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Supporting Information

Chiral Metallacrown Supramolecular Compartments that Template Nanochannels: Self-Assembly and Guest Absorption

Choong-Sun Lim, Joseph Jankolovits, Jeff W. Kampf, and Vincent L. Pecoraro*[a]

asia_200900612_sm_miscellaneous_information.pdf

S1: Dy(III)[15-$MC_{Cu(II),l\text{-}pheHA}$-5] and pimelate assembly.

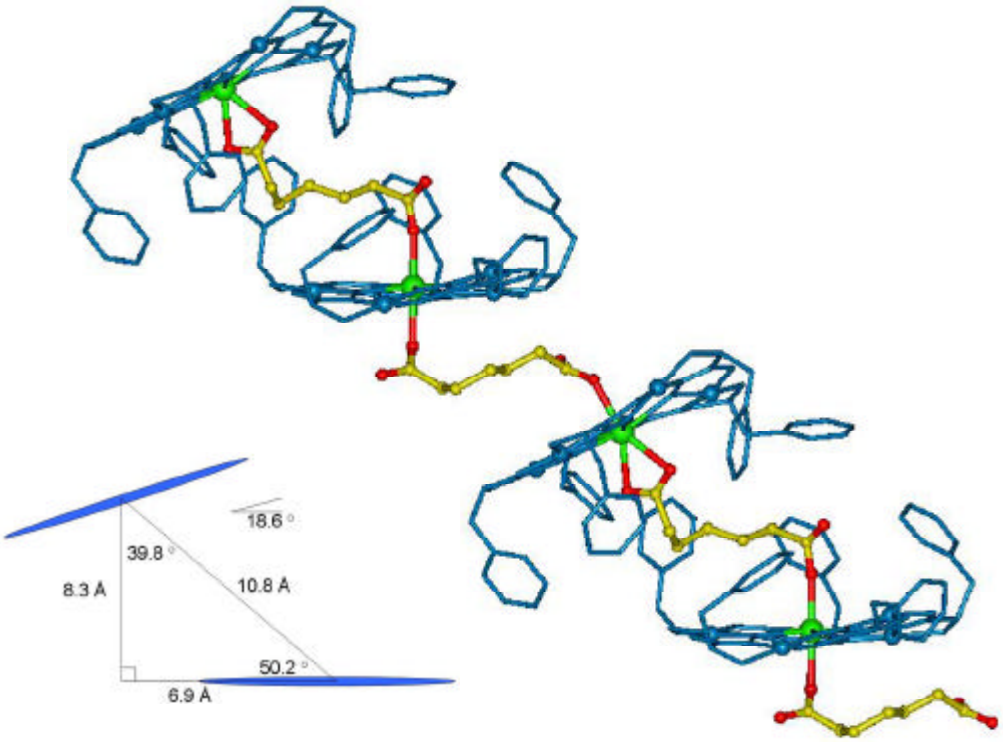

Figure S1: Assembly of Dy(III)[15-$MC_{Cu(II),l\text{-}pheHA}$-5] and pimelate anions. Pimelate bridges the hydrophilic and hydrophobic faces of the metallacrowns. Pimelate is encapsulated in a distorted MC compartment, a result of hydrophobic contacts between the long, flexible guest and metallacrown side chains. This is the first example of a metallacrown binding a satDC on its hydrophobic face. Color scheme: Blue; metallacrown framework. Green; dysprosium. Red, carboxylate oxygens. Yellow, carboxylate carbons. Water, hydrogen atoms, and unbound pimelate anions are removed for clarity. Inset: Diagram displaying the relevant distances and angles for the metallacrown compartment.

S2. Octameric Assembly of Metallacrowns.

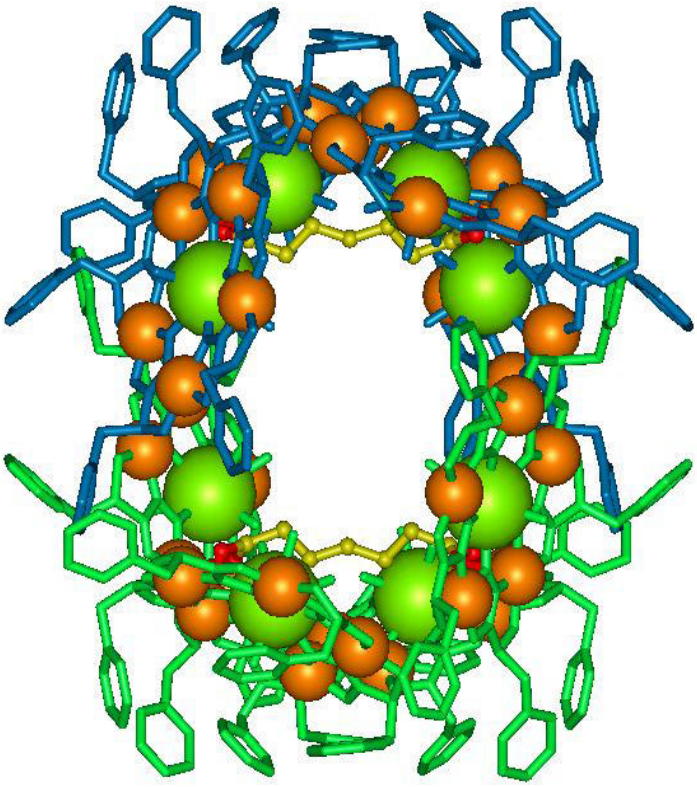

Figure S2. The octameric assembly of metallacrowns held together by two dicarboxylate guest molecules. Each octameric unit is formed by the association of a tetramer that is formed by the guest bridging to one Cu(II) ion of four different metallacrowns. The two tetrameric groups held together by a single dicarboxylate are shown in green or blue. The two guest C7DCs are shown with yellow for carbon atoms and red for oxygen atoms. Metals in the metallacrowns are displayed with CPK radii with green being lanthanum and orange being copper. The opening into the interior of this compartment is 8.9 Å wide by 14.6 Å high.

S3. Copper and Lanthanum Ions in a three fold related structure of Metallacrowns.

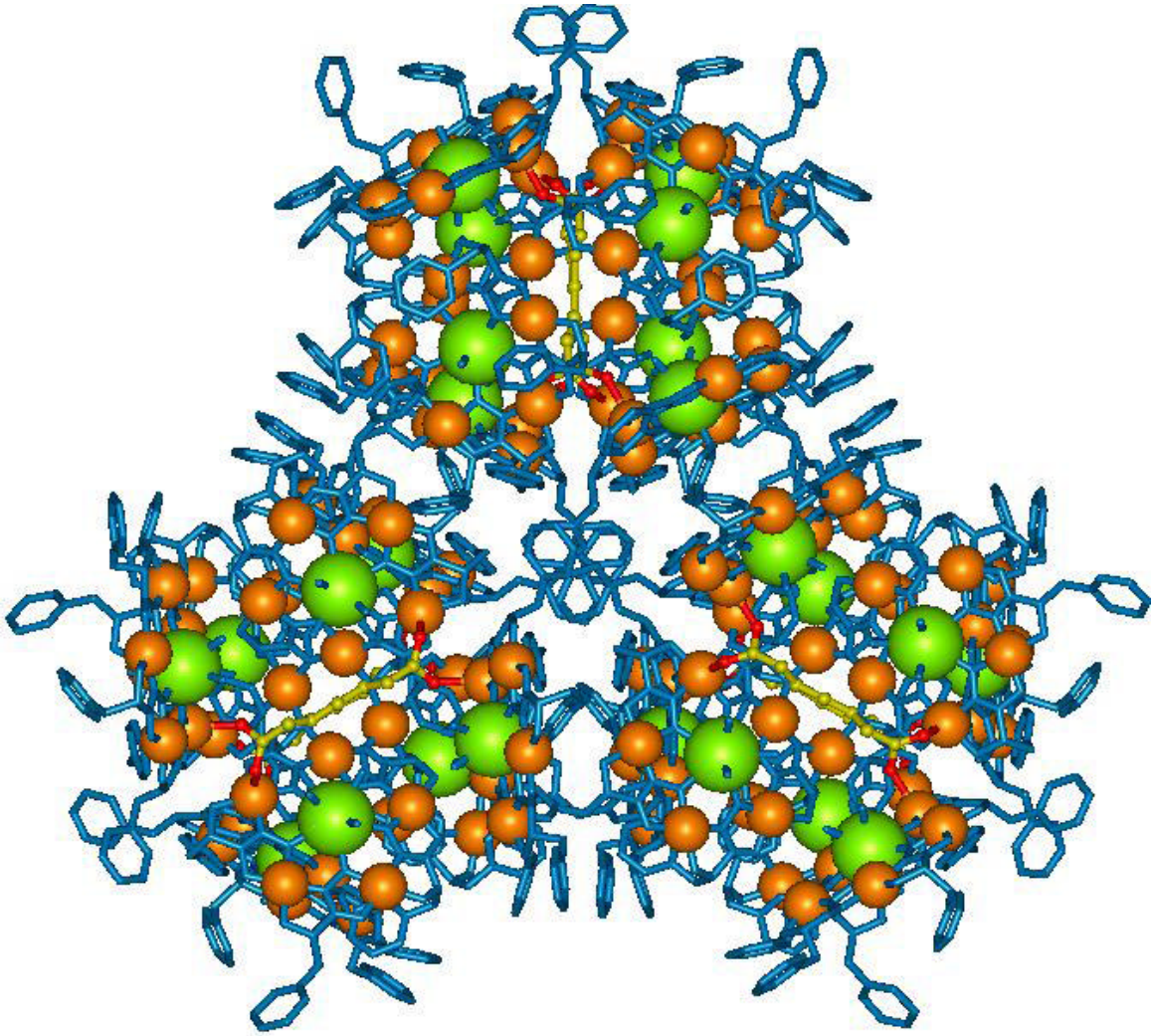

Figure S3. Copper and Lanthanum Ions in a three fold related structure of Metallacrown assemblies that construct the nanochannels. Each metallacrown assembly contains 8 La(III) (Large green) and 40 Cu(II) (Small orange) ions. The nanochannel building blocks are associated by hydrophobic contacts between the phenyl rings of the metallacrown side chains in the 24 metallacrown grouping. Color scheme: Blue; metallacrown framework; Yellow; carboxylate carbon; red; carboxylate oxygen. Orange; copper. Green; lanthanum.

S4. Mesostructured assembly **2** with water and unbound anions included.

