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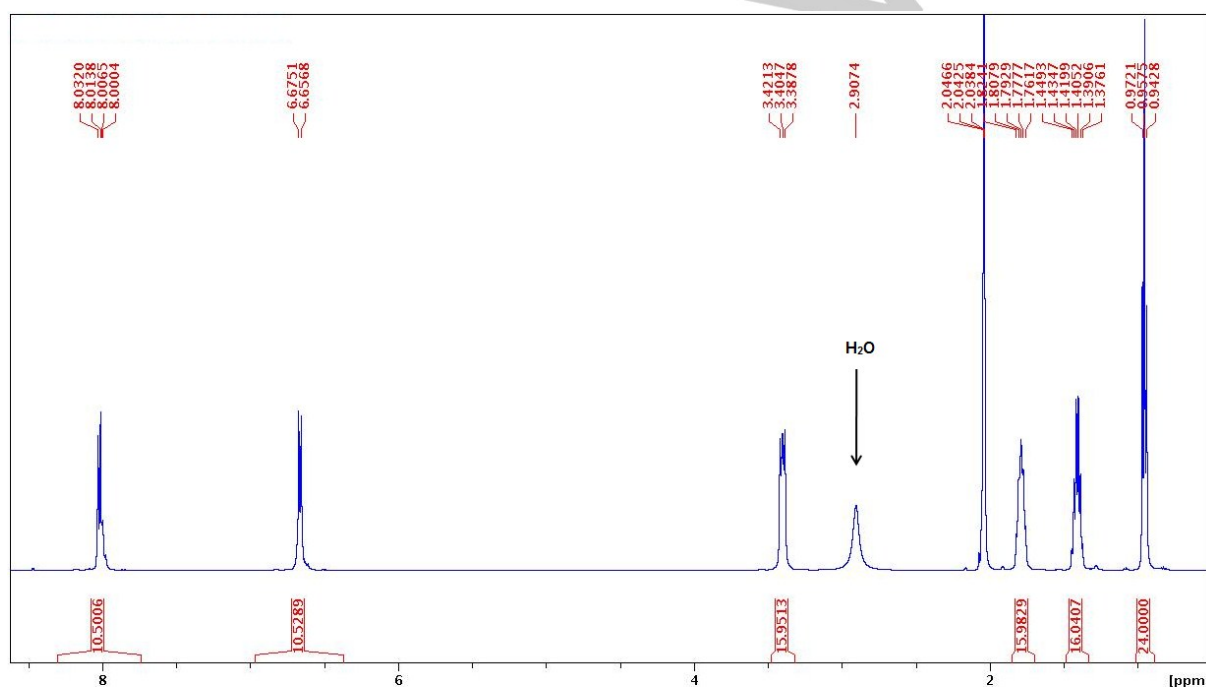
Complexes of {Mo₆I₈} with nitrophenolates: synthesis and luminescence

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Supporting information



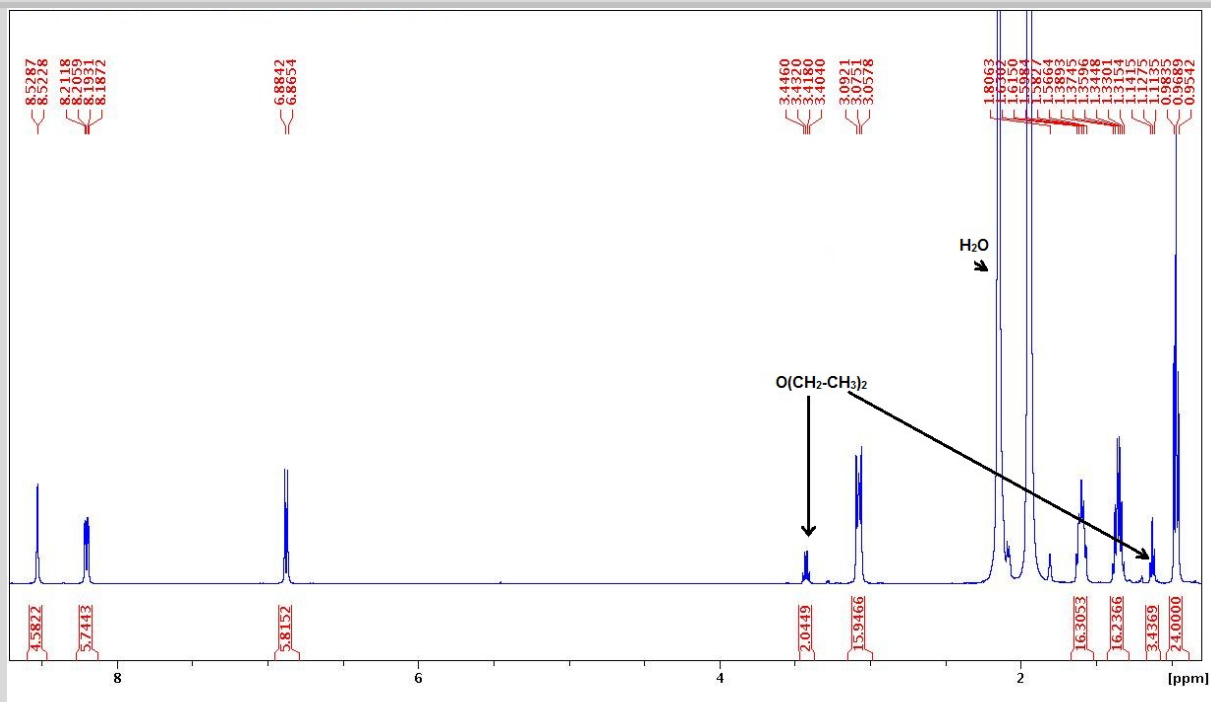


Figure 2S. ^1H NMR spectra (CH_3CN , 25°C) of **2**.

