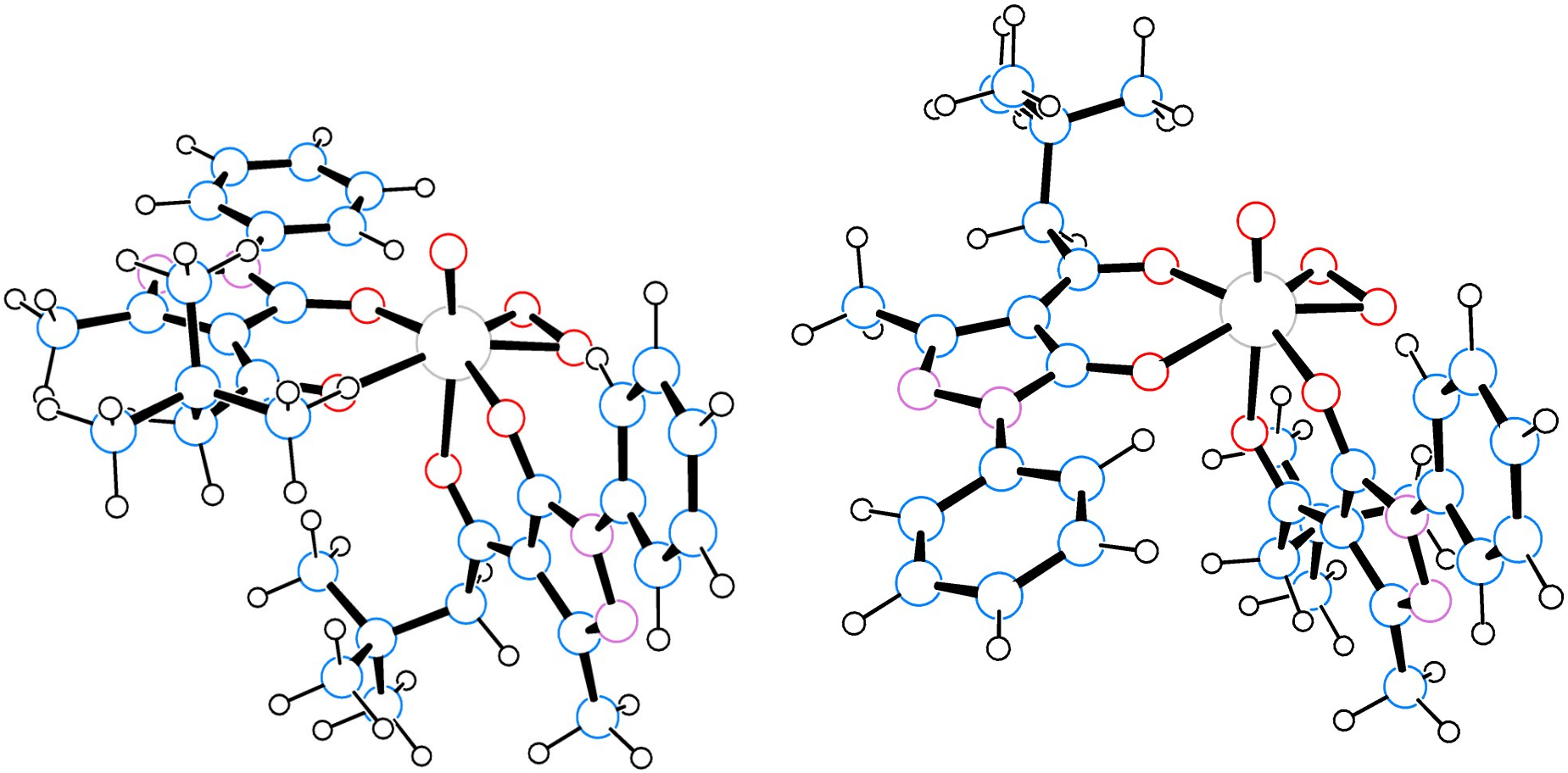
Table S3. Comparison between selected experimental and theoretical structural parameters of the anions of compounds $Ph_4P[Mo(O)(O_2)_2(Q^{nPe})]$, **1**, and $Ph_4P[Mo(O)(O_2)_2(Q^{C2F5})]$, **2**.

Bond distances (Å) and angles (º)	$[Mo(O)(O_2)_2(Q^{nPe})]^-$		$[Mo(O)(O_2)_2(Q^{C2F5})]^-$	
	X-ray	**Calculated**	**X-ray**	**Calculated**
Mo=O	1.686(1)	1.706	1.680(1)	1.704
Mo-O (peroxido)	1.952(1) 1.918(1) 1.921(1) 1.951(1)	1.983 1.973 1.957 1.962	1.904(2) 1.909(2) 1.942(2) 1.947(2)	1.969 1.969 1.958 1.957
Mo-O (Q^R) (*trans* oxido)	2.278(1)	2.422	2.325(2)	2.499
Mo-O (Q^R) (*cis* oxido)	2.081(1)	2.127	2.063(1)	2.127
C=O	1.251(2)	1.240	1.236(3)	1.229
C-O	1.296(2)	1.273	1.288(2)	1.268
O=Mo-O (peroxido)	102.64(7) 102.21(6) 101.27(7) 99.77(7)	103.7 103.5 104.4 104.5	102.84(7) 102.94(7) 101.23(8) 101.31(7)	104.7 104.8 105.0 105.1
O=Mo-O (*trans*)	169.37(6)	171.0	171.30(6)	169.6
O=Mo-O (*cis*)	88.99(6)	93.8	92.21(6)	94.7

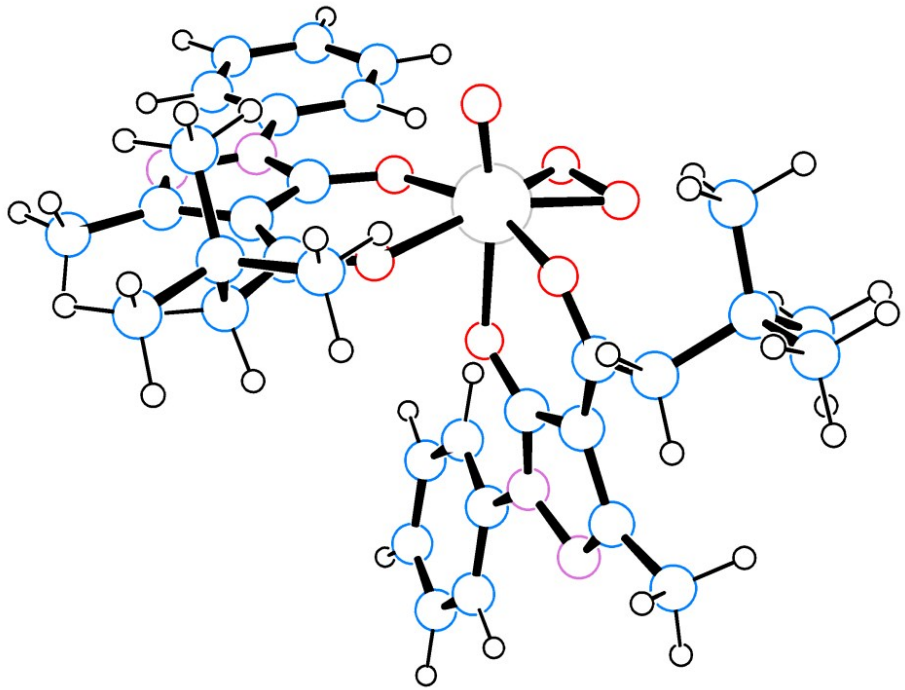
Table S4. Comparison between selected experimental and theoretical structural parameters of compounds $[MoO(O_2)(Q^{nPe})_2]$, **9**, and $[MoO(O_2)(Q^{C6})_2]$, **10**.

Bond distances (Å) and angles (º)	**9**		**10**	
	X-ray	**Isomer C Calculated**	**X-ray**	**Isomer C Calculated**
Mo=O	1.684(2)	1.700	1.687(8)	1.699
Mo-O (peroxido)	1.908(2) 1.912(2)	1.953 1.964	1.885(8) 1.915(5)	1.952 1.962
Mo-O (Q^R) (*trans* oxido)	2.150(2)	2.183	2.138(2)	2.186
Mo-O (Q^R) (*trans* peroxido)	2.121(2)	2.134	2.138(2)	2.138
Mo-O (Q^R) (*cis* oxido)	2.027(2) 2.028(2)	2.073 2.096	2.0380(19)	2.077 2.100
C=O	1.266(3) 1.277(3)	1.273 1.282	1.275(4)	1.272 1.280
C-O	1.289(3) 1.292(4)	1.267 1.282	1.299(4)	1.282 1.267
O=Mo-O (peroxido)	102.16(15) 100.73(13)	102.7 103.5	103.2(2) 102.4(3)	102.9 103.8
O=Mo-O (*trans*)	166.08(11)	166.4	170.5(3)	166.1
O=Mo-O (*cis*)	98.20(11) 89.96(11) 91.50(11)	88.9 92.1 97.4	103.4(2) 90.4(3)	88.89 92.1 97.1

Figure S4 Optimised structures of the four isomers of complex $[MoO(O_2)(Q^{nPe})_2]$, **9**.



