Supporting Information

[3+2] Cycloaddition of azido-bridged molybdenum(II) complex with nitriles and alkynes

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Table S1. Crystal data and structure refinement for $[N(CH_3)_4][(\mu_{1,1}\text{-}N_3)_3\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]$

Empirical formula	$C_{14}H_{22}Mo_2N_{10}O_4$	
Formula weight	586.30	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/m	
Unit cell dimensions	a = 11.3025(7) Å	α = 90°.
	b = 19.3312(12) Å	β = 114.6150(10)°.
	c = 10.8564(7) Å	γ = 90°.
Volume	2156.5(2) $Å^3$	
Z	4	
Density (calculated)	1.806 Mg/m^3	
Absorption coefficient	1.206 mm^{-1}	
F(000)	1168	
Crystal size	0.35 x 0.25 x 0.18 mm^3	
Theta range for data collection	2.06 to 27.50°.	
Index ranges	-14<=h<=14, -25<=k<=25, -14<=l<=14	
Reflections collected	8326	
Independent reflections	2555 [R(int) = 0.0198]	
Completeness to theta = 27.50°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8122 and 0.6776	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2555 / 2 / 172	
Goodness-of-fit on F^2	1.083	
Final R indices [I>2sigma(I)]	R1 = 0.0182, wR2 = 0.0467	
R indices (all data)	R1 = 0.0202, wR2 = 0.0477	
Largest diff. peak and hole	0.350 and -0.389 $e.Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for $[N(CH_3)_4][(\mu_{1,1}\text{-}N_3)_3\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]$

Mo-C(2)	1.9440(18)	N(7)-Mo#1	2.2692(14)
Mo-C(1)	1.9460(18)	N(8)-N(9)	1.148(3)
Mo-N(1)	2.1755(13)	C(1)-O(1)	1.157(2)
Mo-C(4)	2.1994(18)	C(2)-O(2)	1.157(2)
Mo-N(7)	2.2692(14)	C(3)-C(4)	1.407(3)
Mo-N(4)	2.2846(14)	C(4)-C(5)	1.411(3)
Mo-C(3)	2.3007(19)	N(10)-C(9)#2	1.388(17)
Mo-C(5)	2.3159(18)	N(10)-C(9)	1.388(17)
N(1)-N(2)	1.222(3)	N(10)-C(6)#2	1.488(13)
N(1)-Mo#1	2.1755(13)	N(10)-C(6)	1.488(13)
N(2)-N(3)	1.126(3)	N(10)-C(8)#2	1.498(13)
N(4)-N(5)	1.210(3)	N(10)-C(8)	1.498(13)
N(4)-Mo#1	2.2846(14)	N(10)-C(7)#2	1.511(17)
N(5)-N(6)	1.146(3)	N(10)-C(7)	1.511(17)
N(7)-N(8)	1.197(3)		
C(2)-Mo-C(1)	80.38(7)	C(3)-Mo-C(5)	62.32(7)
C(2)-Mo-N(1)	93.68(7)	N(2)-N(1)-Mo#1	129.54(5)
C(1)-Mo-N(1)	94.43(7)	N(2)-N(1)-Mo	129.54(5)
C(2)-Mo-C(4)	104.56(8)	Mo#1-N(1)-Mo	97.20(8)
C(1)-Mo-C(4)	104.26(8)	N(3)-N(2)-N(1)	179.2(2)
N(1)-Mo-C(4)	155.68(7)	N(5)-N(4)-Mo#1	127.58(8)
C(2)-Mo-N(7)	167.07(7)	N(5)-N(4)-Mo	127.58(8)
C(1)-Mo-N(7)	98.65(7)	Mo#1-N(4)-Mo	91.17(7)
N(1)-Mo-N(7)	73.50(6)	N(6)-N(5)-N(4)	178.6(3)
C(4)-Mo-N(7)	88.21(7)	N(8)-N(7)-Mo	130.50(7)
C(2)-Mo-N(4)	104.34(7)	N(8)-N(7)-Mo#1	130.50(7)
C(1)-Mo-N(4)	165.16(6)	Mo-N(7)-Mo#1	91.97(7)
N(1)-Mo-N(4)	71.40(6)	N(9)-N(8)-N(7)	178.3(3)
C(4)-Mo-N(4)	88.34(7)	O(1)-C(1)-Mo	179.28(16)
N(7)-Mo-N(4)	73.54(6)	O(2)-C(2)-Mo	176.59(16)
C(2)-Mo-C(3)	70.54(8)	C(4)-C(3)-Mo	67.90(10)
C(1)-Mo-C(3)	110.03(8)	C(3)-C(4)-C(5)	115.96(19)
N(1)-Mo-C(3)	147.40(7)	C(3)-C(4)-Mo	75.75(11)
C(4)-Mo-C(3)	36.34(7)	C(5)-C(4)-Mo	76.35(11)
N(7)-Mo-C(3)	121.34(8)	C(4)-C(5)-Mo	67.35(10)
N(4)-Mo-C(3)	84.76(7)	C(9)#2-N(10)-C(9)	126.0(15)
C(2)-Mo-C(5)	108.05(8)	C(9)#2-N(10)-C(6)#2	95.6(11)
C(1)-Mo-C(5)	69.54(7)	C(9)-N(10)-C(6)#2	115.5(10)
N(1)-Mo-C(5)	149.66(7)	C(9)#2-N(10)-C(6)	115.5(10)
C(4)-Mo-C(5)	36.30(7)	C(9)-N(10)-C(6)	95.6(11)
N(7)-Mo-C(5)	83.38(6)	C(6)#2-N(10)-C(6)	108.9(11)
N(4)-Mo-C(5)	120.80(7)	C(9)#2-N(10)-C(8)#2	93.8(10)

C(9)-N(10)-C(8)#2	114.4(11)	C(6)-N(10)-C(7)#2	104.3(10)
C(6)#2-N(10)-C(8)#2	108.1(3)	C(8)#2-N(10)-C(7)#2	119.3(10)
C(6)-N(10)-C(8)#2	22.3(7)	C(8)-N(10)-C(7)#2	103.3(9)
C(9)#2-N(10)-C(8)	114.4(11)	C(9)#2-N(10)-C(7)	15.9(14)
C(9)-N(10)-C(8)	93.8(10)	C(9)-N(10)-C(7)	110.1(6)
C(6)#2-N(10)-C(8)	22.3(7)	C(6)#2-N(10)-C(7)	104.3(10)
C(6)-N(10)-C(8)	108.1(3)	C(6)-N(10)-C(7)	123.0(9)
C(8)#2-N(10)-C(8)	116.2(11)	C(8)#2-N(10)-C(7)	103.3(9)
C(9)#2-N(10)-C(7)#2	110.1(6)	C(8)-N(10)-C(7)	119.3(10)
C(9)-N(10)-C(7)#2	15.9(14)	C(7)#2-N(10)-C(7)	94.2(14)
C(6)#2-N(10)-C(7)#2	123.0(9)		

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

Table S3. Crystal data and structure refinement for $[N(CH_3)_4][(\mu\text{-}N_4C\{C(CN)=C(CN)_2\}\text{-}\kappa^2N^2{:}N^3)(\mu_{1,1}\text{-}N_3)_2\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]$

Empirical formula	$C_{20}H_{22}Mo_2N_{14}O_4$	
Formula weight	714.40	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.1748(7) Å	α = 90°.
	b = 11.8254(8) Å	β = 102.6262(14)°.
	c = 21.7960(15) Å	γ = 90°.
Volume	2810.6(3) $Å^3$	
Z	4	
Density (calculated)	1.688 Mg/m^3	
Absorption coefficient	0.946 mm^{-1}	
F(000)	1424	
Crystal size	0.50 x 0.40 x 0.02 mm^3	
Theta range for data collection	1.90 to 27.50°.	
Index ranges	-12<=h<=14, -15<=k<=14, -28<=l<=27	
Reflections collected	17744	
Independent reflections	6456 [R(int) = 0.0480]	
Completeness to theta = 27.50°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9813 and 0.6491	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6456 / 56 / 374	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1025	
R indices (all data)	R1 = 0.0625, wR2 = 0.1098	
Largest diff. peak and hole	1.540 and -0.597 e.$Å^{-3}$	

Table S4. Bond lengths [Å] and angles [°] for $[N(CH_3)_4][(\mu\text{-}N_4C\{C(CN)=C(CN)_2\}\text{-}\kappa^2N^2{:}N^3)(\mu_{1,1}\text{-}N_3)_2\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]$

Mo(1)-C(2)	1.942(5)	N(11)-C(14)	1.131(6)
Mo(1)-C(1)	1.951(5)	N(12)-C(15)	1.135(6)
Mo(1)-N(1)	2.195(3)	N(13)-C(16)	1.127(6)
Mo(1)-C(6)	2.208(5)	C(1)-O(1)	1.148(6)
Mo(1)-N(8)	2.268(3)	C(2)-O(2)	1.150(6)
Mo(1)-N(4)	2.274(3)	C(3)-O(3)	1.156(5)
Mo(1)-C(5)	2.305(5)	C(4)-O(4)	1.157(5)
Mo(1)-C(7)	2.319(5)	C(5)-C(6)	1.394(8)
Mo(2)-C(4)	1.932(4)	C(6)-C(7)	1.417(8)
Mo(2)-C(3)	1.938(5)	C(8)-C(9)	1.397(7)
Mo(2)-N(1)	2.187(3)	C(9)-C(10)	1.393(7)
Mo(2)-C(9)	2.195(4)	C(11)-C(12)	1.446(5)
Mo(2)-N(9)	2.260(3)	C(12)-C(13)	1.355(6)
Mo(2)-N(4)	2.275(3)	C(12)-C(14)	1.443(6)
Mo(2)-C(8)	2.313(5)	C(13)-C(16)	1.434(6)
Mo(2)-C(10)	2.320(4)	C(13)-C(15)	1.435(6)
N(1)-N(2)	1.213(5)	N(14)-C(20)	1.413(10)
N(2)-N(3)	1.129(5)	N(14)-C(18')	1.443(14)
N(4)-N(5)	1.195(5)	N(14)-C(18)	1.486(15)
N(5)-N(6)	1.146(5)	N(14)-C(19')	1.489(13)
N(7)-N(8)	1.320(5)	N(14)-C(17')	1.492(12)
N(7)-C(11)	1.336(5)	N(14)-C(17)	1.500(13)
N(8)-N(9)	1.346(4)	N(14)-C(19)	1.533(14)
N(9)-N(10)	1.319(5)	N(14)-C(20')	1.556(10)
N(10)-C(11)	1.333(5)		

