Electronic Supplementary Information (ESI) for

A Giant Metallo-Supramolecular Cage Encapsulating a Single-Molecule Magnet

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I. Experimental

Synthesis of complex **1**: $Na_9[Ho(W_5O_{18})_2]\cdot xH_2O$ was prepared in situ for synthesizing the silver(I) cluster according to a previously reported method.[1] $Na_2WO_4\cdot 2H_2O$ (4.9 g, 15 mmol) was dissolve in water (12 mL) and pH was adjusted to 7.5 with acetic acid, then aquatic solution (5 mL) of $HoCl_3\cdot 6H_2O$ (570 mg, 1.5 mmol) in water was added. The reaction mixture was heated at 85 °C for 3 hours, filtered and the volume reduced under vacuum and cooled to give $Na_9[Ho(W_5O_{18})_2]\cdot xH_2O$ as a pink solid (2.5 g) which was collected and washed with small quantity of water. The crude solid was dissolved in water (9 mL) and an aliquot of this solution (0.5 mL, ~50 mol Ho, excess) was added to a methanol (15 mL) solution of *t*-BuC≡CAg (95 mg, 500 mol) and $AgCF_3SO_3$ (32 mg, 125 mol) which had been treated in a sonicator for 30 min. The resulting white suspension was sealed and heated at 80 °C for 24 h. After cooling to room temperature, the colorless solution was filtered and the filtrate left to evaporate slowly in dark for 3 weeks to give complex **1** as colorless crystals which were collected and washed with small quantity of methanol and Et_2O (17 mg, 12 %, calculated from Ag). Elemental analysis (%) found: C 21.27, H 3.04, calcd for $C_{168}H_{259}O_{40}Cl_4Ag_{42}HoW_{10}$: C 21.03, H 2.72; IR (KBr, cm^{-1}): 2011 (C≡C); 929, 823, 750, 691, 581, 541, 424 ($[Ho(W_5O_{18})_2]^{9-}$).

[1] M. A. AlDamen, S. Cardona-Serra, J. M. Clemente-Juan , E. Coronado , A. Gaita-Ariño, C. Martí-Gastaldo, F. Luis, O. Montero, *Inorg Chem.*, 2009, **48**, 3467-3479.

II. Physical measurements

General Methods.

All reagents and solvents employed were commercially available and used as received without further purification. Elemental analyses for C, H were performed on a Perkin-Elmer 240C analyzer. Infrared spectra were recorded on a Vector22 Bruker Spectrophotometer with KBr pellets in the 400−4000 cm^{-1} region. UV-vis spectra for solution sample of **1** was measured with a Shimadzu UV-3100 spectrophotometer, for solid sample of **1** was measured with a Perkin-Elmer Lambda 950 UV-vis spectrophotometer. Emission spectra for solid sample of **1** was measured with a Hitachi F-4600 luminescence spectrophotometer. Magnetic susceptibilities for polycrystalline samples were measured with the use of a Quantum Design MPMS-SQUID-VSM magnetometer in the temperature range 1.8–300 K. Field dependences of magnetization were measured using Quantum Design MPMS-SQUID-VSM system in an applied field up to 70 kOe. Diamagnetic corrections were calculated using Pascal's constants and an experimental correction for the diamagnetic sample holder was applied. X-ray powder diffractometry study of the complex was performed on a Bruker D8 ADANCE diffractometer with Cu Kα radiation.

X-ray Crystallography.

The crystal structure was determined on a Bruker AXS SMART APEX II CCD-based diffractometer using monochromated Mo $K\alpha$ radiation (λ = 0.71073 Å) at 123 K. Cell parameters were retrieved using SMART software and refined using SAINT on all observed reflections. Data was collected using a narrow-frame method with scan widths of 0.30° in ω and an exposure time of 10 s/frame. The highly redundant data sets were reduced using SAINT and corrected for Lorentz and polarization effects. Absorption corrections were applied using SADABS supplied by Bruker. Structures were solved by direct methods using the program SHELXL-97. The positions of the metal atoms and their first coordination spheres were located from direct-methods *E* maps, other non-hydrogen atoms were found in alternating difference Fourier syntheses and least-squares refinement cycles and, during the final cycles, refined anisotropically. Hydrogen atoms were placed in calculated positions and refined as riding atoms with a uniform value of U_{iso}.

III. Characterization

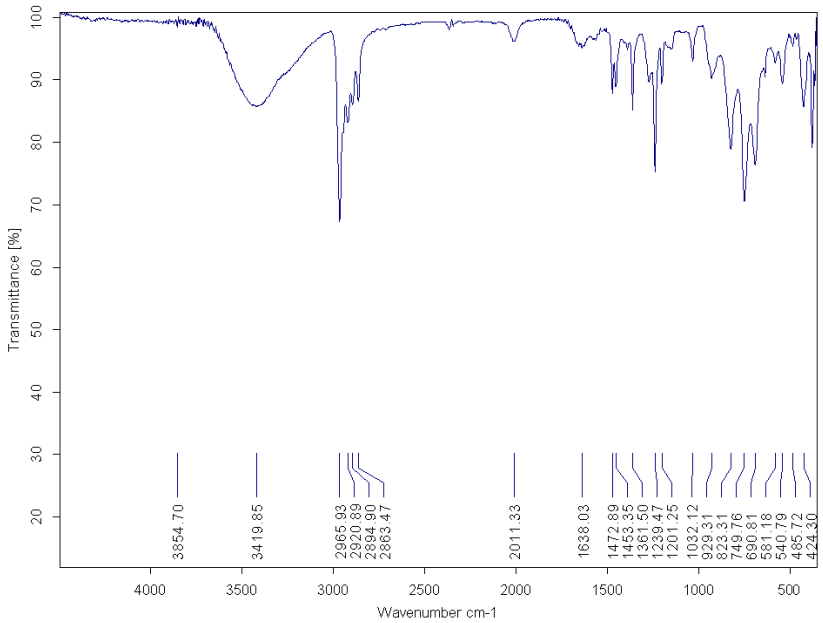

Fig. S1 Broad FTIR (KBr disc) absorption of **1**.

