Appendix A. Full crystal data

Compound 2

Crystal growth	Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method	Oil

Crystal Data

Chemical formula	$C_{40}H_{79}IMo_6N_4O_{18}$
Formula weight	1606.61g mol^{-1}
Temperature	140 K
Crystal size	0.17 x 0.08 x 0.04 mm^3
Crystal description	Orang block
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 12.1154(3) Å α = 93.785(2)°.
	b = 12.1829(4)Å β = 97.680(2)°.
	c = 19.6204(6) Å γ = 93.375(2)°.
Volume	2857.03(15) $Å^3$
Z	2
F(000)	1592
Density (calculated)	1.868 Mg cm^{-3}
Absorption coefficient	1.883 mm^{-1}

Data Collection

Diffractometer	Oxford Diffraction XCalibur 3
Radiation	Mo-*Kα*
2θ range for data collection	2.88 – 32.63°
Reflections collected	23119
Independent reflections	23129 [R(int) = 0.0000]
Transmission coefficients	1.00000
Data corrections	Gaussian
Index ranges	18<=h<=18, -18<=k<=18, -29<=l<=28

Refinement method

Full-matrix least squares on F^2	
Weighting scheme	$w = [\sigma^2(F_o^2) + (0.0587P)^2 + 0.0000P]^{-1}$
	$P = [\max(I_{obs}, 0) + 2F_c^2]/3$
Data / restraints / parameters	23129 / 48 / 652
Data to parameter ratio	35.47
Goodness of fit on F^2	0.994
R indices	$[I_o>2\sigma>(I_o)]$ data R1 = 0.0403, wR2 = 0.0966
	All 2558 data R1 = 0.0626, wR2 = 0.1025
Final difference map	Largest diff. peak + 1.521 and hole -1.530 e.$Å^{-3}$

Bond lengths [Å] and angles [^{o}]

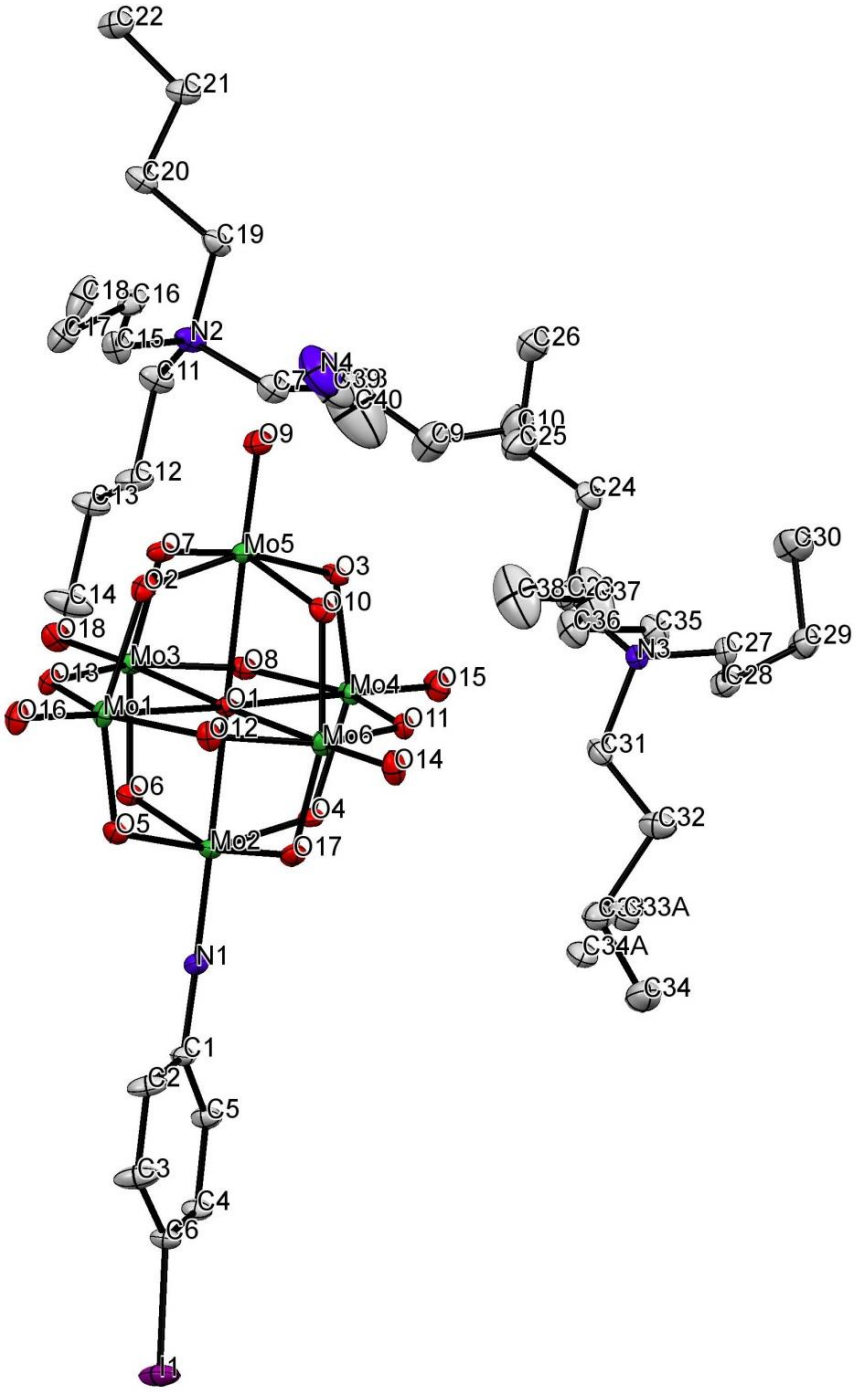
C(1)-C(2)	1.383(6)	O(13)-Mo(1)	1.878(3)
C(1)-C(5)	1.383(6)	O(13)-Mo(3)	1.981(3)
C(1)-N(1)	1.391(5)	O(14)-Mo(6)	1.680(3)
C(2)-C(3)	1.383(6)	O(15)-Mo(4)	1.685(3)
C(3)-C(6)	1.378(6)	O(16)-Mo(1)	1.691(3)
C(4)-C(6)	1.372(6)	O(17)-Mo(6)	1.873(3)
C(4)-C(5)	1.394(6)	O(17)-Mo(2)	1.987(3)
C(6)-I(1)	2.089(4)	O(18)-Mo(3)	1.684(3)
N(1)-Mo(2)	1.743(4)	C(7)-C(8)	1.493(6)
O(1)-Mo(2)	2.199(3)	C(7)-N(2)	1.516(6)
O(1)-Mo(6)	2.327(3)	C(8)-C(9)	1.511(7)
O(1)-Mo(4)	2.334(3)	C(9)-C(10)	1.457(8)
O(1)-Mo(3)	2.335(3)	C(11)-N(2)	1.509(6)
O(1)-Mo(1)	2.343(3)	C(11)-C(12)	1.530(6)
O(1)-Mo(5)	2.375(3)	C(12)-C(13)	1.527(6)
O(2)-Mo(5)	1.882(3)	C(13)-C(14)	1.518(6)
O(2)-Mo(1)	1.974(3)	C(15)-N(2)	1.521(6)
O(3)-Mo(4)	1.882(3)	C(15)-C(16)	1.528(6)
O(3)-Mo(5)	1.958(3)	C(16)-C(17)	1.508(6)
O(4)-Mo(2)	1.903(3)	C(17)-C(18)	1.523(7)
O(4)-Mo(4)	1.942(3)	C(19)-N(2)	1.509(5)
O(5)-Mo(1)	1.870(3)	C(19)-C(20)	1.521(7)
O(5)-Mo(2)	2.005(3)	C(20)-C(21)	1.529(6)
O(6)-Mo(2)	1.905(3)	C(21)-C(22)	1.506(7)
O(6)-Mo(3)	1.946(3)	C(23)-C(24)	1.516(6)
O(7)-Mo(3)	1.884(3)	C(23)-N(3)	1.523(5)
O(7)-Mo(5)	1.968(3)	C(24)-C(25)	1.496(7)
O(8)-Mo(3)	1.894(3)	C(25)-C(26)	1.493(8)
O(8)-Mo(4)	1.984(3)	C(27)-C(28)	1.504(6)
O(9)-Mo(5)	1.682(3)	C(27)-N(3)	1.516(5)
O(10)-Mo(5)	1.881(3)	C(28)-C(29)	1.519(7)
O(10)-Mo(6)	1.977(3)	C(29)-C(30)	1.499(7)
O(11)-Mo(4)	1.890(3)	C(31)-C(32)	1.492(7)
O(11)-Mo(6)	1.985(3)	C(31)-N(3)	1.519(5)

O(12)-Mo(6)	1.889(3)	C(32)-C(33A)	1.458(15)
O(12)-Mo(1)	1.979(3)	C(32)-C(33)	1.632(13)
C(33A)-C(34A)	1.528(13)	Mo(1)-O(5)-Mo(2)	114.12(14)
C(35)-C(36)	1.506(7)	Mo(2)-O(6)-Mo(3)	113.81(14)
C(35)-N(3)	1.524(6)	Mo(3)-O(7)-Mo(5)	117.54(14)
C(36)-C(37)	1.460(8)	Mo(3)-O(8)-Mo(4)	116.90(14)
C(37)-C(38)	1.480(9)	Mo(5)-O(10)-Mo(6)	117.13(14)
C(39)-N(4)	1.126(9)	Mo(4)-O(11)-Mo(6)	116.95(14)
C(39)-C(40)	1.395(11)	Mo(6)-O(12)-Mo(1)	116.79(14)
C(2)-C(1)-C(5)	120.0(4)	Mo(1)-O(13)-Mo(3)	117.58(15)
C(2)-C(1)-N(1)	117.3(4)	Mo(6)-O(17)-Mo(2)	114.64(14)
C(5)-C(1)-N(1)	122.7(4)	O(16)-Mo(1)-O(5)	104.53(15)
C(3)-C(2)-C(1)	119.5(4)	O(16)-Mo(1)-O(13)	104.91(14)
C(6)-C(3)-C(2)	120.6(5)	O(5)-Mo(1)-O(13)	90.32(13)
C(6)-C(4)-C(5)	119.8(4)	O(16)-Mo(1)-O(2)	102.69(15)
C(1)-C(5)-C(4)	119.9(4)	O(5)-Mo(1)-O(2)	152.40(13)
C(4)-C(6)-C(3)	120.0(4)	O(13)-Mo(1)-O(2)	87.04(12)
C(4)-C(6)-I(1)	121.3(3)	O(16)-Mo(1)-O(12)	102.26(13)
C(3)-C(6)-I(1)	118.7(3)	O(5)-Mo(1)-O(12)	87.23(13)
C(1)-N(1)-Mo(2)	164.8(3)	O(13)-Mo(1)-O(12)	152.46(12)
Mo(2)-O(1)-Mo(6)	91.71(10)	O(2)-Mo(1)-O(12)	82.65(12)
Mo(2)-O(1)-Mo(4)	90.90(11)	O(16)-Mo(1)-O(1)	177.60(13)
Mo(6)-O(1)-Mo(4)	90.25(10)	O(5)-Mo(1)-O(1)	76.57(11)
Mo(2)-O(1)-Mo(3)	90.68(10)	O(13)-Mo(1)-O(1)	77.14(11)
Mo(6)-O(1)-Mo(3)	177.58(14)	O(2)-Mo(1)-O(1)	76.06(11)
Mo(4)-O(1)-Mo(3)	90.12(9)	O(12)-Mo(1)-O(1)	75.60(11)
Mo(2)-O(1)-Mo(1)	91.44(10)	N(1)-Mo(2)-O(4)	104.27(15)
Mo(6)-O(1)-Mo(1)	89.76(9)	N(1)-Mo(2)-O(6)	103.80(14)
Mo(4)-O(1)-Mo(1)	177.66(14)	O(4)-Mo(2)-O(6)	91.24(13)
Mo(3)-O(1)-Mo(1)	89.76(10)	N(1)-Mo(2)-O(17)	98.87(15)
Mo(2)-O(1)-Mo(5)	179.29(14)	O(4)-Mo(2)-O(17)	87.90(12)
Mo(6)-O(1)-Mo(5)	88.87(10)	O(6)-Mo(2)-O(17)	156.80(13)
Mo(4)-O(1)-Mo(5)	88.67(9)	N(1)-Mo(2)-O(5)	98.53(15)
Mo(3)-O(1)-Mo(5)	88.76(9)	O(4)-Mo(2)-O(5)	156.67(12)
Mo(1)-O(1)-Mo(5)	88.99(10)	O(6)-Mo(2)-O(5)	88.08(13)
Mo(5)-O(2)-Mo(1)	118.05(16)	O(17)-Mo(2)-O(5)	83.71(12)

Mo(4)-O(3)-Mo(5)	117.96(14)	N(1)-Mo(2)-O(1)	174.72(14)
Mo(2)-O(4)-Mo(4)	114.40(15)	O(4)-Mo(2)-O(1)	79.40(11)
O(17)-Mo(2)-O(1)	77.31(11)	O(6)-Mo(2)-O(1)	79.74(11)
O(5)-Mo(2)-O(1)	77.53(11)	O(2)-Mo(5)-O(3)	152.10(13)
O(18)-Mo(3)-O(7)	104.03(14)	O(9)-Mo(5)-O(7)	103.45(14)
O(18)-Mo(3)-O(8)	105.21(14)	O(10)-Mo(5)-O(7)	152.51(13)
O(7)-Mo(3)-O(8)	89.42(13)	O(2)-Mo(5)-O(7)	86.64(12)
O(18)-Mo(3)-O(6)	102.18(14)	O(3)-Mo(5)-O(7)	83.56(13)
O(7)-Mo(3)-O(6)	153.50(12)	O(9)-Mo(5)-O(1)	177.43(14)
O(8)-Mo(3)-O(6)	87.46(13)	O(10)-Mo(5)-O(1)	77.11(11)
O(18)-Mo(3)-O(13)	102.05(13)	O(2)-Mo(5)-O(1)	76.90(12)
O(7)-Mo(3)-O(13)	87.24(13)	O(3)-Mo(5)-O(1)	75.38(11)
O(8)-Mo(3)-O(13)	152.52(12)	O(7)-Mo(5)-O(1)	75.60(11)
O(6)-Mo(3)-O(13)	83.54(12)	O(14)-Mo(6)-O(17)	104.58(15)
O(18)-Mo(3)-O(1)	176.74(12)	O(14)-Mo(6)-O(12)	103.91(14)
O(7)-Mo(3)-O(1)	78.10(11)	O(17)-Mo(6)-O(12)	91.61(13)
O(8)-Mo(3)-O(1)	77.15(11)	O(14)-Mo(6)-O(10)	102.38(15)
O(6)-Mo(3)-O(1)	75.55(11)	O(17)-Mo(6)-O(10)	152.57(12)
O(13)-Mo(3)-O(1)	75.47(10)	O(12)-Mo(6)-O(10)	86.76(13)
O(15)-Mo(4)-O(3)	103.77(15)	O(14)-Mo(6)-O(11)	102.75(14)
O(15)-Mo(4)-O(11)	103.71(14)	O(17)-Mo(6)-O(11)	86.44(13)
O(3)-Mo(4)-O(11)	90.18(13)	O(12)-Mo(6)-O(11)	152.87(12)
O(15)-Mo(4)-O(4)	103.11(15)	O(10)-Mo(6)-O(11)	82.78(13)
O(3)-Mo(4)-O(4)	152.76(13)	O(14)-Mo(6)-O(1)	178.12(13)
O(11)-Mo(4)-O(4)	87.71(13)	O(17)-Mo(6)-O(1)	76.34(11)
O(15)-Mo(4)-O(8)	103.50(14)	O(12)-Mo(6)-O(1)	77.64(11)
O(3)-Mo(4)-O(8)	85.86(12)	O(10)-Mo(6)-O(1)	76.57(10)
O(11)-Mo(4)-O(8)	152.66(12)	O(11)-Mo(6)-O(1)	75.61(11)
O(4)-Mo(4)-O(8)	83.69(12)	C(8)-C(7)-N(2)	116.6(4)
O(15)-Mo(4)-O(1)	178.19(13)	C(7)-C(8)-C(9)	112.4(4)
O(3)-Mo(4)-O(1)	77.76(11)	C(10)-C(9)-C(8)	114.7(5)
O(11)-Mo(4)-O(1)	77.16(11)	N(2)-C(11)-C(12)	116.9(3)
O(4)-Mo(4)-O(1)	75.30(11)	C(13)-C(12)-C(11)	108.4(4)
O(8)-Mo(4)-O(1)	75.56(11)	C(14)-C(13)-C(12)	111.6(4)
O(9)-Mo(5)-O(10)	103.67(14)	N(2)-C(15)-C(16)	117.7(4)
O(9)-Mo(5)-O(2)	105.49(15)	C(17)-C(16)-C(15)	109.4(4)

O(10)-Mo(5)-O(2)	90.46(13)	C(16)-C(17)-C(18)	111.4(4)
O(9)-Mo(5)-O(3)	102.18(14)	N(2)-C(19)-C(20)	116.9(4)
O(10)-Mo(5)-O(3)	86.41(13)	C(19)-C(20)-C(21)	109.0(4)
C(19)-N(2)-C(11)	108.3(3)	C(22)-C(21)-C(20)	114.1(5)
C(19)-N(2)-C(7)	108.1(3)		
C(11)-N(2)-C(7)	112.0(4)		
C(19)-N(2)-C(15)	111.8(4)		
C(11)-N(2)-C(15)	108.7(3)		
C(7)-N(2)-C(15)	108.1(3)		
C(24)-C(23)-N(3)	116.4(3)		
C(25)-C(24)-C(23)	110.9(4)		
C(26)-C(25)-C(24)	116.5(5)		
C(28)-C(27)-N(3)	116.7(4)		
C(27)-C(28)-C(29)	110.3(4)		
C(30)-C(29)-C(28)	114.1(5)		
C(32)-C(31)-N(3)	117.2(4)		
C(33A)-C(32)-C(31)	122.7(7)		
C(33A)-C(32)-C(33)	24.0(5)		
C(31)-C(32)-C(33)	103.2(5)		
C(34)-C(33)-C(32)	109.6(9)		
C(32)-C(33A)-C(34A)	109.0(10)		
C(36)-C(35)-N(3)	115.2(4)		
C(37)-C(36)-C(35)	112.9(5)		
C(36)-C(37)-C(38)	116.7(6)		
C(27)-N(3)-C(31)	110.4(4)		
C(27)-N(3)-C(23)	110.6(3)		
C(31)-N(3)-C(23)	107.3(3)		
C(27)-N(3)-C(35)	107.7(3)		
C(31)-N(3)-C(35)	110.3(3)		
C(23)-N(3)-C(35)	110.5(4)		
N(4)-C(39)-C(40)	176.6(10)		

ORTEP-1 representation of compound **2**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity.



Compound 3

Crystal growth	Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method	Oil

Crystal Data

Chemical formula	$C_{43}H_{88}Mo_6N_4O_{18}$
Formula weight	1524.81g mol^{-1}
Temperature	293(2) K
Crystal size	0.32 x 0.25 x 0.07 mm^3
Crystal description	Orang plate
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 11.6395(2) Å α = 90°.
	b = 33.6792(5) Å β = 91.5770(10)°.
	c = 14.0382(2) Å γ = 90°.
Volume	5501.02(15) $Å^3$
Z	4
F(000)	3080
Density (calculated)	1.841 Mg cm^{-3}
Absorption coefficient	1.397 mm^{-1}

Data Collection

Diffractometer	Oxford Diffraction XCalibur 3
Radiation	Mo-*Kα*
2θ range for data collection	2.89 – 32.68°
Reflections collected	122706
Independent reflections	18893 [R(int) = 0.0572]
Transmission coefficients	1.00000
Data corrections	Gaussian
Index ranges	-16<=h<=17, -50<=k<=50, -20<=l<=20

Refinement method

Full-matrix least squares on F^2	
Weighting scheme	$w = [\sigma^2(F_o^2) + (0.0000P)^2 + 25.7752P]^{-1}$
	$P = [\max(I_{obs}, 0) + 2F_c^2]/3$
Data / restraints / parameters	18893 / 0 / 639
Data to parameter ratio	29.56
Goodness of fit on F^2	1.191
R indices	$[I_o>2\sigma>(I_o)]$ data R1 = 0.0566, wR2 = 0.0888
	All 2558 data R1 = 0.0758, wR2 = 0.0948
Final difference map	Largest diff. peak + 1.707 and hole -1.884 e.$Å^{-3}$

Bond lengths [Å] and angles [^{o}]

C(1)-N(1)	138.7(5)	C(15)-H(15B)	97.00
C(1)-C(2)	139.4(6)	C(16)-C(17)	152.1(6)
C(1)-C(6)	139.9(5)	C(16)-H(16A)	97.00
C(2)-C(3)	138.0(5)	C(16)-H(16B)	97.00
C(2)-H(2)	93.00	C(17)-C(18)	151.0(8)
C(3)-C(4)	140.1(5)	C(17)-H(17A)	97.00
C(3)-H(3)	93.00	C(17)-H(17B)	97.00
C(4)-C(5)	139.2(5)	C(18)-H(18A)	96.00
C(4)-N(2)	141.1(5)	C(18)-H(18B)	96.00
C(5)-C(6)	138.4(5)	C(18)-H(18C)	96.00
C(5)-H(5)	93.00	C(19)-C(20)	151.4(6)
C(6)-H(6)	93.00	C(19)-N(3)	151.5(5)
C(7)-C(8)	136.1(6)	C(19)-H(19A)	97.00
C(7)-N(2)	138.4(5)	C(19)-H(19B)	97.00
C(7)-H(7)	93.00	C(20)-C(21)	154.3(7)
C(8)-C(9)	141.4(6)	C(20)-H(20A)	97.00
C(8)-H(8)	93.00	C(20)-H(20B)	97.00
C(9)-C(10)	135.9(6)	C(21)-C(22)	149.7(8)
C(9)-H(9)	93.00	C(21)-H(21A)	97.00
C(10)-N(2)	138.1(5)	C(21)-H(21B)	97.00
C(10)-H(10)	93.00	C(22)-H(22A)	96.00
C(11)-C(12)	151.0(6)	C(22)-H(22B)	96.00
C(11)-N(3)	152.1(5)	C(22)-H(22C)	96.00
C(11)-H(11A)	97.00	C(23)-N(3)	151.5(5)
C(11)-H(11B)	97.00	C(23)-C(24)	151.7(6)
C(12)-C(13)	153.6(6)	C(23)-H(23A)	97.00
C(12)-H(12A)	97.00	C(23)-H(23B)	97.00
C(12)-H(12B)	97.00	C(24)-C(25)	152.4(6)
C(13)-C(14)	151.9(6)	C(24)-H(24A)	97.00
C(13)-H(13A)	97.00	C(24)-H(24B)	97.00
C(13)-H(13B)	97.00	C(25)-C(26)	150.7(6)
C(14)-H(14A)	96.00	C(25)-H(25A)	97.00
C(14)-H(14B)	96.00	C(25)-H(25B)	97.00

C(14)-H(14C)	96.00	C(26)-H(26A)	96.00
C(15)-N(3)	151.4(5)	C(26)-H(26B)	96.00
C(15)-C(16)	152.2(6)	C(26)-H(26C)	96.00
C(15)-H(15A)	97.00	C(27)-C(28)	151.8(7)
C(27)-N(4)	152.7(6)	C(38)-H(38C)	96.00
C(27)-H(27A)	97.00	C(39)-C(40)	150.5(6)
C(27)-H(27B)	97.00	C(39)-N(4)	151.4(5)
C(28)-C(29)	152.7(7)	C(39)-H(39A)	97.00
C(28)-H(28A)	97.00	C(39)-H(39B)	97.00
C(28)-H(28B)	97.00	C(40)-C(41)	153.3(6)
C(29)-C(30)	151.7(9)	C(40)-H(40A)	97.00
C(29)-H(29A)	97.00	C(40)-H(40B)	97.00
C(29)-H(29B)	97.00	C(41)-C(42)	151.5(7)
C(30)-H(30A)	96.00	C(41)-H(41A)	97.00
C(30)-H(30B)	96.00	C(41)-H(41B)	97.00
C(30)-H(30C)	96.00	C(42)-H(42A)	96.00
C(31)-C(32)	151.6(6)	C(42)-H(42B)	96.00
C(31)-N(4)	152.0(5)	C(42)-H(42C)	96.00
C(31)-H(31A)	97.00	N(1)-Mo(5)	173.8(3)
C(31)-H(31B)	97.00	O(1)-Mo(5)	220.6(2)
C(32)-C(33)	152.7(6)	O(1)-Mo(4)	233.0(3)
C(32)-H(32A)	97.00	O(1)-Mo(3)	233.4(3)
C(32)-H(32B)	97.00	O(1)-Mo(1)	233.7(3)
C(33)-C(34)	151.5(6)	O(1)-Mo(2)	234.8(3)
C(33)-H(33A)	97.00	O(1)-Mo(6)	236.1(2)
C(33)-H(33B)	97.00	O(2)-Mo(6)	192.3(3)
C(34)-H(34A)	96.00	O(2)-Mo(3)	193.0(3)
C(34)-H(34B)	96.00	O(3)-Mo(6)	190.7(3)
C(34)-H(34C)	96.00	O(3)-Mo(4)	193.7(3)
C(35)-C(36)	150.9(7)	O(4)-Mo(4)	189.2(3)
C(35)-N(4)	151.7(5)	O(4)-Mo(5)	195.5(3)
C(35)-H(35A)	97.00	O(5)-Mo(3)	189.3(3)
C(35)-H(35B)	97.00	O(5)-Mo(5)	194.6(3)
C(36)-C(37)	152.5(6)	O(6)-Mo(5)	190.5(3)
C(36)-H(36A)	97.00	O(6)-Mo(1)	196.2(3)
C(36)-H(36B)	97.00	O(7)-Mo(1)	187.6(3)

C(37)-C(38)	151.4(8)	O(7)-Mo(6)	198.0(3)
C(37)-H(37A)	97.00	O(8)-Mo(6)	186.8(3)
C(37)-H(37B)	97.00	O(8)-Mo(2)	197.4(3)
C(38)-H(38A)	96.00	O(9)-Mo(2)	186.2(3)
C(38)-H(38B)	96.00	O(9)-Mo(5)	200.1(3)
O(10)-Mo(3)	186.8(3)	C(9)-C(8)-H(8)	126.2
O(10)-Mo(1)	201.0(3)	C(10)-C(9)-C(8)	107.6(4)
O(11)-Mo(2)	187.4(3)	C(10)-C(9)-H(9)	126.2
O(11)-Mo(3)	201.5(3)	C(8)-C(9)-H(9)	126.2
O(12)-Mo(4)	187.5(3)	C(9)-C(10)-N(2)	108.4(4)
O(12)-Mo(2)	201.8(3)	C(9)-C(10)-H(10)	125.8
O(13)-Mo(1)	186.7(3)	N(2)-C(10)-H(10)	125.8
O(13)-Mo(4)	200.8(3)	C(12)-C(11)-N(3)	118.3(3)
O(14)-Mo(1)	169.3(3)	C(12)-C(11)-H(11A)	107.7
O(15)-Mo(3)	169.4(3)	N(3)-C(11)-H(11A)	107.7
O(16)-Mo(4)	169.0(3)	C(12)-C(11)-H(11B)	107.7
O(17)-Mo(6)	169.1(3)	N(3)-C(11)-H(11B)	107.7
O(18)-Mo(2)	169.0(3)	H(11A)-C(11)-H(11B)	107.1
N(1)-C(1)-C(2)	121.1(4)	C(11)-C(12)-C(13)	107.4(3)
N(1)-C(1)-C(6)	119.7(4)	C(11)-C(12)-H(12A)	110.2
C(2)-C(1)-C(6)	119.2(4)	C(13)-C(12)-H(12A)	110.2
C(3)-C(2)-C(1)	120.6(4)	C(11)-C(12)-H(12B)	110.2
C(3)-C(2)-H(2)	119.7	C(13)-C(12)-H(12B)	110.2
C(1)-C(2)-H(2)	119.7	H(12A)-C(12)-H(12B)	108.5
C(2)-C(3)-C(4)	120.4(4)	C(14)-C(13)-C(12)	112.9(4)
C(2)-C(3)-H(3)	119.8	C(14)-C(13)-H(13A)	109.0
C(4)-C(3)-H(3)	119.8	C(12)-C(13)-H(13A)	109.0
C(5)-C(4)-C(3)	118.9(3)	C(14)-C(13)-H(13B)	109.0
C(5)-C(4)-N(2)	120.3(3)	C(12)-C(13)-H(13B)	109.0
C(3)-C(4)-N(2)	120.7(3)	H(13A)-C(13)-H(13B)	107.8
C(6)-C(5)-C(4)	120.8(3)	C(13)-C(14)-H(14A)	109.5
C(6)-C(5)-H(5)	119.6	C(13)-C(14)-H(14B)	109.5
C(4)-C(5)-H(5)	119.6	H(14A)-C(14)-H(14B)	109.5
C(5)-C(6)-C(1)	120.0(4)	C(13)-C(14)-H(14C)	109.5
C(5)-C(6)-H(6)	120.0	H(14A)-C(14)-H(14C)	109.5
C(1)-C(6)-H(6)	120.0	H(14B)-C(14)-H(14C)	109.5

C(8)-C(7)-N(2)	108.2(4)	N(3)-C(15)-C(16)	117.4(3)
C(8)-C(7)-H(7)	125.9	N(3)-C(15)-H(15A)	107.9
N(2)-C(7)-H(7)	125.9	C(16)-C(15)-H(15A)	107.9
C(7)-C(8)-C(9)	107.7(4)	N(3)-C(15)-H(15B)	107.9
C(7)-C(8)-H(8)	126.2	C(16)-C(15)-H(15B)	107.9
C(17)-C(16)-C(15)	109.2(4)	H(15A)-C(15)-H(15B)	107.2
C(17)-C(16)-H(16A)	109.8	C(21)-C(22)-H(22B)	109.5
C(15)-C(16)-H(16A)	109.8	H(22A)-C(22)-H(22B)	109.5
C(17)-C(16)-H(16B)	109.8	C(21)-C(22)-H(22C)	109.5
C(15)-C(16)-H(16B)	109.8	H(22A)-C(22)-H(22C)	109.5
H(16A)-C(16)-H(16B)	108.3	H(22B)-C(22)-H(22C)	109.5
C(18)-C(17)-C(16)	113.9(5)	N(3)-C(23)-C(24)	116.6(3)
C(18)-C(17)-H(17A)	108.8	N(3)-C(23)-H(23A)	108.2
C(16)-C(17)-H(17A)	108.8	C(24)-C(23)-H(23A)	108.2
C(18)-C(17)-H(17B)	108.8	N(3)-C(23)-H(23B)	108.2
C(16)-C(17)-H(17B)	108.8	C(24)-C(23)-H(23B)	108.2
H(17A)-C(17)-H(17B)	107.7	H(23A)-C(23)-H(23B)	107.3
C(17)-C(18)-H(18A)	109.5	C(23)-C(24)-C(25)	108.0(3)
C(17)-C(18)-H(18B)	109.5	C(23)-C(24)-H(24A)	110.1
H(18A)-C(18)-H(18B)	109.5	C(25)-C(24)-H(24A)	110.1
C(17)-C(18)-H(18C)	109.5	C(23)-C(24)-H(24B)	110.1
H(18A)-C(18)-H(18C)	109.5	C(25)-C(24)-H(24B)	110.1
H(18B)-C(18)-H(18C)	109.5	H(24A)-C(24)-H(24B)	108.4
C(20)-C(19)-N(3)	118.4(3)	C(26)-C(25)-C(24)	114.6(4)
C(20)-C(19)-H(19A)	107.7	C(26)-C(25)-H(25A)	108.6
N(3)-C(19)-H(19A)	107.7	C(24)-C(25)-H(25A)	108.6
C(20)-C(19)-H(19B)	107.7	C(26)-C(25)-H(25B)	108.6
N(3)-C(19)-H(19B)	107.7	C(24)-C(25)-H(25B)	108.6
H(19A)-C(19)-H(19B)	107.1	H(25A)-C(25)-H(25B)	107.6
C(19)-C(20)-C(21)	107.2(4)	C(25)-C(26)-H(26A)	109.5
C(19)-C(20)-H(20A)	110.3	C(25)-C(26)-H(26B)	109.5
C(21)-C(20)-H(20A)	110.3	H(26A)-C(26)-H(26B)	109.5
C(19)-C(20)-H(20B)	110.3	C(25)-C(26)-H(26C)	109.5
C(21)-C(20)-H(20B)	110.3	H(26A)-C(26)-H(26C)	109.5
H(20A)-C(20)-H(20B)	108.5	H(26B)-C(26)-H(26C)	109.5
C(22)-C(21)-C(20)	114.4(5)	C(28)-C(27)-N(4)	117.1(4)

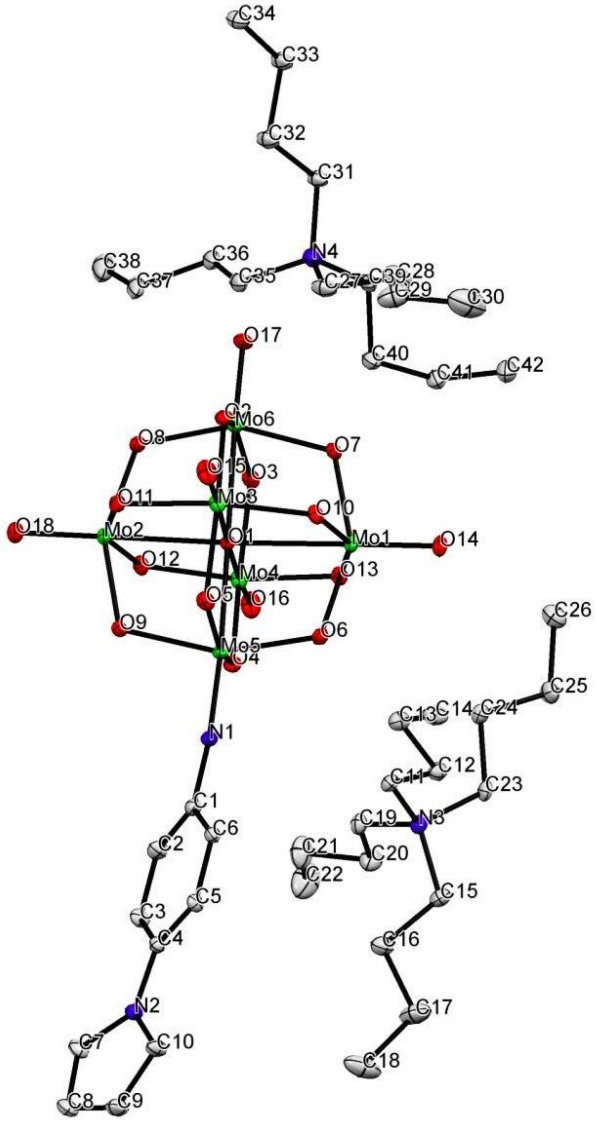
C(22)-C(21)-H(21A)	108.7	C(28)-C(27)-H(27A)	108.0
C(20)-C(21)-H(21A)	108.7	N(4)-C(27)-H(27A)	108.0
C(22)-C(21)-H(21B)	108.7	C(28)-C(27)-H(27B)	108.0
C(20)-C(21)-H(21B)	108.7	N(4)-C(27)-H(27B)	108.0
H(21A)-C(21)-H(21B)	107.6	H(27A)-C(27)-H(27B)	107.3
C(21)-C(22)-H(22A)	109.5	C(27)-C(28)-C(29)	109.0(5)
C(29)-C(28)-H(28A)	109.9	C(27)-C(28)-H(28A)	109.9
C(27)-C(28)-H(28B)	109.9	C(33)-C(34)-H(34C)	109.5
C(29)-C(28)-H(28B)	109.9	H(34A)-C(34)-H(34C)	109.5
H(28A)-C(28)-H(28B)	108.3	H(34B)-C(34)-H(34C)	109.5
C(30)-C(29)-C(28)	113.4(5)	C(36)-C(35)-N(4)	117.6(3)
C(30)-C(29)-H(29A)	108.9	C(36)-C(35)-H(35A)	107.9
C(28)-C(29)-H(29A)	108.9	N(4)-C(35)-H(35A)	107.9
C(30)-C(29)-H(29B)	108.9	C(36)-C(35)-H(35B)	107.9
C(28)-C(29)-H(29B)	108.9	N(4)-C(35)-H(35B)	107.9
H(29A)-C(29)-H(29B)	107.7	H(35A)-C(35)-H(35B)	107.2
C(29)-C(30)-H(30A)	109.5	C(35)-C(36)-C(37)	108.8(4)
C(29)-C(30)-H(30B)	109.5	C(35)-C(36)-H(36A)	109.9
H(30A)-C(30)-H(30B)	109.5	C(37)-C(36)-H(36A)	109.9
C(29)-C(30)-H(30C)	109.5	C(35)-C(36)-H(36B)	109.9
H(30A)-C(30)-H(30C)	109.5	C(37)-C(36)-H(36B)	109.9
H(30B)-C(30)-H(30C)	109.5	H(36A)-C(36)-H(36B)	108.3
C(32)-C(31)-N(4)	116.8(3)	C(38)-C(37)-C(36)	113.3(4)
C(32)-C(31)-H(31A)	108.1	C(38)-C(37)-H(37A)	108.9
N(4)-C(31)-H(31A)	108.1	C(36)-C(37)-H(37A)	108.9
C(32)-C(31)-H(31B)	108.1	C(38)-C(37)-H(37B)	108.9
N(4)-C(31)-H(31B)	108.1	C(36)-C(37)-H(37B)	108.9
H(31A)-C(31)-H(31B)	107.3	H(37A)-C(37)-H(37B)	107.7
C(31)-C(32)-C(33)	109.4(3)	C(37)-C(38)-H(38A)	109.5
C(31)-C(32)-H(32A)	109.8	C(37)-C(38)-H(38B)	109.5
C(33)-C(32)-H(32A)	109.8	H(38A)-C(38)-H(38B)	109.5
C(31)-C(32)-H(32B)	109.8	C(37)-C(38)-H(38C)	109.5
C(33)-C(32)-H(32B)	109.8	H(38A)-C(38)-H(38C)	109.5
H(32A)-C(32)-H(32B)	108.2	H(38B)-C(38)-H(38C)	109.5
C(34)-C(33)-C(32)	111.8(3)	C(40)-C(39)-N(4)	116.5(3)
C(34)-C(33)-H(33A)	109.3	C(40)-C(39)-H(39A)	108.2

C(32)-C(33)-H(33A)	109.3	N(4)-C(39)-H(39A)	108.2
C(34)-C(33)-H(33B)	109.2	C(40)-C(39)-H(39B)	108.2
C(32)-C(33)-H(33B)	109.3	N(4)-C(39)-H(39B)	108.2
H(33A)-C(33)-H(33B)	107.9	H(39A)-C(39)-H(39B)	107.3
C(33)-C(34)-H(34A)	109.5	C(39)-C(40)-C(41)	110.8(4)
C(33)-C(34)-H(34B)	109.5	C(39)-C(40)-H(40A)	109.5
H(34A)-C(34)-H(34B)	109.5	C(41)-C(40)-H(40A)	109.5
C(41)-C(40)-H(40B)	109.5	C(39)-C(40)-H(40B)	109.5
H(40A)-C(40)-H(40B)	108.1	Mo(4)-O(1)-Mo(2)	90.53(9)
C(42)-C(41)-C(40)	114.1(4)	Mo(3)-O(1)-Mo(2)	90.01(9)
C(42)-C(41)-H(41A)	108.7	Mo(1)-O(1)-Mo(2)	177.75(12)
C(40)-C(41)-H(41A)	108.7	Mo(5)-O(1)-Mo(6)	179.71(14)
C(42)-C(41)-H(41B)	108.7	Mo(4)-O(1)-Mo(6)	89.00(9)
C(40)-C(41)-H(41B)	108.7	Mo(3)-O(1)-Mo(6)	89.52(9)
H(41A)-C(41)-H(41B)	107.6	Mo(1)-O(1)-Mo(6)	89.10(9)
C(41)-C(42)-H(42A)	109.5	Mo(2)-O(1)-Mo(6)	88.65(8)
C(41)-C(42)-H(42B)	109.5	Mo(6)-O(2)-Mo(3)	118.19(13)
H(42A)-C(42)-H(42B)	109.5	Mo(6)-O(3)-Mo(4)	117.61(13)
C(41)-C(42)-H(42C)	109.5	Mo(4)-O(4)-Mo(5)	114.27(13)
H(42A)-C(42)-H(42C)	109.5	Mo(3)-O(5)-Mo(5)	114.51(13)
H(42B)-C(42)-H(42C)	109.5	Mo(5)-O(6)-Mo(1)	114.09(13)
C(1)-N(1)-Mo(5)	173.3(3)	Mo(1)-O(7)-Mo(6)	117.40(13)
C(10)-N(2)-C(7)	108.1(3)	Mo(6)-O(8)-Mo(2)	117.80(14)
C(10)-N(2)-C(4)	125.8(3)	Mo(2)-O(9)-Mo(5)	114.62(13)
C(7)-N(2)-C(4)	125.6(3)	Mo(3)-O(10)-Mo(1)	116.50(13)
C(15)-N(3)-C(23)	105.8(3)	Mo(2)-O(11)-Mo(3)	116.64(13)
C(15)-N(3)-C(19)	112.0(3)	Mo(4)-O(12)-Mo(2)	117.12(13)
C(23)-N(3)-C(19)	111.4(3)	Mo(1)-O(13)-Mo(4)	116.01(13)
C(15)-N(3)-C(11)	111.7(3)	O(14)-Mo(1)-O(13)	105.51(13)
C(23)-N(3)-C(11)	111.5(3)	O(14)-Mo(1)-O(7)	103.75(13)
C(19)-N(3)-C(11)	104.5(3)	O(13)-Mo(1)-O(7)	91.88(12)
C(39)-N(4)-C(35)	111.5(3)	O(14)-Mo(1)-O(6)	102.77(13)
C(39)-N(4)-C(31)	105.7(3)	O(13)-Mo(1)-O(6)	88.05(12)
C(35)-N(4)-C(31)	111.9(3)	O(7)-Mo(1)-O(6)	152.46(11)
C(39)-N(4)-C(27)	111.4(3)	O(14)-Mo(1)-O(10)	100.57(12)
C(35)-N(4)-C(27)	105.5(3)	O(13)-Mo(1)-O(10)	153.64(11)

C(31)-N(4)-C(27)	110.9(3)	O(7)-Mo(1)-O(10)	85.51(11)
Mo(5)-O(1)-Mo(4)	90.85(9)	O(6)-Mo(1)-O(10)	82.52(11)
Mo(5)-O(1)-Mo(3)	90.63(9)	O(14)-Mo(1)-O(1)	175.65(12)
Mo(4)-O(1)-Mo(3)	178.41(13)	O(13)-Mo(1)-O(1)	78.37(10)
Mo(5)-O(1)-Mo(1)	91.14(9)	O(7)-Mo(1)-O(1)	77.87(10)
Mo(4)-O(1)-Mo(1)	89.58(9)	O(6)-Mo(1)-O(1)	75.16(10)
Mo(3)-O(1)-Mo(1)	89.83(9)	O(10)-Mo(1)-O(1)	75.44(10)
Mo(5)-O(1)-Mo(2)	91.10(9)	O(18)-Mo(2)-O(9)	103.92(13)
O(9)-Mo(2)-O(11)	92.38(12)	O(18)-Mo(2)-O(11)	105.18(13)
O(18)-Mo(2)-O(8)	103.23(13)	O(3)-Mo(4)-O(13)	83.28(11)
O(9)-Mo(2)-O(8)	151.97(11)	O(16)-Mo(4)-O(1)	177.76(12)
O(11)-Mo(2)-O(8)	87.19(12)	O(12)-Mo(4)-O(1)	77.65(10)
O(18)-Mo(2)-O(12)	102.36(13)	O(4)-Mo(4)-O(1)	76.50(10)
O(9)-Mo(2)-O(12)	86.08(11)	O(3)-Mo(4)-O(1)	76.54(10)
O(11)-Mo(2)-O(12)	151.95(11)	O(13)-Mo(4)-O(1)	75.95(10)
O(8)-Mo(2)-O(12)	81.42(12)	N(1)-Mo(5)-O(6)	104.26(13)
O(18)-Mo(2)-O(1)	176.95(12)	N(1)-Mo(5)-O(5)	102.52(14)
O(9)-Mo(2)-O(1)	76.62(10)	O(6)-Mo(5)-O(5)	89.69(12)
O(11)-Mo(2)-O(1)	77.75(10)	N(1)-Mo(5)-O(4)	100.57(14)
O(8)-Mo(2)-O(1)	75.91(10)	O(6)-Mo(5)-O(4)	89.19(12)
O(12)-Mo(2)-O(1)	74.64(10)	O(5)-Mo(5)-O(4)	156.42(11)
O(15)-Mo(3)-O(10)	104.14(13)	N(1)-Mo(5)-O(9)	98.78(13)
O(15)-Mo(3)-O(5)	104.97(14)	O(6)-Mo(5)-O(9)	156.96(11)
O(10)-Mo(3)-O(5)	90.44(12)	O(5)-Mo(5)-O(9)	85.85(11)
O(15)-Mo(3)-O(2)	102.26(14)	O(4)-Mo(5)-O(9)	86.02(11)
O(10)-Mo(3)-O(2)	89.17(12)	N(1)-Mo(5)-O(1)	176.14(13)
O(5)-Mo(3)-O(2)	152.00(12)	O(6)-Mo(5)-O(1)	79.48(10)
O(15)-Mo(3)-O(11)	102.18(13)	O(5)-Mo(5)-O(1)	78.27(10)
O(10)-Mo(3)-O(11)	153.59(11)	O(4)-Mo(5)-O(1)	78.37(10)
O(5)-Mo(3)-O(11)	84.80(11)	O(9)-Mo(5)-O(1)	77.47(10)
O(2)-Mo(3)-O(11)	83.21(12)	O(17)-Mo(6)-O(8)	104.73(13)
O(15)-Mo(3)-O(1)	177.43(13)	O(17)-Mo(6)-O(3)	103.80(15)
O(10)-Mo(3)-O(1)	78.11(10)	O(8)-Mo(6)-O(3)	89.82(12)
O(5)-Mo(3)-O(1)	76.11(10)	O(17)-Mo(6)-O(2)	103.83(15)
O(2)-Mo(3)-O(1)	76.42(10)	O(8)-Mo(6)-O(2)	88.88(13)
O(11)-Mo(3)-O(1)	75.53(10)	O(3)-Mo(6)-O(2)	151.73(11)

O(16)-Mo(4)-O(12)	104.51(13)	O(17)-Mo(6)-O(7)	102.38(13)
O(16)-Mo(4)-O(4)	103.97(14)	O(8)-Mo(6)-O(7)	152.88(11)
O(12)-Mo(4)-O(4)	90.64(12)	O(3)-Mo(6)-O(7)	84.50(12)
O(16)-Mo(4)-O(3)	102.77(14)	O(2)-Mo(6)-O(7)	83.90(12)
O(12)-Mo(4)-O(3)	88.74(12)	O(17)-Mo(6)-O(1)	177.77(12)
O(4)-Mo(4)-O(3)	152.51(11)	O(8)-Mo(6)-O(1)	77.49(10)
O(16)-Mo(4)-O(13)	101.88(13)	O(3)-Mo(6)-O(1)	76.30(10)
O(12)-Mo(4)-O(13)	153.52(11)	O(2)-Mo(6)-O(1)	75.86(10)
O(4)-Mo(4)-O(13)	85.16(11)	O(7)-Mo(6)-O(1)	75.39(10)

ORTEP-2 representation of compound **3**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity.