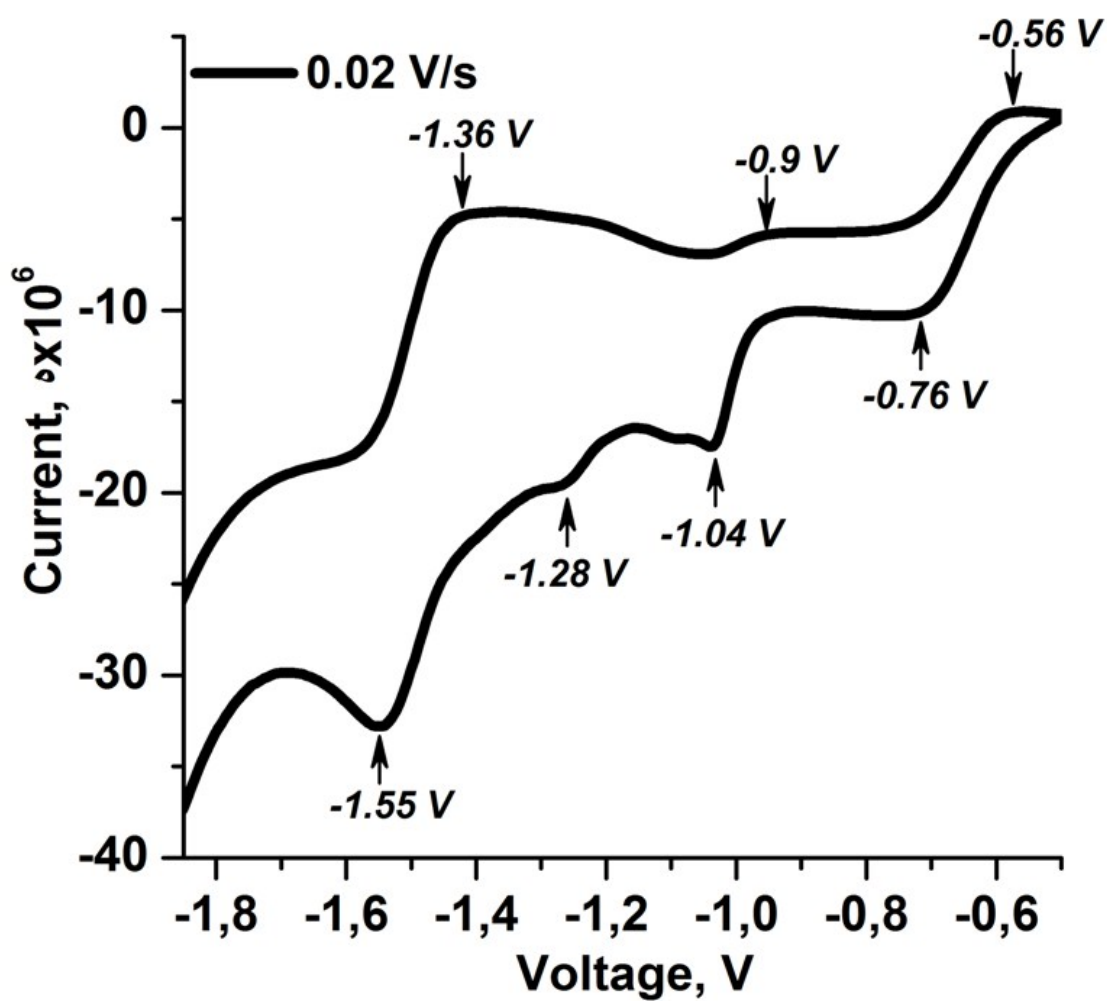


Fig S3. CV of $(\text{Bu}_4\text{N})_2[\{\text{Mo}_6\text{I}_8\}(\text{OC}_6\text{H}_4\text{-p}(\text{NO}_2))_6]$ (1) at negative potentials. 2 mM solution in CH_3CN with 0.05 M Bu_4NBF_4 as supporting electrolyte. Reference electrode Ag/AgCl.

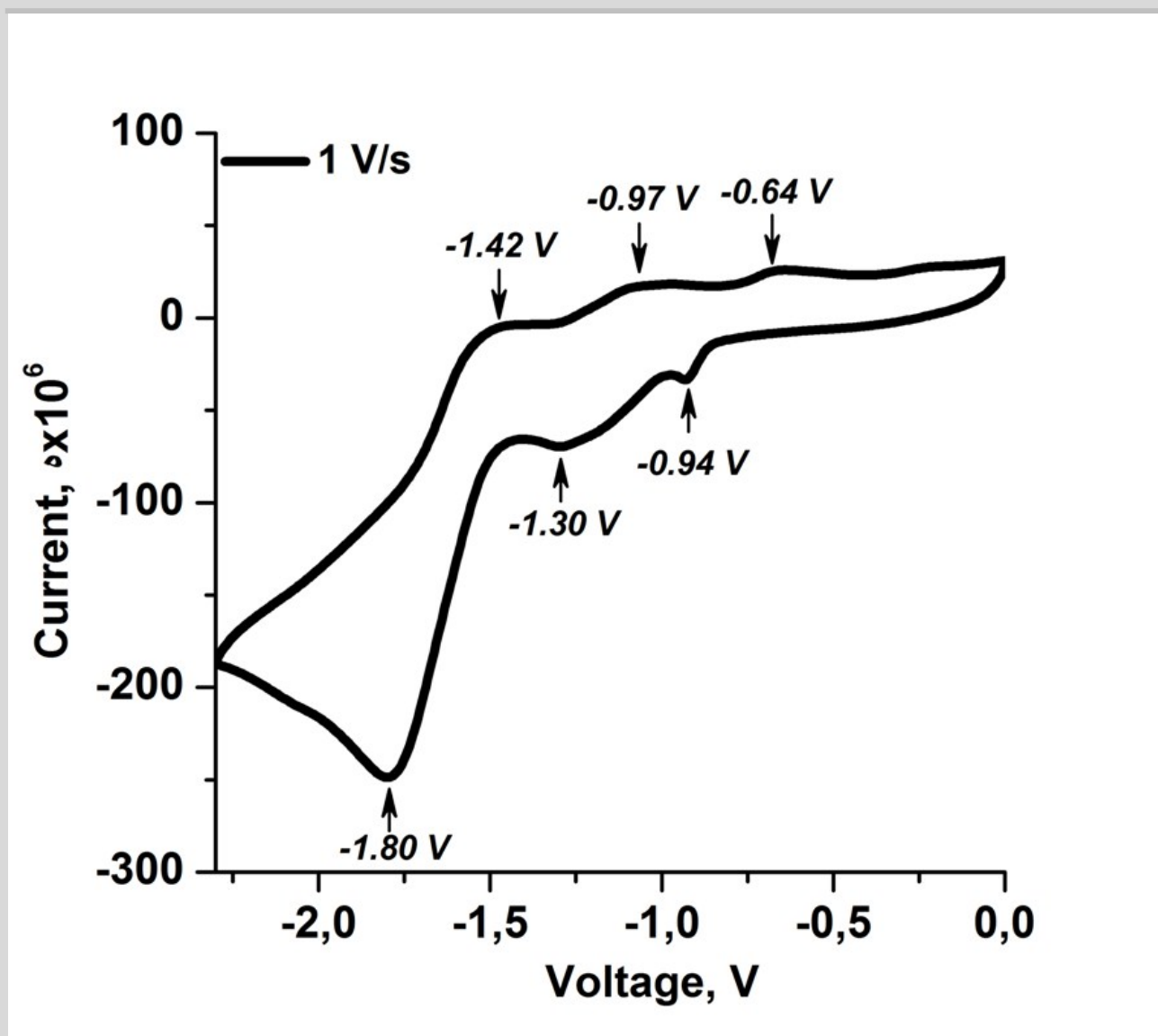


Fig S4. CV of $(\text{Bu}_4\text{N})_2[\{\text{Mo}_6\text{I}_8\}(\text{OC}_6\text{H}_3\text{-}2,4\text{-(NO}_2)_2)_6]$ (**2**) at negative potentials. 0.2 mM solution in CH_3CN with 0.05 M Bu_4NBF_4 as supporting electrolyte. Reference electrode Ag/AgCl .

Table S1. Bond distances and angles in **1**·CH₃CN·H₂O

Bond	d, Å
Mo(1)–Mo(2)#1	2.6612(13)
Mo(1)–Mo(2)	2.6700(13)
Mo(1)–Mo(3)	2.6596(14)
Mo(1)–Mo(3)#1	2.6695(15)
Mo(1)–I(1)	2.7934(12)
Mo(1)–I(2)	2.8015(12)
Mo(1)–I(3)	2.7966(12)
Mo(1)–I(4)#1	2.7913(12)
Mo(1)–O(1)	2.100(8)
Mo(2)–Mo(1)#1	2.6611(13)
Mo(2)–Mo(3)	2.6566(13)
Mo(2)–Mo(3)#1	2.6676(13)
Mo(2)–I(1)	2.8007(13)
Mo(2)–I(2)	2.8104(12)
Mo(2)–I(3)#1	2.7909(13)
Mo(2)–I(4)	2.7980(12)
Mo(2)–O(2)	2.085(7)
Mo(3)–Mo(1)#1	2.6695(15)
Mo(3)–Mo(2)#1	2.6676(13)
Mo(3)–I(1)	2.7986(12)
Mo(3)–I(2)#1	2.7916(12)
Mo(3)–I(3)	2.7910(12)
Mo(3)–I(4)	2.8157(12)
Mo(3)–O(3)	2.095(7)
Mo(4)–Mo(5)#2	2.6589(13)
Mo(4)–Mo(5)	2.6646(16)
Mo(4)–Mo(6)	2.6611(14)
Mo(4)–Mo(6)#2	2.6651(16)
Mo(4)–I(5)	2.7985(13)
Mo(4)–I(6)	2.7988(14)
Mo(4)–I(7)#2	2.7800(13)
Mo(4)–I(8)	2.7990(15)
Mo(4)–O(4)	2.083(8)
Mo(5)–Mo(4)#2	2.6589(13)
Mo(5)–Mo(6)#2	2.6691(14)
Mo(5)–Mo(6)	2.6709(16)
Mo(5)–I(5)	2.7847(14)
Mo(5)–I(6)	2.7918(13)
Mo(5)–I(7)	2.7966(13)
Mo(5)–I(8)#2	2.8014(14)
Mo(5)–O(5)	2.120(9)
Mo(6)–Mo(4)#2	2.6651(16)
Mo(6)–Mo(5)#2	2.6691(14)
Mo(6)–I(5)	2.7987(12)