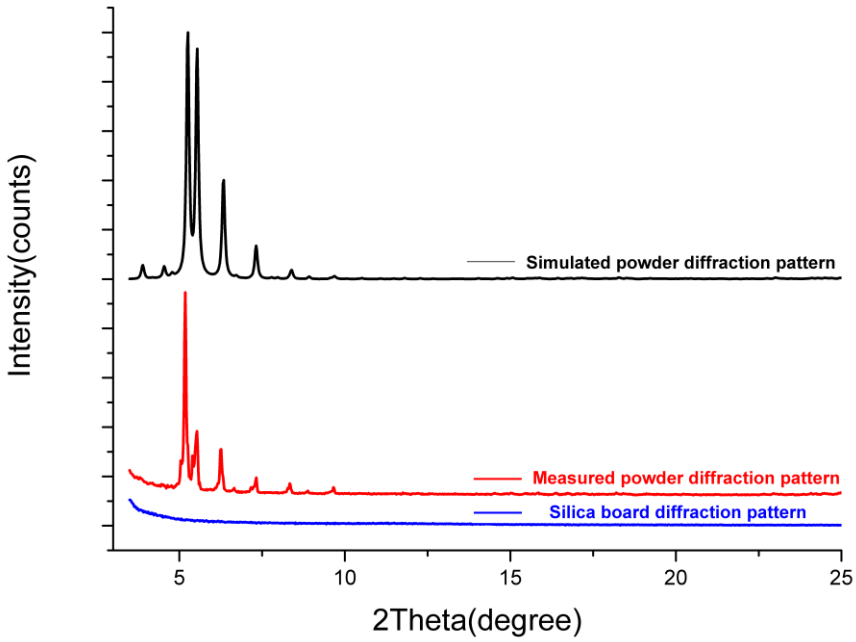

Fig. S2 The measured and simulated X-ray powder diffraction patterns of **1**.

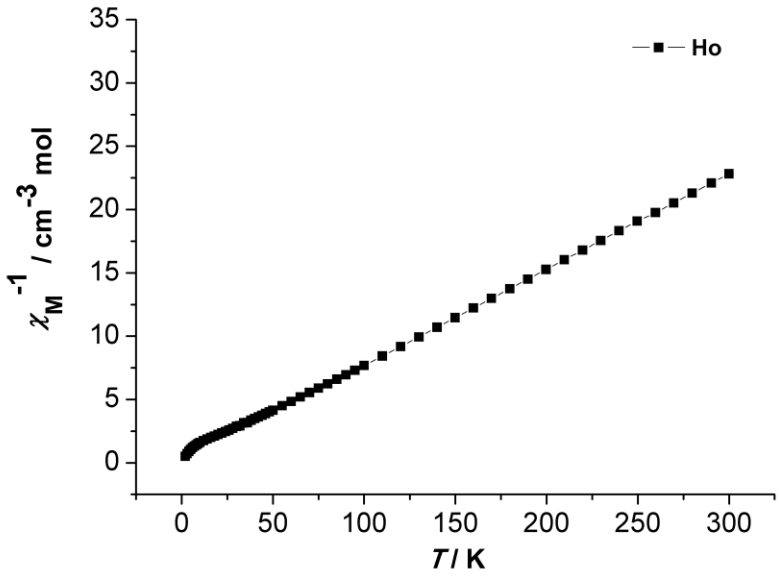

Fig. S3 Plots of χ_M^{-1} determined at 100 Oe upon T from 1.8 to 300 K for **1** with an applied field of 100 Oe.

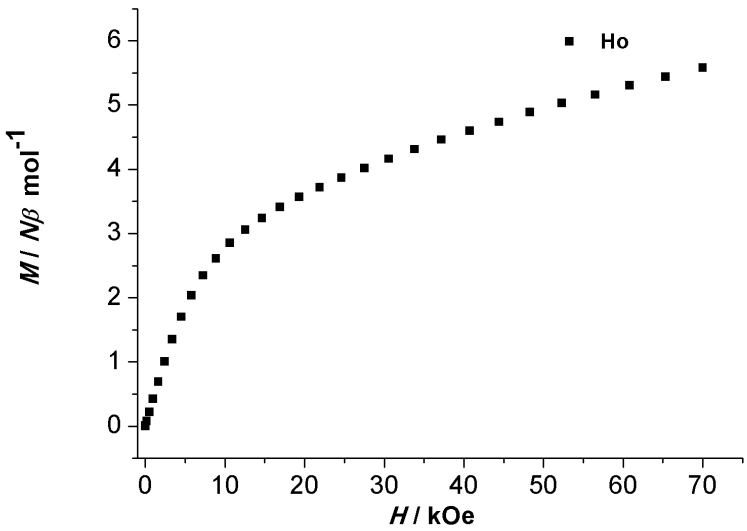

Fig. S4 Plots of magnetization upon magnetic field from 0 to 7 T at 1.8 K for complex **1.**

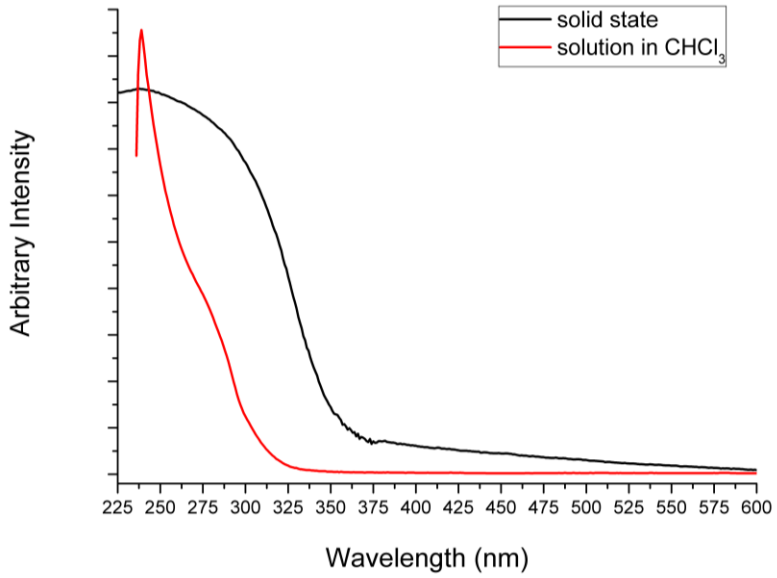

Fig. S5 The UV-vis spectra for complex **1** in solution and solid state.

