Crystal Structure, Dissolution, and Deposition of a 5 nm Functionalized Metal–Organic Great Rhombicuboctahedron

(Supporting Information: 47 pages)

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Synthesis of MOP-18

$Cu_{24}(5OC_{12}H_{25}$-*m*$BDC)_{24}(DMF)_{12}(C_8H_{17}OH)_4(H_2O)_8 \cdot (DMF)_{20}(C_8H_{17}OH)_4(H_2O)_8$, MOP-18. Equimolar amounts of 5-$OC_{12}H_{25}$-*m*$BDCH_2$ (0.147 g, 0.42 mmol) and $Cu(CH_3CO_2)_2 \bullet H_2O$ (0.082 g, 0.41 mmol) in a solvent mixture of DMF (10 mL) were dissolved in a capped vial (20 mL). Blue powder formed immediately was recovered by filtration. The powder (ca. one fifth) was dissolved in hexane (ca. 2 mL) in an uncovered 4 mL vial and a drop of octanol was added to the mixture. After slow evaporation of hexane, blue octahedral crystals were formed, which were then washed with 3 × 5 mL methanol.

FT-IR: (KBr, 3500 – 400 cm^{-1}): 3430 (br), 3089 (w), 2930 (s), 2855 (m), 1669 (m), 1632 (s), 1591 (s), 1457 (m), 1423 (m), 1383 (s), 1321 (w), 1267 (w), 1130 (w), 1103 (w), 1055 (w), 885 (w), 809 (w), 776 (m), 735 (m), 665 (w), 493 (w).

For solvent exchange, MOP-18 was immersed in exchange solvents (i.e. DMSO, BuOH, isoamylalcohol) for a week at room temperature, during which the activation solvent was decanted freshly replenished three times. The solvent was removed under vacuum at room temperature, yielding materials for elemental analyses.

Solubility of MOP-18

As-synthesized MOP-18 powder was washed with acetonitrile several times and the mixture was kept in fresh acetonitrile solution for a week to remove occluded solvents and unreacted organic link. Recovered blue powder was dried under vacuum. The dark blue powder was dissolved in common organic solvents.

Estimated solubility of MOP-18 at room temperature is 5.8 mg mL^{-1} in DEF, 2.7 mg mL^{-1} in DMA, 75 mg mL^{-1} in chloroform, 83 mg mL^{-1} in dichloromethene, 180 mg mL^{-1} in THF, 50 mg mL^{-1} in ethyl acetate, 0.4 mg mL^{-1} in acetone, 9.5 mg mL^{-1} in dioxane, and 38 mg mL^{-1} in toluene. However, MOP-18 powder was insoluble in methanol, ethanol, 1-butanol, isoamylalcohol, hexane, cyclohexane, and DMSO.

Single-Crystal X-ray Diffraction Studies.

A crystal with a suitable size (0.60 mm × 0.24 mm × 0.06 mm) was cut from a large blue prismatic crystal in a mother liquor, and attached on a cryo loop that was coated with Paratone-N oil. It was quickly moved in a $N_2(g)$ stream at 153(2)K (Oxford 700 Series Cryostream) upon mounting on a Bruker SMART APEX CCD diffractometer equipped with a normal focus and graphite monochromated Mo-target X-ray tube (λ = 0.71073 Å) operated at 2000 W power (50 kV, 40 mA). The distance between the detector and crystal was 5.059 cm. Total 1868 frames were collected with varying ω and φ with an exposure time of 40 s/frame. The last 50 frames were collected over the same Ewald sphere as those of the first 50 frames in order to detect possible crystal decay. The frames were integrated with the SAINT software package with a narrow frame algorithm. The final cell constants were based on the *xyz* centroids of 8779 reflections. Analysis of the data showed negligible decay during collection. An absorption correction was applied using SADABS. The structure was solved by direct methods and subsequent difference Fourier syntheses and refined with the SHELX-TL software package. A total of 274510 reflections were collected in the range $0.68° < \theta < 23.33°$ of which 27810 were independent and 12244 were observed ($I > 2\sigma(I)$). All stages of weighted full-matrix least-squares refinement were conducted using F_o^2 data and converged to give $R1$ = 0.1178 ($I > 2\sigma(I)$, 12244 reflections), $wR2$ = 0.3641 (all data) and GOF = 1.066. The diffuse electron density due to the disordered and unidentified moieties was treated with the SQUEEZE routine within the PLATON software package. Statistics prior to treatment of data with SQUEEZE were $R1$ = 0.1564 ($I > 2\sigma(I)$), $wR2$ = 0.5053 (all data) and GOF = 1.543.

The crystal belongs to the tetragonal space group I41/a (No. 88, origin choice 2) with Z' = 4. As the MOP-18 sits on a special position (Wyckoff position a) with 4-fold rotoinversion site symmetry, the asymmetric unit is composed of a quarter of the whole molecule. While the non-hydrogen atoms in a rigid part of the MOP were refined anisotropically, the carbon atoms of the alkyl chains (–OC12H25), a coordinated octanol, and nitrogen and carbon atoms of DMF could not be refined anisotropically due to the large thermal motions. In addition, as the large thermal motion of those atoms resulted in large shifts after refinement, further refinement procedures required restraints to maintain their bonding geometry in optimal status. The carbon…carbon distances of dodecoxy moieties were fixed with 1.54 Å with DFIX instructions. However, most 1,3-nonbonded distances were not restrained except for the particularly unstable cases (C(17A)···C(19A), C(15C)···C(17C), C(16C)···C(18C), C(17C)···C(19C),

C(18C)···C(20C), C(18D)···C(20D), C(11E)···C(13E), C(12F)···C(14F), C(6O)···C(8O)). Although the thermal isotropic parameters of the long alkyl chains were refined by applying group variables, those of the alkyl chains the first three carbon atoms (C(9), C(10), and C(11)) in all the six alkyl chains were refined freely. As the six unique alkyl chains have various conformations with large thermal motions, the anti-bumping restraints (BUMP) has been applied to avoid possible bad contacts among the neighboring chains. Hydrogen atoms were generated with the ideal geometry.

The suitable and stable model for the included solvent molecules and some of the coordinating ligands could not be extracted from diffuse electron density residuals with the current X-ray data. As the total solvent accessible volume was 27160.5 $Å^3$ per unit cell volume 76917.0 $Å^3$ (35.3%), which was calculated by SOLV in the PLATON, 6790 $Å^3$ per asymmetric unit (Z' = 4) was presumed as available room for the unidentified disordered ligand moieties and guests. Although not every species in the asymmetric unit was clearly identified, the crystal formula was used from a reasonable estimate with the aid of elemental microanalysis (EA), thermogravimetric analyses (TGA), and modeling calculation that have been also appended as supporting data. Particularly, with the aid of Forcite program in the MS Modeling 4.0 package O(4O) and O(3O) were designated as DMF oxygen atoms, and O(2S) and O(2O) were as water oxygen atoms The modeling procedure has been described in the modeling part in this supporting material.

Most warning signs from the validation of the CIF file were due to the large thermal motion of the side chains.

Sheldrick, G. M. SHELX-TL, v.6.14; Bruker Analytical X-ray, Madison, WI, 2000.
Sheldirck, G. M. SADABS. Program for Empirical Absorption Correction of Area Detector Data,University of Gottigen: Gottingen, Germany, 1996.
Saint Plus, v.6.01, Bruker Analytical X-ray, Madison, WI, 1999.

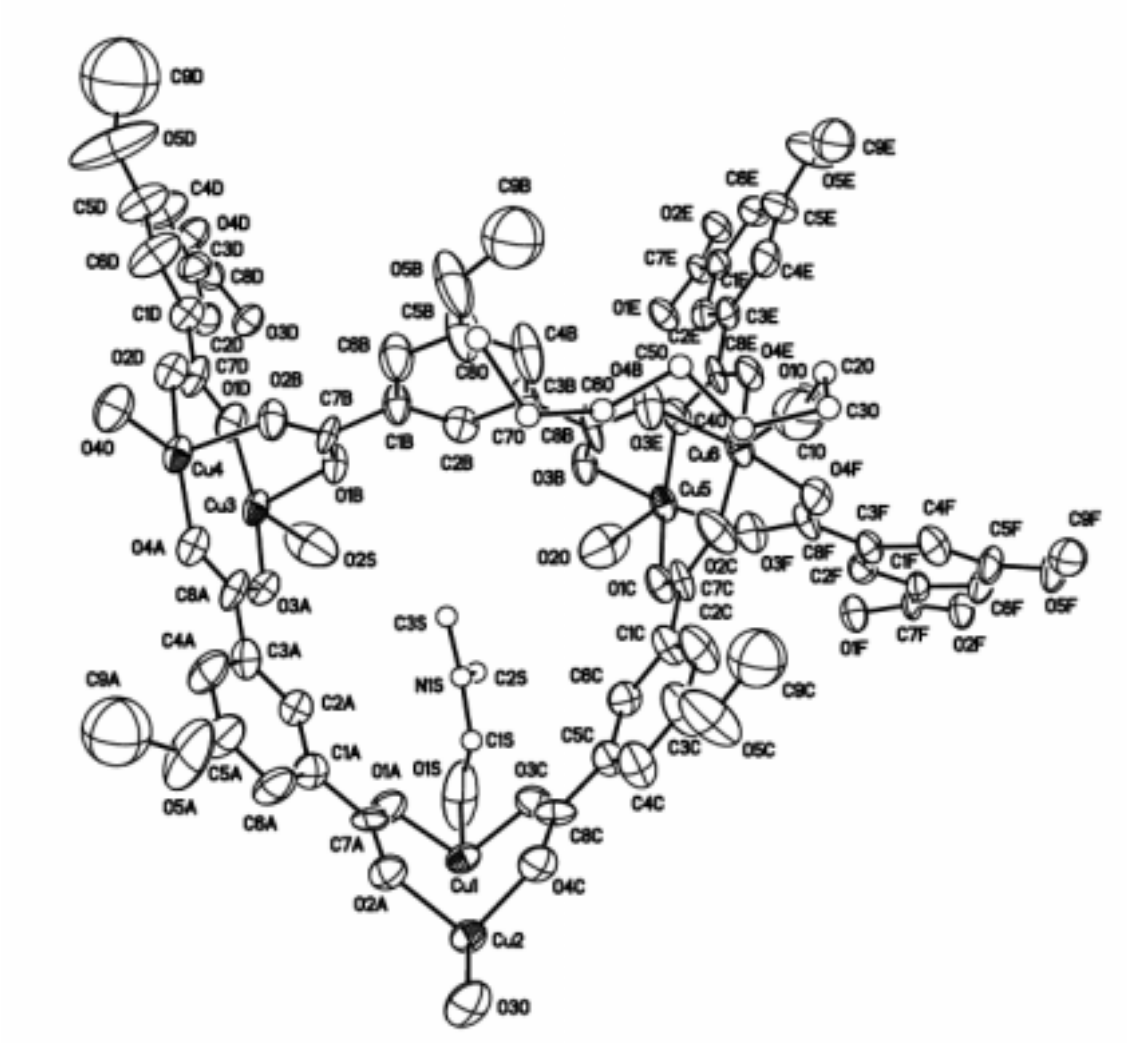

Figure S1. ORTEP drawing of the asymmetric unit of the MOP-18 with atomic numbering scheme. The hydrogen atoms and the carbon atoms in $-OC_{12}H_{25}$ were not shown for clarity.

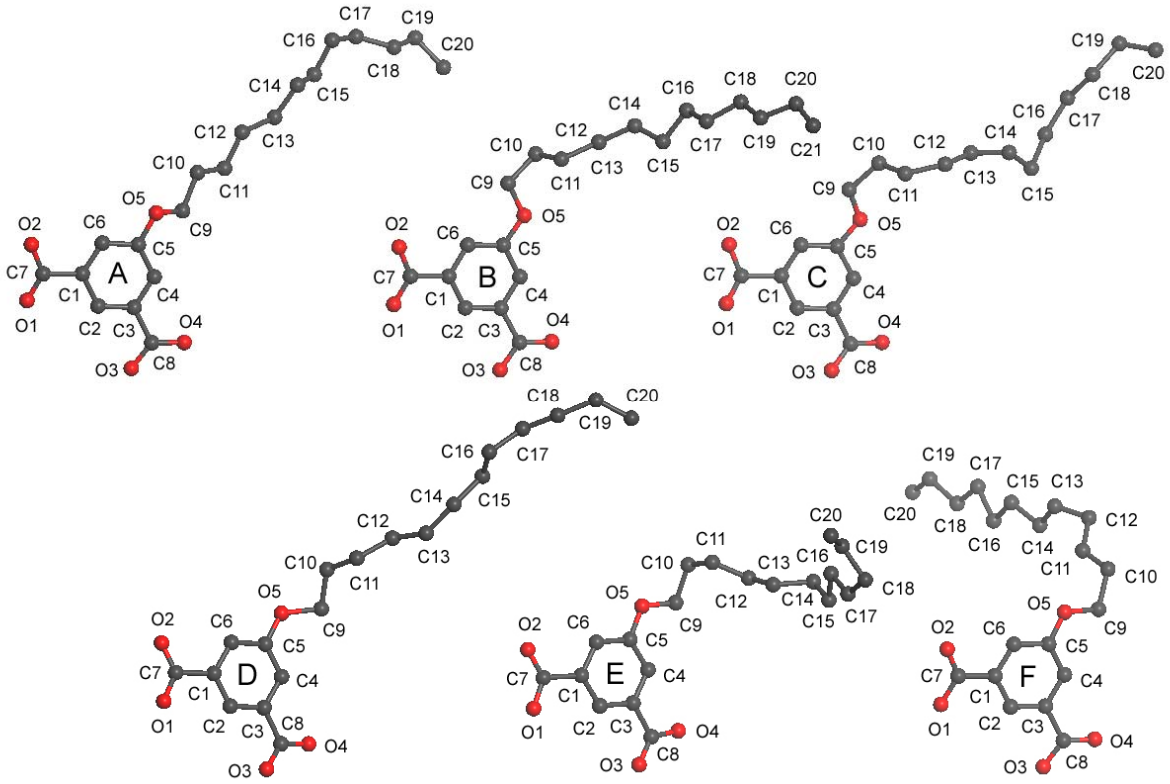

Figure S2. Ball-and-stick drawing of the organic links in the asymmetric unit of the MOP-18 with atomic numbering scheme. The hydrogen atoms were not shown for clarity.

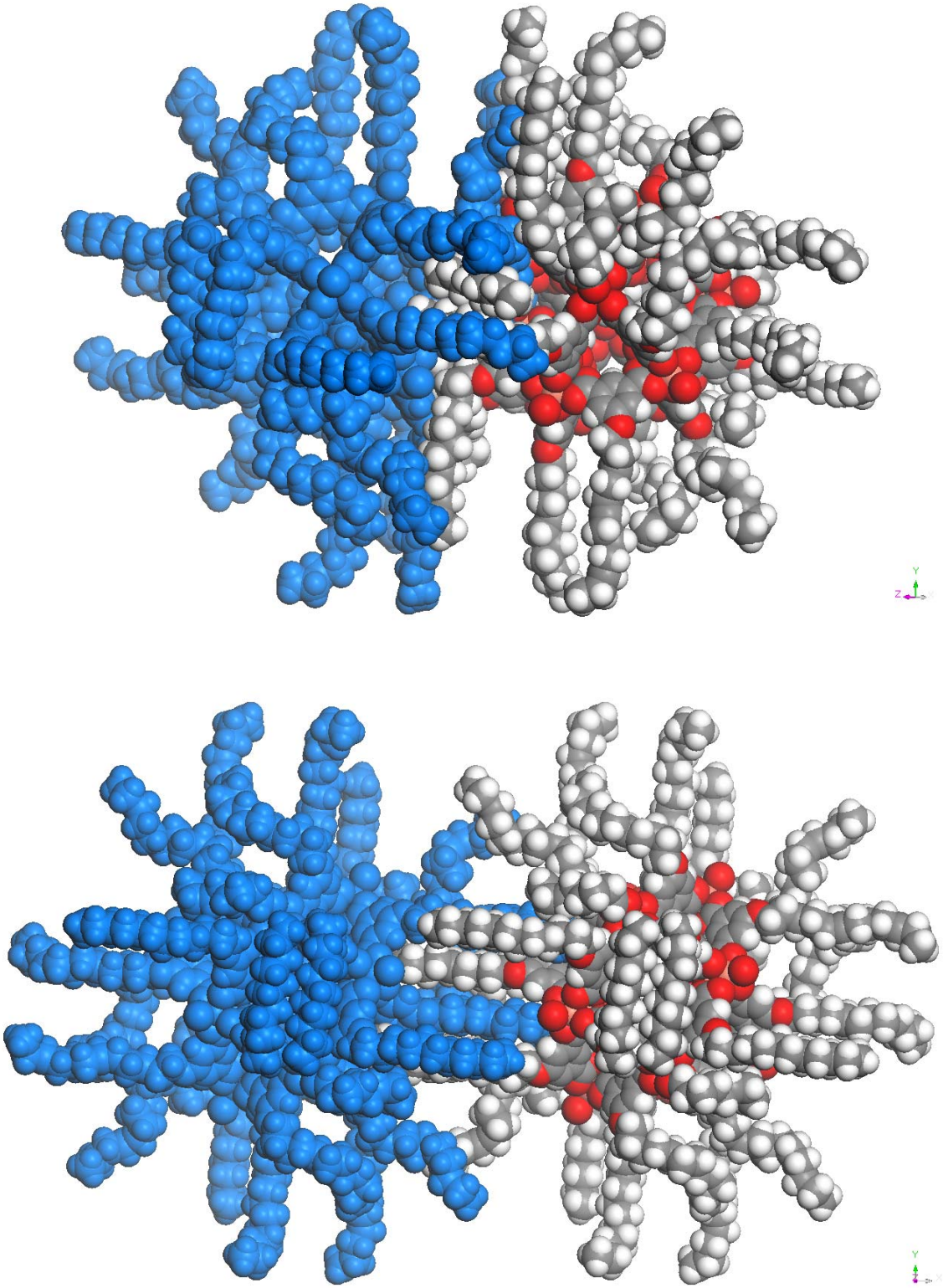

Figure S3. CPK drawings showing contacting modes between two MOPs.