C(2)-Mo(1)-C(1)	77.1(2)	C(1)-Mo(1)-C(5)	112.1(2)
C(2)-Mo(1)-N(1)	94.58(17)	N(1)-Mo(1)-C(5)	149.45(17)
C(1)-Mo(1)-N(1)	90.39(18)	C(6)-Mo(1)-C(5)	35.89(19)
C(2)-Mo(1)-C(6)	104.1(2)	N(8)-Mo(1)-C(5)	117.78(17)
C(1)-Mo(1)-C(6)	105.0(2)	N(4)-Mo(1)-C(5)	85.37(17)
N(1)-Mo(1)-C(6)	157.95(16)	C(2)-Mo(1)-C(7)	104.02(19)
C(2)-Mo(1)-N(8)	170.19(17)	C(1)-Mo(1)-C(7)	69.7(2)
C(1)-Mo(1)-N(8)	99.02(16)	N(1)-Mo(1)-C(7)	148.42(17)
N(1)-Mo(1)-N(8)	76.33(12)	C(6)-Mo(1)-C(7)	36.4(2)
C(6)-Mo(1)-N(8)	85.57(16)	N(8)-Mo(1)-C(7)	82.69(16)
C(2)-Mo(1)-N(4)	102.50(16)	N(4)-Mo(1)-C(7)	127.80(17)
C(1)-Mo(1)-N(4)	160.93(18)	C(5)-Mo(1)-C(7)	62.0(2)
N(1)-Mo(1)-N(4)	70.58(12)	C(4)-Mo(2)-C(3)	78.48(19)
C(6)-Mo(1)-N(4)	93.66(17)	C(4)-Mo(2)-N(1)	93.16(16)
N(8)-Mo(1)-N(4)	78.19(12)	C(3)-Mo(2)-N(1)	93.16(17)
C(2)-Mo(1)-C(5)	72.0(2)	C(4)-Mo(2)-C(9)	104.0(2)

C(3)-Mo(2)-C(9)	103.90(19)	C(5)-C(6)-Mo(1)	75.9(3)
N(1)-Mo(2)-C(9)	157.80(15)	C(7)-C(6)-Mo(1)	76.1(3)
C(4)-Mo(2)-N(9)	99.87(16)	C(6)-C(7)-Mo(1)	67.5(3)
C(3)-Mo(2)-N(9)	169.58(16)	C(9)-C(8)-Mo(2)	67.4(3)
N(1)-Mo(2)-N(9)	76.60(12)	C(10)-C(9)-C(8)	116.2(4)
C(9)-Mo(2)-N(9)	86.50(15)	C(10)-C(9)-Mo(2)	77.0(3)
C(4)-Mo(2)-N(4)	163.81(16)	C(8)-C(9)-Mo(2)	76.6(3)
C(3)-Mo(2)-N(4)	100.79(17)	C(9)-C(10)-Mo(2)	67.2(3)
N(1)-Mo(2)-N(4)	70.69(12)	N(10)-C(11)-N(7)	113.3(3)
C(9)-Mo(2)-N(4)	91.93(16)	N(10)-C(11)-C(12)	124.5(4)
N(9)-Mo(2)-N(4)	77.88(12)	N(7)-C(11)-C(12)	122.2(4)
C(4)-Mo(2)-C(8)	108.92(19)	C(13)-C(12)-C(14)	118.1(4)
C(3)-Mo(2)-C(8)	70.38(19)	C(13)-C(12)-C(11)	125.3(4)
N(1)-Mo(2)-C(8)	148.37(17)	C(14)-C(12)-C(11)	116.6(4)
C(9)-Mo(2)-C(8)	36.00(18)	C(12)-C(13)-C(16)	123.9(4)
N(9)-Mo(2)-C(8)	119.55(16)	C(12)-C(13)-C(15)	120.1(4)
N(4)-Mo(2)-C(8)	85.67(16)	C(16)-C(13)-C(15)	116.0(4)
C(4)-Mo(2)-C(10)	69.9(2)	N(11)-C(14)-C(12)	178.6(6)
C(3)-Mo(2)-C(10)	106.89(19)	N(12)-C(15)-C(13)	177.9(5)
N(1)-Mo(2)-C(10)	149.89(16)	N(13)-C(16)-C(13)	175.1(5)
C(9)-Mo(2)-C(10)	35.82(19)	C(20)-N(14)-C(18')	135.1(11)
N(9)-Mo(2)-C(10)	81.87(14)	C(20)-N(14)-C(18)	118.3(11)
N(4)-Mo(2)-C(10)	124.90(16)	C(18')-N(14)-C(18)	30.9(11)
C(8)-Mo(2)-C(10)	61.53(19)	C(20)-N(14)-C(19')	77.1(9)
N(2)-N(1)-Mo(2)	123.3(3)	C(18')-N(14)-C(19')	99.9(12)
N(2)-N(1)-Mo(1)	128.1(3)	C(18)-N(14)-C(19')	126.0(13)
Mo(2)-N(1)-Mo(1)	107.93(14)	C(20)-N(14)-C(17')	114.1(9)
N(3)-N(2)-N(1)	178.5(5)	C(18')-N(14)-C(17')	101.9(11)
N(5)-N(4)-Mo(1)	130.0(3)	C(18)-N(14)-C(17')	92.6(12)
N(5)-N(4)-Mo(2)	127.6(3)	C(19')-N(14)-C(17')	130.3(11)
Mo(1)-N(4)-Mo(2)	102.31(13)	C(20)-N(14)-C(17)	101.2(10)
N(6)-N(5)-N(4)	179.2(5)	C(18')-N(14)-C(17)	122.3(12)
N(8)-N(7)-C(11)	103.6(3)	C(18)-N(14)-C(17)	119.7(12)
N(7)-N(8)-N(9)	109.7(3)	C(19')-N(14)-C(17)	105.0(11)
N(7)-N(8)-Mo(1)	131.6(3)	C(17')-N(14)-C(17)	27.5(8)
N(9)-N(8)-Mo(1)	118.7(2)	C(20)-N(14)-C(19)	112.5(10)
N(10)-N(9)-N(8)	109.5(3)	C(18')-N(14)-C(19)	74.2(11)
N(10)-N(9)-Mo(2)	131.1(2)	C(18)-N(14)-C(19)	105.0(12)
N(8)-N(9)-Mo(2)	119.4(2)	C(19')-N(14)-C(19)	35.4(9)
N(9)-N(10)-C(11)	103.9(3)	C(17')-N(14)-C(19)	112.7(11)
O(1)-C(1)-Mo(1)	175.5(5)	C(17)-N(14)-C(19)	98.8(11)
O(2)-C(2)-Mo(1)	175.9(4)	C(20)-N(14)-C(20')	38.3(6)
O(3)-C(3)-Mo(2)	175.8(4)	C(18')-N(14)-C(20')	105.7(10)
O(4)-C(4)-Mo(2)	174.8(4)	C(18)-N(14)-C(20')	81.3(10)
C(6)-C(5)-Mo(1)	68.2(3)	C(19')-N(14)-C(20')	107.0(9)
C(5)-C(6)-C(7)	115.7(5)	C(17')-N(14)-C(20')	109.1(9)

C(17)-N(14)-C(20')	114.9(9)	C(19)-N(14)-C(20')	137.2(9)

Symmetry transformations used to generate equivalent atoms:

Table S5. Crystal data and structure refinement for $[N(CH_3)_4][(\mu\text{-}N_4C\{C_6H_4NO_2\}\text{-}\kappa^2N^2{:}N^3)(\mu_{1,1}\text{-}N_3)_2\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]$

Empirical formula	$C_{21}H_{26}Mo_2N_{12}O_6$	
Formula weight	734.42	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 18.9939(4) Å	α = 90°.
	b = 10.7176(2) Å	β = 92.2762(8)°.
	c = 28.9030(5) Å	γ = 90°.
Volume	5879.11(19) $Å^3$	
Z	8	
Density (calculated)	1.659 Mg/m^3	
Absorption coefficient	0.910 mm^{-1}	
F(000)	2944	
Crystal size	0.25 x 0.15 x 0.14 mm^3	
Theta range for data collection	1.41 to 27.50°.	
Index ranges	-24<=h<=24, -11<=k<=13, -21<=l<=37	
Reflections collected	23263	
Independent reflections	6705 [R(int) = 0.0460]	
Completeness to theta = 27.50°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.874 and 0.796	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6705 / 0 / 374	
Goodness-of-fit on F^2	1.020	
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0696	
R indices (all data)	R1 = 0.0568, wR2 = 0.0848	
Largest diff. peak and hole	0.505 and -0.593 $e.Å^{-3}$	

Table S6. Bond lengths [Å] and angles [°] for $[N(CH_3)_4][(\mu\text{-}N_4C\{C_6H_4NO_2\}\text{-}\kappa^2N^2{:}N^3)(\mu_{1,1}\text{-}N_3)_2\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]$