Compound 4

Crystal growth	Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method	Oil

Crystal Data

Chemical formula	$C_{50}H_{84}Mo_6N_4O_{18}$	
Formula weight	1604.85g mol^{-1}	
Temperature	100(2) K	
Crystal size	0.12 x 0.06 x 0.01 mm^3	
Crystal description	Orang blade	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 17.5590(11) Å	α = 90°.
	b = 17.7832(13) Å	β = 90°.
	c = 19.6079(14) Å	γ = 90°.
Volume	6122.7(7) $Å^3$	
Z	4	
F(000)	3232	
Density (calculated)	1.741 Mg cm^{-3}	
Absorption coefficient	1.260 mm^{-1}	

Data Collection

Diffractometer	Rigaku AFC 12 goniometer
Radiation	Mo-*Kα*
2θ range for data collection	2.32 – 27.58 °
Reflections collected	42376
Independent reflections	14052 [R(int) = 0.0827]
Transmission coefficients	0.9875
Data corrections	Gaussian
Index ranges	-21<=h<=22, -14<=k<=23, -16<=l<=25

Refinement method

Full-matrix least squares on F^2		
Weighting scheme	$w = [\sigma^2(F_o^2) + (0.0906P)^2 + 0.0000P]^{-1}$	
	$P = [\max(I_{obs}, 0) + 2F_c^2]/3$	
Data / restraints / parameters	14052 / 357 / 771	
Data to parameter ratio	18.22	
Goodness of fit on F^2	0.914	
R indices	$[I_o>2\sigma>(I_o)]$ data	R1 = 0.0702, wR2 = 0.1543
	All 2558 data	R1 = 0.1716, wR2 = 0.1956
Final difference map	Largest diff. peak + 0.793 and hole - 0.385 e.$Å^{-3}$	

Bond lengths [Å] and angles [^{o}]

Mo(1)-O(15)	1.669(8)	Mo(1)-O(14)	1.866(9)
Mo(1)-O(17)	1.903(9)	Mo(1)-O(8)	1.926(8)
Mo(1)-O(18)	1.937(9)	Mo(1)-O(13)	2.314(7)
Mo(2)-O(11)	1.702(8)	Mo(2)-O(12)	1.862(9)
Mo(2)-O(3)	1.880(11)	Mo(2)-O(9)	1.904(8)
Mo(2)-O(10)	1.950(8)	Mo(2)-O(13)	2.337(7)
Mo(3)-O(4)	1.664(8)	Mo(3)-O(10)	1.898(8)
Mo(3)-O(2)	1.906(9)	Mo(3)-O(5)	1.913(9)
Mo(3)-O(17)	1.930(8)	Mo(3)-O(13)	2.323(8)
Mo(4)-N(1)	1.734(11)	Mo(4)-O(8)	1.913(8)
Mo(4)-O(5)	1.921(8)	Mo(4)-O(12)	1.967(7)
Mo(4)-O(6)	1.983(9)	Mo(4)-O(13)	2.234(7)
Mo(5)-O(1)	1.618(10)	Mo(5)-O(2)	1.911(9)
Mo(5)-O(3)	1.948(9)	Mo(5)-O(16)	1.951(10)
Mo(5)-O(14)	1.957(8)	Mo(5)-O(13)	2.341(8)
Mo(6)-O(7)	1.678(9)	Mo(6)-O(6)	1.861(10)
Mo(6)-O(16)	1.896(11)	Mo(6)-O(18)	1.909(9)
Mo(6)-O(9)	1.963(8)	Mo(6)-O(13)	2.327(8)
N(1)-C(1)	1.321(17)	C(1)-C(6)	1.385(19)
C(1)-C(2)	1.41(2)	C(2)-C(3)	1.37(2)
C(2)-H(2)	0.9500	C(3)-C(4)	1.30(2)
C(3)-H(3)	0.9500	C(4)-C(5)	1.42(2)
C(4)-C(7)	1.43(2)	C(5)-C(6)	1.408(18)
C(5)-H(5)	0.9500	C(6)-H(6)	0.9500
C(7)-C(8)	1.23(2)	C(8)-C(9)	1.45(2)
C(9)-C(10)	1.394(19)	C(9)-C(14)	1.395(19)
C(10)-C(11)	1.337(19)	C(10)-H(10)	0.9500
C(11)-C(12)	1.39(2)	C(11)-H(11)	0.9500
C(12)-C(13)	1.334(18)	C(12)-N(2)	1.421(19)
C(13)-C(14)	1.377(19)	C(13)-H(13)	0.9500
C(14)-H(14)	0.9500	N(2)-C(18)	1.407(17)
N(2)-C(15)	1.410(17)	C(15)-C(16)	1.331(19)
C(15)-H(15)	0.9500	C(16)-C(17)	1.44(3)
C(16)-H(16)	0.9500	C(17)-C(18)	1.332(19)

C(17)-H(17)	0.9500	C(18)-H(18)	0.9500
N(3)-C(22)	1.486(15)	N(3)-C(23)	1.495(16)
N(3)-C(34)	1.509(16)	N(3)-C(30)	1.515(18)
C(19)-C(20)	1.485(19)	C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800	C(19)-H(19C)	0.9800
C(20)-C(21)	1.546(18)	C(20)-H(20A)	0.9900
C(20)-H(20B)	0.9900	C(21)-C(22)	1.517(18)
C(21)-H(21A)	0.9900	C(21)-H(21B)	0.9900
C(22)-H(22A)	0.9900	C(22)-H(22B)	0.9900
C(23)-C(24)	1.508(18)	C(23)-H(23A)	0.9900
C(23)-H(23B)	0.9900	C(24)-C(25)	1.485(19)
C(24)-H(24A)	0.9900	C(24)-H(24B)	0.9900
C(25)-C(26)	1.54(2)	C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900	C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800	C(26)-H(26C)	0.9800
C(27)-C(28)	1.589(16)	C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800	C(27)-H(27C)	0.9800
C(28)-C(29)	1.59(3)	C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900	C(29)-C(30)	1.50(2)
C(29)-H(29A)	0.9900	C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9900	C(30)-H(30B)	0.9900
C(27B)-C(28B)	1.598(16)	C(27B)-H(27D)	0.9800
C(27B)-H(27E)	0.9800	C(27B)-H(27F)	0.9800
C(28B)-C(29B)	1.59(3)	C(28B)-H(28C)	0.9900
C(28B)-H(28D)	0.9900	C(29B)-H(29C)	0.9900
C(29B)-H(29D)	0.9900	C(31)-C(32)	1.48(2)
C(31)-H(31A)	0.9800	C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800	C(32)-C(33)	1.54(2)
C(32)-H(32A)	0.9900	C(32)-H(32B)	0.9900
C(33)-C(34)	1.526(18)	C(33)-H(33A)	0.9900
C(33)-H(33B)	0.9900	C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900	C(35)-C(36)	1.562(18)
C(35)-H(35A)	0.9800	C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800	C(36)-C(37)	1.57(3)
C(36)-H(36A)	0.9900	C(36)-H(36B)	0.9900
C(37)-C(38)	1.54(3)	C(37)-H(37A)	0.9900

C(37)-H(37B)	0.9900	C(38)-N(4)	1.56(2)
C(38)-H(38A)	0.9900	C(38)-H(38B)	0.9900
N(4)-C(50)	1.51(2)	N(4)-C(43)	1.52(2)
N(4)-C(39)	1.54(3)	C(39)-C(40)	1.41(3)
C(39)-H(39A)	0.9900	C(39)-H(39B)	0.9900
C(40)-C(41)	1.49(3)	C(40)-H(40A)	0.9900
C(40)-H(40B)	0.9900	C(41)-C(42)	1.48(3)
C(41)-H(41A)	0.9900	C(41)-H(41B)	0.9900
C(42)-H(42A)	0.9800	C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800	C(39B)-C(40B)	1.41(3)
C(39B)-H(39C)	0.9900	C(39B)-H(39D)	0.9900
C(40B)-C(41B)	1.47(2)	C(40B)-H(40C)	0.9900
C(40B)-H(40D)	0.9900	C(41B)-C(42B)	1.47(3)
C(41B)-H(41C)	0.9900	C(41B)-H(41D)	0.9900
C(42B)-H(42D)	0.9800	C(42B)-H(42E)	0.9800
C(42B)-H(42F)	0.9800	C(43)-C(44)	1.602(17)
C(43)-H(43A)	0.9900	C(43)-H(43B)	0.9900
C(44)-C(45)	1.517(17)	C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900	C(45)-C(46)	1.546(17)
C(45)-H(45A)	0.9900	C(45)-H(45B)	0.9900
C(46)-H(46A)	0.9800	C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800	C(47)-C(48)	1.55(3)
C(47)-H(47A)	0.9800	C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800	C(48)-C(49)	1.56(3)
C(48)-H(48A)	0.9900	C(48)-H(48B)	0.9900
C(49)-C(50)	1.51(3)	C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900	C(50)-H(50A)	0.9900
O(15)-Mo(1)-O(14)	105.6(4)	O(15)-Mo(1)-O(17)	105.2(4)
O(14)-Mo(1)-O(17)	87.7(4)	O(15)-Mo(1)-O(8)	101.1(4)
O(14)-Mo(1)-O(8)	153.3(3)	O(17)-Mo(1)-O(8)	86.1(4)
O(15)-Mo(1)-O(18)	101.7(4)	O(14)-Mo(1)-O(18)	87.3(4)
O(17)-Mo(1)-O(18)	153.1(3)	O(8)-Mo(1)-O(18)	86.6(4)
O(15)-Mo(1)-O(13)	176.8(4)	O(14)-Mo(1)-O(13)	77.2(3)
O(17)-Mo(1)-O(13)	76.2(3)	O(8)-Mo(1)-O(13)	76.1(3)
O(18)-Mo(1)-O(13)	76.8(3)	O(11)-Mo(2)-O(12)	104.4(4)
O(11)-Mo(2)-O(3)	102.1(4)	O(12)-Mo(2)-O(3)	153.4(3)

O(11)-Mo(2)-O(9)	103.7(4)	O(12)-Mo(2)-O(9)	89.3(4)
O(3)-Mo(2)-O(9)	86.3(4)	O(11)-Mo(2)-O(10)	104.1(4)
O(12)-Mo(2)-O(10)	87.7(3)	O(3)-Mo(2)-O(10)	83.9(3)
O(9)-Mo(2)-O(10)	151.9(3)	O(11)-Mo(2)-O(13)	178.7(4)
O(12)-Mo(2)-O(13)	76.8(3)	O(3)-Mo(2)-O(13)	76.6(3)
O(9)-Mo(2)-O(13)	76.5(3)	O(10)-Mo(2)-O(13)	75.5(3)
O(4)-Mo(3)-O(10)	104.0(4)	O(4)-Mo(3)-O(2)	103.8(4)
O(10)-Mo(3)-O(2)	87.2(4)	O(4)-Mo(3)-O(5)	103.0(4)
O(10)-Mo(3)-O(5)	86.9(3)	O(2)-Mo(3)-O(5)	153.2(4)
O(4)-Mo(3)-O(17)	103.6(4)	O(10)-Mo(3)-O(17)	152.4(4)
O(2)-Mo(3)-O(17)	86.9(3)	O(5)-Mo(3)-O(17)	86.3(3)
O(4)-Mo(3)-O(13)	178.8(3)	O(10)-Mo(3)-O(13)	76.8(3)
O(2)-Mo(3)-O(13)	77.0(3)	O(5)-Mo(3)-O(13)	76.2(3)
O(17)-Mo(3)-O(13)	75.5(3)	N(1)-Mo(4)-O(8)	101.7(4)
N(1)-Mo(4)-O(5)	102.8(5)	O(8)-Mo(4)-O(5)	89.1(4)
N(1)-Mo(4)-O(12)	102.5(5)	O(8)-Mo(4)-O(12)	155.7(3)
O(5)-Mo(4)-O(12)	86.8(3)	N(1)-Mo(4)-O(6)	101.8(5)
O(8)-Mo(4)-O(6)	88.2(4)	O(5)-Mo(4)-O(6)	155.2(4)
O(12)-Mo(4)-O(6)	85.6(3)	N(1)-Mo(4)-O(13)	178.9(4)
O(8)-Mo(4)-O(13)	78.3(3)	O(5)-Mo(4)-O(13)	78.3(3)
O(12)-Mo(4)-O(13)	77.5(3)	O(6)-Mo(4)-O(13)	77.0(3)
O(1)-Mo(5)-O(2)	103.1(5)	O(1)-Mo(5)-O(3)	106.2(4)
O(2)-Mo(5)-O(3)	86.4(3)	O(1)-Mo(5)-O(16)	105.1(5)
O(2)-Mo(5)-O(16)	151.7(4)	O(3)-Mo(5)-O(16)	88.0(4)
O(1)-Mo(5)-O(14)	103.6(4)	O(2)-Mo(5)-O(14)	85.7(4)
O(3)-Mo(5)-O(14)	150.2(4)	O(16)-Mo(5)-O(14)	85.5(3)
O(1)-Mo(5)-O(13)	178.5(4)	O(2)-Mo(5)-O(13)	76.4(3)
O(3)-Mo(5)-O(13)	75.2(3)	O(16)-Mo(5)-O(13)	75.3(3)
O(14)-Mo(5)-O(13)	74.9(3)	O(7)-Mo(6)-O(6)	103.9(5)
O(7)-Mo(6)-O(16)	102.4(5)	O(6)-Mo(6)-O(16)	153.6(4)
O(7)-Mo(6)-O(18)	104.1(4)	O(6)-Mo(6)-O(18)	89.3(4)
O(16)-Mo(6)-O(18)	86.7(4)	O(7)-Mo(6)-O(9)	103.1(4)
O(6)-Mo(6)-O(9)	86.9(4)	O(16)-Mo(6)-O(9)	84.8(4)
O(18)-Mo(6)-O(9)	152.7(3)	O(7)-Mo(6)-O(13)	178.5(4)
O(6)-Mo(6)-O(13)	77.0(3)	O(16)-Mo(6)-O(13)	76.7(3)
O(18)-Mo(6)-O(13)	77.0(3)	O(9)-Mo(6)-O(13)	75.7(3)

Mo(3)-O(2)-Mo(5)	117.7(4)	Mo(2)-O(3)-Mo(5)	118.7(3)
Mo(3)-O(5)-Mo(4)	115.1(4)	Mo(6)-O(6)-Mo(4)	115.1(4)
Mo(4)-O(8)-Mo(1)	114.9(3)	Mo(2)-O(9)-Mo(6)	117.4(4)
Mo(3)-O(10)-Mo(2)	117.7(4)	Mo(2)-O(12)-Mo(4)	115.5(4)
Mo(4)-O(13)-Mo(1)	90.7(2)	Mo(4)-O(13)-Mo(3)	90.4(3)
Mo(1)-O(13)-Mo(3)	90.2(3)	Mo(4)-O(13)-Mo(6)	90.7(3)
Mo(1)-O(13)-Mo(6)	89.6(2)	Mo(3)-O(13)-Mo(6)	178.8(4)
Mo(4)-O(13)-Mo(2)	90.2(3)	Mo(1)-O(13)-Mo(2)	179.1(4)
Mo(3)-O(13)-Mo(2)	89.9(2)	Mo(6)-O(13)-Mo(2)	90.2(3)
Mo(4)-O(13)-Mo(5)	179.3(4)	Mo(1)-O(13)-Mo(5)	89.6(3)
Mo(3)-O(13)-Mo(5)	88.9(3)	Mo(6)-O(13)-Mo(5)	89.9(2)
Mo(2)-O(13)-Mo(5)	89.5(2)	Mo(1)-O(14)-Mo(5)	118.2(4)
Mo(6)-O(16)-Mo(5)	118.1(4)	Mo(1)-O(17)-Mo(3)	118.0(4)
Mo(6)-O(18)-Mo(1)	116.5(4)	C(1)-N(1)-Mo(4)	172.7(11)
N(1)-C(1)-C(6)	125.5(16)	N(1)-C(1)-C(2)	120.1(15)
C(6)-C(1)-C(2)	114.3(16)	C(3)-C(2)-C(1)	120.2(17)
C(3)-C(2)-H(2)	119.9	C(1)-C(2)-H(2)	119.9
C(4)-C(3)-C(2)	127.1(19)	C(4)-C(3)-H(3)	116.4
C(2)-C(3)-H(3)	116.4	C(3)-C(4)-C(5)	115.5(16)
C(3)-C(4)-C(7)	123.0(17)	C(5)-C(4)-C(7)	121.5(14)
C(6)-C(5)-C(4)	119.4(15)	C(6)-C(5)-H(5)	120.3
C(4)-C(5)-H(5)	120.3	C(1)-C(6)-C(5)	123.4(15)
C(1)-C(6)-H(6)	118.3	C(5)-C(6)-H(6)	118.3
C(8)-C(7)-C(4)	175.6(17)	C(7)-C(8)-C(9)	174.8(16)
C(10)-C(9)-C(14)	120.6(14)	C(10)-C(9)-C(8)	116.3(14)
C(14)-C(9)-C(8)	123.1(15)	C(11)-C(10)-C(9)	116.9(14)
C(11)-C(10)-H(10)	121.6	C(9)-C(10)-H(10)	121.6
C(10)-C(11)-C(12)	123.2(15)	C(10)-C(11)-H(11)	118.4
C(12)-C(11)-H(11)	118.4	C(13)-C(12)-C(11)	119.7(17)
C(13)-C(12)-N(2)	120.6(16)	C(11)-C(12)-N(2)	119.5(14)
C(12)-C(13)-C(14)	119.8(16)	C(12)-C(13)-H(13)	120.1
C(14)-C(13)-H(13)	120.1	C(13)-C(14)-C(9)	119.6(14)
C(13)-C(14)-H(14)	120.2	C(9)-C(14)-H(14)	120.2
C(18)-N(2)-C(15)	106.6(18)	C(18)-N(2)-C(12)	128.1(14)
C(15)-N(2)-C(12)	125.3(16)	C(16)-C(15)-N(2)	108.4(17)
C(16)-C(15)-H(15)	125.8	N(2)-C(15)-H(15)	125.8

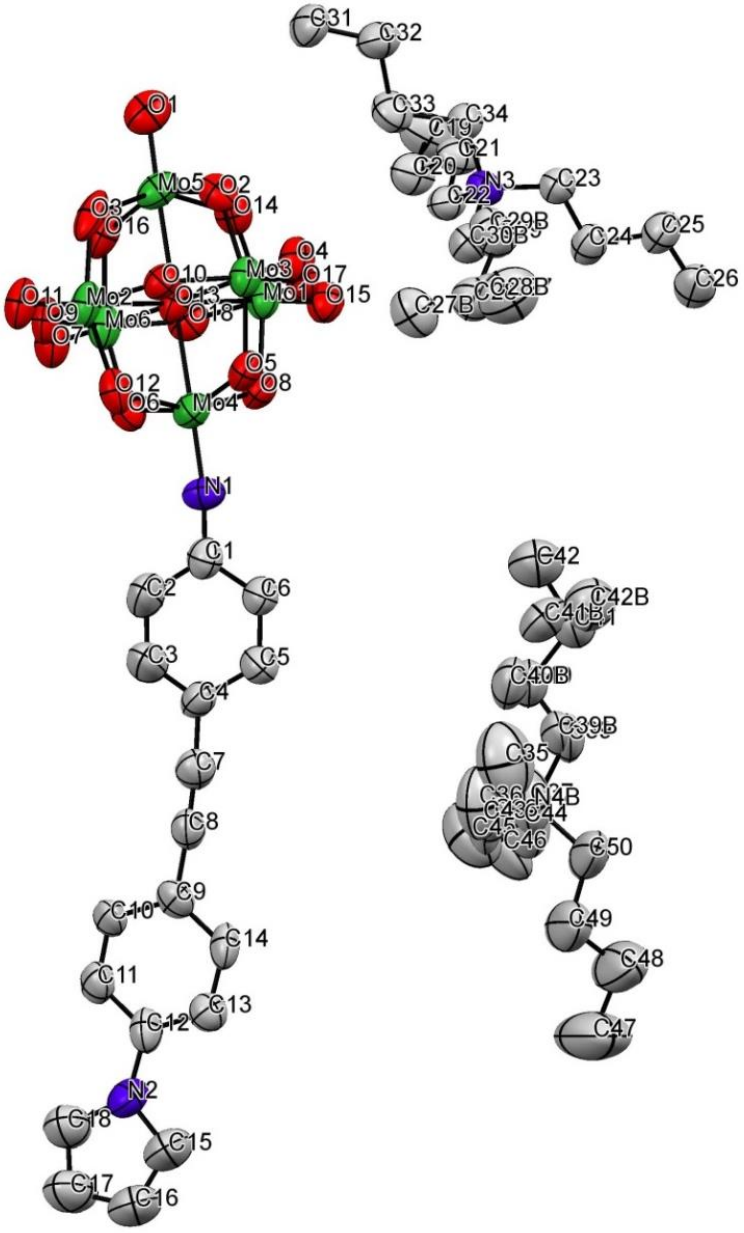
C(15)-C(16)-C(17)	108.5(12)	C(15)-C(16)-H(16)	125.8
C(17)-C(16)-H(16)	125.8	C(18)-C(17)-C(16)	107.2(12)
C(18)-C(17)-H(17)	126.4	C(16)-C(17)-H(17)	126.4
C(17)-C(18)-N(2)	109.4(17)	C(17)-C(18)-H(18)	125.3
N(2)-C(18)-H(18)	125.3	C(22)-N(3)-C(23)	112.3(11)
C(22)-N(3)-C(34)	110.0(11)	C(23)-N(3)-C(34)	107.2(9)
C(22)-N(3)-C(30)	106.0(11)	C(23)-N(3)-C(30)	109.4(11)
C(34)-N(3)-C(30)	112.0(12)	C(20)-C(19)-H(19A)	109.5
C(20)-C(19)-H(19B)	109.5	H(19A)-C(19)-H(19B)	109.5
C(20)-C(19)-H(19C)	109.5	H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5	C(19)-C(20)-C(21)	112.5(13)
C(19)-C(20)-H(20A)	109.1	C(21)-C(20)-H(20A)	109.1
C(19)-C(20)-H(20B)	109.1	C(21)-C(20)-H(20B)	109.1
H(20A)-C(20)-H(20B)	107.8	C(22)-C(21)-C(20)	110.3(12)
C(22)-C(21)-H(21A)	109.6	C(20)-C(21)-H(21A)	109.6
C(22)-C(21)-H(21B)	109.6	C(20)-C(21)-H(21B)	109.6
H(21A)-C(21)-H(21B)	108.1	N(3)-C(22)-C(21)	115.3(11)
N(3)-C(22)-H(22A)	108.4	C(21)-C(22)-H(22A)	108.4
N(3)-C(22)-H(22B)	108.4	C(21)-C(22)-H(22B)	108.4
H(22A)-C(22)-H(22B)	107.5	N(3)-C(23)-C(24)	118.0(11)
N(3)-C(23)-H(23A)	107.8	C(24)-C(23)-H(23A)	107.8
N(3)-C(23)-H(23B)	107.8	C(24)-C(23)-H(23B)	107.8
H(23A)-C(23)-H(23B)	107.1	C(25)-C(24)-C(23)	109.6(13)
C(25)-C(24)-H(24A)	109.8	C(23)-C(24)-H(24A)	109.8
C(25)-C(24)-H(24B)	109.8	C(23)-C(24)-H(24B)	109.8
H(24A)-C(24)-H(24B)	108.2	C(24)-C(25)-C(26)	112.2(14)
C(24)-C(25)-H(25A)	109.2	C(26)-C(25)-H(25A)	109.2
C(24)-C(25)-H(25B)	109.2	C(26)-C(25)-H(25B)	109.2
H(25A)-C(25)-H(25B)	107.9	C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5	H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5	C(28)-C(27)-H(27A)	109.5
C(28)-C(27)-H(27B)	109.5	H(27A)-C(27)-H(27B)	109.5
C(28)-C(27)-H(27C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5	C(27)-C(28)-C(29)	107(2)
C(27)-C(28)-H(28A)	110.4	C(29)-C(28)-H(28A)	110.4

C(27)-C(28)-H(28B)	110.4	C(29)-C(28)-H(28B)	110.4
H(28A)-C(28)-H(28B)	108.6	C(30)-C(29)-C(28)	107.1(19)
C(30)-C(29)-H(29A)	110.3	C(28)-C(29)-H(29A)	110.3
C(30)-C(29)-H(29B)	110.3	C(28)-C(29)-H(29B)	110.3
H(29A)-C(29)-H(29B)	108.6	C(29)-C(30)-N(3)	116.6(16)
C(29)-C(30)-H(30A)	108.1	N(3)-C(30)-H(30A)	108.1
C(29)-C(30)-H(30B)	108.1	N(3)-C(30)-H(30B)	108.1
H(30A)-C(30)-H(30B)	107.3	C(28B)-C(27B)-H(27D)	109.5
C(28B)-C(27B)-H(27E)	109.5	H(27D)-C(27B)-H(27E)	109.5
C(28B)-C(27B)-H(27F)	109.5	H(27D)-C(27B)-H(27F)	109.5
H(27E)-C(27B)-H(27F)	109.5	C(29B)-C(28B)-C(27B)	108(3)
C(29B)-C(28B)-H(28C)	110.1	C(27B)-C(28B)-H(28C)	110.1
C(29B)-C(28B)-H(28D)	110.1	C(27B)-C(28B)-H(28D)	110.1
H(28C)-C(28B)-H(28D)	108.4	C(28B)-C(29B)-H(29C)	109.5
C(28B)-C(29B)-H(29D)	109.5	H(29C)-C(29B)-H(29D)	108.1
C(32)-C(31)-H(31A)	109.5	C(32)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5	C(32)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(31B)-C(31)-H(31C)	109.5
C(31)-C(32)-C(33)	115.8 (14)	C(31)-C(32)-H(32A)	108.3
C(33)-C(32)-H(32A)	108.3	C(31)-C(32)-H(32B)	108.3
C(33)-C(32)-H(32B)	108.3	H(32A)-C(32)-H(32B)	107.4
C(34)-C(33)-C(32)	111.1 (12)	C(34)-C(33)-H(33A)	109.4
C(32)-C(33)-H(33A)	109.4	C(34)-C(33)-H(33B)	109.4
C(32)-C(33)-H(33B)	109.4	H(33A)-C(33)-H(33B)	108.0
N(3)-C(34)-C(33)	117.0 (11)	N(3)-C(34)-H(34A)	108.0
C(33)-C(34)-H(34A)	108.0	N(3)-C(34)-H(34B)	108.0
C(33)-C(34)-H(34B)	108.0	H(34A)-C(34)-H(34B)	107.3
C(36)-C(35)-H(35A)	109.5	C(36)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5	C(36)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5	H(35B)-C(35)-H(35C)	109.5
C(35)-C(36)-C(37)	110 (3)	C(35)-C(36)-H(36A)	109.8
C(37)-C(36)-H(36A)	109.8	C(35)-C(36)-H(36B)	109.8
C(37)-C(36)-H(36B)	109.8	H(36A)-C(36)-H(36B)	108.2
C(38)-C(37)-C(36)	108.6 (19)	C(38)-C(37)-H(37A)	110.0
C(36)-C(37)-H(37A)	110.0	C(38)-C(37)-H(37B)	110.0
C(36)-C(37)-H(37B)	110.0	H(37A)-C(37)-H(37B)	108.3

C(37)-C(38)-N(4)	116.6(18)	C(37)-C(38)-H(38A)	108.1
N(4)-C(38)-H(38A)	108.1	C(37)-C(38)-H(38B)	108.1
N(4)-C(38)-H(38B)	108.1	H(38A)-C(38)-H(38B)	107.3
C(50)-N(4)-C(43)	111 (2)	C(50)-N(4)-C(39)	105(2)
C(43)-N(4)-C(39)	114 (3)	C(50)-N(4)-C(38)	108.8(17)
C(43)-N(4)-C(38)	103.5 (14)	C(39)-N(4)-C(38)	115(3)
C(40)-C(39)-N(4)	117(3)	C(40)-C(39)-H(39A)	107.9
N(4)-C(39)-H(39A)	107.9	C(40)-C(39)-H(39B)	107.9
N(4)-C(39)-H(39B)	107.9	H(39A)-C(39)-H(39B)	107.2
C(39)-C(40)-C(41)	107 (3)	C(39)-C(40)-H(40A)	110.3
C(41)-C(40)-H(40A)	110.3	C(39)-C(40)-H(40B)	110.3
C(41)-C(40)-H(40B)	110.3	H(40A)-C(40)-H(40B)	108.6
C(42)-C(41)-C(40)	111 (3)	C(42)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41A)	109.5	C(42)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41B)	109.5	H(41A)-C(41)-H(41B)	108.1
C(41)-C(42)-H(42A)	109.5	C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5	C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5	H(42B)-C(42)-H(42C)	109.5
C(40B)-C(39B)-H(39C)	108.0	C(40B)-C(39B)-H(39D)	108.0
H(39C)-C(39B)-H(39D)	107.2	C(39B)-C(40B)-C(41B)	108(2)
C(39B)-C(40B)-H(40C)	110.1	C(41B)-C(40B)-H(40C)	110.1
C(39B)-C(40B)-H(40D)	110.1	C(41B)-C(40B)-H(40D)	110.1
H(40C)-C(40B)-H(40D)	108.4	C(40B)-C(41B)-C(42B)	115(3)
C(40B)-C(41B)-H(41C)	108.5	C(42B)-C(41B)-H(41C)	108.5
C(40B)-C(41B)-H(41D)	108.5	C(42B)-C(41B)-H(41D)	108.5
H(41C)-C(41B)-H(41D)	107.5	C(41B)-C(42B)-H(42D)	109.5
C(41B)-C(42B)-H(42E)	109.5	H(42D)-C(42B)-H(42E)	109.5
C(41B)-C(42B)-H(42F)	109.5	H(42D)-C(42B)-H(42F)	109.5
H(42E)-C(42B)-H(42F)	109.5	N(4)-C(43)-C(44)	106.0(15)
N(4)-C(43)-H(43A)	110.5	C(44)-C(43)-H(43A)	110.5
N(4)-C(43)-H(43B)	110.5	C(44)-C(43)-H(43B)	110.5
H(43A)-C(43)-H(43B)	108.7	C(45)-C(44)-C(43)	104.1(17)
C(45)-C(44)-H(44A)	110.9	C(43)-C(44)-H(44A)	110.9
C(45)-C(44)-H(44B)	110.9	C(43)-C(44)-H(44B)	110.9
H(44A)-C(44)-H(44B)	109.0	C(44)-C(45)-C(46)	111.7(19)
C(44)-C(45)-H(45A)	109.3	C(46)-C(45)-H(45A)	109.3

C(44)-C(45)-H(45B)	109.3	C(46)-C(45)-H(45B)	109.3
H(45A)-C(45)-H(45B)	107.9	C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5	H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5	H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5	C(48)-C(47)-H(47A)	109.5
C(48)-C(47)-H(47B)	109.5	H(47A)-C(47)-H(47B)	109.5
C(48)-C(47)-H(47C)	109.5	H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5	C(47)-C(48)-C(49)	113(3)
C(47)-C(48)-H(48A)	109.1	C(49)-C(48)-H(48A)	109.1
C(47)-C(48)-H(48B)	109.1	C(49)-C(48)-H(48B)	109.1
H(48A)-C(48)-H(48B)	107.8	C(50)-C(49)-C(48)	112(2)
C(50)-C(49)-H(49A)	109.3	C(48)-C(49)-H(49A)	109.3
C(50)-C(49)-H(49B)	109.3	C(48)-C(49)-H(49B)	109.3
H(49A)-C(49)-H(49B)	107.9	C(49)-C(50)-N(4)	116.4(18)
C(49)-C(50)-H(50A)	108.2	N(4)-C(50)-H(50A)	108.2
C(49)-C(50)-H(50B)	108.2	N(4)-C(50)-H(50B)	108.2
H(50A)-C(50)-H(50B)	107.3		

ORTEP-3 representation of compound **4**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity



Compound 5

Crystal growth	Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method	Oil

Crystal Data

Chemical formula	$C_{46}H_{82}Mo_6N_4O_{18}$	
Formula weight	1554.79 g mol^{-1}	
Temperature	100(2) K	
Crystal size	0.190 x 0.180 x 0.030 mm^3	
Crystal description	Orang cut blade	
Crystal system	Orthorhombic	
Space group	P212121	
Unit cell dimensions	a = 15.9271(11) Å	α = 90°.
	b = 24.5421(17) Å	β = 90°.
	c = 24.5421(17) Å	γ = 90°.
Volume	11720.3(14) $Å^3$	
Z	8	
F(000)	6256	
Density (calculated)	1.762 Mg cm^{-3}	
Absorption coefficient	1.314 mm^{-1}	

Data Collection

Diffractometer	Rigaku AFC 12 goniometer
Radiation	Mo-*Kα*
2θ range for data collection	1.592 – 27.50°
Reflections collected	153015
Independent reflections	26880 [R(int) = 0.0742]
Transmission coefficients	1.000
Data corrections	Gaussian
Index ranges	-20<=h<=20, -31<=k<=31, -38<=l<=38

Refinement method

Full-matrix least squares on F^2		
Weighting scheme	None	
Data / restraints / parameters	26880 / 2019 / 1627	
Data to parameter ratio	16.52	
Goodness of fit on F^2	0.985	
R indices	[I_o>2σ>(I_o)] data	R1 = 0.0533, wR2 = 0.1442
	All 2558 data	R1 = 0.0558, wR2 = 0.1466
Final difference map	Largest diff. peak + 1.571 and hole - 1.040 e.$Å^{-3}$	

Bond lengths [Å] and angles [°]

Mo(1)-O(1)	1.701(8)	Mo(6)-O(6)	2.196(5)
Mo(1)-O(3)	1.867(6)	Mo(7)-O(20)	1.682(6)
Mo(1)-O(2)	1.905(8)	Mo(7)-O(25)	1.878(7)
Mo(1)-O(4)	1.921(8)	Mo(7)-O(21)	1.889(7)
Mo(1)-O(5)	1.976(8)	Mo(7)-O(22)	1.922(7)
Mo(1)-O(6)	2.353(5)	Mo(7)-O(26)	1.985(6)
Mo(2)-O(7)	1.682(7)	Mo(7)-O(27)	2.358(5)
Mo(2)-O(12)	1.846(8)	Mo(8)-O(30)	1.685(7)
Mo(2)-O(5)	1.864(7)	Mo(8)-O(28)	1.839(7)
Mo(2)-O(16)	1.940(6)	Mo(8)-O(36)	1.857(7)
Mo(2)-O(13)	2.028(8)	Mo(8)-O(25)	1.988(7)
Mo(2)-O(6)	2.334(5)	Mo(8)-O(24)	2.000(7)
Mo(3)-O(10)	1.700(8)	Mo(8)-O(27)	2.328(5)
Mo(3)-O(13)	1.846(8)	Mo(9)-O(23)	1.690(7)
Mo(3)-O(4)	1.892(8)	Mo(9)-O(24)	1.859(7)
Mo(3)-O(15)	1.938(7)	Mo(9)-O(35)	1.884(6)
Mo(3)-O(11)	2.025(7)	Mo(9)-O(21)	1.968(6)
Mo(3)-O(6)	2.339(5)	Mo(9)-O(32)	2.026(7)
Mo(4)-O(9)	1.691(7)	Mo(9)-O(27)	2.322(5)
Mo(4)-O(11)	1.861(7)	Mo(10)-O(19)	1.673(7)
Mo(4)-O(18)	1.869(6)	Mo(10)-O(29)	1.833(7)
Mo(4)-O(3)	1.975(6)	Mo(10)-O(22)	1.901(7)
Mo(4)-O(14)	2.025(7)	Mo(10)-O(33)	1.931(7)
Mo(4)-O(6)	2.339(5)	Mo(10)-O(28)	2.035(7)
Mo(5)-O(8)	1.680(7)	Mo(10)-O(27)	2.352(5)
Mo(5)-O(14)	1.853(7)	Mo(11)-O(31)	1.693(6)
Mo(5)-O(17)	1.890(6)	Mo(11)-O(32)	1.853(7)
Mo(5)-O(2)	1.949(7)	Mo(11)-O(26)	1.881(6)
Mo(5)-O(12)	2.023(7)	Mo(11)-O(34)	1.946(6)
Mo(5)-O(6)	2.339(5)	Mo(11)-O(29)	2.042(6)
Mo(6)-N(1)	1.738(7)	Mo(11)-O(27)	2.341(5)
Mo(6)-O(16)	1.910(6)	Mo(12)-N(5)	1.742(8)
Mo(6)-O(15)	1.912(6)	Mo(12)-O(33)	1.895(6)
Mo(6)-O(17)	1.980(6)	Mo(12)-O(34)	1.904(6)

Mo(6)-O(18)	1.987(6)	Mo(12)-O(35)	1.996(6)
N(1)-C(1)	1.386(10)	C(16)-H(16B)	0.9900
N(2)-C(12)	1.386(11)	C(17)-C(18)	1.517(11)
N(2)-H(02A)	0.75(5)	C(17)-H(17A)	0.9900
N(2)-H(02B)	0.91(3)	C(17)-H(17B)	0.9900
C(1)-C(2)	1.370(13)	C(18)-H(18A)	0.9800
C(1)-C(6)	1.390(13)	C(18)-H(18B)	0.9800
C(2)-C(3)	1.392(13)	C(18)-H(18C)	0.9800
C(2)-H(2)	0.9500	C(19)-C(20)	1.530(16)
C(3)-C(4)	1.371(14)	C(19)-H(19A)	0.9900
C(3)-H(3)	0.9500	C(19)-H(19B)	0.9900
C(4)-C(5)	1.395(14)	C(20)-C(21)	1.517(17)
C(4)-C(7)	1.443(12)	C(20)-H(20A)	0.9900
C(5)-C(6)	1.404(13)	C(20)-H(20B)	0.9900
C(5)-H(5)	0.9500	C(21)-C(22)	1.520(12)
C(6)-H(6)	0.9500	C(21)-H(21A)	0.9900
C(7)-C(8)	1.193(13)	C(21)-H(21B)	0.9900
C(8)-C(9)	1.441(12)	C(22)-H(22A)	0.9800
C(9)-C(10)	1.378(13)	C(22)-H(22B)	0.9800
C(9)-C(14)	1.413(13)	C(22)-H(22C)	0.9800
C(10)-C(11)	1.396(12)	C(23A)-C(24A)	1.465(14)
C(10)-H(10)	0.9500	C(23A)-H(23A)	0.9900
C(11)-C(12)	1.394(12)	C(23A)-H(23B)	0.9900
C(11)-H(11)	0.9500	C(24A)-C(25A)	1.522(13)
C(12)-C(13)	1.378(13)	C(24A)-H(24A)	0.9900
C(13)-C(14)	1.384(12)	C(24A)-H(24B)	0.9900
C(13)-H(13)	0.9500	C(25A)-C(26A)	1.61(4)
C(14)-H(14)	0.9500	C(25A)-H(25A)	0.9900
N(3)-C(15)	1.513(12)	C(25A)-H(25B)	0.9900
N(3)-C(27)	1.511(15)	C(26A)-H(26A)	0.9800
N(3)-C(19)	1.545(15)	C(26A)-H(26B)	0.9800
N(3)-C(23A)	1.547(14)	C(26A)-H(26C)	0.9800
N(3)-C(23B)	1.547(14)	C(23B)-C(24B)	1.465(14)
C(15)-C(16)	1.489(16)	C(23B)-H(23C)	0.9900
C(15)-H(15A)	0.9900	C(23B)-H(23D)	0.9900
C(15)-H(15B)	0.9900	C(24B)-C(25B)	1.485(13)

C(16)-C(17)	1.536(15)	C(24B)-H(24C)	0.9900
C(16)-H(16A)	0.9900	C(24B)-H(24D)	0.9900
C(25B)-C(26B)	1.53(4)	C(34A)-H(34C)	0.9800
C(25B)-H(25C)	0.9900	C(35A)-C(36A)	1.502(14)
C(25B)-H(25D)	0.9900	C(35A)-H(35A)	0.9900
C(26B)-H(26D)	0.9800	C(35A)-H(35B)	0.9900
C(26B)-H(26E)	0.9800	C(36A)-C(37A)	1.517(14)
C(26B)-H(26F)	0.9800	C(36A)-H(36A)	0.9900
C(27)-C(28)	1.540(17)	C(36A)-H(36B)	0.9900
C(27)-H(27A)	0.9900	C(37A)-C(38A)	1.491(14)
C(27)-H(27B)	0.9900	C(37A)-H(37A)	0.9900
C(28)-C(29)	1.550(16)	C(37A)-H(37B)	0.9900
C(28)-H(28A)	0.9900	C(38A)-H(38A)	0.9800
C(28)-H(28B)	0.9900	C(38A)-H(38B)	0.9800
C(29)-C(30)	1.48(2)	C(38A)-H(38C)	0.9800
C(29)-H(29A)	0.9900	C(39A)-C(40A)	1.42(5)
C(29)-H(29B)	0.9900	C(39A)-H(39A)	0.9900
C(30)-H(30A)	0.9800	C(39A)-H(39B)	0.9900
C(30)-H(30B)	0.9800	C(40A)-C(41A)	1.47(4)
C(30)-H(30C)	0.9800	C(40A)-H(40A)	0.9900
N(4)-C(39B)	1.48(4)	C(40A)-H(40B)	0.9900
N(4)-C(31A)	1.497(13)	C(41A)-C(42A)	1.499(14)
N(4)-C(31B)	1.495(13)	C(41A)-H(41A)	0.9900
N(4)-C(35B)	1.511(13)	C(41A)-H(41B)	0.9900
N(4)-C(39A)	1.51(4)	C(42A)-H(42A)	0.9800
N(4)-C(35A)	1.53(3)	C(42A)-H(42B)	0.9800
N(4)-C(43B)	1.542(14)	C(42A)-H(42C)	0.9800
N(4)-C(43A)	1.542(14)	C(43A)-C(44A)	1.58(3)
C(31A)-C(32A)	1.505(14)	C(43A)-H(43A)	0.9900
C(31A)-H(31A)	0.9900	C(43A)-H(43B)	0.9900
C(31A)-H(31B)	0.9900	C(44A)-C(45A)	1.49(3)
C(32A)-C(33A)	1.506(14)	C(44A)-H(44A)	0.9900
C(32A)-H(32A)	0.9900	C(44A)-H(44B)	0.9900
C(32A)-H(32B)	0.9900	C(45A)-C(46A)	1.59(3)
C(33A)-C(34A)	1.512(13)	C(45A)-H(45A)	0.9900
C(33A)-H(33A)	0.9900	C(45A)-H(45B)	0.9900