Table S1. Crystal data and structure refinement for MOP-18.

Empirical formula	$C_{640}\ H_{1072}\ N_{32}\ O_{176}\ Cu_{24}$	
Formula weight	13556.26	
Temperature	153(2) K	
Wavelength	0.71073 Å	
Crystal system	Tetragonal	
Space group	$I4_1/a$	
Unit cell dimensions	a = 33.5715(7) Å	α = 90°.
	b = 33.5715(7) Å	β = 90°.
	c = 68.2468(14) Å	γ = 90°.
Volume	76917(3) $Å^3$	
Z	4	
Density (calculated)	1.171 Mg/m^3	
Absorption coefficient	0.721 mm^{-1}	
F(000)	28960	
Crystal size	0.60 x 0.24 x 0.06 mm^3	
Theta range for data collection	0.68 to 23.33°.	
Index ranges	$-37 \leq h \leq 37$, $-37 \leq k \leq 37$, $-75 \leq l \leq 75$	
Reflections collected	274510	
Independent reflections	27810 [R(int) = 0.1159]	
Completeness to theta = 23.33°	99.7 %	
Absorption correction	SADABS	
Max. and min. transmission	0.9580 and 0.6715	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	27810 / 128 / 1012	
Goodness-of-fit on F^2	1.066	
Final R indices [I>2sigma(I)]	R1 = 0.1178, wR2 = 0.3336	
R indices (all data)	R1 = 0.1830, wR2 = 0.3641	
Largest diff. peak and hole	1.207 and -0.669 $e.Å^{-3}$	

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for MOP-18. U_{eq} is defined as one third of the trace of the orthogonalized U^{ij} tensor.

atom	x	y	z	U_{eq}
		Copper Ions		
Cu(1)	10406(1)	815(1)	2056(1)	61(1)
Cu(2)	10538(1)	285(1)	2331(1)	66(1)
Cu(3)	8741(1)	460(1)	1249(1)	60(1)
Cu(4)	8333(1)	-211(1)	1248(1)	64(1)
Cu(5)	8406(1)	2105(1)	2066(1)	59(1)
Cu(6)	7879(1)	1982(1)	2341(1)	62(1)
		Organic Link A		
benzene-1,3-dicarboxylate moiety				
O(1A)	10093(2)	396(2)	1932(1)	72(2)
O(2A)	10209(2)	-59(2)	2160(1)	75(2)
O(3A)	9060(2)	188(2)	1450(1)	64(2)
O(4A)	8729(2)	-390(2)	1441(1)	70(2)
C(1A)	9768(2)	-217(2)	1904(1)	68(3)
C(2A)	9532(2)	-73(2)	1753(1)	64(3)
C(3A)	9260(2)	-323(2)	1661(1)	70(3)
C(4A)	9225(2)	-717(2)	1720(1)	95(4)
C(5A)	9461(3)	-862(2)	1871(1)	105(4)
C(6A)	9733(2)	-612(2)	1963(1)	92(4)
C(7A)	10042(3)	78(3)	2010(1)	57(3)
C(8A)	8985(3)	-159(3)	1505(1)	62(3)
5-dodecoxy moiety				
O(5A)	9437(4)	-1244(3)	1945(2)	189(6)
C(9A)	9356(8)	-1511(6)	1810(4)	251(11)
C(10A)	9396(10)	-1933(7)	1901(5)	348(17)
C(11A)	9366(11)	-2245(12)	1736(5)	400(20)
C(12A)	9350(20)	-2653(15)	1837(9)	681(6)
C(13A)	9250(20)	-3059(18)	1744(8)	681(6)
C(14A)	9140(20)	-3460(20)	1846(7)	681(6)
C(15A)	9260(20)	-3769(18)	1691(9)	681(6)
C(16A)	9190(20)	-4150(20)	1813(8)	681(6)
C(17A)	9200(20)	-4440(20)	1638(10)	681(6)
C(18A)	8888(14)	-4630(20)	1504(11)	681(6)
C(19A)	8944(18)	-4960(20)	1349(11)	681(6)
C(20A)	8589(18)	-4908(19)	1207(8)	681(6)
		Organic Link B		
benzene-1,3-dicarboxylate moiety				
O(1B)	8368(2)	635(2)	1448(1)	68(2)
O(2B)	8030(2)	55(2)	1463(1)	72(2)
O(3B)	8177(2)	1619(2)	1949(1)	67(2)
O(4B)	7685(2)	1548(2)	2168(1)	90(2)
C(1B)	7863(2)	565(2)	1680(1)	69(3)
C(2B)	7970(2)	924(2)	1767(1)	66(3)
C(3B)	7746(2)	1075(2)	1921(1)	70(3)
C(4B)	7415(2)	867(2)	1989(1)	121(5)

C(5B)	7308(2)	508(2)	1902(1)	137(6)
C(6B)	7532(2)	357(2)	1747(1)	109(4)
C(7B)	8121(3)	395(3)	1519(1)	50(2)
C(8B)	7901(3)	1449(2)	2020(1)	67(3)
5-dodecoxy moiety				
O(5B)	6998(3)	276(3)	1947(2)	178(5)
C(9B)	6697(6)	452(6)	2051(3)	208(9)
C(10B)	6306(8)	213(9)	2054(5)	311(14)
C(11B)	6063(11)	201(12)	1862(5)	430(20)
C(12B)	5811(17)	-159(14)	1790(8)	681(6)
C(13B)	5820(20)	-605(14)	1844(8)	681(6)
C(14B)	5542(13)	-840(20)	1703(9)	681(6)
C(15B)	5777(18)	-1230(15)	1661(6)	681(6)
C(16B)	5587(15)	-1527(11)	1808(9)	681(6)
C(17B)	5212(10)	-1770(11)	1896(9)	681(6)
C(18B)	4764(13)	-1869(17)	1863(8)	681(6)
C(19B)	4445(17)	-2179(13)	1929(6)	681(6)
C(20B)	4208(10)	-2364(12)	1756(8)	681(6)

Organic Link C

benzene-1,3-dicarboxylate moiety				
O(1C)	8748(2)	1766(2)	2228(1)	67(2)
O(2C)	8267(2)	1616(2)	2444(1)	95(3)
O(3C)	9951(2)	951(2)	2221(1)	69(2)
O(4C)	10045(2)	483(2)	2451(1)	75(2)
C(1C)	8876(2)	1279(2)	2470(1)	69(3)
C(2C)	8748(2)	1087(2)	2639(1)	100(4)
C(3C)	8986(2)	798(2)	2726(1)	116(5)
C(4C)	9352(2)	701(2)	2643(1)	93(4)
C(5C)	9480(2)	892(2)	2474(1)	62(3)
C(6C)	9241(2)	1181(2)	2387(1)	65(3)
C(7C)	8604(3)	1576(2)	2369(1)	60(3)
C(8C)	9856(3)	761(3)	2376(2)	58(3)
5-dodecoxy moiety				
O(5C)	8874(3)	588(3)	2889(1)	163(5)
C(9C)	8494(6)	671(5)	2971(3)	178(7)
C(10C)	8461(7)	429(7)	3163(3)	259(11)
C(11C)	8391(9)	0(8)	3091(4)	309(14)
C(12C)	8472(19)	-347(12)	3238(6)	681(6)
C(13C)	8450(20)	-764(11)	3338(7)	681(6)
C(14C)	8509(19)	-1178(14)	3243(6)	681(6)
C(15C)	8320(20)	-1487(11)	3384(7)	681(6)
C(16C)	8230(20)	-1876(13)	3269(5)	681(6)
C(17C)	8180(20)	-2278(12)	3377(5)	681(6)
C(18C)	8149(13)	-2655(12)	3247(5)	681(6)
C(19C)	8120(20)	-3083(13)	3327(5)	681(6)
C(20C)	8133(19)	-3420(12)	3172(7)	681(6)

Organic Link D

benzene-1,3-dicarboxylate moiety				
O(1D)	8356(2)	592(2)	1044(1)	73(2)
O(2D)	7983(2)	42(2)	1057(1)	77(2)
O(3D)	8084(2)	1610(2)	559(1)	69(2)
O(4D)	7639(2)	1502(2)	329(1)	80(2)

C(1D)	7804(2)	543(2)	833(1)	69(3)
C(2D)	7916(2)	892(2)	738(1)	74(3)
C(3D)	7685(2)	1042(2)	586(1)	75(3)
C(4D)	7341(2)	842(3)	529(1)	113(5)
C(5D)	7228(2)	494(3)	624(1)	118(5)
C(6D)	7460(3)	344(2)	776(1)	128(5)
C(7D)	8081(3)	368(3)	988(1)	67(3)
C(8D)	7822(3)	1414(3)	476(2)	60(3)
5-dodecoxy moiety				
O(5D)	6893(4)	297(5)	580(2)	265(9)
C(9D)	6538(12)	481(12)	475(6)	410(20)
C(10D)	6180(13)	235(12)	553(6)	420(20)
C(11D)	5782(18)	440(50)	621(19)	1500(200)
C(12D)	5353(19)	459(17)	533(9)	681(6)
C(13D)	4980(20)	720(12)	566(6)	681(6)
C(14D)	4520(20)	680(13)	568(6)	681(6)
C(15D)	4103(17)	570(20)	484(8)	681(6)
C(16D)	3786(18)	560(20)	649(8)	681(6)
C(17D)	3361(18)	528(19)	560(8)	681(6)
C(18D)	2932(19)	696(14)	566(7)	681(6)
C(19D)	2498(15)	793(15)	494(7)	681(6)
C(20D)	2353(15)	1136(16)	365(9)	681(6)

Organic Link E

benzene-1,3-dicarboxylate moiety				
O(1E)	7704(2)	3441(2)	1450(1)	69(2)
O(2E)	7146(2)	3801(2)	1464(1)	69(2)
O(3E)	7975(2)	2420(2)	1944(1)	68(2)
O(4E)	7558(2)	2362(2)	2193(1)	66(2)
C(1E)	7235(2)	3269(2)	1687(1)	57(2)
C(2E)	7492(1)	2991(2)	1770(1)	63(3)
C(3E)	7372(2)	2773(2)	1933(1)	55(2)
C(4E)	6996(2)	2833(2)	2013(1)	71(3)
C(5E)	6740(1)	3111(2)	1930(1)	74(3)
C(6E)	6859(2)	3329(2)	1768(1)	67(3)
C(7E)	7375(3)	3539(3)	1519(1)	56(3)
C(8E)	7673(3)	2496(2)	2033(1)	51(2)
5-dodecoxy moiety				
O(5E)	6364(2)	3184(3)	1990(1)	111(3)
C(9E)	6224(3)	2949(4)	2136(2)	120(5)
C(10E)	5767(4)	2989(6)	2139(3)	197(8)
C(11E)	5538(11)	2641(9)	2046(7)	560(40)
C(12E)	5569(19)	2272(16)	2179(6)	681(6)
C(13E)	5431(17)	1875(10)	2085(8)	681(6)
C(14E)	5242(18)	1540(18)	2206(6)	681(6)
C(15E)	5256(15)	1161(13)	2081(9)	681(6)
C(16E)	4888(17)	1139(18)	1947(9)	681(6)
C(17E)	4921(19)	745(18)	1833(10)	681(6)
C(18E)	4600(20)	511(16)	1718(10)	681(6)
C(19E)	4346(16)	865(15)	1644(9)	681(6)
C(20E)	4169(17)	852(14)	1434(9)	681(6)

Organic Link F

benzene-1,3-dicarboxylate moiety

O(1F)	9268(2)	3836(2)	2217(1)	73(2)
O(2F)	9158(2)	4284(2)	2456(1)	73(2)
O(3F)	8550(2)	2576(2)	2222(1)	75(2)
O(4F)	8147(2)	2434(2)	2470(1)	72(2)
C(1F)	8879(2)	3645(2)	2484(1)	59(2)
C(2F)	8766(2)	3293(2)	2391(1)	66(3)
C(3F)	8529(2)	3019(2)	2490(1)	56(2)
C(4F)	8404(2)	3096(2)	2680(1)	75(3)
C(5F)	8517(2)	3448(2)	2772(1)	73(3)
C(6F)	8754(2)	3722(2)	2674(1)	67(3)
C(7F)	9115(3)	3954(3)	2379(1)	62(3)
C(8F)	8387(3)	2642(2)	2385(1)	52(2)
5-dodecoxy moiety				
O(5F)	8429(2)	3532(2)	2959(1)	97(2)
C(9F)	8235(3)	3235(3)	3076(2)	89(3)
C(10F)	8221(4)	3397(4)	3289(2)	125(5)
C(11F)	8650(5)	3405(8)	3368(4)	260(11)
C(12F)	8801(15)	3355(18)	3580(4)	681(6)
C(13F)	9252(16)	3437(13)	3594(10)	681(6)
C(14F)	9572(15)	3136(15)	3528(10)	681(6)
C(15F)	9987(15)	3251(18)	3607(9)	681(6)
C(16F)	10326(18)	2976(14)	3537(7)	681(6)
C(17F)	10627(17)	3113(13)	3694(6)	681(6)
C(18F)	10985(17)	2874(19)	3621(9)	681(6)
C(19F)	11385(18)	3000(20)	3709(10)	681(6)
C(20F)	11744(19)	2730(20)	3669(9)	681(6)

Coordinating Molecules

DMF				
O(1S)	10275(4)	1249(2)	1832(1)	192(6)
N(1S)	9613(6)	1351(8)	1726(5)	510(14)
C(1S)	9929(6)	1276(8)	1832(3)	510(14)
C(2S)	9730(8)	1746(9)	1617(5)	510(14)
C(3S)	9228(7)	1209(10)	1698(6)	510(14)
Oxygen atoms of water molecules				
O(2S)	9062(3)	1012(2)	1226(2)	167(5)
O(2O)	8838(3)	2208(3)	1838(1)	146(4)
Oxygen atoms of DMFs				
O(3O)	10634(3)	-184(2)	2554(1)	107(3)
O(4O)	7994(3)	-761(2)	1265(1)	106(3)
Octanol				
O(1O)	7461(2)	1887(2)	2574(1)	63(2)
C(1O)	7431(5)	1521(5)	2674(2)	150(6)
C(2O)	7105(13)	1327(17)	2798(8)	681(6)
C(3O)	7175(19)	986(17)	2944(7)	681(6)
C(4O)	7337(18)	669(11)	2805(7)	681(6)
C(5O)	7064(13)	450(20)	2660(10)	681(6)
C(6O)	7332(19)	140(18)	2556(8)	681(6)
C(7O)	7341(16)	-306(16)	2502(9)	681(6)
C(8O)	7010(17)	-430(15)	2356(8)	681(6)

Table S3. Bond lengths [Å] and angles [°] for MOP-18.