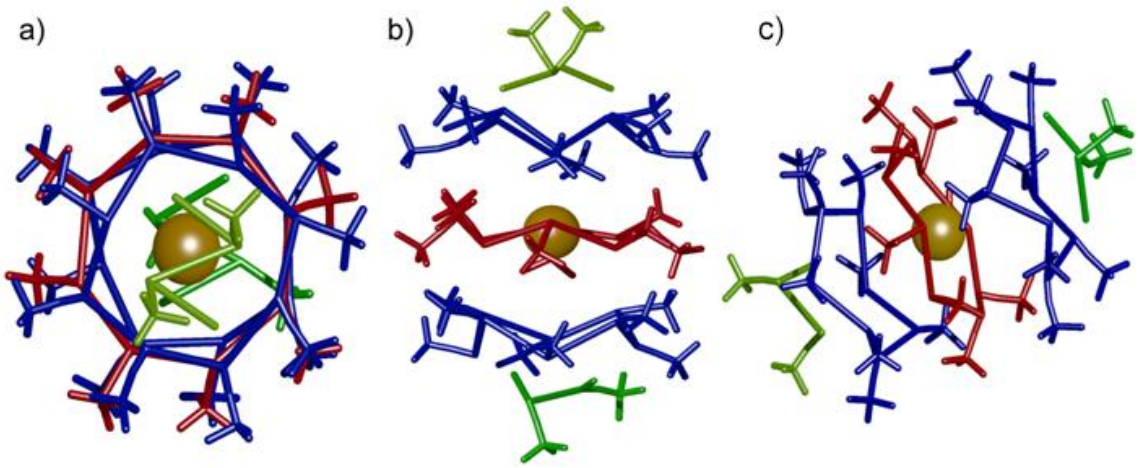

Fig. S6 Representation of the arrangement of *t*-Bu groups on the structure of complex **1**. Atificial bonds are drawn between terminal alkyne carbons to show connectivity; the central Ho atom is shown in CPK representation colored orange. The three "crown-like" layers are colored blue, red, blue and can be seen to be unsymmetrical from top to bottom.

Table S1. Selected bond lengths (Å) and angles (°) for complex **1**.

Ag(1)-C(7)	2.089(9)	Ag(4)-Ag(10)	3.1822(9)	Ag(13)-C(55)	2.175(9)
Ag(1)-C(1)	2.269(9)	Ag(5)-C(31)	2.084(9)	Ag(13)-C(13)	2.212(10)
Ag(1)-C(2)	2.519(10)	Ag(5)-C(1)	2.147(9)	Ag(13)-C(14)	2.654(10)
Ag(1)-O(1)	2.562(6)	Ag(5)-Cl(1)	2.917(2)	Ag(14)-C(67)	2.126(9)
Ag(1)-Ag(3)	3.0046(10)	Ag(5)-Ag(12)	3.1539(9)	Ag(14)-C(37)	2.288(9)
Ag(1)-Ag(4)	3.0977(10)	Ag(5)-Ag(11)	3.3398(10)	Ag(14)-C(38)	2.365(9)
Ag(1)-Ag(5)	3.1972(9)	Ag(6)-C(37)	2.249(9)	Ag(14)-O(10)	2.374(6)
Ag(1)-Ag(2)	3.3221(9)	Ag(6)-C(13)	2.304(10)	Ag(14)-Ag(19)	3.2746(10)
Ag(2)-C(13)	2.124(9)	Ag(6)-Ag(7)	2.8339(10)	Ag(15)-C(79)	2.158(9)
Ag(2)-C(1)	2.181(9)	Ag(6)-Cl(2)	2.876(2)	Ag(15)-C(43)	2.305(9)
Ag(2)-Cl(2)	2.920(2)	Ag(7)-C(37)	2.105(10)	Ag(15)-O(11)	2.444(6)
Ag(2)-Ag(5)	2.9286(9)	Ag(7)-C(19)	2.251(10)	Ag(15)-C(44)	2.531(9)
Ag(2)-Ag(13)	3.1221(10)	Ag(7)-C(20)	2.641(9)	Ag(15)-Ag(21)	2.9953(9)
Ag(2)-Ag(6)	3.2027(10)	Ag(8)-C(19)	2.120(9)	Ag(16)-C(91)	2.143(10)
Ag(3)-C(19)	2.325(10)	Ag(8)-C(43)	2.276(9)	Ag(16)-C(49)	2.300(9)
Ag(3)-C(7)	2.355(10)	Ag(8)-C(44)	2.542(9)	Ag(16)-O(12)	2.349(6)
Ag(3)-Cl(2)	2.543(2)	Ag(8)-Ag(9)	3.0938(10)	Ag(16)-C(50)	2.376(9)
Ag(3)-Ag(8)	2.9042(11)	Ag(9)-C(43)	2.095(9)	Ag(16)-Ag(22)	3.2552(10)
Ag(3)-Ag(7)	3.1372(10)	Ag(9)-C(25)	2.108(9)	Ag(17)-C(103)	2.108(9)
Ag(4)-C(7)	2.246(9)	Ag(10)-C(49)	2.199(9)	Ag(17)-C(55)	2.300(10)
Ag(4)-C(25)	2.278(9)	Ag(10)-C(25)	2.253(8)	Ag(17)-O(13)	2.344(5)
Ag(4)-Cl(1)	2.623(2)	Ag(10)-C(26)	2.489(8)	Ag(17)-C(56)	2.404(9)
Ag(4)-C(8)	2.700(9)	Ag(10)-Ag(11)	2.8079(10)	Ag(17)-Ag(25)	3.3311(10)
Ag(4)-Ag(9)	2.9285(10)	Ag(11)-C(49)	2.228(9)	Ag(18)-C(61)	2.223(9)
Ag(4)-Ag(10)	3.1822(9)	Ag(11)-C(31)	2.371(9)	Ag(18)-C(67)	2.224(8)
Ag(5)-C(31)	2.084(9)	Ag(11)-C(32)	2.673(9)	Ag(18)-O(15)	2.588(5)
Ag(4)-C(7)	2.246(9)	Ag(11)-Cl(1)	2.844(2)	Ag(18)-Ag(19)	3.0348(10)
Ag(4)-C(25)	2.278(9)	Ag(12)-C(31)	2.127(9)	Ag(18)-Ag(25)	3.1127(9)
Ag(4)-Cl(1)	2.623(2)	Ag(12)-C(55)	2.222(8)	Ag(18)-Ag(26)	3.2487(9)
Ag(4)-C(8)	2.700(9)	Ag(12)-C(32)	2.676(10)	Ag(19)-C(67)	2.221(9)
Ag(4)-Ag(9)	2.9285(10)	Ag(12)-Ag(13)	2.7553(10)	Ag(19)-C(73)	2.322(9)
Ag(19)-C(74)	2.556(10)	Ag(24)-Ag(25)	3.0133(9)	Ag(19)-O(34)	2.574(5)
Ag(19)-Ag(20)	3.2104(10)	Ag(28)-C(85)	2.101(9)	Ag(35)-Ag(41)	2.9045(10)
Ag(20)-C(73)	2.193(9)	Ag(28)-C(127)	2.310(9)	Ag(36)-C(109)	2.219(9)