C **D**



E

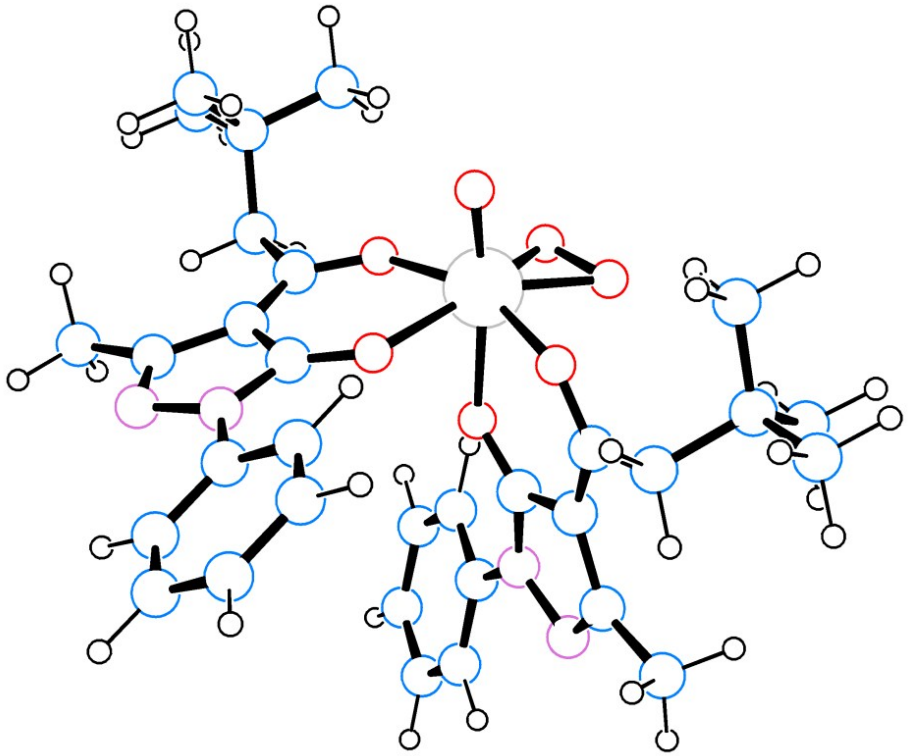


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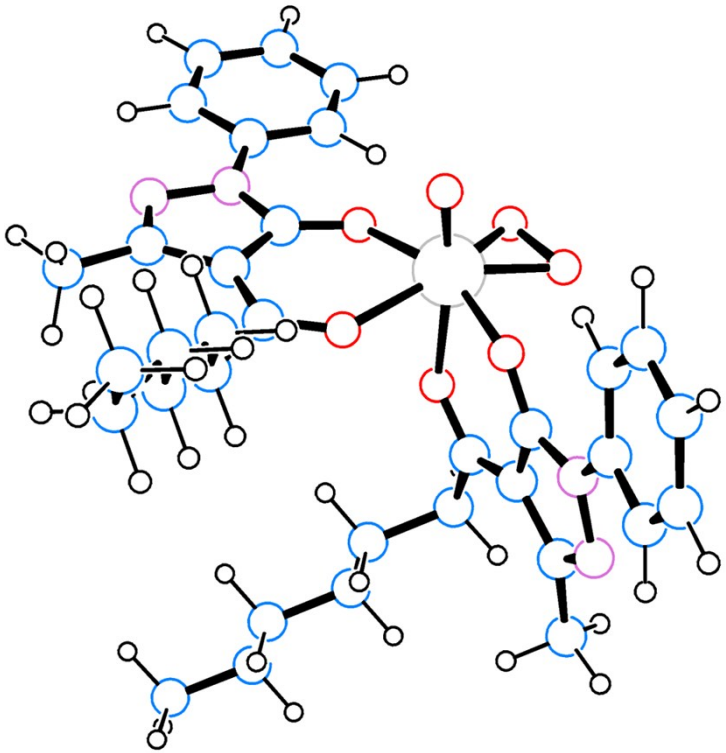
Figure S5 Optimised structures of the four isomers of complex $[MoO(O_2)(Q^{C6})_2]$, **10**.



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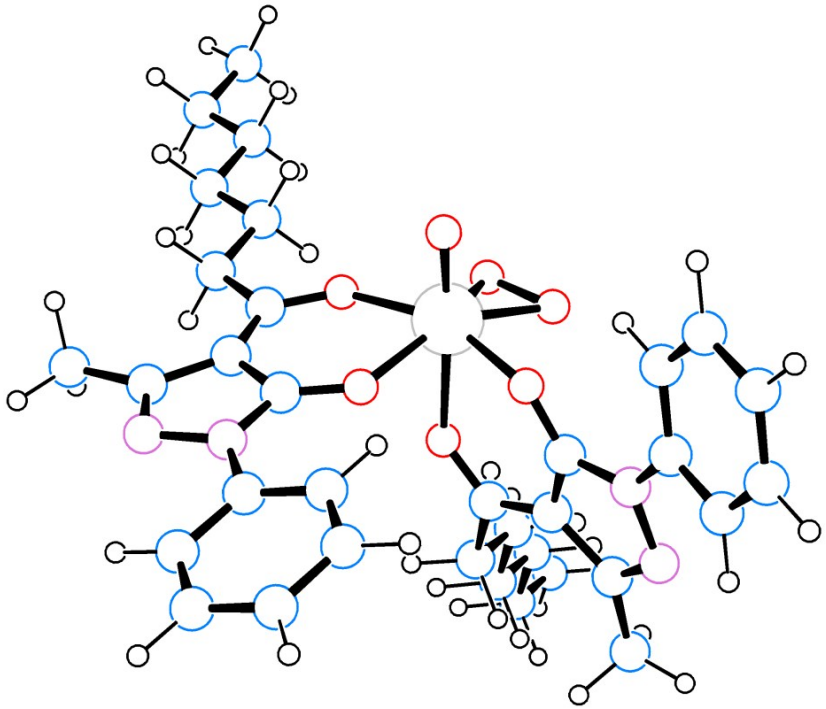

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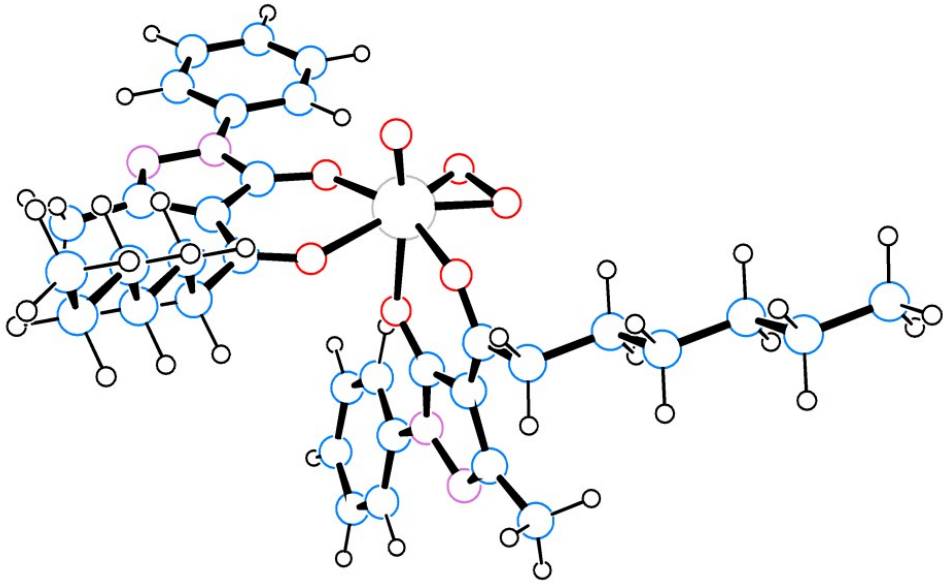