Bond lengths

Cu(1)-O(1F)#1	1.944(6)	Cu(1)-O(1A)	1.951(6)	Cu(1)-O(3C)	1.952(6)
Cu(1)-O(3D)#2	1.961(6)	Cu(1)-O(1S)	2.155(7)	Cu(2)-O(4D)#2	1.953(7)
Cu(2)-O(4C)	1.962(7)	Cu(2)-O(2F)#1	1.963(6)	Cu(2)-O(2A)	1.979(6)
Cu(2)-O(3O)	2.209(7)	Cu(3)-O(1E)#2	1.929(6)	Cu(3)-O(1B)	1.941(6)
Cu(3)-O(1D)	1.957(7)	Cu(3)-O(3A)	1.966(6)	Cu(3)-O(2S)	2.149(7)
Cu(4)-O(2D)	1.953(7)	Cu(4)-O(2E)#2	1.960(6)	Cu(4)-O(4A)	1.963(6)
Cu(4)-O(2B)	1.995(6)	Cu(4)-O(4O)	2.174(7)	Cu(5)-O(1C)	1.959(6)
Cu(5)-O(3F)	1.967(6)	Cu(5)-O(3B)	1.974(6)	Cu(5)-O(3E)	1.976(6)
Cu(5)-O(2O)	2.155(7)	Cu(6)-O(2C)	1.923(7)	Cu(6)-O(4E)	1.954(6)
Cu(6)-O(4F)	1.973(7)	Cu(6)-O(4B)	1.985(7)	Cu(6)-O(1O)	2.146(5)
O(1A)-C(7A)	1.206(10)	O(2A)-C(7A)	1.254(10)	O(3A)-C(8A)	1.250(10)
O(4A)-C(8A)	1.236(10)	O(5A)-C(9A)	1.32(2)	O(5A)-C(5A)	1.382(10)
C(1A)-C(2A)	1.3900	C(1A)-C(6A)	1.3900	C(1A)-C(7A)	1.534(10)
C(2A)-C(3A)	1.3900	C(3A)-C(4A)	1.3900	C(3A)-C(8A)	1.510(11)
C(4A)-C(5A)	1.3900	C(5A)-C(6A)	1.3900	O(1B)-C(7B)	1.254(9)
O(2B)-C(7B)	1.242(9)	O(3B)-C(8B)	1.192(9)	O(4B)-C(8B)	1.283(9)
O(5B)-C(5B)	1.337(9)	O(5B)-C(9B)	1.37(2)	C(1B)-C(2B)	1.3900
C(1B)-C(6B)	1.3900	C(1B)-C(7B)	1.511(9)	C(2B)-C(3B)	1.3900
C(3B)-C(4B)	1.3900	C(3B)-C(8B)	1.519(10)	C(4B)-C(5B)	1.3900
C(5B)-C(6B)	1.3900	O(1C)-C(7C)	1.252(10)	O(2C)-C(7C)	1.249(10)
O(3C)-C(8C)	1.275(10)	O(4C)-C(8C)	1.239(9)	O(5C)-C(3C)	1.371(9)
O(5C)-C(9C)	1.422(18)	C(1C)-C(2C)	1.3900	C(1C)-C(6C)	1.3900
C(1C)-C(7C)	1.518(10)	C(2C)-C(3C)	1.3900	C(3C)-C(4C)	1.3900
C(4C)-C(5C)	1.3900	C(5C)-C(6C)	1.3900	C(5C)-C(8C)	1.498(10)
O(1D)-C(7D)	1.248(10)	O(2D)-C(7D)	1.237(10)	O(3D)-C(8D)	1.236(10)
O(3D)-Cu(1)#3	1.961(6)	O(4D)-C(8D)	1.217(10)	O(4D)-Cu(2)#3	1.953(7)
O(5D)-C(5D)	1.338(11)	O(5D)-C(9D)	1.52(4)	C(1D)-C(2D)	1.3900
C(1D)-C(6D)	1.3900	C(1D)-C(7D)	1.526(11)	C(2D)-C(3D)	1.3900
C(3D)-C(4D)	1.3900	C(3D)-C(8D)	1.529(11)	C(4D)-C(5D)	1.3900
C(5D)-C(6D)	1.3900	O(1E)-C(7E)	1.245(9)	O(1E)-Cu(3)#3	1.929(6)
O(2E)-C(7E)	1.228(10)	O(2E)-Cu(4)#3	1.960(6)	O(3E)-C(8E)	1.208(9)
O(4E)-C(8E)	1.240(9)	O(5E)-C(5E)	1.347(8)	O(5E)-C(9E)	1.353(13)
C(1E)-C(2E)	1.3900	C(1E)-C(6E)	1.3900	C(1E)-C(7E)	1.538(9)
C(2E)-C(3E)	1.3900	C(3E)-C(4E)	1.3900	C(3E)-C(8E)	1.535(10)
C(4E)-C(5E)	1.3900	C(5E)-C(6E)	1.3900	O(1F)-C(7F)	1.281(9)
O(1F)-Cu(1)#1	1.944(6)	O(2F)-C(7F)	1.236(10)	O(2F)-Cu(2)#1	1.963(6)
O(3F)-C(8F)	1.258(9)	O(4F)-C(8F)	1.212(9)	O(5F)-C(5F)	1.335(7)
O(5F)-C(9F)	1.435(12)	C(1F)-C(2F)	1.3900	C(1F)-C(6F)	1.3900
C(1F)-C(7F)	1.490(10)	C(2F)-C(3F)	1.3900	C(3F)-C(4F)	1.3900
C(3F)-C(8F)	1.531(10)	C(4F)-C(5F)	1.3900	C(5F)-C(6F)	1.3900
C(9A)-C(10A)	1.553(10)	C(10A)-C(11A)	1.546(10)	C(11A)-C(12A)	1.536(10)
C(12A)-C(13A)	1.537(10)	C(13A)-C(14A)	1.545(10)	C(14A)-C(15A)	1.547(10)
C(15A)-C(16A)	1.535(10)	C(16A)-C(17A)	1.549(10)	C(17A)-C(18A)	1.535(10)
C(18A)-C(19A)	1.536(10)	C(19A)-C(20A)	1.549(10)	C(9B)-C(10B)	1.540(10)
C(10B)-C(11B)	1.545(10)	C(11B)-C(12B)	1.555(9)	C(12B)-C(13B)	1.543(10)
C(13B)-C(14B)	1.551(10)	C(14B)-C(15B)	1.550(10)	C(15B)-C(16B)	1.554(10)
C(16B)-C(17B)	1.617(8)	C(17B)-C(18B)	1.554(10)	C(18B)-C(19B)	1.561(10)
C(19B)-C(20B)	1.552(10)	C(9C)-C(10C)	1.541(10)	C(10C)-C(11C)	1.540(10)
C(11C)-C(12C)	1.564(10)	C(12C)-C(13C)	1.558(10)	C(13C)-C(14C)	1.546(10)

C(14C)-C(15C)	1.554(10)	C(15C)-C(16C)	1.550(10)	C(16C)-C(17C)	1.550(10)
C(17C)-C(18C)	1.550(10)	C(18C)-C(19C)	1.541(10)	C(19C)-C(20C)	1.554(10)
C(9D)-C(10D)	1.552(10)	C(10D)-C(11D)	1.569(9)	C(11D)-C(12D)	1.562(10)
C(12D)-C(13D)	1.547(10)	C(13D)-C(14D)	1.547(8)	C(14D)-C(15D)	1.558(10)
C(15D)-C(16D)	1.547(10)	C(16D)-C(17D)	1.552(9)	C(17D)-C(18D)	1.549(10)
C(18D)-C(19D)	1.572(10)	C(19D)-C(20D)	1.533(10)	C(9E)-C(10E)	1.544(9)
C(10E)-C(11E)	1.538(10)	C(11E)-C(12E)	1.540(10)	C(12E)-C(13E)	1.546(10)
C(13E)-C(14E)	1.533(10)	C(14E)-C(15E)	1.534(10)	C(15E)-C(16E)	1.541(10)
C(16E)-C(17E)	1.538(10)	C(17E)-C(18E)	1.542(10)	C(18E)-C(19E)	1.552(10)
C(19E)-C(20E)	1.553(10)	C(9F)-C(10F)	1.553(9)	C(10F)-C(11F)	1.541(10)
C(11F)-C(12F)	1.541(10)	C(12F)-C(13F)	1.542(10)	C(13F)-C(14F)	1.540(10)
C(14F)-C(15F)	1.545(10)	C(15F)-C(16F)	1.539(10)	C(16F)-C(17F)	1.537(10)
C(17F)-C(18F)	1.530(10)	C(18F)-C(19F)	1.536(10)	C(19F)-C(20F)	1.535(10)
O(1S)-C(1S)	1.167(17)	N(1S)-C(1S)	1.308(15)	N(1S)-C(3S)	1.389(15)
N(1S)-C(2S)	1.572(18)	O(1O)-C(1O)	1.408(15)	C(1O)-C(2O)	1.528(10)
C(2O)-C(3O)	1.536(10)	C(3O)-C(4O)	1.525(10)	C(4O)-C(5O)	1.538(10)
C(5O)-C(6O)	1.544(10)	C(6O)-C(7O)	1.544(10)	C(7O)-C(8O)	1.548(10)

Bond angles

O(1F)#1-Cu(1)-O(1A)	169.7(3)	O(1F)#1-Cu(1)-O(3C)	88.5(3)
O(1A)-Cu(1)-O(3C)	89.8(3)	O(1F)#1-Cu(1)-O(3D)#2	89.9(3)
O(1A)-Cu(1)-O(3D)#2	89.2(3)	O(3C)-Cu(1)-O(3D)#2	165.9(3)
O(1F)#1-Cu(1)-O(1S)	96.3(3)	O(1A)-Cu(1)-O(1S)	94.0(3)
O(3C)-Cu(1)-O(1S)	95.3(4)	O(3D)#2-Cu(1)-O(1S)	98.8(4)
O(4D)#2-Cu(2)-O(4C)	169.9(3)	O(4D)#2-Cu(2)-O(2F)#1	90.9(3)
O(4C)-Cu(2)-O(2F)#1	90.5(3)	O(4D)#2-Cu(2)-O(2A)	88.1(3)
O(4C)-Cu(2)-O(2A)	88.3(3)	O(2F)#1-Cu(2)-O(2A)	167.2(3)
O(4D)#2-Cu(2)-O(3O)	95.2(3)	O(4C)-Cu(2)-O(3O)	94.5(3)
O(2F)#1-Cu(2)-O(3O)	98.8(3)	O(2A)-Cu(2)-O(3O)	94.1(3)
O(1E)#2-Cu(3)-O(1B)	170.3(3)	O(1E)#2-Cu(3)-O(1D)	87.8(3)
O(1B)-Cu(3)-O(1D)	90.4(3)	O(1E)#2-Cu(3)-O(3A)	89.0(3)
O(1B)-Cu(3)-O(3A)	90.1(3)	O(1D)-Cu(3)-O(3A)	164.7(3)
O(1E)#2-Cu(3)-O(2S)	93.2(3)	O(1B)-Cu(3)-O(2S)	96.5(3)
O(1D)-Cu(3)-O(2S)	94.9(4)	O(3A)-Cu(3)-O(2S)	100.2(4)
O(2D)-Cu(4)-O(2E)#2	89.3(3)	O(2D)-Cu(4)-O(4A)	171.4(3)
O(2E)#2-Cu(4)-O(4A)	89.7(3)	O(2D)-Cu(4)-O(2B)	89.5(3)
O(2E)#2-Cu(4)-O(2B)	166.6(3)	O(4A)-Cu(4)-O(2B)	89.5(3)
O(2D)-Cu(4)-O(4O)	95.1(3)	O(2E)#2-Cu(4)-O(4O)	99.1(3)
O(4A)-Cu(4)-O(4O)	93.4(3)	O(2B)-Cu(4)-O(4O)	94.2(3)
O(1C)-Cu(5)-O(3F)	91.0(3)	O(1C)-Cu(5)-O(3B)	88.6(3)
O(3F)-Cu(5)-O(3B)	168.4(2)	O(1C)-Cu(5)-O(3E)	167.9(2)
O(3F)-Cu(5)-O(3E)	88.7(3)	O(3B)-Cu(5)-O(3E)	89.2(3)
O(1C)-Cu(5)-O(2O)	96.1(3)	O(3F)-Cu(5)-O(2O)	95.6(3)
O(3B)-Cu(5)-O(2O)	95.9(3)	O(3E)-Cu(5)-O(2O)	96.0(3)
O(2C)-Cu(6)-O(4E)	168.7(3)	O(2C)-Cu(6)-O(4F)	91.2(3)
O(4E)-Cu(6)-O(4F)	88.7(3)	O(2C)-Cu(6)-O(4B)	88.4(3)
O(4E)-Cu(6)-O(4B)	89.4(3)	O(4F)-Cu(6)-O(4B)	168.5(3)
O(2C)-Cu(6)-O(1O)	94.5(2)	O(4E)-Cu(6)-O(1O)	96.8(2)
O(4F)-Cu(6)-O(1O)	94.7(2)	O(4B)-Cu(6)-O(1O)	96.8(3)
C(7A)-O(1A)-Cu(1)	121.5(6)	C(7A)-O(2A)-Cu(2)	121.2(6)
C(8A)-O(3A)-Cu(3)	122.2(6)	C(8A)-O(4A)-Cu(4)	121.2(6)
C(9A)-O(5A)-C(5A)	112.7(12)	C(2A)-C(1A)-C(6A)	120.0
C(2A)-C(1A)-C(7A)	117.9(6)	C(6A)-C(1A)-C(7A)	122.0(6)

C(1A)-C(2A)-C(3A)	120.0	C(4A)-C(3A)-C(2A)	120.0
C(4A)-C(3A)-C(8A)	119.9(6)	C(2A)-C(3A)-C(8A)	120.0(6)
C(5A)-C(4A)-C(3A)	120.0	O(5A)-C(5A)-C(4A)	124.2(7)
O(5A)-C(5A)-C(6A)	115.7(7)	C(4A)-C(5A)-C(6A)	120.0
C(5A)-C(6A)-C(1A)	120.0	O(1A)-C(7A)-O(2A)	128.5(9)
O(1A)-C(7A)-C(1A)	116.6(8)	O(2A)-C(7A)-C(1A)	114.6(8)
O(4A)-C(8A)-O(3A)	128.0(9)	O(4A)-C(8A)-C(3A)	116.6(8)
O(3A)-C(8A)-C(3A)	115.2(8)	C(7B)-O(1B)-Cu(3)	120.1(5)
C(7B)-O(2B)-Cu(4)	120.7(6)	C(8B)-O(3B)-Cu(5)	122.2(6)
C(8B)-O(4B)-Cu(6)	118.1(6)	C(5B)-O(5B)-C(9B)	116.0(12)
C(2B)-C(1B)-C(6B)	120.0	C(2B)-C(1B)-C(7B)	119.3(5)
C(6B)-C(1B)-C(7B)	120.7(5)	C(3B)-C(2B)-C(1B)	120.0
C(2B)-C(3B)-C(4B)	120.0	C(2B)-C(3B)-C(8B)	117.1(5)
C(4B)-C(3B)-C(8B)	122.7(5)	C(5B)-C(4B)-C(3B)	120.0
O(5B)-C(5B)-C(6B)	112.4(6)	O(5B)-C(5B)-C(4B)	127.6(6)
C(6B)-C(5B)-C(4B)	120.0	C(5B)-C(6B)-C(1B)	120.0
O(2B)-C(7B)-O(1B)	129.5(8)	O(2B)-C(7B)-C(1B)	115.4(7)
O(1B)-C(7B)-C(1B)	114.6(7)	O(3B)-C(8B)-O(4B)	129.5(9)
O(3B)-C(8B)-C(3B)	118.6(7)	O(4B)-C(8B)-C(3B)	111.8(8)
C(7C)-O(1C)-Cu(5)	120.2(6)	C(7C)-O(2C)-Cu(6)	122.2(6)
C(8C)-O(3C)-Cu(1)	123.9(6)	C(8C)-O(4C)-Cu(2)	121.0(6)
C(3C)-O(5C)-C(9C)	117.8(10)	C(2C)-C(1C)-C(6C)	120.0
C(2C)-C(1C)-C(7C)	119.9(5)	C(6C)-C(1C)-C(7C)	120.0(5)
C(1C)-C(2C)-C(3C)	120.0	O(5C)-C(3C)-C(4C)	116.8(6)
O(5C)-C(3C)-C(2C)	123.2(6)	C(4C)-C(3C)-C(2C)	120.0
C(3C)-C(4C)-C(5C)	120.0	C(4C)-C(5C)-C(6C)	120.0
C(4C)-C(5C)-C(8C)	119.8(6)	C(6C)-C(5C)-C(8C)	120.0(6)
C(5C)-C(6C)-C(1C)	120.0	O(2C)-C(7C)-O(1C)	127.7(9)
O(2C)-C(7C)-C(1C)	115.3(8)	O(1C)-C(7C)-C(1C)	116.9(8)
O(4C)-C(8C)-O(3C)	126.3(9)	O(4C)-C(8C)-C(5C)	117.9(8)
O(3C)-C(8C)-C(5C)	115.8(7)	C(7D)-O(1D)-Cu(3)	124.8(6)
C(7D)-O(2D)-Cu(4)	118.5(7)	C(8D)-O(3D)-Cu(1)#3	122.8(6)
C(8D)-O(4D)-Cu(2)#3	121.9(7)	C(5D)-O(5D)-C(9D)	124.3(19)
C(2D)-C(1D)-C(6D)	120.0	C(2D)-C(1D)-C(7D)	118.8(7)
C(6D)-C(1D)-C(7D)	121.0(7)	C(3D)-C(2D)-C(1D)	120.0
C(2D)-C(3D)-C(4D)	120.0	C(2D)-C(3D)-C(8D)	119.5(7)
C(4D)-C(3D)-C(8D)	120.4(7)	C(5D)-C(4D)-C(3D)	120.0
O(5D)-C(5D)-C(4D)	122.6(8)	O(5D)-C(5D)-C(6D)	117.3(8)
C(4D)-C(5D)-C(6D)	120.0	C(5D)-C(6D)-C(1D)	120.0
O(2D)-C(7D)-O(1D)	127.9(10)	O(2D)-C(7D)-C(1D)	116.1(9)
O(1D)-C(7D)-C(1D)	115.5(8)	O(4D)-C(8D)-O(3D)	127.4(9)
O(4D)-C(8D)-C(3D)	117.0(9)	O(3D)-C(8D)-C(3D)	115.3(8)
C(7E)-O(1E)-Cu(3)#3	121.0(6)	C(7E)-O(2E)-Cu(4)#3	121.4(6)
C(8E)-O(3E)-Cu(5)	121.0(6)	C(8E)-O(4E)-Cu(6)	121.1(6)
C(5E)-O(5E)-C(9E)	116.1(8)	C(2E)-C(1E)-C(6E)	120.0
C(2E)-C(1E)-C(7E)	120.7(5)	C(6E)-C(1E)-C(7E)	119.0(5)
C(1E)-C(2E)-C(3E)	120.0	C(4E)-C(3E)-C(2E)	120.0
C(4E)-C(3E)-C(8E)	120.7(5)	C(2E)-C(3E)-C(8E)	119.1(5)
C(3E)-C(4E)-C(5E)	120.0	O(5E)-C(5E)-C(6E)	114.5(5)
O(5E)-C(5E)-C(4E)	125.4(5)	C(6E)-C(5E)-C(4E)	120.0
C(5E)-C(6E)-C(1E)	120.0	O(2E)-C(7E)-O(1E)	129.1(8)
O(2E)-C(7E)-C(1E)	117.4(7)	O(1E)-C(7E)-C(1E)	113.4(8)
O(3E)-C(8E)-O(4E)	129.0(9)	O(3E)-C(8E)-C(3E)	117.0(7)
O(4E)-C(8E)-C(3E)	113.8(7)	C(7F)-O(1F)-Cu(1)#1	121.7(6)