Ag(20)-C(79)	2.304(9)	Ag(29)-C(109)	2.288(8)	Ag(36)-Ag(41)	3.1761(10)
Ag(20)-O(35)	2.580(5)	Ag(29)-C(110)	2.358(8)	Ag(37)-C(133)	2.219(9)
Ag(20)-C(80)	2.586(9)	Ag(29)-O(31)	2.362(5)	Ag(37)-C(109)	2.256(9)
Ag(20)-Ag(27)	3.1579(10)	Ag(30)-C(115)	2.201(10)	Ag(37)-C(134)	2.684(9)
Ag(20)-Ag(21)	3.2864(10)	Ag(30)-C(133)	2.229(9)	Ag(37)-Cl(3)	2.829(2)
Ag(21)-C(79)	2.081(9)	Ag(30)-O(20)	2.532(5)	Ag(37)-Ag(38)	3.3371(10)
Ag(21)-C(85)	2.236(10)	Ag(30)-Ag(31)	2.7797(10)	Ag(38)-C(133)	2.114(10)
Ag(21)-Ag(28)	3.1862(10)	Ag(30)-Ag(38)	3.0100(10)	Ag(38)-C(157)	2.120(9)
Ag(21)-Ag(22)	3.3305(9)	Ag(31)-C(115)	2.086(9)	Ag(38)-Ag(42)	3.1113(10)
Ag(22)-C(85)	2.202(9)	Ag(31)-C(139)	2.199(9)	Ag(38)-Ag(39)	3.1835(9)
Ag(22)-C(91)	2.254(9)	Ag(31)-C(140)	2.648(10)	Ag(39)-C(139)	2.120(9)
Ag(22)-O(17)	2.538(5)	Ag(31)-Ag(39)	3.0403(10)	Ag(39)-C(157)	2.292(9)
Ag(22)-Ag(23)	3.1354(9)	Ag(32)-C(139)	2.177(9)	Ag(39)-C(158)	2.688(10)
Ag(22)-Ag(28)	3.1527(10)	Ag(32)-C(121)	2.188(9)	Ag(39)-Cl(4)	2.783(2)
Ag(23)-C(91)	2.234(9)	Ag(31)-Ag(39)	3.0403(10)	Ag(39)-Ag(42)	3.1875(10)
Ag(23)-C(97)	2.250(8)	Ag(32)-C(139)	2.177(9)	Ag(40)-C(163)	2.110(8)
Ag(23)-O(36)	2.589(6)	Ag(32)-C(121)	2.188(9)	Ag(40)-C(145)	2.146(9)
Ag(23)-Ag(24)	3.0456(9)	Ag(32)-Ag(33)	2.7868(10)	Ag(40)-Cl(4)	2.825(2)
Ag(24)-C(97)	2.238(9)	Ag(32)-Ag(39)	3.0921(10)	Ag(40)-Ag(41)	3.0763(9)
Ag(24)-C(103)	2.293(8)	Ag(33)-C(121)	2.165(9)	Ag(40)-Ag(42)	3.1778(10)
Ag(24)-O(18)	2.563(5)	Ag(33)-C(145)	2.358(8)	Ag(41)-C(163)	2.259(9)
Ag(25)-C(103)	2.227(9)	Ag(33)-C(146)	2.514(9)	Ag(41)-C(151)	2.276(9)
Ag(25)-C(61)	2.323(10)	Ag(33)-Ag(40)	3.3084(9)	Ag(41)-Cl(3)	2.703(2)
Ag(25)-C(62)	2.616(9)	Ag(34)-C(145)	2.101(9)	Ag(41)-Ag(42)	3.3730(10)
Ag(26)-C(61)	2.061(10)	Ag(34)-C(127)	2.201(9)	Ag(42)-C(157)	2.235(9)
Ag(26)-C(115)	2.305(9)	Ag(34)-Ag(40)	2.8560(10)	Ag(42)-C(163)	2.287(8)
Ag(26)-O(28)	2.354(6)	Ag(34)-Ag(35)	2.9096(9)	Ag(42)-O(19)	2.507(6)
Ag(26)-C(116)	2.374(9)	Ag(35)-C(151)	2.023(8)	Ag(42)-C(164)	2.535(8)
Ag(27)-C(73)	2.173(9)	Ag(35)-C(127)	2.095(9)	C(1)-C(2)	1.231(12)
Ag(27)-C(121)	2.292(9)	Ho(1)-O(18)	2.424(5)	C(7)-C(8)	1.216(12)
Ag(27)-C(122)	2.390(10)	Ho(1)-O(34)	2.391(6)	C(13)-C(14)	1.233(12)
Ag(27)-O(29)	2.401(6)	Ho(1)-O(33)	2.394(5)	C(19)-C(20)	1.255(12)
Ag(28)-O(30)	2.406(5)	Ag(36)-C(151)	2.324(8)	C(25)-C(26)	1.198(11)
Ag(28)-C(128)	2.494(8)	Ag(36)-C(152)	2.590(9)	C(31)-C(32)	1.250(12)
Ag(29)-C(97)	2.128(9)	Ag(36)-Ag(37)	2.8195(10)	C(37)-C(38)	1.202(12)