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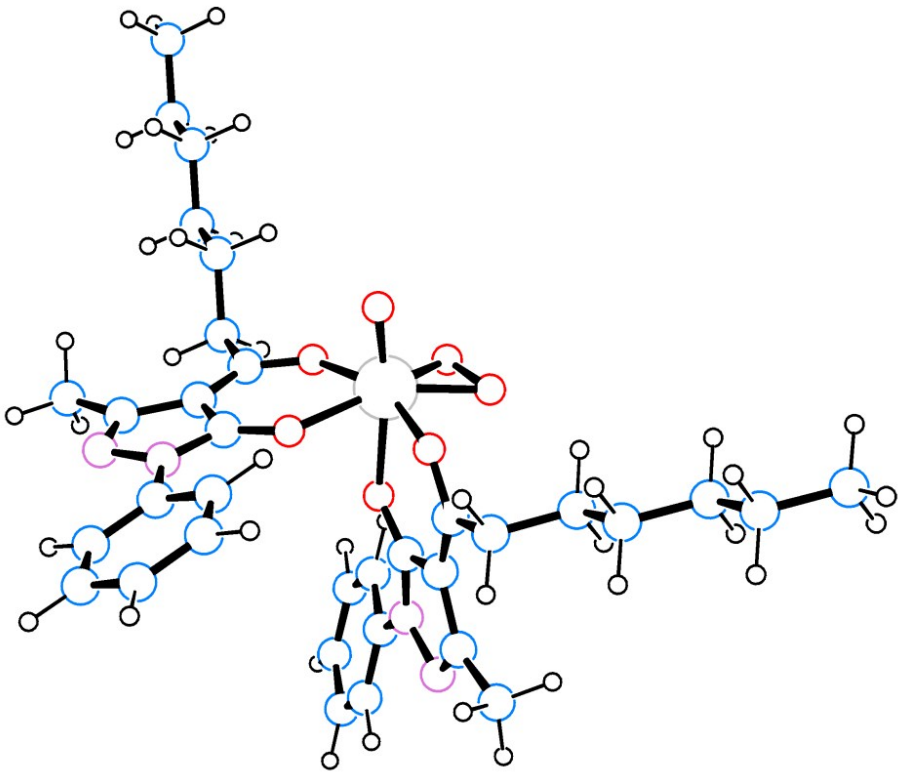

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Figure S6 Isomerisation of complex $[MoO(O_2)(Q^{C6})_2]$, **10**, followed by ^1H NMR ($CDCl_3$): blue line, room temperature (isomer **C**); red line, after heating at 50 ºC for 24h (mixture of isomers **C** and **D**).

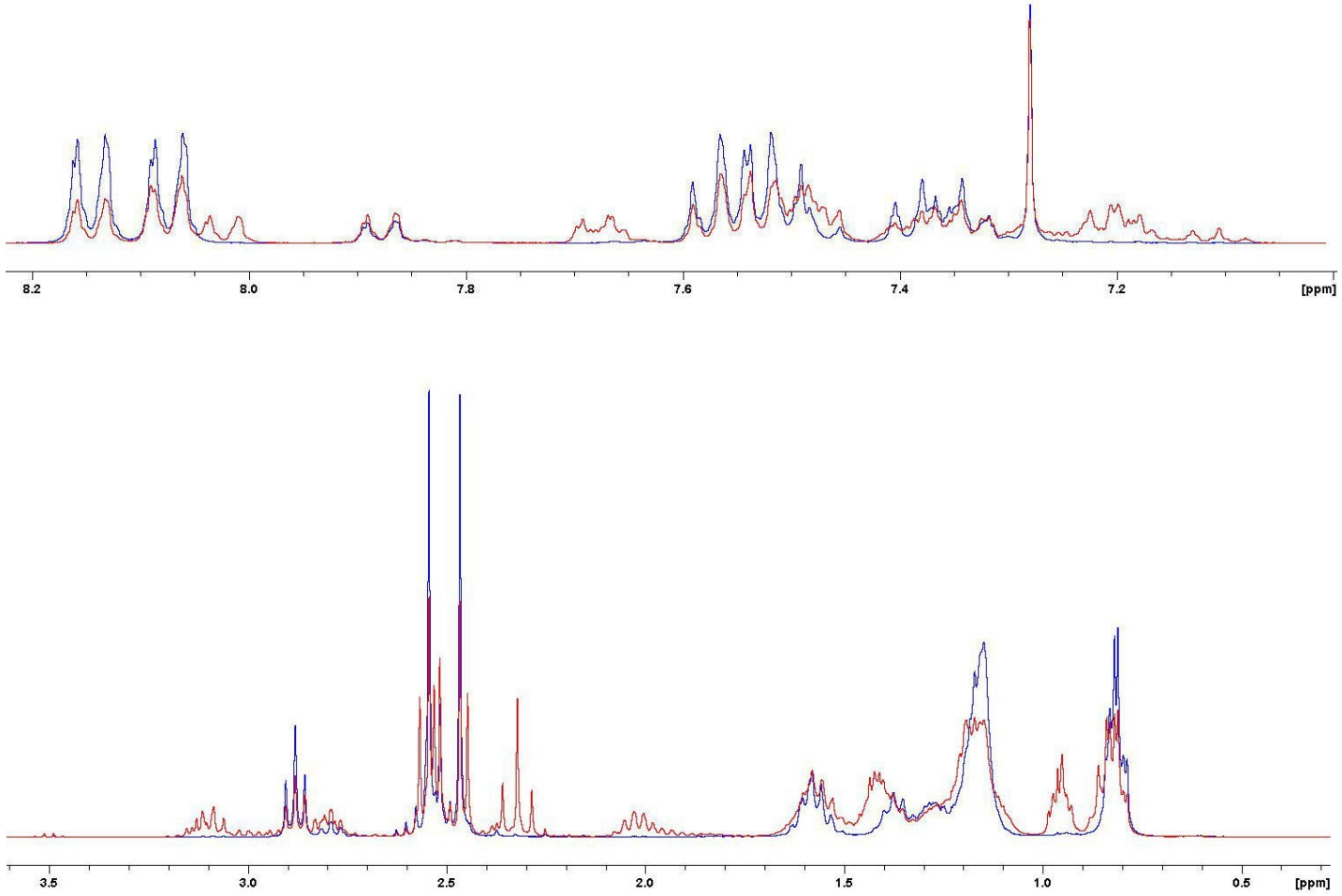

Table S5. Coordinates of the calculated compounds.

Isomer **A** of the anion of complex $Ph_4P[Mo(O)(O_2)_2(Q^{nPe})]$, **1**.

Mo	0.55977900	-2.21768300	-0.00611000
C	0.10041000	4.09002500	-0.69638800
H	-0.71205100	4.81750000	-0.65881400
H	0.59918400	4.17847600	-1.66603200
H	0.82994300	4.34561800	0.07715600
O	-0.96930200	-0.74324400	-0.11778000
O	1.77503900	-0.23427700	-0.68195000
O	-0.50816000	-3.45110500	0.49257100
O	1.11979400	-1.37521600	1.69896300
O	2.07655000	-2.34895300	1.23196800
O	1.63621100	-3.04634200	-1.41466600
O	0.51555700	-2.33150300	-1.97541800
N	-1.77922900	2.64322000	-0.31592300
N	-2.07513500	1.29798900	-0.16029100
C	-0.93570800	0.52296600	-0.24391200
C	0.14280900	1.42770300	-0.46391600
C	-0.47936300	2.72205600	-0.49057800
C	1.49555900	0.97314800	-0.64806100
C	2.65733400	1.94288000	-0.79933700
H	2.30036700	2.96474100	-0.91737600
H	3.17904500	1.66733300	-1.72246300
C	3.68572200	1.90504400	0.37737400
C	4.49274700	0.59365700	0.37235700
H	5.02689600	0.46856800	-0.57566000
H	3.85112600	-0.27642400	0.51097200
H	5.23512700	0.61223900	1.17854300
C	2.96316700	2.05451600	1.73000300
H	2.30815800	1.20201700	1.92604500
H	2.36041100	2.96868700	1.76445100
H	3.69398800	2.10679200	2.54403800
C	4.65021100	3.09026100	0.17790300
H	5.41854300	3.09583500	0.95816400
H	4.12202600	4.04916800	0.22008600
H	5.15852300	3.02742700	-0.79035600
C	-3.41937700	0.91023000	0.05190600
C	-3.78793200	-0.43493600	0.20505100
H	-3.03509100	-1.20603800	0.16506500
C	-5.12637400	-0.76109100	0.41041100
H	-5.39375300	-1.80571000	0.52816700
C	-6.11045100	0.22349100	0.46608500
H	-7.14921200	-0.04368400	0.62674500
C	-5.73720800	1.55841300	0.31266900
H	-6.48702700	2.34193100	0.35286500
C	-4.40661100	1.90607700	0.10706100
H	-4.11148500	2.93826300	-0.01273700

Isomer **B** of the anion of complex $Ph_4P[Mo(O)(O_2)_2(Q^{nPe})]$, **1**.