Mo(1)-C(1)	1.941(3)	N(10)-C(11)	1.343(3)
Mo(1)-C(2)	1.954(3)	N(11)-O(6)	1.228(4)
Mo(1)-N(4)	2.186(2)	N(11)-O(5)	1.232(3)
Mo(1)-C(6)	2.212(3)	N(11)-C(15)	1.475(4)
Mo(1)-N(8)	2.245(2)	C(1)-O(1)	1.165(4)
Mo(1)-N(1)	2.304(2)	C(2)-O(2)	1.162(3)
Mo(1)-C(7)	2.327(3)	C(3)-O(3)	1.161(3)
Mo(1)-C(5)	2.336(3)	C(4)-O(4)	1.162(4)
Mo(2)-C(3)	1.949(3)	C(5)-C(6)	1.406(4)
Mo(2)-C(4)	1.953(3)	C(6)-C(7)	1.406(4)
Mo(2)-N(4)	2.187(2)	C(8)-C(9)	1.402(5)
Mo(2)-C(9)	2.209(3)	C(9)-C(10)	1.413(5)
Mo(2)-N(9)	2.249(2)	C(11)-C(12)	1.464(4)
Mo(2)-N(1)	2.302(2)	C(12)-C(13)	1.387(4)
Mo(2)-C(8)	2.321(3)	C(12)-C(17)	1.400(4)
Mo(2)-C(10)	2.329(3)	C(13)-C(14)	1.385(4)
N(1)-N(2)	1.215(3)	C(14)-C(15)	1.375(4)
N(2)-N(3)	1.144(3)	C(15)-C(16)	1.387(4)
N(4)-N(5)	1.223(3)	C(16)-C(17)	1.378(4)
N(5)-N(6)	1.135(3)	N(12)-C(18)	1.480(4)
N(7)-N(8)	1.338(3)	N(12)-C(19)	1.483(4)
N(7)-C(11)	1.339(4)	N(12)-C(20)	1.494(4)
N(8)-N(9)	1.335(3)	N(12)-C(21)	1.497(4)
N(9)-N(10)	1.330(3)		
C(1)-Mo(1)-C(2)	80.96(12)	C(6)-Mo(1)-C(7)	35.97(11)
C(1)-Mo(1)-N(4)	91.41(10)	N(8)-Mo(1)-C(7)	117.22(10)
C(2)-Mo(1)-N(4)	92.47(10)	N(1)-Mo(1)-C(7)	83.69(10)
C(1)-Mo(1)-C(6)	103.52(12)	C(1)-Mo(1)-C(5)	68.43(12)
C(2)-Mo(1)-C(6)	105.48(12)	C(2)-Mo(1)-C(5)	106.18(12)
N(4)-Mo(1)-C(6)	158.11(11)	N(4)-Mo(1)-C(5)	149.31(10)
C(1)-Mo(1)-N(8)	96.56(10)	C(6)-Mo(1)-C(5)	35.89(11)
C(2)-Mo(1)-N(8)	169.65(11)	N(8)-Mo(1)-C(5)	81.97(10)
N(4)-Mo(1)-N(8)	77.50(8)	N(1)-Mo(1)-C(5)	126.55(10)
C(6)-Mo(1)-N(8)	84.87(10)	C(7)-Mo(1)-C(5)	61.66(11)
C(1)-Mo(1)-N(1)	163.11(11)	C(3)-Mo(2)-C(4)	81.27(12)
C(2)-Mo(1)-N(1)	99.84(10)	C(3)-Mo(2)-N(4)	90.94(10)
N(4)-Mo(1)-N(1)	71.71(9)	C(4)-Mo(2)-N(4)	94.79(11)
C(6)-Mo(1)-N(1)	92.57(11)	C(3)-Mo(2)-C(9)	103.73(13)
N(8)-Mo(1)-N(1)	79.61(8)	C(4)-Mo(2)-C(9)	104.57(13)
C(1)-Mo(1)-C(7)	112.37(12)	N(4)-Mo(2)-C(9)	157.15(11)
C(2)-Mo(1)-C(7)	72.82(12)	C(3)-Mo(2)-N(9)	98.52(10)
N(4)-Mo(1)-C(7)	148.86(10)	C(4)-Mo(2)-N(9)	171.13(11)

N(4)-Mo(2)-N(9)	76.34(8)	O(6)-N(11)-O(5)	123.8(3)
C(9)-Mo(2)-N(9)	84.14(11)	O(6)-N(11)-C(15)	118.5(3)
C(3)-Mo(2)-N(1)	162.40(10)	O(5)-N(11)-C(15)	117.7(3)
C(4)-Mo(2)-N(1)	96.72(10)	O(1)-C(1)-Mo(1)	177.0(3)
N(4)-Mo(2)-N(1)	71.74(9)	O(2)-C(2)-Mo(1)	176.2(3)
C(9)-Mo(2)-N(1)	93.72(11)	O(3)-C(3)-Mo(2)	176.9(3)
N(9)-Mo(2)-N(1)	80.77(8)	O(4)-C(4)-Mo(2)	177.4(2)
C(3)-Mo(2)-C(8)	68.70(13)	C(6)-C(5)-Mo(1)	67.25(16)
C(4)-Mo(2)-C(8)	106.18(12)	C(7)-C(6)-C(5)	116.4(3)
N(4)-Mo(2)-C(8)	147.52(11)	C(7)-C(6)-Mo(1)	76.46(17)
C(9)-Mo(2)-C(8)	35.96(12)	C(5)-C(6)-Mo(1)	76.86(18)
N(9)-Mo(2)-C(8)	81.83(10)	C(6)-C(7)-Mo(1)	67.57(16)
N(1)-Mo(2)-C(8)	128.10(11)	C(9)-C(8)-Mo(2)	67.67(18)
C(3)-Mo(2)-C(10)	112.01(12)	C(8)-C(9)-C(10)	116.3(3)
C(4)-Mo(2)-C(10)	71.47(13)	C(8)-C(9)-Mo(2)	76.4(2)
N(4)-Mo(2)-C(10)	150.24(11)	C(10)-C(9)-Mo(2)	76.55(19)
C(9)-Mo(2)-C(10)	36.17(12)	C(9)-C(10)-Mo(2)	67.28(17)
N(9)-Mo(2)-C(10)	116.44(11)	N(7)-C(11)-N(10)	112.7(2)
N(1)-Mo(2)-C(10)	83.51(10)	N(7)-C(11)-C(12)	123.7(3)
C(8)-Mo(2)-C(10)	61.92(12)	N(10)-C(11)-C(12)	123.3(3)
N(2)-N(1)-Mo(2)	117.61(19)	C(13)-C(12)-C(17)	119.9(3)
N(2)-N(1)-Mo(1)	117.62(19)	C(13)-C(12)-C(11)	119.7(3)
Mo(2)-N(1)-Mo(1)	99.40(9)	C(17)-C(12)-C(11)	120.3(3)
N(3)-N(2)-N(1)	179.0(3)	C(14)-C(13)-C(12)	120.0(3)
N(5)-N(4)-Mo(1)	126.70(19)	C(15)-C(14)-C(13)	118.9(3)
N(5)-N(4)-Mo(2)	124.70(18)	C(14)-C(15)-C(16)	122.6(3)
Mo(1)-N(4)-Mo(2)	106.92(10)	C(14)-C(15)-N(11)	118.4(3)
N(6)-N(5)-N(4)	179.2(3)	C(16)-C(15)-N(11)	119.0(3)
N(8)-N(7)-C(11)	103.8(2)	C(17)-C(16)-C(15)	118.1(3)
N(9)-N(8)-N(7)	109.7(2)	C(16)-C(17)-C(12)	120.5(3)
N(9)-N(8)-Mo(1)	119.00(17)	C(18)-N(12)-C(19)	110.4(3)
N(7)-N(8)-Mo(1)	130.25(17)	C(18)-N(12)-C(20)	108.9(3)
N(10)-N(9)-N(8)	109.7(2)	C(19)-N(12)-C(20)	109.1(2)
N(10)-N(9)-Mo(2)	131.26(18)	C(18)-N(12)-C(21)	109.3(3)
N(8)-N(9)-Mo(2)	118.84(17)	C(19)-N(12)-C(21)	109.7(3)
N(9)-N(10)-C(11)	104.1(2)	C(20)-N(12)-C(21)	109.4(3)

Symmetry transformations used to generate equivalent atoms:

Table S7. Crystal data and structure refinement for $[N(CH_3)_4][(\mu\text{-}N_4C\{C(CN)=C(CN)_2\}\text{-}\kappa^2N^2{:}N^3)_2(\mu_{1,1}\text{-}N_3)\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]\cdot CH_2Cl_2$

Empirical formula	$C_{27}H_{24}Cl_2Mo_2N_{18}O_4$	
Formula weight	927.42	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.2316(4) Å	α = 90°.
	b = 11.6355(4) Å	β = 98.1264(15)°.
	c = 28.9416(10) Å	γ = 90°.
Volume	3744.3(2) $Å^3$	
Z	4	
Density (calculated)	1.645 Mg/m^3	
Absorption coefficient	0.872 mm^{-1}	
F(000)	1848	
Crystal size	0.50 x 0.30 x 0.03 mm^3	
Theta range for data collection	1.42 to 27.50°.	
Index ranges	-14<=h<=14, -15<=k<=14, -37<=l<=37	
Reflections collected	24484	
Independent reflections	8543 [R(int) = 0.0580]	
Completeness to theta = 27.50°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.990 and 0.750	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8543 / 0 / 482	
Goodness-of-fit on F^2	1.028	
Final R indices [I>2sigma(I)]	R1 = 0.0486, wR2 = 0.1148	
R indices (all data)	R1 = 0.0964, wR2 = 0.1337	
Largest diff. peak and hole	1.204 and -1.324 e.$Å^{-3}$	

Table S8. Bond lengths [Å] and angles [°] for $[N(CH_3)_4][(\mu\text{-}N_4C\{C(CN)=C(CN)_2\}\text{-}\kappa^2N^2{:}N^3)_2(\mu_{1,1}\text{-}N_3)\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]\cdot CH_2Cl_2$