C(43)-C(44)	1.215(12)	Ho(1)-O(17)	2.395(5)	C(19)-Ag(3)-Cl(2)	105.3(2)
C(49)-C(50)	1.210(11)	Ho(1)-O(15)	2.398(5)	C(7)-Ag(3)-Cl(2)	115.5(2)
C(55)-C(56)	1.202(11)	Ho(1)-O(16)	2.408(5)	Ag(9)-Ag(4)-Ag(1)	140.06(3)
C(61)-C(62)	1.176(12)	Ho(1)-O(18)	2.424(5)	Ag(9)-Ag(4)-Ag(10)	70.24(2)
C(67)-C(68)	1.193(12)	Ho(1)-O(35)	2.424(6)	Ag(1)-Ag(4)-Ag(10)	123.54(3)
C(73)-C(74)	1.224(12)	Ho(1)-O(36)	2.431(5)	C(31)-Ag(5)-C(1)	162.6(2)
C(79)-C(80)	1.225(12)	C(7)-Ag(1)-C(1)	175.7(3)	C(31)-Ag(5)-Cl(1)	91.9(3)
C(85)-C(86)	1.196(11)	C(7)-Ag(1)-C(2)	146.6(3)	C(1)-Ag(5)-Cl(1)	102.1(2)
C(91)-C(92)	1.187(12)	C(1)-Ag(1)-C(2)	29.2(3)	Ag(2)-Ag(5)-Ag(12)	88.25(3)
C(97)-C(98)	1.220(12)	Ag(3)-Ag(1)-Ag(4)	75.10(3)	Ag(2)-Ag(5)-Ag(1)	65.51(2)
C(103)-C(104)	1.254(11)	Ag(3)-Ag(1)-Ag(5)	126.45(3)	Ag(12)-Ag(5)-Ag(1)	137.72(3)
C(109)-C(110)	1.205(12)	Ag(4)-Ag(1)-Ag(5)	95.67(3)	Ag(2)-Ag(5)-Ag(11)	131.40(3)
C(115)-C(116)	1.206(12)	Ag(3)-Ag(1)-Ag(2)	89.82(3)	Ag(12)-Ag(5)-Ag(11)	64.99(2)
C(121)-C(122)	1.267(12)	Ag(4)-Ag(1)-Ag(2)	126.35(3)	Ag(1)-Ag(5)-Ag(11)	107.35(3)
C(127)-C(128)	1.240(11)	Ag(5)-Ag(1)-Ag(2)	53.35(2)	C(37)-Ag(6)-C(13)	153.1(3)
C(133)-C(134)	1.216(12)	C(13)-Ag(2)-C(1)	162.3(4)	C(37)-Ag(6)-Cl(2)	103.9(2)
C(139)-C(140)	1.196(12)	C(13)-Ag(2)-Cl(2)	92.7(3)	C(13)-Ag(6)-Cl(2)	90.2(2)
C(145)-C(146)	1.210(12)	C(1)-Ag(2)-Cl(2)	99.1(2)	Ag(7)-Ag(6)-Ag(2)	116.41(3)
C(151)-C(152)	1.256(11)	C(1)-Ag(2)-Ag(5)	46.9(2)	C(37)-Ag(7)-C(19)	157.4(2)
C(157)-C(158)	1.181(12)	Ag(3)-Ag(1)-Ag(5)	126.45(3)	C(37)-Ag(7)-C(20)	129.1(2)
C(163)-C(164)	1.201(11)	Ag(4)-Ag(1)-Ag(5)	95.67(3)	C(19)-Ag(7)-C(20)	28.3(3)
Ho(1)-O(34)	2.391(6)	Ag(3)-Ag(1)-Ag(2)	89.82(3)	Ag(6)-Ag(7)-Ag(3)	93.60(3)
Ho(1)-O(33)	2.394(5)	Ag(4)-Ag(1)-Ag(2)	126.35(3)	C(19)-Ag(8)-C(43)	149.5(3)
Ho(1)-O(17)	2.395(5)	Ag(5)-Ag(1)-Ag(2)	53.35(2)	C(19)-Ag(8)-C(44)	122.8(3)
Ho(1)-O(15)	2.398(5)	C(13)-Ag(2)-C(1)	162.3(4)	C(43)-Ag(8)-C(44)	28.5(3)
Ho(1)-O(16)	2.408(5)	C(13)-Ag(2)-Cl(2)	92.7(3)	Ag(4)-Ag(9)-Ag(8)	87.63(3)
Ho(1)-O(35)	2.424(6)	C(1)-Ag(2)-Cl(2)	99.1(2)	C(49)-Ag(10)-C(25)	156.0(3)
Ho(1)-O(36)	2.431(5)	Ag(5)-Ag(2)-Ag(13)	88.58(2)	C(49)-Ag(10)-C(26)	127.5(3)
Ho(1)-O(35)	2.424(6)	Ag(5)-Ag(2)-Ag(6)	132.56(3)	C(25)-Ag(10)-C(26)	28.7(3)
O(1)-Ag(1)-Ag(5)	58.54(14)	Ag(5)-Ag(2)-Ag(6)	132.56(3)	Ag(11)-Ag(10)-Ag(4)	97.34(3)
Ag(6)-Ag(2)-Ag(1)	108.56(3)	Ag(5)-Ag(2)-Ag(1)	61.14(2)	C(49)-Ag(11)-C(31)	154.5(3)
C(19)-Ag(3)-C(7)	138.0(3)	Ag(13)-Ag(2)-Ag(1)	135.07(3)	C(49)-Ag(11)-C(32)	126.6(3)
C(31)-Ag(11)-C(32)	27.9(3)	C(67)-Ag(19)-C(73)	140.9(3)	Ag(24)-Ag(25)-Ag(17)	66.14(2)
C(49)-Ag(11)-Cl(1)	106.9(2)	C(73)-Ag(19)-C(74)	28.6(3)	C(61)-Ag(26)-C(116)	137.5(2)
C(31)-Ag(11)-Cl(1)	88.1(2)	Ag(18)-Ag(19)-Ag(20)	134.22(3)	C(115)-Ag(26)-C(116)	29.8(3)