C(7F)-O(2F)-Cu(2)#1	122.6(6)	C(8F)-O(3F)-Cu(5)	120.9(6)
C(8F)-O(4F)-Cu(6)	122.1(6)	C(5F)-O(5F)-C(9F)	118.9(7)
C(2F)-C(1F)-C(6F)	120.0	C(2F)-C(1F)-C(7F)	121.3(5)
C(6F)-C(1F)-C(7F)	118.6(5)	C(3F)-C(2F)-C(1F)	120.0
C(4F)-C(3F)-C(2F)	120.0	C(4F)-C(3F)-C(8F)	119.9(5)
C(2F)-C(3F)-C(8F)	120.0(5)	C(3F)-C(4F)-C(5F)	120.0
O(5F)-C(5F)-C(6F)	116.5(5)	O(5F)-C(5F)-C(4F)	123.4(5)
C(6F)-C(5F)-C(4F)	120.0	C(5F)-C(6F)-C(1F)	120.0
O(2F)-C(7F)-O(1F)	126.8(9)	O(2F)-C(7F)-C(1F)	118.9(7)
O(1F)-C(7F)-C(1F)	114.3(8)	O(4F)-C(8F)-O(3F)	127.6(8)
O(4F)-C(8F)-C(3F)	117.3(7)	O(3F)-C(8F)-C(3F)	115.0(7)
O(5A)-C(9A)-C(10A)	109(2)	C(11A)-C(10A)-C(9A)	109(3)
C(12A)-C(11A)-C(10A)	106(3)	C(11A)-C(12A)-C(13A)	128(5)
C(12A)-C(13A)-C(14A)	129(5)	C(13A)-C(14A)-C(15A)	102.6(15)
C(16A)-C(15A)-C(14A)	99(5)	C(15A)-C(16A)-C(17A)	96(4)
C(18A)-C(17A)-C(16A)	136(6)	C(17A)-C(18A)-C(19A)	129(3)
C(18A)-C(19A)-C(20A)	105(5)	O(5B)-C(9B)-C(10B)	114(2)
C(9B)-C(10B)-C(11B)	117(3)	C(10B)-C(11B)-C(12B)	125(3)
C(13B)-C(12B)-C(11B)	132(5)	C(12B)-C(13B)-C(14B)	110(5)
C(15B)-C(14B)-C(13B)	104.1(14)	C(14B)-C(15B)-C(16B)	102(4)
C(15B)-C(16B)-C(17B)	152(6)	C(18B)-C(17B)-C(16B)	144(6)
C(17B)-C(18B)-C(19B)	140(5)	C(20B)-C(19B)-C(18B)	113.6(17)
O(5C)-C(9C)-C(10C)	107.1(16)	C(11C)-C(10C)-C(9C)	103.6(19)
C(10C)-C(11C)-C(12C)	118(3)	C(13C)-C(12C)-C(11C)	160(6)
C(14C)-C(13C)-C(12C)	128(3)	C(13C)-C(14C)-C(15C)	106.7(14)
C(16C)-C(15C)-C(14C)	109(4)	C(17C)-C(16C)-C(15C)	121(2)
C(16C)-C(17C)-C(18C)	116(2)	C(19C)-C(18C)-C(17C)	124(2)
C(18C)-C(19C)-C(20C)	116(2)	O(5D)-C(9D)-C(10D)	103(3)
C(9D)-C(10D)-C(11D)	122(8)	C(12D)-C(11D)-C(10D)	134(8)
C(13D)-C(12D)-C(11D)	136(5)	C(12D)-C(13D)-C(14D)	139(3)
C(13D)-C(14D)-C(15D)	156(4)	C(16D)-C(15D)-C(14D)	111(5)
C(15D)-C(16D)-C(17D)	111(5)	C(18D)-C(17D)-C(16D)	145(4)
C(17D)-C(18D)-C(19D)	158(4)	C(20D)-C(19D)-C(18D)	129(2)
O(5E)-C(9E)-C(10E)	107.8(12)	C(11E)-C(10E)-C(9E)	115(2)
C(10E)-C(11E)-C(12E)	110(3)	C(11E)-C(12E)-C(13E)	115(2)
C(14E)-C(13E)-C(12E)	122(4)	C(13E)-C(14E)-C(15E)	107.3(15)
C(14E)-C(15E)-C(16E)	110(4)	C(17E)-C(16E)-C(15E)	107(4)
C(16E)-C(17E)-C(18E)	130(5)	C(17E)-C(18E)-C(19E)	99(4)
C(18E)-C(19E)-C(20E)	119(5)	O(5F)-C(9F)-C(10F)	106.9(9)
C(11F)-C(10F)-C(9F)	108.0(14)	C(10F)-C(11F)-C(12F)	130(3)
C(11F)-C(12F)-C(13F)	111(4)	C(14F)-C(13F)-C(12F)	123(2)
C(13F)-C(14F)-C(15F)	111(5)	C(16F)-C(15F)-C(14F)	114(4)
C(17F)-C(16F)-C(15F)	95.3(14)	C(18F)-C(17F)-C(16F)	97.8(13)
C(17F)-C(18F)-C(19F)	114(4)	C(20F)-C(19F)-C(18F)	117(5)
C(1S)-O(1S)-Cu(1)	104.9(12)	C(1S)-N(1S)-C(3S)	140(2)
C(1S)-N(1S)-C(2S)	102.8(14)	C(3S)-N(1S)-C(2S)	117.1(16)
O(1S)-C(1S)-N(1S)	145(2)	C(1O)-O(1O)-Cu(6)	122.4(8)
O(1O)-C(1O)-C(2O)	134(3)	C(1O)-C(2O)-C(3O)	125(5)
C(4O)-C(3O)-C(2O)	100(4)	C(3O)-C(4O)-C(5O)	122(5)
C(4O)-C(5O)-C(6O)	106(2)	C(7O)-C(6O)-C(5O)	141(7)
C(6O)-C(7O)-C(8O)	114(2)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1/2,z+0 #2 -y+5/4,x-3/4,-z+1/4 #3 y+3/4,-x+5/4,-z+1/4

Table S4. Anisotropic displacement parameters ($Å^2$ x 10^3) for MOP-18. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	64(1)	71(1)	49(1)	10(1)	-10(1)	-4(1)
Cu(2)	73(1)	70(1)	54(1)	12(1)	-8(1)	2(1)
Cu(3)	76(1)	64(1)	40(1)	-11(1)	9(1)	-18(1)
Cu(4)	79(1)	65(1)	49(1)	-11(1)	9(1)	-18(1)
Cu(5)	76(1)	57(1)	45(1)	3(1)	25(1)	6(1)
Cu(6)	79(1)	60(1)	47(1)	3(1)	27(1)	8(1)
O(1A)	86(5)	69(5)	60(4)	12(4)	-19(4)	-4(4)
O(2A)	75(5)	71(5)	79(5)	2(4)	-11(4)	-9(4)
O(3A)	75(4)	67(4)	51(4)	-4(3)	-8(3)	-13(4)
O(4A)	90(5)	64(4)	56(4)	-6(3)	-1(4)	-18(4)
O(5A)	334(16)	56(6)	176(10)	-2(6)	-86(10)	-59(8)
C(1A)	78(7)	72(7)	52(6)	7(5)	1(5)	0(6)
C(2A)	74(7)	60(6)	59(6)	4(5)	0(5)	-7(5)
C(3A)	94(8)	60(7)	56(6)	-8(5)	13(6)	-1(6)
C(4A)	115(10)	67(8)	102(9)	-2(7)	-30(8)	-36(7)
C(5A)	127(11)	90(10)	97(10)	5(8)	-37(8)	-19(8)
C(6A)	109(9)	92(9)	75(8)	12(7)	-42(7)	-6(7)
C(7A)	47(6)	61(7)	64(7)	18(5)	-21(5)	13(5)
C(8A)	92(8)	53(6)	41(6)	-7(5)	0(5)	-36(6)
O(1B)	93(5)	53(4)	57(4)	-20(3)	13(4)	-11(4)
O(2B)	83(5)	65(4)	67(4)	-17(4)	25(4)	-20(4)
O(3B)	90(5)	63(4)	47(4)	-11(3)	34(4)	-10(4)
O(4B)	118(6)	67(5)	86(5)	-21(4)	47(5)	-23(4)
O(5B)	162(9)	126(8)	246(12)	-90(8)	147(9)	-54(7)
C(1B)	85(7)	48(6)	74(7)	-18(5)	29(6)	-21(5)
C(2B)	62(6)	73(7)	63(6)	7(5)	23(5)	-19(5)
C(3B)	87(7)	62(7)	62(6)	-5(5)	43(6)	1(6)
C(4B)	158(12)	71(8)	133(11)	-39(8)	98(10)	-37(8)
C(5B)	146(12)	105(10)	158(13)	-61(9)	120(11)	-67(9)
C(6B)	101(9)	108(10)	118(10)	-48(8)	50(8)	-35(8)
C(7B)	80(7)	41(5)	30(5)	-11(4)	5(4)	-29(5)
C(8B)	101(8)	35(5)	64(6)	-7(5)	66(6)	1(5)
O(1C)	82(5)	70(4)	50(4)	7(3)	31(3)	13(4)
O(2C)	103(6)	109(6)	74(5)	34(4)	53(5)	39(5)
O(3C)	68(4)	69(4)	70(4)	16(4)	-2(4)	11(3)
O(4C)	87(5)	84(5)	55(4)	20(4)	-4(4)	6(4)
O(5C)	176(9)	187(10)	127(8)	92(7)	70(7)	103(8)
C(1C)	86(8)	57(6)	66(7)	11(5)	26(6)	18(6)
C(2C)	120(10)	110(9)	69(7)	27(7)	54(7)	33(8)
C(3C)	170(13)	116(10)	64(8)	47(7)	52(8)	68(10)
C(4C)	128(10)	81(8)	71(8)	15(6)	21(7)	29(7)
C(5C)	80(7)	62(6)	44(6)	11(5)	4(5)	15(5)
C(6C)	69(7)	74(7)	51(6)	8(5)	7(5)	-3(6)
C(7C)	85(7)	36(5)	60(6)	-6(5)	38(6)	8(5)
C(8C)	48(6)	50(6)	77(7)	32(5)	-14(5)	-3(5)
O(1D)	100(5)	69(5)	51(4)	2(3)	1(4)	-20(4)
O(2D)	88(5)	76(5)	66(5)	-5(4)	-1(4)	-13(4)

O(3D)	82(5)	69(4)	56(4)	3(3)	-11(4)	-10(4)
O(4D)	96(5)	90(5)	55(4)	6(4)	-17(4)	-6(4)
O(5D)	197(12)	296(17)	304(17)	168(14)	-156(13)	-172(12)
C(1D)	80(8)	72(7)	57(6)	7(6)	2(6)	-16(6)
C(2D)	71(7)	87(8)	64(7)	-17(6)	-2(6)	-3(6)
C(3D)	62(7)	87(8)	76(8)	-6(6)	0(6)	-16(6)
C(4D)	114(11)	142(12)	83(9)	33(8)	-33(8)	-38(9)
C(5D)	113(11)	141(12)	100(10)	30(9)	-41(9)	-50(10)
C(6D)	148(13)	140(12)	96(10)	35(9)	-45(9)	-65(10)
C(7D)	107(9)	54(7)	41(6)	-3(5)	2(6)	-34(6)
C(8D)	74(7)	44(6)	61(7)	-7(5)	-19(6)	16(5)
O(1E)	77(5)	84(5)	46(4)	16(3)	20(3)	26(4)
O(2E)	72(5)	87(5)	47(4)	10(3)	8(3)	23(4)
O(3E)	83(5)	81(5)	40(4)	11(3)	25(3)	18(4)
O(4E)	72(4)	88(5)	38(4)	3(3)	23(3)	17(4)
O(5E)	66(5)	163(8)	105(6)	81(6)	33(4)	16(5)
C(1E)	70(7)	65(6)	35(5)	0(4)	-4(5)	16(5)
C(2E)	70(7)	64(6)	54(6)	-13(5)	9(5)	-1(5)
C(3E)	69(6)	66(6)	30(5)	-1(4)	14(5)	5(5)
C(4E)	88(8)	85(8)	42(6)	0(5)	16(6)	-14(6)
C(5E)	60(7)	111(9)	51(6)	27(6)	15(5)	21(6)
C(6E)	65(7)	85(7)	52(6)	14(5)	2(5)	10(6)
C(7E)	57(6)	93(8)	20(4)	2(5)	13(4)	23(6)
C(8E)	72(6)	26(5)	54(6)	-4(4)	44(5)	-1(4)
O(1F)	88(5)	63(4)	68(4)	-6(3)	25(4)	-6(4)
O(2F)	83(5)	78(5)	58(4)	-14(4)	21(4)	-7(4)
O(3F)	88(5)	72(4)	64(4)	6(3)	41(4)	-11(4)
O(4F)	72(4)	95(5)	49(4)	1(4)	29(3)	-13(4)
O(5F)	126(6)	117(6)	47(4)	-22(4)	28(4)	-41(5)
C(1F)	58(6)	69(7)	51(6)	-18(5)	10(5)	0(5)
C(2F)	72(7)	80(7)	44(6)	6(5)	2(5)	14(6)
C(3F)	66(6)	62(6)	40(5)	7(5)	19(5)	7(5)
C(4F)	87(8)	83(8)	55(6)	16(6)	37(6)	4(6)
C(5F)	84(7)	97(8)	37(6)	-18(6)	17(5)	-23(6)
C(6F)	80(7)	80(7)	42(6)	-14(5)	12(5)	-26(6)
C(7F)	48(6)	87(8)	51(6)	-33(6)	23(5)	-13(5)
C(8F)	69(6)	32(5)	56(6)	10(4)	38(5)	7(4)
O(1S)	440(20)	81(6)	53(5)	15(4)	-31(8)	78(9)
O(2S)	84(6)	64(5)	355(17)	-11(7)	24(7)	-31(5)
O(1O)	72(4)	71(4)	46(4)	9(3)	26(3)	5(3)
O(2O)	113(7)	258(12)	67(5)	24(6)	26(5)	-49(7)
O(3O)	153(7)	105(6)	62(5)	27(4)	-24(5)	-6(5)
O(4O)	126(7)	82(5)	110(6)	-11(4)	-6(5)	-36(5)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for MOP-18.