Mo	0.98577700	-2.15187000	-0.05008200
C	-0.00851200	4.08246900	-0.56506500
H	-0.82801100	4.79831400	-0.48424800
H	0.47040500	4.21574200	-1.54008500
H	0.73307000	4.31514500	0.20438800
O	-0.99987400	-0.77419400	-0.13139700
O	1.76847700	-0.22430300	-0.51134100

O	2.52063200	-2.90144900	-0.04089700
O	0.41467700	-2.31919900	-1.93365700
O	-0.13734800	-3.36069600	-1.10289300
O	0.14410300	-2.77383800	1.60618800
O	0.80082800	-1.50775500	1.81111800
N	-1.86433600	2.59897100	-0.24629300
N	-2.16069600	1.24629000	-0.12473400
C	-1.01257100	0.46021800	-0.20531700
C	0.07343300	1.40748600	-0.39372300
C	-0.57104700	2.70155400	-0.40413600
C	1.40455600	0.99629400	-0.54907800
C	2.54196000	1.96764600	-0.80025700
H	2.15111500	2.97216300	-0.94656800
H	3.01012700	1.66215700	-1.74325600
C	3.65022000	2.01927900	0.30019800
C	4.52492500	0.75222200	0.28020300
H	4.99547100	0.61907200	-0.69949800
H	3.94479100	-0.14517000	0.49030800
H	5.32137000	0.83662000	1.02796700
C	3.02268500	2.19297300	1.69584100
H	2.40311500	1.33503700	1.96705300
H	2.39782300	3.09083800	1.74631200
H	3.80686600	2.29044100	2.45375800
C	4.53971400	3.23918700	-0.01243100
H	5.36295900	3.31005400	0.70607800
H	3.97091100	4.17390900	0.03590200
H	4.97728400	3.16244700	-1.01351800
C	-3.50184900	0.84479200	0.04429700
C	-3.84901100	-0.51007300	0.17222500
H	-3.07646200	-1.26347600	0.14372900
C	-5.18653200	-0.86178300	0.33342600
H	-5.43872500	-1.91241500	0.43056500
C	-6.19077700	0.10421200	0.37195100
H	-7.22876000	-0.18393000	0.49831400
C	-5.83822300	1.44755900	0.24627900
H	-6.60363500	2.21664200	0.27435200
C	-4.50865000	1.82226600	0.08343700
H	-4.23101500	2.86177700	-0.01500800

Isomer **A** of the anion of complex $Ph_4P[Mo(O)(O_2)_2(Q^{C2F5})]$, **2**.

Mo	0.17337800	2.51551000	-0.01475800
C	-0.77314000	-3.87666900	-0.59402700
H	-0.10517700	-4.73016400	-0.47084600
H	-1.21490700	-3.91726100	-1.59133500
H	-1.58471500	-3.95616700	0.12981100
O	1.23034000	0.66966600	-0.01495200
O	-1.58215700	0.76059800	-0.29963500
O	1.56768200	3.47396200	0.18875000
O	-0.40360300	2.07523800	1.81510500
O	-1.11460200	3.21189500	1.28502800
O	-0.82714100	3.37380200	-1.46124300
O	-0.00720700	2.29976800	-1.96369300
N	1.33133900	-2.79637000	-0.26423800
N	1.89445500	-1.54081100	-0.10888000
C	0.93568800	-0.55635900	-0.14440900
C	-0.31840300	-1.22924900	-0.33849400
C	0.03853500	-2.63021600	-0.40153400
C	-1.52235000	-0.46312200	-0.39480800
C	-2.93332000	-1.11310800	-0.55847000
C	-3.62260200	-1.46601500	0.79034200

C	3.29882200	-1.43332100	0.05284400
C	3.93223400	-0.19709400	0.24668600
H	3.35086000	0.71030800	0.27711400
C	5.31631500	-0.15250100	0.39765000
H	5.79107400	0.81124600	0.54612800
C	6.08521900	-1.31325300	0.36096700
H	7.16207100	-1.26463200	0.47946900
C	5.44830800	-2.53868400	0.16891700
H	6.02789700	-3.45540700	0.13671300
C	4.06798300	-2.60588200	0.01504400
H	3.56910100	-3.55215100	-0.13453000
F	-3.75465100	-0.24918200	-1.19637200
F	-2.90267900	-2.25594800	-1.30651800
F	-2.87522600	-2.33996400	1.49268500
F	-3.81179000	-0.37926500	1.53577700
F	-4.82064100	-2.04270000	0.56998200

Isomer **B** of the anion of complex $Ph_4P[Mo(O)(O_2)_2(Q^{C2F5})]$, **2**.

Mo	-0.50829800	2.44356100	0.01403700
C	-0.36939100	-3.96179700	-0.18774600
H	0.35879300	-4.73157400	0.07087500
H	-0.79977100	-4.19917600	-1.16235700
H	-1.17808800	-3.97966700	0.54414400
O	1.23040800	0.76673300	-0.23164100
O	-1.56345500	0.61523800	-0.41676500
O	-1.91485000	3.39611900	0.13738000
O	-0.04127700	2.56326000	-1.90004100
O	0.70589300	3.49746500	-1.09796100
O	0.53640500	2.90233000	1.60363500
O	-0.27665100	1.73982100	1.84736400
N	1.64220500	-2.67981200	-0.07890900
N	2.11739600	-1.37587800	-0.08788300
C	1.08478200	-0.45700900	-0.20020200
C	-0.13225600	-1.26992200	-0.29165500
C	0.34429900	-2.64310600	-0.20182500
C	-1.36145700	-0.63245400	-0.43673000
C	-2.70318300	-1.37885000	-0.64886900
C	-3.51111900	-1.60926000	0.66243600
C	3.50727100	-1.14392400	0.01685700
C	4.02555000	0.15694800	0.11154600
H	3.35579200	1.00323900	0.10277700
C	5.40249300	0.33802100	0.21218100
H	5.78922700	1.34883300	0.28401800
C	6.27639400	-0.74751000	0.22448700
H	7.34677800	-0.59214500	0.30387000
C	5.75293900	-2.03666100	0.13358800
H	6.41567700	-2.89594300	0.14256500
C	4.38108200	-2.24134500	0.03013100
H	3.97078900	-3.23847900	-0.03824700
F	-3.81720700	-0.45708200	1.25504400
F	-4.65647800	-2.26561300	0.39490500
F	-2.80353800	-2.36032000	1.52743400
F	-3.49986400	-0.65568200	-1.47206800
F	-2.53670200	-2.59922800	-1.23316200

Isomer **C** of complex $[MoO(O_2)(Q^{nPe})_2]$, **9**.

Mo	0.08117600	-0.03122600	-1.37390800
O	2.12589700	0.04789800	-0.99952200

O	0.10387800	-1.02239600	0.51683600
O	-1.94752600	-0.17326000	-0.93190500
O	-0.08797700	1.66877700	0.04054300
O	0.07538600	-1.53596700	-2.16076800
O	0.74707600	1.21291200	-2.71911100
O	-0.66596500	1.18370000	-2.71580600
N	4.16449800	-0.58524100	-0.08239500
N	4.63093600	-1.35856100	0.97378500
N	-4.06833100	0.65729400	-0.49622400
N	-4.65608200	1.76013800	0.10685000
C	3.58817200	-1.84067800	1.59808700
C	2.36466400	-1.40536200	0.96512400
C	2.80593600	-0.59443200	-0.12410000
C	3.81750100	-2.71081500	2.79410300
H	4.89126600	-2.84660000	2.92483000
H	3.35438200	-3.69336200	2.67524000
H	3.41562900	-2.25764000	3.70477500
C	0.99611500	-1.55942800	1.25117300
C	0.47948600	-2.32450900	2.44321900
H	-0.15630300	-1.63468400	3.00937800
H	1.31176900	-2.60131900	3.08731700
C	-0.35745700	-3.60905500	2.12423000
C	0.39878300	-4.51926000	1.13901800
H	1.38992900	-4.78923800	1.51698000
H	0.52492000	-4.04361900	0.16271200
H	-0.15740800	-5.44772300	0.98191500
C	-0.55204600	-4.35224400	3.46008400
H	-1.15857400	-5.25005300	3.31086600
H	-1.06559000	-3.72245300	4.19333900
H	0.40458200	-4.66295700	3.89220700
C	-1.73797300	-3.25026200	1.54768600
H	-2.32181600	-4.16181300	1.38750300
H	-1.66184900	-2.72201900	0.59803200
H	-2.29756700	-2.61328500	2.23987800
C	5.10916200	0.06521100	-0.93235800
C	4.69920500	0.88652600	-1.98936600
H	3.65128000	1.04573700	-2.18567600
C	5.66194900	1.49878400	-2.78845800
H	5.33572100	2.13175400	-3.60574300
C	7.02025900	1.30692700	-2.55044800
H	7.76031900	1.78823700	-3.17916000
C	7.41723300	0.48836600	-1.49455700
H	8.47078100	0.32811100	-1.29520000
C	6.47269500	-0.13310000	-0.68497600
H	6.77510900	-0.76822600	0.13445600
C	-3.68645900	2.54044100	0.51278500
C	-2.39626300	1.97268200	0.19752200
C	-2.71122800	0.74671300	-0.46523000
C	-4.05767400	3.83511500	1.16758900
H	-5.14506900	3.90992800	1.19448100
H	-3.66756900	4.69216200	0.61159800
H	-3.68201600	3.89952700	2.19181900
C	-1.06071200	2.36873300	0.45028100
C	-0.70468000	3.62521000	1.20977400
H	-1.58735900	4.25055900	1.32807800
H	0.00402600	4.17453200	0.58091400
C	-0.04873300	3.41633700	2.61514400
C	1.36647500	2.82422700	2.49068600
H	1.82040200	2.73036500	3.48225900
H	2.01085300	3.46918500	1.88618000
H	1.35376600	1.84018800	2.02202900