C(32)-Ag(11)-Cl(1)	105.71(18)	Ag(18)-Ag(19)-Ag(14)	68.82(2)	C(73)-Ag(27)-C(121)	171.5(2)
Ag(10)-Ag(11)-Ag(5)	115.64(3)	Ag(20)-Ag(19)-Ag(14)	131.13(3)	C(73)-Ag(27)-C(122)	140.3(2)
C(31)-Ag(12)-C(55)	154.7(3)	C(73)-Ag(20)-C(79)	143.5(3)	C(121)-Ag(27)-C(122)	31.3(3)
C(31)-Ag(12)-C(32)	27.2(3)	C(73)-Ag(20)-C(80)	117.7(3)	C(85)-Ag(28)-C(127)	159.2(3)
C(55)-Ag(12)-C(32)	139.3(3)	C(79)-Ag(20)-C(80)	28.3(3)	C(85)-Ag(28)-C(128)	131.7(2)
Ag(13)-Ag(12)-Ag(5)	91.09(3)	Ag(27)-Ag(20)-Ag(19)	71.20(2)	C(127)-Ag(28)-C(128)	29.6(3)
Ag(12)-Ag(13)-Ag(2)	92.07(3)	Ag(27)-Ag(20)-Ag(21)	131.97(3)	Ag(22)-Ag(28)-Ag(21)	63.39(2)
Ag(8)-Ag(3)-Ag(1)	128.39(3)	Ag(19)-Ag(20)-Ag(21)	133.66(3)	C(97)-Ag(29)-C(109)	166.4(2)
Ag(8)-Ag(3)-Ag(7)	68.00(3)	C(79)-Ag(21)-C(85)	147.8(3)	C(97)-Ag(29)-C(110)	136.4(2)
Ag(1)-Ag(3)-Ag(7)	129.50(3)	Ag(15)-Ag(21)-Ag(28)	163.04(3)	C(109)-Ag(29)-C(110)	30.0(3)
C(7)-Ag(4)-C(25)	149.4(2)	Ag(15)-Ag(21)-Ag(20)	67.95(2)	Ag(31)-Ag(30)-Ag(38)	93.47(3)
C(7)-Ag(4)-Cl(1)	106.4(2)	Ag(28)-Ag(21)-Ag(20)	123.15(3)	C(115)-Ag(31)-C(139)	155.6(4)
C(25)-Ag(4)-Cl(1)	101.2(2)	Ag(15)-Ag(21)-Ag(22)	127.56(3)	C(115)-Ag(31)-C(140)	132.7(3)
C(7)-Ag(4)-C(8)	26.5(3)	Ag(28)-Ag(21)-Ag(22)	57.82(2)	C(139)-Ag(31)-C(140)	26.6(3)
C(25)-Ag(4)-C(8)	122.9(2)	Ag(20)-Ag(21)-Ag(22)	129.31(3)	Ag(30)-Ag(31)-Ag(39)	94.11(3)
Cl(1)-Ag(4)-C(8)	129.2(2)	C(85)-Ag(22)-C(91)	140.4(3)	C(139)-Ag(32)-C(121)	156.0(3)
C(67)-Ag(14)-C(37)	171.3(3)	Ag(23)-Ag(22)-Ag(28)	124.55(3)	Ag(33)-Ag(32)-Ag(39)	108.99(3)
C(67)-Ag(14)-C(38)	141.5(3)	Ag(23)-Ag(22)-Ag(16)	66.16(2)	C(121)-Ag(33)-C(145)	157.6(3)
C(37)-Ag(14)-C(38)	29.9(3)	Ag(28)-Ag(22)-Ag(16)	160.57(3)	C(121)-Ag(33)-C(146)	129.3(3)
C(79)-Ag(15)-C(43)	165.3(3)	Ag(23)-Ag(22)-Ag(21)	136.50(3)	C(145)-Ag(33)-C(146)	28.5(3)
C(79)-Ag(15)-C(44)	138.2(3)	Ag(28)-Ag(22)-Ag(21)	58.80(2)	Ag(32)-Ag(33)-Ag(40)	106.44(3)
C(91)-Ag(16)-C(49)	166.7(3)	Ag(16)-Ag(22)-Ag(21)	127.10(3)	C(145)-Ag(34)-C(127)	154.7(3)
C(91)-Ag(16)-C(50)	136.8(3)	C(91)-Ag(23)-C(97)	140.4(3)	Ag(40)-Ag(34)-Ag(35)	97.86(3)
C(49)-Ag(16)-C(50)	29.9(3)	Ag(24)-Ag(23)-Ag(22)	133.38(3)	C(151)-Ag(35)-C(127)	166.9(4)
C(103)-Ag(17)-C(55)	165.3(2)	C(97)-Ag(24)-C(103)	136.1(2)	Ag(41)-Ag(35)-Ag(34)	85.20(3)
C(103)-Ag(17)-C(56)	135.8(2)	Ag(25)-Ag(24)-Ag(23)	137.24(3)	C(109)-Ag(36)-C(151)	157.7(3)
C(55)-Ag(17)-C(56)	29.5(3)	C(103)-Ag(25)-C(61)	136.8(2)	C(109)-Ag(36)-C(152)	130.1(3)
C(61)-Ag(18)-C(67)	138.3(3)	C(103)-Ag(25)-C(62)	115.8(2)	C(151)-Ag(36)-C(152)	29.0(3)
Ag(19)-Ag(18)-Ag(25)	134.57(3)	C(61)-Ag(25)-C(62)	26.7(3)	Ag(37)-Ag(36)-Ag(41)	101.20(3)
Ag(19)-Ag(18)-Ag(26)	127.55(3)	Ag(24)-Ag(25)-Ag(18)	136.54(3)	C(133)-Ag(37)-C(109)	153.3(3)
Ag(25)-Ag(18)-Ag(26)	67.70(2)	Ag(18)-Ag(25)-Ag(17)	127.66(3)	C(133)-Ag(37)-C(134)	26.6(3)
C(67)-Ag(19)-C(74)	117.0(3)	C(61)-Ag(26)-C(115)	167.3(2)	C(109)-Ag(37)-C(134)	127.0(3)
C(133)-Ag(37)-Cl(3)	91.1(3)	Ag(35)-Ag(41)-Ag(40)	93.19(3)	C(20)-C(19)-Ag(7)	93.4(7)
C(109)-Ag(37)-Cl(3)	104.5(2)	Ag(40)-Ag(41)-Ag(36)	140.36(3)	Ag(8)-C(19)-Ag(3)	81.4(3)
C(134)-Ag(37)-Cl(3)	110.8(2)	Ag(35)-Ag(41)-Ag(42)	147.44(3)	Ag(7)-C(19)-Ag(3)	86.6(3)