atom	x	y	z	U_{eq}
H(2AA)	9556	197	1712	77
H(4AA)	9039	-888	1657	113
H(6AA)	9895	-711	2067	111
H(2BA)	8196	1065	1721	79
H(4BA)	7262	970	2094	145
H(6BA)	7459	112	1688	131
H(2CA)	8498	1154	2696	119
H(4CA)	9515	503	2703	112
H(6CA)	9328	1312	2272	77
H(2DA)	8151	1028	777	89
H(4DA)	7183	944	425	135
H(6DA)	7383	106	841	153
H(2EA)	7748	2950	1716	76
H(4EA)	6914	2684	2125	86
H(6EA)	6684	3519	1711	81
H(2FA)	8852	3240	2261	79
H(4FA)	8242	2908	2747	90
H(6FA)	8830	3963	2737	81
H(9AA)	9544	-1483	1699	302
H(9AB)	9082	-1471	1760	302
H(10A)	9656	-1958	1969	417
H(10B)	9182	-1976	1999	417
H(11A)	9123	-2199	1656	481
H(11B)	9601	-2230	1649	481
H(12A)	9150	-2620	1945	817
H(12B)	9608	-2688	1901	817
H(13A)	9482	-3122	1661	817
H(13B)	9026	-3006	1653	817
H(14A)	8852	-3468	1877	817
H(14B)	9294	-3491	1969	817
H(15A)	9082	-3760	1575	817
H(15B)	9539	-3741	1649	817
H(16A)	8932	-4147	1882	817
H(16B)	9410	-4197	1907	817
H(17A)	9383	-4310	1544	817
H(17B)	9351	-4671	1690	817
H(18A)	8762	-4410	1433	817
H(18B)	8681	-4739	1594	817
H(19A)	8939	-5229	1411	817
H(19B)	9201	-4928	1280	817
H(20A)	8559	-5148	1127	817
H(20B)	8638	-4678	1122	817
H(20C)	8344	-4865	1283	817
H(9BA)	6644	718	1993	249
H(9BZ)	6789	493	2187	249
H(10C)	6134	325	2158	374
H(10Z)	6370	-64	2092	374

H(11C)	6254	260	1755	511
H(11Z)	5878	430	1868	511
H(12C)	5532	-75	1813	817
H(12Z)	5845	-156	1645	817
H(13C)	5723	-639	1980	817
H(13D)	6091	-708	1835	817
H(14C)	5283	-902	1766	817
H(14D)	5493	-691	1581	817
H(15B)	6065	-1194	1687	817
H(15C)	5739	-1319	1524	817
H(16C)	5682	-1403	1932	817
H(16D)	5771	-1754	1789	817
H(17C)	5326	-2041	1907	817
H(17D)	5206	-1669	2033	817
H(18B)	4748	-1886	1719	817
H(18C)	4634	-1613	1897	817
H(19B)	4579	-2395	2003	817
H(19Y)	4255	-2048	2020	817
H(20D)	4300	-2638	1734	817
H(20E)	4252	-2205	1638	817
H(20F)	3924	-2367	1788	817
H(9CA)	8281	593	2879	213
H(9CB)	8468	960	2999	213
H(10D)	8710	449	3240	310
H(10E)	8235	523	3244	310
H(11D)	8561	-44	2974	371
H(11E)	8111	-21	3047	371
H(12D)	8766	-340	3227	817
H(12E)	8419	-191	3359	817
H(13E)	8642	-753	3447	817
H(13Q)	8182	-775	3399	817
H(14E)	8796	-1235	3226	817
H(14F)	8379	-1189	3113	817
H(15D)	8501	-1543	3495	817
H(15E)	8066	-1380	3438	817
H(16E)	7988	-1831	3192	817
H(16Q)	8453	-1911	3174	817
H(17E)	7938	-2262	3459	817
H(17Q)	8410	-2314	3467	817
H(18D)	7913	-2616	3163	817
H(18E)	8384	-2651	3159	817
H(19C)	7868	-3108	3402	817
H(19D)	8342	-3126	3421	817
H(20G)	8074	-3676	3234	817
H(20H)	8398	-3431	3112	817
H(20I)	7934	-3367	3070	817
H(9DA)	6564	454	331	498
H(9DB)	6509	767	508	498
H(10F)	6280	78	666	500
H(10G)	6109	41	449	500
H(11F)	5739	329	754	1848
H(11W)	5856	720	640	1848
H(12F)	5402	487	390	817
H(12W)	5251	185	550	817

H(13F)	5021	940	472	817
H(13G)	5034	839	696	817
H(14G)	4459	959	605	817
H(14H)	4497	533	693	817
H(15F)	4024	771	385	817
H(15G)	4117	308	418	817
H(16F)	3807	798	731	817
H(16W)	3836	321	733	817
H(17F)	3422	558	419	817
H(17G)	3307	240	577	817
H(18F)	3005	972	603	817
H(18G)	2855	574	693	817
H(19E)	2407	548	427	817
H(19W)	2337	813	616	817
H(20J)	2249	1028	241	817
H(20K)	2575	1317	337	817
H(20L)	2141	1282	432	817
H(9EA)	6338	3033	2263	144
H(9EB)	6301	2668	2112	144
H(10H)	5679	3017	2277	237
H(10I)	5692	3238	2070	237
H(11G)	5651	2580	1915	678
H(11H)	5254	2715	2029	678
H(12G)	5409	2320	2298	817
H(12V)	5850	2242	2220	817
H(13H)	5239	1945	1981	817
H(13I)	5667	1759	2019	817
H(14I)	4962	1608	2239	817
H(14J)	5391	1501	2330	817
H(15H)	5264	924	2168	817
H(15V)	5502	1161	2001	817
H(16G)	4641	1144	2026	817
H(16H)	4884	1367	1855	817
H(17H)	5027	551	1929	817
H(17V)	5138	789	1737	817
H(18H)	4447	331	1805	817
H(18I)	4718	356	1609	817
H(19F)	4512	1108	1654	817
H(19G)	4121	899	1736	817
H(20M)	3907	981	1433	817
H(20N)	4141	574	1392	817
H(20O)	4348	993	1344	817
H(9FA)	8385	2981	3071	106
H(9FB)	7962	3185	3026	106
H(10J)	8106	3669	3290	150
H(10K)	8052	3223	3371	150
H(11I)	8759	3664	3325	313
H(11Y)	8793	3199	3292	313
H(12H)	8746	3080	3626	817
H(12Y)	8657	3541	3667	817
H(13J)	9302	3685	3520	817
H(13K)	9309	3499	3733	817
H(14K)	9580	3128	3383	817
H(14L)	9500	2867	3576	817

H(15I)	10048	3527	3566	817
H(15J)	9979	3246	3752	817
H(16I)	10258	2690	3549	817
H(16J)	10415	3038	3402	817
H(17I)	10675	3404	3689	817
H(17Y)	10545	3034	3827	817
H(18J)	11001	2899	3477	817
H(18Y)	10941	2589	3652	817
H(19H)	11449	3273	3659	817
H(19I)	11352	3026	3853	817
H(20P)	11991	2885	3682	817
H(20Q)	11724	2623	3536	817
H(20R)	11746	2513	3764	817
H(1SA)	9840	1221	1962	612
H(2SA)	10020	1781	1622	612
H(2SB)	9600	1973	1680	612
H(2SC)	9645	1730	1480	612
H(3SA)	9177	988	1788	612
H(3SB)	9199	1116	1562	612
H(3SC)	9037	1424	1722	612
H(100)	7667	1520	2761	180
H(101)	7489	1320	2572	180
H(102)	6901	1230	2705	817
H(103)	6979	1545	2873	817
H(104)	7372	1060	3046	817
H(105)	6925	900	3008	817
H(106)	7466	463	2888	817
H(107)	7551	796	2728	817
H(108)	6950	638	2564	817
H(109)	6843	316	2730	817
H(110)	7377	268	2428	817
H(111)	7587	172	2628	817
H(112)	7313	-466	2623	817
H(113)	7603	-370	2444	817
H(114)	7117	-623	2263	817
H(115)	6915	-194	2286	817
H(116)	6788	-550	2429	817

Table S6. Torsion angles [°] for IRMOP18.

O(1F)#1-Cu(1)-O(1A)-C(7A)	2(2)	O(3C)-Cu(1)-O(1A)-C(7A)	-79.1(8)
O(3D)#2-Cu(1)-O(1A)-C(7A)	86.8(8)	O(1S)-Cu(1)-O(1A)-C(7A)	-174.4(8)
O(4D)#2-Cu(2)-O(2A)-C(7A)	-90.5(7)	O(4C)-Cu(2)-O(2A)-C(7A)	80.0(7)
O(2F)#1-Cu(2)-O(2A)-C(7A)	-5.0(17)	O(3O)-Cu(2)-O(2A)-C(7A)	174.4(7)
O(1E)#2-Cu(3)-O(3A)-C(8A)	-84.4(7)	O(1B)-Cu(3)-O(3A)-C(8A)	85.9(7)
O(1D)-Cu(3)-O(3A)-C(8A)	-6.2(14)	O(2S)-Cu(3)-O(3A)-C(8A)	-177.5(7)
O(2D)-Cu(4)-O(4A)-C(8A)	6(2)	O(2E)#2-Cu(4)-O(4A)-C(8A)	89.1(7)
O(2B)-Cu(4)-O(4A)-C(8A)	-77.6(7)	O(4O)-Cu(4)-O(4A)-C(8A)	-171.8(7)
C(6A)-C(1A)-C(2A)-C(3A)	0.0	C(7A)-C(1A)-C(2A)-C(3A)	-175.8(7)
C(1A)-C(2A)-C(3A)-C(4A)	0.0	C(1A)-C(2A)-C(3A)-C(8A)	176.1(7)
C(2A)-C(3A)-C(4A)-C(5A)	0.0	C(8A)-C(3A)-C(4A)-C(5A)	-176.1(7)
C(9A)-O(5A)-C(5A)-C(4A)	36(2)	C(9A)-O(5A)-C(5A)-C(6A)	-146.9(15)
C(3A)-C(4A)-C(5A)-O(5A)	177.2(10)	C(3A)-C(4A)-C(5A)-C(6A)	0.0
O(5A)-C(5A)-C(6A)-C(1A)	-177.5(9)	C(4A)-C(5A)-C(6A)-C(1A)	0.0
C(2A)-C(1A)-C(6A)-C(5A)	0.0	C(7A)-C(1A)-C(6A)-C(5A)	175.7(7)
Cu(1)-O(1A)-C(7A)-O(2A)	-10.5(15)	Cu(1)-O(1A)-C(7A)-C(1A)	176.1(5)
Cu(2)-O(2A)-C(7A)-O(1A)	11.7(15)	Cu(2)-O(2A)-C(7A)-C(1A)	-174.7(5)
C(2A)-C(1A)-C(7A)-O(1A)	-14.2(11)	C(6A)-C(1A)-C(7A)-O(1A)	170.0(7)
C(2A)-C(1A)-C(7A)-O(2A)	171.5(6)	C(6A)-C(1A)-C(7A)-O(2A)	-4.3(10)
Cu(4)-O(4A)-C(8A)-O(3A)	-7.8(14)	Cu(4)-O(4A)-C(8A)-C(3A)	176.7(5)
Cu(3)-O(3A)-C(8A)-O(4A)	4.4(14)	Cu(3)-O(3A)-C(8A)-C(3A)	180.0(5)
C(4A)-C(3A)-C(8A)-O(4A)	1.8(10)	C(2A)-C(3A)-C(8A)-O(4A)	-174.3(6)
C(4A)-C(3A)-C(8A)-O(3A)	-174.3(6)	C(2A)-C(3A)-C(8A)-O(3A)	9.6(10)
O(1E)#2-Cu(3)-O(1B)-C(7B)	9(2)	O(1D)-Cu(3)-O(1B)-C(7B)	88.7(7)
O(3A)-Cu(3)-O(1B)-C(7B)	-76.0(7)	O(2S)-Cu(3)-O(1B)-C(7B)	-176.3(7)
O(2D)-Cu(4)-O(2B)-C(7B)	-87.5(7)	O(2E)#2-Cu(4)-O(2B)-C(7B)	-2.6(17)
O(4A)-Cu(4)-O(2B)-C(7B)	84.0(7)	O(4O)-Cu(4)-O(2B)-C(7B)	177.4(7)
O(1C)-Cu(5)-O(3B)-C(8B)	87.3(8)	O(3F)-Cu(5)-O(3B)-C(8B)	-1.1(19)
O(3E)-Cu(5)-O(3B)-C(8B)	-80.8(8)	O(2O)-Cu(5)-O(3B)-C(8B)	-176.7(8)
O(2C)-Cu(6)-O(4B)-C(8B)	-73.5(8)	O(4E)-Cu(6)-O(4B)-C(8B)	95.5(8)
O(4F)-Cu(6)-O(4B)-C(8B)	15(2)	O(1O)-Cu(6)-O(4B)-C(8B)	-167.8(7)
C(6B)-C(1B)-C(2B)-C(3B)	0.0	C(7B)-C(1B)-C(2B)-C(3B)	-176.9(7)
C(1B)-C(2B)-C(3B)-C(4B)	0.0	C(1B)-C(2B)-C(3B)-C(8B)	174.9(7)
C(2B)-C(3B)-C(4B)-C(5B)	0.0	C(8B)-C(3B)-C(4B)-C(5B)	-174.6(8)
C(9B)-O(5B)-C(5B)-C(6B)	-160.4(13)	C(9B)-O(5B)-C(5B)-C(4B)	19(2)
C(3B)-C(4B)-C(5B)-O(5B)	-178.9(12)	C(3B)-C(4B)-C(5B)-C(6B)	0.0
O(5B)-C(5B)-C(6B)-C(1B)	179.1(10)	C(4B)-C(5B)-C(6B)-C(1B)	0.0
C(2B)-C(1B)-C(6B)-C(5B)	0.0	C(7B)-C(1B)-C(6B)-C(5B)	176.9(7)
Cu(4)-O(2B)-C(7B)-O(1B)	7.5(14)	Cu(4)-O(2B)-C(7B)-C(1B)	178.8(5)
Cu(3)-O(1B)-C(7B)-O(2B)	-11.4(14)	Cu(3)-O(1B)-C(7B)-C(1B)	177.2(5)
C(2B)-C(1B)-C(7B)-O(2B)	172.9(6)	C(6B)-C(1B)-C(7B)-O(2B)	-4.0(10)
C(2B)-C(1B)-C(7B)-O(1B)	-14.5(10)	C(6B)-C(1B)-C(7B)-O(1B)	168.6(6)
Cu(5)-O(3B)-C(8B)-O(4B)	5.9(16)	Cu(5)-O(3B)-C(8B)-C(3B)	-179.5(6)
Cu(6)-O(4B)-C(8B)-O(3B)	-13.9(16)	Cu(6)-O(4B)-C(8B)-C(3B)	171.1(6)
C(2B)-C(3B)-C(8B)-O(3B)	8.3(12)	C(4B)-C(3B)-C(8B)-O(3B)	-177.0(8)
C(2B)-C(3B)-C(8B)-O(4B)	-176.2(7)	C(4B)-C(3B)-C(8B)-O(4B)	-1.5(11)
O(3F)-Cu(5)-O(1C)-C(7C)	95.2(7)	O(3B)-Cu(5)-O(1C)-C(7C)	-73.2(7)
O(3E)-Cu(5)-O(1C)-C(7C)	6.7(17)	O(2O)-Cu(5)-O(1C)-C(7C)	-169.1(7)
O(4E)-Cu(6)-O(2C)-C(7C)	10(2)	O(4F)-Cu(6)-O(2C)-C(7C)	-79.2(8)
O(4B)-Cu(6)-O(2C)-C(7C)	89.3(8)	O(1O)-Cu(6)-O(2C)-C(7C)	-174.0(8)