Mo(6)–I(6)#2	2.7871(12)
Mo(6)–I(7)	2.7789(15)
Mo(6)–I(8)	2.8051(15)
Mo(6)–O(6)	2.079(9)
I(2)–Mo(3)#1	2.7916(12)
I(3)–Mo(2)#1	2.7910(13)
I(4)–Mo(1)#1	2.7913(12)
I(6)–Mo(6)#2	2.7871(12)
I(7)–Mo(4)#2	2.7800(13)
I(8)–Mo(5)#2	2.8014(14)
O(1)–C(11)	1.216(13)
O(2)–C(21)	1.221(11)
O(3)–C(31)	1.288(13)
O(4)–C(41)	1.248(13)
O(5)–C(51)	1.283(14)
O(6)–C(61)	1.297(14)
N(1)–O(11)	1.239(13)
N(1)–O(12)	1.255(13)
N(1)–C(14)	1.448(15)
N(2)–O(21)	1.215(14)
N(2)–O(22)	1.237(13)
N(2)–C(24)	1.469(14)
N(3)–O(31)	1.239(19)
N(3)–O(32)	1.211(18)
N(3)–C(34)	1.452(16)
N(4)–O(41)	1.221(16)
N(4)–O(42)	1.207(15)
N(4)–C(44)	1.452(18)
N(5)–O(51)	1.255(17)
N(5)–O(52)	1.213(16)
N(5)–C(54)	1.471(15)
N(6)–O(61)	1.247(13)
N(6)–O(62)	1.213(13)
N(6)–C(64)	1.469(16)
C(11)–C(12)	1.479(16)
C(11)–C(16)	1.395(15)
C(12)–C(13)	1.353(15)
C(13)–C(14)	1.380(16)
C(14)–C(15)	1.383(15)
C(15)–C(16)	1.386(16)
C(21)–C(22)	1.418(14)
C(21)–C(26)	1.437(15)
C(22)–C(23)	1.394(16)
C(23)–C(24)	1.365(17)
C(24)–C(25)	1.401(16)
C(25)–C(26)	1.373(15)
C(31)–C(32)	1.419(16)
C(31)–C(36)	1.410(16)

C(32)–C(33)	1.369(16)
C(33)–C(34)	1.389(19)
C(34)–C(35)	1.389(19)
C(35)–C(36)	1.385(16)
C(41)–C(42)	1.417(17)
C(41)–C(46)	1.458(15)
C(42)–C(43)	1.378(17)
C(43)–C(44)	1.393(16)
C(44)–C(45)	1.362(17)
C(45)–C(46)	1.364(17)
C(51)–C(52)	1.390(16)
C(51)–C(56)	1.391(18)
C(52)–C(53)	1.391(15)
C(53)–C(54)	1.381(18)
C(54)–C(55)	1.371(17)
C(55)–C(56)	1.375(17)
C(61)–C(62)	1.422(17)
C(61)–C(66)	1.399(17)
C(62)–C(63)	1.372(17)
C(63)–C(64)	1.387(17)
C(64)–C(65)	1.375(17)
C(65)–C(66)	1.382(16)
N(11)–C(111)	1.534(14)
N(11)–C(121)	1.526(15)
N(11)–C(131)	1.529(13)
N(11)–C(141)	1.511(15)
C(111)–C(112)	1.466(16)
C(112)–C(113)	1.474(18)
C(113)–C(114)	1.38(2)
C(121)–C(122)	1.468(17)
C(122)–C(123)	1.577(18)
C(123)–C(124)	1.494(18)
C(131)–C(132)	1.516(17)
C(132)–C(133)	1.516(16)
C(133)–C(134)	1.544(17)
C(141)–C(142)	1.460(18)
C(142)–C(143)	1.52(2)
C(143)–C(144)	1.39(2)
N(21)–C(211)	1.49(2)
N(21)–C(221)	1.58(2)
N(21)–C(231)	1.51(2)
N(21)–C(241)	1.54(2)
C(214)–C(213)	1.44(2)
C(211)–C(212)	1.52(2)
C(212)–C(213)	1.57(2)
C(221)–C(222)	1.38(3)
C(222)–C(223)	1.58(3)
C(223)–C(22C)	1.31(4)

C(223)–C(22D)	1.47(4)
C(231)–C(23A)	1.56(6)
C(231)–C(23B)	1.42(2)
C(23A)–C(233)	1.51(6)
C(23B)–C(233)	1.69(3)
C(233)–C(234)	1.47(3)
C(241)–C(242)	1.55(2)
C(242)–C(243)	1.53(3)
C(243)–C(244)	1.53(2)
N(1S)–C(1S)	1.10(2)
C(1S)–C(2S)	1.40(2)
<hr/>	
angle	$\omega, ^\circ$
Mo(2)#1–Mo(1)–Mo(2)	89.90(4)
Mo(2)#1–Mo(1)–Mo(3)#1	59.78(4)
Mo(2)#1–Mo(1)–I(1)	121.87(4)
Mo(2)–Mo(1)–I(1)	61.63(3)
Mo(2)#1–Mo(1)–I(2)	121.06(5)
Mo(2)–Mo(1)–I(2)	61.76(3)
Mo(2)#1–Mo(1)–I(3)	61.45(3)
Mo(2)–Mo(1)–I(3)	121.26(4)
Mo(2)#1–Mo(1)–I(4)#1	61.69(3)
Mo(2)–Mo(1)–I(4)#1	121.96(5)
Mo(3)–Mo(1)–Mo(2)#1	60.18(4)
Mo(3)–Mo(1)–Mo(2)	59.80(3)
Mo(3)#1–Mo(1)–Mo(2)	59.95(4)
Mo(3)–Mo(1)–Mo(3)#1	89.85(4)
Mo(3)–Mo(1)–I(1)	61.70(3)
Mo(3)#1–Mo(1)–I(1)	121.56(4)
Mo(3)–Mo(1)–I(2)	121.55(4)
Mo(3)#1–Mo(1)–I(2)	61.30(3)
Mo(3)–Mo(1)–I(3)	61.47(3)
Mo(3)#1–Mo(1)–I(3)	121.23(4)
Mo(3)–Mo(1)–I(4)#1	121.85(4)
Mo(3)#1–Mo(1)–I(4)#1	62.03(3)
I(1)–Mo(1)–I(2)	90.20(3)
I(1)–Mo(1)–I(3)	90.11(4)
I(3)–Mo(1)–I(2)	176.58(5)
I(4)#1–Mo(1)–I(1)	175.63(5)
I(4)#1–Mo(1)–I(2)	89.69(4)
I(4)#1–Mo(1)–I(3)	89.74(3)
O(1)–Mo(1)–Mo(2)#1	130.7(2)
O(1)–Mo(1)–Mo(2)	139.4(2)
O(1)–Mo(1)–Mo(3)	135.6(2)
O(1)–Mo(1)–Mo(3)#1	134.2(2)
O(1)–Mo(1)–I(1)	91.5(2)
O(1)–Mo(1)–I(2)	90.8(2)
O(1)–Mo(1)–I(3)	85.8(2)