Ag(36)-Ag(37)-Ag(38)	115.68(3)	Ag(40)-Ag(41)-Ag(42)	58.83(2)	C(26)-C(25)-Ag(9)	153.5(8)
C(133)-Ag(38)-C(157)	164.3(4)	Ag(36)-Ag(41)-Ag(42)	116.65(3)	C(26)-C(25)-Ag(10)	86.6(6)
Ag(30)-Ag(38)-Ag(42)	135.52(3)	C(157)-Ag(42)-C(163)	175.6(3)	Ag(9)-C(25)-Ag(10)	107.6(3)
Ag(30)-Ag(38)-Ag(39)	86.97(3)	C(157)-Ag(42)-C(164)	147.5(3)	C(26)-C(25)-Ag(4)	119.6(7)
Ag(30)-Ag(38)-Ag(37)	67.23(2)	C(163)-Ag(42)-C(164)	28.2(3)	Ag(9)-C(25)-Ag(4)	83.7(3)
Ag(42)-Ag(38)-Ag(37)	108.77(3)	Ag(38)-Ag(42)-Ag(40)	129.17(3)	Ag(10)-C(25)-Ag(4)	89.2(3)
Ag(39)-Ag(38)-Ag(37)	129.44(3)	Ag(38)-Ag(42)-Ag(39)	60.70(2)	C(32)-C(31)-Ag(5)	158.6(7)
C(139)-Ag(39)-C(157)	155.0(3)	Ag(40)-Ag(42)-Ag(39)	96.16(3)	C(32)-C(31)-Ag(12)	101.6(7)
C(139)-Ag(39)-C(158)	142.1(3)	Ag(38)-Ag(42)-Ag(41)	97.66(3)	Ag(5)-C(31)-Ag(12)	97.0(4)
C(157)-Ag(39)-C(158)	25.9(3)	Ag(40)-Ag(42)-Ag(41)	55.921(19)	C(32)-C(31)-Ag(11)	89.7(6)
C(139)-Ag(39)-Cl(4)	100.1(2)	Ag(39)-Ag(42)-Ag(41)	123.57(3)	Ag(5)-C(31)-Ag(11)	96.9(4)
C(157)-Ag(39)-Cl(4)	102.2(2)	C(2)-C(1)-Ag(5)	149.7(8)	Ag(12)-C(31)-Ag(11)	101.7(3)
C(158)-Ag(39)-Cl(4)	92.6(2)	C(2)-C(1)-Ag(2)	125.0(7)	C(38)-C(37)-Ag(7)	150.6(8)
Ag(31)-Ag(39)-Ag(32)	68.64(2)	Ag(5)-C(1)-Ag(2)	85.2(3)	C(38)-C(37)-Ag(6)	122.6(8)
Ag(31)-Ag(39)-Ag(38)	85.32(3)	C(2)-C(1)-Ag(1)	86.7(6)	Ag(7)-C(37)-Ag(6)	81.1(3)
Ag(32)-Ag(39)-Ag(38)	134.20(3)	Ag(5)-C(1)-Ag(1)	92.7(3)	C(38)-C(37)-Ag(14)	78.6(6)
Ag(31)-Ag(39)-Ag(42)	134.15(3)	Ag(2)-C(1)-Ag(1)	96.6(4)	Ag(7)-C(37)-Ag(14)	108.3(4)
Ag(32)-Ag(39)-Ag(42)	115.77(3)	Ag(38)-Ag(42)-Ag(41)	97.66(3)	Ag(6)-C(37)-Ag(14)	115.5(3)
Ag(38)-Ag(39)-Ag(42)	58.46(2)	Ag(40)-Ag(42)-Ag(41)	55.921(19)	C(44)-C(43)-Ag(9)	169.0(8)
C(163)-Ag(40)-C(145)	156.5(3)	Ag(39)-Ag(42)-Ag(41)	123.57(3)	C(44)-C(43)-Ag(8)	88.0(7)
C(163)-Ag(40)-Cl(4)	104.3(2)	C(2)-C(1)-Ag(5)	149.7(8)	Ag(9)-C(43)-Ag(8)	90.0(3)
C(145)-Ag(40)-Cl(4)	94.5(2)	C(2)-C(1)-Ag(2)	125.0(7)	C(44)-C(43)-Ag(15)	86.1(7)
Ag(34)-Ag(40)-Ag(41)	83.03(3)	Ag(5)-C(1)-Ag(2)	85.2(3)	Ag(9)-C(43)-Ag(15)	104.8(4)
Ag(34)-Ag(40)-Ag(42)	140.59(3)	C(14)-C(13)-Ag(2)	163.7(9)	Ag(8)-C(43)-Ag(15)	107.2(3)
Ag(41)-Ag(40)-Ag(42)	65.25(2)	C(14)-C(13)-Ag(13)	96.7(7)	C(50)-C(49)-Ag(10)	138.8(7)
Ag(34)-Ag(40)-Ag(33)	68.87(2)	Ag(2)-C(13)-Ag(13)	92.1(4)	C(50)-C(49)-Ag(11)	138.2(8)
Ag(41)-Ag(40)-Ag(33)	128.21(3)	C(14)-C(13)-Ag(6)	99.3(8)	Ag(10)-C(49)-Ag(11)	78.7(3)
Ag(42)-Ag(40)-Ag(33)	112.46(3)	Ag(2)-C(13)-Ag(6)	92.5(3)	C(50)-C(49)-Ag(16)	78.5(6)
C(163)-Ag(41)-C(151)	152.2(3)	Ag(13)-C(13)-Ag(6)	100.8(4)	Ag(10)-C(49)-Ag(16)	104.4(4)
C(163)-Ag(41)-Cl(3)	97.5(2)	C(20)-C(19)-Ag(8)	155.3(8)	Ag(11)-C(49)-Ag(16)	115.0(4)
C(151)-Ag(41)-Cl(3)	100.3(2)	Ag(8)-C(19)-Ag(7)	101.4(4)	C(56)-C(55)-Ag(13)	145.0(8)
Ag(35)-Ag(41)-Ag(36)	73.11(2)	C(20)-C(19)-Ag(3)	119.4(7)	C(56)-C(55)-Ag(12)	134.4(8)
Ag(13)-C(55)-Ag(12)	77.6(3)	C(92)-C(91)-Ag(16)	144.3(9)	Ag(33)-C(121)-Ag(27)	112.2(4)
C(56)-C(55)-Ag(17)	80.1(7)	C(92)-C(91)-Ag(23)	102.0(7)	Ag(32)-C(121)-Ag(27)	112.5(4)
Ag(13)-C(55)-Ag(17)	106.9(4)	Ag(16)-C(91)-Ag(23)	105.7(4)	C(128)-C(127)-Ag(35)	165.7(8)