C(33A)-H(33B)	0.9900	C(46A)-H(46A)	0.9800
C(34A)-H(34A)	0.9800	C(46A)-H(46B)	0.9800
C(34A)-H(34B)	0.9800	C(46A)-H(46C)	0.9800
C(31B)-C(32B)	1.505(14)	C(42B)-H(42E)	0.9800
C(31B)-H(31C)	0.9900	C(42B)-H(42F)	0.9800
C(31B)-H(31D)	0.9900	C(44B)-C(45B)	1.49(4)
C(32B)-C(33B)	1.499(14)	C(44B)-H(44C)	0.9900
C(32B)-H(32C)	0.9900	C(44B)-H(44D)	0.9900
C(32B)-H(32D)	0.9900	C(45B)-C(46B)	1.50(4)
C(33B)-C(34B)	1.501(14)	C(45B)-H(45C)	0.9900
C(33B)-H(33C)	0.9900	C(45B)-H(45D)	0.9900
C(33B)-H(33D)	0.9900	C(46B)-H(46D)	0.9800
C(34B)-H(34D)	0.9800	C(46B)-H(46E)	0.9800
C(34B)-H(34E)	0.9800	C(46B)-H(46F)	0.9800
C(34B)-H(34F)	0.9800	N(5)-C(47)	1.385(12)
C(35B)-C(36B)	1.511(14)	N(6)-C(58)	1.372(11)
C(35B)-H(35C)	0.9900	N(6)-H(06A)	0.92(3)
C(35B)-H(35D)	0.9900	N(6)-H(06B)	0.90(3)
C(36B)-C(37B)	1.510(13)	C(47)-C(48)	1.390(14)
C(36B)-H(36C)	0.9900	C(47)-C(52)	1.417(14)
C(36B)-H(36D)	0.9900	C(48)-C(49)	1.377(13)
C(37B)-C(38B)	1.50(3)	C(48)-H(48)	0.9500
C(37B)-H(37C)	0.9900	C(49)-C(50)	1.403(13)
C(37B)-H(37D)	0.9900	C(49)-H(49)	0.9500
C(38B)-H(38D)	0.9800	C(50)-C(51)	1.366(14)
C(38B)-H(38E)	0.9800	C(50)-C(53)	1.452(12)
C(38B)-H(38F)	0.9800	C(51)-C(52)	1.396(12)
C(39B)-C(40B)	1.59(4)	C(51)-H(51)	0.9500
C(39B)-H(39C)	0.9900	C(52)-H(52)	0.9500
C(39B)-H(39D)	0.9900	C(53)-C(54)	1.201(12)
C(40B)-C(41B)	1.493(14)	C(54)-C(55)	1.436(12)
C(40B)-H(40C)	0.9900	C(55)-C(60)	1.379(13)
C(40B)-H(40D)	0.9900	C(55)-C(56)	1.389(12)
C(41B)-C(42B)	1.499(14)	C(56)-C(57)	1.388(13)
C(41B)-H(41C)	0.9900	C(56)-H(56)	0.9500
C(41B)-H(41D)	0.9900	C(57)-C(58)	1.397(12)

C(43B)-C(44B)	1.517(13)	C(57)-H(57)	0.9500
C(43B)-H(43C)	0.9900	C(58)-C(59)	1.384(12)
C(43B)-H(43D)	0.9900	C(59)-C(60)	1.397(12)
C(42B)-H(42D)	0.9800	C(59)-H(59)	0.9500
C(60)-H(60)	0.9500	C(71)-H(71A)	0.9900
N(7)-C(73B)	1.492(13)	C(71)-H(71B)	0.9900
N(7)-C(73A)	1.502(13)	C(72)-H(72A)	0.9800
N(7)-C(65)	1.505(14)	C(72)-H(72B)	0.9800
N(7)-C(61)	1.508(14)	C(72)-H(72C)	0.9800
N(7)-C(69)	1.539(11)	C(73A)-C(74A)	1.60(3)
C(61)-C(62)	1.526(17)	C(73A)-H(73A)	0.9900
C(61)-H(61A)	0.9900	C(73A)-H(73B)	0.9900
C(61)-H(61B)	0.9900	C(74A)-C(75A)	1.49(4)
C(62)-C(63)	1.51(2)	C(74A)-H(74A)	0.9900
C(62)-H(62A)	0.9900	C(74A)-H(74B)	0.9900
C(62)-H(62B)	0.9900	C(75A)-C(76A)	1.42(4)
C(63)-C(64)	1.481(13)	C(75A)-H(75A)	0.9900
C(63)-H(63A)	0.9900	C(75A)-H(75B)	0.9900
C(63)-H(63B)	0.9900	C(76A)-H(76A)	0.9800
C(64)-H(64A)	0.9800	C(76A)-H(76B)	0.9800
C(64)-H(64B)	0.9800	C(76A)-H(76C)	0.9800
C(64)-H(64C)	0.9800	C(73B)-C(74B)	1.505(14)
C(65)-C(66)	1.542(15)	C(73B)-H(73C)	0.9900
C(65)-H(65A)	0.9900	C(73B)-H(73D)	0.9900
C(65)-H(65B)	0.9900	C(74B)-C(75B)	1.496(14)
C(66)-C(67)	1.52(2)	C(74B)-H(74C)	0.9900
C(66)-H(66A)	0.9900	C(74B)-H(74D)	0.9900
C(66)-H(66B)	0.9900	C(75B)-C(76B)	1.498(14)
C(67)-C(68)	1.50(2)	C(75B)-H(75C)	0.9900
C(67)-H(67A)	0.9900	C(75B)-H(75D)	0.9900
C(67)-H(67B)	0.9900	C(76B)-H(76D)	0.9800
C(68)-H(68A)	0.9800	C(76B)-H(76E)	0.9800
C(68)-H(68B)	0.9800	C(76B)-H(76F)	0.9800
C(68)-H(68C)	0.9800	N(8)-C(81)	1.501(14)
C(69)-C(70)	1.543(16)	N(8)-C(89B)	1.500(11)
C(69)-H(69A)	0.9900	N(8)-C(89A)	1.500(11)

C(69)-H(69B)	0.9900	N(8)-C(77B)	1.54(3)
C(70)-C(71)	1.550(15)	N(8)-C(77A)	1.54(2)
C(70)-H(70A)	0.9900	N(8)-C(85A)	1.541(11)
C(70)-H(70B)	0.9900	N(8)-C(85B)	1.541(11)
C(71)-C(72)	1.504(17)	C(77A)-C(78A)	1.53(3)
C(77A)-H(77A)	0.9900	C(85A)-H(85B)	0.9900
C(77A)-H(77B)	0.9900	C(86A)-C(87A)	1.503(13)
C(78A)-C(79A)	1.52(3)	C(86A)-H(86A)	0.9900
C(78A)-H(78A)	0.9900	C(86A)-H(86B)	0.9900
C(78A)-H(78B)	0.9900	C(87A)-C(88A)	1.482(14)
C(79A)-C(80A)	1.54(3)	C(87A)-H(87A)	0.9900
C(79A)-H(79A)	0.9900	C(87A)-H(87B)	0.9900
C(79A)-H(79B)	0.9900	C(88A)-H(88A)	0.9800
C(80A)-H(80A)	0.9800	C(88A)-H(88B)	0.9800
C(80A)-H(80B)	0.9800	C(88A)-H(88C)	0.9800
C(80A)-H(80C)	0.9800	C(89A)-C(90A)	1.454(12)
C(77B)-C(78B)	1.486(14)	C(89A)-H(89A)	0.9900
C(77B)-H(77C)	0.9900	C(89A)-H(89B)	0.9900
C(77B)-H(77D)	0.9900	C(90A)-C(91A)	1.498(13)
C(78B)-C(79B)	1.503(14)	C(90A)-H(90A)	0.9900
C(78B)-H(78C)	0.9900	C(90A)-H(90B)	0.9900
C(78B)-H(78D)	0.9900	C(91A)-C(92A)	1.491(14)
C(79B)-C(80B)	1.496(14)	C(91A)-H(91A)	0.9900
C(79B)-H(79C)	0.9900	C(91A)-H(91B)	0.9900
C(79B)-H(79D)	0.9900	C(92A)-H(92A)	0.9800
C(80B)-H(80D)	0.9800	C(92A)-H(92B)	0.9800
C(80B)-H(80E)	0.9800	C(92A)-H(92C)	0.9800
C(80B)-H(80F)	0.9800	C(85B)-C(86B)	1.485(12)
C(81)-C(82)	1.526(15)	C(85B)-H(85C)	0.9900
C(81)-H(81A)	0.9900	C(85B)-H(85D)	0.9900
C(81)-H(81B)	0.9900	C(86B)-C(87B)	1.503(13)
C(82)-C(83)	1.524(13)	C(86B)-H(86C)	0.9900
C(82)-H(82A)	0.9900	C(86B)-H(86D)	0.9900
C(82)-H(82B)	0.9900	C(87B)-C(88B)	1.515(14)
C(83)-C(84)	1.500(17)	C(87B)-H(87C)	0.9900
C(83)-H(83A)	0.9900	C(87B)-H(87D)	0.9900

C(83)-H(83B)	0.9900	C(88B)-H(88D)	0.9800
C(84)-H(84A)	0.9800	C(88B)-H(88E)	0.9800
C(84)-H(84B)	0.9800	C(88B)-H(88F)	0.9800
C(84)-H(84C)	0.9800	C(89B)-C(90B)	1.454(12)
C(85A)-C(86A)	1.485(12)	C(89B)-H(89C)	0.9900
C(85A)-H(85A)	0.9900	C(89B)-H(89D)	0.9900
C(90B)-C(91B)	1.530(14)	O(5)-Mo(2)-O(6)	77.2(2)
C(90B)-H(90C)	0.9900	O(16)-Mo(2)-O(6)	75.3(2)
C(90B)-H(90D)	0.9900	O(13)-Mo(2)-O(6)	75.0(2)
C(91B)-C(92B)	1.486(14)	O(10)-Mo(3)-O(13)	105.9(5)
C(91B)-H(91C)	0.9900	O(10)-Mo(3)-O(4)	104.2(4)
C(91B)-H(91D)	0.9900	O(13)-Mo(3)-O(4)	91.2(4)
C(92B)-H(92D)	0.9800	O(10)-Mo(3)-O(15)	102.9(4)
C(92B)-H(92E)	0.9800	O(13)-Mo(3)-O(15)	90.6(3)
C(92B)-H(92F)	0.9800	O(4)-Mo(3)-O(15)	151.2(3)
O(1)-Mo(1)-O(3)	105.3(4)	O(10)-Mo(3)-O(11)	101.3(4)
O(1)-Mo(1)-O(2)	104.3(4)	O(13)-Mo(3)-O(11)	152.7(3)
O(3)-Mo(1)-O(2)	89.7(3)	O(4)-Mo(3)-O(11)	83.9(3)
O(1)-Mo(1)-O(4)	102.5(4)	O(15)-Mo(3)-O(11)	81.5(3)
O(3)-Mo(1)-O(4)	89.0(3)	O(10)-Mo(3)-O(6)	175.5(4)
O(2)-Mo(1)-O(4)	152.5(3)	O(13)-Mo(3)-O(6)	78.2(3)
O(1)-Mo(1)-O(5)	102.3(4)	O(4)-Mo(3)-O(6)	77.2(3)
O(3)-Mo(1)-O(5)	152.3(3)	O(15)-Mo(3)-O(6)	75.1(2)
O(2)-Mo(1)-O(5)	84.8(3)	O(11)-Mo(3)-O(6)	74.5(2)
O(4)-Mo(1)-O(5)	83.6(4)	O(9)-Mo(4)-O(11)	105.1(4)
O(1)-Mo(1)-O(6)	176.9(3)	O(9)-Mo(4)-O(18)	104.0(3)
O(3)-Mo(1)-O(6)	77.6(2)	O(11)-Mo(4)-O(18)	93.1(3)
O(2)-Mo(1)-O(6)	76.6(2)	O(9)-Mo(4)-O(3)	102.8(3)
O(4)-Mo(1)-O(6)	76.3(2)	O(11)-Mo(4)-O(3)	87.2(3)
O(5)-Mo(1)-O(6)	74.7(2)	O(18)-Mo(4)-O(3)	152.2(2)
O(7)-Mo(2)-O(12)	105.2(4)	O(9)-Mo(4)-O(14)	102.0(4)
O(7)-Mo(2)-O(5)	103.1(4)	O(11)-Mo(4)-O(14)	152.5(3)
O(12)-Mo(2)-O(5)	91.7(3)	O(18)-Mo(4)-O(14)	85.2(3)
O(7)-Mo(2)-O(16)	104.0(4)	O(3)-Mo(4)-O(14)	81.9(3)
O(12)-Mo(2)-O(16)	89.3(3)	O(9)-Mo(4)-O(6)	177.2(4)
O(5)-Mo(2)-O(16)	151.6(3)	O(11)-Mo(4)-O(6)	77.5(2)

O(7)-Mo(2)-O(13)	101.7(4)	O(18)-Mo(4)-O(6)	76.9(2)
O(12)-Mo(2)-O(13)	153.0(3)	O(3)-Mo(4)-O(6)	76.0(2)
O(5)-Mo(2)-O(13)	84.3(3)	O(14)-Mo(4)-O(6)	75.4(2)
O(16)-Mo(2)-O(13)	82.1(3)	O(8)-Mo(5)-O(14)	105.4(4)
O(7)-Mo(2)-O(6)	176.7(4)	O(8)-Mo(5)-O(17)	105.0(4)
O(12)-Mo(2)-O(6)	78.1(2)	O(14)-Mo(5)-O(17)	90.9(3)
O(14)-Mo(5)-O(2)	89.9(3)	O(8)-Mo(5)-O(2)	102.3(4)
O(17)-Mo(5)-O(2)	151.4(3)	O(25)-Mo(7)-O(27)	77.2(2)
O(8)-Mo(5)-O(12)	101.3(4)	O(21)-Mo(7)-O(27)	76.5(2)
O(14)-Mo(5)-O(12)	153.2(3)	O(22)-Mo(7)-O(27)	76.3(2)
O(17)-Mo(5)-O(12)	84.8(3)	O(26)-Mo(7)-O(27)	75.7(2)
O(2)-Mo(5)-O(12)	81.7(3)	O(30)-Mo(8)-O(28)	104.8(4)
O(8)-Mo(5)-O(6)	175.9(4)	O(30)-Mo(8)-O(36)	103.9(4)
O(14)-Mo(5)-O(6)	78.5(2)	O(28)-Mo(8)-O(36)	92.8(3)
O(17)-Mo(5)-O(6)	76.0(2)	O(30)-Mo(8)-O(25)	102.4(4)
O(2)-Mo(5)-O(6)	76.2(3)	O(28)-Mo(8)-O(25)	87.5(3)
O(12)-Mo(5)-O(6)	74.7(2)	O(36)-Mo(8)-O(25)	152.7(3)
N(1)-Mo(6)-O(16)	101.8(3)	O(30)-Mo(8)-O(24)	102.1(4)
N(1)-Mo(6)-O(15)	102.1(3)	O(28)-Mo(8)-O(24)	152.4(3)
O(16)-Mo(6)-O(15)	91.9(3)	O(36)-Mo(8)-O(24)	86.6(3)
N(1)-Mo(6)-O(17)	100.9(3)	O(25)-Mo(8)-O(24)	80.8(3)
O(16)-Mo(6)-O(17)	88.4(3)	O(30)-Mo(8)-O(27)	176.8(4)
O(15)-Mo(6)-O(17)	156.5(3)	O(28)-Mo(8)-O(27)	78.0(2)
N(1)-Mo(6)-O(18)	100.6(3)	O(36)-Mo(8)-O(27)	77.4(2)
O(16)-Mo(6)-O(18)	157.3(3)	O(25)-Mo(8)-O(27)	75.9(2)
O(15)-Mo(6)-O(18)	86.6(3)	O(24)-Mo(8)-O(27)	74.9(2)
O(17)-Mo(6)-O(18)	84.2(3)	O(23)-Mo(9)-O(24)	105.2(4)
N(1)-Mo(6)-O(6)	178.2(3)	O(23)-Mo(9)-O(35)	105.5(3)
O(16)-Mo(6)-O(6)	79.3(2)	O(24)-Mo(9)-O(35)	91.9(3)
O(15)-Mo(6)-O(6)	79.2(2)	O(23)-Mo(9)-O(21)	101.6(3)
O(17)-Mo(6)-O(6)	77.8(2)	O(24)-Mo(9)-O(21)	88.6(3)
O(18)-Mo(6)-O(6)	78.2(2)	O(35)-Mo(9)-O(21)	151.7(2)
O(20)-Mo(7)-O(25)	105.2(3)	O(23)-Mo(9)-O(32)	101.8(4)
O(20)-Mo(7)-O(21)	104.5(3)	O(24)-Mo(9)-O(32)	152.7(3)
O(25)-Mo(7)-O(21)	90.4(3)	O(35)-Mo(9)-O(32)	85.0(3)
O(20)-Mo(7)-O(22)	102.5(3)	O(21)-Mo(9)-O(32)	81.8(3)

O(25)-Mo(7)-O(22)	88.1(3)	O(23)-Mo(9)-O(27)	176.3(3)
O(21)-Mo(7)-O(22)	152.4(3)	O(24)-Mo(9)-O(27)	77.6(2)
O(20)-Mo(7)-O(26)	101.9(3)	O(35)-Mo(9)-O(27)	76.6(2)
O(25)-Mo(7)-O(26)	152.8(3)	O(21)-Mo(9)-O(27)	75.9(2)
O(21)-Mo(7)-O(26)	85.6(3)	O(32)-Mo(9)-O(27)	75.3(2)
O(22)-Mo(7)-O(26)	83.3(3)	O(19)-Mo(10)-O(29)	106.1(4)
O(20)-Mo(7)-O(27)	177.4(3)	O(19)-Mo(10)-O(22)	103.9(4)
O(19)-Mo(10)-O(33)	103.7(4)	O(29)-Mo(10)-O(22)	91.0(3)
O(29)-Mo(10)-O(33)	89.8(3)	N(5)-Mo(12)-O(27)	179.0(3)
O(22)-Mo(10)-O(33)	151.0(3)	O(33)-Mo(12)-O(27)	79.2(2)
O(19)-Mo(10)-O(28)	101.3(4)	O(34)-Mo(12)-O(27)	79.5(2)
O(29)-Mo(10)-O(28)	152.5(3)	O(35)-Mo(12)-O(27)	77.2(2)
O(22)-Mo(10)-O(28)	84.4(3)	O(36)-Mo(12)-O(27)	77.6(2)
O(33)-Mo(10)-O(28)	81.7(3)	Mo(1)-O(2)-Mo(5)	117.3(3)
O(19)-Mo(10)-O(27)	175.1(3)	Mo(1)-O(3)-Mo(4)	117.4(3)
O(29)-Mo(10)-O(27)	78.6(2)	Mo(3)-O(4)-Mo(1)	118.1(3)
O(22)-Mo(10)-O(27)	76.8(2)	Mo(2)-O(5)-Mo(1)	118.3(3)
O(33)-Mo(10)-O(27)	74.9(2)	Mo(6)-O(6)-Mo(2)	91.05(19)
O(28)-Mo(10)-O(27)	73.9(2)	Mo(6)-O(6)-Mo(4)	90.73(18)
O(31)-Mo(11)-O(32)	105.5(3)	Mo(2)-O(6)-Mo(4)	178.2(3)
O(31)-Mo(11)-O(26)	103.2(3)	Mo(6)-O(6)-Mo(5)	91.70(17)
O(32)-Mo(11)-O(26)	93.2(3)	Mo(2)-O(6)-Mo(5)	89.98(18)
O(31)-Mo(11)-O(34)	102.8(3)	Mo(4)-O(6)-Mo(5)	89.63(18)
O(32)-Mo(11)-O(34)	88.7(3)	Mo(6)-O(6)-Mo(3)	90.80(19)
O(26)-Mo(11)-O(34)	152.3(3)	Mo(2)-O(6)-Mo(3)	89.82(18)
O(31)-Mo(11)-O(29)	101.3(3)	Mo(4)-O(6)-Mo(3)	90.50(18)
O(32)-Mo(11)-O(29)	152.9(3)	Mo(5)-O(6)-Mo(3)	177.5(2)
O(26)-Mo(11)-O(29)	83.7(3)	Mo(6)-O(6)-Mo(1)	179.1(3)
O(34)-Mo(11)-O(29)	82.2(3)	Mo(2)-O(6)-Mo(1)	89.40(17)
O(31)-Mo(11)-O(27)	176.1(3)	Mo(4)-O(6)-Mo(1)	88.82(18)
O(32)-Mo(11)-O(27)	77.9(2)	Mo(5)-O(6)-Mo(1)	89.11(18)
O(26)-Mo(11)-O(27)	78.0(2)	Mo(3)-O(6)-Mo(1)	88.39(17)
O(34)-Mo(11)-O(27)	75.4(2)	Mo(4)-O(11)-Mo(3)	117.5(3)
O(29)-Mo(11)-O(27)	75.1(2)	Mo(2)-O(12)-Mo(5)	117.2(3)
N(5)-Mo(12)-O(33)	101.7(4)	Mo(3)-O(13)-Mo(2)	116.7(3)
N(5)-Mo(12)-O(34)	100.9(3)	Mo(5)-O(14)-Mo(4)	116.4(3)

O(33)-Mo(12)-O(34)	91.1(3)	Mo(6)-O(15)-Mo(3)	114.1(3)
N(5)-Mo(12)-O(35)	101.9(3)	Mo(6)-O(16)-Mo(2)	114.3(3)
O(33)-Mo(12)-O(35)	156.0(3)	Mo(5)-O(17)-Mo(6)	114.5(3)
O(34)-Mo(12)-O(35)	88.6(3)	Mo(4)-O(18)-Mo(6)	113.7(3)
N(5)-Mo(12)-O(36)	102.0(3)	Mo(7)-O(21)-Mo(9)	117.4(3)
O(33)-Mo(12)-O(36)	87.6(3)	Mo(10)-O(22)-Mo(7)	118.4(3)
O(34)-Mo(12)-O(36)	156.9(3)	Mo(9)-O(24)-Mo(8)	117.1(3)
O(35)-Mo(12)-O(36)	83.4(3)	Mo(7)-O(25)-Mo(8)	117.2(3)
C(5)-C(4)-C(7)	119.1(9)	Mo(11)-O(26)-Mo(7)	116.8(3)
C(4)-C(5)-C(6)	119.6(9)	C(16)-C(15)-H(15A)	108.0
C(4)-C(5)-H(5)	120.2	N(3)-C(15)-H(15A)	108.0
C(6)-C(5)-H(5)	120.2	C(16)-C(15)-H(15B)	108.0
C(1)-C(6)-C(5)	120.0(9)	N(3)-C(15)-H(15B)	108.0
C(1)-C(6)-H(6)	120.0	H(15A)-C(15)-H(15B)	107.2
C(5)-C(6)-H(6)	120.0	C(15)-C(16)-C(17)	111.2(11)
C(8)-C(7)-C(4)	173.7(12)	C(15)-C(16)-H(16A)	109.4
C(7)-C(8)-C(9)	176.7(12)	C(17)-C(16)-H(16A)	109.4
C(10)-C(9)-C(14)	118.7(8)	C(15)-C(16)-H(16B)	109.4
C(10)-C(9)-C(8)	120.6(9)	C(17)-C(16)-H(16B)	109.4
C(14)-C(9)-C(8)	120.6(9)	H(16A)-C(16)-H(16B)	108.0
C(9)-C(10)-C(11)	121.3(9)	C(18)-C(17)-C(16)	112.8(12)
C(9)-C(10)-H(10)	119.4	C(18)-C(17)-H(17A)	109.0
C(11)-C(10)-H(10)	119.4	C(16)-C(17)-H(17A)	109.0
C(12)-C(11)-C(10)	119.5(8)	C(18)-C(17)-H(17B)	109.0
C(12)-C(11)-H(11)	120.3	C(16)-C(17)-H(17B)	109.0
C(10)-C(11)-H(11)	120.3	H(17A)-C(17)-H(17B)	107.8
C(13)-C(12)-N(2)	120.3(8)	C(17)-C(18)-H(18A)	109.5
C(13)-C(12)-C(11)	119.5(8)	C(17)-C(18)-H(18B)	109.5
N(2)-C(12)-C(11)	120.1(8)	H(18A)-C(18)-H(18B)	109.5
C(14)-C(13)-C(12)	121.2(8)	C(17)-C(18)-H(18C)	109.5
C(14)-C(13)-H(13)	119.4	H(18A)-C(18)-H(18C)	109.5
C(12)-C(13)-H(13)	119.4	H(18B)-C(18)-H(18C)	109.5
C(13)-C(14)-C(9)	119.7(8)	C(20)-C(19)-N(3)	117.7(8)
C(13)-C(14)-H(14)	120.2	C(20)-C(19)-H(19A)	107.9
C(9)-C(14)-H(14)	120.2	N(3)-C(19)-H(19A)	107.9
C(15)-N(3)-C(27)	109.6(9)	C(20)-C(19)-H(19B)	107.9

C(15)-N(3)-C(19)	110.7(9)	N(3)-C(19)-H(19B)	107.9
C(27)-N(3)-C(19)	109.4(8)	H(19A)-C(19)-H(19B)	107.2
C(15)-N(3)-C(23A)	107.8(7)	C(21)-C(20)-C(19)	109.1(9)
C(27)-N(3)-C(23A)	109.7(10)	C(21)-C(20)-H(20A)	109.9
C(19)-N(3)-C(23A)	109.6(8)	C(19)-C(20)-H(20A)	109.9
C(15)-N(3)-C(23B)	107.8(7)	C(21)-C(20)-H(20B)	109.9
C(27)-N(3)-C(23B)	109.7(10)	C(19)-C(20)-H(20B)	109.9
C(19)-N(3)-C(23B)	109.6(8)	H(20A)-C(20)-H(20B)	108.3
C(16)-C(15)-N(3)	117.2(11)	C(20)-C(21)-C(22)	112.8(12)
C(22)-C(21)-H(21A)	109.0	C(20)-C(21)-H(21A)	109.0
C(20)-C(21)-H(21B)	109.0	C(24B)-C(23B)-H(23D)	108.3
C(22)-C(21)-H(21B)	109.0	N(3)-C(23B)-H(23D)	108.3
H(21A)-C(21)-H(21B)	107.8	H(23C)-C(23B)-H(23D)	107.4
C(21)-C(22)-H(22A)	109.5	C(23B)-C(24B)-C(25B)	115.6(14)
C(21)-C(22)-H(22B)	109.5	C(23B)-C(24B)-H(24C)	108.4
H(22A)-C(22)-H(22B)	109.5	C(25B)-C(24B)-H(24C)	108.4
C(21)-C(22)-H(22C)	109.5	C(23B)-C(24B)-H(24D)	108.4
H(22A)-C(22)-H(22C)	109.5	C(25B)-C(24B)-H(24D)	108.4
H(22B)-C(22)-H(22C)	109.5	H(24C)-C(24B)-H(24D)	107.4
C(24A)-C(23A)-N(3)	115.9(9)	C(24B)-C(25B)-C(26B)	104.7(17)
C(24A)-C(23A)-H(23A)	108.3	C(24B)-C(25B)-H(25C)	110.8
N(3)-C(23A)-H(23A)	108.3	C(26B)-C(25B)-H(25C)	110.8
C(24A)-C(23A)-H(23B)	108.3	C(24B)-C(25B)-H(25D)	110.8
N(3)-C(23A)-H(23B)	108.3	C(26B)-C(25B)-H(25D)	110.8
H(23A)-C(23A)-H(23B)	107.4	H(25C)-C(25B)-H(25D)	108.9
C(23A)-C(24A)-C(25A)	105.8(15)	C(25B)-C(26B)-H(26D)	109.5
C(23A)-C(24A)-H(24A)	110.6	C(25B)-C(26B)-H(26E)	109.5
C(25A)-C(24A)-H(24A)	110.6	H(26D)-C(26B)-H(26E)	109.5
C(23A)-C(24A)-H(24B)	110.6	C(25B)-C(26B)-H(26F)	109.5
C(25A)-C(24A)-H(24B)	110.6	H(26D)-C(26B)-H(26F)	109.5
H(24A)-C(24A)-H(24B)	108.7	H(26E)-C(26B)-H(26F)	109.5
C(24A)-C(25A)-C(26A)	111(2)	N(3)-C(27)-C(28)	114.5(11)
C(24A)-C(25A)-H(25A)	109.5	N(3)-C(27)-H(27A)	108.6
C(26A)-C(25A)-H(25A)	109.5	C(28)-C(27)-H(27A)	108.6
C(24A)-C(25A)-H(25B)	109.5	N(3)-C(27)-H(27B)	108.6
C(26A)-C(25A)-H(25B)	109.5	C(28)-C(27)-H(27B)	108.6

H(25A)-C(25A)-H(25B)	108.1	H(27A)-C(27)-H(27B)	107.6
C(25A)-C(26A)-H(26A)	109.5	C(27)-C(28)-C(29)	109.4(12)
C(25A)-C(26A)-H(26B)	109.5	C(27)-C(28)-H(28A)	109.8
H(26A)-C(26A)-H(26B)	109.5	C(29)-C(28)-H(28A)	109.8
C(25A)-C(26A)-H(26C)	109.5	C(27)-C(28)-H(28B)	109.8
H(26A)-C(26A)-H(26C)	109.5	C(29)-C(28)-H(28B)	109.8
H(26B)-C(26A)-H(26C)	109.5	H(28A)-C(28)-H(28B)	108.3
C(24B)-C(23B)-N(3)	115.9(9)	C(30)-C(29)-C(28)	110.7(13)
C(24B)-C(23B)-H(23C)	108.3	C(30)-C(29)-H(29A)	109.5
N(3)-C(23B)-H(23C)	108.3	C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5	C(30)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	108.1	H(33A)-C(33A)-H(33B)	107.4
C(29)-C(30)-H(30A)	109.5	C(33A)-C(34A)-H(34A)	109.5
C(29)-C(30)-H(30B)	109.5	C(33A)-C(34A)-H(34B)	109.5
H(30A)-C(30)-H(30B)	109.5	H(34A)-C(34A)-H(34B)	109.5
C(29)-C(30)-H(30C)	109.5	C(33A)-C(34A)-H(34C)	109.5
H(30A)-C(30)-H(30C)	109.5	H(34A)-C(34A)-H(34C)	109.5
H(30B)-C(30)-H(30C)	109.5	H(34B)-C(34A)-H(34C)	109.5
C(39B)-N(4)-C(31B)	101(3)	C(36A)-C(35A)-N(4)	107.1(19)
C(39B)-N(4)-C(35B)	112.2(18)	C(36A)-C(35A)-H(35A)	110.3
C(31B)-N(4)-C(35B)	102(3)	N(4)-C(35A)-H(35A)	110.3
C(31A)-N(4)-C(39A)	123(4)	C(36A)-C(35A)-H(35B)	110.3
C(31A)-N(4)-C(35A)	116(3)	N(4)-C(35A)-H(35B)	110.3
C(39A)-N(4)-C(35A)	99.4(18)	H(35A)-C(35A)-H(35B)	108.6
C(39B)-N(4)-C(43B)	122.2(15)	C(35A)-C(36A)-C(37A)	98(2)
C(31B)-N(4)-C(43B)	108(2)	C(35A)-C(36A)-H(36A)	112.1
C(35B)-N(4)-C(43B)	109(2)	C(37A)-C(36A)-H(36A)	112.1
C(31A)-N(4)-C(43A)	104(2)	C(35A)-C(36A)-H(36B)	112.1
C(39A)-N(4)-C(43A)	102.9(17)	C(37A)-C(36A)-H(36B)	112.1
C(35A)-N(4)-C(43A)	109.9(17)	H(36A)-C(36A)-H(36B)	109.8
N(4)-C(31A)-C(32A)	111(2)	C(38A)-C(37A)-C(36A)	111(2)
N(4)-C(31A)-H(31A)	109.5	C(38A)-C(37A)-H(37A)	109.4
C(32A)-C(31A)-H(31A)	109.5	C(36A)-C(37A)-H(37A)	109.4
N(4)-C(31A)-H(31B)	109.5	C(38A)-C(37A)-H(37B)	109.4
C(32A)-C(31A)-H(31B)	109.5	C(36A)-C(37A)-H(37B)	109.4
H(31A)-C(31A)-H(31B)	108.1	H(37A)-C(37A)-H(37B)	108.0

C(33A)-C(32A)-C(31A)	113(2)	C(37A)-C(38A)-H(38A)	109.5
C(33A)-C(32A)-H(32A)	109.0	C(37A)-C(38A)-H(38B)	109.5
C(31A)-C(32A)-H(32A)	109.0	H(38A)-C(38A)-H(38B)	109.5
C(33A)-C(32A)-H(32B)	109.0	C(37A)-C(38A)-H(38C)	109.5
C(31A)-C(32A)-H(32B)	109.0	H(38A)-C(38A)-H(38C)	109.5
H(32A)-C(32A)-H(32B)	107.8	H(38B)-C(38A)-H(38C)	109.5
C(32A)-C(33A)-C(34A)	116(3)	C(40A)-C(39A)-N(4)	117(2)
C(32A)-C(33A)-H(33A)	108.2	C(40A)-C(39A)-H(39A)	108.1
C(34A)-C(33A)-H(33A)	108.2	N(4)-C(39A)-H(39A)	108.1
C(32A)-C(33A)-H(33B)	108.2	C(40A)-C(39A)-H(39B)	108.1
C(34A)-C(33A)-H(33B)	108.2	N(4)-C(39A)-H(39B)	108.1
C(39A)-C(40A)-C(41A)	117(3)	H(39A)-C(39A)-H(39B)	107.3
C(39A)-C(40A)-H(40A)	108.0	C(45A)-C(46A)-H(46B)	109.5
C(41A)-C(40A)-H(40A)	108.0	H(46A)-C(46A)-H(46B)	109.5
C(39A)-C(40A)-H(40B)	108.0	C(45A)-C(46A)-H(46C)	109.5
C(41A)-C(40A)-H(40B)	108.0	H(46A)-C(46A)-H(46C)	109.5
H(40A)-C(40A)-H(40B)	107.2	H(46B)-C(46A)-H(46C)	109.5
C(40A)-C(41A)-C(42A)	109(3)	N(4)-C(31B)-C(32B)	124(3)
C(40A)-C(41A)-H(41A)	109.8	N(4)-C(31B)-H(31C)	106.3
C(42A)-C(41A)-H(41A)	109.8	C(32B)-C(31B)-H(31C)	106.3
C(40A)-C(41A)-H(41B)	109.8	N(4)-C(31B)-H(31D)	106.3
C(42A)-C(41A)-H(41B)	109.8	C(32B)-C(31B)-H(31D)	106.3
H(41A)-C(41A)-H(41B)	108.3	H(31C)-C(31B)-H(31D)	106.4
C(41A)-C(42A)-H(42A)	109.5	C(31B)-C(32B)-C(33B)	113(3)
C(41A)-C(42A)-H(42B)	109.5	C(31B)-C(32B)-H(32C)	109.1
H(42A)-C(42A)-H(42B)	109.5	C(33B)-C(32B)-H(32C)	109.1
C(41A)-C(42A)-H(42C)	109.5	C(31B)-C(32B)-H(32D)	109.1
H(42A)-C(42A)-H(42C)	109.5	C(33B)-C(32B)-H(32D)	109.1
H(42B)-C(42A)-H(42C)	109.5	H(32C)-C(32B)-H(32D)	107.8
N(4)-C(43A)-C(44A)	119.9(11)	C(34B)-C(33B)-C(32B)	112(3)
N(4)-C(43A)-H(43A)	107.4	C(34B)-C(33B)-H(33C)	109.1
C(44A)-C(43A)-H(43A)	107.4	C(32B)-C(33B)-H(33C)	109.1
N(4)-C(43A)-H(43B)	107.4	C(34B)-C(33B)-H(33D)	109.1
C(44A)-C(43A)-H(43B)	107.4	C(32B)-C(33B)-H(33D)	109.1
H(43A)-C(43A)-H(43B)	106.9	H(33C)-C(33B)-H(33D)	107.8
C(45A)-C(44A)-C(43A)	109.4(16)	C(33B)-C(34B)-H(34D)	109.5

C(45A)-C(44A)-H(44A)	109.8	C(33B)-C(34B)-H(34E)	109.5
C(43A)-C(44A)-H(44A)	109.8	H(34D)-C(34B)-H(34E)	109.5
C(45A)-C(44A)-H(44B)	109.8	C(33B)-C(34B)-H(34F)	109.5
C(43A)-C(44A)-H(44B)	109.8	H(34D)-C(34B)-H(34F)	109.5
H(44A)-C(44A)-H(44B)	108.2	H(34E)-C(34B)-H(34F)	109.5
C(44A)-C(45A)-C(46A)	113.7(19)	N(4)-C(35B)-C(36B)	126.2(17)
C(44A)-C(45A)-H(45A)	108.8	N(4)-C(35B)-H(35C)	105.8
C(46A)-C(45A)-H(45A)	108.8	C(36B)-C(35B)-H(35C)	105.8
C(44A)-C(45A)-H(45B)	108.8	N(4)-C(35B)-H(35D)	105.8
C(46A)-C(45A)-H(45B)	108.8	C(36B)-C(35B)-H(35D)	105.8
H(45A)-C(45A)-H(45B)	107.7	H(35C)-C(35B)-H(35D)	106.2
C(45A)-C(46A)-H(46A)	109.5	C(35B)-C(36B)-C(37B)	116(2)
C(37B)-C(36B)-H(36C)	108.2	C(35B)-C(36B)-H(36C)	108.2
C(35B)-C(36B)-H(36D)	108.2	C(44B)-C(43B)-H(43D)	110.5
C(37B)-C(36B)-H(36D)	108.2	N(4)-C(43B)-H(43D)	110.5
H(36C)-C(36B)-H(36D)	107.3	H(43C)-C(43B)-H(43D)	108.7
C(38B)-C(37B)-C(36B)	111(2)	C(41B)-C(42B)-H(42D)	109.5
C(38B)-C(37B)-H(37C)	109.5	C(41B)-C(42B)-H(42E)	109.5
C(36B)-C(37B)-H(37C)	109.5	H(42D)-C(42B)-H(42E)	109.5
C(38B)-C(37B)-H(37D)	109.5	C(41B)-C(42B)-H(42F)	109.5
C(36B)-C(37B)-H(37D)	109.5	H(42D)-C(42B)-H(42F)	109.5
H(37C)-C(37B)-H(37D)	108.1	H(42E)-C(42B)-H(42F)	109.5
C(37B)-C(38B)-H(38D)	109.5	C(45B)-C(44B)-C(43B)	111(2)
C(37B)-C(38B)-H(38E)	109.5	C(45B)-C(44B)-H(44C)	109.5
H(38D)-C(38B)-H(38E)	109.5	C(43B)-C(44B)-H(44C)	109.5
C(37B)-C(38B)-H(38F)	109.5	C(45B)-C(44B)-H(44D)	109.5
H(38D)-C(38B)-H(38F)	109.5	C(43B)-C(44B)-H(44D)	109.5
H(38E)-C(38B)-H(38F)	109.5	H(44C)-C(44B)-H(44D)	108.1
N(4)-C(39B)-C(40B)	117(3)	C(44B)-C(45B)-C(46B)	103(3)
N(4)-C(39B)-H(39C)	108.1	C(44B)-C(45B)-H(45C)	111.2
C(40B)-C(39B)-H(39C)	108.1	C(46B)-C(45B)-H(45C)	111.2
N(4)-C(39B)-H(39D)	108.1	C(44B)-C(45B)-H(45D)	111.2
C(40B)-C(39B)-H(39D)	108.1	C(46B)-C(45B)-H(45D)	111.2
H(39C)-C(39B)-H(39D)	107.3	H(45C)-C(45B)-H(45D)	109.2
C(41B)-C(40B)-C(39B)	115(2)	C(45B)-C(46B)-H(46D)	109.5
C(41B)-C(40B)-H(40C)	108.6	C(45B)-C(46B)-H(46E)	109.5

C(39B)-C(40B)-H(40C)	108.6	H(46D)-C(46B)-H(46E)	109.5
C(41B)-C(40B)-H(40D)	108.6	C(45B)-C(46B)-H(46F)	109.5
C(39B)-C(40B)-H(40D)	108.6	H(46D)-C(46B)-H(46F)	109.5
H(40C)-C(40B)-H(40D)	107.6	H(46E)-C(46B)-H(46F)	109.5
C(40B)-C(41B)-C(42B)	116(3)	C(47)-N(5)-Mo(12)	175.3(7)
C(40B)-C(41B)-H(41C)	108.2	C(58)-N(6)-H(06A)	103(5)
C(42B)-C(41B)-H(41C)	108.2	C(58)-N(6)-H(06B)	105(5)
C(40B)-C(41B)-H(41D)	108.2	H(06A)-N(6)-H(06B)	107(6)
C(42B)-C(41B)-H(41D)	108.2	N(5)-C(47)-C(48)	121.6(9)
H(41C)-C(41B)-H(41D)	107.3	N(5)-C(47)-C(52)	118.4(9)
C(44B)-C(43B)-N(4)	106.3(14)	C(48)-C(47)-C(52)	119.9(8)
C(44B)-C(43B)-H(43C)	110.5	C(49)-C(48)-C(47)	120.5(9)
N(4)-C(43B)-H(43C)	110.5	C(49)-C(48)-H(48)	119.8
C(48)-C(49)-C(50)	119.4(10)	C(47)-C(48)-H(48)	119.8
C(48)-C(49)-H(49)	120.3	C(73B)-N(7)-C(69)	114.5(16)
C(50)-C(49)-H(49)	120.3	C(73A)-N(7)-C(69)	106.5(12)
C(51)-C(50)-C(49)	120.5(9)	C(65)-N(7)-C(69)	109.8(8)
C(51)-C(50)-C(53)	120.1(9)	C(61)-N(7)-C(69)	106.0(8)
C(49)-C(50)-C(53)	119.4(10)	N(7)-C(61)-C(62)	113.4(9)
C(50)-C(51)-C(52)	120.9(9)	N(7)-C(61)-H(61A)	108.9
C(50)-C(51)-H(51)	119.5	C(62)-C(61)-H(61A)	108.9
C(52)-C(51)-H(51)	119.5	N(7)-C(61)-H(61B)	108.9
C(51)-C(52)-C(47)	118.2(9)	C(62)-C(61)-H(61B)	108.9
C(51)-C(52)-H(52)	120.9	H(61A)-C(61)-H(61B)	107.7
C(47)-C(52)-H(52)	120.9	C(63)-C(62)-C(61)	111.9(13)
C(54)-C(53)-C(50)	175.1(10)	C(63)-C(62)-H(62A)	109.2
C(53)-C(54)-C(55)	176.3(10)	C(61)-C(62)-H(62A)	109.2
C(60)-C(55)-C(56)	118.0(8)	C(63)-C(62)-H(62B)	109.2
C(60)-C(55)-C(54)	121.3(9)	C(61)-C(62)-H(62B)	109.2
C(56)-C(55)-C(54)	120.7(9)	H(62A)-C(62)-H(62B)	107.9
C(57)-C(56)-C(55)	121.4(8)	C(64)-C(63)-C(62)	106.3(18)
C(57)-C(56)-H(56)	119.3	C(64)-C(63)-H(63A)	110.5
C(55)-C(56)-H(56)	119.3	C(62)-C(63)-H(63A)	110.5
C(56)-C(57)-C(58)	120.4(8)	C(64)-C(63)-H(63B)	110.5
C(56)-C(57)-H(57)	119.8	C(62)-C(63)-H(63B)	110.5
C(58)-C(57)-H(57)	119.8	H(63A)-C(63)-H(63B)	108.7

N(6)-C(58)-C(59)	120.9(8)	C(63)-C(64)-H(64A)	109.5
N(6)-C(58)-C(57)	120.9(9)	C(63)-C(64)-H(64B)	109.5
C(59)-C(58)-C(57)	118.1(8)	H(64A)-C(64)-H(64B)	109.5
C(58)-C(59)-C(60)	120.8(8)	C(63)-C(64)-H(64C)	109.5
C(58)-C(59)-H(59)	119.6	H(64A)-C(64)-H(64C)	109.5
C(60)-C(59)-H(59)	119.6	H(64B)-C(64)-H(64C)	109.5
C(55)-C(60)-C(59)	121.1(8)	N(7)-C(65)-C(66)	115.9(8)
C(55)-C(60)-H(60)	119.4	N(7)-C(65)-H(65A)	108.3
C(59)-C(60)-H(60)	119.4	C(66)-C(65)-H(65A)	108.3
C(73B)-N(7)-C(65)	104.7(13)	N(7)-C(65)-H(65B)	108.3
C(73A)-N(7)-C(65)	109.2(16)	C(66)-C(65)-H(65B)	108.3
C(73B)-N(7)-C(61)	109.3(13)	H(65A)-C(65)-H(65B)	107.4
C(73A)-N(7)-C(61)	112.3(16)	C(67)-C(66)-C(65)	108.5(10)
C(65)-N(7)-C(61)	112.7(10)	C(67)-C(66)-H(66A)	110.0
C(67)-C(66)-H(66B)	110.0	C(65)-C(66)-H(66A)	110.0
C(65)-C(66)-H(66B)	110.0	H(72A)-C(72)-H(72C)	109.5
H(66A)-C(66)-H(66B)	108.4	H(72B)-C(72)-H(72C)	109.5
C(68)-C(67)-C(66)	113.9(13)	N(7)-C(73A)-C(74A)	123(2)
C(68)-C(67)-H(67A)	108.8	N(7)-C(73A)-H(73A)	106.6
C(66)-C(67)-H(67A)	108.8	C(74A)-C(73A)-H(73A)	106.6
C(68)-C(67)-H(67B)	108.8	N(7)-C(73A)-H(73B)	106.6
C(66)-C(67)-H(67B)	108.8	C(74A)-C(73A)-H(73B)	106.6
H(67A)-C(67)-H(67B)	107.7	H(73A)-C(73A)-H(73B)	106.6
C(67)-C(68)-H(68A)	109.5	C(75A)-C(74A)-C(73A)	113(3)
C(67)-C(68)-H(68B)	109.5	C(75A)-C(74A)-H(74A)	109.0
H(68A)-C(68)-H(68B)	109.5	C(73A)-C(74A)-H(74A)	109.0
C(67)-C(68)-H(68C)	109.5	C(75A)-C(74A)-H(74B)	109.0
H(68A)-C(68)-H(68C)	109.5	C(73A)-C(74A)-H(74B)	109.0
H(68B)-C(68)-H(68C)	109.5	H(74A)-C(74A)-H(74B)	107.8
N(7)-C(69)-C(70)	115.0(9)	C(76A)-C(75A)-C(74A)	114(3)
N(7)-C(69)-H(69A)	108.5	C(76A)-C(75A)-H(75A)	108.8
C(70)-C(69)-H(69A)	108.5	C(74A)-C(75A)-H(75A)	108.8
N(7)-C(69)-H(69B)	108.5	C(76A)-C(75A)-H(75B)	108.8
C(70)-C(69)-H(69B)	108.5	C(74A)-C(75A)-H(75B)	108.8
H(69A)-C(69)-H(69B)	107.5	H(75A)-C(75A)-H(75B)	107.7
C(71)-C(70)-C(69)	108.7(10)	C(75A)-C(76A)-H(76A)	109.5