O(1)–Mo(1)–I(4)#1	84.1(2)
Mo(1)#1–Mo(2)–Mo(1)	90.11(4)
Mo(1)#1–Mo(2)–Mo(3)#1	59.88(3)
Mo(1)#1–Mo(2)–I(1)	121.89(4)
Mo(1)–Mo(2)–I(1)	61.35(3)
Mo(1)#1–Mo(2)–I(2)	121.07(4)
Mo(1)–Mo(2)–I(2)	61.42(3)
Mo(1)#1–Mo(2)–I(3)#1	61.67(3)
Mo(1)–Mo(2)–I(3)#1	121.45(4)
Mo(1)#1–Mo(2)–I(4)	61.44(3)
Mo(1)–Mo(2)–I(4)	121.99(4)
Mo(3)–Mo(2)–Mo(1)#1	60.26(4)
Mo(3)–Mo(2)–Mo(1)	59.91(4)
Mo(3)#1–Mo(2)–Mo(1)	60.02(4)
Mo(3)–Mo(2)–Mo(3)#1	89.96(4)
Mo(3)–Mo(2)–I(1)	61.64(3)
Mo(3)#1–Mo(2)–I(1)	121.36(4)
Mo(3)–Mo(2)–I(2)	121.32(4)
Mo(3)#1–Mo(2)–I(2)	61.21(3)
Mo(3)–Mo(2)–I(3)#1	121.92(4)
Mo(3)#1–Mo(2)–I(3)#1	61.45(3)
Mo(3)–Mo(2)–I(4)	62.09(3)
Mo(3)#1–Mo(2)–I(4)	121.30(4)
I(1)–Mo(2)–I(2)	89.87(4)
I(3)#1–Mo(2)–I(1)	176.05(4)
I(3)#1–Mo(2)–I(2)	89.37(4)
I(3)#1–Mo(2)–I(4)	89.72(4)
I(4)–Mo(2)–I(1)	90.79(4)
I(4)–Mo(2)–I(2)	176.28(4)
O(2)–Mo(2)–Mo(1)#1	134.9(2)
O(2)–Mo(2)–Mo(1)	134.8(2)
O(2)–Mo(2)–Mo(3)	137.9(2)
O(2)–Mo(2)–Mo(3)#1	132.1(2)
O(2)–Mo(2)–I(1)	90.1(2)
O(2)–Mo(2)–I(2)	86.3(2)
O(2)–Mo(2)–I(3)#1	86.0(2)
O(2)–Mo(2)–I(4)	90.0(2)
Mo(1)–Mo(3)–Mo(1)#1	90.15(4)
Mo(1)–Mo(3)–Mo(2)#1	59.94(3)
Mo(1)–Mo(3)–I(1)	61.50(3)
Mo(1)#1–Mo(3)–I(1)	121.66(4)
Mo(1)–Mo(3)–I(2)#1	121.84(4)
Mo(1)#1–Mo(3)–I(2)#1	61.68(3)
Mo(1)–Mo(3)–I(3)	61.68(3)
Mo(1)#1–Mo(3)–I(3)	121.47(4)
Mo(1)–Mo(3)–I(4)	121.71(4)
Mo(1)#1–Mo(3)–I(4)	61.11(3)
Mo(2)–Mo(3)–Mo(1)	60.30(4)

Mo(2)–Mo(3)–Mo(1)#1	59.95(4)
Mo(2)#1–Mo(3)–Mo(1)#1	60.04(4)
Mo(2)–Mo(3)–Mo(2)#1	90.05(4)
Mo(2)–Mo(3)–I(1)	61.72(3)
Mo(2)#1–Mo(3)–I(1)	121.43(4)
Mo(2)–Mo(3)–I(2)#1	121.61(5)
Mo(2)#1–Mo(3)–I(2)#1	61.92(3)
Mo(2)–Mo(3)–I(3)	121.97(4)
Mo(2)#1–Mo(3)–I(3)	61.45(3)
Mo(2)–Mo(3)–I(4)	61.42(3)
Mo(2)#1–Mo(3)–I(4)	121.13(5)
I(1)–Mo(3)–I(4)	90.47(3)
I(2)#1–Mo(3)–I(1)	175.90(5)
I(2)#1–Mo(3)–I(4)	89.40(4)
I(3)–Mo(3)–I(1)	90.12(4)
I(3)–Mo(3)–I(2)#1	89.75(3)
I(3)–Mo(3)–I(4)	176.27(5)
O(3)–Mo(3)–Mo(1)	132.3(2)
O(3)–Mo(3)–Mo(1)#1	137.4(2)
O(3)–Mo(3)–Mo(2)	131.9(2)
O(3)–Mo(3)–Mo(2)#1	138.0(2)
O(3)–Mo(3)–I(1)	84.2(2)
O(3)–Mo(3)–I(2)#1	91.7(2)
O(3)–Mo(3)–I(3)	88.4(2)
O(3)–Mo(3)–I(4)	88.0(2)
Mo(5)#2–Mo(4)–Mo(5)	90.30(4)
Mo(5)#2–Mo(4)–Mo(6)	60.23(4)
Mo(5)#2–Mo(4)–Mo(6)#2	60.22(4)
Mo(5)–Mo(4)–Mo(6)#2	60.11(4)
Mo(5)#2–Mo(4)–I(5)	121.84(5)
Mo(5)–Mo(4)–I(5)	61.23(4)
Mo(5)#2–Mo(4)–I(6)	121.49(5)
Mo(5)–Mo(4)–I(6)	61.40(4)
Mo(5)#2–Mo(4)–I(7)#2	61.84(3)
Mo(5)–Mo(4)–I(7)#2	121.41(5)
Mo(5)#2–Mo(4)–I(8)	61.70(4)
Mo(5)–Mo(4)–I(8)	121.95(5)
Mo(6)–Mo(4)–Mo(5)	60.20(4)
Mo(6)–Mo(4)–Mo(6)#2	90.36(4)
Mo(6)–Mo(4)–I(5)	61.62(3)
Mo(6)#2–Mo(4)–I(5)	121.32(5)
Mo(6)–Mo(4)–I(6)	121.59(5)
Mo(6)#2–Mo(4)–I(6)	61.28(4)
Mo(6)–Mo(4)–I(7)#2	122.06(4)
Mo(6)#2–Mo(4)–I(7)#2	61.33(4)
Mo(6)–Mo(4)–I(8)	61.76(4)
Mo(6)#2–Mo(4)–I(8)	121.91(4)
I(5)–Mo(4)–I(6)	89.62(4)