Mo(1)-C(1)	1.937(5)	N(13)-N(14)	1.329(4)
Mo(1)-C(2)	1.943(5)	N(14)-C(17)	1.346(5)
Mo(1)-N(1)	2.197(3)	N(15)-C(20)	1.139(6)
Mo(1)-C(6)	2.198(4)	N(16)-C(21)	1.129(5)
Mo(1)-N(5)	2.260(3)	N(17)-C(22)	1.136(6)
Mo(1)-N(12)	2.279(3)	C(1)-O(1)	1.161(5)
Mo(1)-C(7)	2.311(4)	C(2)-O(2)	1.151(5)
Mo(1)-C(5)	2.326(5)	C(3)-O(3)	1.155(5)
Mo(2)-C(4)	1.937(5)	C(4)-O(4)	1.159(5)
Mo(2)-C(3)	1.945(4)	C(5)-C(6)	1.369(7)
Mo(2)-N(1)	2.184(3)	C(6)-C(7)	1.427(7)
Mo(2)-C(9)	2.210(4)	C(8)-C(9)	1.417(7)
Mo(2)-N(6)	2.276(3)	C(9)-C(10)	1.393(8)
Mo(2)-N(13)	2.290(3)	C(11)-C(12)	1.453(5)
Mo(2)-C(8)	2.325(4)	C(12)-C(13)	1.350(6)
Mo(2)-C(10)	2.342(5)	C(12)-C(14)	1.465(6)
N(1)-N(2)	1.225(4)	C(13)-C(16)	1.427(6)
N(2)-N(3)	1.141(5)	C(13)-C(15)	1.449(6)
N(4)-N(5)	1.328(4)	C(17)-C(18)	1.463(5)
N(4)-C(11)	1.334(5)	C(18)-C(19)	1.352(6)
N(5)-N(6)	1.354(4)	C(18)-C(20)	1.445(6)
N(6)-N(7)	1.332(4)	C(19)-C(22)	1.434(6)
N(7)-C(11)	1.336(5)	C(19)-C(21)	1.465(6)
N(8)-C(14)	1.124(5)	N(18)-C(25)	1.479(6)
N(9)-C(15)	1.144(6)	N(18)-C(26)	1.484(6)
N(10)-C(16)	1.138(6)	N(18)-C(23)	1.490(6)
N(11)-N(12)	1.319(4)	N(18)-C(24)	1.492(6)
N(11)-C(17)	1.322(5)	C(27)-Cl(1)	1.743(5)
N(12)-N(13)	1.345(5)	C(27)-Cl(2)	1.766(5)
C(1)-Mo(1)-C(2)	78.73(19)	C(2)-Mo(1)-N(12)	100.03(16)
C(1)-Mo(1)-N(1)	93.48(16)	N(1)-Mo(1)-N(12)	78.03(12)
C(2)-Mo(1)-N(1)	88.73(17)	C(6)-Mo(1)-N(12)	84.93(17)
C(1)-Mo(1)-C(6)	103.6(2)	N(5)-Mo(1)-N(12)	79.55(12)
C(2)-Mo(1)-C(6)	103.2(2)	C(1)-Mo(1)-C(7)	104.64(18)
N(1)-Mo(1)-C(6)	160.72(15)	C(2)-Mo(1)-C(7)	67.6(2)
C(1)-Mo(1)-N(5)	99.58(15)	N(1)-Mo(1)-C(7)	146.08(17)
C(2)-Mo(1)-N(5)	166.02(17)	C(6)-Mo(1)-C(7)	36.80(19)
N(1)-Mo(1)-N(5)	77.47(12)	N(5)-Mo(1)-C(7)	125.78(17)
C(6)-Mo(1)-N(5)	90.73(17)	N(12)-Mo(1)-C(7)	82.44(15)
C(1)-Mo(1)-N(12)	171.47(16)	C(1)-Mo(1)-C(5)	71.6(2)

C(2)-Mo(1)-C(5)	109.91(19)	N(12)-N(11)-C(17)	104.2(3)
N(1)-Mo(1)-C(5)	152.48(16)	N(11)-N(12)-N(13)	109.6(3)
C(6)-Mo(1)-C(5)	35.09(19)	N(11)-N(12)-Mo(1)	126.7(3)
N(5)-Mo(1)-C(5)	82.30(15)	N(13)-N(12)-Mo(1)	123.2(2)
N(12)-Mo(1)-C(5)	116.50(16)	N(14)-N(13)-N(12)	109.6(3)
C(7)-Mo(1)-C(5)	61.44(19)	N(14)-N(13)-Mo(2)	128.2(3)
C(4)-Mo(2)-C(3)	76.77(18)	N(12)-N(13)-Mo(2)	122.1(2)
C(4)-Mo(2)-N(1)	91.43(17)	N(13)-N(14)-C(17)	103.1(3)
C(3)-Mo(2)-N(1)	93.36(14)	O(1)-C(1)-Mo(1)	176.0(4)
C(4)-Mo(2)-C(9)	103.8(2)	O(2)-C(2)-Mo(1)	175.7(4)
C(3)-Mo(2)-C(9)	102.82(18)	O(3)-C(3)-Mo(2)	174.3(4)
N(1)-Mo(2)-C(9)	159.82(16)	O(4)-C(4)-Mo(2)	174.7(4)
C(4)-Mo(2)-N(6)	166.81(17)	C(6)-C(5)-Mo(1)	67.3(3)
C(3)-Mo(2)-N(6)	98.09(14)	C(5)-C(6)-C(7)	115.8(5)
N(1)-Mo(2)-N(6)	76.63(12)	C(5)-C(6)-Mo(1)	77.6(3)
C(9)-Mo(2)-N(6)	89.08(17)	C(7)-C(6)-Mo(1)	75.9(3)
C(4)-Mo(2)-N(13)	100.96(16)	C(6)-C(7)-Mo(1)	67.3(3)
C(3)-Mo(2)-N(13)	170.06(14)	C(9)-C(8)-Mo(2)	67.4(3)
N(1)-Mo(2)-N(13)	76.95(12)	C(10)-C(9)-C(8)	115.9(5)
C(9)-Mo(2)-N(13)	87.12(16)	C(10)-C(9)-Mo(2)	77.4(3)
N(6)-Mo(2)-N(13)	81.99(12)	C(8)-C(9)-Mo(2)	76.3(3)
C(4)-Mo(2)-C(8)	106.96(18)	C(9)-C(10)-Mo(2)	67.1(3)
C(3)-Mo(2)-C(8)	68.79(18)	N(4)-C(11)-N(7)	113.3(3)
N(1)-Mo(2)-C(8)	149.81(15)	N(4)-C(11)-C(12)	121.4(4)
C(9)-Mo(2)-C(8)	36.31(18)	N(7)-C(11)-C(12)	125.2(4)
N(6)-Mo(2)-C(8)	81.89(14)	C(13)-C(12)-C(11)	125.6(4)
N(13)-Mo(2)-C(8)	120.90(15)	C(13)-C(12)-C(14)	119.7(4)
C(4)-Mo(2)-C(10)	70.7(2)	C(11)-C(12)-C(14)	114.7(4)
C(3)-Mo(2)-C(10)	106.42(17)	C(12)-C(13)-C(16)	124.1(4)
N(1)-Mo(2)-C(10)	148.81(16)	C(12)-C(13)-C(15)	119.7(4)
C(9)-Mo(2)-C(10)	35.49(19)	C(16)-C(13)-C(15)	116.2(4)
N(6)-Mo(2)-C(10)	122.52(17)	N(8)-C(14)-C(12)	178.3(5)
N(13)-Mo(2)-C(10)	81.57(15)	N(9)-C(15)-C(13)	179.2(6)
C(8)-Mo(2)-C(10)	61.37(18)	N(10)-C(16)-C(13)	174.7(5)
N(2)-N(1)-Mo(2)	117.9(3)	N(11)-C(17)-N(14)	113.6(3)
N(2)-N(1)-Mo(1)	119.7(3)	N(11)-C(17)-C(18)	121.0(4)
Mo(2)-N(1)-Mo(1)	122.02(14)	N(14)-C(17)-C(18)	125.3(4)
N(3)-N(2)-N(1)	179.6(5)	C(19)-C(18)-C(20)	119.3(4)
N(5)-N(4)-C(11)	104.2(3)	C(19)-C(18)-C(17)	124.2(4)
N(4)-N(5)-N(6)	109.3(3)	C(20)-C(18)-C(17)	116.4(4)
N(4)-N(5)-Mo(1)	128.5(2)	C(18)-C(19)-C(22)	123.1(4)
N(6)-N(5)-Mo(1)	122.2(2)	C(18)-C(19)-C(21)	120.1(4)
N(7)-N(6)-N(5)	109.2(3)	C(22)-C(19)-C(21)	116.7(4)
N(7)-N(6)-Mo(2)	126.7(2)	N(15)-C(20)-C(18)	177.5(5)
N(5)-N(6)-Mo(2)	124.0(2)	N(16)-C(21)-C(19)	176.7(5)
N(6)-N(7)-C(11)	104.0(3)	N(17)-C(22)-C(19)	177.3(5)

C(25)-N(18)-C(26)	108.2(4)	C(26)-N(18)-C(24)	109.1(4)
C(25)-N(18)-C(23)	109.2(4)	C(23)-N(18)-C(24)	110.8(4)
C(26)-N(18)-C(23)	109.8(4)	Cl(1)-C(27)-Cl(2)	108.3(3)
C(25)-N(18)-C(24)	109.7(4)		

Symmetry transformations used to generate equivalent atoms:

Table S9. Crystal data and structure refinement for $[N(CH_3)_4][(\mu\text{-}N_4C\{C_6H_4NO_2\}\text{-}\kappa^2N^2{:}N^3)_2(\mu_{1,1}\text{-}N_3)\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]\cdot(THF)$

Empirical formula	$C_{32}H_{38}Mo_2N_{14}O_9$	
Formula weight	954.64	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.3540(6) Å	α = 66.3975(12)°.
	b = 12.9495(7) Å	β = 70.1697(10)°.
	c = 14.5236(7) Å	γ = 77.6550(11)°.
Volume	1994.63(17) $Å^3$	
Z	2	
Density (calculated)	1.589 Mg/m^3	
Absorption coefficient	0.698 mm^{-1}	
F(000)	968	
Crystal size	0.28 x 0.15 x 0.15 mm^3	
Theta range for data collection	1.76 to 27.50°.	
Index ranges	-16<=h<=16, -16<=k<=16, -18<=l<=18	
Reflections collected	26034	
Independent reflections	9151 [R(int) = 0.0489]	
Completeness to theta = 27.50°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9026 and 0.8286	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9151 / 17 / 509	
Goodness-of-fit on F^2	1.099	
Final R indices [I>2sigma(I)]	R1 = 0.0581, wR2 = 0.1361	
R indices (all data)	R1 = 0.0769, wR2 = 0.1456	
Largest diff. peak and hole	1.551 and -0.699 $e.Å^{-3}$	

Table S10. Bond lengths [Å] and angles [°] for $[N(CH_3)_4][(\mu\text{-}N_4C\{C_6H_4NO_2\}\text{-}\kappa^2N^2{:}N^3)_2(\mu_{1,1}\text{-}N_3)\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]\cdot(THF)$