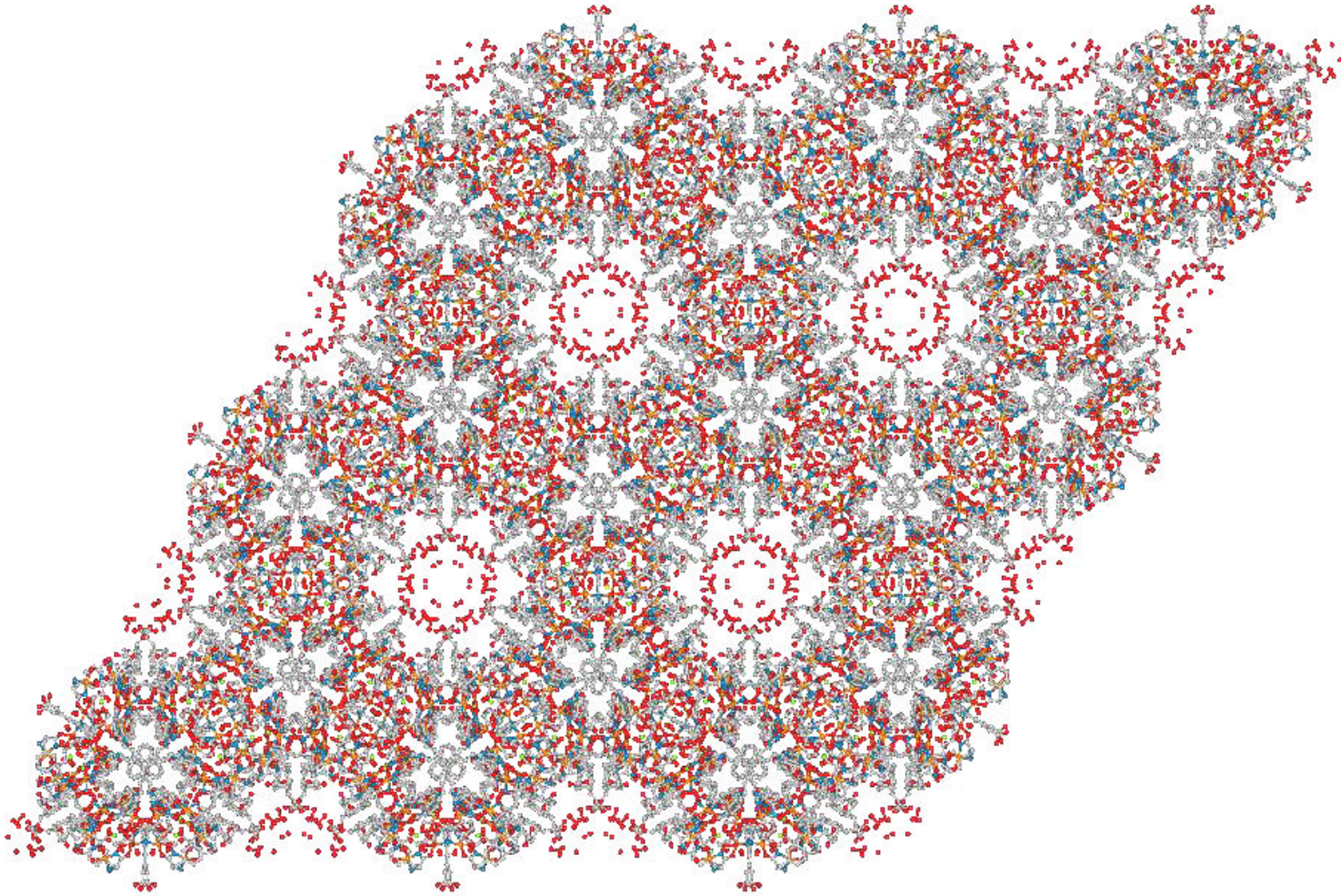

Figure S4. Packing diagram for **2** highlighting the 2.4 nm solvent and anion filled channels through the chiral solid.

S5. Mesostructured assembly **2** with water and unbound anions excluded.

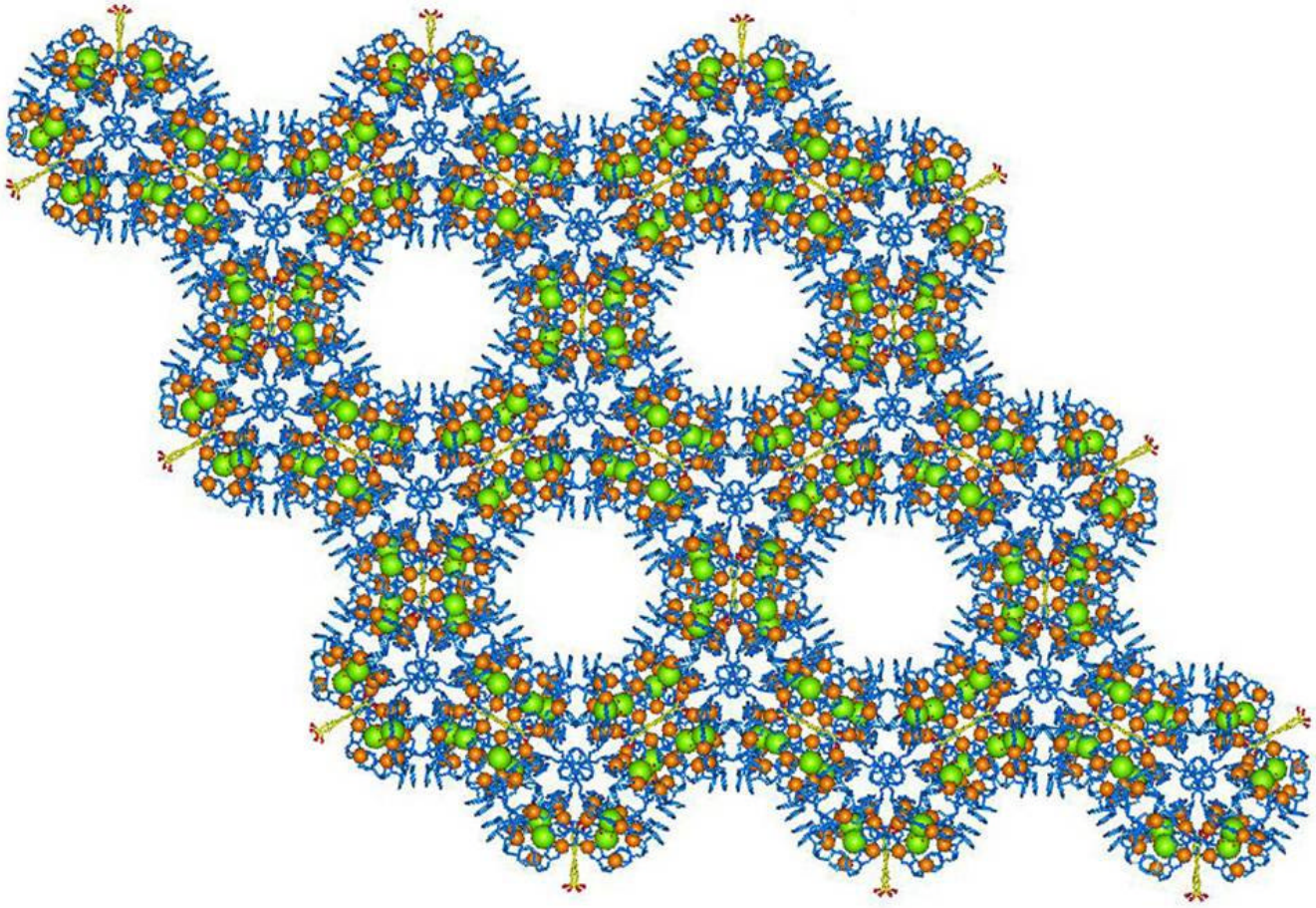

Figure S5: Packing diagram of **2** displaying the 2.4 nm solvent channels. Metal ions are highlighted with CPK radii. Solvent and unbound anions were removed for clarity. Color scheme: green: lanthanum; orange: copper; blue: MC framework; yellow: C7DC carbon chain; red: C7DC oxygen.

S6. PXRD patterns of **2**, **3**, and La(III)[15-$MC_{Cu(II),\ LpheHA}$-5](NO_3).

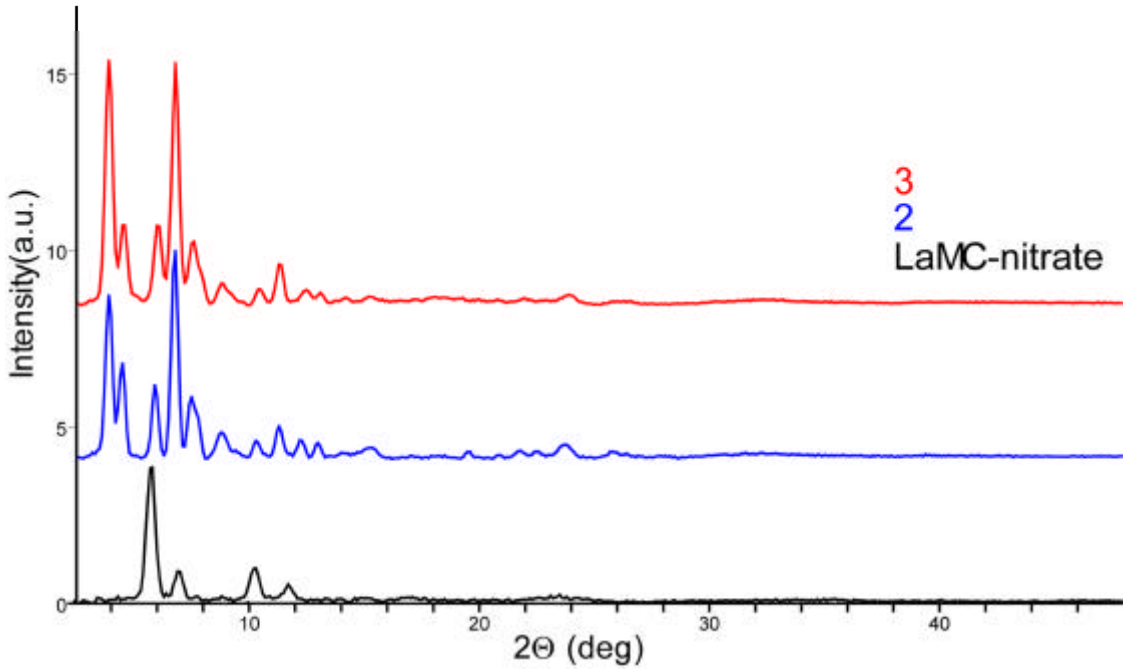

Figure S6. PXRD data for 2 (blue), 3 (red), and La(III)[15-$MC_{Cu(II),\ LpheHA}$-5](NO_3). The data for 2 and 3 match, and are in sharp contrast with the observations for the metallacrown without the satDC guest, revealing the need for the appropriate guest in order to realize the mesostructured material.

Structure Determination for 1.

Blue plates of **1** were grown from a water solution at 25 deg. C. A crystal of dimensions 0.34 x 0.20 x 0.11 mm was mounted on a Bruker SMART APEX CCD-based X-ray diffractometer equipped with a low temperature device and fine focus Mo-target X-ray tube (λ = 0.71073 A) operated at 1500 W power (50 kV, 30 mA). The X-ray intensities were measured at 85(1) K; the detector was placed at a distance 5.055 cm from the crystal. A total of 5190 frames were collected with a scan width of 0.5° in ω and 0.45° in phi with an exposure time of 20 s/frame. The integration of the data yielded a total of 117140 reflections to a maximum 2θ value of 56.72° of which 37759 were independent and 34737 were greater than $2\sigma(I)$. The final cell constants (Table 1) were based on the xyz centroids of 9001 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection; the data were processed with SADABS and corrected for absorption. The structure was solved and refined with the Bruker SHELXTL (version 2008/3) software package, using the space group P1 with Z = 1 for the formula $C_{111}H_{178}N_{20}O_{56}Cu_{10}Dy_2$. All non-hydrogen atoms were refined anisotropically with the hydrogen atoms placed in idealized positions. Full matrix least-squares refinement based on F^2 converged at R1 = 0.0448 and wR2 = 0.1260 [based on I > 2sigma(I)], R1 = 0.0508 and wR2 = 0.1337 for all data. Additional details are presented in Table S1 and are given as Supporting Information in a CIF file.

Sheldrick, G.M. SHELXTL, v. 2008/3; Bruker Analytical X-ray, Madison, WI, 2008.

Sheldrick, G.M. SADABS, v. 2008/1. Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen: Gottingen, Germany, 2008.

Saint Plus, v. 7.54a, Bruker Analytical X-ray, Madison, WI, 2008.

Table S1. Crystal data and structure refinement for **1**.