I(5)–Mo(4)–I(8)	90.39(4)
I(6)–Mo(4)–I(8)	175.98(5)
I(7)#2–Mo(4)–I(5)	176.02(5)
I(7)#2–Mo(4)–I(6)	89.37(4)
I(7)#2–Mo(4)–I(8)	90.34(4)
O(4)–Mo(4)–Mo(5)#2	138.5(2)
O(4)–Mo(4)–Mo(5)	131.2(2)
O(4)–Mo(4)–Mo(6)	134.5(3)
O(4)–Mo(4)–Mo(6)#2	134.9(3)
O(4)–Mo(4)–I(5)	85.4(2)
O(4)–Mo(4)–I(6)	85.8(3)
O(4)–Mo(4)–I(7)#2	90.7(2)
O(4)–Mo(4)–I(8)	90.2(3)
Mo(4)#2–Mo(5)–Mo(4)	89.70(4)
Mo(4)#2–Mo(5)–Mo(6)#2	59.93(4)
Mo(4)–Mo(5)–Mo(6)#2	59.96(4)
Mo(4)#2–Mo(5)–Mo(6)	60.00(4)
Mo(4)–Mo(5)–Mo(6)	59.83(4)
Mo(4)#2–Mo(5)–I(5)	121.68(5)
Mo(4)–Mo(5)–I(5)	61.76(4)
Mo(4)#2–Mo(5)–I(6)	121.25(5)
Mo(4)–Mo(5)–I(6)	61.67(4)
Mo(4)#2–Mo(5)–I(7)	61.21(3)
Mo(4)–Mo(5)–I(7)	120.87(5)
Mo(4)#2–Mo(5)–I(8)#2	61.61(4)
Mo(4)–Mo(5)–I(8)#2	121.59(5)
Mo(6)#2–Mo(5)–Mo(6)	90.06(5)
Mo(6)#2–Mo(5)–I(5)	121.69(5)
Mo(6)–Mo(5)–I(5)	61.68(4)
Mo(6)#2–Mo(5)–I(6)	61.33(3)
Mo(6)–Mo(5)–I(6)	121.49(5)
Mo(6)#2–Mo(5)–I(7)	121.13(4)
Mo(6)–Mo(5)–I(7)	61.04(4)
Mo(6)#2–Mo(5)–I(8)#2	61.64(4)
Mo(6)–Mo(5)–I(8)#2	121.60(4)
I(5)–Mo(5)–I(6)	90.05(4)
I(5)–Mo(5)–I(7)	89.91(4)
I(5)–Mo(5)–I(8)#2	175.95(5)
I(6)–Mo(5)–I(7)	176.94(5)
I(6)–Mo(5)–I(8)#2	89.87(4)
I(7)–Mo(5)–I(8)#2	89.95(4)
O(5)–Mo(5)–Mo(4)#2	132.9(2)
O(5)–Mo(5)–Mo(4)	137.3(2)
O(5)–Mo(5)–Mo(6)#2	136.4(3)
O(5)–Mo(5)–Mo(6)	133.5(3)
O(5)–Mo(5)–I(5)	88.4(3)
O(5)–Mo(5)–I(6)	90.8(2)
O(5)–Mo(5)–I(7)	86.1(2)

O(5)–Mo(5)–I(8)#2	87.5(3)
Mo(4)–Mo(6)–Mo(4)#2	89.64(4)
Mo(4)–Mo(6)–Mo(5)#2	59.85(4)
Mo(4)#2–Mo(6)–Mo(5)#2	59.94(4)
Mo(4)–Mo(6)–Mo(5)	59.96(4)
Mo(4)#2–Mo(6)–Mo(5)	59.77(4)
Mo(4)–Mo(6)–I(5)	61.61(3)
Mo(4)#2–Mo(6)–I(5)	120.92(5)
Mo(4)–Mo(6)–I(6)#2	121.34(5)
Mo(4)#2–Mo(6)–I(6)#2	61.72(4)
Mo(4)–Mo(6)–I(7)	121.67(5)
Mo(4)#2–Mo(6)–I(7)	61.37(4)
Mo(4)–Mo(6)–I(8)	61.54(4)
Mo(4)#2–Mo(6)–I(8)	121.43(5)
Mo(5)#2–Mo(6)–Mo(5)	89.94(5)
Mo(5)#2–Mo(6)–I(5)	121.45(5)
Mo(5)–Mo(6)–I(5)	61.16(4)
Mo(5)#2–Mo(6)–I(6)#2	61.50(3)
Mo(5)–Mo(6)–I(6)#2	121.48(5)
Mo(5)#2–Mo(6)–I(7)	121.29(5)
Mo(5)–Mo(6)–I(7)	61.71(4)
Mo(5)#2–Mo(6)–I(8)	61.50(4)
Mo(5)–Mo(6)–I(8)	121.49(5)
I(5)–Mo(6)–I(8)	90.27(4)
I(6)#2–Mo(6)–I(5)	176.57(5)
I(6)#2–Mo(6)–I(8)	89.90(4)
I(7)–Mo(6)–I(5)	89.99(4)
I(7)–Mo(6)–I(6)#2	89.63(4)
I(7)–Mo(6)–I(8)	176.31(5)
O(6)–Mo(6)–Mo(4)	130.7(2)
O(6)–Mo(6)–Mo(4)#2	139.6(2)
O(6)–Mo(6)–Mo(5)#2	135.0(3)
O(6)–Mo(6)–Mo(5)	134.8(2)
O(6)–Mo(6)–I(5)	85.3(2)
O(6)–Mo(6)–I(6)#2	91.3(2)
O(6)–Mo(6)–I(7)	91.2(3)
O(6)–Mo(6)–I(8)	85.1(3)
Mo(1)–I(1)–Mo(2)	57.02(3)
Mo(1)–I(1)–Mo(3)	56.80(3)
Mo(3)–I(1)–Mo(2)	56.65(3)
Mo(1)–I(2)–Mo(2)	56.82(3)
Mo(3)#1–I(2)–Mo(1)	57.02(3)
Mo(3)#1–I(2)–Mo(2)	56.87(3)
Mo(2)#1–I(3)–Mo(1)	56.88(3)
Mo(2)#1–I(3)–Mo(3)	57.10(3)
Mo(3)–I(3)–Mo(1)	56.85(3)
Mo(1)#1–I(4)–Mo(2)	56.86(3)
Mo(1)#1–I(4)–Mo(3)	56.86(3)

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Mo(2)–I(4)–Mo(3)	56.49(3)
Mo(4)–I(5)–Mo(6)	56.78(3)
Mo(5)–I(5)–Mo(4)	57.01(4)
Mo(5)–I(5)–Mo(6)	57.16(3)
Mo(5)–I(6)–Mo(4)	56.93(4)
Mo(6)#2–I(6)–Mo(4)	56.99(3)
Mo(6)#2–I(6)–Mo(5)	57.17(3)
Mo(4)#2–I(7)–Mo(5)	56.95(3)
Mo(6)–I(7)–Mo(4)#2	57.30(4)
Mo(6)–I(7)–Mo(5)	57.25(4)
Mo(4)–I(8)–Mo(5)#2	56.69(3)
Mo(4)–I(8)–Mo(6)	56.70(4)
Mo(5)#2–I(8)–Mo(6)	56.86(4)
C(11)–O(1)–Mo(1)	141.0(7)
C(21)–O(2)–Mo(2)	143.4(7)
C(31)–O(3)–Mo(3)	132.2(7)
C(41)–O(4)–Mo(4)	142.3(7)
C(51)–O(5)–Mo(5)	135.3(8)
C(61)–O(6)–Mo(6)	146.7(8)
O(11)–N(1)–O(12)	121.0(11)
O(11)–N(1)–C(14)	120.4(11)
O(12)–N(1)–C(14)	118.5(11)
O(21)–N(2)–O(22)	123.4(11)
O(21)–N(2)–C(24)	119.1(11)
O(22)–N(2)–C(24)	117.2(11)
O(31)–N(3)–C(34)	120.0(16)
O(32)–N(3)–O(31)	122.7(13)
O(32)–N(3)–C(34)	117.2(17)
O(41)–N(4)–C(44)	117.7(13)
O(42)–N(4)–O(41)	125.7(15)
O(42)–N(4)–C(44)	116.5(14)
O(51)–N(5)–C(54)	117.5(13)
O(52)–N(5)–O(51)	125.3(13)
O(52)–N(5)–C(54)	117.1(14)
O(61)–N(6)–C(64)	115.9(12)
O(62)–N(6)–O(61)	124.4(12)
O(62)–N(6)–C(64)	119.7(11)
O(1)–C(11)–C(12)	123.5(10)
O(1)–C(11)–C(16)	124.5(11)
C(16)–C(11)–C(12)	111.9(11)
C(13)–C(12)–C(11)	123.3(11)
C(12)–C(13)–C(14)	119.4(11)
C(13)–C(14)–N(1)	118.8(10)
C(13)–C(14)–C(15)	121.9(11)
C(15)–C(14)–N(1)	119.2(11)
C(14)–C(15)–C(16)	117.2(11)
C(15)–C(16)–C(11)	126.1(11)
O(2)–C(21)–C(22)	120.4(10)