C	-0.91964500	2.49802400	3.49201100
H	-1.00539800	1.49480400	3.06543400
H	-1.93065400	2.89778400	3.61542200
H	-0.48048200	2.39957500	4.48915800
C	0.04942600	4.80539000	3.27452200
H	0.52791300	4.73111000	4.25558600
H	-0.93918500	5.25236700	3.41770300
H	0.64501200	5.49152700	2.66465500
C	-4.90119800	-0.37749500	-1.01116100
C	-6.23248700	-0.43632800	-0.58531500
H	-6.59437600	0.29896800	0.11900900
C	-7.07183900	-1.42770600	-1.08248300
H	-8.10253100	-1.46550900	-0.74826700
C	-6.59774300	-2.36436900	-1.99953300
H	-7.25501300	-3.13563800	-2.38411200
C	-5.27175900	-2.29633800	-2.42021200
H	-4.89087500	-3.01378000	-3.13815100
C	-4.41710900	-1.30896300	-1.93607600
H	-3.39303700	-1.26376100	-2.27217300

Isomer **D** of complex $[MoO(O_2)(Q^{nPe})_2]$, **9**.

Mo	-0.44435000	-0.60957100	-1.28127600
O	-0.49368500	1.08291400	-0.03329600
O	-2.48623000	-0.64408300	-0.78359600
O	1.56335400	-0.14605200	-1.07857900
O	-0.09495600	-1.51712300	0.72505400
O	-0.62208700	0.32046800	-2.69089000
O	-1.03493200	-2.38442200	-1.83200200
O	0.36601100	-2.26579800	-1.96159700
N	-1.39896200	2.76684100	1.28936500
N	-2.64531700	3.13224400	1.78868000
N	3.75047100	-0.40560600	-0.35626100
N	4.44733700	-1.02365300	0.67184400
C	-3.51348800	2.25733400	1.35480200
C	-2.86806900	1.25794400	0.53170700
C	-1.49027300	1.64232600	0.53154400
C	-4.94538600	2.41700600	1.75919700
H	-5.03534300	3.31108300	2.37640900
H	-5.29708200	1.55997300	2.34051300
H	-5.60140700	2.52657400	0.89228800
C	-3.30134000	0.11146500	-0.14665900
C	-4.73473600	-0.35274200	-0.17419500
H	-5.31559300	0.21696000	0.54907000
H	-4.73030800	-1.39752200	0.15422700
C	3.56857800	-1.65707600	1.40694900
C	2.23204500	-1.47727000	0.89104200
C	2.41497900	-0.64842600	-0.25666800
C	4.06884500	-2.41131100	2.60003800
H	5.15492700	-2.32220200	2.63493000
H	3.80957700	-3.47138400	2.54970000
H	3.66102100	-2.00876400	3.53155500
C	0.94892900	-1.88703600	1.33533800
C	0.73514900	-2.76223500	2.54613600
H	-0.00670800	-2.25665700	3.17345900
H	1.65372800	-2.84183500	3.12395000
C	-0.26020200	3.55914600	1.61740400
C	0.96177800	3.38366600	0.95785700
C	-0.38919900	4.53409200	2.61290200
C	2.04477700	4.18780000	1.30516400
H	1.06525700	2.63539200	0.18805300

C	0.70406100	5.32740100	2.94422300
H	-1.34101200	4.66377100	3.10709000
C	1.92622100	5.16005400	2.29516100
H	2.98726000	4.04807200	0.78829200
H	0.59547700	6.08122600	3.71580500
H	2.77484800	5.78137600	2.55666000
C	4.46837900	0.38262300	-1.30159900
C	5.79129900	0.73326400	-1.00809400
C	3.88553600	0.79206600	-2.50648700
C	6.52232900	1.49005800	-1.91746400
H	6.23101100	0.40155900	-0.07870800
C	4.63318200	1.55190100	-3.40304000
H	2.86804600	0.52230700	-2.74097300
C	5.94966900	1.90559900	-3.11852300
H	7.54692400	1.75507500	-1.68188800
H	4.17502100	1.86289700	-4.33499800
H	6.52322200	2.49518300	-3.82430900
C	0.21096100	-4.20689100	2.23988900
C	-1.23320600	-4.17840600	1.70799800
H	-1.30659100	-3.66033000	0.75165800
H	-1.59649100	-5.20186100	1.57078100
H	-1.90119100	-3.67764800	2.41618800
C	0.24017200	-4.98097300	3.57162100
H	-0.13933800	-5.99733300	3.43091800
H	1.25690600	-5.05618700	3.97010900
H	-0.38368400	-4.49420500	4.32793800
C	1.12236900	-4.91155800	1.21829300
H	1.11967100	-4.39973800	0.25259700
H	2.15664900	-4.96698300	1.57186000
H	0.77732800	-5.93579800	1.04945300
C	-5.45541800	-0.28093800	-1.56372900
C	-6.94153600	-0.59499700	-1.30371600
H	-7.50155100	-0.58784200	-2.24306800
H	-7.06459800	-1.58322400	-0.85004100
H	-7.39856200	0.14293300	-0.63681000
C	-4.89003700	-1.32156100	-2.54628500
H	-3.84091400	-1.14091500	-2.77922400
H	-4.96873200	-2.33328900	-2.13776400
H	-5.45675100	-1.29209300	-3.48199400
C	-5.33095700	1.12838200	-2.17008900
H	-5.89368300	1.18590400	-3.10603000
H	-5.72970000	1.89483700	-1.49831300
H	-4.29191500	1.38241100	-2.39623200

Isomer **E** of complex $[MoO(O_2)(Q^{nPe})_2]$, **9**.

Mo	-0.25255400	-0.54747100	-1.32975500
O	1.78187600	-0.25538400	-1.05901300
O	-0.06750600	-1.48364400	0.57912600
O	-0.46408500	1.14774200	0.03010000
O	-2.25951900	-0.83618300	-0.79848500
O	-0.15863500	-2.08252100	-2.05453800
O	0.22045400	0.67299100	-2.78008300
O	-1.17968500	0.51861000	-2.69364900
N	3.89501400	-0.55874600	-0.14595500
N	4.47094100	-1.17424400	0.95808600
N	-1.64429000	2.77648400	1.19752000
N	-2.95506200	3.02350500	1.59101500
C	3.50678100	-1.72996000	1.64464900
C	2.22920300	-1.50895200	1.00763600
C	2.54785600	-0.73926700	-0.15150300