Empirical formula	C111 H178 Cu10 Dy2 N20 O56

Formula weight	3649.13
Temperature	85(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P1
Unit cell dimensions	a = 14.8653(10) A alpha = 76.069(1) deg.
	b = 15.0643(10) A beta = 87.081(1) deg.
	c = 17.8253(12) A gamma = 79.311(1) deg.
Volume	3807.0(4) A^3
Z, Calculated density	1, 1.592 Mg/m^3
Absorption coefficient	2.422 mm^-1
F(000)	1854
Crystal size	0.34 x 0.20 x 0.11 mm
Theta range for data collection	1.61 to 28.36 deg.
Limiting indices	-19<=h<=19, -20<=k<=20, -23<=l<=23
Reflections collected / unique	177140 / 37759 [R(int) = 0.0316]
Completeness to theta = 28.36	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7765 and 0.4931
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	37759 / 491 / 1999
Goodness-of-fit on F^2	1.090
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.1260
R indices (all data)	R1 = 0.0508, wR2 = 0.1337
Absolute structure parameter	-0.030(6)
Largest diff. peak and hole	1.149 and -0.819 e.A^-3

Table S2. Bond lengths [A] and angles [deg] for **1**.

Dy(1)-O(25)	2.191(4)

Dy(1)-O(100)	2.290(5)
Dy(1)-O(4)	2.361(3)
Dy(1)-O(8)	2.370(3)
Dy(1)-O(10)	2.377(3)
Dy(1)-O(6)	2.382(3)
Dy(1)-O(2)	2.391(4)
Dy(2)-O(102)#1	2.293(4)
Dy(2)-O(20)	2.336(4)
Dy(2)-O(16)	2.389(4)
Dy(2)-O(27)	2.396(5)
Dy(2)-O(18)	2.422(5)
Dy(2)-O(28)	2.428(5)
Dy(2)-O(12)	2.432(4)
Dy(2)-O(14)	2.447(5)
Dy(2)-C(97)	2.748(6)
Cu(1)-N(2)	1.899(4)
Cu(1)-O(10)	1.921(3)
Cu(1)-O(9)	1.947(4)
Cu(1)-N(1)	1.995(5)
Cu(2)-N(4)	1.902(4)
Cu(2)-O(2)	1.916(4)
Cu(2)-O(1)	1.946(4)
Cu(2)-N(3)	1.984(4)
Cu(3)-N(6)	1.888(4)
Cu(3)-O(3)	1.921(4)
Cu(3)-O(4)	1.932(3)
Cu(3)-N(5)	2.021(5)
Cu(4)-N(8)	1.915(5)
Cu(4)-O(5)	1.944(4)
Cu(4)-O(6)	1.946(4)
Cu(4)-N(7)	2.038(5)
Cu(4)-O(29)	2.250(6)
Cu(5)-N(10)	1.886(4)
Cu(5)-O(8)	1.910(4)
Cu(5)-O(7)	1.918(4)
Cu(5)-N(9)	2.011(5)
Cu(6)-N(12)	1.884(6)
Cu(6)-O(19)	1.932(5)
Cu(6)-O(20)	1.932(4)
Cu(6)-N(11)	2.010(5)
Cu(6)-O(24)	2.368(6)
Cu(7)-N(14)	1.915(5)
Cu(7)-O(11)	1.929(4)
Cu(7)-O(12)	1.929(5)
Cu(7)-N(13)	2.004(6)
Cu(8)-N(16)	1.892(7)
Cu(8)-O(13)	1.909(5)
Cu(8)-O(14)	1.910(4)
Cu(8)-N(15)	1.993(5)
Cu(9)-N(18)	1.903(6)
Cu(9)-O(16)	1.930(5)
Cu(9)-O(15)	1.944(6)

Cu(9)-N(17)	1.985(7)
Cu(10)-N(20)	1.903(5)
Cu(10)-O(18)	1.922(5)
Cu(10)-O(17)	1.953(4)
Cu(10)-N(19)	2.000(6)
Cu(10)-O(21)	2.312(4)
O(1)-C(1)	1.305(6)
O(2)-N(2)	1.396(6)
O(3)-C(10)	1.295(6)
O(4)-N(4)	1.391(5)
O(5)-C(19)	1.285(7)
O(6)-N(6)	1.389(5)
O(7)-C(28)	1.266(7)
O(8)-N(8)	1.384(6)
O(9)-C(37)	1.304(7)
O(10)-N(10)	1.388(5)
O(11)-C(46)	1.315(8)
O(12)-N(12)	1.402(6)
O(13)-C(55)	1.299(7)
O(14)-N(14)	1.387(6)
O(15)-C(64)	1.274(11)
O(16)-N(16)	1.382(8)
O(17)-C(73)	1.287(9)
O(18)-N(18)	1.372(6)
O(19)-C(82)	1.317(7)
O(20)-N(20)	1.390(7)
O(25)-C(91)	1.241(7)
O(26)-C(91)	1.235(8)
C(91)-C(92)	1.565(9)
C(92)-C(93)	1.545(8)
C(93)-C(94)	1.504(11)
C(94)-C(95)	1.562(8)
C(95)-C(96)	1.500(8)
C(96)-C(97)	1.546(10)
C(97)-O(28)	1.218(8)
C(97)-O(27)	1.221(7)
N(1)-C(2)	1.477(7)
N(2)-C(1)	1.289(6)
N(3)-C(11)	1.456(8)
N(4)-C(10)	1.269(6)
N(5)-C(20)	1.466(8)
N(6)-C(19)	1.282(7)
N(7)-C(29)	1.486(9)
N(8)-C(28)	1.292(7)
N(9)-C(38)	1.474(8)
N(10)-C(37)	1.283(7)
N(11)-C(47)	1.497(9)
N(12)-C(46)	1.274(8)
N(13)-C(56)	1.513(9)
N(14)-C(55)	1.265(9)
N(15)-C(65)	1.506(12)
N(16)-C(64)	1.314(8)

N(17)-C(74)	1.467(10)
N(18)-C(73)	1.287(9)
N(19)-C(83)	1.491(7)
N(20)-C(82)	1.256(8)
C(1)-C(2)	1.504(7)
C(2)-C(3)	1.522(8)
C(3)-C(4)	1.497(9)
C(4)-C(5)	1.381(9)
C(4)-C(9)	1.421(9)
C(5)-C(6)	1.377(11)
C(6)-C(7)	1.393(11)
C(7)-C(8)	1.399(11)
C(8)-C(9)	1.348(11)
C(10)-C(11)	1.528(7)
C(11)-C(12)	1.544(8)
C(12)-C(13)	1.517(8)
C(13)-C(14)	1.384(8)
C(13)-C(18)	1.412(8)
C(14)-C(15)	1.377(9)
C(15)-C(16)	1.403(10)
C(16)-C(17)	1.363(10)
C(17)-C(18)	1.381(9)
C(19)-C(20)	1.543(8)
C(20)-C(21)	1.548(9)
C(21)-C(22)	1.505(10)
C(22)-C(23)	1.333(12)
C(22)-C(27)	1.360(12)
C(23)-C(24)	1.377(14)
C(24)-C(25)	1.335(14)
C(25)-C(26)	1.270(16)
C(26)-C(27)	1.362(16)
C(28)-C(29)	1.516(8)
C(29)-C(30)	1.543(8)
C(30)-C(31)	1.492(8)
C(31)-C(36)	1.370(12)
C(31)-C(32)	1.379(12)
C(32)-C(33)	1.394(10)
C(33)-C(34)	1.400(16)
C(34)-C(35)	1.307(17)
C(35)-C(36)	1.439(11)
C(37)-C(38)	1.512(7)
C(38)-C(39)	1.549(9)
C(39)-C(40)	1.490(9)
C(40)-C(41)	1.383(8)
C(40)-C(45)	1.410(8)
C(41)-C(42)	1.417(10)
C(42)-C(43)	1.384(9)
C(43)-C(44)	1.390(9)
C(44)-C(45)	1.373(10)
C(46)-C(47)	1.514(8)
C(47)-C(48)	1.522(8)
C(48)-C(49)	1.521(8)

C(49)-C(54)	1.385(10)
C(49)-C(50)	1.392(9)
C(50)-C(51)	1.369(10)
C(51)-C(52)	1.351(11)
C(52)-C(53)	1.363(12)
C(53)-C(54)	1.381(10)
C(55)-C(56)	1.522(9)
C(56)-C(57)	1.460(11)
C(57)-C(58)	1.501(10)
C(58)-C(59)	1.377(9)
C(58)-C(63)	1.433(10)
C(59)-C(60)	1.347(10)
C(60)-C(61)	1.420(12)
C(61)-C(62)	1.365(13)
C(62)-C(63)	1.353(12)
C(64)-C(65)	1.533(12)
C(65)-C(66)	1.535(12)
C(66)-C(67)	1.508(15)
C(67)-C(72)	1.368(17)
C(67)-C(68)	1.409(15)
C(68)-C(69)	1.318(18)
C(69)-C(70)	1.44(2)
C(70)-C(71)	1.428(19)
C(71)-C(72)	1.428(17)
C(73)-C(74)	1.544(9)
C(74)-C(75)	1.517(10)
C(75)-C(76)	1.457(12)
C(76)-C(77)	1.404(10)
C(76)-C(81)	1.446(11)
C(77)-C(78)	1.374(11)
C(78)-C(79)	1.413(10)
C(79)-C(80)	1.364(16)
C(80)-C(81)	1.320(17)
C(82)-C(83)	1.540(9)
C(83)-C(84)	1.530(8)
C(84)-C(85)	1.500(9)
C(85)-C(86)	1.391(8)
C(85)-C(90)	1.399(10)
C(86)-C(87)	1.414(11)
C(87)-C(88)	1.361(14)
C(88)-C(89)	1.370(13)
C(89)-C(90)	1.399(11)
O(100)-C(100)	1.286(11)
O(100)-C(10A)	1.287(15)
O(101)-C(100)	1.331(14)
C(100)-C(101)	1.568(14)
C(101)-C(102)	1.479(15)
C(102)-C(103)	1.483(15)
C(103)-C(104)	1.584(17)
C(104)-C(105)	1.482(17)
C(105)-C(106)	1.537(15)
O(10A)-C(10A)	1.328(16)

C(10A)-C(10B)	1.580(18)
C(10B)-C(10C)	1.494(17)
C(10C)-C(10D)	1.527(18)
C(10D)-C(10E)	1.614(18)
C(10E)-C(10F)	1.507(18)
C(10F)-C(106)	1.520(15)
C(106)-O(103)	1.246(10)
C(106)-O(102)	1.263(9)
O(102)-Dy(2)#2	2.293(4)
O(300)-C(300)	1.212(11)
O(301)-C(300)	1.292(11)
C(300)-C(301)	1.585(13)
C(301)-C(302)	1.440(15)
C(302)-C(303)	1.583(15)
C(303)-C(304)	1.628(16)
C(304)-C(305)	1.548(14)
C(305)-C(306)	1.502(15)
C(306)-O(303)	1.279(14)
C(306)-O(302)	1.312(15)