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O(2)–C(21)–C(26)	126.1(9)
C(22)–C(21)–C(26)	113.5(9)
C(23)–C(22)–C(21)	124.7(12)
C(24)–C(23)–C(22)	117.6(11)
C(23)–C(24)–N(2)	119.5(11)
C(23)–C(24)–C(25)	122.2(10)
C(25)–C(24)–N(2)	118.2(11)
C(26)–C(25)–C(24)	118.7(11)
C(25)–C(26)–C(21)	123.2(11)
O(3)–C(31)–C(32)	121.4(11)
O(3)–C(31)–C(36)	121.1(11)
C(36)–C(31)–C(32)	117.5(11)
C(33)–C(32)–C(31)	121.3(13)
C(32)–C(33)–C(34)	118.9(13)
C(33)–C(34)–N(3)	119.9(14)
C(35)–C(34)–N(3)	117.4(14)
C(35)–C(34)–C(33)	122.7(12)
C(36)–C(35)–C(34)	117.6(13)
C(35)–C(36)–C(31)	122.1(13)
O(4)–C(41)–C(42)	125.2(10)
O(4)–C(41)–C(46)	118.7(11)
C(42)–C(41)–C(46)	115.9(11)
C(43)–C(42)–C(41)	121.4(11)
C(42)–C(43)–C(44)	120.8(12)
C(43)–C(44)–N(4)	119.4(13)
C(45)–C(44)–N(4)	121.3(12)
C(45)–C(44)–C(43)	119.3(12)
C(44)–C(45)–C(46)	122.4(12)
C(45)–C(46)–C(41)	120.2(12)
O(5)–C(51)–C(52)	121.4(12)
O(5)–C(51)–C(56)	122.4(12)
C(52)–C(51)–C(56)	116.2(11)
C(51)–C(52)–C(53)	122.8(12)
C(54)–C(53)–C(52)	117.5(12)
C(53)–C(54)–N(5)	119.6(12)
C(55)–C(54)–N(5)	118.2(13)
C(55)–C(54)–C(53)	122.2(11)
C(54)–C(55)–C(56)	118.3(13)
C(55)–C(56)–C(51)	122.9(13)
O(6)–C(61)–C(62)	116.6(12)
O(6)–C(61)–C(66)	124.5(11)
C(66)–C(61)–C(62)	118.9(12)
C(63)–C(62)–C(61)	120.0(13)
C(62)–C(63)–C(64)	119.7(13)
C(63)–C(64)–N(6)	120.0(12)
C(65)–C(64)–N(6)	118.7(12)
C(65)–C(64)–C(63)	121.4(12)
C(64)–C(65)–C(66)	119.9(12)

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C(65)–C(66)–C(61)	120.1(12)
C(121)–N(11)–C(111)	108.4(9)
C(121)–N(11)–C(131)	110.9(9)
C(131)–N(11)–C(111)	108.4(9)
C(141)–N(11)–C(111)	110.7(9)
C(141)–N(11)–C(121)	108.9(9)
C(141)–N(11)–C(131)	109.5(9)
C(112)–C(111)–N(11)	116.5(10)
C(111)–C(112)–C(113)	112.6(12)
C(114)–C(113)–C(112)	119.0(17)
C(122)–C(121)–N(11)	113.9(10)
C(121)–C(122)–C(123)	110.3(11)
C(124)–C(123)–C(122)	110.2(12)
C(132)–C(131)–N(11)	115.2(11)
C(133)–C(132)–C(131)	113.0(11)
C(132)–C(133)–C(134)	114.7(10)
C(142)–C(141)–N(11)	118.9(12)
C(141)–C(142)–C(143)	109.6(14)
C(144)–C(143)–C(142)	119(2)
C(211)–N(21)–C(221)	109.6(13)
C(211)–N(21)–C(231)	109.6(17)
C(211)–N(21)–C(241)	112.2(15)
C(231)–N(21)–C(221)	112.1(14)
C(231)–N(21)–C(241)	109.4(13)
C(241)–N(21)–C(221)	103.9(15)
N(21)–C(211)–C(212)	111.1(16)
C(211)–C(212)–C(213)	105.7(16)
C(214)–C(213)–C(212)	110.1(18)
C(222)–C(221)–N(21)	115(2)
C(221)–C(222)–C(223)	108(2)
C(22C)–C(223)–C(222)	126(3)
C(22C)–C(223)–C(22D)	56(2)
C(22D)–C(223)–C(222)	125(3)
N(21)–C(231)–C(23A)	148(3)
C(23B)–C(231)–N(21)	116.6(17)
C(23B)–C(231)–C(23A)	70(2)
C(233)–C(23A)–C(231)	105(4)
C(231)–C(23B)–C(233)	101.9(17)
C(23A)–C(233)–C(23B)	64(2)
C(234)–C(233)–C(23A)	151(3)
C(234)–C(233)–C(23B)	102(2)
N(21)–C(241)–C(242)	117.4(14)
C(243)–C(242)–C(241)	108.3(15)
C(242)–C(243)–C(244)	111(2)
N(1S)–C(1S)–C(2S)	177(2)

Symmetry transformations used to generate equivalent atoms:

#1 $-x, -y + 2, -z + 2$ #2 $-x, -y + 1, -z + 1$

Table S2. Bond distances and angles in 2·3THF

Bond	d, Å
Mo(1)–Mo(2)#1	2.6444(15)
Mo(1)–Mo(2)	2.6822(14)
Mo(1)–Mo(3)	2.6591(14)
Mo(1)–Mo(3)#1	2.6734(17)
Mo(1)–I(1)	2.7858(14)
Mo(1)–I(2)	2.7786(13)
Mo(1)–I(3)#1	2.7823(14)
Mo(1)–I(4)	2.7942(13)
Mo(1)–O(11)	2.105(8)
Mo(2)–Mo(1)#1	2.6444(15)
Mo(2)–Mo(3)#1	2.6622(15)
Mo(2)–Mo(3)	2.6640(15)
Mo(2)–I(1)	2.7939(16)
Mo(2)–I(2)	2.7778(12)
Mo(2)–I(3)	2.7871(13)
Mo(2)–I(4)#1	2.8026(16)
Mo(2)–O(21)	2.069(7)
Mo(3)–Mo(1)#1	2.6734(17)
Mo(3)–Mo(2)#1	2.6623(15)
Mo(3)–I(1)	2.7918(13)
Mo(3)–I(2)#1	2.7713(13)
Mo(3)–I(3)	2.7624(13)
Mo(3)–I(4)	2.7769(13)
Mo(3)–O(31)	2.090(9)
I(2)–Mo(3)#1	2.7713(13)
I(3)–Mo(1)#1	2.7825(14)
I(4)–Mo(2)#1	2.8025(16)
O(11)–C(11)	1.289(13)
O(12)–N(11)	1.233(14)
O(13)–N(11)	1.226(14)
O(14A)–N(12)	1.23(2)
O(15A)–N(12)	1.206(18)
O(14B)–N(12)	1.22(3)
O(15B)–N(12)	1.26(3)
O(21)–C(21)	1.276(13)
O(22)–N(21)	1.251(14)
O(23)–N(21)	1.221(15)
O(24)–N(22)	1.219(14)
O(25)–N(22)	1.211(13)
O(31)–C(31)	1.268(15)
O(32)–N(31)	1.224(16)
O(33)–N(31)	1.244(15)
O(34)–N(32)	1.235(14)
O(35)–N(32)	1.228(14)