C	3.86302900	-2.45322400	2.90566700
H	4.94634700	-2.42958600	3.02536100
H	3.53903700	-3.49642000	2.88127000
H	3.41087800	-1.98017000	3.78197500
C	0.89845300	-1.83397800	1.33032500
C	0.50641900	-2.58066300	2.58069800
H	-0.23122700	-1.95729100	3.09786300
H	1.36956000	-2.67383100	3.23669600
C	-3.68969800	2.04410000	1.13438200
C	-2.88332400	1.08685100	0.40486800
C	-1.54917000	1.61814900	0.48570900
C	-5.15819400	2.07426600	1.42566400
H	-5.38311300	2.98920300	1.97430000
H	-5.46653700	1.22182600	2.03789500
H	-5.75445000	2.06315300	0.51021400
C	-3.16721900	-0.12750500	-0.23524800
C	-4.54696600	-0.73313500	-0.30212100
H	-4.45927300	-1.75701100	0.07683900
H	-5.21721200	-0.19507300	0.36495900
C	4.73795800	0.12975700	-1.06962000
C	6.11964300	0.11664300	-0.84480900
C	4.21315100	0.80836800	-2.17603300
C	6.96754200	0.77885800	-1.72583200
H	6.51094400	-0.40887400	0.01364800
C	5.08035600	1.46438300	-3.04666500
H	3.15046800	0.82431000	-2.35588800
C	6.45582400	1.45617200	-2.83128500
H	8.03606800	0.76203900	-1.54326700
H	4.66557200	1.98566200	-3.90181200
H	7.12086600	1.96989300	-3.51569900
C	-0.61926100	3.68552500	1.58000900
C	-0.85510100	4.55235800	2.65220600
C	0.59852200	3.73045500	0.89239800
C	0.13064300	5.45531700	3.03679700
H	-1.80723400	4.51519000	3.16232000
C	1.57546800	4.63767800	1.29518000
H	0.77709700	3.06756300	0.05950200
C	1.35116100	5.50167600	2.36471200
H	-0.05927400	6.12484000	3.86814800
H	2.51668900	4.66923100	0.75820300
H	2.11686700	6.20604000	2.66851400
C	-5.19799100	-0.79418300	-1.72620200
C	-6.66295000	-1.22634400	-1.52170700
H	-7.21572200	-0.50059200	-0.91672200
H	-7.17251600	-1.31499500	-2.48538800
H	-6.72365400	-2.19845200	-1.02217800
C	-5.15969800	0.58773600	-2.40344800
H	-5.66007200	1.34934900	-1.79746700
H	-4.13481600	0.91946200	-2.58849900
H	-5.67199600	0.54727500	-3.36907200
C	-4.49332200	-1.82819300	-2.62241300
H	-3.45598900	-1.55895000	-2.81976400
H	-4.50028200	-2.82010700	-2.16035900
H	-5.01362300	-1.90161600	-3.58239900
C	-0.11550200	-4.00123700	2.36600300
C	-1.51905500	-3.91152500	1.74068000
H	-1.49607700	-3.46955000	0.74487400
H	-1.95412000	-4.91259500	1.66161200
H	-2.18502600	-3.30483800	2.36246900
C	-0.23016100	-4.64903100	3.75925900
H	-0.68475100	-5.64095600	3.68285900

H	0.75096800	-4.76677000	4.22962200
H	-0.85464200	-4.04706800	4.42681200
C	0.79522700	-4.86507500	1.47459400
H	0.88868400	-4.45040600	0.46743100
H	1.79996400	-4.96113900	1.89754500
H	0.38169600	-5.87294600	1.37768800

Isomer **F** of complex $[MoO(O_2)(Q^{nPe})_2]$, **9**.

Mo	0.08052400	-0.16305000	-1.73568800
O	0.34903300	-1.35567000	-0.01414000
O	2.09694600	0.28013200	-1.38489200
O	-0.26672100	1.30654400	-0.13483900
O	-1.87189800	-0.71536100	-1.26761000
O	0.34582400	-1.50658800	-2.74341500
O	0.42950100	1.34178200	-2.92888400
O	-0.94571600	1.03423300	-2.91250500
N	1.42717300	-2.21309100	1.85557800
N	2.67120700	-2.11792300	2.47188700
N	-1.57234900	2.54228900	1.33749700
N	-2.87833600	2.54354500	1.81569300
C	3.41062300	-1.33142100	1.73531000
C	2.67309500	-0.86250300	0.58123500
C	1.38200600	-1.46290900	0.72314700
C	4.80949500	-1.04649300	2.18412200
H	4.99225500	-1.58245700	3.11570400
H	4.96259800	0.02127900	2.36432200
H	5.54735300	-1.37229300	1.44696800
C	2.97445000	-0.03062200	-0.50424300
C	4.33050000	0.58423000	-0.73599600
H	4.94264500	0.46385500	0.15590300
C	-3.51416600	1.57550100	1.21179000
C	-2.64113800	0.87459100	0.29049700
C	-1.37471500	1.54733500	0.42617300
C	-4.95402500	1.35923700	1.56132100
H	-5.25031600	2.11680000	2.28730600
H	-5.11649000	0.37378000	2.00724700
H	-5.60370100	1.44439400	0.68704200
C	-2.82278200	-0.22348200	-0.55865800
C	-4.13473800	-0.95071800	-0.71362000
H	-3.92773800	-2.01331000	-0.54878000
H	4.16602800	1.65656100	-0.88353500
H	-4.82577300	-0.62958300	0.06252200
C	0.41336700	-3.01430900	2.45137000
C	0.51524800	-3.32503100	3.81086500
C	-0.65624800	-3.50219100	1.69362500
C	-0.45577600	-4.12204300	4.40809800
H	1.35513300	-2.94943300	4.37801400
C	-1.61934200	-4.29790400	2.30934300
H	-0.73049000	-3.26707500	0.64269500
C	-1.52819700	-4.61094500	3.66369800
H	-0.37095400	-4.36023300	5.46225900
H	-2.44274000	-4.68139600	1.71736500
H	-2.28154000	-5.23277600	4.13322100
C	-0.64805800	3.50058000	1.83392800
C	-0.90391200	4.10852300	3.06722200
C	0.48825000	3.85267700	1.09729500
C	-0.01914600	5.06116800	3.56194600
H	-1.79494000	3.83671500	3.61549800
C	1.36489600	4.80537600	1.61056300
H	0.67902200	3.38908600	0.14099100

C	1.12035600	5.41328700	2.84013500
H	-0.22446400	5.52935600	4.51803200
H	2.24110900	5.07964800	1.03373400
H	1.80640100	6.15686600	3.22906500
C	-4.83776900	-0.80068600	-2.10587600
C	-6.24274100	-1.41651900	-1.95791300
H	-6.83886700	-0.88368700	-1.21033700
H	-6.78101800	-1.37013400	-2.90891500
H	-6.18617100	-2.46781100	-1.65821400
C	-4.07451300	-1.55960200	-3.20620900
H	-3.07737800	-1.15115400	-3.36910100
H	-3.96582200	-2.61845300	-2.95211700
H	-4.62529100	-1.49613600	-4.14979600
C	-4.96745600	0.68299000	-2.49600700
H	-5.50841900	1.25509200	-1.73603300
H	-3.99019800	1.15032800	-2.64152100
H	-5.52087600	0.77699100	-3.43472000
C	5.13013700	0.03879400	-1.96784300
C	5.25693900	-1.49370300	-1.89915600
H	5.73642500	-1.81823300	-0.97043200
H	4.28292500	-1.98561300	-1.96714500
H	5.86751300	-1.85872800	-2.72987200
C	6.53415200	0.67001200	-1.89522900
H	7.14160000	0.34545200	-2.74482700
H	6.47892800	1.76253500	-1.92367000
H	7.05897500	0.38109100	-0.97915800
C	4.46873500	0.44718100	-3.29593200
H	3.47608800	0.01269900	-3.41353700
H	4.36360300	1.53362200	-3.36712600
H	5.08782100	0.11373000	-4.13448700

Isomer **C** of complex $[MoO(O_2)(Q^{C6})_2]$, **10**.

Mo	0.12431000	-0.35020300	-1.81967000
O	2.07914500	-0.87387700	-1.32823600
O	-0.18765900	-0.83562200	0.23380900
O	-1.84174400	0.27789300	-1.50854100
O	0.55341100	1.56873800	-0.79942500
O	-0.39259600	-1.90390700	-2.26676000
O	1.16385200	0.27063000	-3.34695000
O	-0.17568600	0.71077000	-3.43699000
N	3.78239700	-1.92488100	-0.14273500
N	3.95671200	-2.54737700	1.08854600
N	-3.58292400	1.76380500	-1.12561800
N	-3.76565000	3.06334300	-0.66917000
C	2.81431200	-2.48876300	1.72163500
C	1.81789800	-1.82066800	0.91998500
C	2.50417400	-1.48345700	-0.28487800
C	2.71634900	-3.09071700	3.08807600
H	3.66308300	-3.57548400	3.32706800
H	1.91876800	-3.83616900	3.14355800
H	2.51896900	-2.33023100	3.84911900
C	0.48102000	-1.44586600	1.12925100
C	-0.28659700	-1.73358800	2.39333300
H	-0.79383600	-0.80623700	2.67761200
H	0.38399000	-2.01265700	3.20487100
C	4.88892100	-1.84970900	-1.04123500
C	4.78651700	-1.19573200	-2.27485600
H	3.86076100	-0.73151600	-2.57439900
C	5.89637900	-1.15119200	-3.11533500
H	5.80803800	-0.64455800	-4.06955000