Mo(1)-C(1)	1.951(5)	N(13')-C(22)	1.502(19)
Mo(1)-C(2)	1.955(5)	O(1)-C(1)	1.151(6)
Mo(1)-C(6)	2.196(5)	O(2)-C(2)	1.152(6)
Mo(1)-N(5)	2.197(4)	O(3)-C(3)	1.156(6)
Mo(1)-N(1)	2.246(4)	O(4)-C(4)	1.149(7)
Mo(1)-N(11)	2.264(3)	C(5)-C(6)	1.403(7)
Mo(1)-C(7)	2.315(5)	C(6)-C(7)	1.407(7)
Mo(1)-C(5)	2.315(5)	C(8)-C(9)	1.403(8)
Mo(2)-C(3)	1.949(6)	C(9)-C(10)	1.402(8)
Mo(2)-C(4)	1.950(6)	C(11)-C(12)	1.466(6)
Mo(2)-N(6)	2.201(4)	C(12)-C(17)	1.390(6)
Mo(2)-C(9)	2.204(5)	C(12)-C(13)	1.396(6)
Mo(2)-N(10)	2.249(4)	C(13)-C(14)	1.382(6)
Mo(2)-N(1)	2.255(4)	C(14)-C(15)	1.376(6)
Mo(2)-C(10)	2.302(5)	C(15)-C(16)	1.379(6)
Mo(2)-C(8)	2.314(6)	C(16)-C(17)	1.379(6)
N(1)-N(2)	1.204(5)	C(18)-C(19)	1.472(6)
N(2)-N(3)	1.145(6)	C(19)-C(24)	1.372(7)
N(4)-N(5)	1.342(5)	C(19)-C(20)	1.393(7)
N(4)-C(11)	1.343(5)	C(20)-C(21)	1.391(7)
N(5)-N(6)	1.335(5)	C(21)-C(22)	1.346(9)
N(6)-N(7)	1.326(5)	C(22)-C(23)	1.397(9)
N(7)-C(11)	1.321(6)	C(23)-C(24)	1.384(7)
N(8)-O(5)	1.210(5)	N(14)-C(28')	1.40(3)
N(8)-O(6)	1.228(5)	N(14)-C(27)	1.442(9)
N(8)-C(15)	1.473(6)	N(14)-C(26')	1.45(3)
N(9)-N(10)	1.333(5)	N(14)-C(28)	1.469(9)
N(9)-C(18)	1.338(6)	N(14)-C(25)	1.487(6)
N(10)-N(11)	1.332(5)	N(14)-C(26)	1.545(10)
N(11)-N(12)	1.329(5)	N(14)-C(27')	1.61(3)
N(12)-C(18)	1.340(6)	O(9)-C(29)	1.497(13)
N(13)-O(7)	1.21(3)	O(9)-C(32)	1.540(13)
N(13)-O(8)	1.243(18)	C(29)-C(30)	1.361(15)
N(13)-C(22)	1.498(16)	C(30)-C(31)	1.482(15)
N(13')-O(7')	1.18(4)	C(31)-C(32)	1.503(14)
N(13')-O(8')	1.25(2)		

C(1)-Mo(1)-C(2)	79.8(2)	C(1)-Mo(1)-N(1)	164.97(17)
C(1)-Mo(1)-C(6)	102.6(2)	C(2)-Mo(1)-N(1)	95.27(19)
C(2)-Mo(1)-C(6)	104.5(2)	C(6)-Mo(1)-N(1)	92.39(17)
C(1)-Mo(1)-N(5)	88.25(16)	N(5)-Mo(1)-N(1)	77.60(13)
C(2)-Mo(1)-N(5)	91.39(18)	C(1)-Mo(1)-N(11)	102.11(17)
C(6)-Mo(1)-N(5)	161.99(17)	C(2)-Mo(1)-N(11)	169.75(17)

C(6)-Mo(1)-N(11)	84.96(17)	Mo(1)-N(1)-Mo(2)	116.01(16)
N(5)-Mo(1)-N(11)	78.66(13)	N(3)-N(2)-N(1)	178.6(5)
N(1)-Mo(1)-N(11)	80.28(13)	N(5)-N(4)-C(11)	103.7(3)
C(1)-Mo(1)-C(7)	68.21(19)	N(6)-N(5)-N(4)	109.1(3)
C(2)-Mo(1)-C(7)	108.3(2)	N(6)-N(5)-Mo(1)	124.8(3)
C(6)-Mo(1)-C(7)	36.24(19)	N(4)-N(5)-Mo(1)	125.9(3)
N(5)-Mo(1)-C(7)	145.21(16)	N(7)-N(6)-N(5)	109.6(3)
N(1)-Mo(1)-C(7)	126.71(16)	N(7)-N(6)-Mo(2)	126.6(3)
N(11)-Mo(1)-C(7)	81.63(15)	N(5)-N(6)-Mo(2)	123.9(3)
C(1)-Mo(1)-C(5)	107.57(19)	C(11)-N(7)-N(6)	104.8(4)
C(2)-Mo(1)-C(5)	70.5(2)	O(5)-N(8)-O(6)	123.3(4)
C(6)-Mo(1)-C(5)	36.12(19)	O(5)-N(8)-C(15)	118.4(4)
N(5)-Mo(1)-C(5)	152.75(17)	O(6)-N(8)-C(15)	118.3(4)
N(1)-Mo(1)-C(5)	83.77(17)	N(10)-N(9)-C(18)	104.1(3)
N(11)-Mo(1)-C(5)	117.75(17)	N(11)-N(10)-N(9)	109.6(3)
C(7)-Mo(1)-C(5)	61.91(18)	N(11)-N(10)-Mo(2)	123.3(3)
C(3)-Mo(2)-C(4)	81.6(3)	N(9)-N(10)-Mo(2)	126.4(3)
C(3)-Mo(2)-N(6)	87.92(18)	N(12)-N(11)-N(10)	109.6(3)
C(4)-Mo(2)-N(6)	89.6(2)	N(12)-N(11)-Mo(1)	126.4(3)
C(3)-Mo(2)-C(9)	104.4(2)	N(10)-N(11)-Mo(1)	123.5(3)
C(4)-Mo(2)-C(9)	104.8(2)	N(11)-N(12)-C(18)	104.3(3)
N(6)-Mo(2)-C(9)	162.08(18)	O(7)-N(13)-O(8)	124(2)
C(3)-Mo(2)-N(10)	165.85(19)	O(7)-N(13)-C(22)	110.9(19)
C(4)-Mo(2)-N(10)	94.8(2)	O(8)-N(13)-C(22)	124.7(12)
N(6)-Mo(2)-N(10)	78.32(13)	O(7')-N(13')-O(8')	124(3)
C(9)-Mo(2)-N(10)	89.74(17)	O(7')-N(13')-C(22)	129(2)
C(3)-Mo(2)-N(1)	100.0(2)	O(8')-N(13')-C(22)	106.7(16)
C(4)-Mo(2)-N(1)	167.6(2)	O(1)-C(1)-Mo(1)	176.2(4)
N(6)-Mo(2)-N(1)	78.15(14)	O(2)-C(2)-Mo(1)	178.6(5)
C(9)-Mo(2)-N(1)	86.80(19)	O(3)-C(3)-Mo(2)	177.2(6)
N(10)-Mo(2)-N(1)	80.52(13)	O(4)-C(4)-Mo(2)	178.4(6)
C(3)-Mo(2)-C(10)	110.0(2)	C(6)-C(5)-Mo(1)	67.3(3)
C(4)-Mo(2)-C(10)	70.6(2)	C(5)-C(6)-C(7)	115.8(5)
N(6)-Mo(2)-C(10)	150.3(2)	C(5)-C(6)-Mo(1)	76.6(3)
C(9)-Mo(2)-C(10)	36.2(2)	C(7)-C(6)-Mo(1)	76.5(3)
N(10)-Mo(2)-C(10)	81.39(18)	C(6)-C(7)-Mo(1)	67.3(3)
N(1)-Mo(2)-C(10)	119.61(19)	C(9)-C(8)-Mo(2)	67.7(3)
C(3)-Mo(2)-C(8)	69.8(2)	C(10)-C(9)-C(8)	115.1(6)
C(4)-Mo(2)-C(8)	108.7(2)	C(10)-C(9)-Mo(2)	75.7(3)
N(6)-Mo(2)-C(8)	147.95(19)	C(8)-C(9)-Mo(2)	76.2(3)
C(9)-Mo(2)-C(8)	36.07(19)	C(9)-C(10)-Mo(2)	68.1(3)
N(10)-Mo(2)-C(8)	124.10(17)	N(7)-C(11)-N(4)	112.7(4)
N(1)-Mo(2)-C(8)	83.3(2)	N(7)-C(11)-C(12)	123.7(4)
C(10)-Mo(2)-C(8)	61.7(2)	N(4)-C(11)-C(12)	123.5(4)
N(2)-N(1)-Mo(1)	118.4(3)	C(17)-C(12)-C(13)	119.5(4)
N(2)-N(1)-Mo(2)	121.8(3)	C(17)-C(12)-C(11)	122.0(4)