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N(11)–C(14)	1.452(16)
N(12)–C(12)	1.463(16)
N(21)–C(24)	1.445(16)
N(22)–C(22)	1.458(17)
N(31)–C(34)	1.451(17)
N(32)–C(32)	1.451(16)
C(11)–C(12)	1.403(17)
C(11)–C(16)	1.414(17)
C(12)–C(13)	1.377(17)
C(13)–C(14)	1.396(18)
C(14)–C(15)	1.361(18)
C(15)–C(16)	1.390(18)
C(21)–C(22)	1.445(17)
C(21)–C(26)	1.433(17)
C(22)–C(23)	1.369(17)
C(23)–C(24)	1.393(18)
C(24)–C(25)	1.404(18)
C(25)–C(26)	1.343(17)
C(31)–C(32)	1.447(18)
C(31)–C(36)	1.426(17)
C(32)–C(33)	1.375(18)
C(33)–C(34)	1.367(18)
C(34)–C(35)	1.403(19)
C(35)–C(36)	1.361(18)
N(1)–C(111)	1.502(16)
N(1)–C(121)	1.543(16)
N(1)–C(131)	1.506(17)
N(1)–C(141)	1.511(19)
C(111)–C(112)	1.53(2)
C(112)–C(113)	1.541(19)
C(113)–C(114)	1.49(2)
C(121)–C(122)	1.505(19)
C(122)–C(123)	1.535(18)
C(123)–C(124)	1.49(2)
C(131)–C(132)	1.548(18)
C(132)–C(133)	1.55(2)
C(133)–C(134)	1.48(2)
C(141)–C(142)	1.508(19)
C(142)–C(143)	1.49(2)
C(143)–C(144)	1.50(2)
O(1S)–C(1S)	1.46(2)
O(1S)–C(4S)	1.44(2)
C(1S)–C(2SA)	1.52(6)
C(1S)–C(2SB)	1.40(4)
C(2SA)–C(3S)	1.49(6)
C(2SB)–C(3S)	1.64(4)
C(3S)–C(4S)	1.44(3)
O(2S)–C(5S)	1.36(4)

O(2S)–C(8S)	1.27(4)
C(5S)–C(6S)	1.45(4)
C(6S)–C(7S)	1.32(5)
C(7S)–C(8S)	1.50(5)
Angle	$\omega, ^\circ$
Mo(2)#1–Mo(1)–Mo(2)	89.87(4)
Mo(2)#1–Mo(1)–Mo(3)	60.26(4)
Mo(2)#1–Mo(1)–Mo(3)#1	60.13(4)
Mo(2)#1–Mo(1)–I(1)	121.90(5)
Mo(2)–Mo(1)–I(1)	61.42(4)
Mo(2)#1–Mo(1)–I(2)	121.18(5)
Mo(2)–Mo(1)–I(2)	61.12(3)
Mo(2)#1–Mo(1)–I(3)#1	61.74(4)
Mo(2)–Mo(1)–I(3)#1	120.39(5)
Mo(2)#1–Mo(1)–I(4)	61.96(4)
Mo(2)–Mo(1)–I(4)	120.98(4)
Mo(3)–Mo(1)–Mo(2)	59.83(4)
Mo(3)#1–Mo(1)–Mo(2)	59.61(4)
Mo(3)–Mo(1)–Mo(3)#1	89.99(5)
Mo(3)–Mo(1)–I(1)	61.64(4)
Mo(3)#1–Mo(1)–I(1)	121.01(5)
Mo(3)–Mo(1)–I(2)	120.94(5)
Mo(3)#1–Mo(1)–I(2)	61.07(4)
Mo(3)–Mo(1)–I(3)#1	122.01(5)
Mo(3)#1–Mo(1)–I(3)#1	60.80(4)
Mo(3)–Mo(1)–I(4)	61.16(4)
Mo(3)#1–Mo(1)–I(4)	122.09(5)
I(1)–Mo(1)–I(4)	89.66(4)
I(2)–Mo(1)–I(1)	89.33(4)
I(2)–Mo(1)–I(3)#1	89.00(4)
I(2)–Mo(1)–I(4)	176.66(5)
I(3)#1–Mo(1)–I(1)	176.30(5)
I(3)#1–Mo(1)–I(4)	91.83(4)
O(11)–Mo(1)–Mo(2)#1	137.8(2)
O(11)–Mo(1)–Mo(2)	132.4(2)
O(11)–Mo(1)–Mo(3)	134.8(2)
O(11)–Mo(1)–Mo(3)#1	135.1(2)
O(11)–Mo(1)–I(1)	86.1(2)
O(11)–Mo(1)–I(2)	86.7(2)
O(11)–Mo(1)–I(3)#1	90.5(2)
O(11)–Mo(1)–I(4)	90.1(2)
Mo(1)#1–Mo(2)–Mo(1)	90.13(4)
Mo(1)#1–Mo(2)–Mo(3)#1	60.14(4)
Mo(1)#1–Mo(2)–Mo(3)	60.48(4)
Mo(1)#1–Mo(2)–I(1)	121.95(5)
Mo(1)–Mo(2)–I(1)	61.12(4)
Mo(1)#1–Mo(2)–I(2)	121.34(5)

Mo(1)–Mo(2)–I(2)	61.15(3)
Mo(1)#1–Mo(2)–I(3)	61.57(4)
Mo(1)–Mo(2)–I(3)	120.48(5)
Mo(1)#1–Mo(2)–I(4)#1	61.65(4)
Mo(1)–Mo(2)–I(4)#1	121.03(5)
Mo(3)#1–Mo(2)–Mo(1)	60.03(4)
Mo(3)–Mo(2)–Mo(1)	59.65(4)
Mo(3)#1–Mo(2)–Mo(3)	90.13(5)
Mo(3)#1–Mo(2)–I(1)	121.12(5)
Mo(3)–Mo(2)–I(1)	61.47(4)
Mo(3)#1–Mo(2)–I(2)	61.21(4)
Mo(3)–Mo(2)–I(2)	120.79(5)
Mo(3)#1–Mo(2)–I(3)	121.71(5)
Mo(3)–Mo(2)–I(3)	60.85(3)
Mo(3)#1–Mo(2)–I(4)#1	61.02(4)
Mo(3)–Mo(2)–I(4)#1	122.12(5)
I(1)–Mo(2)–I(4)#1	176.27(5)
I(2)–Mo(2)–I(1)	89.18(4)
I(2)–Mo(2)–I(3)	177.00(5)
I(2)–Mo(2)–I(4)#1	89.47(4)
I(3)–Mo(2)–I(1)	89.63(4)
I(3)–Mo(2)–I(4)#1	91.55(4)
O(21)–Mo(2)–Mo(1)#1	129.6(2)
O(21)–Mo(2)–Mo(1)	140.2(2)
O(21)–Mo(2)–Mo(3)#1	134.7(3)
O(21)–Mo(2)–Mo(3)	134.7(2)
O(21)–Mo(2)–I(1)	91.9(3)
O(21)–Mo(2)–I(2)	92.2(2)
O(21)–Mo(2)–I(3)	85.0(2)
O(21)–Mo(2)–I(4)#1	84.7(3)
Mo(1)–Mo(3)–Mo(1)#1	90.01(5)
Mo(1)–Mo(3)–Mo(2)#1	59.59(4)
Mo(1)–Mo(3)–Mo(2)	60.51(4)
Mo(1)–Mo(3)–I(1)	61.41(4)
Mo(1)#1–Mo(3)–I(1)	120.95(5)
Mo(1)–Mo(3)–I(2)#1	121.04(5)
Mo(1)#1–Mo(3)–I(2)#1	61.34(4)
Mo(1)–Mo(3)–I(3)	122.28(5)
Mo(1)#1–Mo(3)–I(3)	61.55(4)
Mo(1)–Mo(3)–I(4)	61.82(4)
Mo(1)#1–Mo(3)–I(4)	122.32(5)
Mo(2)#1–Mo(3)–Mo(1)#1	60.36(4)
Mo(2)–Mo(3)–Mo(1)#1	59.40(4)
Mo(2)#1–Mo(3)–Mo(2)	89.88(5)
Mo(2)#1–Mo(3)–I(1)	121.00(4)
Mo(2)–Mo(3)–I(1)	61.55(4)
Mo(2)#1–Mo(3)–I(2)#1	61.45(3)
Mo(2)–Mo(3)–I(2)#1	120.73(5)