Ag(12)-C(55)-Ag(17)	106.7(4)	C(92)-C(91)-Ag(22)	107.4(8)	C(128)-C(127)-Ag(34)	102.7(7)
C(62)-C(61)-Ag(26)	143.4(8)	Ag(16)-C(91)-Ag(22)	95.5(3)	Ag(35)-C(127)-Ag(34)	85.2(3)
C(62)-C(61)-Ag(18)	114.3(8)	Ag(23)-C(91)-Ag(22)	88.6(3)	C(128)-C(127)-Ag(28)	83.4(6)
Ag(26)-C(61)-Ag(18)	98.6(4)	C(98)-C(97)-Ag(29)	142.5(7)	Ag(35)-C(127)-Ag(28)	105.6(4)
C(62)-C(61)-Ag(25)	90.7(8)	C(98)-C(97)-Ag(24)	99.4(7)	Ag(34)-C(127)-Ag(28)	108.2(4)
Ag(26)-C(61)-Ag(25)	107.8(4)	Ag(29)-C(97)-Ag(24)	106.4(4)	C(134)-C(133)-Ag(38)	156.9(8)
Ag(18)-C(61)-Ag(25)	86.4(3)	C(98)-C(97)-Ag(23)	107.1(6)	C(134)-C(133)-Ag(37)	98.5(7)
C(68)-C(67)-Ag(14)	119.0(8)	Ag(29)-C(97)-Ag(23)	101.7(4)	Ag(38)-C(133)-Ag(37)	100.7(4)
C(68)-C(67)-Ag(19)	122.8(8)	Ag(24)-C(97)-Ag(23)	85.5(3)	C(134)-C(133)-Ag(30)	99.6(7)
Ag(14)-C(67)-Ag(19)	97.7(4)	C(104)-C(103)-Ag(17)	140.7(7)	Ag(38)-C(133)-Ag(30)	87.7(3)
C(68)-C(67)-Ag(18)	115.5(7)	C(104)-C(103)-Ag(25)	112.9(7)	Ag(37)-C(133)-Ag(30)	104.8(4)
Ag(14)-C(67)-Ag(18)	110.3(4)	Ag(17)-C(103)-Ag(25)	100.4(3)	C(140)-C(139)-Ag(39)	151.6(8)
Ag(19)-C(67)-Ag(18)	86.1(3)	C(104)-C(103)-Ag(24)	100.1(6)	C(140)-C(139)-Ag(32)	112.1(7)
C(74)-C(73)-Ag(27)	137.3(8)	Ag(17)-C(103)-Ag(24)	104.1(4)	Ag(39)-C(139)-Ag(32)	92.0(4)
C(74)-C(73)-Ag(20)	127.0(8)	Ag(25)-C(103)-Ag(24)	83.6(3)	C(140)-C(139)-Ag(31)	98.2(8)
Ag(27)-C(73)-Ag(20)	92.6(3)	C(110)-C(109)-Ag(36)	142.6(8)	Ag(39)-C(139)-Ag(31)	89.5(3)
C(74)-C(73)-Ag(19)	86.4(7)	C(110)-C(109)-Ag(37)	136.8(8)	Ag(32)-C(139)-Ag(31)	104.4(3)
Ag(27)-C(73)-Ag(19)	111.1(4)	Ag(36)-C(109)-Ag(37)	78.1(3)	C(146)-C(145)-Ag(34)	142.4(8)
Ag(20)-C(73)-Ag(19)	90.6(3)	C(110)-C(109)-Ag(29)	78.2(6)	C(146)-C(145)-Ag(40)	132.5(8)
C(80)-C(79)-Ag(21)	142.4(8)	Ag(36)-C(109)-Ag(29)	103.0(3)	Ag(34)-C(145)-Ag(40)	84.5(3)
C(80)-C(79)-Ag(15)	124.7(7)	Ag(37)-C(109)-Ag(29)	112.3(3)	C(146)-C(145)-Ag(33)	82.9(6)
Ag(21)-C(79)-Ag(15)	89.9(4)	C(116)-C(115)-Ag(31)	144.1(8)	Ag(34)-C(145)-Ag(33)	103.5(3)
C(80)-C(79)-Ag(20)	88.8(7)	C(116)-C(115)-Ag(30)	131.0(7)	Ag(40)-C(145)-Ag(33)	94.4(3)
Ag(21)-C(79)-Ag(20)	97.0(3)	Ag(31)-C(115)-Ag(30)	80.8(3)	C(152)-C(151)-Ag(35)	149.8(8)
Ag(15)-C(79)-Ag(20)	104.1(4)	C(116)-C(115)-Ag(26)	78.2(7)	C(152)-C(151)-Ag(41)	119.6(7)
C(86)-C(85)-Ag(28)	140.9(8)	Ag(31)-C(115)-Ag(26)	111.4(4)	Ag(35)-C(151)-Ag(41)	84.8(3)
C(86)-C(85)-Ag(22)	111.9(7)	Ag(30)-C(115)-Ag(26)	107.0(4)	C(152)-C(151)-Ag(36)	87.3(6)
Ag(28)-C(85)-Ag(22)	94.2(3)	C(122)-C(121)-Ag(33)	141.6(8)	Ag(35)-C(151)-Ag(36)	113.0(4)
C(86)-C(85)-Ag(21)	109.8(8)	C(122)-C(121)-Ag(32)	132.0(8)	Ag(41)-C(151)-Ag(36)	87.3(3)
Ag(28)-C(85)-Ag(21)	94.5(4)	Ag(33)-C(121)-Ag(32)	79.6(3)	C(158)-C(157)-Ag(38)	165.2(9)
Ag(22)-C(85)-Ag(21)	97.2(4)	C(122)-C(121)-Ag(27)	78.6(6)	C(158)-C(157)-Ag(42)	101.0(8)
Ag(38)-C(157)-Ag(42)	91.2(3)	Ag(41)-Cl(3)-Ag(37)	113.93(8)	O(16)-Ho(1)-O(18)	120.53(19)
C(158)-C(157)-Ag(39)	96.2(7)	Ag(39)-Cl(4)-Ag(40)	115.23(8)	O(34)-Ho(1)-O(35)	75.30(19)
Ag(38)-C(157)-Ag(39)	92.3(3)	O(34)-Ho(1)-O(33)	75.8(2)	O(33)-Ho(1)-O(35)	119.45(19)
Ag(42)-C(157)-Ag(39)	89.5(3)	O(34)-Ho(1)-O(17)	140.47(19)	O(17)-Ho(1)-O(35)	73.68(19)

C(164)-C(163)-Ag(40)	165.3(8)	O(33)-Ho(1)-O(17)	141.8(2)	O(15)-Ho(1)-O(35)	141.28(19)
C(164)-C(163)-Ag(41)	105.2(7)	O(34)-Ho(1)-O(15)	74.2(2)	O(16)-Ho(1)-O(35)	73.04(19)
Ag(40)-C(163)-Ag(41)	89.4(3)	O(33)-Ho(1)-O(15)	74.91(19)	O(18)-Ho(1)-O(35)	140.9(2)
C(164)-C(163)-Ag(42)	87.4(6)	O(17)-Ho(1)-O(15)	118.90(18)	O(34)-Ho(1)-O(36)	119.76(19)
Ag(40)-C(163)-Ag(42)	92.5(3)	O(34)-Ho(1)-O(16)	72.82(19)	O(33)-Ho(1)-O(36)	74.54(19)
Ag(41)-C(163)-Ag(42)	95.8(3)	O(33)-Ho(1)-O(16)	141.5(2)	O(17)-Ho(1)-O(36)	74.95(19)
Ag(4)-Cl(1)-Ag(11)	110.90(9)	O(17)-Ho(1)-O(16)	75.12(19)	O(15)-Ho(1)-O(36)	141.28(18)
Ag(4)-Cl(1)-Ag(5)	114.64(9)	O(15)-Ho(1)-O(16)	75.54(19)	O(16)-Ho(1)-O(36)	141.49(19)
Ag(11)-Cl(1)-Ag(5)	70.84(5)	O(34)-Ho(1)-O(18)	142.08(19)	O(18)-Ho(1)-O(36)	73.72(19)
Ag(3)-Cl(2)-Ag(6)	106.91(8)	O(33)-Ho(1)-O(18)	74.51(19)	O(35)-Ho(1)-O(36)	75.69(19)
Ag(3)-Cl(2)-Ag(2)	109.70(8)	O(17)-Ho(1)-O(18)	75.30(19)		
Ag(6)-Cl(2)-Ag(2)	67.08(5)	O(15)-Ho(1)-O(18)	75.63(18)		