O(1F)#1-Cu(1)-O(3C)-C(8C)	-89.2(7)	O(1A)-Cu(1)-O(3C)-C(8C)	80.7(7)
O(3D)#2-Cu(1)-O(3C)-C(8C)	-5.4(16)	O(1S)-Cu(1)-O(3C)-C(8C)	174.7(7)
O(4D)#2-Cu(2)-O(4C)-C(8C)	-16(2)	O(2F)#1-Cu(2)-O(4C)-C(8C)	82.3(7)
O(2A)-Cu(2)-O(4C)-C(8C)	-85.0(7)	O(3O)-Cu(2)-O(4C)-C(8C)	-178.9(7)
C(6C)-C(1C)-C(2C)-C(3C)	0.0	C(7C)-C(1C)-C(2C)-C(3C)	176.3(7)
C(9C)-O(5C)-C(3C)-C(4C)	-177.4(11)	C(9C)-O(5C)-C(3C)-C(2C)	0.5(17)
C(1C)-C(2C)-C(3C)-O(5C)	-177.8(10)	C(1C)-C(2C)-C(3C)-C(4C)	0.0
O(5C)-C(3C)-C(4C)-C(5C)	178.0(9)	C(2C)-C(3C)-C(4C)-C(5C)	0.0
C(3C)-C(4C)-C(5C)-C(6C)	0.0	C(3C)-C(4C)-C(5C)-C(8C)	-174.5(7)
C(4C)-C(5C)-C(6C)-C(1C)	0.0	C(8C)-C(5C)-C(6C)-C(1C)	174.5(7)
C(2C)-C(1C)-C(6C)-C(5C)	0.0	C(7C)-C(1C)-C(6C)-C(5C)	-176.3(7)
Cu(6)-O(2C)-C(7C)-O(1C)	3.1(15)	Cu(6)-O(2C)-C(7C)-C(1C)	179.2(5)
Cu(5)-O(1C)-C(7C)-O(2C)	-11.9(14)	Cu(5)-O(1C)-C(7C)-C(1C)	172.1(5)
C(2C)-C(1C)-C(7C)-O(2C)	-2.9(10)	C(6C)-C(1C)-C(7C)-O(2C)	173.4(7)
C(2C)-C(1C)-C(7C)-O(1C)	173.6(6)	C(6C)-C(1C)-C(7C)-O(1C)	-10.1(10)
Cu(2)-O(4C)-C(8C)-O(3C)	-0.9(14)	Cu(2)-O(4C)-C(8C)-C(5C)	179.3(5)
Cu(1)-O(3C)-C(8C)-O(4C)	4.4(14)	Cu(1)-O(3C)-C(8C)-C(5C)	-175.7(5)
C(4C)-C(5C)-C(8C)-O(4C)	-0.4(11)	C(6C)-C(5C)-C(8C)-O(4C)	-175.0(7)
C(4C)-C(5C)-C(8C)-O(3C)	179.7(6)	C(6C)-C(5C)-C(8C)-O(3C)	5.2(10)
O(1E)#2-Cu(3)-O(1D)-C(7D)	86.3(8)	O(1B)-Cu(3)-O(1D)-C(7D)	-84.2(8)
O(3A)-Cu(3)-O(1D)-C(7D)	7.9(15)	O(2S)-Cu(3)-O(1D)-C(7D)	179.3(8)
O(2E)#2-Cu(4)-O(2D)-C(7D)	75.1(7)	O(4A)-Cu(4)-O(2D)-C(7D)	8(2)
O(2B)-Cu(4)-O(2D)-C(7D)	91.6(7)	O(4O)-Cu(4)-O(2D)-C(7D)	-174.3(7)
C(6D)-C(1D)-C(2D)-C(3D)	0.0	C(7D)-C(1D)-C(2D)-C(3D)	175.0(7)
C(1D)-C(2D)-C(3D)-C(4D)	0.0	C(1D)-C(2D)-C(3D)-C(8D)	-176.9(7)
C(2D)-C(3D)-C(4D)-C(5D)	0.0	C(8D)-C(3D)-C(4D)-C(5D)	176.9(7)
C(9D)-O(5D)-C(5D)-C(4D)	-20(3)	C(9D)-O(5D)-C(5D)-C(6D)	157(2)
C(3D)-C(4D)-C(5D)-O(5D)	177.4(14)	C(3D)-C(4D)-C(5D)-C(6D)	0.0
O(5D)-C(5D)-C(6D)-C(1D)	-177.6(13)	C(4D)-C(5D)-C(6D)-C(1D)	0.0
C(2D)-C(1D)-C(6D)-C(5D)	0.0	C(7D)-C(1D)-C(6D)-C(5D)	-174.9(7)
Cu(4)-O(2D)-C(7D)-O(1D)	-10.6(15)	Cu(4)-O(2D)-C(7D)-C(1D)	177.8(5)
Cu(3)-O(1D)-C(7D)-O(2D)	5.2(15)	Cu(3)-O(1D)-C(7D)-C(1D)	176.9(5)
C(2D)-C(1D)-C(7D)-O(2D)	-174.5(7)	C(6D)-C(1D)-C(7D)-O(2D)	0.4(11)
C(2D)-C(1D)-C(7D)-O(1D)	12.8(11)	C(6D)-C(1D)-C(7D)-O(1D)	-172.3(7)
Cu(2)#3-O(4D)-C(8D)-O(3D)	8.6(15)	Cu(2)#3-O(4D)-C(8D)-C(3D)	-178.7(5)
Cu(1)#3-O(3D)-C(8D)-O(4D)	-8.4(14)	Cu(1)#3-O(3D)-C(8D)-C(3D)	178.9(5)
C(2D)-C(3D)-C(8D)-O(4D)	170.4(7)	C(4D)-C(3D)-C(8D)-O(4D)	-6.4(11)
C(2D)-C(3D)-C(8D)-O(3D)	-16.0(10)	C(4D)-C(3D)-C(8D)-O(3D)	167.1(7)
O(1C)-Cu(5)-O(3E)-C(8E)	14.1(17)	O(3F)-Cu(5)-O(3E)-C(8E)	-74.6(7)
O(3B)-Cu(5)-O(3E)-C(8E)	94.0(7)	O(2O)-Cu(5)-O(3E)-C(8E)	-170.2(7)
O(2C)-Cu(6)-O(4E)-C(8E)	-1(2)	O(4F)-Cu(6)-O(4E)-C(8E)	88.8(7)
O(4B)-Cu(6)-O(4E)-C(8E)	-79.8(7)	O(1O)-Cu(6)-O(4E)-C(8E)	-176.6(7)
C(6E)-C(1E)-C(2E)-C(3E)	0.0	C(7E)-C(1E)-C(2E)-C(3E)	174.4(6)
C(1E)-C(2E)-C(3E)-C(4E)	0.0	C(1E)-C(2E)-C(3E)-C(8E)	-174.5(6)
C(2E)-C(3E)-C(4E)-C(5E)	0.0	C(8E)-C(3E)-C(4E)-C(5E)	174.4(6)
C(9E)-O(5E)-C(5E)-C(6E)	173.6(8)	C(9E)-O(5E)-C(5E)-C(4E)	-3.9(13)
C(3E)-C(4E)-C(5E)-O(5E)	177.3(8)	C(3E)-C(4E)-C(5E)-C(6E)	0.0
O(5E)-C(5E)-C(6E)-C(1E)	-177.6(7)	C(4E)-C(5E)-C(6E)-C(1E)	0.0
C(2E)-C(1E)-C(6E)-C(5E)	0.0	C(7E)-C(1E)-C(6E)-C(5E)	-174.5(6)
Cu(4)#3-O(2E)-C(7E)-O(1E)	-5.0(14)	Cu(4)#3-O(2E)-C(7E)-C(1E)	179.8(5)
Cu(3)#3-O(1E)-C(7E)-O(2E)	9.3(14)	Cu(3)#3-O(1E)-C(7E)-C(1E)	-175.4(5)
C(2E)-C(1E)-C(7E)-O(2E)	-173.8(6)	C(6E)-C(1E)-C(7E)-O(2E)	0.6(10)
C(2E)-C(1E)-C(7E)-O(1E)	10.3(10)	C(6E)-C(1E)-C(7E)-O(1E)	-175.3(6)
Cu(5)-O(3E)-C(8E)-O(4E)	-10.0(13)	Cu(5)-O(3E)-C(8E)-C(3E)	174.7(5)

Cu(6)-O(4E)-C(8E)-O(3E)	1.3(13)	Cu(6)-O(4E)-C(8E)-C(3E)	176.8(4)
C(4E)-C(3E)-C(8E)-O(3E)	171.3(6)	C(2E)-C(3E)-C(8E)-O(3E)	-14.3(9)
C(4E)-C(3E)-C(8E)-O(4E)	-4.8(9)	C(2E)-C(3E)-C(8E)-O(4E)	169.7(6)
O(1C)-Cu(5)-O(3F)-C(8F)	-80.0(7)	O(3B)-Cu(5)-O(3F)-C(8F)	8.2(18)
O(3E)-Cu(5)-O(3F)-C(8F)	87.9(7)	O(2O)-Cu(5)-O(3F)-C(8F)	-176.2(7)
O(2C)-Cu(6)-O(4F)-C(8F)	95.5(7)	O(4E)-Cu(6)-O(4F)-C(8F)	-73.2(7)
O(4B)-Cu(6)-O(4F)-C(8F)	8(2)	O(1O)-Cu(6)-O(4F)-C(8F)	-169.9(7)
C(6F)-C(1F)-C(2F)-C(3F)	0.0	C(7F)-C(1F)-C(2F)-C(3F)	-176.9(7)
C(1F)-C(2F)-C(3F)-C(4F)	0.0	C(1F)-C(2F)-C(3F)-C(8F)	176.7(6)
C(2F)-C(3F)-C(4F)-C(5F)	0.0	C(8F)-C(3F)-C(4F)-C(5F)	-176.7(6)
C(9F)-O(5F)-C(5F)-C(6F)	-171.1(7)	C(9F)-O(5F)-C(5F)-C(4F)	4.8(11)
C(3F)-C(4F)-C(5F)-O(5F)	-175.8(8)	C(3F)-C(4F)-C(5F)-C(6F)	0.0
O(5F)-C(5F)-C(6F)-C(1F)	176.0(7)	C(4F)-C(5F)-C(6F)-C(1F)	0.0
C(2F)-C(1F)-C(6F)-C(5F)	0.0	C(7F)-C(1F)-C(6F)-C(5F)	177.0(7)
Cu(2)#1-O(2F)-C(7F)-O(1F)	3.1(15)	Cu(2)#1-O(2F)-C(7F)-C(1F)	-179.8(5)
Cu(1)#1-O(1F)-C(7F)-O(2F)	-2.1(14)	Cu(1)#1-O(1F)-C(7F)-C(1F)	-179.3(5)
C(2F)-C(1F)-C(7F)-O(2F)	169.4(7)	C(6F)-C(1F)-C(7F)-O(2F)	-7.5(11)
C(2F)-C(1F)-C(7F)-O(1F)	-13.1(10)	C(6F)-C(1F)-C(7F)-O(1F)	170.0(6)
Cu(6)-O(4F)-C(8F)-O(3F)	-12.3(14)	Cu(6)-O(4F)-C(8F)-C(3F)	171.4(5)
Cu(5)-O(3F)-C(8F)-O(4F)	3.4(14)	Cu(5)-O(3F)-C(8F)-C(3F)	179.8(5)
C(4F)-C(3F)-C(8F)-O(4F)	4.3(10)	C(2F)-C(3F)-C(8F)-O(4F)	-172.4(6)
C(4F)-C(3F)-C(8F)-O(3F)	-172.5(6)	C(2F)-C(3F)-C(8F)-O(3F)	10.8(10)
C(5A)-O(5A)-C(9A)-C(10A)	171.8(19)	O(5A)-C(9A)-C(10A)-C(11A)	-171(2)
C(9A)-C(10A)-C(11A)-C(12A)	-172(3)	C(10A)-C(11A)-C(12A)-C(13A)	170(7)
C(11A)-C(12A)-C(13A)-C(14A)	-166(6)	C(12A)-C(13A)-C(14A)-C(15A)	-156(7)
C(13A)-C(14A)-C(15A)-C(16A)	173(6)	C(14A)-C(15A)-C(16A)-C(17A)	165(6)
C(15A)-C(16A)-C(17A)-C(18A)	-95(11)	C(16A)-C(17A)-C(18A)-C(19A)	-172(6)
C(17A)-C(18A)-C(19A)-C(20A)	-157(8)	C(5B)-O(5B)-C(9B)-C(10B)	165.3(19)
O(5B)-C(9B)-C(10B)-C(11B)	-72(4)	C(9B)-C(10B)-C(11B)-C(12B)	146(4)
C(10B)-C(11B)-C(12B)-C(13B)	-19(11)	C(11B)-C(12B)-C(13B)-C(14B)	-171(6)
C(12B)-C(13B)-C(14B)-C(15B)	140(5)	C(13B)-C(14B)-C(15B)-C(16B)	97(5)
C(14B)-C(15B)-C(16B)-C(17B)	60(10)	C(15B)-C(16B)-C(17B)-C(18B)	6(14)
C(16B)-C(17B)-C(18B)-C(19B)	162(6)	C(17B)-C(18B)-C(19B)-C(20B)	-131(7)
C(3C)-O(5C)-C(9C)-C(10C)	-174.4(14)	O(5C)-C(9C)-C(10C)-C(11C)	-75(2)
C(9C)-C(10C)-C(11C)-C(12C)	162(3)	C(10C)-C(11C)-C(12C)-C(13C)	155(11)
C(11C)-C(12C)-C(13C)-C(14C)	53(19)	C(12C)-C(13C)-C(14C)-C(15C)	-161(7)
C(13C)-C(14C)-C(15C)-C(16C)	160(6)	C(14C)-C(15C)-C(16C)-C(17C)	159(6)
C(15C)-C(16C)-C(17C)-C(18C)	-173(5)	C(16C)-C(17C)-C(18C)-C(19C)	177(6)
C(17C)-C(18C)-C(19C)-C(20C)	-174(6)	C(5D)-O(5D)-C(9D)-C(10D)	-152(3)
O(5D)-C(9D)-C(10D)-C(11D)	135(6)	C(9D)-C(10D)-C(11D)-C(12D)	108(18)
C(10D)-C(11D)-C(12D)-C(13D)	-164(10)	C(11D)-C(12D)-C(13D)-C(14D)	-144(12)
C(12D)-C(13D)-C(14D)-C(15D)	-55(11)	C(13D)-C(14D)-C(15D)-C(16D)	164(7)
C(14D)-C(15D)-C(16D)-C(17D)	169(5)	C(15D)-C(16D)-C(17D)-C(18D)	-132(10)
C(16D)-C(17D)-C(18D)-C(19D)	160(9)	C(17D)-C(18D)-C(19D)-C(20D)	-83(15)
C(5E)-O(5E)-C(9E)-C(10E)	-163.1(11)	O(5E)-C(9E)-C(10E)-C(11E)	102(3)
C(9E)-C(10E)-C(11E)-C(12E)	71(5)	C(10E)-C(11E)-C(12E)-C(13E)	-168(5)
C(11E)-C(12E)-C(13E)-C(14E)	-148(6)	C(12E)-C(13E)-C(14E)-C(15E)	-164(5)
C(13E)-C(14E)-C(15E)-C(16E)	-87(7)	C(14E)-C(15E)-C(16E)-C(17E)	-178(5)
C(15E)-C(16E)-C(17E)-C(18E)	163(7)	C(16E)-C(17E)-C(18E)-C(19E)	32(11)
C(17E)-C(18E)-C(19E)-C(20E)	141(5)	C(5F)-O(5F)-C(9F)-C(10F)	173.1(9)
O(5F)-C(9F)-C(10F)-C(11F)	-68.8(15)	C(9F)-C(10F)-C(11F)-C(12F)	-150(4)
C(10F)-C(11F)-C(12F)-C(13F)	-173(3)	C(11F)-C(12F)-C(13F)-C(14F)	-77(9)
C(12F)-C(13F)-C(14F)-C(15F)	-165(5)	C(13F)-C(14F)-C(15F)-C(16F)	-177(6)
C(14F)-C(15F)-C(16F)-C(17F)	-164(6)	C(15F)-C(16F)-C(17F)-C(18F)	-176(5)

C(16F)-C(17F)-C(18F)-C(19F)	166(6)	C(17F)-C(18F)-C(19F)-C(20F)	170(5)
O(1F)#1-Cu(1)-O(1S)-C(1S)	-120.4(15)	O(1A)-Cu(1)-O(1S)-C(1S)	58.9(16)
O(3C)-Cu(1)-O(1S)-C(1S)	-31.3(16)	O(3D)#2-Cu(1)-O(1S)-C(1S)	148.8(15)
Cu(1)-O(1S)-C(1S)-N(1S)	-150(4)	C(3S)-N(1S)-C(1S)-O(1S)	138(6)
C(2S)-N(1S)-C(1S)-O(1S)	-49(5)	O(2C)-Cu(6)-O(1O)-C(1O)	-30.1(10)
O(4E)-Cu(6)-O(1O)-C(1O)	149.1(9)	O(4F)-Cu(6)-O(1O)-C(1O)	-121.7(9)
O(4B)-Cu(6)-O(1O)-C(1O)	58.8(10)	Cu(6)-O(1O)-C(1O)-C(2O)	-159(4)
O(1O)-C(1O)-C(2O)-C(3O)	-161(4)	C(1O)-C(2O)-C(3O)-C(4O)	-61(8)
C(2O)-C(3O)-C(4O)-C(5O)	-73(7)	C(3O)-C(4O)-C(5O)-C(6O)	-177(4)
C(4O)-C(5O)-C(6O)-C(7O)	131(6)	C(5O)-C(6O)-C(7O)-C(8O)	64(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y+1/2,z+0 #2 -y+5/4,x-3/4,-z+1/4 #3 y+3/4,-x+5/4,-z+1/4

Modeling X-Ray Data.