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Mo(2)#1–Mo(3)–I(3)	121.88(5)
Mo(2)–Mo(3)–I(3)	61.78(3)
Mo(2)#1–Mo(3)–I(4)	61.99(4)
Mo(2)–Mo(3)–I(4)	122.31(4)
I(2)#1–Mo(3)–I(1)	177.09(6)
I(2)#1–Mo(3)–I(4)	90.13(4)
I(3)–Mo(3)–I(1)	90.18(4)
I(3)–Mo(3)–I(2)#1	89.56(4)
I(3)–Mo(3)–I(4)	175.13(5)
I(4)–Mo(3)–I(1)	89.89(4)
O(31)–Mo(3)–Mo(1)	133.7(2)
O(31)–Mo(3)–Mo(1)#1	136.0(2)
O(31)–Mo(3)–Mo(2)#1	139.1(2)
O(31)–Mo(3)–Mo(2)	131.0(2)
O(31)–Mo(3)–I(1)	84.8(2)
O(31)–Mo(3)–I(2)#1	92.3(2)
O(31)–Mo(3)–I(3)	85.6(2)
O(31)–Mo(3)–I(4)	89.5(2)
Mo(1)–I(1)–Mo(2)	57.46(4)
Mo(1)–I(1)–Mo(3)	56.95(3)
Mo(3)–I(1)–Mo(2)	56.97(3)
Mo(2)–I(2)–Mo(1)	57.73(3)
Mo(3)#1–I(2)–Mo(1)	57.59(4)
Mo(3)#1–I(2)–Mo(2)	57.34(3)
Mo(1)#1–I(3)–Mo(2)	56.69(3)
Mo(3)–I(3)–Mo(1)#1	57.65(4)
Mo(3)–I(3)–Mo(2)	57.37(3)
Mo(1)–I(4)–Mo(2)#1	56.39(3)
Mo(3)–I(4)–Mo(1)	57.02(3)
Mo(3)–I(4)–Mo(2)#1	57.00(4)
C(11)–O(11)–Mo(1)	137.3(8)
C(21)–O(21)–Mo(2)	166.1(8)
C(31)–O(31)–Mo(3)	146.7(9)
O(12)–N(11)–C(14)	117.7(11)
O(13)–N(11)–O(12)	124.7(11)
O(13)–N(11)–C(14)	117.6(11)
O(14A)–N(12)–O(15B)	108(2)
O(14A)–N(12)–C(12)	117.1(13)
O(15A)–N(12)–O(14A)	122.3(15)
O(15A)–N(12)–O(14B)	111.2(16)
O(15A)–N(12)–O(15B)	43.5(14)
O(15A)–N(12)–C(12)	120.3(12)
O(14B)–N(12)–O(14A)	30.4(14)
O(14B)–N(12)–O(15B)	121(2)
O(14B)–N(12)–C(12)	116.8(15)
O(15B)–N(12)–C(12)	120.8(16)
O(22)–N(21)–C(24)	118.1(12)
O(23)–N(21)–O(22)	123.6(12)

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O(23)–N(21)–C(24)	118.3(11)
O(24)–N(22)–C(22)	117.0(11)
O(25)–N(22)–O(24)	123.2(12)
O(25)–N(22)–C(22)	119.7(12)
O(32)–N(31)–O(33)	122.7(12)
O(32)–N(31)–C(34)	119.3(13)
O(33)–N(31)–C(34)	117.9(13)
O(34)–N(32)–C(32)	117.4(11)
O(35)–N(32)–O(34)	123.8(12)
O(35)–N(32)–C(32)	118.7(12)
O(11)–C(11)–C(12)	122.8(11)
O(11)–C(11)–C(16)	120.4(11)
C(12)–C(11)–C(16)	116.8(11)
C(11)–C(12)–N(12)	121.2(11)
C(13)–C(12)–N(12)	117.1(11)
C(13)–C(12)–C(11)	121.7(11)
C(12)–C(13)–C(14)	119.8(12)
C(13)–C(14)–N(11)	119.3(11)
C(15)–C(14)–N(11)	120.4(12)
C(15)–C(14)–C(13)	119.9(11)
C(14)–C(15)–C(16)	120.7(13)
C(15)–C(16)–C(11)	120.8(12)
O(21)–C(21)–C(22)	123.4(12)
O(21)–C(21)–C(26)	121.9(11)
C(26)–C(21)–C(22)	114.7(10)
C(21)–C(22)–N(22)	120.6(11)
C(23)–C(22)–N(22)	116.6(11)
C(23)–C(22)–C(21)	122.7(12)
C(22)–C(23)–C(24)	119.1(12)
C(23)–C(24)–N(21)	119.1(11)
C(23)–C(24)–C(25)	120.2(11)
C(25)–C(24)–N(21)	120.6(12)
C(26)–C(25)–C(24)	120.5(12)
C(25)–C(26)–C(21)	122.6(12)
O(31)–C(31)–C(32)	121.9(12)
O(31)–C(31)–C(36)	123.9(12)
C(36)–C(31)–C(32)	114.0(12)
C(31)–C(32)–N(32)	118.9(11)
C(33)–C(32)–N(32)	118.5(12)
C(33)–C(32)–C(31)	122.6(12)
C(34)–C(33)–C(32)	119.4(12)
C(33)–C(34)–N(31)	118.1(13)
C(33)–C(34)–C(35)	121.5(12)
C(35)–C(34)–N(31)	120.4(12)
C(36)–C(35)–C(34)	118.8(13)
C(35)–C(36)–C(31)	123.6(13)
C(111)–N(1)–C(121)	110.7(10)
C(111)–N(1)–C(131)	105.7(11)

C(111)–N(1)–C(141)	112.0(11)
C(131)–N(1)–C(121)	110.3(10)
C(131)–N(1)–C(141)	110.7(10)
C(141)–N(1)–C(121)	107.5(11)
N(1)–C(111)–C(112)	115.8(12)
C(111)–C(112)–C(113)	110.9(13)
C(114)–C(113)–C(112)	112.0(14)
C(122)–C(121)–N(1)	114.7(11)
C(121)–C(122)–C(123)	110.2(12)
C(124)–C(123)–C(122)	109.5(12)
N(1)–C(131)–C(132)	115.6(11)
C(133)–C(132)–C(131)	109.1(11)
C(134)–C(133)–C(132)	113.6(13)
C(142)–C(141)–N(1)	115.2(13)
C(143)–C(142)–C(141)	114.1(14)
C(142)–C(143)–C(144)	113.6(14)
C(4S)–O(1S)–C(1S)	106.5(16)
O(1S)–C(1S)–C(2SA)	109(3)
C(2SB)–C(1S)–O(1S)	104(2)
C(2SB)–C(1S)–C(2SA)	36(3)
C(3S)–C(2SA)–C(1S)	102(4)
C(1S)–C(2SB)–C(3S)	100(3)
C(2SA)–C(3S)–C(2SB)	33(2)
C(4S)–C(3S)–C(2SA)	108(3)
C(4S)–C(3S)–C(2SB)	103(2)
C(3S)–C(4S)–O(1S)	107.7(18)
C(8S)–O(2S)–C(5S)	105(3)
O(2S)–C(5S)–C(6S)	109(3)
C(7S)–C(6S)–C(5S)	100(3)
C(6S)–C(7S)–C(8S)	110(4)
O(2S)–C(8S)–C(7S)	105(3)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+1/2, -y + 3/2, -z$