C(13)-C(12)-C(11)	118.5(4)	C(28')-N(14)-C(26')	105.5(17)
C(14)-C(13)-C(12)	120.3(4)	C(27)-N(14)-C(26')	60.4(13)
C(15)-C(14)-C(13)	118.6(4)	C(28')-N(14)-C(28)	50.2(12)
C(14)-C(15)-C(16)	122.4(4)	C(27)-N(14)-C(28)	113.1(7)
C(14)-C(15)-N(8)	118.4(4)	C(26')-N(14)-C(28)	138.1(12)
C(16)-C(15)-N(8)	119.2(4)	C(28')-N(14)-C(25)	109.5(11)
C(17)-C(16)-C(15)	118.6(4)	C(27)-N(14)-C(25)	110.5(5)
C(16)-C(17)-C(12)	120.5(4)	C(26')-N(14)-C(25)	109.4(12)
N(9)-C(18)-N(12)	112.4(4)	C(28)-N(14)-C(25)	111.1(5)
N(9)-C(18)-C(19)	124.3(4)	C(28')-N(14)-C(26)	59.8(12)
N(12)-C(18)-C(19)	123.3(4)	C(27)-N(14)-C(26)	105.7(6)
C(24)-C(19)-C(20)	120.3(5)	C(26')-N(14)-C(26)	48.2(12)
C(24)-C(19)-C(18)	120.8(4)	C(28)-N(14)-C(26)	106.7(7)
C(20)-C(19)-C(18)	118.9(4)	C(25)-N(14)-C(26)	109.5(5)
C(21)-C(20)-C(19)	119.0(5)	C(28')-N(14)-C(27')	120.5(15)
C(22)-C(21)-C(20)	119.3(6)	C(27)-N(14)-C(27')	45.6(9)
C(21)-C(22)-C(23)	123.4(5)	C(26')-N(14)-C(27')	104.8(16)
C(21)-C(22)-N(13)	109.6(8)	C(28)-N(14)-C(27')	73.4(10)
C(23)-C(22)-N(13)	127.1(8)	C(25)-N(14)-C(27')	106.7(9)
C(21)-C(22)-N(13')	131.4(9)	C(26)-N(14)-C(27')	140.5(10)
C(23)-C(22)-N(13')	105.2(9)	C(29)-O(9)-C(32)	105.6(11)
N(13)-C(22)-N(13')	22.0(7)	C(30)-C(29)-O(9)	92.5(14)
C(24)-C(23)-C(22)	116.6(6)	C(29)-C(30)-C(31)	102.6(17)
C(19)-C(24)-C(23)	121.4(6)	C(30)-C(31)-C(32)	103.4(15)
C(28')-N(14)-C(27)	140.0(12)	C(31)-C(32)-O(9)	97.3(12)

Symmetry transformations used to generate equivalent atoms:

Table S11.Crystal data and structure refinement for $[N(CH_3)_4][(\mu\text{-}N_3C_2\{CO_2CH_3\}_2\text{-}\kappa^2N^1{:}N^2)(\mu_{1,1}\text{-}N_3)_2\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]$

Empirical formula	$C_{20}H_{28}Mo_2N_{10}O_8$	
Formula weight	728.40	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.3722(7) Å	α = 79.3555(13)°.
	b = 12.2607(8) Å	β = 68.3190(12)°.
	c = 13.1324(9) Å	γ = 69.1996(12)°.
Volume	1448.00(17) $Å^3$	
Z	2	
Density (calculated)	1.671 Mg/m^3	
Absorption coefficient	0.926 mm^{-1}	
F(000)	732	
Crystal size	0.38 x 0.35 x 0.30 mm^3	
Theta range for data collection	1.67 to 27.50°.	
Index ranges	-13<=h<=13, -15<=k<=15, -17<=l<=17	
Reflections collected	18748	
Independent reflections	6638 [R(int) = 0.0202]	
Completeness to theta = 27.50°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7686 and 0.7199	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6638 / 0 / 367	
Goodness-of-fit on F^2	1.052	
Final R indices [I>2sigma(I)]	R1 = 0.0218, wR2 = 0.0544	
R indices (all data)	R1 = 0.0246, wR2 = 0.0556	
Largest diff. peak and hole	0.422 and -0.355 $e.Å^{-3}$	

Table S12. Bond lengths [Å] and angles [°] for $[N(CH_3)_4][(\mu\text{-}N_3C_2\{CO_2CH_3\}_2\text{-}\kappa^2N^1{:}N^2)(\mu_{1,1}\text{-}N_3)_2\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]$

Mo(1)-C(1)	1.9455(19)	N(9)-C(12)	1.342(2)
Mo(1)-C(2)	1.9548(19)	C(1)-O(1)	1.159(2)
Mo(1)-C(6)	2.2020(18)	C(2)-O(2)	1.151(2)
Mo(1)-N(7)	2.2180(14)	C(3)-O(3)	1.156(2)
Mo(1)-N(4)	2.2598(15)	C(4)-O(4)	1.150(2)
Mo(1)-N(1)	2.2962(15)	C(5)-C(6)	1.408(3)
Mo(1)-C(7)	2.3058(18)	C(6)-C(7)	1.407(3)
Mo(1)-C(5)	2.3194(19)	C(8)-C(9)	1.398(3)
Mo(2)-C(3)	1.9382(19)	C(9)-C(10)	1.395(4)
Mo(2)-C(4)	1.939(2)	C(11)-C(12)	1.384(2)
Mo(2)-N(8)	2.1733(14)	C(11)-C(13)	1.491(2)
Mo(2)-C(9)	2.1941(19)	C(12)-C(15)	1.477(2)
Mo(2)-N(4)	2.2726(15)	C(13)-O(5)	1.198(2)
Mo(2)-N(1)	2.2828(15)	C(13)-O(6)	1.313(2)
Mo(2)-C(10)	2.299(2)	C(14)-O(6)	1.449(2)
Mo(2)-C(8)	2.308(2)	C(15)-O(7)	1.197(2)
N(1)-N(2)	1.206(2)	C(15)-O(8)	1.331(2)
N(2)-N(3)	1.140(2)	C(16)-O(8)	1.449(2)
N(4)-N(5)	1.201(2)	N(10)-C(19)	1.473(3)
N(5)-N(6)	1.144(2)	N(10)-C(20)	1.484(3)
N(7)-C(11)	1.341(2)	N(10)-C(17)	1.491(3)
N(7)-N(8)	1.3576(19)	N(10)-C(18)	1.494(2)
N(8)-N(9)	1.316(2)		

C(1)-Mo(1)-C(2)	79.96(8)	N(7)-Mo(1)-C(7)	149.60(6)
C(1)-Mo(1)-C(6)	102.66(8)	N(4)-Mo(1)-C(7)	83.52(6)
C(2)-Mo(1)-C(6)	103.27(8)	N(1)-Mo(1)-C(7)	119.02(7)
C(1)-Mo(1)-N(7)	91.50(6)	C(1)-Mo(1)-C(5)	68.25(8)
C(2)-Mo(1)-N(7)	92.12(6)	C(2)-Mo(1)-C(5)	106.90(8)
C(6)-Mo(1)-N(7)	160.59(7)	C(6)-Mo(1)-C(5)	36.18(7)
C(1)-Mo(1)-N(4)	168.36(7)	N(7)-Mo(1)-C(5)	148.53(6)
C(2)-Mo(1)-N(4)	101.90(7)	N(4)-Mo(1)-C(5)	121.33(7)
C(6)-Mo(1)-N(4)	88.18(7)	N(1)-Mo(1)-C(5)	84.00(7)
N(7)-Mo(1)-N(4)	76.98(5)	C(7)-Mo(1)-C(5)	61.86(7)
C(1)-Mo(1)-N(1)	103.07(7)	C(3)-Mo(2)-C(4)	78.89(8)
C(2)-Mo(1)-N(1)	168.94(7)	C(3)-Mo(2)-N(8)	88.90(7)
C(6)-Mo(1)-N(1)	86.56(7)	C(4)-Mo(2)-N(8)	88.31(7)
N(7)-Mo(1)-N(1)	77.25(5)	C(3)-Mo(2)-C(9)	104.02(8)
N(4)-Mo(1)-N(1)	73.01(5)	C(4)-Mo(2)-C(9)	104.75(9)
C(1)-Mo(1)-C(7)	107.72(7)	N(8)-Mo(2)-C(9)	163.04(7)
C(2)-Mo(1)-C(7)	69.20(7)	C(3)-Mo(2)-N(4)	166.59(7)
C(6)-Mo(1)-C(7)	36.27(7)	C(4)-Mo(2)-N(4)	99.22(7)

N(8)-Mo(2)-N(4)	77.75(5)	O(1)-C(1)-Mo(1)	177.60(16)
C(9)-Mo(2)-N(4)	89.32(7)	O(2)-C(2)-Mo(1)	176.52(17)
C(3)-Mo(2)-N(1)	105.12(7)	O(3)-C(3)-Mo(2)	175.88(16)
C(4)-Mo(2)-N(1)	163.27(7)	O(4)-C(4)-Mo(2)	177.2(2)
N(8)-Mo(2)-N(1)	75.66(5)	C(6)-C(5)-Mo(1)	67.37(10)
C(9)-Mo(2)-N(1)	90.18(8)	C(7)-C(6)-C(5)	115.25(19)
N(4)-Mo(2)-N(1)	73.03(5)	C(7)-C(6)-Mo(1)	75.88(11)
C(3)-Mo(2)-C(10)	107.50(8)	C(5)-C(6)-Mo(1)	76.46(11)
C(4)-Mo(2)-C(10)	70.49(9)	C(6)-C(7)-Mo(1)	67.84(10)
N(8)-Mo(2)-C(10)	149.41(8)	C(9)-C(8)-Mo(2)	67.51(11)
C(9)-Mo(2)-C(10)	36.08(9)	C(10)-C(9)-C(8)	115.7(2)
N(4)-Mo(2)-C(10)	84.02(7)	C(10)-C(9)-Mo(2)	76.07(12)
N(1)-Mo(2)-C(10)	122.07(8)	C(8)-C(9)-Mo(2)	76.43(12)
C(3)-Mo(2)-C(8)	70.22(8)	C(9)-C(10)-Mo(2)	67.85(12)
C(4)-Mo(2)-C(8)	109.34(8)	N(7)-C(11)-C(12)	107.47(15)
N(8)-Mo(2)-C(8)	148.61(8)	N(7)-C(11)-C(13)	123.53(15)
C(9)-Mo(2)-C(8)	36.07(9)	C(12)-C(11)-C(13)	128.99(15)
N(4)-Mo(2)-C(8)	122.41(7)	N(9)-C(12)-C(11)	108.42(15)
N(1)-Mo(2)-C(8)	87.15(7)	N(9)-C(12)-C(15)	120.43(16)
C(10)-Mo(2)-C(8)	61.77(9)	C(11)-C(12)-C(15)	131.12(16)
N(2)-N(1)-Mo(2)	122.08(12)	O(5)-C(13)-O(6)	126.39(17)
N(2)-N(1)-Mo(1)	126.94(12)	O(5)-C(13)-C(11)	123.13(16)
Mo(2)-N(1)-Mo(1)	101.92(6)	O(6)-C(13)-C(11)	110.47(14)
N(3)-N(2)-N(1)	179.5(2)	O(7)-C(15)-O(8)	124.68(17)
N(5)-N(4)-Mo(1)	130.31(12)	O(7)-C(15)-C(12)	124.60(17)
N(5)-N(4)-Mo(2)	125.79(12)	O(8)-C(15)-C(12)	110.72(16)
Mo(1)-N(4)-Mo(2)	103.38(6)	C(13)-O(6)-C(14)	116.72(14)
N(6)-N(5)-N(4)	178.71(19)	C(15)-O(8)-C(16)	114.35(15)
C(11)-N(7)-N(8)	106.01(13)	C(19)-N(10)-C(20)	110.2(2)
C(11)-N(7)-Mo(1)	136.29(12)	C(19)-N(10)-C(17)	110.56(19)
N(8)-N(7)-Mo(1)	117.69(10)	C(20)-N(10)-C(17)	108.68(17)
N(9)-N(8)-N(7)	111.51(13)	C(19)-N(10)-C(18)	109.71(18)
N(9)-N(8)-Mo(2)	126.00(11)	C(20)-N(10)-C(18)	108.32(16)
N(7)-N(8)-Mo(2)	122.24(10)	C(17)-N(10)-C(18)	109.32(16)
N(8)-N(9)-C(12)	106.59(14)		