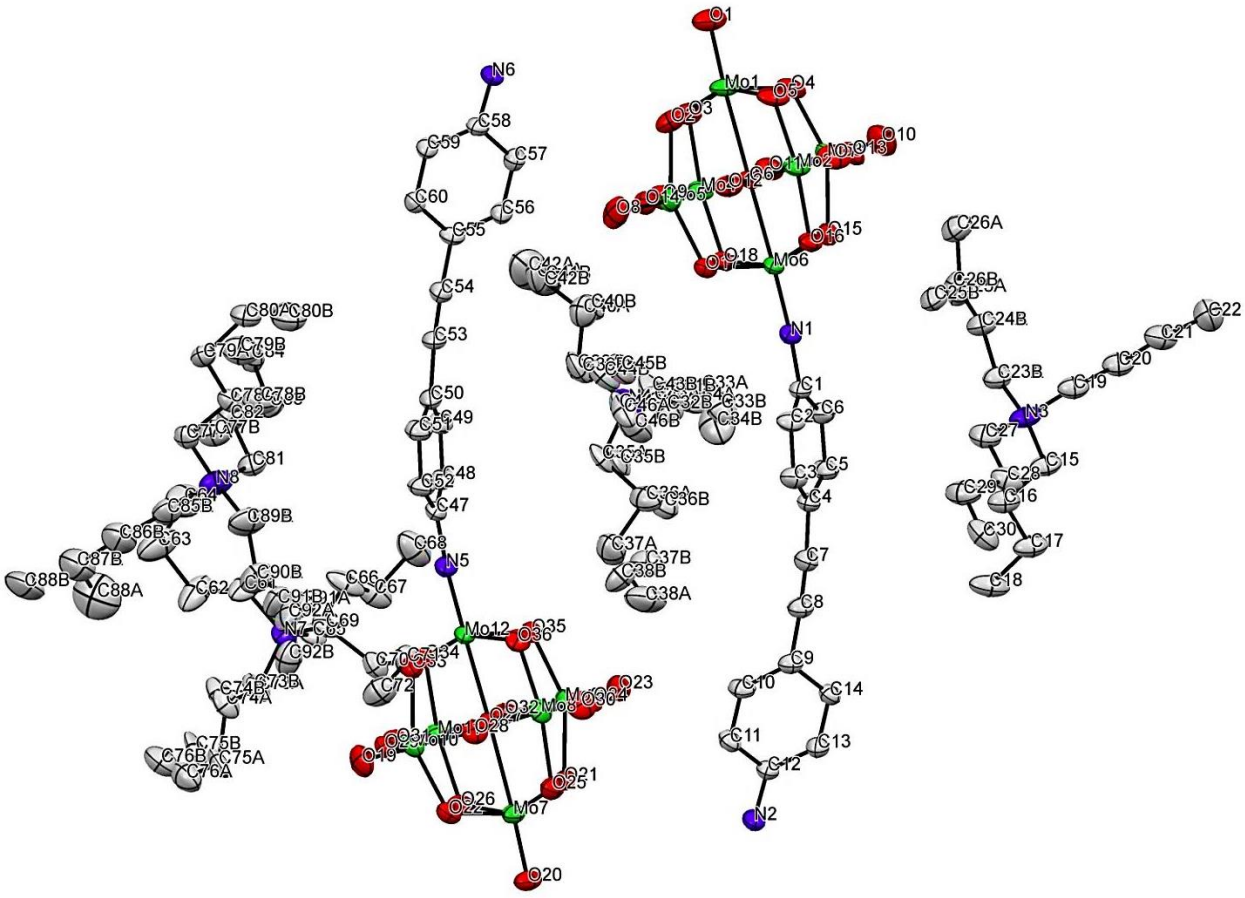
C(71)-C(70)-H(70A)	110.0	C(75A)-C(76A)-H(76B)	109.5
C(69)-C(70)-H(70A)	110.0	H(76A)-C(76A)-H(76B)	109.5
C(71)-C(70)-H(70B)	110.0	C(75A)-C(76A)-H(76C)	109.5
C(69)-C(70)-H(70B)	110.0	H(76A)-C(76A)-H(76C)	109.5
H(70A)-C(70)-H(70B)	108.3	H(76B)-C(76A)-H(76C)	109.5
C(72)-C(71)-C(70)	112.5(12)	N(7)-C(73B)-C(74B)	113.6(15)
C(72)-C(71)-H(71A)	109.1	N(7)-C(73B)-H(73C)	108.9
C(70)-C(71)-H(71A)	109.1	C(74B)-C(73B)-H(73C)	108.9
C(72)-C(71)-H(71B)	109.1	N(7)-C(73B)-H(73D)	108.9
C(70)-C(71)-H(71B)	109.1	C(74B)-C(73B)-H(73D)	108.9
H(71A)-C(71)-H(71B)	107.8	H(73C)-C(73B)-H(73D)	107.7
C(71)-C(72)-H(72A)	109.5	C(75B)-C(74B)-C(73B)	115(2)
C(71)-C(72)-H(72B)	109.5	C(75B)-C(74B)-H(74C)	108.6
H(72A)-C(72)-H(72B)	109.5	C(73B)-C(74B)-H(74C)	108.6
C(71)-C(72)-H(72C)	109.5	C(75B)-C(74B)-H(74D)	108.6
H(74C)-C(74B)-H(74D)	107.6	C(73B)-C(74B)-H(74D)	108.6
C(76B)-C(75B)-C(74B)	120(3)	C(80A)-C(79A)-C(78A)	111.3(19)
C(76B)-C(75B)-H(75C)	107.4	C(80A)-C(79A)-H(79A)	109.4
C(74B)-C(75B)-H(75C)	107.4	C(78A)-C(79A)-H(79A)	109.4
C(76B)-C(75B)-H(75D)	107.4	C(80A)-C(79A)-H(79B)	109.4
C(74B)-C(75B)-H(75D)	107.4	C(78A)-C(79A)-H(79B)	109.4
H(75C)-C(75B)-H(75D)	107.0	H(79A)-C(79A)-H(79B)	108.0
C(75B)-C(76B)-H(76D)	109.5	C(79A)-C(80A)-H(80A)	109.5
C(75B)-C(76B)-H(76E)	109.5	C(79A)-C(80A)-H(80B)	109.5
H(76D)-C(76B)-H(76E)	109.5	H(80A)-C(80A)-H(80B)	109.5
C(75B)-C(76B)-H(76F)	109.5	C(79A)-C(80A)-H(80C)	109.5
H(76D)-C(76B)-H(76F)	109.5	H(80A)-C(80A)-H(80C)	109.5
H(76E)-C(76B)-H(76F)	109.5	H(80B)-C(80A)-H(80C)	109.5
C(81)-N(8)-C(89B)	109.4(12)	C(78B)-C(77B)-N(8)	129(2)
C(81)-N(8)-C(89A)	109.4(12)	C(78B)-C(77B)-H(77C)	105.1
C(81)-N(8)-C(77B)	103.1(13)	N(8)-C(77B)-H(77C)	105.1
C(89B)-N(8)-C(77B)	99.7(14)	C(78B)-C(77B)-H(77D)	105.1
C(81)-N(8)-C(77A)	115.4(11)	N(8)-C(77B)-H(77D)	105.1
C(89A)-N(8)-C(77A)	114.8(12)	H(77C)-C(77B)-H(77D)	105.9
C(81)-N(8)-C(85A)	107.0(9)	C(77B)-C(78B)-C(79B)	112(3)
C(89A)-N(8)-C(85A)	109.9(11)	C(77B)-C(78B)-H(78C)	109.3

C(77A)-N(8)-C(85A)	99.5(12)	C(79B)-C(78B)-H(78C)	109.3
C(81)-N(8)-C(85B)	107.0(9)	C(77B)-C(78B)-H(78D)	109.3
C(89B)-N(8)-C(85B)	109.9(11)	C(79B)-C(78B)-H(78D)	109.3
C(77B)-N(8)-C(85B)	126.7(14)	H(78C)-C(78B)-H(78D)	107.9
C(78A)-C(77A)-N(8)	106.6(16)	C(80B)-C(79B)-C(78B)	110(3)
C(78A)-C(77A)-H(77A)	110.4	C(80B)-C(79B)-H(79C)	109.6
N(8)-C(77A)-H(77A)	110.4	C(78B)-C(79B)-H(79C)	109.6
C(78A)-C(77A)-H(77B)	110.4	C(80B)-C(79B)-H(79D)	109.6
N(8)-C(77A)-H(77B)	110.4	C(78B)-C(79B)-H(79D)	109.6
H(77A)-C(77A)-H(77B)	108.6	H(79C)-C(79B)-H(79D)	108.1
C(77A)-C(78A)-C(79A)	109.3(18)	C(79B)-C(80B)-H(80D)	109.5
C(77A)-C(78A)-H(78A)	109.8	C(79B)-C(80B)-H(80E)	109.5
C(79A)-C(78A)-H(78A)	109.8	H(80D)-C(80B)-H(80E)	109.5
C(77A)-C(78A)-H(78B)	109.8	C(79B)-C(80B)-H(80F)	109.5
C(79A)-C(78A)-H(78B)	109.8	H(80D)-C(80B)-H(80F)	109.5
H(78A)-C(78A)-H(78B)	108.3	H(80E)-C(80B)-H(80F)	109.5
N(8)-C(81)-H(81A)	108.2	N(8)-C(81)-C(82)	116.3(9)
C(82)-C(81)-H(81A)	108.2	C(86A)-C(87A)-H(87A)	107.9
N(8)-C(81)-H(81B)	108.2	C(88A)-C(87A)-H(87B)	107.9
C(82)-C(81)-H(81B)	108.2	C(86A)-C(87A)-H(87B)	107.9
H(81A)-C(81)-H(81B)	107.4	H(87A)-C(87A)-H(87B)	107.2
C(83)-C(82)-C(81)	110.9(10)	C(87A)-C(88A)-H(88A)	109.5
C(83)-C(82)-H(82A)	109.5	C(87A)-C(88A)-H(88B)	109.5
C(81)-C(82)-H(82A)	109.5	H(88A)-C(88A)-H(88B)	109.5
C(83)-C(82)-H(82B)	109.5	C(87A)-C(88A)-H(88C)	109.5
C(81)-C(82)-H(82B)	109.5	H(88A)-C(88A)-H(88C)	109.5
H(82A)-C(82)-H(82B)	108.0	H(88B)-C(88A)-H(88C)	109.5
C(84)-C(83)-C(82)	112.6(10)	C(90A)-C(89A)-N(8)	122.5(13)
C(84)-C(83)-H(83A)	109.1	C(90A)-C(89A)-H(89A)	106.7
C(82)-C(83)-H(83A)	109.1	N(8)-C(89A)-H(89A)	106.7
C(84)-C(83)-H(83B)	109.1	C(90A)-C(89A)-H(89B)	106.7
C(82)-C(83)-H(83B)	109.1	N(8)-C(89A)-H(89B)	106.7
H(83A)-C(83)-H(83B)	107.8	H(89A)-C(89A)-H(89B)	106.6
C(83)-C(84)-H(84A)	109.5	C(89A)-C(90A)-C(91A)	114.4(17)
C(83)-C(84)-H(84B)	109.5	C(89A)-C(90A)-H(90A)	108.7
H(84A)-C(84)-H(84B)	109.5	C(91A)-C(90A)-H(90A)	108.7

C(83)-C(84)-H(84C)	109.5	C(89A)-C(90A)-H(90B)	108.7
H(84A)-C(84)-H(84C)	109.5	C(91A)-C(90A)-H(90B)	108.7
H(84B)-C(84)-H(84C)	109.5	H(90A)-C(90A)-H(90B)	107.6
C(86A)-C(85A)-N(8)	130.4(13)	C(90A)-C(91A)-C(92A)	109(2)
C(86A)-C(85A)-H(85A)	104.7	C(90A)-C(91A)-H(91A)	109.9
N(8)-C(85A)-H(85A)	104.7	C(92A)-C(91A)-H(91A)	109.9
C(86A)-C(85A)-H(85B)	104.7	C(90A)-C(91A)-H(91B)	109.9
N(8)-C(85A)-H(85B)	104.7	C(92A)-C(91A)-H(91B)	109.9
H(85A)-C(85A)-H(85B)	105.7	H(91A)-C(91A)-H(91B)	108.3
C(85A)-C(86A)-C(87A)	119.3(16)	C(91A)-C(92A)-H(92A)	109.5
C(85A)-C(86A)-H(86A)	107.5	C(91A)-C(92A)-H(92B)	109.5
C(87A)-C(86A)-H(86A)	107.5	H(92A)-C(92A)-H(92B)	109.5
C(85A)-C(86A)-H(86B)	107.5	C(91A)-C(92A)-H(92C)	109.5
C(87A)-C(86A)-H(86B)	107.5	H(92A)-C(92A)-H(92C)	109.5
H(86A)-C(86A)-H(86B)	107.0	H(92B)-C(92A)-H(92C)	109.5
C(88A)-C(87A)-C(86A)	117(3)	C(86B)-C(85B)-N(8)	130.4(13)
C(88A)-C(87A)-H(87A)	107.9	C(86B)-C(85B)-H(85C)	104.7
C(86B)-C(85B)-H(85D)	104.7	N(8)-C(85B)-H(85C)	104.7
N(8)-C(85B)-H(85D)	104.7	C(90B)-C(91B)-H(91D)	112.3
H(85C)-C(85B)-H(85D)	105.7	H(91C)-C(91B)-H(91D)	109.9
C(85B)-C(86B)-C(87B)	119.3(16)	C(91B)-C(92B)-H(92D)	109.5
C(85B)-C(86B)-H(86C)	107.5	C(91B)-C(92B)-H(92E)	109.5
C(87B)-C(86B)-H(86C)	107.5	H(92D)-C(92B)-H(92E)	109.5
C(85B)-C(86B)-H(86D)	107.5	C(91B)-C(92B)-H(92F)	109.5
C(87B)-C(86B)-H(86D)	107.5	H(92D)-C(92B)-H(92F)	109.5
H(86C)-C(86B)-H(86D)	107.0	H(92E)-C(92B)-H(92F)	109.5
C(86B)-C(87B)-C(88B)	121(3)	C(90B)-C(91B)-H(91D)	112.3
C(86B)-C(87B)-H(87C)	107.2	Mo(12)-O(27)-Mo(9)	91.94(19)
C(88B)-C(87B)-H(87C)	107.2	Mo(12)-O(27)-Mo(8)	90.77(17)
C(86B)-C(87B)-H(87D)	107.2	Mo(9)-O(27)-Mo(8)	90.12(17)
C(88B)-C(87B)-H(87D)	107.2	Mo(12)-O(27)-Mo(11)	90.68(18)
H(87C)-C(87B)-H(87D)	106.8	Mo(9)-O(27)-Mo(11)	90.13(17)
C(87B)-C(88B)-H(88D)	109.5	Mo(8)-O(27)-Mo(11)	178.5(3)
C(87B)-C(88B)-H(88E)	109.5	Mo(12)-O(27)-Mo(10)	90.13(18)
H(88D)-C(88B)-H(88E)	109.5	Mo(9)-O(27)-Mo(10)	177.9(2)
C(87B)-C(88B)-H(88F)	109.5	Mo(8)-O(27)-Mo(10)	90.33(17)

H(88D)-C(88B)-H(88F)	109.5	Mo(11)-O(27)-Mo(10)	89.38(17)
H(88E)-C(88B)-H(88F)	109.5	Mo(12)-O(27)-Mo(7)	178.5(3)
C(90B)-C(89B)-N(8)	122.5(13)	Mo(9)-O(27)-Mo(7)	89.52(17)
C(90B)-C(89B)-H(89C)	106.7	Mo(8)-O(27)-Mo(7)	89.55(17)
N(8)-C(89B)-H(89C)	106.7	Mo(11)-O(27)-Mo(7)	88.99(16)
C(90B)-C(89B)-H(89D)	106.7	Mo(10)-O(27)-Mo(7)	88.41(17)
N(8)-C(89B)-H(89D)	106.7	Mo(8)-O(28)-Mo(10)	117.8(3)
H(89C)-C(89B)-H(89D)	106.6	Mo(10)-O(29)-Mo(11)	116.7(3)
C(89B)-C(90B)-C(91B)	101.6(16)	Mo(11)-O(32)-Mo(9)	116.6(3)
C(89B)-C(90B)-H(90C)	111.4	Mo(12)-O(33)-Mo(10)	115.2(3)
C(91B)-C(90B)-H(90C)	111.4	Mo(12)-O(34)-Mo(11)	114.4(3)
C(89B)-C(90B)-H(90D)	111.4	Mo(9)-O(35)-Mo(12)	114.2(3)
C(91B)-C(90B)-H(90D)	111.4	Mo(12)-O(27)-Mo(9)	91.94(19)
H(90C)-C(90B)-H(90D)	109.3	Mo(12)-O(27)-Mo(8)	90.77(17)
C(92B)-C(91B)-C(90B)	97(2)	Mo(9)-O(27)-Mo(8)	90.12(17)
C(92B)-C(91B)-H(91C)	112.3	Mo(12)-O(27)-Mo(11)	90.68(18)
C(90B)-C(91B)-H(91C)	112.3	Mo(9)-O(27)-Mo(11)	90.13(17)
C(92B)-C(91B)-H(91D)	112.3	Mo(8)-O(36)-Mo(12)	113.6(3)
C(12)-N(2)-H(02A)	120(4)	C(1)-N(1)-Mo(6)	176.1(7)
C(12)-N(2)-H(02B)	108(4)		
H(02A)-N(2)-H(02B)	121(7)		
C(2)-C(1)-N(1)	121.0(8)		
C(2)-C(1)-C(6)	119.6(8)		
N(1)-C(1)-C(6)	119.4(9)		
C(1)-C(2)-C(3)	119.4(8)		
C(1)-C(2)-H(2)	120.3		
C(3)-C(2)-H(2)	120.3		
C(4)-C(3)-C(2)	121.8(9)		
C(4)-C(3)-H(3)	119.1		
C(2)-C(3)-H(3)	119.1		
C(3)-C(4)-C(5)	118.6(8)		
C(3)-C(4)-C(7)	122.2(9)		

ORTEP-4 representation of compound **5**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity.



Compound 6

Crystal growth Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method Oil

Crystal Data

Chemical formula	$C_{40}H_{77}Mo_6N_3O_{18}$	
Formula weight	1463.69 g mol^{-1}	
Temperature	140 (2) K	
Crystal size	0.30 x 0.25 x 0.15 mm^3	
Crystal description	Orang block	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.3617(2) Å	α = 107.135(2)°.
	b = 19.1579(3) Å	β = 94.4450(10)°.
	c = 25.2441(4) Å	γ = 100.8150(10)°.
	Volume	5555.14(15) $Å^3$
Z	4	
F(000)	2936	
Density (calculated)	1.750 Mg cm^{-3}	
Absorption coefficient	1.379 mm^{-1}	

Data Collection

Diffractometer	Oxford Diffraction XCalibur 3
Radiation	Mo-*Kα*
2θ range for data collection	3.07 – 32.73°
Reflections collected	112337
Independent reflections	36262 [R(int) = 0.0577]
Transmission coefficients	1.0000
Data corrections	Gaussian
Index ranges	-17<=h<=18, -29<=k<=28, -37<=l<=37

Refinement method

Full-matrix least squares on F^2

Weighting scheme	$w = [\sigma^2(F_o^2) + (0.0664P)^2 + 0.0000P]^{-1}$	
	$P = [\max(I_{obs}, 0) + 2F_c^2]/3$	
Data / restraints / parameters	36262 / 515 / 1330	
Data to parameter ratio	27.26	
Goodness of fit on F^2	1.019	
R indices	$[I_o>2\sigma>(I_o)]$ data	R1 = 0.0585, wR2 = 0.1283
	All 2558 data	R1 = 0.1201, wR2 = 0.1445
Final difference map	Largest diff. peak + 1.917 and hole - 1.102 $e.Å^{-3}$	

Bond lengths [Å] and angles [°]

C(1)-C(2)	1.373(8)	Mo(4A)-O(17A)	1.694(7)
C(1)-N(1)	1.382(6)	Mo(4A)-O(5)	1.782(5)
C(1)-C(6)	1.426(7)	Mo(4A)-O(13A)	1.873(8)
C(2)-C(3)	1.389(8)	Mo(4A)-O(12A)	1.975(8)
C(2)-H(2)	0.9300	Mo(4A)-O(4)	2.091(6)
C(3)-C(4)	1.393(9)	Mo(4A)-O(1)	2.341(3)
C(3)-H(3)	0.9300	Mo(6A)-O(18A)	1.684(8)
C(4)-C(5)	1.394(9)	Mo(6A)-O(12A)	1.868(9)
C(4)-C(7)	1.433(9)	Mo(6A)-O(9)	1.902(4)
C(5)-C(6)	1.382(8)	Mo(6A)-O(8)	1.958(5)
C(5)-H(5)	0.9300	Mo(6A)-O(11A)	1.988(11)
C(6)-H(6)	0.9300	Mo(6A)-O(1)	2.287(4)
C(7)-C(8)	1.177(9)	Mo(2B)-O(14B)	1.683(9)
C(8)-H(8)	0.9300	Mo(2B)-O(11B)	1.859(11)
Mo(1)-N(1)	1.726(4)	Mo(2B)-O(2)	1.888(6)
Mo(1)-O(9)	1.893(3)	Mo(2B)-O(3)	1.959(7)
Mo(1)-O(5)	1.905(4)	Mo(2B)-O(10B)	1.994(9)
Mo(1)-O(2)	1.946(3)	Mo(2B)-O(1)	2.328(5)
Mo(1)-O(6)	1.980(4)	Mo(3B)-O(16B)	1.679(8)
Mo(1)-O(1)	2.220(3)	Mo(3B)-O(10B)	1.875(10)
Mo(1)-Mo(4A)	3.130(2)	Mo(3B)-O(7)	1.875(5)
Mo(1)-Mo(6A)	3.158(3)	Mo(3B)-O(6)	1.950(5)
Mo(2A)-O(14A)	1.679(9)	Mo(3B)-O(13B)	1.985(8)
Mo(2A)-O(11A)	1.860(10)	Mo(3B)-O(1)	2.280(4)
Mo(2A)-O(2)	1.908(6)	Mo(3B)-Mo(5)	3.179(3)
Mo(2A)-O(3)	1.949(6)	Mo(4B)-O(17B)	1.693(7)
Mo(2A)-O(10A)	1.981(10)	Mo(4B)-O(4)	1.729(5)
Mo(2A)-O(1)	2.300(5)	Mo(4B)-O(13B)	1.880(8)
Mo(3A)-O(16A)	1.676(8)	Mo(4B)-O(12B)	1.979(8)
Mo(3A)-O(6)	1.801(5)	Mo(4B)-O(5)	2.111(5)
Mo(3A)-O(10A)	1.871(9)	Mo(4B)-O(1)	2.327(3)
Mo(3A)-O(13A)	1.978(9)	Mo(4B)-Mo(5)	3.153(2)
Mo(3A)-O(7)	2.092(5)	Mo(6B)-O(18B)	1.683(7)

Mo(3A)-O(1)	2.365(4)	Mo(6B)-O(8)	1.849(4)
Mo(6B)-O(1)	2.386(4)	Mo(12)-O(30)	1.955(3)
Mo(5)-O(15)	1.681(3)	Mo(12)-O(19)	2.335(3)
Mo(5)-O(7)	1.859(3)	Mo(11)-O(32)	1.691(3)
Mo(5)-O(3)	1.883(4)	Mo(11)-O(28)	1.900(3)
Mo(5)-O(4)	1.930(4)	Mo(11)-O(23)	1.919(3)
Mo(5)-O(8)	1.962(4)	Mo(11)-O(26)	1.923(3)
Mo(5)-O(1)	2.360(3)	Mo(11)-O(27)	1.941(3)
C(9)-C(10)	1.381(7)	Mo(11)-O(19)	2.323(3)
C(9)-N(2)	1.386(6)	Mo(10)-O(35)	1.699(3)
C(9)-C(14)	1.395(7)	Mo(10)-O(21)	1.898(3)
C(10)-C(11)	1.382(6)	Mo(10)-O(27)	1.918(3)
C(10)-H(10)	0.9300	Mo(10)-O(29)	1.928(3)
C(11)-C(12)	1.388(7)	Mo(10)-O(24)	1.952(3)
C(11)-H(11)	0.9300	Mo(10)-O(19)	2.329(3)
C(12)-C(13)	1.386(7)	Mo(9)-O(34)	1.700(3)
C(12)-C(15)	1.418(7)	Mo(9)-O(30)	1.882(3)
C(13)-C(14)	1.386(8)	Mo(9)-O(31)	1.916(3)
C(13)-H(13)	0.9300	Mo(9)-O(29)	1.921(3)
C(14)-H(14)	0.9300	Mo(9)-O(28)	1.959(3)
C(15)-C(16)	1.190(7)	Mo(9)-O(19)	2.336(3)
C(16)-H(16)	0.9300	C(17)-C(18)	1.516(8)
Mo(7)-N(2)	1.738(4)	C(17)-N(3)	1.530(7)
Mo(7)-O(23)	1.923(3)	C(17)-H(17A)	0.9700
Mo(7)-O(21)	1.951(3)	C(17)-H(17B)	0.9700
Mo(7)-O(22)	1.951(3)	C(18)-C(19)	1.504(8)
Mo(7)-O(20)	1.967(3)	C(18)-H(18A)	0.9700
Mo(7)-O(19)	2.220(3)	C(18)-H(18B)	0.9700
Mo(8)-O(33)	1.694(4)	C(19)-C(20)	1.480(9)
Mo(8)-O(22)	1.901(3)	C(19)-H(19A)	0.9700
Mo(8)-O(25)	1.921(4)	C(19)-H(19B)	0.9700
Mo(8)-O(31)	1.925(3)	C(20)-H(20A)	0.9600
Mo(8)-O(26)	1.936(4)	C(20)-H(20B)	0.9600
Mo(8)-O(19)	2.333(3)	C(20)-H(20C)	0.9600
Mo(12)-O(36)	1.691(3)	C(21)-C(22)	1.496(7)
Mo(12)-O(20)	1.876(3)	C(21)-N(3)	1.528(5)

Mo(12)-O(24)	1.916(3)	C(21)-H(21A)	0.9700
Mo(12)-O(25)	1.937(3)	C(21)-H(21B)	0.9700
C(22)-C(23)	1.537(6)	C(33)-H(33A)	0.9700
C(22)-H(22A)	0.9700	C(33)-H(33B)	0.9700
C(22)-H(22B)	0.9700	C(34)-C(35)	1.464(9)
C(23)-C(24)	1.512(7)	C(34)-H(34A)	0.9700
C(23)-H(23A)	0.9700	C(34)-H(34B)	0.9700
C(23)-H(23B)	0.9700	C(35)-C(36)	1.457(5)
C(24)-H(24A)	0.9600	C(35)-H(35A)	0.9700
C(24)-H(24B)	0.9600	C(35)-H(35B)	0.9700
C(24)-H(24C)	0.9600	C(36)-H(36A)	0.9600
C(25)-C(26)	1.505(6)	C(36)-H(36B)	0.9600
C(25)-N(3)	1.522(6)	C(36)-H(36C)	0.9600
C(25)-H(25A)	0.9700	C(37)-C(38)	1.489(9)
C(25)-H(25B)	0.9700	C(37)-N(4)	1.530(8)
C(26)-C(27)	1.533(7)	C(37)-H(37A)	0.9700
C(26)-H(26A)	0.9700	C(37)-H(37B)	0.9700
C(26)-H(26B)	0.9700	C(38)-C(39)	1.515(10)
C(27)-C(28)	1.500(7)	C(38)-H(38A)	0.9700
C(27)-H(27A)	0.9700	C(38)-H(38B)	0.9700
C(27)-H(27B)	0.9700	C(39)-C(40)	1.479(5)
C(28)-H(28A)	0.9600	C(39)-H(39A)	0.9700
C(28)-H(28B)	0.9600	C(39)-H(39B)	0.9700
C(28)-H(28C)	0.9600	C(40)-H(40A)	0.9600
C(29)-N(3)	1.510(7)	C(40)-H(40B)	0.9600
C(29)-C(30)	1.545(8)	C(40)-H(40C)	0.9600
C(29)-H(29A)	0.9700	C(41)-N(4)	1.505(7)
C(29)-H(29B)	0.9700	C(41)-C(42)	1.522(9)
C(30)-C(31)	1.486(11)	C(41)-H(41A)	0.9700
C(30)-H(30A)	0.9700	C(41)-H(41B)	0.9700
C(30)-H(30B)	0.9700	C(42)-C(43)	1.470(10)
C(31)-C(32)	1.476(5)	C(42)-H(42A)	0.9700
C(31)-H(31A)	0.9700	C(42)-H(42B)	0.9700
C(31)-H(31B)	0.9700	C(43)-C(44)	1.413(11)
C(32)-H(32A)	0.9600	C(43)-H(43A)	0.9700
C(32)-H(32B)	0.9600	C(43)-H(43B)	0.9700

C(32)-H(32C)	0.9600	C(44)-H(44A)	0.9600
C(33)-N(4)	1.506(7)	C(44)-H(44B)	0.9600
C(33)-C(34)	1.526(9)	C(44)-H(44C)	0.9600
C(45)-C(46)	1.514(8)	C(56)-H(56B)	0.9600
C(45)-N(4)	1.520(8)	C(56)-H(56C)	0.9600
C(45)-H(45A)	0.9700	C(57)-N(5)	1.517(6)
C(45)-H(45B)	0.9700	C(57)-C(58)	1.518(9)
C(46)-C(47)	1.491(9)	C(57)-H(57A)	0.9700
C(46)-H(46A)	0.9700	C(57)-H(57B)	0.9700
C(46)-H(46B)	0.9700	C(58)-C(59)	1.488(9)
C(47)-C(48)	1.502(8)	C(58)-H(58A)	0.9700
C(47)-H(47A)	0.9700	C(58)-H(58B)	0.9700
C(47)-H(47B)	0.9700	C(59)-C(60)	1.519(13)
C(48)-H(48A)	0.9600	C(59)-H(59A)	0.9700
C(48)-H(48B)	0.9600	C(59)-H(59B)	0.9700
C(48)-H(48C)	0.9600	C(60)-H(60A)	0.9600
C(49)-N(5)	1.531(7)	C(60)-H(60B)	0.9600
C(49)-C(50)	1.548(8)	C(60)-H(60C)	0.9600
C(49)-H(49A)	0.9700	C(61)-C(62)	1.506(10)
C(49)-H(49B)	0.9700	C(61)-N(5)	1.521(8)
C(50)-C(51)	1.526(10)	C(61)-H(61A)	0.9700
C(50)-H(50A)	0.9700	C(61)-H(61B)	0.9700
C(50)-H(50B)	0.9700	C(62)-C(63)	1.502(10)
C(51)-C(52)	1.466(12)	C(62)-H(62A)	0.9700
C(51)-H(51A)	0.9700	C(62)-H(62B)	0.9700
C(51)-H(51B)	0.9700	C(63)-C(64)	1.503(12)
C(52)-H(52A)	0.9600	C(63)-H(63A)	0.9700
C(52)-H(52B)	0.9600	C(63)-H(63B)	0.9700
C(52)-H(52C)	0.9600	C(64)-H(64A)	0.9600
C(53)-C(54)	1.490(10)	C(64)-H(64B)	0.9600
C(53)-N(5)	1.509(9)	C(64)-H(64C)	0.9600
C(53)-H(53A)	0.9700	C(65)-C(66)	1.507(6)
C(53)-H(53B)	0.9700	C(65)-N(6)	1.525(5)
C(54)-C(55)	1.536(11)	C(65)-H(65A)	0.9700
C(54)-H(54A)	0.9700	C(65)-H(65B)	0.9700
C(54)-H(54B)	0.9700	C(66)-C(67)	1.535(6)

C(55)-C(56)	1.442(13)	C(66)-H(66A)	0.9700
C(55)-H(55A)	0.9700	C(66)-H(66B)	0.9700
C(55)-H(55B)	0.9700	C(67)-C(68)	1.527(7)
C(56)-H(56A)	0.9600	C(67)-H(67A)	0.9700
C(67)-H(67B)	0.9700	C(79)-C(80)	1.498(8)
C(68)-H(68A)	0.9600	C(79)-H(79A)	0.9700
C(68)-H(68B)	0.9600	C(79)-H(79B)	0.9700
C(68)-H(68C)	0.9600	C(80)-H(80A)	0.9600
C(69)-C(70)	1.495(6)	C(80)-H(80B)	0.9600
C(69)-N(6)	1.546(5)	C(80)-H(80C)	0.9600
C(69)-H(69A)	0.9700	C(2)-C(1)-N(1)	119.8(5)
C(69)-H(69B)	0.9700	C(2)-C(1)-C(6)	121.0(5)
C(70)-C(71)	1.517(6)	N(1)-C(1)-C(6)	119.1(5)
C(70)-H(70A)	0.9700	C(1)-C(2)-C(3)	119.8(5)
C(70)-H(70B)	0.9700	C(1)-C(2)-H(2)	120.1
C(71)-C(72)	1.518(7)	C(3)-C(2)-H(2)	120.1
C(71)-H(71A)	0.9700	C(2)-C(3)-C(4)	120.6(6)
C(71)-H(71B)	0.9700	C(2)-C(3)-H(3)	119.7
C(72)-H(72A)	0.9600	C(4)-C(3)-H(3)	119.7
C(72)-H(72B)	0.9600	C(3)-C(4)-C(5)	118.9(6)
C(72)-H(72C)	0.9600	C(3)-C(4)-C(7)	120.5(7)
C(73)-N(6)	1.513(6)	C(5)-C(4)-C(7)	120.6(7)
C(73)-C(74)	1.519(7)	C(6)-C(5)-C(4)	121.8(6)
C(73)-H(73A)	0.9700	C(6)-C(5)-H(5)	119.1
C(73)-H(73B)	0.9700	C(4)-C(5)-H(5)	119.1
C(74)-C(75)	1.513(7)	C(5)-C(6)-C(1)	117.6(6)
C(74)-H(74A)	0.9700	C(5)-C(6)-H(6)	121.2
C(74)-H(74B)	0.9700	C(1)-C(6)-H(6)	121.2
C(75)-C(76)	1.519(8)	C(8)-C(7)-C(4)	177.6(8)
C(75)-H(75A)	0.9700	C(7)-C(8)-H(8)	180.0
C(75)-H(75B)	0.9700	N(1)-Mo(1)-O(9)	103.70(16)
C(76)-H(76A)	0.9600	N(1)-Mo(1)-O(5)	102.06(18)
C(76)-H(76B)	0.9600	O(9)-Mo(1)-O(5)	90.77(18)
C(76)-H(76C)	0.9600	N(1)-Mo(1)-O(2)	101.62(16)
C(77)-C(78)	1.508(7)	O(9)-Mo(1)-O(2)	88.59(16)
C(77)-N(6)	1.517(6)	O(5)-Mo(1)-O(2)	155.77(14)

C(77)-H(77A)	0.9700	N(1)-Mo(1)-O(6)	100.23(17)
C(77)-H(77B)	0.9700	O(9)-Mo(1)-O(6)	156.02(14)
C(78)-C(79)	1.536(7)	O(5)-Mo(1)-O(6)	85.7(2)
C(78)-H(78A)	0.9700	O(2)-Mo(1)-O(6)	85.11(18)
C(78)-H(78B)	0.9700	O(6)-Mo(3A)-O(13A)	79.1(4)
N(1)-Mo(1)-O(1)	176.87(15)	O(10A)-Mo(3A)-O(13A)	152.8(5)
O(9)-Mo(1)-O(1)	79.33(12)	O(16A)-Mo(3A)-O(7)	103.4(5)
O(5)-Mo(1)-O(1)	78.53(13)	O(6)-Mo(3A)-O(7)	146.7(2)
O(2)-Mo(1)-O(1)	77.55(11)	O(10A)-Mo(3A)-O(7)	89.6(5)
O(6)-Mo(1)-O(1)	76.72(13)	O(13A)-Mo(3A)-O(7)	80.7(3)
N(1)-Mo(1)-Mo(4A)	131.93(15)	O(16A)-Mo(3A)-O(1)	176.7(5)
O(9)-Mo(1)-Mo(4A)	89.51(13)	O(6)-Mo(3A)-O(1)	76.37(17)
O(5)-Mo(1)-Mo(4A)	30.70(11)	O(10A)-Mo(3A)-O(1)	76.7(4)
O(2)-Mo(1)-Mo(4A)	125.07(10)	O(13A)-Mo(3A)-O(1)	76.1(3)
O(6)-Mo(1)-Mo(4A)	75.47(16)	O(7)-Mo(3A)-O(1)	73.26(14)
O(1)-Mo(1)-Mo(4A)	48.28(9)	O(17A)-Mo(4A)-O(5)	101.9(3)
N(1)-Mo(1)-Mo(6A)	136.72(14)	O(17A)-Mo(4A)-O(13A)	103.3(4)
O(9)-Mo(1)-Mo(6A)	33.79(10)	O(5)-Mo(4A)-O(13A)	95.1(3)
O(5)-Mo(1)-Mo(6A)	78.03(18)	O(17A)-Mo(4A)-O(12A)	103.5(4)
O(2)-Mo(1)-Mo(6A)	88.22(14)	O(5)-Mo(4A)-O(12A)	77.3(3)
O(6)-Mo(1)-Mo(6A)	122.71(12)	O(13A)-Mo(4A)-O(12A)	153.1(4)
O(1)-Mo(1)-Mo(6A)	46.39(9)	O(17A)-Mo(4A)-O(4)	106.5(4)
Mo(4A)-Mo(1)-Mo(6A)	62.88(5)	O(5)-Mo(4A)-O(4)	147.2(2)
O(14A)-Mo(2A)-O(11A)	105.3(6)	O(13A)-Mo(4A)-O(4)	94.0(3)
O(14A)-Mo(2A)-O(2)	107.6(5)	O(12A)-Mo(4A)-O(4)	80.4(3)
O(11A)-Mo(2A)-O(2)	92.4(8)	O(17A)-Mo(4A)-O(1)	178.1(4)
O(14A)-Mo(2A)-O(3)	99.2(5)	O(5)-Mo(4A)-O(1)	77.69(14)
O(11A)-Mo(2A)-O(3)	93.1(8)	O(13A)-Mo(4A)-O(1)	78.6(3)
O(2)-Mo(2A)-O(3)	150.1(3)	O(12A)-Mo(4A)-O(1)	74.6(3)
O(14A)-Mo(2A)-O(10A)	101.9(5)	O(4)-Mo(4A)-O(1)	73.40(15)
O(11A)-Mo(2A)-O(10A)	152.8(5)	O(17A)-Mo(4A)-Mo(1)	134.7(3)
O(2)-Mo(2A)-O(10A)	80.3(5)	O(5)-Mo(4A)-Mo(1)	33.09(11)
O(3)-Mo(2A)-O(10A)	81.5(5)	O(13A)-Mo(4A)-Mo(1)	83.0(3)
O(14A)-Mo(2A)-O(1)	175.5(6)	O(12A)-Mo(4A)-Mo(1)	76.7(3)
O(11A)-Mo(2A)-O(1)	76.5(4)	O(4)-Mo(4A)-Mo(1)	117.90(13)
O(2)-Mo(2A)-O(1)	76.3(2)	O(1)-Mo(4A)-Mo(1)	45.06(8)

O(3)-Mo(2A)-O(1)	76.5(2)	O(18A)-Mo(6A)-O(12A)	104.3(4)
O(10A)-Mo(2A)-O(1)	76.3(3)	O(18A)-Mo(6A)-O(9)	102.5(4)
O(16A)-Mo(3A)-O(6)	106.8(5)	O(12A)-Mo(6A)-O(9)	89.9(3)
O(16A)-Mo(3A)-O(10A)	103.6(5)	O(18A)-Mo(6A)-O(8)	102.0(4)
O(6)-Mo(3A)-O(10A)	96.5(5)	O(12A)-Mo(6A)-O(8)	99.5(4)
O(16A)-Mo(3A)-O(13A)	103.4(5)	O(10B)-Mo(3B)-O(7)	82.9(5)
O(9)-Mo(6A)-O(8)	150.6(2)	O(16B)-Mo(3B)-O(6)	103.9(4)
O(18A)-Mo(6A)-O(11A)	103.4(5)	O(10B)-Mo(3B)-O(6)	86.6(5)
O(12A)-Mo(6A)-O(11A)	151.6(4)	O(7)-Mo(3B)-O(6)	154.5(2)
O(9)-Mo(6A)-O(11A)	78.3(7)	O(16B)-Mo(3B)-O(13B)	102.7(4)
O(8)-Mo(6A)-O(11A)	80.4(7)	O(10B)-Mo(3B)-O(13B)	152.0(4)
O(18A)-Mo(6A)-O(1)	177.8(4)	O(7)-Mo(3B)-O(13B)	84.0(3)
O(12A)-Mo(6A)-O(1)	77.8(3)	O(6)-Mo(3B)-O(13B)	94.8(4)
O(9)-Mo(6A)-O(1)	77.43(15)	O(16B)-Mo(3B)-O(1)	177.7(4)
O(8)-Mo(6A)-O(1)	77.43(16)	O(10B)-Mo(3B)-O(1)	78.2(3)
O(11A)-Mo(6A)-O(1)	74.4(3)	O(7)-Mo(3B)-O(1)	79.25(17)
O(18A)-Mo(6A)-Mo(1)	135.6(4)	O(6)-Mo(3B)-O(1)	75.87(16)
O(12A)-Mo(6A)-Mo(1)	77.2(3)	O(13B)-Mo(3B)-O(1)	75.1(3)
O(9)-Mo(6A)-Mo(1)	33.60(10)	O(16B)-Mo(3B)-Mo(5)	132.5(4)
O(8)-Mo(6A)-Mo(1)	121.77(15)	O(10B)-Mo(3B)-Mo(5)	80.1(4)
O(11A)-Mo(6A)-Mo(1)	78.9(6)	O(7)-Mo(3B)-Mo(5)	31.50(11)
O(1)-Mo(6A)-Mo(1)	44.65(9)	O(6)-Mo(3B)-Mo(5)	123.61(16)
Mo(3A)-O(10A)-Mo(2A)	117.2(6)	O(13B)-Mo(3B)-Mo(5)	75.8(3)
Mo(2A)-O(11A)-Mo(6A)	117.4(6)	O(1)-Mo(3B)-Mo(5)	47.82(9)
Mo(6A)-O(12A)-Mo(4A)	117.2(4)	O(17B)-Mo(4B)-O(4)	101.9(3)
Mo(4A)-O(13A)-Mo(3A)	116.8(4)	O(17B)-Mo(4B)-O(13B)	104.5(4)
O(14B)-Mo(2B)-O(11B)	105.5(5)	O(4)-Mo(4B)-O(13B)	79.9(4)
O(14B)-Mo(2B)-O(2)	101.8(5)	O(17B)-Mo(4B)-O(12B)	102.7(4)
O(11B)-Mo(2B)-O(2)	87.0(8)	O(4)-Mo(4B)-O(12B)	93.6(3)
O(14B)-Mo(2B)-O(3)	106.8(5)	O(13B)-Mo(4B)-O(12B)	152.8(4)
O(11B)-Mo(2B)-O(3)	83.2(8)	O(17B)-Mo(4B)-O(5)	105.5(3)
O(2)-Mo(2B)-O(3)	151.3(3)	O(4)-Mo(4B)-O(5)	150.6(2)
O(14B)-Mo(2B)-O(10B)	101.3(5)	O(13B)-Mo(4B)-O(5)	83.2(3)
O(11B)-Mo(2B)-O(10B)	152.7(6)	O(12B)-Mo(4B)-O(5)	90.5(3)
O(2)-Mo(2B)-O(10B)	92.3(5)	O(17B)-Mo(4B)-O(1)	177.7(3)
O(3)-Mo(2B)-O(10B)	84.4(5)	O(4)-Mo(4B)-O(1)	80.35(15)