C	7.10102500	-1.74362700	-2.74601800
H	7.95769400	-1.70268900	-3.40864300
C	7.19237500	-2.39011700	-1.51460200
H	8.12280600	-2.85667800	-1.21131700
C	6.09626600	-2.44733400	-0.66082500
H	6.16159500	-2.94728800	0.29420600
C	-2.57907000	3.55443100	-0.41948500
C	-1.54705000	2.58426700	-0.69389500
C	-2.26092000	1.43493900	-1.15183300
C	-2.48151500	4.96246300	0.07924400
H	-3.48904200	5.36176200	0.19792300
H	-1.93969300	5.60087400	-0.62440900
H	-1.96993000	5.01638500	1.04393500
C	-0.14343400	2.59205500	-0.53542900
C	0.62490900	3.77956400	-0.00848600
H	0.05653500	4.70149600	-0.12473300
H	1.52848200	3.86186100	-0.61964900
C	-4.72648000	0.97872100	-1.45047500
C	-5.99051300	1.45992900	-1.08955000
H	-6.06782800	2.40840300	-0.57837000
C	-7.12551600	0.71881600	-1.40024200
H	-8.09987000	1.10094200	-1.11708300
C	-7.01800700	-0.50021600	-2.06773400
H	-7.90560700	-1.07379800	-2.30833900
C	-5.75700700	-0.97044000	-2.42537500
H	-5.65600300	-1.91382700	-2.94988000
C	-4.60816000	-0.24262900	-2.12429000
H	-3.63746600	-0.61765200	-2.40703400
C	-1.34060300	-2.83856900	2.16376600
H	-1.98237300	-2.54036300	1.33002600
H	-0.83571300	-3.76166700	1.85588700
C	-2.19190500	-3.10797100	3.40896400
H	-1.54150700	-3.39906000	4.24403800
H	-2.68694100	-2.17801400	3.71605200
C	-3.24896200	-4.19521800	3.18572000
H	-3.89610900	-3.90232200	2.34951900
H	-2.75392600	-5.12456200	2.87570400
C	-4.11458800	-4.47241100	4.42036400
H	-4.60646500	-3.54292600	4.73178800
H	-3.46877200	-4.76975900	5.25568100
C	-5.17257800	-5.55384700	4.18310000
H	-5.77301500	-5.72828300	5.08011500
H	-5.85514400	-5.26817900	3.37671100
H	-4.71008900	-6.50541500	3.90264400
C	1.02956400	3.58673900	1.46796400
H	1.57580700	2.64280800	1.56012300
H	0.12769700	3.49006300	2.08427700
C	1.89159200	4.73874000	1.99529700
H	1.34259100	5.68352900	1.89171300
H	2.78564000	4.83497800	1.36670800
C	2.31624700	4.55749700	3.45675400
H	2.86574700	3.61278800	3.55882000
H	1.42224300	4.45929700	4.08641700
C	3.18339900	5.70461800	3.98852000
H	2.63297000	6.64821000	3.89016600
H	4.07405000	5.80498500	3.35667700
C	3.61098500	5.51306600	5.44640100
H	4.19708000	4.59686300	5.56949100
H	4.22440200	6.34815400	5.79550200
H	2.74168500	5.44059900	6.10775400

Isomer **D** of complex $[MoO(O_2)(Q^{C6})_2]$, **10**.

Mo	0.07422700	-0.40355100	-1.41126500
O	-0.66389700	-1.61601600	0.13909500
O	1.91127200	-1.22209100	-0.76447100
O	-1.90679900	0.18017700	-1.28994500
O	0.24790100	0.94959000	0.37401800
O	-0.22625500	-1.57698800	-2.60020900
O	1.42301100	0.73726900	-2.23245800
O	0.13150400	1.26155800	-2.44965000
N	-0.62320200	-3.16944500	1.87625800
N	0.32014400	-3.93218700	2.55824300
N	-3.65436300	1.65242900	-0.88742700
N	-3.93674300	2.74948800	-0.08630300
C	1.48710700	-3.66801700	2.03064100
C	1.36095300	-2.70688900	0.96224600
C	-0.03334700	-2.41700500	0.90776700
C	2.70261600	-4.35646900	2.56440700
H	2.40923000	-5.00454400	3.39032600
H	3.44349600	-3.63972400	2.92874700
H	3.18529800	-4.96910600	1.79780700
C	2.27625000	-2.08066900	0.10398000
C	-2.85813800	2.99980700	0.61313400
C	-1.80629800	2.06414700	0.30031200
C	-2.38297900	1.21147600	-0.68559900
C	-2.87981600	4.15885600	1.56053100
H	-3.82854800	4.68403200	1.44762400
H	-2.06690600	4.86087900	1.35890900
H	-2.79145200	3.83143800	2.60053100
C	-0.49798900	1.87011500	0.81055000
C	0.10495900	2.75014300	1.87801900
H	0.67836500	2.09651800	2.54165300
H	-0.66453300	3.24171300	2.47212800
C	-1.99398200	-3.25717200	2.25590700
C	-3.00481100	-2.71016300	1.45729500
C	-2.31691500	-3.91327300	3.44894400
C	-4.33193400	-2.82612700	1.86413300
H	-2.76038000	-2.20468300	0.53630500
C	-3.64831300	-4.01953900	3.83671400
H	-1.52604300	-4.33662100	4.05094200
C	-4.66307900	-3.47722000	3.04985200
H	-5.10983600	-2.40234300	1.23937600
H	-3.89020400	-4.53066100	4.76173200
H	-5.69907900	-3.56305200	3.35638000
C	-4.67576100	1.12818200	-1.73060600
C	-6.00303200	1.48809000	-1.47294500
C	-4.37245000	0.28423900	-2.80455900
C	-7.01965600	1.00072100	-2.28741300
H	-6.21910400	2.15056700	-0.64705600
C	-5.40432900	-0.19673500	-3.60693900
H	-3.35036600	0.00660000	-3.00974400
C	-6.72853800	0.15484400	-3.35657100
H	-8.04530800	1.28572700	-2.08173500
H	-5.16186500	-0.84927300	-4.43792900
H	-7.52401000	-0.22336100	-3.98817000
C	3.76046000	-2.37081700	0.15544900
H	4.11406800	-2.10194400	1.15865900
H	3.89216800	-3.45608400	0.08078200
C	4.59715400	-1.65793100	-0.90887700
H	4.45731500	-0.57737300	-0.81882000
H	4.22525900	-1.92582500	-1.90222300

C	6.08573100	-2.00656700	-0.79764800
H	6.21525700	-3.09360400	-0.88358400
H	6.45148900	-1.73529600	0.20172200
C	6.95076200	-1.31213800	-1.85505100
H	6.82114100	-0.22554000	-1.77273100
H	6.58922100	-1.58511300	-2.85456800
C	8.44128500	-1.65355700	-1.74558900
H	8.56916600	-2.74004200	-1.82568500
H	8.80185000	-1.37803700	-0.74684900
C	9.30013500	-0.95980300	-2.80679000
H	9.21875700	0.12912600	-2.73169300
H	10.35636700	-1.22185300	-2.69965600
H	8.98799100	-1.24475600	-3.81637500
C	1.05187000	3.80073000	1.25788700
H	1.80599600	3.28096400	0.65915200
H	0.48893900	4.43475800	0.56327200
C	1.73250100	4.67462200	2.31632700
H	0.96823600	5.18429700	2.91736200
H	2.28829700	4.03251400	3.01155900
C	2.68365400	5.71680000	1.71733500
H	3.44606100	5.20676100	1.11483700
H	2.12777000	6.35856600	1.02178600
C	3.37349100	6.59251200	2.76954900
H	3.92919100	5.95094000	3.46429300
H	2.61109300	7.10258100	3.37110900
C	4.32240600	7.63040700	2.16322600
H	3.78850600	8.30978100	1.49138200
H	4.79872200	8.23705300	2.93837000
H	5.11628400	7.14957100	1.58307600

Isomer **E** of complex $[MoO(O_2)(Q^{C6})_2]$, **10**.