In order to find out the reasonable structural model of the ambiguous coordinating ligands in the X-ray structure, modeling studies by using Forcite program in the MS Modeling package 4.0 (Accelrys) was performed. In the crystal structure refinement processes only the structural models of a DMF and an octanol were incorporated based on the electron densities in the difference Fourier maps. As there should be six coordinating ligands in the asymmetric unit, the remaining four oxygen atoms attached to the copper atoms had possibilities of the oxygen atoms in DMF, octanol, or water molecules. A DMF inside MOP-18 had been included in the refinement processes, and the remaining two oxygen atoms could be originated from water or DMF molecules; due to the limited volume inside MOP-18, the octanol was excluded from the candidates. However, when a coordinating oxygen atom was replaced with a DMF by using MS Modeling program, bad non-bonded contacts with the already-present DMF molecule was found. Therefore two oxygen atoms inside MOP-18 were designated as water molecules. As the EA and TGA analyses indicated that two coordinating water molecules per asymmetric unit, which are 8 H_2O in MOP-18, the remaining two oxygen atoms outside MOP-18 were regarded as DMF oxygen atoms. Through these procedures the initial structural model was established for the geometry optimization calculation which was carried out by Forcite program in MS Modeling package. The original space group and unit cell parameters were maintained during the calculation, and the fractional coordinates of copper atoms were not allowed to move during the optimization processes. Universal force-field and SMART algorithm were used for the energy and geometry optimization, and the maximum iteration number was 3000. Although the calculation accuracy was not so high, the resulting structure was sufficiently reasonable without strange bond geometry and bad non-bonding contacts. As the guest molecules in the void space between MOP-18s were not included in the structural model, the conformation of the terminal alkyl chains in the organic links were slightly changed compared to the initial crystal structure. The conditions and results of the calculation have been listed in the following ***Table S7***. The optimized structure of MOP-18 has been also presented as various drawings in ***Figures S4 and S5***. The final atomic coordinates with the SHELX res format have been also listed in ***Table S8***.

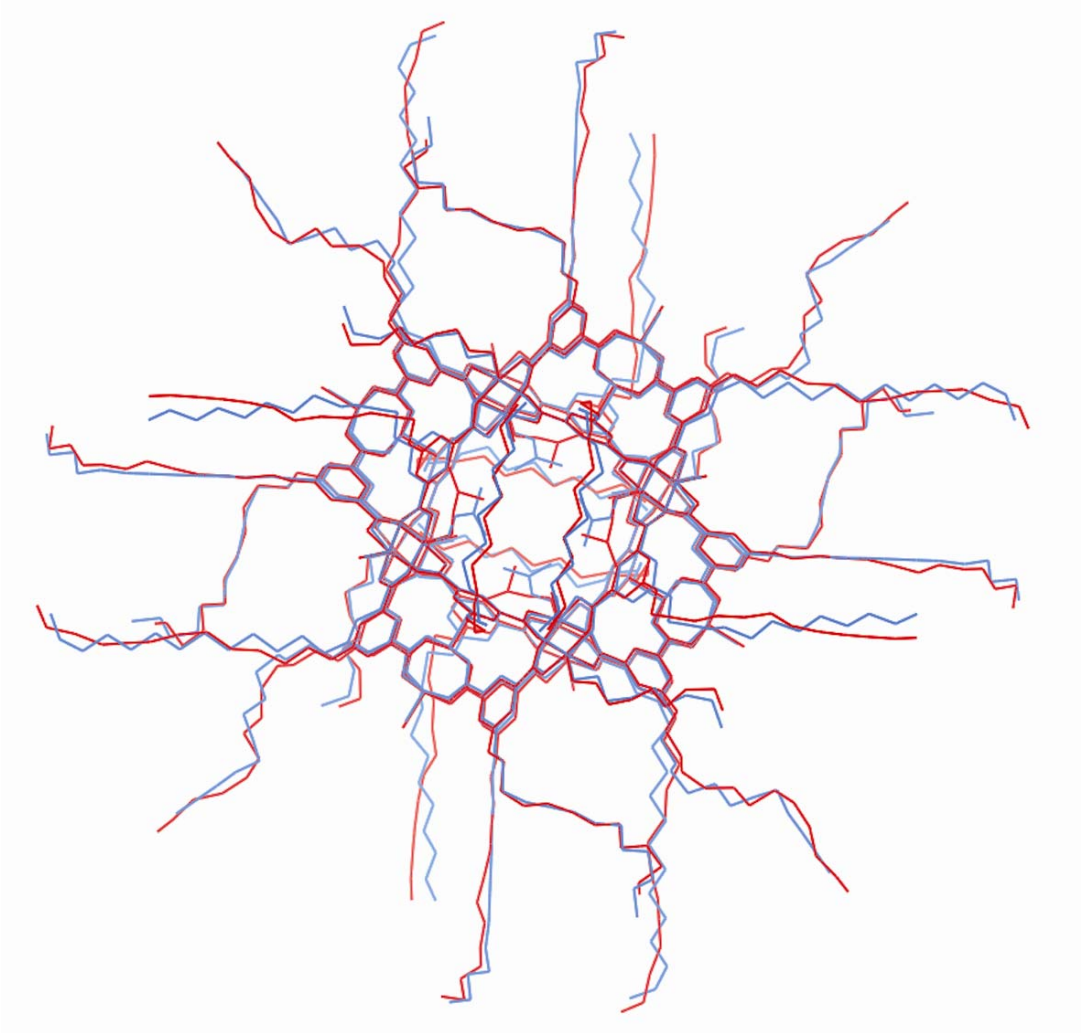

Figure S4. Superposition of two structural models; red: X-ray structure, blue: geometry-optimized structure by Forcite program. The supersposition was calculated by 'Superpose Structures' utility in MS Modeling package. To match the exact number of atoms, the C and N atoms of 8 DMF molecules outside MOP-18 were removed in the geometry-optimized model (Blue). The calculated RMS was 0.713 Å.

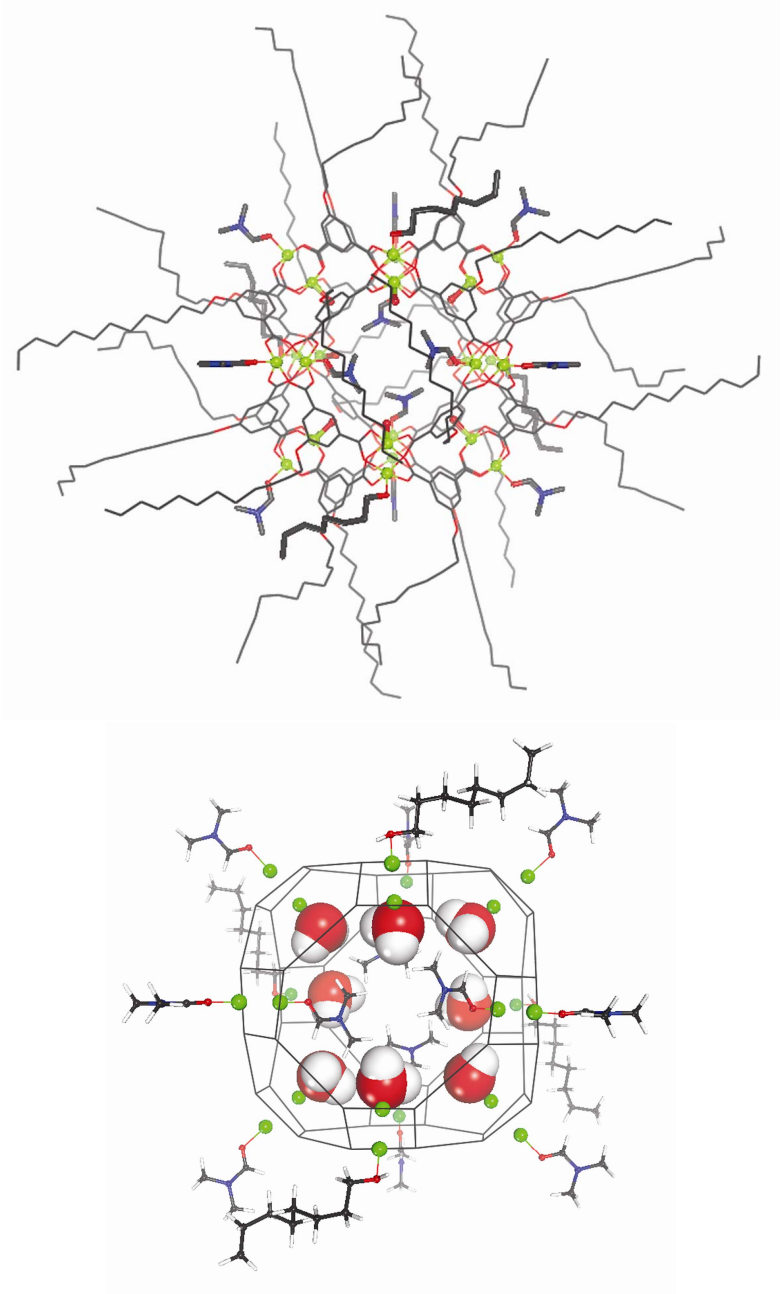

Figure S5. (Top) Molecular Structure of MOP-18 after geometry minimization with the incorporated ligand models (2 DMF and 2 H_2O molecules per asymmetric unit). The ligands (12 DMF, 4 octanol, and 8 H_2O molecules) were shown as sticks and the framework organic links as lines. (Bottom) The ligands were highlighted without the MOP-18 framework links which are represneted as polyhedron. Water molecules were drawn as CPK models to show the volume they occupy inside MOP-18. Copper atoms are shown as green balls.

Table S7. The conditions and results of the Forcite calculation in the MS Modeling package.

Forcite

Task : Geometry Optimization

Version : 4.0

---- Geometry optimization parameters ----

Algorithm : Smart

Convergence tolerance:

Energy : 0.001 kcal/mol

Force : 0.5 kcal/mol/A

Maximum number of iterations : 3000

External pressure : 0 GPa

Motion groups rigid : NO

Optimize cell : NO

---- Energy parameters ----

Forcefield : Universal

Electrostatic terms:

Summation method : Ewald

Accuracy : 0.001 kcal/mol

Buffer width : 0.5 A

van der Waals terms:

Summation method : Ewald

Accuracy : 0.001 kcal/mol

Repulsive cutoff : 6 A

Buffer width : 0.5 A

---- Initial structure ----

Total enthalpy : 5038500675.236310 kcal/mol

External pressure term : 0.000000 kcal/mol

Total energy : 5038500675.236310 kcal/mol

Contributions to total energy (kcal/mol):

Valence energy (diag. terms) : 17764.656

Bond : 1541.467

Angle : 15132.519

Torsion	:	1083.505
Inversion	:	7.165
Valence energy (cross terms)	:	0.000
Stretch-Stretch	:	0.000
Stretch-Bend-Stretch	:	0.000
Stretch-Torsion-Stretch	:	0.000
Separated-Stretch-Stretch	:	0.000
Torsion-Stretch	:	0.000
Bend-Bend	:	0.000
Torsion-Bend-Bend	:	0.000
Bend-Torsion-Bend	:	0.000
Non-bond energy	:	5038482910.580
Hydrogen bond	:	0.000
van der Waals	:	5038482910.580
Electrostatic	:	0.000

rms force : 3.598E+008 kcal/mol A
max force : 7.494E+009 kcal/mol A

Cell parameters: a: 33.571500 A b: 33.571500 A c: 68.246800 A
alpha: 90.000 deg beta: 90.000 deg gamma: 90.000 deg

---- Final structure ----

Total enthalpy	: 14633.168641 kcal/mol
External pressure term	: 0.000000 kcal/mol
Total energy	: 14633.168641 kcal/mol

Contributions to total energy (kcal/mol):

Valence energy (diag. terms)	:	15930.968
Bond	:	529.704
Angle	:	14513.235
Torsion	:	882.778
Inversion	:	5.250
Valence energy (cross terms)	:	0.000
Stretch-Stretch	:	0.000
Stretch-Bend-Stretch	:	0.000

Stretch-Torsion-Stretch	:	0.000
Separated-Stretch-Stretch	:	0.000
Torsion-Stretch	:	0.000
Bend-Bend	:	0.000
Torsion-Bend-Bend	:	0.000
Bend-Torsion-Bend	:	0.000
Non-bond energy	:	-1297.799
Hydrogen bond	:	0.000
van der Waals	:	-1297.799
Electrostatic	:	0.000

rms force : 4.584E-002 kcal/mol A
max force : 3.707E-001 kcal/mol A

Cell parameters: a: 33.571500 A b: 33.571500 A c: 68.246800 A
alpha: 90.000 deg beta: 90.000 deg gamma: 90.000 deg

Termination status : Normal

Table S8. Geometry-optimized atomic coordinates (x 10^4) for MOP-18. The coordinates were saved to a SHELX res file by MS Modeling program.

```
TITL MOP-18 geometry optimized
CELL    0.0000   33.5715   33.5715   68.2468   90.0000   90.0000   90.0000
LATT 2
SYMM -X+1/2,-Y,Z+1/2
SYMM -Y+3/4,X+1/4,Z+1/4
SYMM Y+3/4,-X+3/4,Z+3/4
SFAC  C Cu  H  N  O
CU1   2     1.04075    0.08114    0.20566    1.00000    0.06375    0.07104 =
                0.04895    0.00972   -0.01013   -0.00348
CU2   2     1.05403    0.02856    0.23343    1.00000    0.07307    0.07040 =
                0.05358    0.01174   -0.00796    0.00181
CU3   2     0.87181    0.04872    0.12359    1.00000    0.07595    0.06419 =
                0.03945   -0.01097    0.00943   -0.01764
CU4   2     0.83331   -0.01946    0.12395    1.00000    0.07865    0.06529 =
                0.04889   -0.01119    0.00917   -0.01816
CU5   2     0.84116    0.20676    0.20724    1.00000    0.07545    0.05658 =
                0.04457    0.00288    0.02485    0.00551
CU6   2     0.78711    0.19508    0.23487    1.00000    0.07940    0.06012 =
                0.04730    0.00308    0.02725    0.00800
O7    5     1.01099    0.04461    0.19238    1.00000    0.08568    0.06911 =
                0.06033    0.01156   -0.01905   -0.00356
O8    5     1.02018    0.00128    0.21572    1.00000    0.07484    0.07053 =
                0.07914    0.00158   -0.01127   -0.00865
O9    5     0.90138    0.02184    0.14263    1.00000    0.07471    0.06697 =
                0.05122   -0.00441   -0.00772   -0.01323
O10   5     0.86997   -0.03476    0.14260    1.00000    0.09030    0.06405 =
                0.05634   -0.00633   -0.00140   -0.01783
O11   5     0.94284   -0.12146    0.19358    1.00000    0.33396    0.05618 =
                0.17611   -0.00226   -0.08566   -0.05926
C12   1     0.97598   -0.01654    0.18954    1.00000    0.07847    0.07176 =
                0.05249    0.00736    0.00099   -0.00019
C13   1     0.95259   -0.00305    0.17371    1.00000    0.07355    0.06044 =
                0.05890    0.00351    0.00009   -0.00657
H14   3     0.95538    0.02749    0.16878    1.00000    0.07716
C15   1     0.92445   -0.02824    0.16476    1.00000    0.09429    0.06048 =
                0.05611   -0.00799    0.01263   -0.00090
C16   1     0.92109   -0.06776    0.17130    1.00000    0.11530    0.06655 =
                0.10166   -0.00189   -0.02980   -0.03650
H17   3     0.89907   -0.08696    0.16467    1.00000    0.11340
C18   1     0.94526   -0.08210    0.18661    1.00000    0.12685    0.09022 =
                0.09748    0.00455   -0.03698   -0.01913
C19   1     0.97130   -0.05590    0.19609    1.00000    0.10948    0.09206 =
                0.07513    0.01216   -0.04189   -0.00621
H20   3     0.98858   -0.06676    0.20839    1.00000    0.11067
C21   1     1.00394    0.01095    0.19961    1.00000    0.04740    0.06061 =
                0.06377    0.01754   -0.02136    0.01283
C22   1     0.89749   -0.01309    0.14918    1.00000    0.09234    0.05334 =
                0.04060   -0.00652    0.00003   -0.03554
O23   5     0.83763    0.06574    0.14272    1.00000    0.09250    0.05334 =
                0.05699   -0.01964    0.01279   -0.01070
```