O(14B)-Mo(2B)-O(1)	175.3(4)	O(13B)-Mo(4B)-O(1)	75.8(3)
O(11B)-Mo(2B)-O(1)	78.6(4)	O(12B)-Mo(4B)-O(1)	77.0(2)
O(2)-Mo(2B)-O(1)	76.0(2)	O(5)-Mo(4B)-O(1)	72.24(14)
O(3)-Mo(2B)-O(1)	75.7(2)	O(17B)-Mo(4B)-Mo(5)	134.1(3)
O(10B)-Mo(2B)-O(1)	74.8(4)	O(4)-Mo(4B)-Mo(5)	32.38(12)
O(16B)-Mo(3B)-O(10B)	104.1(5)	O(13B)-Mo(4B)-Mo(5)	77.7(3)
O(16B)-Mo(3B)-O(7)	101.2(4)	O(15)-Mo(5)-Mo(4B)	132.18(15)
O(12B)-Mo(4B)-Mo(5)	82.8(2)	O(7)-Mo(5)-Mo(4B)	84.69(14)
O(5)-Mo(4B)-Mo(5)	120.09(12)	O(3)-Mo(5)-Mo(4B)	123.18(10)
O(1)-Mo(4B)-Mo(5)	48.17(8)	O(4)-Mo(5)-Mo(4B)	28.68(12)
O(18B)-Mo(6B)-O(8)	105.9(4)	O(8)-Mo(5)-Mo(4B)	76.04(18)
O(18B)-Mo(6B)-O(12B)	104.3(4)	O(1)-Mo(5)-Mo(4B)	47.28(8)
O(8)-Mo(6B)-O(12B)	81.5(3)	O(15)-Mo(5)-Mo(3B)	135.45(15)
O(18B)-Mo(6B)-O(11B)	103.3(5)	O(7)-Mo(5)-Mo(3B)	31.81(11)
O(8)-Mo(6B)-O(11B)	92.2(8)	O(3)-Mo(5)-Mo(3B)	83.65(13)
O(12B)-Mo(6B)-O(11B)	152.3(4)	O(4)-Mo(5)-Mo(3B)	78.87(17)
O(18B)-Mo(6B)-O(9)	104.5(3)	O(8)-Mo(5)-Mo(3B)	121.21(13)
O(8)-Mo(6B)-O(9)	148.8(2)	O(1)-Mo(5)-Mo(3B)	45.71(9)
O(12B)-Mo(6B)-O(9)	84.3(3)	Mo(4B)-Mo(5)-Mo(3B)	62.91(7)
O(11B)-Mo(6B)-O(9)	87.6(8)	C(1)-N(1)-Mo(1)	169.9(4)
O(18B)-Mo(6B)-O(1)	176.9(4)	Mo(1)-O(1)-Mo(3B)	93.75(14)
O(8)-Mo(6B)-O(1)	76.93(16)	Mo(1)-O(1)-Mo(6A)	88.96(12)
O(12B)-Mo(6B)-O(1)	77.4(3)	Mo(3B)-O(1)-Mo(6A)	168.67(15)
O(11B)-Mo(6B)-O(1)	75.0(4)	Mo(1)-O(1)-Mo(2A)	91.06(17)
O(9)-Mo(6B)-O(1)	72.87(14)	Mo(3B)-O(1)-Mo(2A)	99.30(14)
Mo(3B)-O(10B)-Mo(2B)	116.0(5)	Mo(6A)-O(1)-Mo(2A)	91.64(13)
Mo(2B)-O(11B)-Mo(6B)	117.9(6)	Mo(1)-O(1)-Mo(4B)	95.04(12)
Mo(6B)-O(12B)-Mo(4B)	116.7(4)	Mo(3B)-O(1)-Mo(4B)	91.65(12)
Mo(4B)-O(13B)-Mo(3B)	117.5(5)	Mo(6A)-O(1)-Mo(4B)	77.15(10)
O(15)-Mo(5)-O(7)	103.73(17)	Mo(2A)-O(1)-Mo(4B)	167.10(18)
O(15)-Mo(5)-O(3)	104.16(17)	Mo(1)-O(1)-Mo(2B)	90.95(17)
O(7)-Mo(5)-O(3)	89.11(16)	Mo(3B)-O(1)-Mo(2B)	90.83(14)
O(15)-Mo(5)-O(4)	103.77(18)	Mo(6A)-O(1)-Mo(2B)	100.14(16)
O(7)-Mo(5)-O(4)	87.54(19)	Mo(2A)-O(1)-Mo(2B)	8.50(17)
O(3)-Mo(5)-O(4)	151.86(15)	Mo(4B)-O(1)-Mo(2B)	173.4(2)
O(15)-Mo(5)-O(8)	103.20(18)	Mo(1)-O(1)-Mo(4A)	86.65(13)

O(7)-Mo(5)-O(8)	153.02(15)	Mo(3B)-O(1)-Mo(4A)	78.93(11)
O(3)-Mo(5)-O(8)	85.92(19)	Mo(6A)-O(1)-Mo(4A)	90.27(11)
O(4)-Mo(5)-O(8)	84.5(2)	Mo(2A)-O(1)-Mo(4A)	177.0(2)
O(15)-Mo(5)-O(1)	178.74(15)	Mo(4B)-O(1)-Mo(4A)	15.74(4)
O(7)-Mo(5)-O(1)	77.45(12)	Mo(2B)-O(1)-Mo(4A)	169.28(19)
O(3)-Mo(5)-O(1)	76.23(11)	Mo(1)-O(1)-Mo(5)	179.54(16)
O(4)-Mo(5)-O(1)	75.77(13)	Mo(3B)-O(1)-Mo(5)	86.47(12)
O(8)-Mo(5)-O(1)	75.60(13)	Mo(5)-O(7)-Mo(3B)	116.69(18)
Mo(6A)-O(1)-Mo(5)	90.74(13)	Mo(5)-O(7)-Mo(3A)	117.09(17)
Mo(2A)-O(1)-Mo(5)	89.30(17)	Mo(3B)-O(7)-Mo(3A)	11.24(11)
Mo(4B)-O(1)-Mo(5)	84.55(11)	Mo(6B)-O(8)-Mo(6A)	14.75(8)
Mo(2B)-O(1)-Mo(5)	89.45(17)	Mo(6B)-O(8)-Mo(5)	119.2(2)
Mo(4A)-O(1)-Mo(5)	93.00(13)	Mo(6A)-O(8)-Mo(5)	115.1(2)
Mo(1)-O(1)-Mo(3A)	89.20(14)	Mo(1)-O(9)-Mo(6A)	112.62(16)
Mo(3B)-O(1)-Mo(3A)	10.77(8)	Mo(1)-O(9)-Mo(6B)	115.53(16)
Mo(6A)-O(1)-Mo(3A)	177.78(19)	Mo(6A)-O(9)-Mo(6B)	14.17(9)
Mo(2A)-O(1)-Mo(3A)	89.64(13)	C(10)-C(9)-N(2)	120.3(5)
Mo(4B)-O(1)-Mo(3A)	101.78(12)	C(10)-C(9)-C(14)	120.2(4)
Mo(2B)-O(1)-Mo(3A)	81.13(14)	N(2)-C(9)-C(14)	119.5(5)
Mo(4A)-O(1)-Mo(3A)	88.39(11)	C(9)-C(10)-C(11)	118.8(5)
Mo(5)-O(1)-Mo(3A)	91.09(13)	C(9)-C(10)-H(10)	120.6
Mo(1)-O(1)-Mo(6B)	92.08(11)	C(11)-C(10)-H(10)	120.6
Mo(3B)-O(1)-Mo(6B)	174.13(17)	C(10)-C(11)-C(12)	122.3(5)
Mo(6A)-O(1)-Mo(6B)	12.06(7)	C(10)-C(11)-H(11)	118.9
Mo(2A)-O(1)-Mo(6B)	79.94(13)	C(12)-C(11)-H(11)	118.9
Mo(4B)-O(1)-Mo(6B)	88.47(11)	C(13)-C(12)-C(11)	118.0(5)
Mo(2B)-O(1)-Mo(6B)	88.44(14)	C(13)-C(12)-C(15)	119.5(5)
Mo(4A)-O(1)-Mo(6B)	102.07(11)	C(11)-C(12)-C(15)	122.4(4)
Mo(5)-O(1)-Mo(6B)	87.70(12)	C(14)-C(13)-C(12)	120.8(5)
Mo(3A)-O(1)-Mo(6B)	169.52(14)	C(14)-C(13)-H(13)	119.6
Mo(2B)-O(2)-Mo(2A)	10.4(2)	C(12)-C(13)-H(13)	119.6
Mo(2B)-O(2)-Mo(1)	115.5(2)	C(13)-C(14)-C(9)	119.8(5)
Mo(2A)-O(2)-Mo(1)	113.7(2)	C(13)-C(14)-H(14)	120.1
Mo(5)-O(3)-Mo(2A)	117.4(2)	C(9)-C(14)-H(14)	120.1
Mo(5)-O(3)-Mo(2B)	118.3(2)	C(16)-C(15)-C(12)	176.9(6)
Mo(2A)-O(3)-Mo(2B)	10.1(2)	C(15)-C(16)-H(16)	180.0

Mo(4B)-O(4)-Mo(5)	118.94(19)	N(2)-Mo(7)-O(23)	103.46(17)
Mo(4B)-O(4)-Mo(4A)	15.93(10)	N(2)-Mo(7)-O(21)	100.54(17)
Mo(5)-O(4)-Mo(4A)	115.95(19)	O(23)-Mo(7)-O(21)	89.10(14)
Mo(4A)-O(5)-Mo(1)	116.21(18)	N(2)-Mo(7)-O(22)	102.63(17)
Mo(4A)-O(5)-Mo(4B)	16.23(7)	O(23)-Mo(7)-O(22)	87.85(15)
Mo(1)-O(5)-Mo(4B)	113.15(18)	O(21)-Mo(7)-O(22)	156.71(13)
Mo(3A)-O(6)-Mo(3B)	12.83(11)	N(2)-Mo(7)-O(20)	99.85(17)
Mo(3A)-O(6)-Mo(1)	116.7(2)	O(23)-Mo(7)-O(20)	156.68(13)
Mo(3B)-O(6)-Mo(1)	113.4(2)	O(32)-Mo(11)-O(28)	103.66(16)
O(21)-Mo(7)-O(20)	86.31(14)	O(32)-Mo(11)-O(23)	102.74(16)
O(22)-Mo(7)-O(20)	87.41(15)	O(28)-Mo(11)-O(23)	153.60(13)
N(2)-Mo(7)-O(19)	177.67(17)	O(32)-Mo(11)-O(26)	104.16(19)
O(23)-Mo(7)-O(19)	78.68(12)	O(28)-Mo(11)-O(26)	87.13(14)
O(21)-Mo(7)-O(19)	78.49(11)	O(23)-Mo(11)-O(26)	87.06(15)
O(22)-Mo(7)-O(19)	78.27(12)	O(32)-Mo(11)-O(27)	102.53(17)
O(20)-Mo(7)-O(19)	78.00(11)	O(28)-Mo(11)-O(27)	87.82(13)
O(33)-Mo(8)-O(22)	104.10(18)	O(23)-Mo(11)-O(27)	85.90(14)
O(33)-Mo(8)-O(25)	102.9(2)	O(26)-Mo(11)-O(27)	153.28(14)
O(22)-Mo(8)-O(25)	88.00(15)	O(32)-Mo(11)-O(19)	178.58(15)
O(33)-Mo(8)-O(31)	102.69(18)	O(28)-Mo(11)-O(19)	77.43(11)
O(22)-Mo(8)-O(31)	153.21(14)	O(23)-Mo(11)-O(19)	76.17(12)
O(25)-Mo(8)-O(31)	86.50(14)	O(26)-Mo(11)-O(19)	76.75(13)
O(33)-Mo(8)-O(26)	104.5(2)	O(27)-Mo(11)-O(19)	76.54(11)
O(22)-Mo(8)-O(26)	87.05(15)	O(35)-Mo(10)-O(21)	104.76(16)
O(25)-Mo(8)-O(26)	152.45(14)	O(35)-Mo(10)-O(27)	102.97(16)
O(31)-Mo(8)-O(26)	85.82(14)	O(21)-Mo(10)-O(27)	87.73(14)
O(33)-Mo(8)-O(19)	179.02(19)	O(35)-Mo(10)-O(29)	101.87(16)
O(22)-Mo(8)-O(19)	76.42(12)	O(21)-Mo(10)-O(29)	153.34(13)
O(25)-Mo(8)-O(19)	76.21(11)	O(27)-Mo(10)-O(29)	87.42(13)
O(31)-Mo(8)-O(19)	76.81(12)	O(35)-Mo(10)-O(24)	103.97(16)
O(26)-Mo(8)-O(19)	76.29(12)	O(21)-Mo(10)-O(24)	86.80(13)
O(36)-Mo(12)-O(20)	104.65(16)	O(27)-Mo(10)-O(24)	153.03(13)
O(36)-Mo(12)-O(24)	104.03(17)	O(29)-Mo(10)-O(24)	85.74(13)
O(20)-Mo(12)-O(24)	88.61(14)	O(35)-Mo(10)-O(19)	178.44(15)
O(36)-Mo(12)-O(25)	103.28(17)	O(21)-Mo(10)-O(19)	76.79(11)
O(20)-Mo(12)-O(25)	88.29(14)	O(27)-Mo(10)-O(19)	76.82(11)

O(24)-Mo(12)-O(25)	152.40(13)	O(29)-Mo(10)-O(19)	76.58(11)
O(36)-Mo(12)-O(30)	102.36(15)	O(24)-Mo(10)-O(19)	76.21(11)
O(20)-Mo(12)-O(30)	152.97(13)	O(34)-Mo(9)-O(30)	104.00(15)
O(24)-Mo(12)-O(30)	85.97(13)	O(34)-Mo(9)-O(31)	103.14(16)
O(25)-Mo(12)-O(30)	84.45(14)	O(30)-Mo(9)-O(31)	88.13(15)
O(36)-Mo(12)-O(19)	178.27(15)	O(34)-Mo(9)-O(29)	103.38(15)
O(20)-Mo(12)-O(19)	76.88(12)	O(30)-Mo(9)-O(29)	88.29(14)
O(24)-Mo(12)-O(19)	76.72(11)	O(31)-Mo(9)-O(29)	153.32(13)
O(25)-Mo(12)-O(19)	75.87(12)	O(34)-Mo(9)-O(28)	102.57(14)
O(30)-Mo(12)-O(19)	76.10(11)	C(18)-C(17)-H(17A)	108.1
O(30)-Mo(9)-O(28)	153.43(13)	N(3)-C(17)-H(17A)	108.1
O(31)-Mo(9)-O(28)	85.76(14)	C(18)-C(17)-H(17B)	108.1
O(29)-Mo(9)-O(28)	85.72(13)	N(3)-C(17)-H(17B)	108.1
O(34)-Mo(9)-O(19)	178.61(13)	H(17A)-C(17)-H(17B)	107.3
O(30)-Mo(9)-O(19)	77.39(12)	C(19)-C(18)-C(17)	114.0(5)
O(31)-Mo(9)-O(19)	76.89(12)	C(19)-C(18)-H(18A)	108.8
O(29)-Mo(9)-O(19)	76.53(11)	C(17)-C(18)-H(18A)	108.8
O(28)-Mo(9)-O(19)	76.04(11)	C(19)-C(18)-H(18B)	108.8
C(9)-N(2)-Mo(7)	170.8(4)	C(17)-C(18)-H(18B)	108.8
Mo(7)-O(19)-Mo(11)	90.64(10)	H(18A)-C(18)-H(18B)	107.6
Mo(7)-O(19)-Mo(10)	90.51(10)	C(20)-C(19)-C(18)	113.0(5)
Mo(11)-O(19)-Mo(10)	89.88(9)	C(20)-C(19)-H(19A)	109.0
Mo(7)-O(19)-Mo(8)	90.75(10)	C(18)-C(19)-H(19A)	109.0
Mo(11)-O(19)-Mo(8)	89.96(10)	C(20)-C(19)-H(19B)	109.0
Mo(10)-O(19)-Mo(8)	178.73(14)	C(18)-C(19)-H(19B)	109.0
Mo(7)-O(19)-Mo(12)	90.49(10)	H(19A)-C(19)-H(19B)	107.8
Mo(11)-O(19)-Mo(12)	178.87(14)	C(19)-C(20)-H(20A)	109.5
Mo(10)-O(19)-Mo(12)	90.03(10)	C(19)-C(20)-H(20B)	109.5
Mo(8)-O(19)-Mo(12)	90.11(9)	H(20A)-C(20)-H(20B)	109.5
Mo(7)-O(19)-Mo(9)	179.62(14)	C(19)-C(20)-H(20C)	109.5
Mo(11)-O(19)-Mo(9)	89.72(10)	H(20A)-C(20)-H(20C)	109.5
Mo(10)-O(19)-Mo(9)	89.60(10)	H(20B)-C(20)-H(20C)	109.5
Mo(8)-O(19)-Mo(9)	89.14(9)	C(22)-C(21)-N(3)	116.2(4)
Mo(12)-O(19)-Mo(9)	89.15(9)	C(22)-C(21)-H(21A)	108.2
Mo(10)-O(21)-Mo(7)	114.15(15)	N(3)-C(21)-H(21A)	108.2
Mo(8)-O(22)-Mo(7)	114.56(16)	C(22)-C(21)-H(21B)	108.2

Mo(9)-O(31)-Mo(8)	117.12(16)	N(3)-C(21)-H(21B)	108.2
Mo(9)-O(29)-Mo(10)	117.27(15)	H(21A)-C(21)-H(21B)	107.4
Mo(12)-O(20)-Mo(7)	114.63(15)	C(21)-C(22)-C(23)	110.3(4)
Mo(12)-O(24)-Mo(10)	117.01(15)	C(21)-C(22)-H(22A)	109.6
Mo(9)-O(30)-Mo(12)	117.36(15)	C(23)-C(22)-H(22A)	109.6
Mo(8)-O(25)-Mo(12)	117.79(15)	C(21)-C(22)-H(22B)	109.6
Mo(11)-O(23)-Mo(7)	114.51(15)	C(23)-C(22)-H(22B)	109.6
Mo(11)-O(26)-Mo(8)	117.00(17)	H(22A)-C(22)-H(22B)	108.1
Mo(11)-O(28)-Mo(9)	116.81(15)	C(24)-C(23)-C(22)	112.6(5)
Mo(10)-O(27)-Mo(11)	116.71(14)	C(24)-C(23)-H(23A)	109.1
C(18)-C(17)-N(3)	116.9(4)	N(3)-C(29)-H(29B)	108.2
C(22)-C(23)-H(23A)	109.1	C(30)-C(29)-H(29B)	108.2
C(24)-C(23)-H(23B)	109.1	H(29A)-C(29)-H(29B)	107.4
C(22)-C(23)-H(23B)	109.1	C(31)-C(30)-C(29)	108.1(6)
H(23A)-C(23)-H(23B)	107.8	C(31)-C(30)-H(30A)	110.1
C(23)-C(24)-H(24A)	109.5	C(29)-C(30)-H(30A)	110.1
C(23)-C(24)-H(24B)	109.5	C(31)-C(30)-H(30B)	110.1
H(24A)-C(24)-H(24B)	109.5	C(29)-C(30)-H(30B)	110.1
C(23)-C(24)-H(24C)	109.5	H(30A)-C(30)-H(30B)	108.4
H(24A)-C(24)-H(24C)	109.5	C(32)-C(31)-C(30)	127.8(8)
H(24B)-C(24)-H(24C)	109.5	C(32)-C(31)-H(31A)	105.4
C(26)-C(25)-N(3)	117.8(4)	C(30)-C(31)-H(31A)	105.4
C(26)-C(25)-H(25A)	107.9	C(32)-C(31)-H(31B)	105.4
N(3)-C(25)-H(25A)	107.9	C(30)-C(31)-H(31B)	105.4
C(26)-C(25)-H(25B)	107.9	H(31A)-C(31)-H(31B)	106.0
N(3)-C(25)-H(25B)	107.9	C(31)-C(32)-H(32A)	109.5
H(25A)-C(25)-H(25B)	107.2	C(31)-C(32)-H(32B)	109.5
C(25)-C(26)-C(27)	109.1(4)	H(32A)-C(32)-H(32B)	109.5
C(25)-C(26)-H(26A)	109.9	C(31)-C(32)-H(32C)	109.5
C(27)-C(26)-H(26A)	109.9	H(32A)-C(32)-H(32C)	109.5
C(25)-C(26)-H(26B)	109.9	H(32B)-C(32)-H(32C)	109.5
C(27)-C(26)-H(26B)	109.9	C(29)-N(3)-C(25)	108.1(4)
H(26A)-C(26)-H(26B)	108.3	C(29)-N(3)-C(21)	111.0(4)
C(28)-C(27)-C(26)	113.3(5)	C(25)-N(3)-C(21)	108.0(3)
C(28)-C(27)-H(27A)	108.9	C(29)-N(3)-C(17)	111.1(4)
C(26)-C(27)-H(27A)	108.9	C(25)-N(3)-C(17)	110.3(4)

C(28)-C(27)-H(27B)	108.9	C(21)-N(3)-C(17)	108.3(4)
C(26)-C(27)-H(27B)	108.9	N(4)-C(33)-C(34)	116.6(5)
H(27A)-C(27)-H(27B)	107.7	N(4)-C(33)-H(33A)	108.1
C(27)-C(28)-H(28A)	109.5	C(34)-C(33)-H(33A)	108.1
C(27)-C(28)-H(28B)	109.5	N(4)-C(33)-H(33B)	108.1
H(28A)-C(28)-H(28B)	109.5	C(34)-C(33)-H(33B)	108.1
C(27)-C(28)-H(28C)	109.5	H(33A)-C(33)-H(33B)	107.3
H(28A)-C(28)-H(28C)	109.5	C(35)-C(34)-C(33)	111.3(6)
H(28B)-C(28)-H(28C)	109.5	C(35)-C(34)-H(34A)	109.4
N(3)-C(29)-C(30)	116.2(5)	C(33)-C(34)-H(34A)	109.4
N(3)-C(29)-H(29A)	108.2	C(35)-C(34)-H(34B)	109.4
C(30)-C(29)-H(29A)	108.2	H(40B)-C(40)-H(40C)	109.5
C(33)-C(34)-H(34B)	109.4	N(4)-C(41)-C(42)	114.9(5)
H(34A)-C(34)-H(34B)	108.0	N(4)-C(41)-H(41A)	108.5
C(36)-C(35)-C(34)	120.4(8)	C(42)-C(41)-H(41A)	108.5
C(36)-C(35)-H(35A)	107.2	N(4)-C(41)-H(41B)	108.5
C(34)-C(35)-H(35A)	107.2	C(42)-C(41)-H(41B)	108.5
C(36)-C(35)-H(35B)	107.2	H(41A)-C(41)-H(41B)	107.5
C(34)-C(35)-H(35B)	107.2	C(43)-C(42)-C(41)	109.8(6)
H(35A)-C(35)-H(35B)	106.8	C(43)-C(42)-H(42A)	109.7
C(35)-C(36)-H(36A)	109.5	C(41)-C(42)-H(42A)	109.7
C(35)-C(36)-H(36B)	109.5	C(43)-C(42)-H(42B)	109.7
H(36A)-C(36)-H(36B)	109.5	C(41)-C(42)-H(42B)	109.7
C(35)-C(36)-H(36C)	109.5	H(42A)-C(42)-H(42B)	108.2
H(36A)-C(36)-H(36C)	109.5	C(44)-C(43)-C(42)	116.8(8)
H(36B)-C(36)-H(36C)	109.5	C(44)-C(43)-H(43A)	108.1
C(38)-C(37)-N(4)	118.3(5)	C(42)-C(43)-H(43A)	108.1
C(38)-C(37)-H(37A)	107.7	C(44)-C(43)-H(43B)	108.1
N(4)-C(37)-H(37A)	107.7	C(42)-C(43)-H(43B)	108.1
C(38)-C(37)-H(37B)	107.7	H(43A)-C(43)-H(43B)	107.3
N(4)-C(37)-H(37B)	107.7	C(43)-C(44)-H(44A)	109.5
H(37A)-C(37)-H(37B)	107.1	C(43)-C(44)-H(44B)	109.5
C(37)-C(38)-C(39)	106.6(6)	H(44A)-C(44)-H(44B)	109.5
C(37)-C(38)-H(38A)	110.4	C(43)-C(44)-H(44C)	109.5
C(39)-C(38)-H(38A)	110.4	H(44A)-C(44)-H(44C)	109.5
C(37)-C(38)-H(38B)	110.4	H(44B)-C(44)-H(44C)	109.5

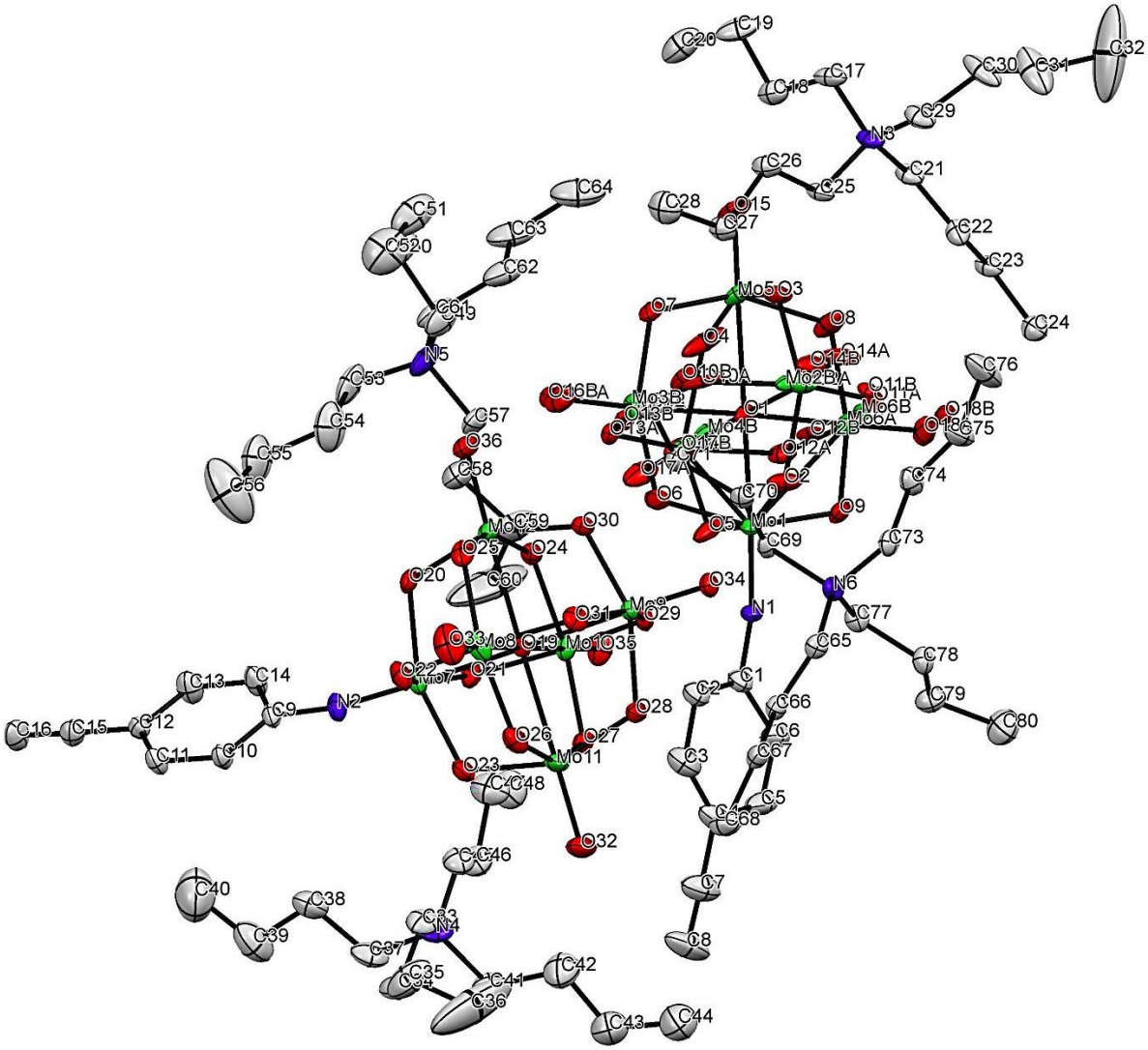
C(39)-C(38)-H(38B)	110.4	C(46)-C(45)-N(4)	115.1(5)
H(38A)-C(38)-H(38B)	108.6	C(46)-C(45)-H(45A)	108.5
C(40)-C(39)-C(38)	113.4(8)	N(4)-C(45)-H(45A)	108.5
C(40)-C(39)-H(39A)	108.9	C(46)-C(45)-H(45B)	108.5
C(38)-C(39)-H(39A)	108.9	N(4)-C(45)-H(45B)	108.5
C(40)-C(39)-H(39B)	108.9	H(45A)-C(45)-H(45B)	107.5
C(38)-C(39)-H(39B)	108.9	C(47)-C(46)-C(45)	111.4(5)
H(39A)-C(39)-H(39B)	107.7	C(47)-C(46)-H(46A)	109.3
C(39)-C(40)-H(40A)	109.5	C(45)-C(46)-H(46A)	109.3
C(39)-C(40)-H(40B)	109.5	C(47)-C(46)-H(46B)	109.3
H(40A)-C(40)-H(40B)	109.5	C(45)-C(46)-H(46B)	109.3
C(39)-C(40)-H(40C)	109.5	H(46A)-C(46)-H(46B)	108.0
H(40A)-C(40)-H(40C)	109.5	C(51)-C(52)-H(52B)	109.5
C(46)-C(47)-C(48)	111.1(6)	H(52A)-C(52)-H(52B)	109.5
C(46)-C(47)-H(47A)	109.4	C(51)-C(52)-H(52C)	109.5
C(48)-C(47)-H(47A)	109.4	H(52A)-C(52)-H(52C)	109.5
C(46)-C(47)-H(47B)	109.4	H(52B)-C(52)-H(52C)	109.5
C(48)-C(47)-H(47B)	109.4	C(54)-C(53)-N(5)	114.2(5)
H(47A)-C(47)-H(47B)	108.0	C(54)-C(53)-H(53A)	108.7
C(47)-C(48)-H(48A)	109.5	N(5)-C(53)-H(53A)	108.7
C(47)-C(48)-H(48B)	109.5	C(54)-C(53)-H(53B)	108.7
H(48A)-C(48)-H(48B)	109.5	N(5)-C(53)-H(53B)	108.7
C(47)-C(48)-H(48C)	109.5	H(53A)-C(53)-H(53B)	107.6
H(48A)-C(48)-H(48C)	109.5	C(53)-C(54)-C(55)	114.1(6)
H(48B)-C(48)-H(48C)	109.5	C(53)-C(54)-H(54A)	108.7
C(41)-N(4)-C(33)	111.0(5)	C(55)-C(54)-H(54A)	108.7
C(41)-N(4)-C(45)	111.0(5)	C(53)-C(54)-H(54B)	108.7
C(33)-N(4)-C(45)	107.8(4)	C(55)-C(54)-H(54B)	108.7
C(41)-N(4)-C(37)	106.7(4)	H(54A)-C(54)-H(54B)	107.6
C(33)-N(4)-C(37)	111.2(5)	C(56)-C(55)-C(54)	117.0(8)
C(45)-N(4)-C(37)	109.1(5)	C(56)-C(55)-H(55A)	108.0
N(5)-C(49)-C(50)	113.7(5)	C(54)-C(55)-H(55A)	108.0
N(5)-C(49)-H(49A)	108.8	C(56)-C(55)-H(55B)	108.0
C(50)-C(49)-H(49A)	108.8	C(54)-C(55)-H(55B)	108.0
N(5)-C(49)-H(49B)	108.8	H(55A)-C(55)-H(55B)	107.3
C(50)-C(49)-H(49B)	108.8	C(55)-C(56)-H(56A)	109.5

H(49A)-C(49)-H(49B)	107.7	C(55)-C(56)-H(56B)	109.5
C(51)-C(50)-C(49)	111.9(6)	H(56A)-C(56)-H(56B)	109.5
C(51)-C(50)-H(50A)	109.2	C(55)-C(56)-H(56C)	109.5
C(49)-C(50)-H(50A)	109.2	H(56A)-C(56)-H(56C)	109.5
C(51)-C(50)-H(50B)	109.2	H(56B)-C(56)-H(56C)	109.5
C(49)-C(50)-H(50B)	109.2	N(5)-C(57)-C(58)	115.3(5)
H(50A)-C(50)-H(50B)	107.9	N(5)-C(57)-H(57A)	108.4
C(52)-C(51)-C(50)	112.7(9)	C(58)-C(57)-H(57A)	108.4
C(52)-C(51)-H(51A)	109.0	N(5)-C(57)-H(57B)	108.4
C(50)-C(51)-H(51A)	109.0	C(58)-C(57)-H(57B)	108.4
C(52)-C(51)-H(51B)	109.0	H(57A)-C(57)-H(57B)	107.5
C(50)-C(51)-H(51B)	109.0	C(59)-C(58)-C(57)	114.2(6)
H(51A)-C(51)-H(51B)	107.8	C(59)-C(58)-H(58A)	108.7
C(51)-C(52)-H(52A)	109.5	C(63)-C(64)-H(64C)	109.5
C(57)-C(58)-H(58A)	108.7	H(64A)-C(64)-H(64C)	109.5
C(59)-C(58)-H(58B)	108.7	H(64B)-C(64)-H(64C)	109.5
C(57)-C(58)-H(58B)	108.7	C(53)-N(5)-C(57)	111.3(5)
H(58A)-C(58)-H(58B)	107.6	C(53)-N(5)-C(61)	108.5(5)
C(58)-C(59)-C(60)	109.9(9)	C(57)-N(5)-C(61)	109.2(5)
C(58)-C(59)-H(59A)	109.7	C(53)-N(5)-C(49)	110.8(5)
C(60)-C(59)-H(59A)	109.7	C(57)-N(5)-C(49)	108.3(4)
C(58)-C(59)-H(59B)	109.7	C(61)-N(5)-C(49)	108.7(5)
C(60)-C(59)-H(59B)	109.7	C(66)-C(65)-N(6)	116.0(3)
H(59A)-C(59)-H(59B)	108.2	C(66)-C(65)-H(65A)	108.3
C(59)-C(60)-H(60A)	109.5	N(6)-C(65)-H(65A)	108.3
C(59)-C(60)-H(60B)	109.5	C(66)-C(65)-H(65B)	108.3
H(60A)-C(60)-H(60B)	109.5	N(6)-C(65)-H(65B)	108.3
C(59)-C(60)-H(60C)	109.5	H(65A)-C(65)-H(65B)	107.4
H(60A)-C(60)-H(60C)	109.5	C(65)-C(66)-C(67)	109.3(4)
H(60B)-C(60)-H(60C)	109.5	C(65)-C(66)-H(66A)	109.8
C(62)-C(61)-N(5)	116.8(5)	C(67)-C(66)-H(66A)	109.8
C(62)-C(61)-H(61A)	108.1	C(65)-C(66)-H(66B)	109.8
N(5)-C(61)-H(61A)	108.1	C(67)-C(66)-H(66B)	109.8
C(62)-C(61)-H(61B)	108.1	H(66A)-C(66)-H(66B)	108.3
N(5)-C(61)-H(61B)	108.1	C(68)-C(67)-C(66)	112.0(4)
H(61A)-C(61)-H(61B)	107.3	C(68)-C(67)-H(67A)	109.2

C(63)-C(62)-C(61)	111.6(6)	C(66)-C(67)-H(67A)	109.2
C(63)-C(62)-H(62A)	109.3	C(68)-C(67)-H(67B)	109.2
C(61)-C(62)-H(62A)	109.3	C(66)-C(67)-H(67B)	109.2
C(63)-C(62)-H(62B)	109.3	H(67A)-C(67)-H(67B)	107.9
C(61)-C(62)-H(62B)	109.3	C(67)-C(68)-H(68A)	109.5
H(62A)-C(62)-H(62B)	108.0	C(67)-C(68)-H(68B)	109.5
C(62)-C(63)-C(64)	113.3(8)	H(68A)-C(68)-H(68B)	109.5
C(62)-C(63)-H(63A)	108.9	C(67)-C(68)-H(68C)	109.5
C(64)-C(63)-H(63A)	108.9	H(68A)-C(68)-H(68C)	109.5
C(62)-C(63)-H(63B)	108.9	H(68B)-C(68)-H(68C)	109.5
C(64)-C(63)-H(63B)	108.9	C(70)-C(69)-N(6)	117.4(4)
H(63A)-C(63)-H(63B)	107.7	C(70)-C(69)-H(69A)	108.0
C(63)-C(64)-H(64A)	109.5	N(6)-C(69)-H(69A)	108.0
C(63)-C(64)-H(64B)	109.5	C(70)-C(69)-H(69B)	108.0
H(64A)-C(64)-H(64B)	109.5	H(75A)-C(75)-H(75B)	107.8
N(6)-C(69)-H(69B)	108.0	C(75)-C(76)-H(76A)	109.5
H(69A)-C(69)-H(69B)	107.2	C(75)-C(76)-H(76B)	109.5
C(69)-C(70)-C(71)	109.9(4)	H(76A)-C(76)-H(76B)	109.5
C(69)-C(70)-H(70A)	109.7	C(75)-C(76)-H(76C)	109.5
C(71)-C(70)-H(70A)	109.7	H(76A)-C(76)-H(76C)	109.5
C(69)-C(70)-H(70B)	109.7	H(76B)-C(76)-H(76C)	109.5
C(71)-C(70)-H(70B)	109.7	C(78)-C(77)-N(6)	115.6(4)
H(70A)-C(70)-H(70B)	108.2	C(78)-C(77)-H(77A)	108.4
C(70)-C(71)-C(72)	113.3(4)	N(6)-C(77)-H(77A)	108.4
C(70)-C(71)-H(71A)	108.9	C(78)-C(77)-H(77B)	108.4
C(72)-C(71)-H(71A)	108.9	N(6)-C(77)-H(77B)	108.4
C(70)-C(71)-H(71B)	108.9	H(77A)-C(77)-H(77B)	107.5
C(72)-C(71)-H(71B)	108.9	C(77)-C(78)-C(79)	108.3(4)
H(71A)-C(71)-H(71B)	107.7	C(77)-C(78)-H(78A)	110.0
C(71)-C(72)-H(72A)	109.5	C(79)-C(78)-H(78A)	110.0
C(71)-C(72)-H(72B)	109.5	C(77)-C(78)-H(78B)	110.0
H(72A)-C(72)-H(72B)	109.5	C(79)-C(78)-H(78B)	110.0
C(71)-C(72)-H(72C)	109.5	H(78A)-C(78)-H(78B)	108.4
H(72A)-C(72)-H(72C)	109.5	C(80)-C(79)-C(78)	111.5(5)
H(72B)-C(72)-H(72C)	109.5	C(80)-C(79)-H(79A)	109.3
N(6)-C(73)-C(74)	115.5(4)	C(78)-C(79)-H(79A)	109.3

N(6)-C(73)-H(73A)	108.4	C(80)-C(79)-H(79B)	109.3
C(74)-C(73)-H(73A)	108.4	C(78)-C(79)-H(79B)	109.3
N(6)-C(73)-H(73B)	108.4	H(79A)-C(79)-H(79B)	108.0
C(74)-C(73)-H(73B)	108.4	C(79)-C(80)-H(80A)	109.5
H(73A)-C(73)-H(73B)	107.5	C(79)-C(80)-H(80B)	109.5
C(75)-C(74)-C(73)	110.4(4)	H(80A)-C(80)-H(80B)	109.5
C(75)-C(74)-H(74A)	109.6	C(79)-C(80)-H(80C)	109.5
C(73)-C(74)-H(74A)	109.6	H(80A)-C(80)-H(80C)	109.5
C(75)-C(74)-H(74B)	109.6	H(80B)-C(80)-H(80C)	109.5
C(73)-C(74)-H(74B)	109.6	C(73)-N(6)-C(77)	111.7(4)
H(74A)-C(74)-H(74B)	108.1	C(73)-N(6)-C(65)	107.1(3)
C(74)-C(75)-C(76)	112.7(5)	C(77)-N(6)-C(65)	111.4(3)
C(74)-C(75)-H(75A)	109.0	C(73)-N(6)-C(69)	110.5(3)
C(76)-C(75)-H(75A)	109.0	C(77)-N(6)-C(69)	106.5(3)
C(74)-C(75)-H(75B)	109.0	C(65)-N(6)-C(69)	109.6(3)
C(76)-C(75)-H(75B)	109.0		

ORTEP-5 representation of compound **6**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity.



Compound 8

Crystal growth Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method Oil

Crystal Data

Chemical formula	$C_{47}H_{82.50}Mo_6N_4O_{20.25}$	
Formula weight	1603.31 g mol^{-1}	
Temperature	100 (2) K	
Crystal size	0.150 x 0.090 x 0.040 mm^3	
Crystal description	Red-orange block	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 11.4858(3) Å	α = 90°.
	b = 38.1339(10) Å	β = 94.4450(10)°.
	c = 14.2817(5) Å	γ = 100.8150(10)°.
	Volume	6252.8(3) $Å^3$
Z	4	
F(000)	2936	
Density (calculated)	1.703 Mg cm^{-3}	
Absorption coefficient	1.236 mm^{-1}	

Data Collection

Diffractometer	Rigaku AFC 12 goniometer
Radiation	Mo-*Kα*
2θ range for data collection	2.136 – 27.499°.
Reflections collected	86181
Independent reflections	14275 [R(int) = 0.0724]
Transmission coefficients	1.000
Data corrections	Gaussian
Index ranges	-14<=h<=14, -49<=k<=49, -18<=l<=18

Refinement method

Full-matrix least squares on F^2		
Weighting scheme	$w = [\sigma^2(F_o^2) + (0.0085P)^2 + 76.1899P]^{-1}$	
	$P = [\max(I_{obs}, 0) + 2F_c^2]/3$	
Data / restraints / parameters	14275 / 8 / 758	
Data to parameter ratio	18.83	
Goodness of fit on F^2	1.204	
R indices	$[I_o>2\sigma>(I_o)]$ data	R1 = 0.0707, wR2 = 0.1380
	All 2558 data	R1 = 0.0779, wR2 = 0.1405
Final difference map	Largest diff. peak +1.361 and hole -1.655e.$Å^{-3}$	

Bond lengths [Å] and angles [^{o}]

Mo(1)-O(14)	1.701(5)	C(5)-C(6)	1.388(10)
Mo(1)-O(8)	1.848(5)	C(5)-H(5)	0.9500
Mo(1)-O(17)	1.874(5)	C(6)-H(6)	0.9500
Mo(1)-O(12)	1.965(5)	C(7)-C(8)	1.160(12)
Mo(1)-O(6)	2.068(5)	C(8)-C(9)	1.450(12)
Mo(1)-O(1)	2.361(4)	C(9)-C(11)	1.413(13)
Mo(2)-O(4)	1.705(5)	C(9)-C(10)	1.416(11)
Mo(2)-O(6)	1.849(5)	C(10)-C(12)	1.374(12)
Mo(2)-O(13)	1.871(4)	C(10)-H(10)	0.9500
Mo(2)-O(16)	1.976(4)	C(11)-C(13)	1.373(14)
Mo(2)-O(10)	2.050(5)	C(11)-H(11)	0.9500
Mo(2)-O(1)	2.362(4)	C(12)-C(14)	1.372(13)
Mo(3)-O(2)	1.690(5)	C(12)-H(12)	0.9500
Mo(3)-O(15)	1.851(5)	C(13)-C(14)	1.404(13)
Mo(3)-O(10)	1.861(5)	C(13)-H(13)	0.9500
Mo(3)-O(5)	1.987(5)	C(14)-N(2)	1.489(12)
Mo(3)-O(11)	2.065(5)	N(2)-O(20)	1.216(11)
Mo(3)-O(1)	2.350(4)	N(2)-O(19A)	1.26(3)
Mo(4)-O(7)	1.698(5)	N(2)-O(19B)	1.29(4)
Mo(4)-O(11)	1.852(5)	N(3)-C(19)	1.517(9)
Mo(4)-O(18)	1.889(5)	N(3)-C(23)	1.524(9)
Mo(4)-O(3)	1.948(5)	N(3)-C(27B)	1.526(9)
Mo(4)-O(8)	2.052(5)	N(3)-C(27A)	1.526(9)
Mo(4)-O(1)	2.367(4)	N(3)-C(15)	1.532(9)
Mo(5)-O(9)	1.689(5)	C(15)-C(16)	1.516(10)
Mo(5)-O(5)	1.861(5)	C(15)-H(15A)	0.9900
Mo(5)-O(16)	1.888(5)	C(15)-H(15B)	0.9900
Mo(5)-O(17)	1.984(5)	C(16)-C(17)	1.547(10)
Mo(5)-O(18)	1.997(5)	C(16)-H(16A)	0.9900
Mo(5)-O(1)	2.352(4)	C(16)-H(16B)	0.9900
Mo(6)-N(1)	1.745(6)	C(17)-C(18)	1.525(11)
Mo(6)-O(12)	1.885(5)	C(17)-H(17A)	0.9900
Mo(6)-O(3)	1.919(5)	C(17)-H(17B)	0.9900
Mo(6)-O(13)	2.026(5)	C(18)-H(18A)	0.9800

Mo(6)-O(15)	2.032(5)	C(18)-H(18B)	0.9800
Mo(6)-O(1)	2.188(4)	C(18)-H(18C)	0.9800
N(1)-C(1)	1.381(9)	C(19)-C(20)	1.523(10)
C(1)-C(2)	1.408(11)	C(19)-H(19A)	0.9900
C(1)-C(6)	1.412(10)	C(19)-H(19B)	0.9900
C(2)-C(3)	1.369(11)	C(20)-C(21)	1.527(10)
C(2)-H(2)	0.9500	C(20)-H(20A)	0.9900
C(3)-C(4)	1.406(11)	C(20)-H(20B)	0.9900
C(3)-H(3)	0.9500	C(21)-C(22)	1.510(11)
C(4)-C(5)	1.405(11)	C(21)-H(21A)	0.9900
C(4)-C(7)	1.457(11)	C(21)-H(21B)	0.9900
C(23)-C(24)	1.523(10)	C(33)-H(33A)	0.9900
C(23)-H(23A)	0.9900	C(33)-H(33B)	0.9900
C(23)-H(23B)	0.9900	C(34)-H(34A)	0.9800
C(24)-C(25)	1.528(10)	C(34)-H(34B)	0.9800
C(24)-H(24A)	0.9900	C(34)-H(34C)	0.9800
C(24)-H(24B)	0.9900	C(35)-C(36)	1.521(12)
C(25)-C(26)	1.530(11)	C(35)-H(35A)	0.9900
C(25)-H(25A)	0.9900	C(35)-H(35B)	0.9900
C(25)-H(25B)	0.9900	C(36)-C(37)	1.535(12)
C(26)-H(26A)	0.9800	C(36)-H(36A)	0.9900
C(26)-H(26B)	0.9800	C(36)-H(36B)	0.9900
C(26)-H(26C)	0.9800	C(37)-C(38)	1.516(13)
C(27A)-C(28A)	1.517(11)	C(37)-H(37A)	0.9900
C(27A)-H(27A)	0.9900	C(37)-H(37B)	0.9900
C(27A)-H(27B)	0.9900	C(38)-H(38A)	0.9800
C(28A)-C(29A)	1.497(13)	C(38)-H(38B)	0.9800
C(28A)-H(28A)	0.9900	C(38)-H(38C)	0.9800
C(28A)-H(28B)	0.9900	C(39A)-C(40A)	1.507(13)
C(29A)-C(30A)	1.485(9)	C(39A)-H(39A)	0.9900
C(29A)-H(29A)	0.9900	C(39A)-H(39B)	0.9900
C(29A)-H(29B)	0.9900	C(40A)-C(41A)	1.518(9)
C(30A)-H(30A)	0.9800	C(40A)-H(40A)	0.9900
C(30A)-H(30B)	0.9800	C(40A)-H(40B)	0.9900
C(30A)-H(30C)	0.9800	C(41A)-C(42A)	1.502(9)
C(27B)-C(28B)	1.517(11)	C(41A)-H(41A)	0.9900

C(27B)-H(27C)	0.9900	C(41A)-H(41B)	0.9900
C(27B)-H(27D)	0.9900	C(42A)-H(42A)	0.9800
C(28B)-C(29B)	1.497(13)	C(42A)-H(42B)	0.9800
C(28B)-H(28C)	0.9900	C(42A)-H(42C)	0.9800
C(28B)-H(28D)	0.9900	C(39B)-C(40B)	1.507(13)
C(29B)-C(30B)	1.485(10)	C(39B)-H(39C)	0.9900
C(29B)-H(29C)	0.9900	C(39B)-H(39D)	0.9900
C(29B)-H(29D)	0.9900	C(40B)-C(41B)	1.500(9)
C(30B)-H(30D)	0.9800	C(40B)-H(40C)	0.9900
C(30B)-H(30E)	0.9800	C(40B)-H(40D)	0.9900
C(30B)-H(30F)	0.9800	C(41B)-C(42B)	1.494(10)
N(4)-C(31)	1.512(9)	C(41B)-H(41C)	0.9900
N(4)-C(43)	1.521(11)	C(41B)-H(41D)	0.9900
N(4)-C(39B)	1.526(10)	C(42B)-H(42D)	0.9800
N(4)-C(39A)	1.526(10)	C(42B)-H(42E)	0.9800
N(4)-C(35)	1.532(9)	C(42B)-H(42F)	0.9800
C(31)-C(32)	1.517(10)	C(43)-C(44)	1.528(11)
C(31)-H(31A)	0.9900	C(43)-H(43A)	0.9900
C(31)-H(31B)	0.9900	C(43)-H(43B)	0.9900
C(32)-C(33)	1.531(10)	C(44)-C(45)	1.528(14)
C(32)-H(32A)	0.9900	C(44)-H(44A)	0.9900
C(32)-H(32B)	0.9900	C(44)-H(44B)	0.9900
C(33)-C(34)	1.518(12)	C(45)-C(46)	1.547(13)
C(45)-H(45A)	0.9900	O(10)-Mo(2)-O(1)	74.80(17)
C(45)-H(45B)	0.9900	O(2)-Mo(3)-O(15)	105.2(2)
C(46)-H(46A)	0.9800	O(2)-Mo(3)-O(10)	105.1(2)
C(46)-H(46B)	0.9800	O(15)-Mo(3)-O(10)	94.2(2)
C(46)-H(46C)	0.9800	O(2)-Mo(3)-O(5)	101.8(2)
O(21)-C(47)	1.36(4)	O(15)-Mo(3)-O(5)	151.2(2)
O(21)-C(49)	1.37(3)	O(10)-Mo(3)-O(5)	88.15(19)
C(47)-C(48)	1.45(4)	O(2)-Mo(3)-O(11)	101.7(2)
C(47)-H(47A)	0.9900	O(15)-Mo(3)-O(11)	85.0(2)
C(47)-H(47B)	0.9900	O(10)-Mo(3)-O(11)	152.43(19)
C(48)-H(48A)	0.9800	O(5)-Mo(3)-O(11)	79.97(19)
C(48)-H(48B)	0.9800	O(2)-Mo(3)-O(1)	175.6(2)
C(48)-H(48C)	0.9800	O(15)-Mo(3)-O(1)	76.82(18)

C(49)-C(50)	1.505(10)	O(10)-Mo(3)-O(1)	78.50(18)
C(49)-H(49A)	0.9900	O(5)-Mo(3)-O(1)	75.55(17)
C(49)-H(49B)	0.9900	O(11)-Mo(3)-O(1)	74.48(16)
C(50)-H(50A)	0.9800	O(7)-Mo(4)-O(11)	105.6(2)
C(50)-H(50B)	0.9800	O(7)-Mo(4)-O(18)	104.2(2)
C(50)-H(50C)	0.9800	O(11)-Mo(4)-O(18)	92.0(2)
O(14)-Mo(1)-O(8)	104.8(2)	O(7)-Mo(4)-O(3)	103.3(2)
O(14)-Mo(1)-O(17)	105.3(3)	O(11)-Mo(4)-O(3)	89.4(2)
O(8)-Mo(1)-O(17)	93.8(2)	O(18)-Mo(4)-O(3)	151.03(19)
O(14)-Mo(1)-O(12)	102.5(3)	O(7)-Mo(4)-O(8)	101.4(2)
O(8)-Mo(1)-O(12)	89.3(2)	O(11)-Mo(4)-O(8)	152.8(2)
O(17)-Mo(1)-O(12)	150.2(2)	O(18)-Mo(4)-O(8)	83.8(2)
O(14)-Mo(1)-O(6)	102.2(2)	O(3)-Mo(4)-O(8)	81.8(2)
O(8)-Mo(1)-O(6)	152.63(19)	O(7)-Mo(4)-O(1)	176.2(2)
O(17)-Mo(1)-O(6)	83.4(2)	O(11)-Mo(4)-O(1)	77.85(18)
O(12)-Mo(1)-O(6)	80.37(19)	O(18)-Mo(4)-O(1)	77.14(17)
O(14)-Mo(1)-O(1)	175.4(2)	O(3)-Mo(4)-O(1)	74.92(17)
O(8)-Mo(1)-O(1)	78.87(18)	O(8)-Mo(4)-O(1)	75.03(17)
O(17)-Mo(1)-O(1)	77.05(18)	O(9)-Mo(5)-O(5)	104.9(2)
O(12)-Mo(1)-O(1)	74.49(17)	O(9)-Mo(5)-O(16)	103.6(2)
O(6)-Mo(1)-O(1)	73.96(16)	O(5)-Mo(5)-O(16)	91.4(2)
O(4)-Mo(2)-O(6)	105.5(2)	O(9)-Mo(5)-O(17)	101.9(2)
O(4)-Mo(2)-O(13)	104.1(2)	O(5)-Mo(5)-O(17)	152.8(2)
O(6)-Mo(2)-O(13)	93.6(2)	O(16)-Mo(5)-O(17)	86.6(2)
O(4)-Mo(2)-O(16)	102.4(2)	O(9)-Mo(5)-O(18)	102.7(2)
O(6)-Mo(2)-O(16)	88.9(2)	O(5)-Mo(5)-O(18)	87.4(2)
O(13)-Mo(2)-O(16)	151.62(19)	O(16)-Mo(5)-O(18)	153.1(2)
O(4)-Mo(2)-O(10)	101.8(2)	O(17)-Mo(5)-O(18)	82.37(19)
O(6)-Mo(2)-O(10)	152.24(19)	O(9)-Mo(5)-O(1)	176.9(2)
O(13)-Mo(2)-O(10)	84.51(19)	O(5)-Mo(5)-O(1)	77.76(18)
O(16)-Mo(2)-O(10)	80.39(19)	O(16)-Mo(5)-O(1)	77.86(17)
O(4)-Mo(2)-O(1)	176.4(2)	O(17)-Mo(5)-O(1)	75.31(17)
O(6)-Mo(2)-O(1)	77.80(17)	O(18)-Mo(5)-O(1)	75.58(17)
O(13)-Mo(2)-O(1)	76.91(18)	N(1)-Mo(6)-O(12)	104.3(3)
O(16)-Mo(2)-O(1)	76.01(17)	N(1)-Mo(6)-O(3)	105.3(2)
O(12)-Mo(6)-O(3)	92.6(2)	C(2)-C(3)-H(3)	120.1

N(1)-Mo(6)-O(13)	96.0(2)	C(4)-C(3)-H(3)	120.1
O(12)-Mo(6)-O(13)	89.0(2)	C(5)-C(4)-C(3)	120.1(7)
O(3)-Mo(6)-O(13)	157.45(19)	C(5)-C(4)-C(7)	118.4(7)
N(1)-Mo(6)-O(15)	97.6(3)	C(3)-C(4)-C(7)	121.4(7)
O(12)-Mo(6)-O(15)	157.4(2)	C(6)-C(5)-C(4)	120.7(7)
O(3)-Mo(6)-O(15)	86.8(2)	C(6)-C(5)-H(5)	119.7
O(13)-Mo(6)-O(15)	83.29(19)	C(4)-C(5)-H(5)	119.7
N(1)-Mo(6)-O(1)	172.6(2)	C(5)-C(6)-C(1)	118.4(7)
O(12)-Mo(6)-O(1)	80.32(19)	C(5)-C(6)-H(6)	120.8
O(3)-Mo(6)-O(1)	79.91(18)	C(1)-C(6)-H(6)	120.8
O(13)-Mo(6)-O(1)	78.18(17)	C(8)-C(7)-C(4)	174.8(10)
O(15)-Mo(6)-O(1)	77.31(17)	C(7)-C(8)-C(9)	173.8(10)
Mo(6)-O(1)-Mo(3)	91.72(16)	C(11)-C(9)-C(10)	119.2(8)
Mo(6)-O(1)-Mo(5)	179.6(2)	C(11)-C(9)-C(8)	118.8(8)
Mo(3)-O(1)-Mo(5)	88.66(15)	C(10)-C(9)-C(8)	122.0(8)
Mo(6)-O(1)-Mo(1)	90.36(16)	C(12)-C(10)-C(9)	120.9(8)
Mo(3)-O(1)-Mo(1)	177.9(2)	C(12)-C(10)-H(10)	119.5
Mo(5)-O(1)-Mo(1)	89.26(15)	C(9)-C(10)-H(10)	119.5
Mo(6)-O(1)-Mo(2)	91.03(16)	C(13)-C(11)-C(9)	120.6(9)
Mo(3)-O(1)-Mo(2)	89.88(15)	C(13)-C(11)-H(11)	119.7
Mo(5)-O(1)-Mo(2)	88.82(15)	C(9)-C(11)-H(11)	119.7
Mo(1)-O(1)-Mo(2)	90.52(15)	C(14)-C(12)-C(10)	117.5(8)
Mo(6)-O(1)-Mo(4)	90.89(16)	C(14)-C(12)-H(12)	121.3
Mo(3)-O(1)-Mo(4)	90.39(15)	C(10)-C(12)-H(12)	121.3
Mo(5)-O(1)-Mo(4)	89.26(15)	C(11)-C(13)-C(14)	117.2(9)
Mo(1)-O(1)-Mo(4)	89.14(15)	C(11)-C(13)-H(13)	121.4
Mo(2)-O(1)-Mo(4)	178.1(2)	C(14)-C(13)-H(13)	121.4
Mo(6)-O(3)-Mo(4)	114.3(2)	C(12)-C(14)-C(13)	124.6(9)
Mo(5)-O(5)-Mo(3)	117.2(2)	C(12)-C(14)-N(2)	118.6(8)
Mo(2)-O(6)-Mo(1)	117.7(2)	C(13)-C(14)-N(2)	116.8(9)
Mo(1)-O(8)-Mo(4)	116.5(2)	O(20)-N(2)-O(19A)	124.1(17)
Mo(3)-O(10)-Mo(2)	116.6(2)	O(20)-N(2)-O(19B)	118(2)
Mo(4)-O(11)-Mo(3)	117.3(2)	O(20)-N(2)-C(14)	117.8(9)
Mo(6)-O(12)-Mo(1)	114.0(2)	O(19A)-N(2)-C(14)	116.5(17)
Mo(2)-O(13)-Mo(6)	112.9(2)	O(19B)-N(2)-C(14)	118(2)
Mo(3)-O(15)-Mo(6)	114.0(2)	C(19)-N(3)-C(23)	110.6(5)

Mo(5)-O(16)-Mo(2)	117.2(2)	C(19)-N(3)-C(27B)	106.7(5)
Mo(1)-O(17)-Mo(5)	118.2(2)	C(23)-N(3)-C(27B)	111.1(5)
Mo(4)-O(18)-Mo(5)	117.1(2)	C(19)-N(3)-C(27A)	106.7(5)
C(1)-N(1)-Mo(6)	163.4(6)	C(23)-N(3)-C(27A)	111.1(5)
N(1)-C(1)-C(2)	119.4(7)	C(19)-N(3)-C(15)	111.0(5)
N(1)-C(1)-C(6)	119.8(7)	C(23)-N(3)-C(15)	106.5(5)
C(2)-C(1)-C(6)	120.7(7)	C(27B)-N(3)-C(15)	111.0(5)
C(3)-C(2)-C(1)	120.2(7)	C(27A)-N(3)-C(15)	111.0(5)
C(3)-C(2)-H(2)	119.9	C(16)-C(15)-N(3)	117.0(6)
C(1)-C(2)-H(2)	119.9	C(16)-C(15)-H(15A)	108.0
C(2)-C(3)-C(4)	119.8(7)	N(3)-C(15)-H(15A)	108.0
C(16)-C(15)-H(15B)	108.0	C(24)-C(23)-H(23B)	108.2
N(3)-C(15)-H(15B)	108.0	N(3)-C(23)-H(23B)	108.2
H(15A)-C(15)-H(15B)	107.3	H(23A)-C(23)-H(23B)	107.3
C(15)-C(16)-C(17)	110.4(6)	C(23)-C(24)-C(25)	109.4(6)
C(15)-C(16)-H(16A)	109.6	C(23)-C(24)-H(24A)	109.8
C(17)-C(16)-H(16A)	109.6	C(25)-C(24)-H(24A)	109.8
C(15)-C(16)-H(16B)	109.6	C(23)-C(24)-H(24B)	109.8
C(17)-C(16)-H(16B)	109.6	C(25)-C(24)-H(24B)	109.8
H(16A)-C(16)-H(16B)	108.1	H(24A)-C(24)-H(24B)	108.2
C(18)-C(17)-C(16)	114.3(7)	C(24)-C(25)-C(26)	111.2(6)
C(18)-C(17)-H(17A)	108.7	C(24)-C(25)-H(25A)	109.4
C(16)-C(17)-H(17A)	108.7	C(26)-C(25)-H(25A)	109.4
C(18)-C(17)-H(17B)	108.7	C(24)-C(25)-H(25B)	109.4
C(16)-C(17)-H(17B)	108.7	C(26)-C(25)-H(25B)	109.4
H(17A)-C(17)-H(17B)	107.6	H(25A)-C(25)-H(25B)	108.0
C(17)-C(18)-H(18A)	109.5	C(25)-C(26)-H(26A)	109.5
C(17)-C(18)-H(18B)	109.5	C(25)-C(26)-H(26B)	109.5
H(18A)-C(18)-H(18B)	109.5	H(26A)-C(26)-H(26B)	109.5
C(17)-C(18)-H(18C)	109.5	C(25)-C(26)-H(26C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(18B)-C(18)-H(18C)	109.5	H(26B)-C(26)-H(26C)	109.5
N(3)-C(19)-C(20)	115.8(5)	C(28A)-C(27A)-N(3)	115.6(6)
N(3)-C(19)-H(19A)	108.3	C(28A)-C(27A)-H(27A)	108.4
C(20)-C(19)-H(19A)	108.3	N(3)-C(27A)-H(27A)	108.4
N(3)-C(19)-H(19B)	108.3	C(28A)-C(27A)-H(27B)	108.4

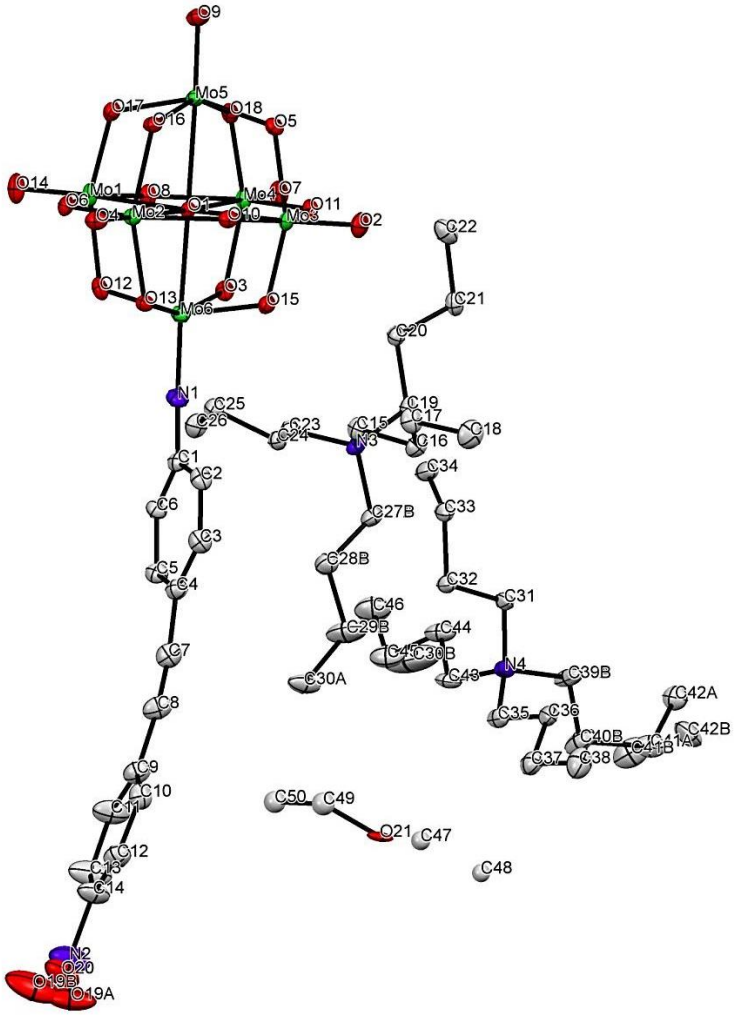
C(20)-C(19)-H(19B)	108.3	N(3)-C(27A)-H(27B)	108.4
H(19A)-C(19)-H(19B)	107.4	H(27A)-C(27A)-H(27B)	107.4
C(19)-C(20)-C(21)	109.7(6)	C(29A)-C(28A)-C(27A)	111.7(7)
C(19)-C(20)-H(20A)	109.7	C(29A)-C(28A)-H(28A)	109.3
C(21)-C(20)-H(20A)	109.7	C(27A)-C(28A)-H(28A)	109.3
C(19)-C(20)-H(20B)	109.7	C(29A)-C(28A)-H(28B)	109.3
C(21)-C(20)-H(20B)	109.7	C(27A)-C(28A)-H(28B)	109.3
H(20A)-C(20)-H(20B)	108.2	H(28A)-C(28A)-H(28B)	107.9
C(22)-C(21)-C(20)	111.2(6)	C(30A)-C(29A)-C(28A)	118.3(11)
C(22)-C(21)-H(21A)	109.4	C(30A)-C(29A)-H(29A)	107.7
C(20)-C(21)-H(21A)	109.4	C(28A)-C(29A)-H(29A)	107.7
C(22)-C(21)-H(21B)	109.4	C(30A)-C(29A)-H(29B)	107.7
C(20)-C(21)-H(21B)	109.4	C(28A)-C(29A)-H(29B)	107.7
H(21A)-C(21)-H(21B)	108.0	H(29A)-C(29A)-H(29B)	107.1
C(21)-C(22)-H(22A)	109.5	C(29A)-C(30A)-H(30A)	109.5
C(21)-C(22)-H(22B)	109.5	C(29A)-C(30A)-H(30B)	109.5
H(22A)-C(22)-H(22B)	109.5	H(30A)-C(30A)-H(30B)	109.5
C(21)-C(22)-H(22C)	109.5	C(29A)-C(30A)-H(30C)	109.5
H(22A)-C(22)-H(22C)	109.5	H(30A)-C(30A)-H(30C)	109.5
H(22B)-C(22)-H(22C)	109.5	H(30B)-C(30A)-H(30C)	109.5
C(24)-C(23)-N(3)	116.4(5)	C(28B)-C(27B)-N(3)	115.6(6)
C(24)-C(23)-H(23A)	108.2	C(28B)-C(27B)-H(27C)	108.4
N(3)-C(23)-H(23A)	108.2	N(3)-C(27B)-H(27C)	108.4
C(28B)-C(27B)-H(27D)	108.4	C(33)-C(34)-H(34A)	109.5
N(3)-C(27B)-H(27D)	108.4	C(33)-C(34)-H(34B)	109.5
H(27C)-C(27B)-H(27D)	107.4	H(34A)-C(34)-H(34B)	109.5
C(29B)-C(28B)-C(27B)	111.7(7)	C(33)-C(34)-H(34C)	109.5
C(29B)-C(28B)-H(28C)	109.3	H(34A)-C(34)-H(34C)	109.5
C(27B)-C(28B)-H(28C)	109.3	H(34B)-C(34)-H(34C)	109.5
C(29B)-C(28B)-H(28D)	109.3	C(36)-C(35)-N(4)	117.1(7)
C(27B)-C(28B)-H(28D)	109.3	C(36)-C(35)-H(35A)	108.0
H(28C)-C(28B)-H(28D)	107.9	N(4)-C(35)-H(35A)	108.0
C(30B)-C(29B)-C(28B)	128.5(15)	C(36)-C(35)-H(35B)	108.0
C(30B)-C(29B)-H(29C)	105.2	N(4)-C(35)-H(35B)	108.0
C(28B)-C(29B)-H(29C)	105.2	H(35A)-C(35)-H(35B)	107.3
C(30B)-C(29B)-H(29D)	105.2	C(35)-C(36)-C(37)	111.0(7)

C(28B)-C(29B)-H(29D)	105.2	C(35)-C(36)-H(36A)	109.4
H(29C)-C(29B)-H(29D)	105.9	C(37)-C(36)-H(36A)	109.4
C(29B)-C(30B)-H(30D)	109.5	C(35)-C(36)-H(36B)	109.4
C(29B)-C(30B)-H(30E)	109.5	C(37)-C(36)-H(36B)	109.4
H(30D)-C(30B)-H(30E)	109.5	H(36A)-C(36)-H(36B)	108.0
C(29B)-C(30B)-H(30F)	109.5	C(38)-C(37)-C(36)	113.7(8)
H(30D)-C(30B)-H(30F)	109.5	C(38)-C(37)-H(37A)	108.8
H(30E)-C(30B)-H(30F)	109.5	C(36)-C(37)-H(37A)	108.8
C(31)-N(4)-C(43)	111.5(6)	C(38)-C(37)-H(37B)	108.8
C(31)-N(4)-C(39B)	106.8(6)	C(36)-C(37)-H(37B)	108.8
C(43)-N(4)-C(39B)	110.2(7)	H(37A)-C(37)-H(37B)	107.7
C(31)-N(4)-C(39A)	106.8(6)	C(37)-C(38)-H(38A)	109.5
C(43)-N(4)-C(39A)	110.2(7)	C(37)-C(38)-H(38B)	109.5
C(31)-N(4)-C(35)	110.8(6)	H(38A)-C(38)-H(38B)	109.5
C(43)-N(4)-C(35)	106.4(6)	C(37)-C(38)-H(38C)	109.5
C(39B)-N(4)-C(35)	111.2(6)	H(38A)-C(38)-H(38C)	109.5
C(39A)-N(4)-C(35)	111.2(6)	H(38B)-C(38)-H(38C)	109.5
N(4)-C(31)-C(32)	115.5(6)	C(40A)-C(39A)-N(4)	117.2(8)
N(4)-C(31)-H(31A)	108.4	C(40A)-C(39A)-H(39A)	108.0
C(32)-C(31)-H(31A)	108.4	N(4)-C(39A)-H(39A)	108.0
N(4)-C(31)-H(31B)	108.4	C(40A)-C(39A)-H(39B)	108.0
C(32)-C(31)-H(31B)	108.4	N(4)-C(39A)-H(39B)	108.0
H(31A)-C(31)-H(31B)	107.5	H(39A)-C(39A)-H(39B)	107.2
C(31)-C(32)-C(33)	111.7(6)	C(39A)-C(40A)-C(41A)	109.4(11)
C(31)-C(32)-H(32A)	109.3	C(39A)-C(40A)-H(40A)	109.8
C(33)-C(32)-H(32A)	109.3	C(41A)-C(40A)-H(40A)	109.8
C(31)-C(32)-H(32B)	109.3	C(39A)-C(40A)-H(40B)	109.8
C(33)-C(32)-H(32B)	109.3	C(41A)-C(40A)-H(40B)	109.8
H(32A)-C(32)-H(32B)	107.9	H(40A)-C(40A)-H(40B)	108.2
C(34)-C(33)-C(32)	113.3(7)	C(42A)-C(41A)-C(40A)	117.8(13)
C(34)-C(33)-H(33A)	108.9	C(42A)-C(41A)-H(41A)	107.8
C(32)-C(33)-H(33A)	108.9	C(40A)-C(41A)-H(41A)	107.8
C(34)-C(33)-H(33B)	108.9	C(42A)-C(41A)-H(41B)	107.9
C(32)-C(33)-H(33B)	108.9	C(40A)-C(41A)-H(41B)	107.9
H(33A)-C(33)-H(33B)	107.7	H(41A)-C(41A)-H(41B)	107.2
C(41A)-C(42A)-H(42A)	109.5	C(45)-C(46)-H(46A)	109.5

C(41A)-C(42A)-H(42B)	109.5	C(45)-C(46)-H(46B)	109.5
H(42A)-C(42A)-H(42B)	109.5	H(46A)-C(46)-H(46B)	109.5
C(41A)-C(42A)-H(42C)	109.5	C(45)-C(46)-H(46C)	109.5
H(42A)-C(42A)-H(42C)	109.5	H(46A)-C(46)-H(46C)	109.5
H(42B)-C(42A)-H(42C)	109.5	H(46B)-C(46)-H(46C)	109.5
C(40B)-C(39B)-N(4)	117.2(8)	C(47)-O(21)-C(49)	118(2)
C(40B)-C(39B)-H(39C)	108.0	O(21)-C(47)-C(48)	116(3)
N(4)-C(39B)-H(39C)	108.0	O(21)-C(47)-H(47A)	108.3
C(40B)-C(39B)-H(39D)	108.0	C(48)-C(47)-H(47A)	108.3
N(4)-C(39B)-H(39D)	108.0	O(21)-C(47)-H(47B)	108.3
H(39C)-C(39B)-H(39D)	107.2	C(48)-C(47)-H(47B)	108.3
C(41B)-C(40B)-C(39B)	123.9(12)	H(47A)-C(47)-H(47B)	107.4
C(41B)-C(40B)-H(40C)	106.3	C(47)-C(48)-H(48A)	109.5
C(39B)-C(40B)-H(40C)	106.3	C(47)-C(48)-H(48B)	109.5
C(41B)-C(40B)-H(40D)	106.3	H(48A)-C(48)-H(48B)	109.5
C(39B)-C(40B)-H(40D)	106.3	C(47)-C(48)-H(48C)	109.5
H(40C)-C(40B)-H(40D)	106.4	H(48A)-C(48)-H(48C)	109.5
C(42B)-C(41B)-C(40B)	97.7(15)	H(48B)-C(48)-H(48C)	109.5
C(42B)-C(41B)-H(41C)	112.2	O(21)-C(49)-C(50)	120(2)
C(40B)-C(41B)-H(41C)	112.2	O(21)-C(49)-H(49A)	107.3
C(42B)-C(41B)-H(41D)	112.2	C(50)-C(49)-H(49A)	107.3
C(40B)-C(41B)-H(41D)	112.2	O(21)-C(49)-H(49B)	107.3
H(41C)-C(41B)-H(41D)	109.8	C(50)-C(49)-H(49B)	107.3
C(41B)-C(42B)-H(42D)	109.5	H(49A)-C(49)-H(49B)	106.9
C(41B)-C(42B)-H(42E)	109.5	C(49)-C(50)-H(50A)	109.5
H(42D)-C(42B)-H(42E)	109.5	C(49)-C(50)-H(50B)	109.5
C(41B)-C(42B)-H(42F)	109.5	H(50A)-C(50)-H(50B)	109.5
H(42D)-C(42B)-H(42F)	109.5	C(49)-C(50)-H(50C)	109.5
H(42E)-C(42B)-H(42F)	109.5	H(50A)-C(50)-H(50C)	109.5
N(4)-C(43)-C(44)	116.4(7)	H(50B)-C(50)-H(50C)	109.5
N(4)-C(43)-H(43A)	108.2	C(45)-C(46)-H(46A)	109.5
C(44)-C(43)-H(43A)	108.2	C(45)-C(46)-H(46B)	109.5
N(4)-C(43)-H(43B)	108.2	H(46A)-C(46)-H(46B)	109.5
C(44)-C(43)-H(43B)	108.2	C(45)-C(46)-H(46C)	109.5
H(43A)-C(43)-H(43B)	107.3	H(46A)-C(46)-H(46C)	109.5
C(45)-C(44)-C(43)	109.2(7)	H(46B)-C(46)-H(46C)	109.5

C(45)-C(44)-H(44A)	109.8	C(47)-O(21)-C(49)	118(2)
C(43)-C(44)-H(44A)	109.8	O(21)-C(47)-C(48)	116(3)
C(45)-C(44)-H(44B)	109.8	O(21)-C(47)-H(47A)	108.3
C(43)-C(44)-H(44B)	109.8	C(48)-C(47)-H(47A)	108.3
H(44A)-C(44)-H(44B)	108.3	O(21)-C(47)-H(47B)	108.3
C(44)-C(45)-C(46)	113.4(9)	C(48)-C(47)-H(47B)	108.3
C(44)-C(45)-H(45A)	108.9	H(47A)-C(47)-H(47B)	107.4
C(46)-C(45)-H(45A)	108.9	C(47)-C(48)-H(48A)	109.5
C(44)-C(45)-H(45B)	108.9	C(47)-C(48)-H(48B)	109.5
C(46)-C(45)-H(45B)	108.9	H(48A)-C(48)-H(48B)	109.5
H(45A)-C(45)-H(45B)	107.7	C(47)-C(48)-H(48C)	109.5

ORTEP-6 representation of compound **8**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity.



Compound 9

Crystal growth Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method Oil

Crystal Data

Chemical formula	$C_{50.50}H_{91.75}Mo_6N_{4.25}O_{18.50}$	
Formula weight	1630.17 g mol^{-1}	
Temperature	100 (2) K	
Crystal size	0.340 x 0.050 x 0.020 mm^3	
Crystal description	Red needle	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 11.4858(3) Å	α = 90°.
	b = 38.1339(10) Å	β = 103.573(2)°.
	c = 14.2817(5) Å	γ = 90°.
	Volume	6329.36(19) $Å^3$
Z	4	
F(000)	3298	
Density (calculated)	1.711 Mg cm^{-3}	
Absorption coefficient	1.221 mm^{-1}	

Data Collection

Diffractometer	Rigaku AFC 12 goniometer
Radiation	Mo-*Kα*
2θ range for data collection	1.888 – 27.499°.
Reflections collected	89587
Independent reflections	14538 [R(int) = 0.0506]
Transmission coefficients	1.000
Data corrections	Gaussian
Index ranges	-16<=h<=16, -30<=k<=30, -28<=l<=28

Refinement method

Full-matrix least squares on F^2		
Weighting scheme	$w = [\sigma^2(F_o^2) + (0.0599P)^2 + 6.6257P]^{-1}$	
	$P = [\max(I_{obs}, 0) + 2F_c^2]/3$	
Data / restraints / parameters	14538 / 2 / 730	
Data to parameter ratio	19.91	
Goodness of fit on F^2	0.990	
R indices	$[I_o>2\sigma>(I_o)]$ data	R1 = 0.0384, wR2 = 0.0972
	All 2558 data	R1 = 0.0512, wR2 = 0.1032
Final difference map	Largest diff. peak +1.440 and hole -0.807 e.$Å^{-3}$	

Bond lengths [Å] and angles [°]

Mo(1)-N(1)	1.737(3)	Mo(6)-O(9)	2.355(2)
Mo(1)-O(3)	1.882(2)	N(1)-C(1)	1.395(4)
Mo(1)-O(8)	1.930(2)	N(2)-C(14)	1.368(4)
Mo(1)-O(2)	1.951(2)	N(2)-C(15)	1.452(5)
Mo(1)-O(1)	2.023(2)	N(2)-C(16)	1.452(5)
Mo(1)-O(9)	2.219(2)	C(1)-C(4)	1.382(5)
Mo(1)-Mo(2)	3.2194(4)	C(1)-C(2)	1.388(5)
Mo(2)-O(5)	1.684(2)	C(2)-C(3)	1.381(5)
Mo(2)-O(12)	1.894(2)	C(2)-H(2)	0.9500
Mo(2)-O(8)	1.906(2)	C(3)-C(6)	1.394(5)
Mo(2)-O(11)	1.915(2)	C(3)-H(3)	0.9500
Mo(2)-O(4)	1.990(2)	C(4)-C(5)	1.389(5)
Mo(2)-O(9)	2.313(2)	C(4)-H(4)	0.9500
Mo(3)-O(17)	1.691(3)	C(5)-C(6)	1.389(5)
Mo(3)-O(10)	1.861(2)	C(5)-H(5)	0.9500
Mo(3)-O(6)	1.886(3)	C(6)-C(7)	1.433(5)
Mo(3)-O(3)	1.966(2)	C(7)-C(8)	1.208(5)
Mo(3)-O(12)	1.993(2)	C(8)-C(9)	1.429(5)
Mo(3)-O(9)	2.340(2)	C(9)-C(10)	1.402(5)
Mo(4)-O(14)	1.686(3)	C(9)-C(12)	1.405(5)
Mo(4)-O(16)	1.882(2)	C(10)-C(11)	1.391(5)
Mo(4)-O(2)	1.891(2)	C(10)-H(10)	0.9500
Mo(4)-O(7)	1.942(2)	C(11)-C(14)	1.405(5)
Mo(4)-O(6)	1.992(2)	C(11)-H(11)	0.9500
Mo(4)-O(9)	2.330(2)	C(12)-C(13)	1.380(5)
Mo(5)-O(15)	1.689(3)	C(12)-H(12)	0.9500
Mo(5)-O(1)	1.842(2)	C(13)-C(14)	1.417(5)
Mo(5)-O(4)	1.886(2)	C(13)-H(13)	0.9500
Mo(5)-O(16)	1.983(2)	C(15)-H(15A)	0.9800
Mo(5)-O(13)	2.010(2)	C(15)-H(15B)	0.9800
Mo(5)-O(9)	2.343(2)	C(15)-H(15C)	0.9800
Mo(6)-O(18)	1.684(3)	C(16)-H(16A)	0.9800
Mo(6)-O(13)	1.856(3)	C(16)-H(16B)	0.9800

Mo(6)-O(7)	1.897(3)	C(16)-H(16C)	0.9800
Mo(6)-O(11)	1.932(3)	N(3)-C(29)	1.503(5)
Mo(6)-O(10)	1.996(3)	N(3)-C(25)	1.522(4)
N(3)-C(21)	1.527(5)	C(29)-C(30)	1.498(6)
C(17)-C(18)	1.521(5)	C(29)-H(29A)	0.9900
C(17)-H(17A)	0.9900	C(29)-H(29B)	0.9900
C(17)-H(17B)	0.9900	C(30)-C(31)	1.523(6)
C(18)-C(19)	1.518(6)	C(30)-H(30A)	0.9900
C(18)-H(18A)	0.9900	C(30)-H(30B)	0.9900
C(18)-H(18B)	0.9900	C(31)-C(32)	1.430(8)
C(19)-C(20)	1.499(7)	C(31)-H(31A)	0.9900
C(19)-H(19A)	0.9900	C(31)-H(31B)	0.9900
C(19)-H(19B)	0.9900	C(32)-H(32A)	0.9800
C(20)-H(20A)	0.9800	C(32)-H(32B)	0.9800
C(20)-H(20B)	0.9800	C(32)-H(32C)	0.9800
C(20)-H(20C)	0.9800	N(4)-C(45)	1.515(4)
C(21)-C(22)	1.510(6)	N(4)-C(33)	1.515(4)
C(21)-H(21A)	0.9900	N(4)-C(41)	1.518(4)
C(21)-H(21B)	0.9900	N(4)-C(37)	1.521(4)
C(22)-C(23)	1.525(6)	C(33)-C(34)	1.514(5)
C(22)-H(22A)	0.9900	C(33)-H(33A)	0.9900
C(22)-H(22B)	0.9900	C(33)-H(33B)	0.9900
C(23)-C(24)	1.515(6)	C(34)-C(35)	1.513(5)
C(23)-H(23A)	0.9900	C(34)-H(34A)	0.9900
C(23)-H(23B)	0.9900	C(34)-H(34B)	0.9900
C(24)-H(24A)	0.9800	C(35)-C(36)	1.517(6)
C(24)-H(24B)	0.9800	C(35)-H(35A)	0.9900
C(24)-H(24C)	0.9800	C(35)-H(35B)	0.9900
C(25)-C(26)	1.511(5)	C(36)-H(36A)	0.9800
C(25)-H(25A)	0.9900	C(36)-H(36B)	0.9800
C(25)-H(25B)	0.9900	C(36)-H(36C)	0.9800
C(26)-C(27)	1.518(5)	C(37)-C(38)	1.501(5)
C(26)-H(26A)	0.9900	C(37)-H(37A)	0.9900
C(26)-H(26B)	0.9900	C(37)-H(37B)	0.9900
C(27)-C(28)	1.520(6)	C(38)-C(39)	1.529(5)
C(27)-H(27A)	0.9900	C(38)-H(38A)	0.9900

C(27)-H(27B)	0.9900	C(38)-H(38B)	0.9900
C(28)-H(28A)	0.9800	C(39)-C(40)	1.515(6)
C(28)-H(28B)	0.9800	C(39)-H(39A)	0.9900
C(28)-H(28C)	0.9800	C(39)-H(39B)	0.9900
C(40)-H(40A)	0.9800	C(03)-H(03B)	0.9900
C(40)-H(40B)	0.9800	C(04)-H(04A)	0.9800
C(40)-H(40C)	0.9800	C(04)-H(04B)	0.9800
C(41)-C(42)	1.516(5)	C(04)-H(04C)	0.9800
C(41)-H(41A)	0.9900	N(01)-C(06)	1.13(4)
C(41)-H(41B)	0.9900	C(05)-C(06)	1.53(3)
C(42)-C(43)	1.536(5)	C(05)-H(05A)	0.9800
C(42)-H(42A)	0.9900	C(05)-H(05B)	0.9800
C(42)-H(42B)	0.9900	C(05)-H(05C)	0.9800
C(43)-C(44)	1.512(5)	N(1)-Mo(1)-O(3)	103.83(12)
C(43)-H(43A)	0.9900	N(1)-Mo(1)-O(8)	100.24(11)
C(43)-H(43B)	0.9900	O(3)-Mo(1)-O(8)	91.78(10)
C(44)-H(44A)	0.9800	N(1)-Mo(1)-O(2)	103.22(12)
C(44)-H(44B)	0.9800	O(3)-Mo(1)-O(2)	89.09(10)
C(44)-H(44C)	0.9800	O(8)-Mo(1)-O(2)	155.60(9)
C(45)-C(46)	1.513(5)	N(1)-Mo(1)-O(1)	99.36(11)
C(45)-H(45A)	0.9900	O(3)-Mo(1)-O(1)	156.79(9)
C(45)-H(45B)	0.9900	O(8)-Mo(1)-O(1)	85.09(10)
C(46)-C(47)	1.519(5)	O(2)-Mo(1)-O(1)	84.59(10)
C(46)-H(46A)	0.9900	N(1)-Mo(1)-O(9)	176.28(11)
C(46)-H(46B)	0.9900	O(3)-Mo(1)-O(9)	79.71(9)
C(47)-C(48)	1.489(6)	O(8)-Mo(1)-O(9)	78.34(8)
C(47)-H(47A)	0.9900	O(2)-Mo(1)-O(9)	77.83(9)
C(47)-H(47B)	0.9900	O(1)-Mo(1)-O(9)	77.14(8)
C(48)-H(48A)	0.9800	N(1)-Mo(1)-Mo(2)	132.87(10)
C(48)-H(48B)	0.9800	O(3)-Mo(1)-Mo(2)	82.12(7)
C(48)-H(48C)	0.9800	O(8)-Mo(1)-Mo(2)	32.70(6)
O(01)-C(01)	1.444(16)	O(2)-Mo(1)-Mo(2)	123.76(7)
O(01)-C(03)	1.490(18)	O(1)-Mo(1)-Mo(2)	82.92(7)
C(01)-C(02)	1.481(19)	O(9)-Mo(1)-Mo(2)	45.93(5)
C(01)-H(01A)	0.9900	O(5)-Mo(2)-O(12)	104.70(12)
C(01)-H(01B)	0.9900	O(5)-Mo(2)-O(8)	102.54(11)

C(02)-H(02A)	0.9800	O(12)-Mo(2)-O(8)	89.54(10)
C(02)-H(02B)	0.9800	O(5)-Mo(2)-O(11)	103.86(12)
C(02)-H(02C)	0.9800	O(12)-Mo(2)-O(11)	89.07(11)
C(03)-C(04)	1.60(2)	O(8)-Mo(2)-O(11)	153.04(10)
C(03)-H(03A)	0.9900	O(5)-Mo(2)-O(4)	101.25(12)
O(12)-Mo(2)-O(4)	154.04(10)	O(2)-Mo(4)-O(6)	85.33(10)
O(8)-Mo(2)-O(4)	84.78(10)	O(7)-Mo(4)-O(6)	83.77(10)
O(11)-Mo(2)-O(4)	84.78(11)	O(14)-Mo(4)-O(9)	178.00(11)
O(5)-Mo(2)-O(9)	176.95(11)	O(16)-Mo(4)-O(9)	77.55(9)
O(12)-Mo(2)-O(9)	78.22(9)	O(2)-Mo(4)-O(9)	76.25(8)
O(8)-Mo(2)-O(9)	76.47(8)	O(7)-Mo(4)-O(9)	76.46(9)
O(11)-Mo(2)-O(9)	76.89(9)	O(6)-Mo(4)-O(9)	75.95(9)
O(4)-Mo(2)-O(9)	75.82(8)	O(15)-Mo(5)-O(1)	105.02(12)
O(5)-Mo(2)-Mo(1)	135.63(9)	O(15)-Mo(5)-O(4)	104.47(12)
O(12)-Mo(2)-Mo(1)	79.63(7)	O(1)-Mo(5)-O(4)	92.30(10)
O(8)-Mo(2)-Mo(1)	33.17(7)	O(15)-Mo(5)-O(16)	102.81(12)
O(11)-Mo(2)-Mo(1)	120.46(7)	O(1)-Mo(5)-O(16)	88.30(10)
O(4)-Mo(2)-Mo(1)	81.86(7)	O(4)-Mo(5)-O(16)	151.55(10)
O(9)-Mo(2)-Mo(1)	43.58(5)	O(15)-Mo(5)-O(13)	101.73(12)
O(17)-Mo(3)-O(10)	105.05(13)	O(1)-Mo(5)-O(13)	152.92(10)
O(17)-Mo(3)-O(6)	103.56(13)	O(4)-Mo(5)-O(13)	85.00(11)
O(10)-Mo(3)-O(6)	91.20(11)	O(16)-Mo(5)-O(13)	81.73(11)
O(17)-Mo(3)-O(3)	102.12(12)	O(15)-Mo(5)-O(9)	176.93(11)
O(10)-Mo(3)-O(3)	152.51(10)	O(1)-Mo(5)-O(9)	77.53(9)
O(6)-Mo(3)-O(3)	86.41(11)	O(4)-Mo(5)-O(9)	76.98(9)
O(17)-Mo(3)-O(12)	102.84(13)	O(16)-Mo(5)-O(9)	75.40(8)
O(10)-Mo(3)-O(12)	87.11(11)	O(13)-Mo(5)-O(9)	75.61(9)
O(6)-Mo(3)-O(12)	153.06(10)	O(18)-Mo(6)-O(13)	105.10(13)
O(3)-Mo(3)-O(12)	82.89(10)	O(18)-Mo(6)-O(7)	103.28(12)
O(17)-Mo(3)-O(9)	176.98(11)	O(13)-Mo(6)-O(7)	91.11(11)
O(10)-Mo(3)-O(9)	77.62(9)	O(18)-Mo(6)-O(11)	104.13(12)
O(6)-Mo(3)-O(9)	77.63(9)	O(13)-Mo(6)-O(11)	88.99(11)
O(3)-Mo(3)-O(9)	75.12(8)	O(7)-Mo(6)-O(11)	151.57(10)
O(12)-Mo(3)-O(9)	75.75(8)	O(18)-Mo(6)-O(10)	101.92(13)
O(14)-Mo(4)-O(16)	104.37(12)	O(13)-Mo(6)-O(10)	152.94(10)
O(14)-Mo(4)-O(2)	104.18(12)	O(7)-Mo(6)-O(10)	84.05(11)

O(16)-Mo(4)-O(2)	90.59(10)	O(11)-Mo(6)-O(10)	83.05(11)
O(14)-Mo(4)-O(7)	102.93(12)	O(18)-Mo(6)-O(9)	176.76(12)
O(16)-Mo(4)-O(7)	87.92(11)	O(13)-Mo(6)-O(9)	78.14(9)
O(2)-Mo(4)-O(7)	152.34(10)	O(7)-Mo(6)-O(9)	76.64(9)
O(14)-Mo(4)-O(6)	102.11(12)	O(11)-Mo(6)-O(9)	75.57(8)
O(16)-Mo(4)-O(6)	153.40(10)	O(10)-Mo(6)-O(9)	74.84(8)
Mo(5)-O(1)-Mo(1)	114.40(11)	C(2)-C(3)-C(6)	120.8(3)
Mo(4)-O(2)-Mo(1)	115.05(11)	C(2)-C(3)-H(3)	119.6
Mo(1)-O(3)-Mo(3)	114.64(11)	C(6)-C(3)-H(3)	119.6
Mo(5)-O(4)-Mo(2)	116.76(11)	C(1)-C(4)-C(5)	119.9(3)
Mo(3)-O(6)-Mo(4)	116.46(11)	C(1)-C(4)-H(4)	120.1
Mo(6)-O(7)-Mo(4)	117.41(12)	C(5)-C(4)-H(4)	120.1
Mo(2)-O(8)-Mo(1)	114.13(11)	C(4)-C(5)-C(6)	120.6(3)
Mo(1)-O(9)-Mo(2)	90.49(7)	C(4)-C(5)-H(5)	119.7
Mo(1)-O(9)-Mo(4)	90.86(7)	C(6)-C(5)-H(5)	119.7
Mo(2)-O(9)-Mo(4)	178.65(10)	C(5)-C(6)-C(3)	118.7(3)
Mo(1)-O(9)-Mo(3)	90.51(7)	C(5)-C(6)-C(7)	120.4(3)
Mo(2)-O(9)-Mo(3)	90.07(7)	C(3)-C(6)-C(7)	120.8(3)
Mo(4)-O(9)-Mo(3)	89.84(7)	C(8)-C(7)-C(6)	179.8(5)
Mo(1)-O(9)-Mo(5)	90.81(7)	C(7)-C(8)-C(9)	177.9(4)
Mo(2)-O(9)-Mo(5)	90.31(7)	C(10)-C(9)-C(12)	117.6(3)
Mo(4)-O(9)-Mo(5)	89.75(7)	C(10)-C(9)-C(8)	121.2(3)
Mo(3)-O(9)-Mo(5)	178.62(10)	C(12)-C(9)-C(8)	121.2(3)
Mo(1)-O(9)-Mo(6)	179.76(10)	C(11)-C(10)-C(9)	121.6(3)
Mo(2)-O(9)-Mo(6)	89.75(7)	C(11)-C(10)-H(10)	119.2
Mo(4)-O(9)-Mo(6)	88.90(7)	C(9)-C(10)-H(10)	119.2
Mo(3)-O(9)-Mo(6)	89.50(7)	C(10)-C(11)-C(14)	120.8(3)
Mo(5)-O(9)-Mo(6)	89.18(7)	C(10)-C(11)-H(11)	119.6
Mo(3)-O(10)-Mo(6)	117.88(12)	C(14)-C(11)-H(11)	119.6
Mo(2)-O(11)-Mo(6)	117.78(12)	C(13)-C(12)-C(9)	121.2(4)
Mo(2)-O(12)-Mo(3)	115.73(12)	C(13)-C(12)-H(12)	119.4
Mo(6)-O(13)-Mo(5)	117.06(12)	C(9)-C(12)-H(12)	119.4
Mo(4)-O(16)-Mo(5)	117.07(12)	C(12)-C(13)-C(14)	121.3(4)
C(1)-N(1)-Mo(1)	168.3(3)	C(12)-C(13)-H(13)	119.3
C(14)-N(2)-C(15)	121.2(3)	C(14)-C(13)-H(13)	119.3
C(14)-N(2)-C(16)	119.6(3)	N(2)-C(14)-C(11)	121.5(3)

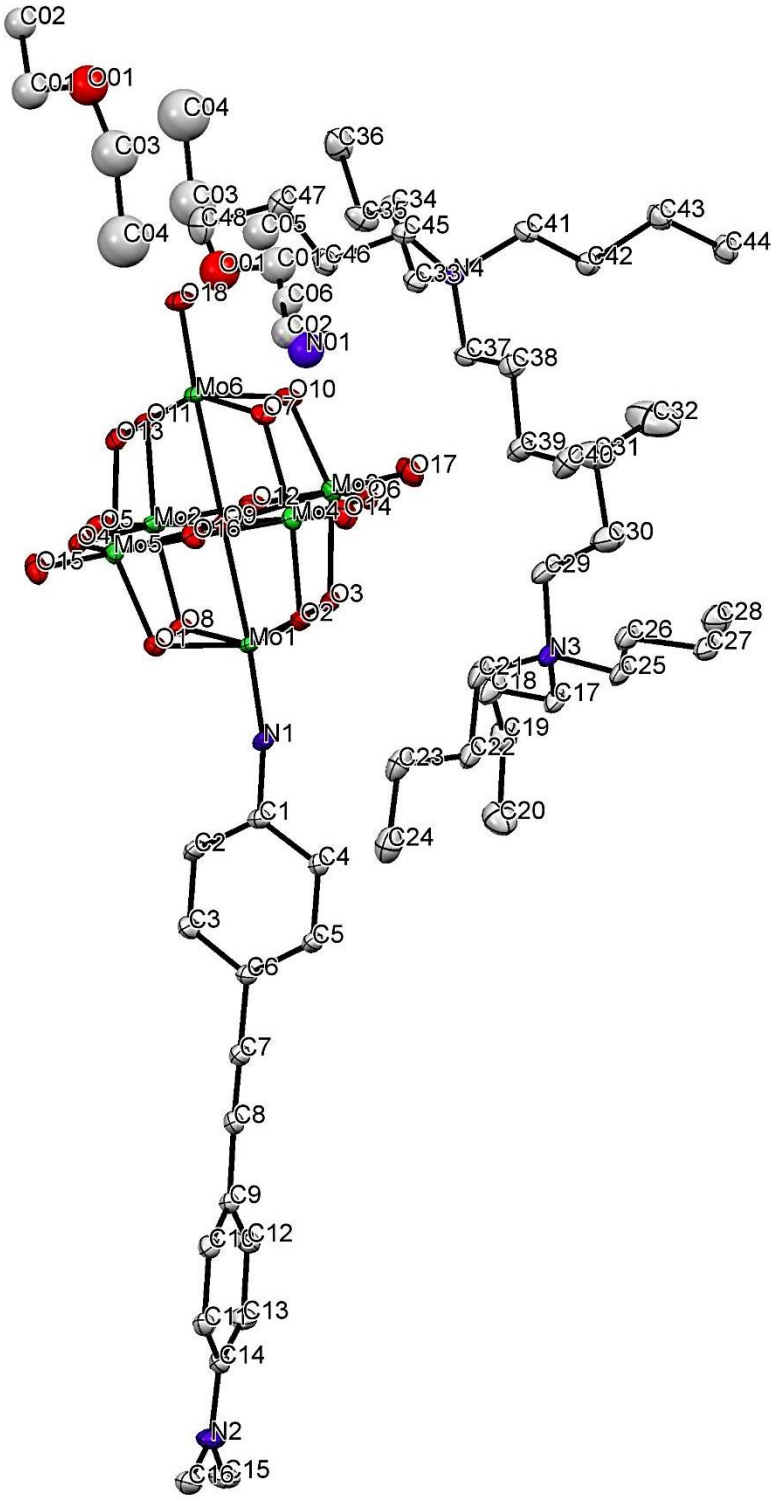
C(15)-N(2)-C(16)	119.2(3)	N(2)-C(14)-C(13)	121.1(3)
C(4)-C(1)-C(2)	120.1(3)	C(11)-C(14)-C(13)	117.4(3)
C(4)-C(1)-N(1)	120.3(3)	N(2)-C(15)-H(15A)	109.5
C(2)-C(1)-N(1)	119.6(3)	N(2)-C(15)-H(15B)	109.5
C(3)-C(2)-C(1)	119.8(3)	H(15A)-C(15)-H(15B)	109.5
C(3)-C(2)-H(2)	120.1	N(2)-C(15)-H(15C)	109.5
C(1)-C(2)-H(2)	120.1	H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5	C(22)-C(21)-N(3)	116.5(3)
N(2)-C(16)-H(16A)	109.5	C(22)-C(21)-H(21A)	108.2
N(2)-C(16)-H(16B)	109.5	N(3)-C(21)-H(21A)	108.2
H(16A)-C(16)-H(16B)	109.5	C(22)-C(21)-H(21B)	108.2
N(2)-C(16)-H(16C)	109.5	N(3)-C(21)-H(21B)	108.2
H(16A)-C(16)-H(16C)	109.5	H(21A)-C(21)-H(21B)	107.3
H(16B)-C(16)-H(16C)	109.5	C(21)-C(22)-C(23)	110.5(3)
C(29)-N(3)-C(25)	111.7(3)	C(21)-C(22)-H(22A)	109.5
C(29)-N(3)-C(17)	110.7(3)	C(23)-C(22)-H(22A)	109.5
C(25)-N(3)-C(17)	105.8(3)	C(21)-C(22)-H(22B)	109.5
C(29)-N(3)-C(21)	106.2(3)	C(23)-C(22)-H(22B)	109.5
C(25)-N(3)-C(21)	111.4(3)	H(22A)-C(22)-H(22B)	108.1
C(17)-N(3)-C(21)	111.2(3)	C(24)-C(23)-C(22)	112.6(4)
C(18)-C(17)-N(3)	115.8(3)	C(24)-C(23)-H(23A)	109.1
C(18)-C(17)-H(17A)	108.3	C(22)-C(23)-H(23A)	109.1
N(3)-C(17)-H(17A)	108.3	C(24)-C(23)-H(23B)	109.1
C(18)-C(17)-H(17B)	108.3	C(22)-C(23)-H(23B)	109.1
N(3)-C(17)-H(17B)	108.3	H(23A)-C(23)-H(23B)	107.8
H(17A)-C(17)-H(17B)	107.4	C(23)-C(24)-H(24A)	109.5
C(19)-C(18)-C(17)	110.8(3)	C(23)-C(24)-H(24B)	109.5
C(19)-C(18)-H(18A)	109.5	H(24A)-C(24)-H(24B)	109.5
C(17)-C(18)-H(18A)	109.5	C(23)-C(24)-H(24C)	109.5
C(19)-C(18)-H(18B)	109.5	H(24A)-C(24)-H(24C)	109.5
C(17)-C(18)-H(18B)	109.5	H(24B)-C(24)-H(24C)	109.5
H(18A)-C(18)-H(18B)	108.1	C(26)-C(25)-N(3)	116.1(3)
C(20)-C(19)-C(18)	113.2(4)	C(26)-C(25)-H(25A)	108.3
C(20)-C(19)-H(19A)	108.9	N(3)-C(25)-H(25A)	108.3
C(18)-C(19)-H(19A)	108.9	C(26)-C(25)-H(25B)	108.3
C(20)-C(19)-H(19B)	108.9	N(3)-C(25)-H(25B)	108.3

C(18)-C(19)-H(19B)	108.9	H(25A)-C(25)-H(25B)	107.4
H(19A)-C(19)-H(19B)	107.8	C(25)-C(26)-C(27)	109.0(3)
C(19)-C(20)-H(20A)	109.5	C(25)-C(26)-H(26A)	109.9
C(19)-C(20)-H(20B)	109.5	C(27)-C(26)-H(26A)	109.9
H(20A)-C(20)-H(20B)	109.5	C(25)-C(26)-H(26B)	109.9
C(19)-C(20)-H(20C)	109.5	C(27)-C(26)-H(26B)	109.9
H(20A)-C(20)-H(20C)	109.5	H(26A)-C(26)-H(26B)	108.3
H(20B)-C(20)-H(20C)	109.5	C(26)-C(27)-C(28)	112.7(3)
C(26)-C(27)-H(27A)	109.1	C(33)-N(4)-C(41)	111.2(3)
C(28)-C(27)-H(27A)	109.1	C(45)-N(4)-C(37)	110.7(3)
C(26)-C(27)-H(27B)	109.1	C(33)-N(4)-C(37)	106.4(2)
C(28)-C(27)-H(27B)	109.1	C(41)-N(4)-C(37)	111.6(3)
H(27A)-C(27)-H(27B)	107.8	C(34)-C(33)-N(4)	115.5(3)
C(27)-C(28)-H(28A)	109.5	C(34)-C(33)-H(33A)	108.4
C(27)-C(28)-H(28B)	109.5	N(4)-C(33)-H(33A)	108.4
H(28A)-C(28)-H(28B)	109.5	C(34)-C(33)-H(33B)	108.4
C(27)-C(28)-H(28C)	109.5	N(4)-C(33)-H(33B)	108.4
H(28A)-C(28)-H(28C)	109.5	H(33A)-C(33)-H(33B)	107.5
H(28B)-C(28)-H(28C)	109.5	C(35)-C(34)-C(33)	111.0(3)
C(30)-C(29)-N(3)	116.5(3)	C(35)-C(34)-H(34A)	109.4
C(30)-C(29)-H(29A)	108.2	C(33)-C(34)-H(34A)	109.4
N(3)-C(29)-H(29A)	108.2	C(35)-C(34)-H(34B)	109.4
C(30)-C(29)-H(29B)	108.2	C(33)-C(34)-H(34B)	109.4
N(3)-C(29)-H(29B)	108.2	H(34A)-C(34)-H(34B)	108.0
H(29A)-C(29)-H(29B)	107.3	C(34)-C(35)-C(36)	111.8(3)
C(29)-C(30)-C(31)	109.6(4)	C(34)-C(35)-H(35A)	109.3
C(29)-C(30)-H(30A)	109.8	C(36)-C(35)-H(35A)	109.3
C(31)-C(30)-H(30A)	109.8	C(34)-C(35)-H(35B)	109.3
C(29)-C(30)-H(30B)	109.8	C(36)-C(35)-H(35B)	109.3
C(31)-C(30)-H(30B)	109.8	H(35A)-C(35)-H(35B)	107.9
H(30A)-C(30)-H(30B)	108.2	C(35)-C(36)-H(36A)	109.5
C(32)-C(31)-C(30)	113.5(5)	C(35)-C(36)-H(36B)	109.5
C(32)-C(31)-H(31A)	108.9	H(36A)-C(36)-H(36B)	109.5
C(30)-C(31)-H(31A)	108.9	C(35)-C(36)-H(36C)	109.5
C(32)-C(31)-H(31B)	108.9	H(36A)-C(36)-H(36C)	109.5
C(30)-C(31)-H(31B)	108.9	H(36B)-C(36)-H(36C)	109.5

H(31A)-C(31)-H(31B)	107.7	C(38)-C(37)-N(4)	116.4(3)
C(31)-C(32)-H(32A)	109.5	C(38)-C(37)-H(37A)	108.2
C(31)-C(32)-H(32B)	109.5	N(4)-C(37)-H(37A)	108.2
H(32A)-C(32)-H(32B)	109.5	C(38)-C(37)-H(37B)	108.2
C(31)-C(32)-H(32C)	109.5	N(4)-C(37)-H(37B)	108.2
H(32A)-C(32)-H(32C)	109.5	H(37A)-C(37)-H(37B)	107.3
H(32B)-C(32)-H(32C)	109.5	C(37)-C(38)-C(39)	109.6(3)
C(45)-N(4)-C(33)	111.6(3)	C(37)-C(38)-H(38A)	109.7
C(45)-N(4)-C(41)	105.4(3)	C(39)-C(38)-H(38A)	109.7
C(37)-C(38)-H(38B)	109.7	H(44A)-C(44)-H(44C)	109.5
C(39)-C(38)-H(38B)	109.7	H(44B)-C(44)-H(44C)	109.5
H(38A)-C(38)-H(38B)	108.2	C(46)-C(45)-N(4)	117.6(3)
C(40)-C(39)-C(38)	111.9(3)	C(46)-C(45)-H(45A)	107.9
C(40)-C(39)-H(39A)	109.2	N(4)-C(45)-H(45A)	107.9
C(38)-C(39)-H(39A)	109.2	C(46)-C(45)-H(45B)	107.9
C(40)-C(39)-H(39B)	109.2	N(4)-C(45)-H(45B)	107.9
C(38)-C(39)-H(39B)	109.2	H(45A)-C(45)-H(45B)	107.2
H(39A)-C(39)-H(39B)	107.9	C(45)-C(46)-C(47)	109.0(3)
C(39)-C(40)-H(40A)	109.5	C(45)-C(46)-H(46A)	109.9
C(39)-C(40)-H(40B)	109.5	C(47)-C(46)-H(46A)	109.9
H(40A)-C(40)-H(40B)	109.5	C(45)-C(46)-H(46B)	109.9
C(39)-C(40)-H(40C)	109.5	C(47)-C(46)-H(46B)	109.9
H(40A)-C(40)-H(40C)	109.5	H(46A)-C(46)-H(46B)	108.3
H(40B)-C(40)-H(40C)	109.5	C(48)-C(47)-C(46)	113.3(4)
C(42)-C(41)-N(4)	116.8(3)	C(48)-C(47)-H(47A)	108.9
C(42)-C(41)-H(41A)	108.1	C(46)-C(47)-H(47A)	108.9
N(4)-C(41)-H(41A)	108.1	C(48)-C(47)-H(47B)	108.9
C(42)-C(41)-H(41B)	108.1	C(46)-C(47)-H(47B)	108.9
N(4)-C(41)-H(41B)	108.1	H(47A)-C(47)-H(47B)	107.7
H(41A)-C(41)-H(41B)	107.3	C(47)-C(48)-H(48A)	109.5
C(41)-C(42)-C(43)	109.3(3)	C(47)-C(48)-H(48B)	109.5
C(41)-C(42)-H(42A)	109.8	H(48A)-C(48)-H(48B)	109.5
C(43)-C(42)-H(42A)	109.8	C(47)-C(48)-H(48C)	109.5
C(41)-C(42)-H(42B)	109.8	H(48A)-C(48)-H(48C)	109.5
C(43)-C(42)-H(42B)	109.8	H(48B)-C(48)-H(48C)	109.5
H(42A)-C(42)-H(42B)	108.3	C(01)-O(01)-C(03)	120.9(12)

C(44)-C(43)-C(42)	112.3(3)	O(01)-C(01)-C(02)	115.9(12)
C(44)-C(43)-H(43A)	109.1	O(01)-C(01)-H(01A)	108.3
C(42)-C(43)-H(43A)	109.1	C(02)-C(01)-H(01A)	108.3
C(44)-C(43)-H(43B)	109.1	O(01)-C(01)-H(01B)	108.3
C(42)-C(43)-H(43B)	109.1	C(02)-C(01)-H(01B)	108.3
H(43A)-C(43)-H(43B)	107.9	H(01A)-C(01)-H(01B)	107.4
C(43)-C(44)-H(44A)	109.5	C(01)-C(02)-H(02A)	109.5
C(43)-C(44)-H(44B)	109.5	C(01)-C(02)-H(02B)	109.5
H(44A)-C(44)-H(44B)	109.5	H(02A)-C(02)-H(02B)	109.5
C(43)-C(44)-H(44C)	109.5	C(01)-C(02)-H(02C)	109.5
H(02A)-C(02)-H(02C)	109.5		
H(02B)-C(02)-H(02C)	109.5		
O(01)-C(03)-C(04)	136.6(16)		
O(01)-C(03)-H(03A)	103.0		
C(04)-C(03)-H(03A)	103.0		
O(01)-C(03)-H(03B)	103.0		
C(04)-C(03)-H(03B)	103.0		
H(03A)-C(03)-H(03B)	105.1		
C(03)-C(04)-H(04A)	109.5		
C(03)-C(04)-H(04B)	109.5		
H(04A)-C(04)-H(04B)	109.5		
C(03)-C(04)-H(04C)	109.5		
H(04A)-C(04)-H(04C)	109.5		
H(04B)-C(04)-H(04C)	109.5		
C(06)-C(05)-H(05A)	109.5		
C(06)-C(05)-H(05B)	109.5		
H(05A)-C(05)-H(05B)	109.5		
C(06)-C(05)-H(05C)	109.5		
H(05A)-C(05)-H(05C)	109.5		
H(05B)-C(05)-H(05C)	109.5		
N(01)-C(06)-C(05)	176(3)		

ORTEP-7 representation of compound **9**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity.



Compound 10

Crystal growth Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method Oil

Crystal Data

Chemical formula	$C_{40}H_{32}Mo_6N_4O_{18}$	
Formula weight	1482.7 g mol^{-1}	
Temperature	100 (2) K	
Crystal size	0.190 × 0.040 × 0.040 mm^3	
Crystal description	Dark red prism	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 17.3560(11) Å	α = 90°.
	b = 15.6450(11) Å	β = 104.2520(10)°.
	c = 20.4840(14) Å	γ = 90°.
	Volume	5390.9(6) $Å^3$
Z	4	
F(000)	2984	
Density (calculated)	1.827 Mg cm^{-3}	
Absorption coefficient	1.42 mm^{-1}	

Data Collection

Diffractometer	Oxford Diffraction XCalibur 3
Radiation	Mo-*Kα*
2θ range for data collection	2.2 – 27.5°.
Reflections collected	69741
Independent reflections	12362 [R(int) = 0.049]
Transmission coefficients	1.000
Data corrections	Gaussian
Index ranges	-20<=h<=22, -20<=k<=20, -26<=l<=26

Refinement method

Full-matrix least squares on F^2		
Weighting scheme	$w = [\sigma^2(F_o^2) + (0.0377P)^2 + 13.6058P]^{-1}$	
	$P = [\max(I_{obs}, 0) + 2F_c^2]/3$	
Data / restraints / parameters	12362 / 0 / 615	
Data to parameter ratio	20.10	
Goodness of fit on F^2	1.220	
R indices	$[I_o>2\sigma>(I_o)]$ data	R1 = 0.039, wR2 = 0.100
	All 2558 data	R1 = 0.040, wR2 = 0.100
Final difference map	Largest diff. peak +1.24 and hole -1.30 e.$Å^{-3}$	

Bond lengths [Å] and angles [^{o}]

(1)–N(1)	1.441(6)	C(17)–N(3)	1.525(5)
C(1)–H(1A)	0.9800	C(17)–H(17A)	0.9900
C(1)–H(1B)	0.9800	C(17)–H(17B)	0.9900
C(1)–H(1C)	0.9800	C(18)–C(19)	1.528(5)
C(2)–N(1)	1.467(5)	C(18)–H(18A)	0.9900
C(2)–H(2A)	0.9800	C(18)–H(18B)	0.9900
C(2)–H(2B)	0.9800	C(19)–C(20)	1.516(6)
C(2)–H(2C)	0.9800	C(19)–H(19A)	0.9900
C(3)–N(1)	1.375(5)	C(19)–H(19B)	0.9900
C(3)–C(8)	1.418(6)	C(20)–H(20A)	0.9800
C(3)–C(4)	1.424(5)	C(20)–H(20B)	0.9800
C(4)–C(5)	1.352(5)	C(20)–H(20C)	0.9800
C(4)–H(4)	0.9500	C(21)–N(3)	1.518(4)
C(5)–C(6)	1.414(5)	C(21)–C(22)	1.522(5)
C(5)–H(5)	0.9500	C(21)–H(21A)	0.9900
C(6)–N(2)	1.383(5)	C(21)–H(21B)	0.9900
C(6)–C(7)	1.398(5)	C(22)–C(23)	1.522(5)
C(7)–C(8)	1.359(6)	C(22)–H(22A)	0.9900
C(7)–H(7)	0.9500	C(22)–H(22B)	0.9900
C(8)–H(8)	0.9500	C(23)–C(24)	1.516(5)
C(9)–N(3)	1.515(5)	C(23)–H(23A)	0.9900
C(9)–C(10)	1.515(5)	C(23)–H(23B)	0.9900
C(9)–H(9A)	0.9900	C(24)–H(24A)	0.9800
C(9)–H(9B)	0.9900	C(24)–H(24B)	0.9800
C(10)–C(11)	1.520(6)	C(24)–H(24C)	0.9800
C(10)–H(10A)	0.9900	C(25)–C(26)	1.468(8)
C(10)–H(10B)	0.9900	C(25)–H(25A)	0.9800
C(11)–C(12)	1.522(6)	C(25)–H(25B)	0.9800
C(11)–H(11A)	0.9900	C(25)–H(25C)	0.9800
C(11)–H(11B)	0.9900	C(26)–C(27)	1.519(8)
C(12)–H(12A)	0.9800	C(26)–H(26A)	0.9900
C(12)–H(12B)	0.9800	C(26)–H(26B)	0.9900
C(12)–H(12C)	0.9800	C(27)–C(28)	1.526(6)

C(13)–C(14)	1.520(5)	C(27)–H(27A)	0.9900
C(13)–N(3)	1.526(4)	C(27)–H(27B)	0.9900
C(13)–H(13A)	0.9900	C(28)–N(4)	1.519(5)
C(13)–H(13B)	0.9900	C(28)–H(28A)	0.9900
C(14)–C(15)	1.531(5)	C(28)–H(28B)	0.9900
C(14)–H(14A)	0.9900	C(29)–C(30)	1.482(6)
C(14)–H(14B)	0.9900	C(29)–H(29A)	0.9800
C(15)–C(16)	1.522(5)	C(29)–H(29B)	0.9800
C(15)–H(15A)	0.9900	C(29)–H(29C)	0.9800
C(15)–H(15B)	0.9900	C(30)–C(31)	1.484(6)
C(16)–H(16A)	0.9800	C(30)–H(30A)	0.9900
C(16)–H(16B)	0.9800	C(30)–H(30B)	0.9900
C(16)–H(16C)	0.9800	C(31)–C(32)	1.497(6)
C(17)–C(18)	1.515(5)	C(31)–H(31A)	0.9900
C(32)–N(4)	1.530(5)	O(12)–Mo(5)	2.323(2)
C(32)–H(32A)	0.9900	O(12)–Mo(4)	2.330(2)
C(32)–H(32B)	0.9900	O(12)–Mo(3)	2.336(2)
C(33)–N(4)	1.526(5)	O(12)–Mo(2)	2.349(2)
C(33)–C(34)	1.528(6)	O(12)–Mo(1)	2.350(2)
C(33)–H(33A)	0.9900	O(13)–Mo(2)	1.852(2)
C(33)–H(33B)	0.9900	O(13)–Mo(6)	2.016(2)
C(34)–C(35)	1.501(6)	O(14)–Mo(6)	1.917(2)
C(34)–H(34A)	0.9900	O(14)–Mo(4)	1.943(2)
C(34)–H(34B)	0.9900	O(15)–Mo(6)	1.891(2)
C(35)–C(36)	1.522(6)	O(15)–Mo(3)	1.957(2)
C(35)–H(35A)	0.9900	O(16)–Mo(5)	1.857(2)
C(35)–H(35B)	0.9900	O(16)–Mo(6)	1.998(3)
C(36)–H(36A)	0.9800	O(17)–Mo(2)	1.893(3)
C(36)–H(36B)	0.9800	O(17)–Mo(3)	1.974(2)
C(36)–H(36C)	0.9800	O(18)–Mo(4)	1.894(3)
C(37)–C(38)	1.500(6)	O(18)–Mo(5)	1.977(3)
C(37)–N(4)	1.511(5)	N(1)–C(1)–H(1A)	109.5
C(37)–H(37A)	0.9900	N(1)–C(1)–H(1B)	109.5
C(37)–H(37B)	0.9900	H(1A)–C(1)–H(1B)	109.5
C(38)–C(39)	1.532(7)	N(1)–C(1)–H(1C)	109.5
C(38)–H(38A)	0.9900	H(1A)–C(1)–H(1C)	109.5

C(38)–H(38B)	0.9900	H(1B)–C(1)–H(1C)	109.5
C(39)–C(40)	1.485(7)	N(1)–C(2)–H(2A)	109.5
C(39)–H(39A)	0.9900	N(1)–C(2)–H(2B)	109.5
C(39)–H(39B)	0.9900	H(2A)–C(2)–H(2B)	109.5
C(40)–H(40A)	0.9800	N(1)–C(2)–H(2C)	109.5
C(40)–H(40B)	0.9800	H(2A)–C(2)–H(2C)	109.5
C(40)–H(40C)	0.9800	H(2B)–C(2)–H(2C)	109.5
N(2)–Mo(6)	1.737(3)	N(1)–C(3)–C(8)	121.4(4)
O(1)–Mo(1)	1.684(3)	N(1)–C(3)–C(4)	122.6(4)
O(2)–Mo(3)	1.873(3)	C(8)–C(3)–C(4)	116.0(3)
O(2)–Mo(1)	1.978(3)	C(5)–C(4)–C(3)	122.1(4)
O(3)–Mo(4)	1.894(2)	C(5)–C(4)–H(4)	118.9
O(3)–Mo(1)	1.961(3)	C(3)–C(4)–H(4)	118.9
O(4)–Mo(1)	1.865(2)	C(4)–C(5)–C(6)	120.8(4)
O(4)–Mo(2)	1.982(2)	C(4)–C(5)–H(5)	119.6
O(5)–Mo(1)	1.877(3)	C(6)–C(5)–H(5)	119.6
O(5)–Mo(5)	1.972(2)	N(2)–C(6)–C(7)	121.7(3)
O(6)–Mo(4)	1.691(3)	N(2)–C(6)–C(5)	120.4(3)
O(7)–Mo(3)	1.686(3)	C(7)–C(6)–C(5)	117.9(3)
O(8)–Mo(3)	1.898(2)	C(8)–C(7)–C(6)	121.4(4)
O(8)–Mo(4)	1.966(3)	C(8)–C(7)–H(7)	119.3
O(9)–Mo(5)	1.688(3)	C(6)–C(7)–H(7)	119.3
O(10)–Mo(5)	1.900(3)	C(7)–C(8)–C(3)	121.8(4)
O(10)–Mo(2)	1.989(3)	C(7)–C(8)–H(8)	119.1
O(11)–Mo(2)	1.687(3)	C(3)–C(8)–H(8)	119.1
O(12)–Mo(6)	2.211(2)	N(3)–C(9)–C(10)	115.3(3)
N(3)–C(9)–H(9A)	108.4	C(18)–C(17)–N(3)	116.9(3)
C(10)–C(9)–H(9A)	108.4	C(18)–C(17)–H(17A)	108.1
N(3)–C(9)–H(9B)	108.4	N(3)–C(17)–H(17A)	108.1
C(10)–C(9)–H(9B)	108.4	C(18)–C(17)–H(17B)	108.1
H(9A)–C(9)–H(9B)	107.5	N(3)–C(17)–H(17B)	108.1
C(9)–C(10)–C(11)	110.1(3)	H(17A)–C(17)–H(17B)	107.3
C(9)–C(10)–H(10A)	109.6	C(17)–C(18)–C(19)	108.9(3)
C(11)–C(10)–H(10A)	109.6	C(17)–C(18)–H(18A)	109.9
C(9)–C(10)–H(10B)	109.6	C(19)–C(18)–H(18A)	109.9
C(11)–C(10)–H(10B)	109.6	C(17)–C(18)–H(18B)	109.9

H(10A)–C(10)–H(10B)	108.1	C(19)–C(18)–H(18B)	109.9
C(10)–C(11)–C(12)	111.7(4)	H(18A)–C(18)–H(18B)	108.3
C(10)–C(11)–H(11A)	109.3	C(20)–C(19)–C(18)	113.3(3)
C(12)–C(11)–H(11A)	109.3	C(20)–C(19)–H(19A)	108.9
C(10)–C(11)–H(11B)	109.3	C(18)–C(19)–H(19A)	108.9
C(12)–C(11)–H(11B)	109.3	C(20)–C(19)–H(19B)	108.9
H(11A)–C(11)–H(11B)	107.9	C(18)–C(19)–H(19B)	108.9
C(11)–C(12)–H(12A)	109.5	H(19A)–C(19)–H(19B)	107.7
C(11)–C(12)–H(12B)	109.5	C(19)–C(20)–H(20A)	109.5
H(12A)–C(12)–H(12B)	109.5	C(19)–C(20)–H(20B)	109.5
C(11)–C(12)–H(12C)	109.5	H(20A)–C(20)–H(20B)	109.5
H(12A)–C(12)–H(12C)	109.5	C(19)–C(20)–H(20C)	109.5
H(12B)–C(12)–H(12C)	109.5	H(20A)–C(20)–H(20C)	109.5
C(14)–C(13)–N(3)	117.3(3)	H(20B)–C(20)–H(20C)	109.5
C(14)–C(13)–H(13A)	108.0	N(3)–C(21)–C(22)	116.0(3)
N(3)–C(13)–H(13A)	108.0	N(3)–C(21)–H(21A)	108.3
C(14)–C(13)–H(13B)	108.0	C(22)–C(21)–H(21A)	108.3
N(3)–C(13)–H(13B)	108.0	N(3)–C(21)–H(21B)	108.3
H(13A)–C(13)–H(13B)	107.2	C(22)–C(21)–H(21B)	108.3
C(13)–C(14)–C(15)	108.3(3)	H(21A)–C(21)–H(21B)	107.4
C(13)–C(14)–H(14A)	110.0	C(21)–C(22)–C(23)	109.1(3)
C(15)–C(14)–H(14A)	110.0	C(21)–C(22)–H(22A)	109.9
C(13)–C(14)–H(14B)	110.0	C(23)–C(22)–H(22A)	109.9
C(15)–C(14)–H(14B)	110.0	C(21)–C(22)–H(22B)	109.9
H(14A)–C(14)–H(14B)	108.4	C(23)–C(22)–H(22B)	109.9
C(16)–C(15)–C(14)	111.7(3)	H(22A)–C(22)–H(22B)	108.3
C(16)–C(15)–H(15A)	109.3	C(24)–C(23)–C(22)	112.4(3)
C(14)–C(15)–H(15A)	109.3	C(24)–C(23)–H(23A)	109.1
C(16)–C(15)–H(15B)	109.3	C(22)–C(23)–H(23A)	109.1
C(14)–C(15)–H(15B)	109.3	C(24)–C(23)–H(23B)	109.1
H(15A)–C(15)–H(15B)	107.9	C(22)–C(23)–H(23B)	109.1
C(15)–C(16)–H(16A)	109.5	H(23A)–C(23)–H(23B)	107.9
C(15)–C(16)–H(16B)	109.5	C(23)–C(24)–H(24A)	109.5
H(16A)–C(16)–H(16B)	109.5	C(23)–C(24)–H(24B)	109.5
C(15)–C(16)–H(16C)	109.5	H(24A)–C(24)–H(24B)	109.5
H(16A)–C(16)–H(16C)	109.5	C(23)–C(24)–H(24C)	109.5

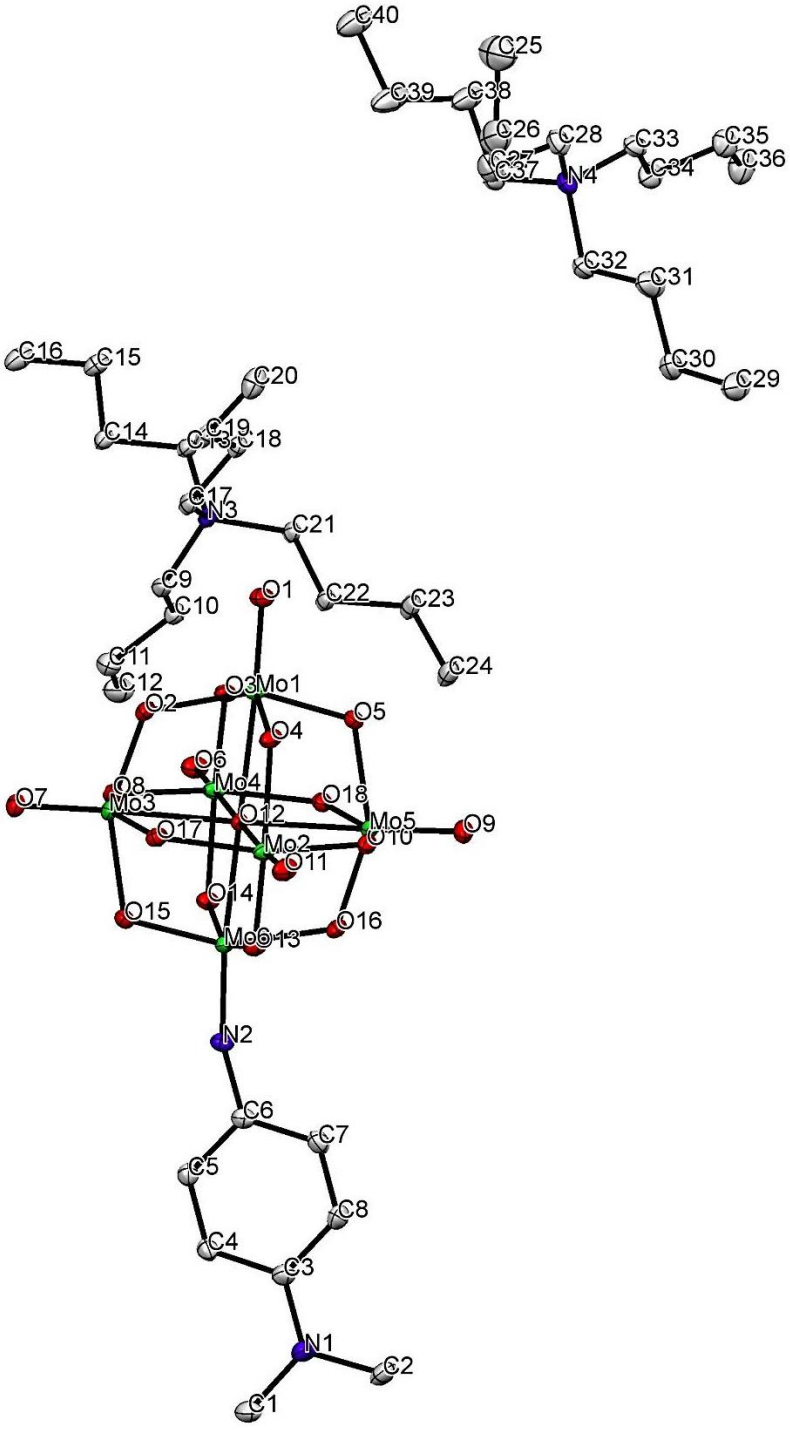
H(16B)–C(16)–H(16C)	109.5	H(24A)–C(24)–H(24C)	109.5
C(26)–C(25)–H(25A)	109.5	H(24B)–C(24)–H(24C)	109.5
C(26)–C(25)–H(25B)	109.5	N(4)–C(33)–C(34)	115.6(3)
H(25A)–C(25)–H(25B)	109.5	N(4)–C(33)–H(33A)	108.4
C(26)–C(25)–H(25C)	109.5	C(34)–C(33)–H(33A)	108.4
H(25A)–C(25)–H(25C)	109.5	N(4)–C(33)–H(33B)	108.4
H(25B)–C(25)–H(25C)	109.5	C(34)–C(33)–H(33B)	108.4
C(25)–C(26)–C(27)	113.7(5)	H(33A)–C(33)–H(33B)	107.4
C(25)–C(26)–H(26A)	108.8	C(35)–C(34)–C(33)	109.8(3)
C(27)–C(26)–H(26A)	108.8	C(35)–C(34)–H(34A)	109.7
C(25)–C(26)–H(26B)	108.8	C(33)–C(34)–H(34A)	109.7
C(27)–C(26)–H(26B)	108.8	C(35)–C(34)–H(34B)	109.7
H(26A)–C(26)–H(26B)	107.7	C(33)–C(34)–H(34B)	109.7
C(26)–C(27)–C(28)	110.8(4)	H(34A)–C(34)–H(34B)	108.2
C(26)–C(27)–H(27A)	109.5	C(34)–C(35)–C(36)	112.5(4)
C(28)–C(27)–H(27A)	109.5	C(34)–C(35)–H(35A)	109.1
C(26)–C(27)–H(27B)	109.5	C(36)–C(35)–H(35A)	109.1
C(28)–C(27)–H(27B)	109.5	C(34)–C(35)–H(35B)	109.1
H(27A)–C(27)–H(27B)	108.1	C(36)–C(35)–H(35B)	109.1
N(4)–C(28)–C(27)	115.2(3)	H(35A)–C(35)–H(35B)	107.8
N(4)–C(28)–H(28A)	108.5	C(35)–C(36)–H(36A)	109.5
C(27)–C(28)–H(28A)	108.5	C(35)–C(36)–H(36B)	109.5
N(4)–C(28)–H(28B)	108.5	H(36A)–C(36)–H(36B)	109.5
C(27)–C(28)–H(28B)	108.5	C(35)–C(36)–H(36C)	109.5
H(28A)–C(28)–H(28B)	107.5	H(36A)–C(36)–H(36C)	109.5
C(30)–C(29)–H(29A)	109.5	H(36B)–C(36)–H(36C)	109.5
C(30)–C(29)–H(29B)	109.5	C(38)–C(37)–N(4)	115.1(3)
H(29A)–C(29)–H(29B)	109.5	C(38)–C(37)–H(37A)	108.5
C(30)–C(29)–H(29C)	109.5	N(4)–C(37)–H(37A)	108.5
H(29A)–C(29)–H(29C)	109.5	C(38)–C(37)–H(37B)	108.5
H(29B)–C(29)–H(29C)	109.5	N(4)–C(37)–H(37B)	108.5
C(29)–C(30)–C(31)	116.1(4)	H(37A)–C(37)–H(37B)	107.5
C(29)–C(30)–H(30A)	108.2	C(37)–C(38)–C(39)	111.1(4)
C(31)–C(30)–H(30A)	108.2	C(37)–C(38)–H(38A)	109.4
C(29)–C(30)–H(30B)	108.2	C(39)–C(38)–H(38A)	109.4
C(31)–C(30)–H(30B)	108.2	C(37)–C(38)–H(38B)	109.4

H(30A)–C(30)–H(30B)	107.4	C(39)–C(38)–H(38B)	109.4
C(30)–C(31)–C(32)	113.8(4)	H(38A)–C(38)–H(38B)	108.0
C(30)–C(31)–H(31A)	108.8	C(40)–C(39)–C(38)	112.4(4)
C(32)–C(31)–H(31A)	108.8	C(40)–C(39)–H(39A)	109.1
C(30)–C(31)–H(31B)	108.8	C(38)–C(39)–H(39A)	109.1
C(32)–C(31)–H(31B)	108.8	C(40)–C(39)–H(39B)	109.1
H(31A)–C(31)–H(31B)	107.7	C(38)–C(39)–H(39B)	109.1
C(31)–C(32)–N(4)	115.2(3)	H(39A)–C(39)–H(39B)	107.9
C(31)–C(32)–H(32A)	108.5	C(39)–C(40)–H(40A)	109.5
N(4)–C(32)–H(32A)	108.5	C(39)–C(40)–H(40B)	109.5
C(31)–C(32)–H(32B)	108.5	H(40A)–C(40)–H(40B)	109.5
N(4)–C(32)–H(32B)	108.5	C(39)–C(40)–H(40C)	109.5
H(32A)–C(32)–H(32B)	107.5	H(40A)–C(40)–H(40C)	109.5
C(3)–N(1)–C(1)	122.5(4)	H(40B)–C(40)–H(40C)	109.5
C(3)–N(1)–C(2)	120.0(4)	O(5)–Mo(1)–O(3)	86.97(11)
C(1)–N(1)–C(2)	115.8(3)	O(1)–Mo(1)–O(2)	101.91(12)
C(6)–N(2)–Mo(6)	162.6(3)	O(4)–Mo(1)–O(2)	86.17(11)
C(9)–N(3)–C(21)	110.3(3)	O(5)–Mo(1)–O(2)	153.15(10)
C(9)–N(3)–C(17)	106.5(3)	O(3)–Mo(1)–O(2)	83.05(11)
C(21)–N(3)–C(17)	111.9(3)	O(1)–Mo(1)–O(12)	176.93(11)
C(9)–N(3)–C(13)	111.6(3)	O(4)–Mo(1)–O(12)	77.20(9)
C(21)–N(3)–C(13)	106.5(3)	O(5)–Mo(1)–O(12)	77.89(9)
C(17)–N(3)–C(13)	110.1(3)	O(3)–Mo(1)–O(12)	75.40(9)
C(37)–N(4)–C(28)	111.4(3)	O(2)–Mo(1)–O(12)	75.49(9)
C(37)–N(4)–C(33)	111.7(3)	O(11)–Mo(2)–O(13)	104.57(12)
C(28)–N(4)–C(33)	107.0(3)	O(11)–Mo(2)–O(17)	104.62(12)
C(37)–N(4)–C(32)	107.3(3)	O(13)–Mo(2)–O(17)	91.48(11)
C(28)–N(4)–C(32)	109.9(3)	O(11)–Mo(2)–O(4)	102.80(12)
C(33)–N(4)–C(32)	109.6(3)	O(13)–Mo(2)–O(4)	152.28(11)
Mo(3)–O(2)–Mo(1)	117.51(12)	O(17)–Mo(2)–O(4)	85.80(11)
Mo(4)–O(3)–Mo(1)	117.63(12)	O(11)–Mo(2)–O(10)	102.64(12)
Mo(1)–O(4)–Mo(2)	118.33(12)	O(13)–Mo(2)–O(10)	87.84(11)
Mo(1)–O(5)–Mo(5)	116.22(12)	O(17)–Mo(2)–O(10)	151.98(10)
Mo(3)–O(8)–Mo(4)	117.11(12)	O(4)–Mo(2)–O(10)	81.99(11)
Mo(5)–O(10)–Mo(2)	116.38(12)	O(11)–Mo(2)–O(12)	177.34(11)
Mo(6)–O(12)–Mo(5)	91.29(8)	O(13)–Mo(2)–O(12)	77.36(9)

Mo(6)–O(12)–Mo(4)	90.38(8)	O(17)–Mo(2)–O(12)	77.03(9)
Mo(5)–O(12)–Mo(4)	90.32(8)	O(4)–Mo(2)–O(12)	75.14(9)
Mo(6)–O(12)–Mo(3)	90.68(8)	O(10)–Mo(2)–O(12)	75.50(9)
Mo(5)–O(12)–Mo(3)	178.02(11)	O(7)–Mo(3)–O(2)	103.97(12)
Mo(4)–O(12)–Mo(3)	89.91(8)	O(7)–Mo(3)–O(8)	104.22(12)
Mo(6)–O(12)–Mo(2)	90.69(8)	O(2)–Mo(3)–O(8)	90.29(11)
Mo(5)–O(12)–Mo(2)	90.03(8)	O(7)–Mo(3)–O(15)	103.12(12)
Mo(4)–O(12)–Mo(2)	178.87(11)	O(2)–Mo(3)–O(15)	152.62(10)
Mo(3)–O(12)–Mo(2)	89.71(8)	O(8)–Mo(3)–O(15)	86.89(11)
Mo(6)–O(12)–Mo(1)	179.96(13)	O(7)–Mo(3)–O(17)	102.91(12)
Mo(5)–O(12)–Mo(1)	88.75(8)	O(2)–Mo(3)–O(17)	86.55(10)
Mo(4)–O(12)–Mo(1)	89.60(8)	O(8)–Mo(3)–O(17)	152.65(10)
Mo(3)–O(12)–Mo(1)	89.29(7)	O(15)–Mo(3)–O(17)	83.63(10)
Mo(2)–O(12)–Mo(1)	89.33(8)	O(7)–Mo(3)–O(12)	177.92(11)
Mo(2)–O(13)–Mo(6)	113.97(12)	O(2)–Mo(3)–O(12)	77.72(9)
Mo(6)–O(14)–Mo(4)	113.22(12)	O(8)–Mo(3)–O(12)	76.90(9)
Mo(6)–O(15)–Mo(3)	114.44(12)	O(15)–Mo(3)–O(12)	75.12(9)
Mo(5)–O(16)–Mo(6)	114.46(12)	O(17)–Mo(3)–O(12)	75.88(9)
Mo(2)–O(17)–Mo(3)	117.38(12)	O(6)–Mo(4)–O(3)	103.13(12)
Mo(4)–O(18)–Mo(5)	116.94(13)	O(6)–Mo(4)–O(18)	103.97(13)
O(1)–Mo(1)–O(4)	104.40(12)	O(3)–Mo(4)–O(18)	89.76(11)
O(1)–Mo(1)–O(5)	104.59(12)	O(6)–Mo(4)–O(14)	103.29(12)
O(4)–Mo(1)–O(5)	91.35(11)	O(3)–Mo(4)–O(14)	153.38(10)
O(1)–Mo(1)–O(3)	102.79(12)	O(18)–Mo(4)–O(14)	87.01(11)
O(4)–Mo(1)–O(3)	152.28(10)	O(6)–Mo(4)–O(8)	103.20(12)
O(18)–Mo(4)–O(8)	152.74(11)	O(3)–Mo(4)–O(8)	86.18(11)
O(14)–Mo(4)–O(8)	84.73(11)		
O(6)–Mo(4)–O(12)	178.97(12)		
O(3)–Mo(4)–O(12)	77.09(9)		
O(18)–Mo(4)–O(12)	77.02(9)		
O(14)–Mo(4)–O(12)	76.44(9)		
O(8)–Mo(4)–O(12)	75.79(9)		
O(9)–Mo(5)–O(16)	104.04(12)		
O(9)–Mo(5)–O(10)	104.29(13)		
O(16)–Mo(5)–O(10)	90.70(11)		
O(9)–Mo(5)–O(5)	101.95(12)		

O(16)–Mo(5)–O(5)	153.77(11)
O(10)–Mo(5)–O(5)	86.32(11)
O(9)–Mo(5)–O(18)	102.15(13)
O(16)–Mo(5)–O(18)	87.66(11)
O(10)–Mo(5)–O(18)	153.11(11)
O(5)–Mo(5)–O(18)	83.45(11)
O(9)–Mo(5)–O(12)	177.60(12)
O(16)–Mo(5)–O(12)	77.07(9)
O(10)–Mo(5)–O(12)	77.76(9)
O(5)–Mo(5)–O(12)	76.83(9)
O(18)–Mo(5)–O(12)	75.71(9)
N(2)–Mo(6)–O(15)	105.36(13)
N(2)–Mo(6)–O(14)	103.63(12)
O(15)–Mo(6)–O(14)	92.26(11)
N(2)–Mo(6)–O(16)	97.63(13)
O(15)–Mo(6)–O(16)	156.19(10)
O(14)–Mo(6)–O(16)	88.25(11)
N(2)–Mo(6)–O(13)	98.32(12)
O(15)–Mo(6)–O(13)	87.60(11)
O(14)–Mo(6)–O(13)	157.25(10)
O(16)–Mo(6)–O(13)	82.95(11)
N(2)–Mo(6)–O(12)	173.69(12)
O(15)–Mo(6)–O(12)	79.49(9)
O(14)–Mo(6)–O(12)	79.95(9)
O(16)–Mo(6)–O(12)	77.16(9)
O(13)–Mo(6)–O(12)	77.66(9)

ORTEP-8 representation of compound **10**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity.



Compound 14

Crystal growth Diffusion of ether into an acetonitrile solution at room temperature.
Mounting method Oil

Crystal Data		
Chemical formula	C41H85Mo6N5O18	
Formula weight	1511.77 g mol-1	
Temperature	100 (2) K	
Crystal size	0.110 × 0.060 × 0.010 mm3	
Crystal description	Light yellow plate	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 18.8960(13) Å	α = 90°.
	b = 16.5079(11) Å	β = 90.224(2)°.
	c = 18.4858 (13) Å	γ = 90°.
Volume	5766.3(7) Å3	
Z	4	
F(000)	3048	
Density (calculated)	1.741 Mg cm-3	
Absorption coefficient	1.332 mm-1	
Data Collection		
Diffractometer	Rigaku AFC 12 goniometer	
Radiation	Mo-Kα	
2θ range for data collection	3.089 – 27.485°.	
Reflections collected	65963	
Independent reflections	13088 [Rint = 0.0741]	
Transmission coefficients	1.000	
Data corrections	Gaussian	
Index ranges	-24<=h<=24, -20<=k<=21, -23<=l<=24	
Refinement method		
Full-matrix least squares on F2		
Weighting scheme	None	
3		
Data / restraints / parameters	13088 / 3369 / 967	
Data to parameter ratio	13.53	
Goodness of fit on F2	1.122	
R indices	[Io>2σ>(Io)] data	R1 = 0.0700, wR2 = 0.1795
	All 2558 data	R1 = 0.0958, wR2 = 0.1934
Final difference map	Largest diff. peak +2.896 and hole -1.814 e.Å-3	

Bond lengths [Å] and angles [°]

C1–N1	1.466(11)	Mo6–O7	1.955(6)
C1–C2	1.523(10)	Mo6–O6	1.984(5)
C1–H1A	0.9900	Mo6–O1	2.365(6)
C1–H1B	0.9900	C11–C12	1.526(11)
C2–C3	1.527(11)	C11–N11	1.529(9)
C2–H2A	0.9900	C11–H11A	0.9900
C2–H2B	0.9900	C11–H11B	0.9900
C3–N2	1.477(9)	C12–C13	1.531(11)
C3–H3A	0.9900	C12–H12A	0.9900
C3–H3B	0.9900	C12–H12B	0.9900
C4–N2	1.360(12)	C13–C14	1.538(13)
C4–C5	1.376(13)	C13–H13A	0.9900
C4–H4	0.9500	C13–H13B	0.9900
C5–C6	1.400(17)	C14–H14A	0.9800
C5–H5	0.9500	C14–H14B	0.9800
C6–C7	1.381(14)	C14–H14C	0.9800
C6–H6	0.9500	C15–C16	1.516(13)
C7–N2	1.354(12)	C15–N11	1.519(11)
C7–H7	0.9500	C15–H15A	0.9900
Mo1–N1	1.725(7)	C15–H15B	0.9900
Mo1–O3	1.909(6)	C16–C17	1.545(14)
Mo1–O2	1.925(5)	C16–H16A	0.9900
Mo1–O5	2.013(5)	C16–H16B	0.9900
Mo1–O4	2.013(5)	C17–C18	1.428(17)
Mo1–O1	2.214(6)	C17–H17A	0.9900
Mo2–O14	1.688(5)	C17–H17B	0.9900
Mo2–O10	1.851(5)	C18–H18A	0.9800
Mo2–O6	1.881(6)	C18–H18B	0.9800
Mo2–O2	1.946(6)	C18–H18C	0.9800
Mo2–O13	2.040(5)	C19–C20	1.507(13)
Mo2–O1	2.328(4)	C19–N11	1.534(10)
Mo3–O15	1.681(6)	C19–H19A	0.9900
Mo3–O11	1.857(5)	C19–H19B	0.9900
Mo3–O7	1.895(6)	C20–C21	1.490(13)

Mo3–O3	1.953(6)	C20–H20A	0.9900
Mo3–O10	2.061(5)	C20–H20B	0.9900
Mo3–O1	2.345(5)	C21–C22	1.531(15)
Mo4–O16	1.678(5)	C21–H21A	0.9900
Mo4–O12	1.839(5)	C21–H21B	0.9900
Mo4–O4	1.865(6)	C22–H22A	0.9800
Mo4–O8	1.988(6)	C22–H22B	0.9800
Mo4–O11	2.034(6)	C22–H22C	0.9800
Mo4–O1	2.338(4)	C23–C24	1.526(10)
Mo5–O17	1.683(5)	C23–N11	1.533(11)
Mo5–O5	1.865(6)	C23–H23A	0.9900
Mo5–O13	1.870(5)	C23–H23B	0.9900
Mo5–O9	1.965(6)	C24–C25	1.523(13)
Mo5–O12	2.050(5)	C24–H24A	0.9900
Mo5–O1	2.353(5)	C24–H24B	0.9900
Mo6–O18	1.679(7)	C25–C26	1.546(12)
Mo6–O8	1.880(5)	C25–H25A	0.9900
Mo6–O9	1.899(6)	C25–H25B	0.9900
C31–H31B	0.9900	C102–C103	1.527(15)
C32–C33	1.515(13)	C102–H10C	0.9900
C32–H32A	0.9900	C102–H10D	0.9900
C32–H32B	0.9900	C103–N102	1.478(13)
C33–C34	1.554(12)	C103–H10E	0.9900
C33–H33A	0.9900	C103–H10F	0.9900
C33–H33B	0.9900	C104–N102	1.361(15)
C34–H34A	0.9800	C104–C105	1.377(16)
C34–H34B	0.9800	C104–H104	0.9500
C34–H34C	0.9800	C105–C106	1.40(2)
C35–C36	1.492(14)	C105–H105	0.9500
C35–N31	1.535(11)	C106–C107	1.383(17)
C35–H35A	0.9900	C106–H106	0.9500
C35–H35B	0.9900	C107–N102	1.356(15)
C36–C37	1.532(15)	C107–H107	0.9500
C36–H36A	0.9900	Mo11–N101	1.734(11)
C36–H36B	0.9900	Mo11–O102	1.917(9)
C37–C38	1.508(18)	Mo11–O103	1.914(10)

C37–H37A	0.9900	Mo11–O105	2.010(10)
C37–H37B	0.9900	Mo11–O104	2.020(10)
C38–H38A	0.9800	Mo11–O101	2.211(9)
C38–H38B	0.9800	Mo11–Mo12	3.221(7)
C38–H38C	0.9800	Mo12–O114	1.688(9)
C39–N31	1.528(12)	Mo12–O110	1.853(10)
C39–C40	1.534(12)	Mo12–O106	1.885(10)
C39–H39A	0.9900	Mo12–O102	1.948(10)
C39–H39B	0.9900	Mo12–O113	2.040(10)
C40–C41	1.513(13)	Mo12–O101	2.327(8)
C40–H40A	0.9900	Mo13–O115	1.680(10)
C40–H40B	0.9900	Mo13–O111	1.858(10)
C41–C42	1.530(15)	Mo13–O107	1.894(11)
C41–H41A	0.9900	Mo13–O103	1.951(11)
C41–H41B	0.9900	Mo13–O110	2.063(10)
C42–H42A	0.9800	Mo13–O101	2.343(9)
C42–H42B	0.9800	Mo14–O116	1.680(10)
C42–H42C	0.9800	Mo14–O112	1.833(10)
C43–C44	1.505(12)	Mo14–O104	1.861(11)
C43–N31	1.539(10)	Mo14–O108	1.990(11)
C43–H43A	0.9900	Mo14–O111	2.037(10)
C43–H43B	0.9900	Mo14–O101	2.336(8)
C44–C45	1.539(13)	Mo15–O117	1.685(10)
C44–H44A	0.9900	Mo15–O105	1.863(10)
C44–H44B	0.9900	Mo15–O113	1.867(10)
C45–C46	1.539(15)	Mo15–O109	1.970(11)
C45–H45A	0.9900	Mo15–O112	2.050(10)
C45–H45B	0.9900	Mo15–O101	2.348(9)
C46–H46A	0.9800	Mo16–O118	1.682(11)
C46–H46B	0.9800	Mo16–O108	1.879(10)
C46–H46C	0.9800	Mo16–O109	1.893(10)
C51–N51	1.171(17)	Mo16–O107	1.957(10)
C51–C52	1.450(17)	Mo16–O106	1.985(10)
C52–H52A	0.9800	Mo16–O101	2.364(10)
C52–H52B	0.9800	C201–N201	1.479(14)
C52–H52C	0.9800	C201–C202	1.522(14)

C101–N101	1.496(14)	C201–H20C	0.9900
C101–C102	1.522(14)	C201–H20D	0.9900
C101–H10A	0.9900	C202–C203	1.527(15)
C101–H10B	0.9900	C202–H20E	0.9900
C202–H20F	0.9900		
C203–N202	1.480(14)		
C203–H20G	0.9900		
C203–H20H	0.9900		
C204–N202	1.362(15)		
C204–C205	1.377(16)		
C204–H204	0.9500		
C205–C206	1.40(2)		
C205–H205	0.9500		
C206–C207	1.383(17)		
C206–H206	0.9500		
C207–N202	1.357(15)		
C207–H207	0.9500		
Mo21–N201	1.727(11)		
Mo21–O203	1.912(10)		
Mo21–O202	1.921(9)		
Mo21–O205	2.013(10)		
Mo21–O204	2.017(10)		
Mo21–O201	2.215(9)		
Mo21–Mo22	3.226(7)		
Mo22–O214	1.689(9)		
Mo22–O210	1.853(10)		
Mo22–O206	1.882(10)		
Mo22–O202	1.949(10)		
Mo22–O213	2.039(10)		
Mo22–O201	2.326(8)		
Mo23–O215	1.680(10)		
Mo23–O211	1.856(10)		
Mo23–O207	1.892(11)		
Mo23–O203	1.954(11)		
Mo23–O210	2.065(10)		
Mo23–O201	2.344(9)		

Mo24–O216	1.680(10)	Mo25–O213	1.869(10)
Mo24–O212	1.834(10)	Mo25–O205	1.866(10)
Mo24–O204	1.865(11)	Mo25–O209	1.968(11)
Mo24–O208	1.989(11)	Mo25–O212	2.049(10)
Mo24–O211	2.036(10)	Mo25–O201	2.349(9)
Mo24–O201	2.335(9)	Mo26–O218	1.680(11)
Mo25–O217	1.685(10)	Mo26–O208	1.879(10)
Mo26–O209	1.899(10)	Mo26–O201	2.368(10)
Mo26–O207	1.953(10)	Mo26–O206	1.985(10)
N1–C1–C2	109.7(6)	O15–Mo3–O11	104.3(3)
N1–C1–H1A	109.7	O15–Mo3–O7	104.4(3)
C2–C1–H1A	109.7	O11–Mo3–O7	92.9(3)
N1–C1–H1B	109.7	O15–Mo3–O3	103.1(3)
C2–C1–H1B	109.7	O11–Mo3–O3	89.1(2)
H1A–C1–H1B	108.2	O7–Mo3–O3	151.1(2)
C1–C2–C3	112.1(6)	O15–Mo3–O10	102.7(2)
C1–C2–H2A	109.2	O11–Mo3–O10	152.8(2)
C3–C2–H2A	109.2	O7–Mo3–O10	83.9(2)
C1–C2–H2B	109.2	O3–Mo3–O10	81.4(2)
C3–C2–H2B	109.2	O15–Mo3–O1	177.2(2)
H2A–C2–H2B	107.9	O11–Mo3–O1	78.2(2)
N2–C3–C2	111.7(7)	O7–Mo3–O1	76.8(2)
N2–C3–H3A	109.3	O3–Mo3–O1	75.4(2)
C2–C3–H3A	109.3	O10–Mo3–O1	74.76(19)
N2–C3–H3B	109.3	O16–Mo4–O12	103.7(3)
C2–C3–H3B	109.3	O16–Mo4–O4	104.0(3)
H3A–C3–H3B	107.9	O12–Mo4–O4	93.4(3)
N2–C4–C5	107.2(10)	O16–Mo4–O8	102.2(3)
N2–C4–H4	126.4	O12–Mo4–O8	88.2(3)
C5–C4–H4	126.4	O4–Mo4–O8	152.6(2)
C4–C5–C6	107.6(9)	O16–Mo4–O11	102.0(3)
C4–C5–H5	126.2	O12–Mo4–O11	153.8(2)
C6–C5–H5	126.2	O4–Mo4–O11	85.3(2)
C7–C6–C5	107.4(9)	O8–Mo4–O11	81.5(2)
C7–C6–H6	126.3	O16–Mo4–O1	176.7(3)
C5–C6–H6	126.3	O12–Mo4–O1	79.10(19)
N2–C7–C6	107.3(10)	O4–Mo4–O1	77.5(2)

N2–C7–H7	126.4	O8–Mo4–O1	75.9(2)
C6–C7–H7	126.4	O11–Mo4–O1	75.09(19)
N1–Mo1–O3	105.2(3)	O17–Mo5–O5	103.9(3)
N1–Mo1–O2	102.4(3)	O17–Mo5–O13	104.7(2)
O3–Mo1–O2	92.4(2)	O5–Mo5–O13	93.1(2)
N1–Mo1–O5	98.1(3)	O17–Mo5–O9	103.1(3)
O3–Mo1–O5	156.2(2)	O5–Mo5–O9	151.6(2)
O2–Mo1–O5	86.9(2)	O13–Mo5–O9	88.8(2)
N1–Mo1–O4	100.1(3)	O17–Mo5–O12	101.9(2)
O3–Mo1–O4	88.4(2)	O5–Mo5–O12	84.7(2)
O2–Mo1–O4	156.4(2)	O13–Mo5–O12	153.0(2)
O5–Mo1–O4	83.0(2)	O9–Mo5–O12	81.0(2)
N1–Mo1–O1	174.8(3)	O17–Mo5–O1	176.8(2)
O3–Mo1–O1	79.5(2)	O5–Mo5–O1	76.4(2)
O2–Mo1–O1	79.3(2)	O13–Mo5–O1	78.4(2)
O5–Mo1–O1	77.0(2)	O9–Mo5–O1	76.2(2)
O4–Mo1–O1	77.7(2)	O12–Mo5–O1	74.89(19)
O14–Mo2–O10	105.0(2)	O18–Mo6–O8	105.0(3)
O14–Mo2–O6	103.7(3)	O18–Mo6–O9	104.5(3)
O10–Mo2–O6	93.4(3)	O8–Mo6–O9	89.9(2)
O14–Mo2–O2	101.2(3)	O18–Mo6–O7	103.1(3)
O10–Mo2–O2	90.0(2)	O8–Mo6–O7	87.2(2)
O6–Mo2–O2	153.0(2)	O9–Mo6–O7	152.1(3)
O14–Mo2–O13	100.0(2)	O18–Mo6–O6	102.2(3)
O10–Mo2–O13	154.8(2)	O8–Mo6–O6	152.6(3)
O6–Mo2–O13	84.2(2)	O9–Mo6–O6	86.6(2)
O2–Mo2–O13	81.5(2)	O7–Mo6–O6	83.5(2)
O14–Mo2–O1	175.3(3)	O18–Mo6–O1	177.2(3)
O10–Mo2–O1	79.02(19)	O8–Mo6–O1	77.2(2)
O6–Mo2–O1	78.3(2)	O9–Mo6–O1	77.1(2)
O2–Mo2–O1	76.0(2)	O7–Mo6–O1	75.2(2)
O13–Mo2–O1	75.87(18)	O6–Mo6–O1	75.5(2)
C1–N1–Mo1	167.8(5)	H15A–C15–H15B	107.2
C7–N2–C4	110.5(8)	C15–C16–C17	110.1(8)
C7–N2–C3	123.1(8)	C15–C16–H16A	109.6
C4–N2–C3	126.2(8)	C17–C16–H16A	109.6
Mo1–O1–Mo2	90.69(18)	C15–C16–H16B	109.6

Mo1–O1–Mo4	91.03(18)	C17–C16–H16B	109.6
Mo2–O1–Mo4	178.2(3)	H16A–C16–H16B	108.1
Mo1–O1–Mo3	90.71(18)	C18–C17–C16	115.0(11)
Mo2–O1–Mo3	90.26(17)	C18–C17–H17A	108.5
Mo4–O1–Mo3	90.07(17)	C16–C17–H17A	108.5
Mo1–O1–Mo5	91.3(2)	C18–C17–H17B	108.5
Mo2–O1–Mo5	90.06(17)	C16–C17–H17B	108.5
Mo4–O1–Mo5	89.56(16)	H17A–C17–H17B	107.5
Mo3–O1–Mo5	178.0(3)	C17–C18–H18A	109.5
Mo1–O1–Mo6	179.7(3)	C17–C18–H18B	109.5
Mo2–O1–Mo6	89.15(17)	H18A–C18–H18B	109.5
Mo4–O1–Mo6	89.12(17)	C17–C18–H18C	109.5
Mo3–O1–Mo6	89.1(2)	H18A–C18–H18C	109.5
Mo5–O1–Mo6	88.95(17)	H18B–C18–H18C	109.5
Mo1–O2–Mo2	113.2(3)	C20–C19–N11	115.9(7)
Mo1–O3–Mo3	114.3(3)	C20–C19–H19A	108.3
Mo4–O4–Mo1	113.7(3)	N11–C19–H19A	108.3
Mo5–O5–Mo1	114.7(3)	C20–C19–H19B	108.3
Mo2–O6–Mo6	116.9(3)	N11–C19–H19B	108.3
Mo3–O7–Mo6	118.1(3)	H19A–C19–H19B	107.4
Mo6–O8–Mo4	117.1(3)	C21–C20–C19	111.4(8)
Mo6–O9–Mo5	117.6(3)	C21–C20–H20A	109.3
Mo2–O10–Mo3	115.6(2)	C19–C20–H20A	109.3
Mo3–O11–Mo4	116.7(3)	C21–C20–H20B	109.3
Mo4–O12–Mo5	116.2(2)	C19–C20–H20B	109.3
Mo5–O13–Mo2	115.7(2)	H20A–C20–H20B	108.0
C12–C11–N11	114.5(6)	C20–C21–C22	114.9(9)
C12–C11–H11A	108.6	C20–C21–H21A	108.5
N11–C11–H11A	108.6	C22–C21–H21A	108.5
C12–C11–H11B	108.6	C20–C21–H21B	108.5
N11–C11–H11B	108.6	C22–C21–H21B	108.5
H11A–C11–H11B	107.6	H21A–C21–H21B	107.5
C11–C12–C13	109.7(7)	C21–C22–H22A	109.5
C11–C12–H12A	109.7	C21–C22–H22B	109.5
C13–C12–H12A	109.7	H22A–C22–H22B	109.5
C11–C12–H12B	109.7	C21–C22–H22C	109.5
C13–C12–H12B	109.7	H22A–C22–H22C	109.5

H12A–C12–H12B	108.2	H22B–C22–H22C	109.5
C12–C13–C14	112.1(8)	C24–C23–N11	114.9(6)
C12–C13–H13A	109.2	C24–C23–H23A	108.5
C14–C13–H13A	109.2	N11–C23–H23A	108.5
C12–C13–H13B	109.2	C24–C23–H23B	108.5
C14–C13–H13B	109.2	N11–C23–H23B	108.5
H13A–C13–H13B	107.9	H23A–C23–H23B	107.5
C13–C14–H14A	109.5	C25–C24–C23	110.1(7)
C13–C14–H14B	109.5	C25–C24–H24A	109.6
H14A–C14–H14B	109.5	C23–C24–H24A	109.6
C13–C14–H14C	109.5	C25–C24–H24B	109.6
H14A–C14–H14C	109.5	C23–C24–H24B	109.6
H14B–C14–H14C	109.5	H24A–C24–H24B	108.1
C16–C15–N11	117.2(7)	C24–C25–C26	112.7(8)
C16–C15–H15A	108.0	C24–C25–H25A	109.0
N11–C15–H15A	108.0	C26–C25–H25A	109.0
C16–C15–H15B	108.0	C24–C25–H25B	109.0
N11–C15–H15B	108.0	C26–C25–H25B	109.0
H25A–C25–H25B	107.8	H38B–C38–H38C	109.5
C25–C26–H26A	109.5	N31–C39–C40	115.3(6)
C25–C26–H26B	109.5	N31–C39–H39A	108.5
H26A–C26–H26B	109.5	C40–C39–H39A	108.5
C25–C26–H26C	109.5	N31–C39–H39B	108.5
H26A–C26–H26C	109.5	C40–C39–H39B	108.5
H26B–C26–H26C	109.5	H39A–C39–H39B	107.5
C15–N11–C11	109.0(6)	C41–C40–C39	109.4(7)
C15–N11–C23	110.4(7)	C41–C40–H40A	109.8
C11–N11–C23	108.1(6)	C39–C40–H40A	109.8
C15–N11–C19	107.2(6)	C41–C40–H40B	109.8
C11–N11–C19	110.8(7)	C39–C40–H40B	109.8
C23–N11–C19	111.3(6)	H40A–C40–H40B	108.2
N31–C31–C32	115.3(7)	C40–C41–C42	112.5(8)
N31–C31–H31A	108.4	C40–C41–H41A	109.1
C32–C31–H31A	108.4	C42–C41–H41A	109.1
N31–C31–H31B	108.4	C40–C41–H41B	109.1
C32–C31–H31B	108.4	C42–C41–H41B	109.1
H31A–C31–H31B	107.5	H41A–C41–H41B	107.8

C33–C32–C31	110.1(7)	C41–C42–H42A	109.5
C33–C32–H32A	109.6	C41–C42–H42B	109.5
C31–C32–H32A	109.6	H42A–C42–H42B	109.5
C33–C32–H32B	109.6	C41–C42–H42C	109.5
C31–C32–H32B	109.6	H42A–C42–H42C	109.5
H32A–C32–H32B	108.2	H42B–C42–H42C	109.5
C32–C33–C34	110.3(7)	C44–C43–N31	114.4(6)
C32–C33–H33A	109.6	C44–C43–H43A	108.7
C34–C33–H33A	109.6	N31–C43–H43A	108.7
C32–C33–H33B	109.6	C44–C43–H43B	108.7
C34–C33–H33B	109.6	N31–C43–H43B	108.7
H33A–C33–H33B	108.1	H43A–C43–H43B	107.6
C33–C34–H34A	109.5	C43–C44–C45	111.2(7)
C33–C34–H34B	109.5	C43–C44–H44A	109.4
H34A–C34–H34B	109.5	C45–C44–H44A	109.4
C33–C34–H34C	109.5	C43–C44–H44B	109.4
H34A–C34–H34C	109.5	C45–C44–H44B	109.4
H34B–C34–H34C	109.5	H44A–C44–H44B	108.0
C36–C35–N31	114.9(7)	C46–C45–C44	111.6(9)
C36–C35–H35A	108.5	C46–C45–H45A	109.3
N31–C35–H35A	108.5	C44–C45–H45A	109.3
C36–C35–H35B	108.5	C46–C45–H45B	109.3
N31–C35–H35B	108.5	C44–C45–H45B	109.3
H35A–C35–H35B	107.5	H45A–C45–H45B	108.0
C35–C36–C37	110.3(9)	C45–C46–H46A	109.5
C35–C36–H36A	109.6	C45–C46–H46B	109.5
C37–C36–H36A	109.6	H46A–C46–H46B	109.5
C35–C36–H36B	109.6	C45–C46–H46C	109.5
C37–C36–H36B	109.6	H46A–C46–H46C	109.5
H36A–C36–H36B	108.1	H46B–C46–H46C	109.5
C38–C37–C36	111.4(11)	C31–N31–C39	109.7(7)
C38–C37–H37A	109.3	C31–N31–C35	111.0(6)
C36–C37–H37A	109.3	C39–N31–C35	107.1(6)
C38–C37–H37B	109.3	C31–N31–C43	108.1(6)
C36–C37–H37B	109.3	C39–N31–C43	110.4(6)
H37A–C37–H37B	108.0	C35–N31–C43	110.6(7)
C37–C38–H38A	109.5	N51–C51–C52	179.3(18)

C37–C38–H38B	109.5	C51–C52–H52A	109.5
H38A–C38–H38B	109.5	C51–C52–H52B	109.5
C37–C38–H38C	109.5	H52A–C52–H52B	109.5
H38A–C38–H38C	109.5	C51–C52–H52C	109.5
H52A–C52–H52C	109.5	O110–Mo12–O113	154.7(5)
H52B–C52–H52C	109.5	O106–Mo12–O113	84.1(7)
N101–C101–C102	108.4(16)	O102–Mo12–O113	81.6(6)
N101–C101–H10A	110.0	O114–Mo12–O101	175.4(9)
C102–C101–H10A	110.0	O110–Mo12–O101	78.9(4)
N101–C101–H10B	110.0	O106–Mo12–O101	78.2(5)
C102–C101–H10B	110.0	O102–Mo12–O101	76.2(4)
H10A–C101–H10B	108.4	O113–Mo12–O101	76.0(4)
C101–C102–C103	112.2(16)	O114–Mo12–Mo11	134.5(8)
C101–C102–H10C	109.2	O110–Mo12–Mo11	79.8(5)
C103–C102–H10C	109.2	O106–Mo12–Mo11	121.5(4)
C101–C102–H10D	109.2	O102–Mo12–Mo11	33.2(3)
C103–C102–H10D	109.2	O113–Mo12–Mo11	80.4(4)
H10C–C102–H10D	107.9	O101–Mo12–Mo11	43.3(2)
N102–C103–C102	111.6(17)	O115–Mo13–O111	104.2(9)
N102–C103–H10E	109.3	O115–Mo13–O107	104.3(9)
C102–C103–H10E	109.3	O111–Mo13–O107	92.9(8)
N102–C103–H10F	109.3	O115–Mo13–O103	103.1(9)
C102–C103–H10F	109.3	O111–Mo13–O103	89.2(7)
H10E–C103–H10F	108.0	O107–Mo13–O103	151.1(6)
N102–C104–C105	107.2(14)	O115–Mo13–O110	102.9(8)
N102–C104–H104	126.4	O111–Mo13–O110	152.6(6)
C105–C104–H104	126.4	O107–Mo13–O110	83.9(7)
C104–C105–C106	107.4(15)	O103–Mo13–O110	81.1(6)
C104–C105–H105	126.3	O115–Mo13–O101	177.2(9)
C106–C105–H105	126.3	O111–Mo13–O101	78.1(5)
C107–C106–C105	106.9(17)	O107–Mo13–O101	77.0(5)
C107–C106–H106	126.6	O103–Mo13–O101	75.2(5)
C105–C106–H106	126.6	O110–Mo13–O101	74.6(4)
N102–C107–C106	106.9(17)	O116–Mo14–O112	103.5(9)
N102–C107–H107	126.6	O116–Mo14–O104	104.2(9)
C106–C107–H107	126.6	O112–Mo14–O104	93.7(8)
N101–Mo11–O102	104.8(8)	O116–Mo14–O108	101.9(9)

N101–Mo11–O103	102.9(8)	O112–Mo14–O108	88.5(7)
O102–Mo11–O103	92.7(7)	O104–Mo14–O108	152.6(6)
N101–Mo11–O105	100.2(8)	O116–Mo14–O111	101.8(9)
O102–Mo11–O105	87.1(6)	O112–Mo14–O111	154.1(6)
O103–Mo11–O105	156.2(6)	O104–Mo14–O111	85.4(7)
N101–Mo11–O104	97.8(7)	O108–Mo14–O111	81.0(7)
O102–Mo11–O104	156.6(6)	O116–Mo14–O101	176.4(9)
O103–Mo11–O104	88.1(7)	O112–Mo14–O101	79.5(5)
O105–Mo11–O104	82.9(6)	O104–Mo14–O101	77.5(5)
N101–Mo11–O101	174.9(8)	O108–Mo14–O101	76.0(5)
O102–Mo11–O101	79.7(4)	O111–Mo14–O101	75.0(4)
O103–Mo11–O101	79.2(5)	O117–Mo15–O105	105.8(9)
O105–Mo11–O101	77.3(5)	O117–Mo15–O113	105.5(8)
O104–Mo11–O101	77.5(5)	O105–Mo15–O113	93.4(7)
N101–Mo11–Mo12	138.4(7)	O117–Mo15–O109	100.6(9)
O102–Mo11–Mo12	33.9(3)	O105–Mo15–O109	151.8(6)
O103–Mo11–Mo12	81.6(4)	O113–Mo15–O109	88.8(7)
O105–Mo11–Mo12	85.2(4)	O117–Mo15–O112	100.4(8)
O104–Mo11–Mo12	123.8(4)	O105–Mo15–O112	85.0(7)
O101–Mo11–Mo12	46.2(2)	O113–Mo15–O112	153.5(6)
O114–Mo12–O110	105.2(9)	O109–Mo15–O112	80.8(7)
O114–Mo12–O106	103.5(8)	O117–Mo15–O101	174.8(9)
O110–Mo12–O106	93.2(8)	O105–Mo15–O101	76.8(5)
O114–Mo12–O102	101.4(8)	O113–Mo15–O101	78.6(5)
O110–Mo12–O102	90.2(7)	O109–Mo15–O101	76.2(5)
O106–Mo12–O102	153.0(6)	O112–Mo15–O101	75.2(4)
O114–Mo12–O113	99.9(8)	O118–Mo16–O108	105.0(9)
O118–Mo16–O109	104.6(9)	N202–C203–H20H	109.4
O108–Mo16–O109	89.8(7)	C202–C203–H20H	109.4
O118–Mo16–O107	102.6(9)	H20G–C203–H20H	108.0
O108–Mo16–O107	87.3(7)	N202–C204–C205	107.2(14)
O109–Mo16–O107	152.4(6)	N202–C204–H204	126.4
O118–Mo16–O106	102.0(9)	C205–C204–H204	126.4
O108–Mo16–O106	152.8(6)	C204–C205–C206	107.3(15)
O109–Mo16–O106	86.6(7)	C204–C205–H205	126.3
O107–Mo16–O106	83.5(7)	C206–C205–H205	126.3
O118–Mo16–O101	176.9(9)	C207–C206–C205	106.7(17)

O108–Mo16–O101	77.4(5)	C207–C206–H206	126.6
O109–Mo16–O101	77.2(5)	C205–C206–H206	126.6
O107–Mo16–O101	75.4(5)	N202–C207–C206	106.6(17)
O106–Mo16–O101	75.5(4)	N202–C207–H207	126.7
C101–N101–Mo11	138.8(16)	C206–C207–H207	126.7
C107–N102–C104	110.1(13)	N201–Mo21–O203	104.0(8)
C107–N102–C103	122.9(19)	N201–Mo21–O202	103.7(8)
C104–N102–C103	126(2)	O203–Mo21–O202	92.7(7)
Mo11–O101–Mo12	90.4(4)	N201–Mo21–O205	99.4(8)
Mo11–O101–Mo14	91.2(4)	O203–Mo21–O205	156.0(6)
Mo12–O101–Mo14	178.2(5)	O202–Mo21–O205	86.9(6)
Mo11–O101–Mo13	91.0(4)	N201–Mo21–O204	98.9(8)
Mo12–O101–Mo13	90.5(4)	O203–Mo21–O204	88.2(7)
Mo14–O101–Mo13	90.2(4)	O202–Mo21–O204	156.4(6)
Mo11–O101–Mo15	91.0(4)	O205–Mo21–O204	82.9(7)
Mo12–O101–Mo15	90.0(4)	N201–Mo21–O201	175.3(8)
Mo14–O101–Mo15	89.3(4)	O203–Mo21–O201	79.1(5)
Mo13–O101–Mo15	177.9(5)	O202–Mo21–O201	79.5(4)
Mo11–O101–Mo16	179.7(5)	O205–Mo21–O201	77.2(5)
Mo12–O101–Mo16	89.3(4)	O204–Mo21–O201	77.5(5)
Mo14–O101–Mo16	89.1(4)	N201–Mo21–Mo22	137.4(7)
Mo13–O101–Mo16	89.0(4)	O203–Mo21–Mo22	81.5(4)
Mo15–O101–Mo16	89.0(4)	O202–Mo21–Mo22	33.8(3)
Mo11–O102–Mo12	112.9(6)	O205–Mo21–Mo22	85.0(4)
Mo11–O103–Mo13	114.5(6)	O204–Mo21–Mo22	123.7(4)
Mo14–O104–Mo11	113.7(6)	O201–Mo21–Mo22	46.1(2)
Mo15–O105–Mo11	114.2(6)	O214–Mo22–O210	105.2(9)
Mo12–O106–Mo16	116.8(6)	O214–Mo22–O206	103.8(8)
Mo13–O107–Mo16	117.8(7)	O210–Mo22–O206	93.3(8)
Mo16–O108–Mo14	116.8(7)	O214–Mo22–O202	101.1(8)
Mo16–O109–Mo15	117.5(7)	O210–Mo22–O202	90.0(7)
Mo12–O110–Mo13	115.6(6)	O206–Mo22–O202	153.1(6)
Mo13–O111–Mo14	116.6(6)	O214–Mo22–O213	99.8(8)
Mo14–O112–Mo15	115.8(6)	O210–Mo22–O213	154.7(5)
Mo15–O113–Mo12	115.4(6)	O206–Mo22–O213	84.2(7)
N201–C201–C202	109.1(17)	O202–Mo22–O213	81.5(6)
N201–C201–H20C	109.9	O214–Mo22–O201	175.2(9)

C202–C201–H20C	109.9	O210–Mo22–O201	78.9(5)
N201–C201–H20D	109.9	O206–Mo22–O201	78.3(5)
C202–C201–H20D	109.9	O202–Mo22–O201	76.2(4)
H20C–C201–H20D	108.3	O213–Mo22–O201	76.0(4)
C201–C202–C203	112.3(14)	O214–Mo22–Mo21	134.3(8)
C201–C202–H20E	109.1	O210–Mo22–Mo21	79.6(5)
C203–C202–H20E	109.1	O206–Mo22–Mo21	121.6(4)
C201–C202–H20F	109.1	O202–Mo22–Mo21	33.2(3)
C203–C202–H20F	109.1	O213–Mo22–Mo21	80.4(4)
H20E–C202–H20F	107.9	O201–Mo22–Mo21	43.4(2)
N202–C203–C202	111.3(17)	O215–Mo23–O211	104.4(9)
N202–C203–H20G	109.4	O215–Mo23–O207	104.4(9)
C202–C203–H20G	109.4	O211–Mo23–O207	93.2(8)
O215–Mo23–O203	102.9(9)	C204–N202–C203	126(2)
O211–Mo23–O203	89.0(7)	Mo21–O201–Mo22	90.5(4)
O207–Mo23–O203	151.1(6)	Mo21–O201–Mo24	91.2(4)
O215–Mo23–O210	102.9(8)	Mo22–O201–Mo24	178.1(5)
O211–Mo23–O210	152.4(6)	Mo21–O201–Mo23	91.0(4)
O207–Mo23–O210	84.0(7)	Mo22–O201–Mo23	90.6(4)
O203–Mo23–O210	80.9(6)	Mo24–O201–Mo23	90.2(4)
O215–Mo23–O201	176.9(9)	Mo21–O201–Mo25	91.1(4)
O211–Mo23–O201	78.1(5)	Mo22–O201–Mo25	90.0(4)
O207–Mo23–O201	77.2(5)	Mo24–O201–Mo25	89.2(4)
O203–Mo23–O201	75.1(5)	Mo23–O201–Mo25	177.8(5)
O210–Mo23–O201	74.5(4)	Mo21–O201–Mo26	179.6(5)
O216–Mo24–O212	103.5(9)	Mo22–O201–Mo26	89.2(4)
O216–Mo24–O204	104.1(9)	Mo24–O201–Mo26	89.0(4)
O212–Mo24–O204	93.5(8)	Mo23–O201–Mo26	88.7(4)
O216–Mo24–O208	101.9(9)	Mo25–O201–Mo26	89.2(4)
O212–Mo24–O208	88.7(7)	Mo21–O202–Mo22	113.0(6)
O204–Mo24–O208	152.6(6)	Mo21–O203–Mo23	114.6(6)
O216–Mo24–O211	101.7(9)	Mo24–O204–Mo21	113.7(6)
O212–Mo24–O211	154.2(6)	Mo25–O205–Mo21	114.3(6)
O204–Mo24–O211	85.3(7)	Mo22–O206–Mo26	117.0(6)
O208–Mo24–O211	81.1(7)	Mo23–O207–Mo26	117.8(7)
O216–Mo24–O201	176.3(9)	Mo26–O208–Mo24	117.0(7)
O212–Mo24–O201	79.6(5)	Mo26–O209–Mo25	117.9(7)

O204–Mo24–O201	77.5(5)	Mo22–O210–Mo23	115.6(6)
O208–Mo24–O201	76.1(5)	Mo23–O211–Mo24	116.7(6)
O211–Mo24–O201	75.0(4)	Mo24–O212–Mo25	115.8(6)
O217–Mo25–O213	104.9(9)	Mo25–O213–Mo22	115.4(6)
O217–Mo25–O205	105.0(9)		
O213–Mo25–O205	93.1(7)		
O217–Mo25–O209	101.8(9)		
O213–Mo25–O209	88.9(7)		
O205–Mo25–O209	151.6(6)		
O217–Mo25–O212	101.1(8)		
O213–Mo25–O212	153.5(6)		
O205–Mo25–O212	85.0(7)		
O209–Mo25–O212	80.8(7)		
O217–Mo25–O201	175.9(9)		
O213–Mo25–O201	78.6(5)		
O205–Mo25–O201	76.7(5)		
O209–Mo25–O201	76.0(5)		
O212–Mo25–O201	75.2(4)		
O218–Mo26–O208	105.0(9)		
O218–Mo26–O209	104.6(9)		
O208–Mo26–O209	89.5(7)		
O218–Mo26–O207	102.9(9)		
O208–Mo26–O207	87.5(7)		
O209–Mo26–O207	152.1(6)		
O218–Mo26–O206	102.3(9)		
O208–Mo26–O206	152.5(6)		
O209–Mo26–O206	86.4(7)		
O207–Mo26–O206	83.7(7)		
O218–Mo26–O201	177.2(9)		
O208–Mo26–O201	77.2(5)		
O209–Mo26–O201	76.8(5)		
O207–Mo26–O201	75.5(5)		
O206–Mo26–O201	75.4(4)		
C201–N201–Mo21	151(3)		
C207–N202–C204	109.8(13)		
C207–N202–C203	122.2(19)		

ORTEP-9 representation of compound **14**: thermal ellipsoids at 30% probability, hydrogen atoms are omitted for clarity.