Symmetry transformations used to generate equivalent atoms:

Table S13. Crystal data and structure refinement for $[N(CH_3)_4][(\mu\text{-}N_3C_2\{CO_2CH_2CH_3\}_2\text{-}\kappa^2N^1{:}N^2)(\mu_{1,1}\text{-}N_3)_2\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]\cdot 1/2(THF)$

Empirical formula	$C_{24}H_{36}Mo_2N_{10}O_{8.50}$	
Formula weight	792.51	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.4046(3) Å	α = 90°.
	b = 29.2236(6) Å	β = 90.5145(10)°.
	c = 17.1632(3) Å	γ = 90°.
Volume	6723.1(2) $Å^3$	
Z	8	
Density (calculated)	1.566 Mg/m^3	
Absorption coefficient	0.806 mm^{-1}	
F(000)	3216	
Crystal size	0.18 x 0.15 x 0.10 mm^3	
Theta range for data collection	1.38 to 27.50°.	
Index ranges	-17<=h<=17, -37<=k<=37, -22<=l<=22	
Reflections collected	42118	
Independent reflections	15379 [R(int) = 0.0450]	
Completeness to theta = 27.50°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.926 and 0.829	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	15379 / 0 / 814	
Goodness-of-fit on F^2	1.062	
Final R indices [I>2sigma(I)]	R1 = 0.0428, wR2 = 0.1126	
R indices (all data)	R1 = 0.0786, wR2 = 0.1226	
Largest diff. peak and hole	1.367 and -0.590 $e.Å^{-3}$	

Table S14. Bond lengths [Å] and angles [°] for $[N(CH_3)_4][(\mu\text{-}N_3C_2\{CO_2CH_2CH_3\}_2\text{-}\kappa^2N^1{:}N^2)(\mu_{1,1}\text{-}N_3)_2\{Mo(\eta^3\text{-}C_3H_5)(CO)_2\}_2]\cdot 1/2(THF)$

Mo(1)-C(1)	1.961(4)	Mo(3)-C(20)	1.953(4)
Mo(1)-C(2)	1.972(5)	Mo(3)-C(19)	1.954(4)
Mo(1)-C(6)	2.197(4)	Mo(3)-C(24)	2.195(4)
Mo(1)-N(7)	2.233(3)	Mo(3)-N(16)	2.224(3)
Mo(1)-N(4)	2.255(3)	Mo(3)-N(13)	2.246(3)
Mo(1)-N(1)	2.266(3)	Mo(3)-N(10)	2.276(3)
Mo(1)-C(5)	2.304(4)	Mo(3)-C(25)	2.302(4)
Mo(1)-C(7)	2.318(4)	Mo(3)-C(23)	2.317(4)
Mo(2)-C(4)	1.941(4)	Mo(4)-C(21)	1.942(5)
Mo(2)-C(3)	1.947(5)	Mo(4)-C(22)	1.966(4)
Mo(2)-N(8)	2.206(3)	Mo(4)-N(17)	2.196(3)
Mo(2)-C(9)	2.208(4)	Mo(4)-C(27)	2.202(4)
Mo(2)-N(4)	2.250(3)	Mo(4)-N(13)	2.260(3)
Mo(2)-N(1)	2.275(3)	Mo(4)-N(10)	2.267(3)
Mo(2)-C(10)	2.315(4)	Mo(4)-C(26)	2.304(4)
Mo(2)-C(8)	2.318(4)	Mo(4)-C(28)	2.316(4)
N(1)-N(2)	1.184(4)	N(10)-N(11)	1.186(5)
N(2)-N(3)	1.155(4)	N(11)-N(12)	1.140(5)
N(4)-N(5)	1.208(4)	N(13)-N(14)	1.190(4)
N(5)-N(6)	1.145(5)	N(14)-N(15)	1.147(5)
N(7)-C(11)	1.337(4)	N(16)-C(29)	1.340(4)
N(7)-N(8)	1.346(4)	N(16)-N(17)	1.359(4)
N(8)-N(9)	1.323(4)	N(17)-N(18)	1.318(4)
N(9)-C(12)	1.350(5)	N(18)-C(30)	1.350(5)
C(1)-O(1)	1.150(5)	C(19)-O(9)	1.153(4)
C(2)-O(2)	1.144(5)	C(20)-O(10)	1.154(5)
C(3)-O(3)	1.156(5)	C(21)-O(11)	1.165(5)
C(4)-O(4)	1.158(5)	C(22)-O(12)	1.154(5)
C(5)-C(6)	1.410(6)	C(23)-C(24)	1.384(6)
C(6)-C(7)	1.398(6)	C(24)-C(25)	1.406(6)
C(8)-C(9)	1.398(7)	C(26)-C(27)	1.385(6)
C(9)-C(10)	1.414(7)	C(27)-C(28)	1.415(6)
C(11)-C(12)	1.379(5)	C(29)-C(30)	1.385(5)
C(11)-C(13)	1.500(5)	C(29)-C(31)	1.499(5)
C(12)-C(16)	1.498(5)	C(30)-C(34)	1.479(5)
C(13)-O(5)	1.205(4)	C(31)-O(13)	1.186(5)
C(13)-O(6)	1.330(5)	C(31)-O(14)	1.334(5)
C(14)-O(6)	1.459(5)	C(32)-O(14)	1.466(5)
C(14)-C(15)	1.505(6)	C(32)-C(33)	1.490(7)
C(16)-O(7)	1.196(5)	C(34)-O(15)	1.203(5)
C(16)-O(8)	1.330(5)	C(34)-O(16)	1.320(5)
C(17)-O(8)	1.451(4)	C(35)-O(16)	1.452(4)
C(17)-C(18)	1.508(6)	C(35)-C(36)	1.489(6)

N(19)-C(37)	1.440(6)	N(20)-C(41)	1.693(8)
N(19)-C(40)	1.454(6)	O(17)-C(48)	1.394(6)
N(19)-C(39)	1.468(6)	O(17)-C(45)	1.417(7)
N(19)-C(38)	1.576(7)	C(45)-C(46)	1.364(8)
N(20)-C(42)	1.430(6)	C(46)-C(47)	1.499(8)
N(20)-C(43)	1.448(6)	C(47)-C(48)	1.488(7)
N(20)-C(44)	1.453(5)		

C(1)-Mo(1)-C(2)	82.26(17)	C(4)-Mo(2)-N(1)	166.61(15)
C(1)-Mo(1)-C(6)	102.82(16)	C(3)-Mo(2)-N(1)	104.64(16)
C(2)-Mo(1)-C(6)	103.06(17)	N(8)-Mo(2)-N(1)	76.23(11)
C(1)-Mo(1)-N(7)	92.11(14)	C(9)-Mo(2)-N(1)	87.79(14)
C(2)-Mo(1)-N(7)	92.24(15)	N(4)-Mo(2)-N(1)	73.60(11)
C(6)-Mo(1)-N(7)	159.81(14)	C(4)-Mo(2)-C(10)	70.03(17)
C(1)-Mo(1)-N(4)	169.22(14)	C(3)-Mo(2)-C(10)	107.74(18)
C(2)-Mo(1)-N(4)	99.51(15)	N(8)-Mo(2)-C(10)	150.32(16)
C(6)-Mo(1)-N(4)	87.20(14)	C(9)-Mo(2)-C(10)	36.32(17)
N(7)-Mo(1)-N(4)	77.22(11)	N(4)-Mo(2)-C(10)	83.61(15)
C(1)-Mo(1)-N(1)	102.69(15)	N(1)-Mo(2)-C(10)	119.99(15)
C(2)-Mo(1)-N(1)	168.32(15)	C(4)-Mo(2)-C(8)	108.61(17)
C(6)-Mo(1)-N(1)	86.29(14)	C(3)-Mo(2)-C(8)	69.90(18)
N(7)-Mo(1)-N(1)	77.13(11)	N(8)-Mo(2)-C(8)	147.50(15)
N(4)-Mo(1)-N(1)	73.66(11)	C(9)-Mo(2)-C(8)	35.87(17)
C(1)-Mo(1)-C(5)	107.25(16)	N(4)-Mo(2)-C(8)	122.05(15)
C(2)-Mo(1)-C(5)	68.19(16)	N(1)-Mo(2)-C(8)	84.58(14)
C(6)-Mo(1)-C(5)	36.42(15)	C(10)-Mo(2)-C(8)	62.16(18)
N(7)-Mo(1)-C(5)	149.57(13)	N(2)-N(1)-Mo(1)	126.8(3)
N(4)-Mo(1)-C(5)	83.15(13)	N(2)-N(1)-Mo(2)	130.9(3)
N(1)-Mo(1)-C(5)	119.30(14)	Mo(1)-N(1)-Mo(2)	101.91(12)
C(1)-Mo(1)-C(7)	68.89(16)	N(3)-N(2)-N(1)	178.6(4)
C(2)-Mo(1)-C(7)	108.95(17)	N(5)-N(4)-Mo(2)	125.5(3)
C(6)-Mo(1)-C(7)	35.95(15)	N(5)-N(4)-Mo(1)	124.9(3)
N(7)-Mo(1)-C(7)	148.51(14)	Mo(2)-N(4)-Mo(1)	103.01(12)
N(4)-Mo(1)-C(7)	119.89(14)	N(6)-N(5)-N(4)	178.9(5)
N(1)-Mo(1)-C(7)	82.73(14)	C(11)-N(7)-N(8)	107.0(3)
C(5)-Mo(1)-C(7)	61.92(15)	C(11)-N(7)-Mo(1)	134.6(3)
C(4)-Mo(2)-C(3)	78.68(18)	N(8)-N(7)-Mo(1)	117.9(2)
C(4)-Mo(2)-N(8)	90.93(14)	N(9)-N(8)-N(7)	111.3(3)
C(3)-Mo(2)-N(8)	89.69(15)	N(9)-N(8)-Mo(2)	127.5(2)
C(4)-Mo(2)-C(9)	104.19(17)	N(7)-N(8)-Mo(2)	120.9(2)
C(3)-Mo(2)-C(9)	103.50(18)	N(8)-N(9)-C(12)	106.0(3)
N(8)-Mo(2)-C(9)	161.51(14)	O(1)-C(1)-Mo(1)	177.4(4)
C(4)-Mo(2)-N(4)	100.20(15)	O(2)-C(2)-Mo(1)	178.2(4)
C(3)-Mo(2)-N(4)	167.10(15)	O(3)-C(3)-Mo(2)	176.1(4)
N(8)-Mo(2)-N(4)	77.45(11)	O(4)-C(4)-Mo(2)	177.8(4)
C(9)-Mo(2)-N(4)	89.27(16)	C(6)-C(5)-Mo(1)	67.7(2)