O(25)-Dy(1)-O(100)	174.89(17)
O(25)-Dy(1)-O(4)	98.42(15)
O(100)-Dy(1)-O(4)	86.15(15)
O(25)-Dy(1)-O(8)	90.32(16)
O(100)-Dy(1)-O(8)	84.64(17)
O(4)-Dy(1)-O(8)	142.61(11)
O(25)-Dy(1)-O(10)	93.53(14)
O(100)-Dy(1)-O(10)	84.08(17)
O(4)-Dy(1)-O(10)	142.90(12)
O(8)-Dy(1)-O(10)	71.72(11)
O(25)-Dy(1)-O(6)	87.05(15)
O(100)-Dy(1)-O(6)	92.20(19)
O(4)-Dy(1)-O(6)	72.27(12)
O(8)-Dy(1)-O(6)	71.97(12)
O(10)-Dy(1)-O(6)	143.69(11)
O(25)-Dy(1)-O(2)	90.50(17)
O(100)-Dy(1)-O(2)	93.0(2)
O(4)-Dy(1)-O(2)	73.14(12)
O(8)-Dy(1)-O(2)	143.45(12)
O(10)-Dy(1)-O(2)	71.76(12)
O(6)-Dy(1)-O(2)	144.55(12)
O(102)#1-Dy(2)-O(20)	92.17(17)
O(102)#1-Dy(2)-O(16)	80.44(17)
O(20)-Dy(2)-O(16)	143.25(16)
O(102)#1-Dy(2)-O(27)	154.19(16)
O(20)-Dy(2)-O(27)	88.74(16)
O(16)-Dy(2)-O(27)	113.17(17)
O(102)#1-Dy(2)-O(18)	82.09(16)
O(20)-Dy(2)-O(18)	70.75(14)
O(16)-Dy(2)-O(18)	72.59(16)
O(27)-Dy(2)-O(18)	122.25(15)
O(102)#1-Dy(2)-O(28)	153.11(17)

O(20)-Dy(2)-O(28)	90.2(2)
O(16)-Dy(2)-O(28)	81.7(2)
O(27)-Dy(2)-O(28)	52.62(16)
O(18)-Dy(2)-O(28)	73.44(15)
O(102)#1-Dy(2)-O(12)	80.78(15)
O(20)-Dy(2)-O(12)	72.94(14)
O(16)-Dy(2)-O(12)	139.44(15)
O(27)-Dy(2)-O(12)	74.84(15)
O(18)-Dy(2)-O(12)	138.95(14)
O(28)-Dy(2)-O(12)	125.31(17)
O(102)#1-Dy(2)-O(14)	86.16(18)
O(20)-Dy(2)-O(14)	144.35(13)
O(16)-Dy(2)-O(14)	71.51(15)
O(27)-Dy(2)-O(14)	78.29(15)
O(18)-Dy(2)-O(14)	143.58(13)
O(28)-Dy(2)-O(14)	106.96(18)
O(12)-Dy(2)-O(14)	71.64(13)
O(102)#1-Dy(2)-C(97)	177.6(2)
O(20)-Dy(2)-C(97)	90.1(2)
O(16)-Dy(2)-C(97)	97.4(2)
O(27)-Dy(2)-C(97)	26.34(17)
O(18)-Dy(2)-C(97)	98.22(17)
O(28)-Dy(2)-C(97)	26.30(18)
O(12)-Dy(2)-C(97)	100.39(17)
O(14)-Dy(2)-C(97)	92.24(19)
N(2)-Cu(1)-O(10)	90.12(16)
N(2)-Cu(1)-O(9)	172.3(2)
O(10)-Cu(1)-O(9)	85.39(15)
N(2)-Cu(1)-N(1)	82.2(2)
O(10)-Cu(1)-N(1)	171.3(2)
O(9)-Cu(1)-N(1)	101.77(19)
N(4)-Cu(2)-O(2)	90.65(17)
N(4)-Cu(2)-O(1)	174.57(19)
O(2)-Cu(2)-O(1)	85.55(16)
N(4)-Cu(2)-N(3)	81.84(19)
O(2)-Cu(2)-N(3)	172.48(18)
O(1)-Cu(2)-N(3)	101.96(18)
N(6)-Cu(3)-O(3)	170.82(18)
N(6)-Cu(3)-O(4)	90.39(16)
O(3)-Cu(3)-O(4)	84.91(15)
N(6)-Cu(3)-N(5)	82.32(18)
O(3)-Cu(3)-N(5)	102.02(17)
O(4)-Cu(3)-N(5)	172.43(18)
N(8)-Cu(4)-O(5)	168.1(2)
N(8)-Cu(4)-O(6)	89.00(17)
O(5)-Cu(4)-O(6)	84.59(16)
N(8)-Cu(4)-N(7)	82.7(2)
O(5)-Cu(4)-N(7)	100.6(2)
O(6)-Cu(4)-N(7)	162.6(3)
N(8)-Cu(4)-O(29)	95.3(2)
O(5)-Cu(4)-O(29)	95.7(2)
O(6)-Cu(4)-O(29)	100.21(19)

N(7)-Cu(4)-O(29)	95.8(3)
N(10)-Cu(5)-O(8)	89.26(16)
N(10)-Cu(5)-O(7)	171.68(19)
O(8)-Cu(5)-O(7)	85.80(16)
N(10)-Cu(5)-N(9)	82.15(19)
O(8)-Cu(5)-N(9)	170.68(18)
O(7)-Cu(5)-N(9)	103.15(19)
N(12)-Cu(6)-O(19)	170.8(2)
N(12)-Cu(6)-O(20)	91.47(19)
O(19)-Cu(6)-O(20)	85.49(18)
N(12)-Cu(6)-N(11)	82.7(2)
O(19)-Cu(6)-N(11)	98.6(2)
O(20)-Cu(6)-N(11)	167.7(2)
N(12)-Cu(6)-O(24)	91.8(2)
O(19)-Cu(6)-O(24)	97.0(2)
O(20)-Cu(6)-O(24)	92.4(2)
N(11)-Cu(6)-O(24)	98.6(3)
N(14)-Cu(7)-O(11)	176.2(2)
N(14)-Cu(7)-O(12)	91.4(2)
O(11)-Cu(7)-O(12)	85.48(18)
N(14)-Cu(7)-N(13)	82.4(2)
O(11)-Cu(7)-N(13)	100.3(2)
O(12)-Cu(7)-N(13)	169.9(2)
N(16)-Cu(8)-O(13)	174.7(2)
N(16)-Cu(8)-O(14)	90.3(2)
O(13)-Cu(8)-O(14)	85.88(18)
N(16)-Cu(8)-N(15)	85.0(3)
O(13)-Cu(8)-N(15)	98.5(3)
O(14)-Cu(8)-N(15)	172.7(2)
N(18)-Cu(9)-O(16)	91.1(2)
N(18)-Cu(9)-O(15)	170.4(3)
O(16)-Cu(9)-O(15)	85.1(2)
N(18)-Cu(9)-N(17)	82.9(3)
O(16)-Cu(9)-N(17)	173.8(3)
O(15)-Cu(9)-N(17)	101.1(3)
N(20)-Cu(10)-O(18)	88.3(2)
N(20)-Cu(10)-O(17)	166.38(19)
O(18)-Cu(10)-O(17)	84.32(19)
N(20)-Cu(10)-N(19)	82.6(2)
O(18)-Cu(10)-N(19)	165.9(2)
O(17)-Cu(10)-N(19)	102.4(2)
N(20)-Cu(10)-O(21)	94.0(2)
O(18)-Cu(10)-O(21)	99.18(18)
O(17)-Cu(10)-O(21)	98.45(18)
N(19)-Cu(10)-O(21)	92.2(2)
C(1)-O(1)-Cu(2)	106.7(3)
N(2)-O(2)-Cu(2)	107.8(3)
N(2)-O(2)-Dy(1)	125.2(3)
Cu(2)-O(2)-Dy(1)	125.83(18)
C(10)-O(3)-Cu(3)	107.6(3)
N(4)-O(4)-Cu(3)	107.8(3)
N(4)-O(4)-Dy(1)	124.7(3)

Cu(3)-O(4)-Dy(1)	127.41(16)
C(19)-O(5)-Cu(4)	107.0(4)
N(6)-O(6)-Cu(4)	108.2(3)
N(6)-O(6)-Dy(1)	125.2(3)
Cu(4)-O(6)-Dy(1)	125.10(16)
C(28)-O(7)-Cu(5)	107.3(3)
N(8)-O(8)-Cu(5)	107.0(3)
N(8)-O(8)-Dy(1)	125.4(3)
Cu(5)-O(8)-Dy(1)	127.57(17)
C(37)-O(9)-Cu(1)	106.1(3)
N(10)-O(10)-Cu(1)	107.5(3)
N(10)-O(10)-Dy(1)	124.2(3)
Cu(1)-O(10)-Dy(1)	128.16(16)
C(46)-O(11)-Cu(7)	106.3(3)
N(12)-O(12)-Cu(7)	107.7(3)
N(12)-O(12)-Dy(2)	123.2(3)
Cu(7)-O(12)-Dy(2)	126.14(18)
C(55)-O(13)-Cu(8)	106.8(4)
N(14)-O(14)-Cu(8)	107.2(3)
N(14)-O(14)-Dy(2)	125.2(3)
Cu(8)-O(14)-Dy(2)	126.7(2)
C(64)-O(15)-Cu(9)	107.1(4)
N(16)-O(16)-Cu(9)	107.4(3)
N(16)-O(16)-Dy(2)	125.5(4)
Cu(9)-O(16)-Dy(2)	126.2(2)
C(73)-O(17)-Cu(10)	107.2(4)
N(18)-O(18)-Cu(10)	108.7(4)
N(18)-O(18)-Dy(2)	124.4(4)
Cu(10)-O(18)-Dy(2)	124.01(18)
C(82)-O(19)-Cu(6)	105.4(4)
N(20)-O(20)-Cu(6)	108.2(3)
N(20)-O(20)-Dy(2)	124.0(3)
Cu(6)-O(20)-Dy(2)	127.6(2)
C(91)-O(25)-Dy(1)	168.2(4)
O(26)-C(91)-O(25)	124.2(5)
O(26)-C(91)-C(92)	121.2(6)
O(25)-C(91)-C(92)	113.7(6)
C(93)-C(92)-C(91)	106.3(5)
C(94)-C(93)-C(92)	112.1(6)
C(93)-C(94)-C(95)	113.6(7)
C(96)-C(95)-C(94)	113.7(7)
C(95)-C(96)-C(97)	105.3(7)
O(28)-C(97)-O(27)	122.5(6)
O(28)-C(97)-C(96)	118.2(6)
O(27)-C(97)-C(96)	118.4(6)
O(28)-C(97)-Dy(2)	62.0(3)
O(27)-C(97)-Dy(2)	60.5(3)
C(96)-C(97)-Dy(2)	167.2(5)
C(97)-O(27)-Dy(2)	93.1(4)
C(97)-O(28)-Dy(2)	91.7(4)
C(2)-N(1)-Cu(1)	111.5(4)
C(1)-N(2)-O(2)	116.1(4)

C(1)-N(2)-Cu(1)	117.0(4)
O(2)-N(2)-Cu(1)	123.9(3)
C(11)-N(3)-Cu(2)	111.6(3)
C(10)-N(4)-O(4)	115.5(4)
C(10)-N(4)-Cu(2)	119.4(3)
O(4)-N(4)-Cu(2)	124.9(3)
C(20)-N(5)-Cu(3)	111.4(3)
C(19)-N(6)-O(6)	114.8(4)
C(19)-N(6)-Cu(3)	120.9(4)
O(6)-N(6)-Cu(3)	124.2(3)
C(29)-N(7)-Cu(4)	110.8(4)
C(28)-N(8)-O(8)	115.7(5)
C(28)-N(8)-Cu(4)	119.6(4)
O(8)-N(8)-Cu(4)	124.1(3)
C(38)-N(9)-Cu(5)	107.7(3)
C(37)-N(10)-O(10)	116.0(4)
C(37)-N(10)-Cu(5)	117.9(3)
O(10)-N(10)-Cu(5)	125.5(3)
C(47)-N(11)-Cu(6)	111.3(4)
C(46)-N(12)-O(12)	114.9(5)
C(46)-N(12)-Cu(6)	120.8(4)
O(12)-N(12)-Cu(6)	124.2(4)
C(56)-N(13)-Cu(7)	112.4(4)
C(55)-N(14)-O(14)	116.1(5)
C(55)-N(14)-Cu(7)	119.5(4)
O(14)-N(14)-Cu(7)	124.1(4)
C(65)-N(15)-Cu(8)	108.6(5)
C(64)-N(16)-O(16)	115.6(6)
C(64)-N(16)-Cu(8)	118.3(6)
O(16)-N(16)-Cu(8)	125.9(4)
C(74)-N(17)-Cu(9)	109.2(4)
C(73)-N(18)-O(18)	115.7(6)
C(73)-N(18)-Cu(9)	118.7(4)
O(18)-N(18)-Cu(9)	125.0(4)
C(83)-N(19)-Cu(10)	111.4(4)
C(82)-N(20)-O(20)	114.6(5)
C(82)-N(20)-Cu(10)	119.5(4)
O(20)-N(20)-Cu(10)	124.9(4)
N(2)-C(1)-O(1)	123.2(5)
N(2)-C(1)-C(2)	117.6(5)
O(1)-C(1)-C(2)	119.1(4)
N(1)-C(2)-C(1)	107.6(4)
N(1)-C(2)-C(3)	113.7(5)
C(1)-C(2)-C(3)	114.3(5)
C(4)-C(3)-C(2)	115.7(4)
C(5)-C(4)-C(9)	118.9(6)
C(5)-C(4)-C(3)	120.4(6)
C(9)-C(4)-C(3)	120.7(6)
C(6)-C(5)-C(4)	121.0(6)
C(5)-C(6)-C(7)	120.1(6)
C(6)-C(7)-C(8)	118.7(7)
C(9)-C(8)-C(7)	121.7(7)

C(8)-C(9)-C(4)	119.7(6)
N(4)-C(10)-O(3)	124.1(4)
N(4)-C(10)-C(11)	115.0(5)
O(3)-C(10)-C(11)	120.8(4)
N(3)-C(11)-C(10)	108.4(4)
N(3)-C(11)-C(12)	113.1(5)
C(10)-C(11)-C(12)	109.8(5)
C(13)-C(12)-C(11)	113.9(4)
C(14)-C(13)-C(18)	118.7(5)
C(14)-C(13)-C(12)	120.7(5)
C(18)-C(13)-C(12)	120.6(5)
C(15)-C(14)-C(13)	120.5(6)
C(14)-C(15)-C(16)	120.3(6)
C(17)-C(16)-C(15)	119.6(6)
C(16)-C(17)-C(18)	120.8(6)
C(17)-C(18)-C(13)	120.1(6)
N(6)-C(19)-O(5)	125.4(5)
N(6)-C(19)-C(20)	114.4(5)
O(5)-C(19)-C(20)	120.2(5)
N(5)-C(20)-C(19)	109.5(4)
N(5)-C(20)-C(21)	113.0(5)
C(19)-C(20)-C(21)	110.3(5)
C(22)-C(21)-C(20)	115.4(5)
C(23)-C(22)-C(27)	115.5(8)
C(23)-C(22)-C(21)	123.8(7)
C(27)-C(22)-C(21)	120.8(8)
C(22)-C(23)-C(24)	124.0(9)
C(25)-C(24)-C(23)	117.0(9)
C(26)-C(25)-C(24)	120.8(10)
C(25)-C(26)-C(27)	122.7(9)
C(22)-C(27)-C(26)	119.9(10)
O(7)-C(28)-N(8)	123.9(5)
O(7)-C(28)-C(29)	120.3(5)
N(8)-C(28)-C(29)	115.8(5)
N(7)-C(29)-C(28)	110.7(4)
N(7)-C(29)-C(30)	112.2(6)
C(28)-C(29)-C(30)	110.9(4)
C(31)-C(30)-C(29)	113.9(5)
C(36)-C(31)-C(32)	117.8(6)
C(36)-C(31)-C(30)	121.7(7)
C(32)-C(31)-C(30)	120.3(7)
C(31)-C(32)-C(33)	122.1(9)
C(32)-C(33)-C(34)	117.3(9)
C(35)-C(34)-C(33)	122.8(8)
C(34)-C(35)-C(36)	118.9(10)
C(31)-C(36)-C(35)	120.6(9)
N(10)-C(37)-O(9)	123.8(4)
N(10)-C(37)-C(38)	115.4(5)
O(9)-C(37)-C(38)	120.8(5)
N(9)-C(38)-C(37)	108.0(5)
N(9)-C(38)-C(39)	111.6(5)
C(37)-C(38)-C(39)	111.8(5)

C(40)-C(39)-C(38)	113.1(5)
C(41)-C(40)-C(45)	117.4(6)
C(41)-C(40)-C(39)	120.6(5)
C(45)-C(40)-C(39)	121.9(5)
C(40)-C(41)-C(42)	121.6(5)
C(43)-C(42)-C(41)	119.0(6)
C(42)-C(43)-C(44)	120.2(6)
C(45)-C(44)-C(43)	120.1(6)
C(44)-C(45)-C(40)	121.8(5)
N(12)-C(46)-O(11)	124.6(5)
N(12)-C(46)-C(47)	115.8(6)
O(11)-C(46)-C(47)	119.6(5)
N(11)-C(47)-C(46)	109.1(5)
N(11)-C(47)-C(48)	113.1(5)
C(46)-C(47)-C(48)	109.7(5)
C(49)-C(48)-C(47)	114.9(5)
C(54)-C(49)-C(50)	116.3(6)
C(54)-C(49)-C(48)	122.1(5)
C(50)-C(49)-C(48)	121.5(6)
C(51)-C(50)-C(49)	121.3(7)
C(52)-C(51)-C(50)	120.9(7)
C(51)-C(52)-C(53)	119.8(7)
C(52)-C(53)-C(54)	119.7(8)
C(53)-C(54)-C(49)	121.9(7)
N(14)-C(55)-O(13)	123.8(6)
N(14)-C(55)-C(56)	117.7(5)
O(13)-C(55)-C(56)	118.5(6)
C(57)-C(56)-N(13)	115.4(6)
C(57)-C(56)-C(55)	112.9(5)
N(13)-C(56)-C(55)	107.4(6)
C(56)-C(57)-C(58)	112.8(5)
C(59)-C(58)-C(63)	118.6(6)
C(59)-C(58)-C(57)	122.3(6)
C(63)-C(58)-C(57)	119.1(6)
C(60)-C(59)-C(58)	120.5(7)
C(59)-C(60)-C(61)	120.2(7)
C(62)-C(61)-C(60)	120.2(7)
C(63)-C(62)-C(61)	119.7(7)
C(62)-C(63)-C(58)	120.7(7)
O(15)-C(64)-N(16)	123.4(7)
O(15)-C(64)-C(65)	122.6(6)
N(16)-C(64)-C(65)	113.9(7)
N(15)-C(65)-C(64)	109.7(5)
N(15)-C(65)-C(66)	111.3(8)
C(64)-C(65)-C(66)	108.3(8)
C(67)-C(66)-C(65)	113.9(6)
C(72)-C(67)-C(68)	118.0(11)
C(72)-C(67)-C(66)	121.8(9)
C(68)-C(67)-C(66)	120.1(11)
C(69)-C(68)-C(67)	124.6(13)
C(68)-C(69)-C(70)	117.6(13)
C(71)-C(70)-C(69)	121.4(13)

C(72)-C(71)-C(70)	116.1(14)
C(67)-C(72)-C(71)	122.2(11)
N(18)-C(73)-O(17)	123.6(6)
N(18)-C(73)-C(74)	113.3(6)
O(17)-C(73)-C(74)	122.9(6)
N(17)-C(74)-C(75)	111.6(7)
N(17)-C(74)-C(73)	110.0(6)
C(75)-C(74)-C(73)	113.5(5)
C(76)-C(75)-C(74)	113.1(6)
C(77)-C(76)-C(81)	115.4(8)
C(77)-C(76)-C(75)	120.7(6)
C(81)-C(76)-C(75)	123.8(7)
C(78)-C(77)-C(76)	121.5(6)
C(77)-C(78)-C(79)	119.0(8)
C(80)-C(79)-C(78)	120.8(9)
C(81)-C(80)-C(79)	119.8(8)
C(80)-C(81)-C(76)	123.3(9)
N(20)-C(82)-O(19)	126.3(6)
N(20)-C(82)-C(83)	115.3(5)
O(19)-C(82)-C(83)	118.2(5)
N(19)-C(83)-C(84)	111.9(5)
N(19)-C(83)-C(82)	106.9(5)
C(84)-C(83)-C(82)	108.2(5)
C(85)-C(84)-C(83)	113.3(5)
C(86)-C(85)-C(90)	120.2(6)
C(86)-C(85)-C(84)	120.2(6)
C(90)-C(85)-C(84)	119.5(5)
C(85)-C(86)-C(87)	119.2(7)
C(88)-C(87)-C(86)	119.6(7)
C(87)-C(88)-C(89)	121.8(8)
C(88)-C(89)-C(90)	120.0(8)
C(89)-C(90)-C(85)	119.1(7)
C(100)-O(100)-C(10A)	13(2)
C(100)-O(100)-Dy(1)	135.0(6)
C(10A)-O(100)-Dy(1)	122(2)
O(100)-C(100)-O(101)	126.5(13)
O(100)-C(100)-C(101)	121.6(11)
O(101)-C(100)-C(101)	111.5(13)
C(102)-C(101)-C(100)	111.6(11)
C(101)-C(102)-C(103)	120.9(15)
C(102)-C(103)-C(104)	108.5(15)
C(105)-C(104)-C(103)	117.3(16)
C(104)-C(105)-C(106)	110.4(15)
O(100)-C(10A)-O(10A)	128(2)
O(100)-C(10A)-C(10B)	111.8(19)
O(10A)-C(10A)-C(10B)	112(2)
C(10C)-C(10B)-C(10A)	114(2)
C(10B)-C(10C)-C(10D)	109.1(19)
C(10C)-C(10D)-C(10E)	106.6(16)
C(10F)-C(10E)-C(10D)	107.9(17)
C(10E)-C(10F)-C(106)	112.8(18)
O(103)-C(106)-O(102)	126.3(8)

O(103)-C(106)-C(10F)	112.8(10)
O(102)-C(106)-C(10F)	118.3(10)
O(103)-C(106)-C(105)	107.1(10)
O(102)-C(106)-C(105)	126.5(12)
C(10F)-C(106)-C(105)	14.9(17)
C(106)-O(102)-Dy(2)#2	135.2(5)
O(300)-C(300)-O(301)	125.7(10)
O(300)-C(300)-C(301)	120.7(11)
O(301)-C(300)-C(301)	111.9(10)
C(302)-C(301)-C(300)	116.5(12)
C(301)-C(302)-C(303)	113.6(12)
C(302)-C(303)-C(304)	104.9(12)
C(305)-C(304)-C(303)	108.1(11)
C(306)-C(305)-C(304)	122.8(12)
O(303)-C(306)-O(302)	114.9(15)
O(303)-C(306)-C(305)	120.6(15)
O(302)-C(306)-C(305)	124.2(12)

Symmetry transformations used to generate equivalent atoms:
#1 x,y+1,z-1 #2 x,y-1,z+1

Structure Determination for 2.

Blue needles of **2** were crystallized from a water solution at 23 deg. C. A crystal of dimensions 0.37 x 0.10 x 0.10 mm was mounted on a standard Bruker SMART-APEX CCD-based X-ray diffractometer equipped with a low temperature device and fine focus Mo-target X-ray tube (λ = 0.71073 A) operated at 1500 W power (50 kV, 30 mA). The X-ray intensities were measured at 85(2) K; the detector was placed at a distance 5.055 cm from the crystal. A total of 3365 frames were collected with a scan width of 0.5° in ω and 0.45° in ϕ with an exposure time of 60 s/frame. The frames were integrated with the Bruker SAINT software package with a narrow frame algorithm. The integration of the data yielded a total of 333062 reflections to a maximum 2θ value of 35.08° of which 11288 were independent and 10653 were greater than $2\sigma(I)$. The final cell constants (Table 1) were based on the xyz centroids of 9854 reflections above $10\sigma(I)$. Analysis of the data showed negligible decay during data collection; the data were processed with SADABS and corrected for absorption. The structure was solved and refined with the Bruker SHELXTL (version 2008/4) software package, using the space group P6(2)22 with Z = 12 for the formula $C_{45}H_{50}N_{10}O_{10}Cu_5La(C_7H_{10}O_4)_{1.5}(H_2O)_{28}$(solvent). This limited resolution and considerable disorder resulted in formidable refinement challenges. Full-matrix least-squares refinement based on F^2 converged at R1 = 0.0935 and wR2 = 0.2516 [based on I > 2sigma(I)], R1 = 0.0970 and wR2 = 0.2558 for all data. Additional details are presented in Table S3 with further detail given as Supporting Information in a CIF file.

Sheldrick, G.M. SHELXTL, v. 2008/4; Bruker Analytical X-ray, Madison, WI, 2008.

Saint Plus, v. 7.60A, Bruker Analytical X-ray, Madison, WI, 2009.

Sheldrick, G.M. SADABS, v. 2008/1. Program for Empirical Absorption Correction of Area Detector Data, University of Gottingen: Gottingen, Germany, 2008.

Table S3. Crystal data and structure refinement for **2**.

Empirical formula	C111 H186 Cu10 La2 N20 O60
Formula weight	3674.02
Temperature	85(2) K
Wavelength	0.71073 A
Crystal system, space group	Hexagonal, P6(2)22

Unit cell dimensions	a = 45.328(2) A alpha = 90 deg.
	b = 45.328(2) A beta = 90 deg.
	c = 29.754(3) A gamma = 120 deg.
Volume	52943(6) A^3
Z, Calculated density	12, 1.383 Mg/m^3
Absorption coefficient	1.730 mm^-1
F(000)	22512
Crystal size	0.37 x 0.10 x 0.10 mm
Theta range for data collection	1.53 to 17.54 deg.
Limiting indices	-38<=h<=38, -38<=k<=38, -25<=l<=25
Reflections collected / unique	383062 / 11288 [R(int) = 0.0888]
Completeness to theta = 17.54	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8461 and 0.5672
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11288 / 612 / 1227
Goodness-of-fit on F^2	1.044
Final R indices [I>2sigma(I)]	R1 = 0.0935, wR2 = 0.2516
R indices (all data)	R1 = 0.0970, wR2 = 0.2558
Absolute structure parameter	0.08(4)
Largest diff. peak and hole	0.827 and -0.934 e.A^-3

Table S4. Bond lengths [A] and angles [deg] for **2**.

La(1)-O(8)	2.538(12)
La(1)-O(32)	2.539(15)
La(1)-O(4)	2.553(10)
La(1)-O(10)	2.564(10)
La(1)-O(2)	2.568(10)
La(1)-O(30)	2.568(12)
La(1)-O(6)	2.573(10)
La(1)-O(33)	2.590(12)
La(1)-O(31)	2.589(12)
Cu(1)-N(10)	1.886(14)
Cu(1)-O(2)	1.924(9)
Cu(1)-O(1)	1.949(12)
Cu(1)-N(9)	2.009(11)

O(1)-C(1)	1.273(17)
O(2)-N(2)	1.409(17)
N(1)-C(2)	1.554(19)
N(1)-Cu(2)	2.024(15)
N(2)-C(1)	1.318(18)
N(2)-Cu(2)	1.900(11)
C(1)-C(2)	1.47(3)
C(2)-C(3)	1.529(10)
C(3)-C(4)	1.56(2)
C(4)-C(5)	1.3900
C(4)-C(9)	1.3900
C(5)-C(6)	1.3900
C(6)-C(7)	1.3900
C(7)-C(8)	1.3900
C(8)-C(9)	1.3900
Cu(2)-O(4)	1.894(12)
Cu(2)-O(3)	1.946(10)
O(3)-C(10)	1.258(17)
O(4)-N(4)	1.362(14)
N(3)-C(11)	1.43(3)
N(3)-Cu(3)	1.997(15)
N(4)-C(10)	1.319(18)
N(4)-Cu(3)	1.886(14)
C(10)-C(11)	1.59(2)
C(11)-C(12)	1.524(11)
C(12)-C(13)	1.46(2)
C(13)-C(14)	1.3900
C(13)-C(18)	1.3900
C(14)-C(15)	1.3900
C(15)-C(16)	1.3900
C(16)-C(17)	1.3900
C(17)-C(18)	1.3900
Cu(3)-O(5)	1.912(13)
Cu(3)-O(6)	1.911(11)
O(5)-C(19)	1.23(2)
O(6)-N(6)	1.35(2)
N(5)-C(20)	1.48(3)
N(5)-Cu(4)	1.955(15)
N(6)-C(19)	1.27(2)
N(6)-Cu(4)	1.916(16)
C(19)-C(20)	1.53(3)
C(20)-C(21)	1.58(2)
C(21)-C(22)	1.48(3)
C(22)-C(27)	1.34(3)
C(22)-C(23)	1.37(3)
C(23)-C(24)	1.55(4)
C(24)-C(25)	1.38(3)
C(25)-C(26)	1.37(3)
C(26)-C(27)	1.44(3)
Cu(4)-O(7)	1.867(13)
Cu(4)-O(8)	1.910(11)
O(7)-C(28)	1.364(18)

O(8)-N(8)	1.396(16)
N(7)-C(29)	1.482(9)
N(7)-Cu(5)	2.049(13)
N(8)-C(28)	1.28(2)
N(8)-Cu(5)	1.881(12)
C(28)-C(29)	1.522(9)
C(29)-C(30)	1.525(8)
C(30)-C(31)	1.59(2)
C(31)-C(32)	1.3900
C(31)-C(36)	1.3900
C(32)-C(33)	1.3900
C(33)-C(34)	1.3900
C(34)-C(35)	1.3900
C(35)-C(36)	1.3900
Cu(5)-O(10)	1.897(12)
Cu(5)-O(9)	1.947(10)
Cu(5)-O(121)	2.454(15)
O(9)-C(37)	1.24(2)
O(10)-N(10)	1.384(16)
N(9)-C(38)	1.48(2)
N(10)-C(37)	1.37(2)
C(37)-C(38)	1.51(2)
C(38)-C(39)	1.59(2)
C(39)-C(40)	1.558(19)
C(40)-C(41)	1.30(2)
C(40)-C(45)	1.40(2)
C(41)-C(42)	1.35(2)
C(42)-C(43)	1.31(3)
C(43)-C(44)	1.35(3)
C(44)-C(45)	1.33(2)
La(2)-O(12)	2.500(14)
La(2)-O(36)	2.509(18)
La(2)-O(14)	2.511(15)
La(2)-O(35)	2.539(17)
La(2)-O(18)	2.550(18)
La(2)-O(16)	2.561(14)
La(2)-O(20)	2.574(19)
La(2)-O(101)	2.59(2)
La(2)-O(100)	2.59(2)
Cu(6)-N(20)	1.78(3)
Cu(6)-O(11)	1.90(2)
Cu(6)-O(12)	1.915(15)
Cu(6)-N(19)	2.045(15)
O(11)-C(46)	1.32(2)
O(12)-N(12)	1.37(3)
N(11)-C(47)	1.55(3)
N(11)-Cu(7)	2.017(15)
N(12)-C(46)	1.36(2)
N(12)-Cu(7)	1.87(2)
C(46)-C(47)	1.46(3)
C(47)-C(48)	1.504(10)
C(48)-C(49)	1.501(10)

C(49)-C(50)	1.3900
C(49)-C(54)	1.3900
C(50)-C(51)	1.3900
C(51)-C(52)	1.3900
C(52)-C(53)	1.3900
C(53)-C(54)	1.3900
Cu(7)-O(14)	1.870(14)
Cu(7)-O(13)	1.937(13)
O(13)-C(55)	1.28(2)
O(14)-N(14)	1.398(19)
N(13)-C(56)	1.506(19)
N(13)-Cu(8)	2.025(13)
N(14)-C(55)	1.29(2)
N(14)-Cu(8)	1.935(14)
C(55)-C(56)	1.56(2)
C(56)-C(57)	1.52(2)
C(57)-C(58)	1.493(19)
C(58)-C(59)	1.3900
C(58)-C(63)	1.3900
C(59)-C(60)	1.3900
C(60)-C(61)	1.3900
C(61)-C(62)	1.3900
C(62)-C(63)	1.3900
Cu(8)-O(16)	1.864(14)
Cu(8)-O(15)	1.941(12)
Cu(8)-O(120)	2.490(11)
O(15)-C(64)	1.22(3)
O(16)-N(16)	1.36(2)
N(15)-C(65)	1.563(11)
N(15)-Cu(9)	1.876(18)
N(16)-C(64)	1.41(3)
N(16)-Cu(9)	1.933(18)
C(64)-C(65)	1.50(4)
C(65)-C(66)	1.50(3)
C(66)-C(67)	1.523(11)
C(67)-C(68)	1.3900
C(67)-C(72)	1.3900
C(68)-C(69)	1.3900
C(69)-C(70)	1.3900
C(70)-C(71)	1.3900
C(71)-C(72)	1.3900
Cu(9)-O(18)	1.854(18)
Cu(9)-O(17)	1.942(16)
O(17)-C(73)	1.24(3)
O(18)-N(18)	1.42(3)
N(17)-C(74)	1.47(3)
N(17)-Cu(10)	1.91(2)
N(18)-C(73)	1.35(3)
N(18)-Cu(10)	1.87(2)
C(73)-C(74)	1.518(11)
C(74)-C(75)	1.62(3)
C(75)-C(76)	1.524(10)

C(76)-C(81)	1.26(2)
C(76)-C(77)	1.37(3)
C(77)-C(78)	1.49(3)
C(78)-C(79)	1.22(2)
C(79)-C(80)	1.29(3)
C(80)-C(81)	1.34(3)
Cu(10)-O(20)	1.92(2)
Cu(10)-O(19)	1.939(18)
O(19)-C(82)	1.27(3)
O(20)-N(20)	1.42(3)
N(19)-C(83)	1.599(19)
N(20)-C(82)	1.42(4)
C(82)-C(83)	1.503(11)
C(83)-C(84)	1.525(10)
C(84)-C(85)	1.524(9)
C(85)-C(86)	1.3900
C(85)-C(90)	1.3900
C(86)-C(87)	1.3900
C(87)-C(88)	1.3900
C(88)-C(89)	1.3900
C(89)-C(90)	1.3900
O(120)-C(121)	1.398(13)
O(121)-C(121)	1.412(13)
C(121)-C(122)	1.532(11)
C(122)-C(123)	1.520(10)
C(123)-C(124)	1.521(6)
C(124)-C(123)#1	1.521(6)
O(999)-C(999)	1.356(13)
O(998)-C(999)	1.389(12)
C(999)-C(998)	1.516(7)
C(998)-C(997)	1.402(11)
C(997)-C(996)	1.604(13)
C(996)-C(995)	1.523(9)
C(995)-C(994)	1.586(12)
C(994)-C(993)	1.506(12)
C(993)-O(997)	1.375(12)
C(993)-O(996)	1.378(11)
O(99A)-C(99A)	1.356(15)
O(99B)-C(99A)	1.397(15)
C(99A)-C(99B)	1.517(12)
C(99B)-C(99C)	1.402(15)
C(99C)-C(99D)	1.604(15)
C(99D)-C(99E)	1.523(13)
C(99E)-C(99F)	1.586(16)
C(99F)-C(99G)	1.507(14)
C(99G)-O(99D)	1.379(15)
C(99G)-O(99C)	1.381(14)
O(207)-C(900)	1.349(19)
O(208)-C(900)	1.35(2)
C(900)-C(901)	1.520(15)
C(901)-C(902)	1.516(16)
C(902)-C(903)	1.525(16)

C(903)-C(904)	1.519(13)
C(904)-C(905)	1.522(14)
C(905)-C(906)	1.526(15)
C(906)-O(228)	1.36(2)
C(906)-O(227)	1.37(2)

O(8)-La(1)-O(32)	74.2(6)
O(8)-La(1)-O(4)	137.0(3)
O(32)-La(1)-O(4)	136.1(5)
O(8)-La(1)-O(10)	69.8(4)
O(32)-La(1)-O(10)	70.4(4)
O(4)-La(1)-O(10)	139.7(3)
O(8)-La(1)-O(2)	128.1(4)
O(32)-La(1)-O(2)	118.5(5)
O(4)-La(1)-O(2)	70.8(3)
O(10)-La(1)-O(2)	69.2(3)
O(8)-La(1)-O(30)	76.9(5)
O(32)-La(1)-O(30)	143.8(6)
O(4)-La(1)-O(30)	80.1(4)
O(10)-La(1)-O(30)	79.5(4)
O(2)-La(1)-O(30)	65.6(4)
O(8)-La(1)-O(6)	68.9(4)
O(32)-La(1)-O(6)	111.5(5)
O(4)-La(1)-O(6)	70.8(4)
O(10)-La(1)-O(6)	136.0(4)
O(2)-La(1)-O(6)	129.8(3)
O(30)-La(1)-O(6)	77.0(4)
O(8)-La(1)-O(33)	99.8(5)
O(32)-La(1)-O(33)	61.3(5)
O(4)-La(1)-O(33)	80.4(5)
O(10)-La(1)-O(33)	131.5(4)
O(2)-La(1)-O(33)	131.2(5)
O(30)-La(1)-O(33)	146.3(4)
O(6)-La(1)-O(33)	70.8(4)
O(8)-La(1)-O(31)	142.8(4)
O(32)-La(1)-O(31)	69.5(6)
O(4)-La(1)-O(31)	78.1(4)
O(10)-La(1)-O(31)	90.2(4)
O(2)-La(1)-O(31)	66.4(4)
O(30)-La(1)-O(31)	131.5(5)
O(6)-La(1)-O(31)	132.9(4)
O(33)-La(1)-O(31)	69.7(4)
N(10)-Cu(1)-O(2)	92.5(5)
N(10)-Cu(1)-O(1)	174.3(5)
O(2)-Cu(1)-O(1)	83.3(4)
N(10)-Cu(1)-N(9)	81.3(5)
O(2)-Cu(1)-N(9)	173.5(5)
O(1)-Cu(1)-N(9)	102.8(5)
C(1)-O(1)-Cu(1)	109.1(10)
N(2)-O(2)-Cu(1)	109.0(8)
N(2)-O(2)-La(1)	121.5(7)
Cu(1)-O(2)-La(1)	125.2(5)

C(2)-N(1)-Cu(2)	109.7(11)
C(1)-N(2)-O(2)	113.7(12)
C(1)-N(2)-Cu(2)	120.3(11)
O(2)-N(2)-Cu(2)	125.9(9)
O(1)-C(1)-N(2)	122.4(16)
O(1)-C(1)-C(2)	121.5(13)
N(2)-C(1)-C(2)	115.9(13)
C(1)-C(2)-C(3)	114.1(16)
C(1)-C(2)-N(1)	107.7(11)
C(3)-C(2)-N(1)	113.2(12)
C(2)-C(3)-C(4)	109.9(12)
C(5)-C(4)-C(9)	120.0
C(5)-C(4)-C(3)	118.5(12)
C(9)-C(4)-C(3)	121.5(12)
C(4)-C(5)-C(6)	120.0
C(7)-C(6)-C(5)	120.0
C(6)-C(7)-C(8)	120.0
C(7)-C(8)-C(9)	120.0
C(8)-C(9)-C(4)	120.0
O(4)-Cu(2)-N(2)	94.4(5)
O(4)-Cu(2)-O(3)	82.6(5)
N(2)-Cu(2)-O(3)	162.9(5)
O(4)-Cu(2)-N(1)	171.3(5)
N(2)-Cu(2)-N(1)	81.7(5)
O(3)-Cu(2)-N(1)	103.4(5)
C(10)-O(3)-Cu(2)	107.9(8)
N(4)-O(4)-Cu(2)	113.4(9)
N(4)-O(4)-La(1)	121.8(9)
Cu(2)-O(4)-La(1)	124.6(4)
C(11)-N(3)-Cu(3)	111.5(13)
C(10)-N(4)-O(4)	110.4(12)
C(10)-N(4)-Cu(3)	119.1(9)
O(4)-N(4)-Cu(3)	128.4(10)
O(3)-C(10)-N(4)	125.1(11)
O(3)-C(10)-C(11)	122.5(14)
N(4)-C(10)-C(11)	112.3(14)
N(3)-C(11)-C(12)	114.5(17)
N(3)-C(11)-C(10)	104.9(15)
C(12)-C(11)-C(10)	108.1(12)
C(13)-C(12)-C(11)	113.6(15)
C(14)-C(13)-C(18)	120.0
C(14)-C(13)-C(12)	118.7(9)
C(18)-C(13)-C(12)	121.3(9)
C(13)-C(14)-C(15)	120.0
C(14)-C(15)-C(16)	120.0
C(17)-C(16)-C(15)	120.0
C(16)-C(17)-C(18)	120.0
C(17)-C(18)-C(13)	120.0
N(4)-Cu(3)-O(5)	173.1(5)
N(4)-Cu(3)-O(6)	93.4(5)
O(5)-Cu(3)-O(6)	80.5(5)
N(4)-Cu(3)-N(3)	80.3(6)

O(5)-Cu(3)-N(3)	105.7(6)
O(6)-Cu(3)-N(3)	173.2(6)
C(19)-O(5)-Cu(3)	113.3(12)
N(6)-O(6)-Cu(3)	110.7(8)
N(6)-O(6)-La(1)	125.5(9)
Cu(3)-O(6)-La(1)	122.8(6)
C(20)-N(5)-Cu(4)	114.3(13)
C(19)-N(6)-O(6)	115.3(17)
C(19)-N(6)-Cu(4)	120.2(16)
O(6)-N(6)-Cu(4)	124.5(10)
O(5)-C(19)-N(6)	120(2)
O(5)-C(19)-C(20)	124.8(16)
N(6)-C(19)-C(20)	115.0(18)
N(5)-C(20)-C(19)	107.3(15)
N(5)-C(20)-C(21)	114.7(17)
C(19)-C(20)-C(21)	108.6(15)
C(22)-C(21)-C(20)	109.6(13)
C(27)-C(22)-C(23)	119(2)
C(27)-C(22)-C(21)	122(2)
C(23)-C(22)-C(21)	119.0(17)
C(22)-C(23)-C(24)	121(2)
C(25)-C(24)-C(23)	114(2)
C(26)-C(25)-C(24)	125(2)
C(25)-C(26)-C(27)	117(2)
C(22)-C(27)-C(26)	124(2)
O(7)-Cu(4)-O(8)	84.7(5)
O(7)-Cu(4)-N(6)	176.6(6)
O(8)-Cu(4)-N(6)	93.0(6)
O(7)-Cu(4)-N(5)	100.4(7)
O(8)-Cu(4)-N(5)	173.8(7)
N(6)-Cu(4)-N(5)	81.8(7)
C(28)-O(7)-Cu(4)	110.2(10)
N(8)-O(8)-Cu(4)	110.2(9)
N(8)-O(8)-La(1)	122.8(8)
Cu(4)-O(8)-La(1)	126.5(5)
C(29)-N(7)-Cu(5)	112.7(7)
C(28)-N(8)-O(8)	114.7(11)
C(28)-N(8)-Cu(5)	118.6(9)
O(8)-N(8)-Cu(5)	126.7(10)
N(8)-C(28)-O(7)	119.7(10)
N(8)-C(28)-C(29)	119.8(12)
O(7)-C(28)-C(29)	120.3(13)
N(7)-C(29)-C(28)	106.4(10)
N(7)-C(29)-C(30)	114.4(10)
C(28)-C(29)-C(30)	111.1(9)
C(29)-C(30)-C(31)	113.2(11)
C(32)-C(31)-C(36)	120.0
C(32)-C(31)-C(30)	118.8(7)
C(36)-C(31)-C(30)	121.2(7)
C(31)-C(32)-C(33)	120.0
C(34)-C(33)-C(32)	120.0
C(35)-C(34)-C(33)	120.0

C(34)-C(35)-C(36)	120.0
C(35)-C(36)-C(31)	120.0
N(8)-Cu(5)-O(10)	92.9(5)
N(8)-Cu(5)-O(9)	162.8(5)
O(10)-Cu(5)-O(9)	83.9(4)
N(8)-Cu(5)-N(7)	82.5(5)
O(10)-Cu(5)-N(7)	174.8(4)
O(9)-Cu(5)-N(7)	99.6(4)
N(8)-Cu(5)-O(121)	98.9(5)
O(10)-Cu(5)-O(121)	94.9(5)
O(9)-Cu(5)-O(121)	98.2(4)
N(7)-Cu(5)-O(121)	88.5(5)
C(37)-O(9)-Cu(5)	108.7(9)
N(10)-O(10)-Cu(5)	112.1(8)
N(10)-O(10)-La(1)	123.5(8)
Cu(5)-O(10)-La(1)	124.3(5)
C(38)-N(9)-Cu(1)	111.0(9)
C(37)-N(10)-O(10)	110.5(12)
C(37)-N(10)-Cu(1)	121.8(10)
O(10)-N(10)-Cu(1)	126.8(9)
O(9)-C(37)-N(10)	124.5(13)
O(9)-C(37)-C(38)	123.5(15)
N(10)-C(37)-C(38)	110.3(15)
N(9)-C(38)-C(37)	111.1(13)
N(9)-C(38)-C(39)	111.1(13)
C(37)-C(38)-C(39)	110.3(13)
C(40)-C(39)-C(38)	109.8(10)
C(41)-C(40)-C(45)	116.1(14)
C(41)-C(40)-C(39)	123.1(15)
C(45)-C(40)-C(39)	120.8(15)
C(40)-C(41)-C(42)	119.5(18)
C(43)-C(42)-C(41)	123(2)
C(42)-C(43)-C(44)	120(2)
C(45)-C(44)-C(43)	116(2)
C(44)-C(45)-C(40)	124.8(19)
O(12)-La(2)-O(36)	101.9(6)
O(12)-La(2)-O(14)	68.8(5)
O(36)-La(2)-O(14)	68.0(6)
O(12)-La(2)-O(35)	78.6(5)
O(36)-La(2)-O(35)	137.3(6)
O(14)-La(2)-O(35)	72.8(5)
O(12)-La(2)-O(18)	134.7(5)
O(36)-La(2)-O(18)	122.6(6)
O(14)-La(2)-O(18)	132.9(6)
O(35)-La(2)-O(18)	74.5(6)
O(12)-La(2)-O(16)	137.8(5)
O(36)-La(2)-O(16)	74.5(5)
O(14)-La(2)-O(16)	71.1(4)
O(35)-La(2)-O(16)	77.4(5)
O(18)-La(2)-O(16)	69.3(5)
O(12)-La(2)-O(20)	67.6(6)
O(36)-La(2)-O(20)	140.5(8)

O(14)-La(2)-O(20)	132.1(6)
O(35)-La(2)-O(20)	79.9(7)
O(18)-La(2)-O(20)	72.3(6)
O(16)-La(2)-O(20)	139.3(6)
O(12)-La(2)-O(101)	80.4(6)
O(36)-La(2)-O(101)	70.4(7)
O(14)-La(2)-O(101)	120.4(7)
O(35)-La(2)-O(101)	148.3(6)
O(18)-La(2)-O(101)	105.2(7)
O(16)-La(2)-O(101)	133.1(5)
O(20)-La(2)-O(101)	70.2(8)
O(12)-La(2)-O(100)	124.4(9)
O(36)-La(2)-O(100)	68.2(7)
O(14)-La(2)-O(100)	136.0(6)
O(35)-La(2)-O(100)	145.8(8)
O(18)-La(2)-O(100)	71.5(9)
O(16)-La(2)-O(100)	94.0(8)
O(20)-La(2)-O(100)	86.3(7)
O(101)-La(2)-O(100)	44.2(9)
N(20)-Cu(6)-O(11)	167.4(12)
N(20)-Cu(6)-O(12)	91.1(9)
O(11)-Cu(6)-O(12)	86.8(7)
N(20)-Cu(6)-N(19)	90.7(8)
O(11)-Cu(6)-N(19)	88.7(6)
O(12)-Cu(6)-N(19)	167.6(8)
C(46)-O(11)-Cu(6)	108.5(12)
N(12)-O(12)-Cu(6)	109.0(11)
N(12)-O(12)-La(2)	123.5(11)
Cu(6)-O(12)-La(2)	126.2(9)
C(47)-N(11)-Cu(7)	112.2(14)
O(12)-N(12)-C(46)	115.0(16)
O(12)-N(12)-Cu(7)	127.1(12)
C(46)-N(12)-Cu(7)	117.6(15)
O(11)-C(46)-N(12)	120.8(16)
O(11)-C(46)-C(47)	120.3(18)
N(12)-C(46)-C(47)	118.7(18)
C(46)-C(47)-C(48)	117.8(15)
C(46)-C(47)-N(11)	106.8(17)
C(48)-C(47)-N(11)	112.6(16)
C(49)-C(48)-C(47)	116.7(12)
C(50)-C(49)-C(54)	120.0
C(50)-C(49)-C(48)	109.4(6)
C(54)-C(49)-C(48)	130.6(6)
C(49)-C(50)-C(51)	120.0
C(52)-C(51)-C(50)	120.0
C(51)-C(52)-C(53)	120.0
C(54)-C(53)-C(52)	120.0
C(53)-C(54)-C(49)	120.0
O(14)-Cu(7)-N(12)	90.6(7)
O(14)-Cu(7)-O(13)	85.5(6)
N(12)-Cu(7)-O(13)	173.6(8)
O(14)-Cu(7)-N(11)	173.4(6)

N(12)-Cu(7)-N(11)	83.5(8)
O(13)-Cu(7)-N(11)	100.2(6)
C(55)-O(13)-Cu(7)	106.5(11)
N(14)-O(14)-Cu(7)	109.8(11)
N(14)-O(14)-La(2)	121.4(10)
Cu(7)-O(14)-La(2)	126.9(7)
C(56)-N(13)-Cu(8)	113.8(9)
C(55)-N(14)-O(14)	113.1(14)
C(55)-N(14)-Cu(8)	119.4(12)
O(14)-N(14)-Cu(8)	127.5(12)
O(13)-C(55)-N(14)	124.9(17)
O(13)-C(55)-C(56)	117.7(16)
N(14)-C(55)-C(56)	117.3(15)
N(13)-C(56)-C(57)	109.4(14)
N(13)-C(56)-C(55)	107.0(12)
C(57)-C(56)-C(55)	108.3(12)
C(58)-C(57)-C(56)	112.7(10)
C(59)-C(58)-C(63)	120.0
C(59)-C(58)-C(57)	117.0(10)
C(63)-C(58)-C(57)	123.0(10)
C(60)-C(59)-C(58)	120.0
C(61)-C(60)-C(59)	120.0
C(62)-C(61)-C(60)	120.0
C(61)-C(62)-C(63)	120.0
C(62)-C(63)-C(58)	120.0
O(16)-Cu(8)-N(14)	92.0(6)
O(16)-Cu(8)-O(15)	83.5(6)
N(14)-Cu(8)-O(15)	167.3(6)
O(16)-Cu(8)-N(13)	174.2(5)
N(14)-Cu(8)-N(13)	82.5(6)
O(15)-Cu(8)-N(13)	101.4(5)
O(16)-Cu(8)-O(120)	90.3(6)
N(14)-Cu(8)-O(120)	94.4(6)
O(15)-Cu(8)-O(120)	97.5(5)
N(13)-Cu(8)-O(120)	92.1(5)
C(64)-O(15)-Cu(8)	112.7(14)
N(16)-O(16)-Cu(8)	112.2(11)
N(16)-O(16)-La(2)	122.4(11)
Cu(8)-O(16)-La(2)	125.4(7)
C(65)-N(15)-Cu(9)	116.6(13)
O(16)-N(16)-C(64)	113.3(17)
O(16)-N(16)-Cu(9)	127.1(12)
C(64)-N(16)-Cu(9)	119.5(16)
O(15)-C(64)-N(16)	118(2)
O(15)-C(64)-C(65)	127(2)
N(16)-C(64)-C(65)	111(2)
C(64)-C(65)-C(66)	113.8(17)
C(64)-C(65)-N(15)	105.4(19)
C(66)-C(65)-N(15)	124(2)
C(65)-C(66)-C(67)	103.9(13)
C(68)-C(67)-C(72)	120.0
C(68)-C(67)-C(66)	116.7(16)

C(72)-C(67)-C(66)	123.3(16)
C(69)-C(68)-C(67)	120.0
C(68)-C(69)-C(70)	120.0
C(71)-C(70)-C(69)	120.0
C(70)-C(71)-C(72)	120.0
C(71)-C(72)-C(67)	120.0
O(18)-Cu(9)-N(15)	169.6(9)
O(18)-Cu(9)-N(16)	91.4(7)
N(15)-Cu(9)-N(16)	81.6(7)
O(18)-Cu(9)-O(17)	83.2(7)
N(15)-Cu(9)-O(17)	103.5(7)
N(16)-Cu(9)-O(17)	174.6(7)
C(73)-O(17)-Cu(9)	111.9(13)
N(18)-O(18)-Cu(9)	112.3(14)
N(18)-O(18)-La(2)	118.6(15)
Cu(9)-O(18)-La(2)	127.2(8)
C(74)-N(17)-Cu(10)	115.1(13)
C(73)-N(18)-O(18)	111.8(18)
C(73)-N(18)-Cu(10)	118.1(15)
O(18)-N(18)-Cu(10)	130.2(16)
O(17)-C(73)-N(18)	120.7(16)
O(17)-C(73)-C(74)	125(2)
N(18)-C(73)-C(74)	114(2)
N(17)-C(74)-C(73)	107.5(19)
N(17)-C(74)-C(75)	112.0(15)
C(73)-C(74)-C(75)	107.5(19)
C(76)-C(75)-C(74)	111.5(10)
C(81)-C(76)-C(77)	119.6(17)
C(81)-C(76)-C(75)	129.7(15)
C(77)-C(76)-C(75)	110.7(12)
C(76)-C(77)-C(78)	113.7(16)
C(79)-C(78)-C(77)	118(2)
C(78)-C(79)-C(80)	129(2)
C(79)-C(80)-C(81)	113.2(17)
C(76)-C(81)-C(80)	127(2)
N(18)-Cu(10)-N(17)	84.0(9)
N(18)-Cu(10)-O(20)	93.7(9)
N(17)-Cu(10)-O(20)	176.2(9)
N(18)-Cu(10)-O(19)	176.6(9)
N(17)-Cu(10)-O(19)	98.2(8)
O(20)-Cu(10)-O(19)	84.1(8)
C(82)-O(19)-Cu(10)	104.7(14)
N(20)-O(20)-Cu(10)	115.6(16)
N(20)-O(20)-La(2)	121.8(16)
Cu(10)-O(20)-La(2)	122.4(9)
C(83)-N(19)-Cu(6)	89.8(7)
C(82)-N(20)-O(20)	102.2(19)
C(82)-N(20)-Cu(6)	129.9(17)
O(20)-N(20)-Cu(6)	127.8(18)
O(19)-C(82)-N(20)	129.6(19)
O(19)-C(82)-C(83)	134(3)
N(20)-C(82)-C(83)	90.9(19)

C(82)-C(83)-C(84)	88.1(15)
C(82)-C(83)-N(19)	136.8(18)
C(84)-C(83)-N(19)	107.5(9)
C(85)-C(84)-C(83)	102.0(9)
C(86)-C(85)-C(90)	120.0
C(86)-C(85)-C(84)	119.6(7)
C(90)-C(85)-C(84)	120.4(7)
C(87)-C(86)-C(85)	120.0
C(86)-C(87)-C(88)	120.0
C(89)-C(88)-C(87)	120.0
C(88)-C(89)-C(90)	120.0
C(89)-C(90)-C(85)	120.0
C(121)-O(120)-Cu(8)	139.9(8)
C(121)-O(121)-Cu(5)	123.1(12)
O(120)-C(121)-O(121)	109.4(10)
O(120)-C(121)-C(122)	114.1(8)
O(121)-C(121)-C(122)	135.5(11)
C(123)-C(122)-C(121)	113.4(10)
C(122)-C(123)-C(124)	114.1(8)
C(123)#1-C(124)-C(123)	124.6(9)
O(999)-C(999)-O(998)	126.1(8)
O(999)-C(999)-C(998)	117.7(10)
O(998)-C(999)-C(998)	115.8(10)
C(997)-C(998)-C(999)	121.1(8)
C(998)-C(997)-C(996)	115.3(10)
C(995)-C(996)-C(997)	108.6(7)
C(996)-C(995)-C(994)	109.4(6)
C(993)-C(994)-C(995)	110.7(7)
O(997)-C(993)-O(996)	126.2(11)
O(997)-C(993)-C(994)	115.9(10)
O(996)-C(993)-C(994)	116.4(8)
O(99A)-C(99A)-O(99B)	124.7(14)
O(99A)-C(99A)-C(99B)	117.8(13)
O(99B)-C(99A)-C(99B)	116.2(14)
C(99C)-C(99B)-C(99A)	120.9(16)
C(99B)-C(99C)-C(99D)	115.9(13)
C(99E)-C(99D)-C(99C)	108.7(11)
C(99D)-C(99E)-C(99F)	109.0(13)
C(99G)-C(99F)-C(99E)	111.3(14)
O(99D)-C(99G)-O(99C)	126.1(18)
O(99D)-C(99G)-C(99F)	115.5(14)
O(99C)-C(99G)-C(99F)	115.9(14)
O(208)-C(900)-O(207)	105(2)
O(208)-C(900)-C(901)	145(2)
O(207)-C(900)-C(901)	105.4(19)
C(902)-C(901)-C(900)	115(2)
C(901)-C(902)-C(903)	116.1(19)
C(904)-C(903)-C(902)	111.0(15)
C(903)-C(904)-C(905)	118.3(18)
C(904)-C(905)-C(906)	110.8(13)
O(228)-C(906)-O(227)	141(5)
O(228)-C(906)-C(905)	109(3)

O(227)-C(906)-C(905)	103(2)	

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