Mo	0.03083200	-0.28597000	-1.37942800
O	-2.04614000	-0.30046900	-1.33533300
O	-0.23997700	1.26300100	0.06905100
O	-0.13498700	-1.41193400	0.48757200
O	1.99142700	0.01100700	-0.68685400
O	0.20690300	0.90821800	-2.57494900
O	-0.42862200	-1.89192500	-2.38996600
O	0.96153000	-1.82710600	-2.15841900
N	-4.18723400	0.51624700	-0.94139500
N	-4.79081000	1.54289500	-0.22416000
N	0.68483800	-2.57350100	2.33248600
N	1.89759800	-2.74099100	2.99427100
C	-3.84150000	2.20210600	0.38722500
C	-2.54866000	1.63647700	0.08730700
C	-2.83678300	0.54535800	-0.78471700
C	-4.21447600	3.37192200	1.24226600
H	-5.28723900	3.54396100	1.15282000
H	-3.68859900	4.27981700	0.93585000
H	-3.98394400	3.18854100	2.29570900
C	-1.23690700	1.92444900	0.50069300
C	-0.88822600	3.02941300	1.46441500
H	-0.15551400	2.61866700	2.16569300
H	-1.76207100	3.33839800	2.03666900
C	2.78945600	-2.03351900	2.35258300
C	2.19741300	-1.35666100	1.21966500
C	0.81566600	-1.74691700	1.25567200
C	4.20119500	-2.04359600	2.84992600
H	4.27008300	-2.73243000	3.69220400
H	4.51597100	-1.05265400	3.19025100

H	4.90050700	-2.36947100	2.07552700
C	2.70855300	-0.48586900	0.24970000
C	4.15351100	-0.05958200	0.18788100
H	4.16295100	0.99668600	-0.09514400
H	4.63006800	-0.15169000	1.16329500
C	-5.00832900	-0.37019100	-1.70089000
C	-6.39008200	-0.14624200	-1.71750500
C	-4.46220600	-1.44284400	-2.41593700
C	-7.21680400	-0.99328700	-2.44734000
H	-6.79796700	0.68422000	-1.16051700
C	-5.30819900	-2.27836700	-3.14154300
H	-3.39917300	-1.62167900	-2.40873500
C	-6.68362300	-2.06338100	-3.16380200
H	-8.28553900	-0.81120600	-2.45382000
H	-4.87671400	-3.10522400	-3.69399500
H	-7.33192200	-2.72003900	-3.73226000
C	-0.47740000	-3.22268000	2.83300600
C	-0.48074900	-3.66897400	4.15873100
C	-1.59540400	-3.42931300	2.01735200
C	-1.60459500	-4.31387800	4.66468300
H	0.39695300	-3.51549300	4.77045900
C	-2.71332700	-4.07236200	2.54310800
H	-1.58881600	-3.09241500	0.99196200
C	-2.72725500	-4.51656600	3.86338200
H	-1.59990200	-4.65833300	5.69271900
H	-3.57629100	-4.23065900	1.90635000
H	-3.60097000	-5.01876700	4.26233900
C	-0.27191200	4.24280000	0.73568300
H	0.59062000	3.90253600	0.15509800
H	-0.99576400	4.64018900	0.01472500
C	0.15184400	5.35159000	1.70461600
H	-0.71683700	5.67783400	2.29100000
H	0.87107500	4.94449100	2.42672400
C	0.77090100	6.56391000	1.00018800
H	1.63952100	6.23737500	0.41438600
H	0.05237300	6.96935000	0.27621200
C	1.19962100	7.67725300	1.96296700
H	0.33044200	8.00388000	2.54685900
H	1.91661800	7.27147100	2.68707400
C	1.81946000	8.88415600	1.25288800
H	2.11477600	9.65831600	1.96632600
H	2.71118600	8.59572900	0.68758400
H	1.11334200	9.33421400	0.54801900
C	4.93403300	-0.87442900	-0.86642200
H	4.42878200	-0.77465700	-1.83169400
H	4.89716800	-1.93795200	-0.60426400
C	6.39314100	-0.42344800	-0.99064500
H	6.88918000	-0.51465200	-0.01547500
H	6.42088800	0.64269800	-1.24907800
C	7.18201000	-1.21939300	-2.03636900
H	6.68620600	-1.12650200	-3.01085300
H	7.15028100	-2.28628700	-1.78035200
C	8.64343100	-0.77576700	-2.16883100
H	9.13926200	-0.87014600	-1.19486600
H	8.67495500	0.29046900	-2.42405800
C	9.42361200	-1.57402900	-3.21727000
H	8.97379200	-1.46933500	-4.20953100
H	10.46109200	-1.23544800	-3.28596600
H	9.43797800	-2.64077500	-2.97248000

Isomer **F** of complex $[MoO(O_2)(Q^{C6})_2]$, **10**.

Mo	-0.08670700	1.42931100	-0.07962300
O	-0.28516800	-0.11051700	1.35612300
O	-2.11770800	1.01261100	-0.39608200
O	0.21822600	-0.36912300	-1.31555500
O	1.89311600	1.05904400	0.47032200
O	-0.31910500	2.61391000	1.11626300
O	-0.49822000	2.38939000	-1.72744800
O	0.88651700	2.42117700	-1.46850200
N	-1.35085700	-1.76037600	2.60254400
N	-2.61968300	-2.32554900	2.70359800
N	1.50467400	-1.98480900	-2.38727600
N	2.81723600	-2.44791400	-2.36430800
C	-3.38580600	-1.71663600	1.83804400
C	-2.64572500	-0.70493700	1.11755800
C	-1.32460600	-0.78079100	1.65914000
C	-4.82196500	-2.12354800	1.73730000
H	-5.02317100	-2.88928600	2.48666500
H	-5.05349100	-2.53731300	0.75155400
H	-5.49337300	-1.27894500	1.91314500
C	-2.97413900	0.20433700	0.10687000
C	-4.35485300	0.34617500	-0.47647000
H	-4.94524000	-0.55116000	-0.29529800
C	3.46787800	-1.72120500	-1.49551100
C	2.60189500	-0.72843700	-0.89526400
C	1.32238600	-0.95387700	-1.51255200
C	4.92009900	-2.00615300	-1.27257100
H	5.23185900	-2.79081700	-1.96232300
H	5.10889100	-2.35168600	-0.25189400
H	5.53885800	-1.12235500	-1.44789500
C	2.81638400	0.26689400	0.06298800
C	4.15744200	0.54084800	0.69568800
H	3.97039700	0.82386000	1.73493400
H	-4.23251600	0.45859100	-1.55744800
H	4.77805000	-0.35473100	0.69624400
C	-0.30324800	-2.25287700	3.43027000
C	-0.46711300	-3.49598300	4.05036600
C	0.86430300	-1.51032300	3.63773000
C	0.53702700	-3.99070700	4.87572000
H	-1.37881300	-4.05253300	3.88701200
C	1.85852400	-2.02306800	4.46752700
H	0.98897900	-0.54964800	3.16233400
C	1.70504000	-3.26039500	5.08858800
H	0.40240400	-4.95442700	5.35361700
H	2.75846000	-1.44105600	4.63149500
H	2.48407500	-3.64946500	5.73383300
C	0.56289200	-2.60065800	-3.25477100
C	0.81558800	-3.89704800	-3.71471000
C	-0.58879300	-1.91971400	-3.66434200
C	-0.08674600	-4.50882400	-4.57886200
H	1.71776300	-4.40269000	-3.40027700
C	-1.48251400	-2.54959900	-4.52690600
H	-0.77739400	-0.91594300	-3.31440600
C	-1.24070800	-3.84199800	-4.98782400
H	0.11601600	-5.51334900	-4.93279800
H	-2.37040100	-2.01578700	-4.84684500
H	-1.94034400	-4.32244500	-5.66200600
C	-5.08667800	1.58590100	0.08297600
H	-4.47233000	2.47144400	-0.10444600
H	-5.18090500	1.49288600	1.17119900

C	4.88938300	1.69585600	-0.02196000
H	4.23887000	2.57571100	-0.02672600
H	5.05412700	1.42568400	-1.07117100
C	-6.47364400	1.76852700	-0.54176300
H	-7.07648300	0.86871100	-0.36284000
H	-6.36916900	1.85468200	-1.63060200
C	-7.22268200	2.99387000	-0.00593600
H	-6.62159200	3.89364300	-0.18785300
H	-7.32360700	2.91089500	1.08399100
C	-8.61137600	3.17902300	-0.62821100
H	-9.21150300	2.27925700	-0.44528900
H	-8.50998000	3.26074100	-1.71717300
C	-9.35474100	4.40583400	-0.09199900
H	-8.79487300	5.32511000	-0.29028900
H	-10.33925200	4.51031600	-0.55615600
H	-9.50363900	4.33705200	0.99025600
C	6.22847100	2.04029500	0.63873200
H	6.86606000	1.14682300	0.66144200
H	6.05398900	2.31770300	1.68596400
C	6.97388600	3.17642600	-0.07009200
H	6.33467900	4.06798400	-0.09597200
H	7.14804700	2.89769500	-1.11739000
C	8.31269700	3.53388100	0.58583100
H	8.95024500	2.64165800	0.61457900
H	8.13816400	3.81649500	1.63110900
C	9.05290700	4.66633800	-0.13148700
H	8.45581900	5.58352700	-0.14444500
H	10.00273200	4.89581300	0.35931800
H	9.27165400	4.40032800	-1.17045300