C(7)-C(6)-C(5)	115.7(4)	C(20)-Mo(3)-C(23)	69.49(15)
C(7)-C(6)-Mo(1)	76.8(2)	C(19)-Mo(3)-C(23)	109.22(15)
C(5)-C(6)-Mo(1)	75.9(2)	C(24)-Mo(3)-C(23)	35.58(15)
C(6)-C(7)-Mo(1)	67.3(2)	N(16)-Mo(3)-C(23)	151.03(13)
C(9)-C(8)-Mo(2)	67.8(2)	N(13)-Mo(3)-C(23)	82.56(13)
C(8)-C(9)-C(10)	116.6(4)	N(10)-Mo(3)-C(23)	118.17(14)
C(8)-C(9)-Mo(2)	76.3(3)	C(25)-Mo(3)-C(23)	61.77(16)
C(10)-C(9)-Mo(2)	76.0(3)	C(21)-Mo(4)-C(22)	81.27(17)
C(9)-C(10)-Mo(2)	67.7(2)	C(21)-Mo(4)-N(17)	89.29(14)
N(7)-C(11)-C(12)	107.0(3)	C(22)-Mo(4)-N(17)	90.49(14)
N(7)-C(11)-C(13)	123.3(3)	C(21)-Mo(4)-C(27)	104.03(17)
C(12)-C(11)-C(13)	129.7(3)	C(22)-Mo(4)-C(27)	104.68(16)
N(9)-C(12)-C(11)	108.7(3)	N(17)-Mo(4)-C(27)	161.03(14)
N(9)-C(12)-C(16)	120.7(3)	C(21)-Mo(4)-N(13)	166.59(14)
C(11)-C(12)-C(16)	130.4(4)	C(22)-Mo(4)-N(13)	98.92(14)
O(5)-C(13)-O(6)	125.7(4)	N(17)-Mo(4)-N(13)	77.30(11)
O(5)-C(13)-C(11)	122.8(4)	C(27)-Mo(4)-N(13)	88.95(15)
O(6)-C(13)-C(11)	111.5(3)	C(21)-Mo(4)-N(10)	103.24(15)
O(6)-C(14)-C(15)	107.7(4)	C(22)-Mo(4)-N(10)	165.77(14)
O(7)-C(16)-O(8)	126.1(4)	N(17)-Mo(4)-N(10)	76.19(11)
O(7)-C(16)-C(12)	124.5(4)	C(27)-Mo(4)-N(10)	87.48(14)
O(8)-C(16)-C(12)	109.4(3)	N(13)-Mo(4)-N(10)	73.53(11)
O(8)-C(17)-C(18)	106.1(3)	C(21)-Mo(4)-C(26)	107.45(17)
C(13)-O(6)-C(14)	115.0(3)	C(22)-Mo(4)-C(26)	70.30(16)
C(16)-O(8)-C(17)	115.7(3)	N(17)-Mo(4)-C(26)	151.60(15)
C(20)-Mo(3)-C(19)	82.31(17)	C(27)-Mo(4)-C(26)	35.71(15)
C(20)-Mo(3)-C(24)	103.42(16)	N(13)-Mo(4)-C(26)	85.03(14)
C(19)-Mo(3)-C(24)	104.37(15)	N(10)-Mo(4)-C(26)	119.94(14)
C(20)-Mo(3)-N(16)	92.32(13)	C(21)-Mo(4)-C(28)	70.04(17)
C(19)-Mo(3)-N(16)	89.53(13)	C(22)-Mo(4)-C(28)	111.04(17)
C(24)-Mo(3)-N(16)	160.12(13)	N(17)-Mo(4)-C(28)	146.54(15)
C(20)-Mo(3)-N(13)	99.22(14)	C(27)-Mo(4)-C(28)	36.39(17)
C(19)-Mo(3)-N(13)	167.72(13)	N(13)-Mo(4)-C(28)	121.63(15)
C(24)-Mo(3)-N(13)	87.19(13)	N(10)-Mo(4)-C(28)	83.12(14)
N(16)-Mo(3)-N(13)	78.25(11)	C(26)-Mo(4)-C(28)	61.85(17)
C(20)-Mo(3)-N(10)	167.90(14)	N(11)-N(10)-Mo(4)	127.8(3)
C(19)-Mo(3)-N(10)	102.61(15)	N(11)-N(10)-Mo(3)	130.1(3)
C(24)-Mo(3)-N(10)	86.22(14)	Mo(4)-N(10)-Mo(3)	101.84(13)
N(16)-Mo(3)-N(10)	76.79(11)	N(12)-N(11)-N(10)	179.4(5)
N(13)-Mo(3)-N(10)	73.63(11)	N(14)-N(13)-Mo(3)	127.2(3)
C(20)-Mo(3)-C(25)	109.16(16)	N(14)-N(13)-Mo(4)	124.7(3)
C(19)-Mo(3)-C(25)	69.91(15)	Mo(3)-N(13)-Mo(4)	103.03(12)
C(24)-Mo(3)-C(25)	36.34(14)	N(15)-N(14)-N(13)	178.9(4)
N(16)-Mo(3)-C(25)	147.19(14)	C(29)-N(16)-N(17)	106.8(3)
N(13)-Mo(3)-C(25)	120.36(13)	C(29)-N(16)-Mo(3)	135.8(2)
N(10)-Mo(3)-C(25)	82.94(14)	N(17)-N(16)-Mo(3)	117.1(2)

N(18)-N(17)-N(16)	110.9(3)	O(14)-C(31)-C(29)	109.2(3)
N(18)-N(17)-Mo(4)	127.2(2)	O(14)-C(32)-C(33)	107.2(4)
N(16)-N(17)-Mo(4)	121.7(2)	O(15)-C(34)-O(16)	125.2(4)
N(17)-N(18)-C(30)	106.8(3)	O(15)-C(34)-C(30)	124.4(4)
O(9)-C(19)-Mo(3)	178.9(4)	O(16)-C(34)-C(30)	110.4(3)
O(10)-C(20)-Mo(3)	178.2(3)	O(16)-C(35)-C(36)	106.3(4)
O(11)-C(21)-Mo(4)	177.0(4)	C(31)-O(14)-C(32)	115.2(3)
O(12)-C(22)-Mo(4)	179.0(4)	C(34)-O(16)-C(35)	116.4(3)
C(24)-C(23)-Mo(3)	67.4(2)	C(37)-N(19)-C(40)	114.1(4)
C(23)-C(24)-C(25)	116.4(4)	C(37)-N(19)-C(39)	110.5(4)
C(23)-C(24)-Mo(3)	77.0(2)	C(40)-N(19)-C(39)	112.2(4)
C(25)-C(24)-Mo(3)	76.0(2)	C(37)-N(19)-C(38)	107.1(5)
C(24)-C(25)-Mo(3)	67.7(2)	C(40)-N(19)-C(38)	105.1(4)
C(27)-C(26)-Mo(4)	68.1(2)	C(39)-N(19)-C(38)	107.4(4)
C(26)-C(27)-C(28)	116.0(4)	C(42)-N(20)-C(43)	118.4(4)
C(26)-C(27)-Mo(4)	76.2(2)	C(42)-N(20)-C(44)	117.5(4)
C(28)-C(27)-Mo(4)	76.2(3)	C(43)-N(20)-C(44)	112.9(4)
C(27)-C(28)-Mo(4)	67.4(2)	C(42)-N(20)-C(41)	98.4(5)
N(16)-C(29)-C(30)	107.2(3)	C(43)-N(20)-C(41)	102.2(4)
N(16)-C(29)-C(31)	123.7(3)	C(44)-N(20)-C(41)	103.3(4)
C(30)-C(29)-C(31)	129.0(3)	C(48)-O(17)-C(45)	107.3(5)
N(18)-C(30)-C(29)	108.3(3)	C(46)-C(45)-O(17)	109.1(6)
N(18)-C(30)-C(34)	121.3(3)	C(45)-C(46)-C(47)	104.2(6)
C(29)-C(30)-C(34)	130.4(4)	C(48)-C(47)-C(46)	104.4(5)
O(13)-C(31)-O(14)	126.7(4)	O(17)-C(48)-C(47)	106.6(5)
O(13)-C(31)-C(29)	124.1(4)		

Symmetry transformations used to generate equivalent atoms: