Electronic Supplementary Information for Dalton Transactions

Table C.1. Crystal data and structure refinement for $[cis\text{-}Mo_2(mhp)_2(CH_3CN)_4]^{2+}(BF_4^-)_2$ (**1**)

File: Chisholm 1449.

Empirical formula	C22 H24 Mo2 N6 O2, 2(C2 H3 N), 2(B F4)	
Formula weight	828.06	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$P2_1nm$	
Unit cell dimensions	a = 7.26150(10) Å	α= 90°.
	b = 12.0539(2) Å	β= 90°.
	c = 19.1113(3) Å	γ = 90°.
Volume	1672.9(4) $Å^3$	
Z	2	
Density (calculated)	1.644 Mg/m^3	
Absorption coefficient	0.830 mm^{-1}	
F(000)	824	
Crystal size	0.04 x 0.08 x 0.38 mm^3	
Theta range for data collection	3.28 to 27.49°.	
Index ranges	-9≤h≤9, 0≤k≤15, 0≤l≤24	
Reflections collected	19161	
Independent reflections	3950 [R(int) = 0.0336]	
Completeness to theta = 27.49°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3950 / 1 / 221	
Goodness-of-fit on F^2	1.034	
Final R indices [I>2sigma(I)]	R1 = 0.0282, wR2 = 0.0671	
R indices (all data)	R1 = 0.0324, wR2 = 0.0687	
Absolute structure parameter	0.02(4)	
Largest diff. peak and hole	0.544 and -0.381 $e.Å^{-3}$	

Table C.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Chisholm 1449. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	867(1)	3500(1)	0	17(1)
Mo(2)	-1482(1)	2450(1)	0	18(1)
N(1)	-307(3)	4476(2)	837(1)	20(1)
N(2)	-718(4)	1208(2)	769(1)	25(1)
N(3)	2598(4)	2748(2)	787(1)	22(1)
O(1)	-2789(3)	3327(2)	763(1)	23(1)
C(1)	2467(5)	5650(3)	934(2)	40(1)
C(2)	567(4)	5337(3)	1174(2)	25(1)
C(3)	-261(5)	5902(3)	1713(2)	32(1)
C(4)	-2022(5)	5606(3)	1933(2)	34(1)
C(5)	-2896(5)	4727(3)	1617(2)	29(1)
C(6)	-2013(4)	4166(2)	1068(2)	21(1)
C(7)	-552(5)	473(3)	1136(2)	28(1)
C(8)	-381(6)	-484(3)	1602(2)	44(1)
C(9)	3514(5)	2379(2)	1205(1)	23(1)
C(10)	4671(5)	1867(3)	1732(2)	29(1)
B(1)	9701(6)	1770(3)	3001(2)	35(1)
F(1)	10953(5)	1751(3)	2480(2)	81(1)
F(3)	10374(5)	2293(2)	3580(2)	69(1)
F(2)	9295(7)	705(2)	3182(2)	113(2)
F(4)	8096(5)	2278(3)	2797(2)	97(1)
N(4)	5680(6)	1064(3)	0	32(1)
C(21)	4814(7)	275(4)	0	28(1)
C(22)	3703(10)	-735(5)	0	50(2)
N(5)	9485(11)	8128(8)	0	89(3)
C(31)	8398(10)	7478(5)	0	45(1)
C(32)	6943(8)	6650(4)	0	38(1)

Table C.3. Bond lengths [Å] and angles [°] for Chisholm 1449.

Mo(1)-Mo(2)	2.1242(5)
Mo(1)-N(3)	2.160(3)
Mo(1)-N(1)	2.161(2)
Mo(2)-O(1)	2.035(2)
Mo(2)-N(2)	2.170(3)
N(1)-C(6)	1.367(4)
N(1)-C(2)	1.376(4)
N(2)-C(7)	1.137(4)
N(3)-C(9)	1.130(4)
O(1)-C(6)	1.297(4)
C(1)-C(2)	1.502(5)
C(2)-C(3)	1.373(5)
C(3)-C(4)	1.392(6)
C(4)-C(5)	1.374(5)
C(5)-C(6)	1.403(4)
C(7)-C(8)	1.462(5)
C(9)-C(10)	1.450(4)
B(1)-F(1)	1.349(5)
B(1)-F(3)	1.363(5)
B(1)-F(2)	1.361(5)
B(1)-F(4)	1.373(5)
N(4)-C(21)	1.140(6)
C(21)-C(22)	1.461(7)
N(5)-C(31)	1.112(10)
C(31)-C(32)	1.454(9)
Mo(2)-Mo(1)-N(3)	102.54(7)
Mo(2)-Mo(1)-N(3)*	102.54(7)
N(3)-Mo(1)-N(3)*	88.29(14)
Mo(2)-Mo(1)-N(1)	90.43(7)
N(3)-Mo(1)-N(1)	86.70(10)
N(3)*-Mo(1)-N(1)	166.84(10)
Mo(2)-Mo(1)-N(1)*	90.43(7)

N(3)-Mo(1)-N(1)*	166.84(10)
N(3)*-Mo(1)-N(1)*	86.70(10)
N(1)-Mo(1)-N(1)*	95.53(13)
O(1)-Mo(2)-O(1)*	91.47(13)
O(1)-Mo(2)-Mo(1)	93.73(6)
O(1)*-Mo(2)-Mo(1)	93.73(6)
O(1)-Mo(2)-N(2)*	164.25(9)
O(1)*-Mo(2)-N(2)*	89.58(10)
Mo(1)-Mo(2)-N(2)*	101.88(7)
O(1)-Mo(2)-N(2)	89.58(10)
O(1)*-Mo(2)-N(2)	164.25(9)
Mo(1)-Mo(2)-N(2)	101.88(7)
N(2)*-Mo(2)-N(2)	85.24(15)
C(6)-N(1)-C(2)	118.2(3)
C(6)-N(1)-Mo(1)	116.6(2)
C(2)-N(1)-Mo(1)	125.1(2)
C(7)-N(2)-Mo(2)	169.5(3)
C(9)-N(3)-Mo(1)	178.3(3)
C(6)-O(1)-Mo(2)	121.67(19)
C(3)-C(2)-N(1)	121.6(3)
C(3)-C(2)-C(1)	120.4(3)
N(1)-C(2)-C(1)	118.0(3)
C(2)-C(3)-C(4)	120.1(3)
C(5)-C(4)-C(3)	119.3(3)
C(4)-C(5)-C(6)	119.2(3)
O(1)-C(6)-N(1)	117.5(3)
O(1)-C(6)-C(5)	120.9(3)
N(1)-C(6)-C(5)	121.6(3)
N(2)-C(7)-C(8)	178.5(4)
N(3)-C(9)-C(10)	178.0(3)
F(1)-B(1)-F(3)	111.4(4)
F(1)-B(1)-F(2)	108.5(4)
F(3)-B(1)-F(2)	107.9(4)
F(1)-B(1)-F(4)	111.7(4)
F(3)-B(1)-F(4)	109.2(4)

F(2)-B(1)-F(4)	108.0(4)
N(4)-C(21)-C(22)	180.0(6)
N(5)-C(31)-C(32)	178.6(9)

Symmetry transformations used to generate equivalent atoms:

* x,y,-z

Table C.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for Chisholm 1449. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	14(1)	21(1)	16(1)	0	0	-1(1)
Mo(2)	18(1)	20(1)	16(1)	0	0	-2(1)
N(1)	20(1)	21(1)	18(1)	-1(1)	-1(1)	-2(1)
N(2)	26(1)	28(1)	22(1)	2(1)	-1(1)	-2(1)
N(3)	20(1)	24(1)	21(1)	-1(1)	1(1)	0(1)
O(1)	20(1)	28(1)	21(1)	-2(1)	3(1)	-3(1)
C(1)	30(2)	39(2)	49(2)	-14(2)	-1(2)	-11(2)
C(2)	25(2)	25(2)	24(1)	-1(1)	-4(1)	-2(1)
C(3)	38(2)	31(2)	27(2)	-10(2)	-7(2)	1(2)
C(4)	43(2)	38(2)	22(2)	-8(1)	1(1)	3(2)
C(5)	30(2)	35(2)	22(2)	-3(1)	7(1)	2(1)
C(6)	22(2)	23(2)	18(1)	0(1)	-1(1)	3(1)
C(7)	28(2)	30(2)	26(2)	-2(1)	-5(1)	-6(1)
C(8)	59(2)	39(2)	33(2)	13(2)	-8(2)	-3(2)
C(9)	19(1)	30(2)	21(1)	-1(1)	2(2)	-6(1)
C(10)	29(2)	37(2)	21(1)	11(1)	0(1)	0(2)
B(1)	26(2)	33(2)	46(2)	-6(2)	2(2)	0(2)
F(1)	55(2)	130(3)	57(2)	-18(2)	22(2)	-4(2)
F(3)	81(2)	74(2)	51(2)	-17(1)	-14(2)	-6(2)
F(2)	180(5)	42(2)	116(3)	-17(2)	38(3)	-24(2)
F(4)	59(2)	138(3)	94(3)	-29(2)	-24(2)	47(2)
N(4)	31(2)	32(2)	34(2)	0	0	3(2)
C(21)	26(2)	31(3)	25(2)	0	0	3(2)
C(22)	60(4)	47(3)	42(3)	0	0	-21(3)
N(5)	78(5)	127(6)	60(4)	0	0	-56(5)
C(31)	43(3)	61(4)	31(2)	0	0	-7(3)
C(32)	42(3)	39(3)	33(3)	0	0	4(2)

Table C.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for Chisholm 1449.

	x	y	z	U(eq)
H(1A)	2840	5163	549	59
H(1B)	3334	5570	1324	59
H(1C)	2465	6422	773	59
H(3)	368	6496	1936	39
H(4)	-2612	6007	2297	41
H(5)	-4084	4502	1769	35
H(8A)	-260	-228	2086	65
H(8B)	710	-916	1472	65
H(8C)	-1481	-951	1559	65
H(10A)	4824	1078	1625	43
H(10B)	4092	1948	2193	43
H(10C)	5879	2230	1735	43
H(22A)	4252	-1279	-319	75
H(22B)	2450	-561	-155	75
H(22C)	3662	-1044	474	75
H(32A)	7452	5930	139	57
H(32B)	6415	6592	-471	57
H(32C)	5980	6870	331	57

Table 6. Torsion angles [°] for Chisholm 1449.

N(3)-Mo(1)-Mo(2)-O(1)	88.62(9)
N(3)*-Mo(1)-Mo(2)-O(1)	179.66(11)
N(1)-Mo(1)-Mo(2)-O(1)	1.91(9)
N(1)*-Mo(1)-Mo(2)-O(1)	-93.63(10)
N(3)-Mo(1)-Mo(2)-O(1)*	-179.66(11)
N(3)*-Mo(1)-Mo(2)-O(1)*	-88.62(9)
N(1)-Mo(1)-Mo(2)-O(1)*	93.63(10)
N(1)*-Mo(1)-Mo(2)-O(1)*	-1.91(9)
N(3)-Mo(1)-Mo(2)-N(2)*	-89.31(11)
N(3)*-Mo(1)-Mo(2)-N(2)*	1.73(10)
N(1)-Mo(1)-Mo(2)-N(2)*	-176.02(10)
N(1)*-Mo(1)-Mo(2)-N(2)*	88.44(10)
N(3)-Mo(1)-Mo(2)-N(2)	-1.73(10)
N(3)*-Mo(1)-Mo(2)-N(2)	89.31(11)
N(1)-Mo(1)-Mo(2)-N(2)	-88.44(10)
N(1)*-Mo(1)-Mo(2)-N(2)	176.02(10)
Mo(2)-Mo(1)-N(1)-C(6)	-1.3(2)
N(3)-Mo(1)-N(1)-C(6)	-103.9(2)
N(3)*-Mo(1)-N(1)-C(6)	-171.6(4)
N(1)*-Mo(1)-N(1)-C(6)	89.2(2)
Mo(2)-Mo(1)-N(1)-C(2)	175.1(2)
N(3)-Mo(1)-N(1)-C(2)	72.6(2)
N(3)*-Mo(1)-N(1)-C(2)	4.8(6)
N(1)*-Mo(1)-N(1)-C(2)	-94.4(2)
O(1)-Mo(2)-N(2)-C(7)	96.0(15)
O(1)*-Mo(2)-N(2)-C(7)	2.1(17)
Mo(1)-Mo(2)-N(2)-C(7)	-170.3(15)
N(2)*-Mo(2)-N(2)-C(7)	-69.1(15)
Mo(2)-Mo(1)-N(3)-C(9)	-139(9)
N(3)*-Mo(1)-N(3)-C(9)	118(9)
N(1)-Mo(1)-N(3)-C(9)	-50(9)
N(1)*-Mo(1)-N(3)-C(9)	51(9)
O(1)*-Mo(2)-O(1)-C(6)	-97.2(2)

Mo(1)-Mo(2)-O(1)-C(6)	-3.4(2)
N(2)*-Mo(2)-O(1)-C(6)	169.2(3)
N(2)-Mo(2)-O(1)-C(6)	98.5(2)
C(6)-N(1)-C(2)-C(3)	-2.2(5)
Mo(1)-N(1)-C(2)-C(3)	-178.6(2)
C(6)-N(1)-C(2)-C(1)	178.1(3)
Mo(1)-N(1)-C(2)-C(1)	1.7(4)
N(1)-C(2)-C(3)-C(4)	0.3(5)
C(1)-C(2)-C(3)-C(4)	-179.9(3)
C(2)-C(3)-C(4)-C(5)	1.6(5)
C(3)-C(4)-C(5)-C(6)	-1.7(5)
Mo(2)-O(1)-C(6)-N(1)	2.9(4)
Mo(2)-O(1)-C(6)-C(5)	-176.7(2)
C(2)-N(1)-C(6)-O(1)	-177.5(3)
Mo(1)-N(1)-C(6)-O(1)	-0.8(3)
C(2)-N(1)-C(6)-C(5)	2.2(4)
Mo(1)-N(1)-C(6)-C(5)	178.9(2)
C(4)-C(5)-C(6)-O(1)	179.4(3)
C(4)-C(5)-C(6)-N(1)	-0.3(5)
Mo(2)-N(2)-C(7)-C(8)	-2(17)
Mo(1)-N(3)-C(9)-C(10)	178(100)

Symmetry transformations used to generate equivalent atoms:

* x,y,-z