O24	5	0.80637	0.00913	0.14335	1.00000	0.08257	0.06494 =
		0.06736	-0.01710	0.02537	-0.02015		
O25	5	0.82047	0.15814	0.19918	1.00000	0.08961	0.06299 =
		0.04734	-0.01085	0.03387	-0.00986		
O26	5	0.76663	0.15846	0.21681	1.00000	0.11805	0.06666 =
		0.08559	-0.02096	0.04710	-0.02264		
O27	5	0.69167	0.03036	0.19159	1.00000	0.16180	0.12553 =
		0.24592	-0.09015	0.14716	-0.05382		
C28	1	0.78541	0.05893	0.16591	1.00000	0.08522	0.04824 =
		0.07411	-0.01756	0.02903	-0.02120		
C29	1	0.79588	0.09342	0.17634	1.00000	0.06214	0.07343 =
		0.06271	0.00664	0.02273	-0.01930		
H30	3	0.82296	0.10895	0.17232	1.00000	0.07931	
C31	1	0.77274	0.10773	0.19210	1.00000	0.08711	0.06162 =
		0.06182	-0.00502	0.04317	0.00110		
C32	1	0.73741	0.08757	0.19733	1.00000	0.15836	0.07118 =
		0.13264	-0.03877	0.09765	-0.03686		
H33	3	0.71995	0.09801	0.20963	1.00000	0.14487	
C34	1	0.72547	0.05319	0.18698	1.00000	0.14635	0.10518 =
		0.15838	-0.06090	0.12023	-0.06655		
C35	1	0.75098	0.03828	0.17113	1.00000	0.10116	0.10837 =
		0.11780	-0.04783	0.04970	-0.03549		
H36	3	0.74230	0.01142	0.16344	1.00000	0.13093	
C37	1	0.81094	0.04400	0.14986	1.00000	0.08008	0.04141 =
		0.02994	-0.01102	0.00520	-0.02915		
C38	1	0.78700	0.14315	0.20322	1.00000	0.10146	0.03466 =
		0.06355	-0.00683	0.06644	0.00068		
O39	5	0.87767	0.18216	0.22510	1.00000	0.08184	0.06965 =
		0.05016	0.00688	0.03123	0.01346		
O40	5	0.82492	0.15671	0.24166	1.00000	0.10347	0.10893 =
		0.07391	0.03371	0.05274	0.03887		
O41	5	0.99799	0.09051	0.22255	1.00000	0.06822	0.06883 =
		0.06980	0.01554	-0.00156	0.01098		
O42	5	1.00879	0.04700	0.24557	1.00000	0.08693	0.08431 =
		0.05460	0.01961	-0.00397	0.00565		
O43	5	0.87840	0.03614	0.28193	1.00000	0.17635	0.18670 =
		0.12651	0.09169	0.07022	0.10329		
C44	1	0.88582	0.12150	0.24594	1.00000	0.08556	0.05714 =
		0.06578	0.01087	0.02625	0.01805		
C45	1	0.86928	0.09494	0.25975	1.00000	0.11960	0.11019 =
		0.06880	0.02726	0.05438	0.03337		
H46	3	0.83850	0.09876	0.26393	1.00000	0.11944	
C47	1	0.89233	0.06365	0.26780	1.00000	0.16965	0.11615 =
		0.06359	0.04695	0.05195	0.06769		
C48	1	0.93160	0.05881	0.26140	1.00000	0.12839	0.08068 =
		0.07060	0.01519	0.02112	0.02911		
H49	3	0.94882	0.03426	0.26726	1.00000	0.11187	
C50	1	0.94814	0.08384	0.24707	1.00000	0.08025	0.06216 =
		0.04408	0.01052	0.00409	0.01488		
C51	1	0.92528	0.11564	0.23971	1.00000	0.06896	0.07383 =
		0.05092	0.00762	0.00661	-0.00328		
H52	3	0.93779	0.13507	0.22863	1.00000	0.07748	
C53	1	0.86135	0.15424	0.23749	1.00000	0.08501	0.03614 =
		0.06016	-0.00581	0.03835	0.00810		

C54 1 0.98722 0.07382 0.23825 1.00000 0.04760 0.05027 =
0.07713 0.03167 -0.01425 -0.00283
O55 5 0.83381 0.05970 0.10473 1.00000 0.09985 0.06893 =
0.05119 0.00150 0.00122 -0.02003
O56 5 0.80096 0.00390 0.10489 1.00000 0.08783 0.07638 =
0.06631 -0.00486 -0.00105 -0.01263
O57 5 0.80663 0.16356 0.05391 1.00000 0.08168 0.06921 =
0.05572 0.00349 -0.01093 -0.00951
O58 5 0.76352 0.15153 0.03093 1.00000 0.09581 0.09036 =
0.05460 0.00632 -0.01731 -0.00611
O59 5 0.67855 0.03768 0.06254 1.00000 0.19667 0.29595 =
0.30357 0.16792 -0.15581 -0.17230
C60 1 0.77926 0.05519 0.08283 1.00000 0.07978 0.07202 =
0.05665 0.00658 0.00185 -0.01597
C61 1 0.79059 0.08973 0.07254 1.00000 0.07115 0.08670 =
0.06393 -0.01692 -0.00156 -0.00279
H62 3 0.81924 0.10329 0.07553 1.00000 0.08871
C63 1 0.76587 0.10638 0.05805 1.00000 0.06187 0.08739 =
0.07590 -0.00605 0.00008 -0.01576
C64 1 0.72856 0.08899 0.05446 1.00000 0.11374 0.14166 =
0.08257 0.03269 -0.03265 -0.03772
H65 3 0.70924 0.10189 0.04350 1.00000 0.13519
C66 1 0.71617 0.05523 0.06514 1.00000 0.11336 0.14126 =
0.09968 0.02957 -0.04068 -0.04991
C67 1 0.74221 0.03779 0.07871 1.00000 0.14760 0.13980 =
0.09628 0.03482 -0.04460 -0.06549
H68 3 0.73265 0.01153 0.08664 1.00000 0.15347
C69 1 0.80584 0.03858 0.09819 1.00000 0.10702 0.05375 =
0.04073 -0.00265 0.00227 -0.03423
C70 1 0.77912 0.14216 0.04706 1.00000 0.07413 0.04355 =
0.06086 -0.00683 -0.01874 0.01608
O71 5 0.77667 0.34703 0.14528 1.00000 0.07680 0.08360 =
0.04631 0.01581 0.02035 0.02609
O72 5 0.72000 0.37868 0.14534 1.00000 0.07233 0.08713 =
0.04729 0.01042 0.00843 0.02265
O73 5 0.80028 0.23471 0.19509 1.00000 0.08337 0.08147 =
0.03964 0.01149 0.02479 0.01846
O74 5 0.75963 0.23186 0.21990 1.00000 0.07167 0.08802 =
0.03759 0.00349 0.02321 0.01745
O75 5 0.63459 0.30710 0.19487 1.00000 0.06646 0.16312 =
0.10491 0.08059 0.03275 0.01611
C76 1 0.72807 0.32452 0.16759 1.00000 0.07021 0.06493 =
0.03454 -0.00045 -0.00446 0.01562
C77 1 0.75436 0.29730 0.17633 1.00000 0.07013 0.06449 =
0.05439 -0.01313 0.00911 -0.00050
H78 3 0.78486 0.29471 0.17131 1.00000 0.07560
C79 1 0.74103 0.27366 0.19330 1.00000 0.06943 0.06598 =
0.03002 -0.00117 0.01374 0.00464
C80 1 0.70246 0.28009 0.20034 1.00000 0.08814 0.08452 =
0.04161 -0.00011 0.01564 -0.01405
H81 3 0.69383 0.26560 0.21356 1.00000 0.08571
C82 1 0.67542 0.30474 0.19029 1.00000 0.06043 0.11110 =
0.05079 0.02681 0.01476 0.02108
C83 1 0.68860 0.32662 0.17417 1.00000 0.06486 0.08517 =

		0.05192	0.01437	0.00225	0.01031		
H84	3	0.66756	0.34574	0.16677	1.00000	0.08078	
C85	1	0.74206	0.35120	0.15190	1.00000	0.05678	0.09264 =
		0.01960	0.00238	0.01341	0.02257		
C86	1	0.76822	0.24528	0.20316	1.00000	0.07249	0.02558 =
		0.05357	-0.00426	0.04374	-0.00131		
O87	5	0.92746	0.38373	0.21905	1.00000	0.08756	0.06253 =
		0.06759	-0.00634	0.02543	-0.00642		
O88	5	0.91835	0.42652	0.24264	1.00000	0.08288	0.07805 =
		0.05800	-0.01402	0.02078	-0.00710		
O89	5	0.85044	0.25331	0.22088	1.00000	0.08800	0.07201 =
		0.06365	0.00577	0.04148	-0.01142		
O90	5	0.81477	0.23777	0.24639	1.00000	0.07157	0.09480 =
		0.04946	0.00074	0.02858	-0.01313		
O91	5	0.84602	0.35120	0.29590	1.00000	0.12556	0.11674 =
		0.04725	-0.02241	0.02840	-0.04100		
C92	1	0.88795	0.36256	0.24612	1.00000	0.05764	0.06870 =
		0.05069	-0.01824	0.01013	-0.00004		
C93	1	0.87681	0.32615	0.23740	1.00000	0.07235	0.08031 =
		0.04428	0.00617	0.00159	0.01371		
H94	3	0.88641	0.31956	0.22260	1.00000	0.07878	
C95	1	0.85191	0.29905	0.24742	1.00000	0.06582	0.06247 =
		0.03956	0.00724	0.01949	0.00742		
C96	1	0.83917	0.30870	0.26641	1.00000	0.08706	0.08292 =
		0.05465	0.01641	0.03686	0.00433		
H97	3	0.81817	0.28985	0.27365	1.00000	0.08985	
C98	1	0.85319	0.34299	0.27598	1.00000	0.08440	0.09718 =
		0.03738	-0.01776	0.01746	-0.02297		
C99	1	0.87613	0.37030	0.26548	1.00000	0.07963	0.08037 =
		0.04190	-0.01426	0.01162	-0.02630		
H100	3	0.88614	0.39707	0.27282	1.00000	0.08076	
C101	1	0.91242	0.39227	0.23539	1.00000	0.04828	0.08655 =
		0.05066	-0.03277	0.02311	-0.01343		
C102	1	0.83844	0.26152	0.23786	1.00000	0.06866	0.03184 =
		0.05610	0.01002	0.03766	0.00659		
C103	1	0.93951	-0.15205	0.17907	1.00000	0.25130	
H104	3	0.96472	-0.14972	0.16854	1.00000	0.30156	
H105	3	0.91084	-0.14968	0.17107	1.00000	0.30156	
C106	1	0.94092	-0.19266	0.18910	1.00000	0.34782	
H107	3	0.96896	-0.19501	0.19768	1.00000	0.41738	
H108	3	0.91534	-0.19497	0.19940	1.00000	0.41738	
C109	1	0.93892	-0.22667	0.17412	1.00000	0.40052	
H110	3	0.91134	-0.22358	0.16524	1.00000	0.48062	
H111	3	0.96507	-0.22489	0.16416	1.00000	0.48062	
C112	1	0.93865	-0.26721	0.18444	1.00000	0.68069	
H113	3	0.91207	-0.26905	0.19414	1.00000	0.81683	
H114	3	0.96579	-0.26999	0.19367	1.00000	0.81683	
C115	1	0.93751	-0.30160	0.16966	1.00000	0.68069	
H116	3	0.96444	-0.30037	0.16018	1.00000	0.81683	
H117	3	0.91067	-0.29851	0.16023	1.00000	0.81683	
C118	1	0.93608	-0.34180	0.18030	1.00000	0.68069	
H119	3	0.90903	-0.34292	0.18970	1.00000	0.81683	
H120	3	0.96275	-0.34473	0.18987	1.00000	0.81683	
C121	1	0.93518	-0.37667	0.16581	1.00000	0.68069	

H122	3	0.90980	-0.37256	0.15555	1.00000	0.81683
H123	3	0.96336	-0.37695	0.15724	1.00000	0.81683
C124	1	0.93032	-0.41637	0.17676	1.00000	0.68069
H125	3	0.90064	-0.41772	0.18385	1.00000	0.81683
H126	3	0.95273	-0.41797	0.18866	1.00000	0.81683
C127	1	0.93600	-0.45285	0.16349	1.00000	0.68069
H128	3	0.96567	-0.45140	0.15630	1.00000	0.81683
H129	3	0.93569	-0.47978	0.17295	1.00000	0.81683
C130	1	0.90310	-0.45689	0.14801	1.00000	0.68069
H131	3	0.90503	-0.43173	0.13749	1.00000	0.81683
H132	3	0.87346	-0.45601	0.15526	1.00000	0.81683
C133	1	0.90736	-0.49610	0.13671	1.00000	0.68069
H134	3	0.90534	-0.52164	0.14704	1.00000	0.81683
H135	3	0.93691	-0.49708	0.12936	1.00000	0.81683
C136	1	0.87485	-0.50038	0.12125	1.00000	0.68069
H137	3	0.87882	-0.52905	0.11339	1.00000	0.81683
H138	3	0.87667	-0.47570	0.11045	1.00000	0.81683
H139	3	0.84496	-0.50019	0.12823	1.00000	0.81683
C140	1	0.65769	0.05076	0.19912	1.00000	0.20766
H141	3	0.65551	0.08119	0.19296	1.00000	0.24919
H142	3	0.66001	0.05245	0.21532	1.00000	0.24919
C143	1	0.62004	0.02771	0.19353	1.00000	0.31125
H144	3	0.59509	0.03744	0.20312	1.00000	0.37350
H145	3	0.62535	-0.00449	0.19606	1.00000	0.37350
C146	1	0.60865	0.03522	0.17202	1.00000	0.42556
H147	3	0.63504	0.03129	0.16235	1.00000	0.51067
H148	3	0.59898	0.06675	0.17062	1.00000	0.51067
C149	1	0.57436	0.00841	0.16499	1.00000	0.68069
H150	3	0.55124	0.00576	0.17658	1.00000	0.81683
H151	3	0.56032	0.02317	0.15213	1.00000	0.81683
C152	1	0.58876	-0.03326	0.15882	1.00000	0.68069
H153	3	0.59921	-0.04967	0.17196	1.00000	0.81683
H154	3	0.61414	-0.03017	0.14846	1.00000	0.81683
C155	1	0.55518	-0.05679	0.14874	1.00000	0.68069
H156	3	0.53048	-0.06216	0.15921	1.00000	0.81683
H157	3	0.54285	-0.03833	0.13664	1.00000	0.81683
C158	1	0.56977	-0.09615	0.13959	1.00000	0.68069
H159	3	0.59682	-0.09005	0.13067	1.00000	0.81683
H160	3	0.54701	-0.10714	0.12911	1.00000	0.81683
C161	1	0.57981	-0.12908	0.15454	1.00000	0.68069
H162	3	0.60177	-0.11756	0.16528	1.00000	0.81683
H163	3	0.59480	-0.15387	0.14663	1.00000	0.81683
C164	1	0.54377	-0.14616	0.16573	1.00000	0.68069
H165	3	0.55544	-0.16770	0.17669	1.00000	0.81683
H166	3	0.52828	-0.12233	0.17402	1.00000	0.81683
C167	1	0.51408	-0.16802	0.15236	1.00000	0.68069
H168	3	0.53041	-0.18990	0.14315	1.00000	0.81683
H169	3	0.49893	-0.14624	0.14263	1.00000	0.81683
C170	1	0.48241	-0.19005	0.16441	1.00000	0.68069
H171	3	0.49703	-0.21263	0.17390	1.00000	0.81683
H172	3	0.46630	-0.16857	0.17395	1.00000	0.81683
C173	1	0.45229	-0.21098	0.15118	1.00000	0.68069
H174	3	0.46763	-0.23215	0.14122	1.00000	0.81683
H175	3	0.43562	-0.18878	0.14232	1.00000	0.81683

H176	3	0.43074	-0.22794	0.16028	1.00000	0.81683
C177	1	0.83901	0.04020	0.28966	1.00000	0.17784
H178	3	0.81708	0.02844	0.27897	1.00000	0.21341
H179	3	0.83252	0.07196	0.29300	1.00000	0.21341
C180	1	0.83578	0.01803	0.30923	1.00000	0.25854
H181	3	0.86383	0.02252	0.31746	1.00000	0.31025
H182	3	0.81113	0.03151	0.31789	1.00000	0.31025
C183	1	0.82811	-0.02690	0.30741	1.00000	0.30876
H184	3	0.85049	-0.04060	0.29748	1.00000	0.37051
H185	3	0.79786	-0.03165	0.30119	1.00000	0.37051
C186	1	0.83110	-0.04615	0.32787	1.00000	0.68069
H187	3	0.86267	-0.04621	0.33281	1.00000	0.81683
H188	3	0.81411	-0.02762	0.33849	1.00000	0.81683
C189	1	0.81391	-0.08844	0.32899	1.00000	0.68069
H190	3	0.81020	-0.09594	0.34476	1.00000	0.81683
H191	3	0.78391	-0.08912	0.32221	1.00000	0.81683
C192	1	0.84054	-0.12009	0.31937	1.00000	0.68069
H193	3	0.87179	-0.11655	0.32449	1.00000	0.81683
H194	3	0.83976	-0.11621	0.30320	1.00000	0.81683
C195	1	0.82583	-0.16199	0.32484	1.00000	0.68069
H196	3	0.82929	-0.16637	0.34091	1.00000	0.81683
H197	3	0.79372	-0.16462	0.32116	1.00000	0.81683
C198	1	0.84865	-0.19479	0.31398	1.00000	0.68069
H199	3	0.84386	-0.19121	0.29795	1.00000	0.81683
H200	3	0.88105	-0.19202	0.31707	1.00000	0.81683
C201	1	0.83403	-0.23609	0.32049	1.00000	0.68069
H202	3	0.80108	-0.23761	0.31890	1.00000	0.81683
H203	3	0.84161	-0.24062	0.33620	1.00000	0.81683
C204	1	0.85283	-0.26942	0.30822	1.00000	0.68069
H205	3	0.84509	-0.26477	0.29253	1.00000	0.81683
H206	3	0.88580	-0.26834	0.30976	1.00000	0.81683
C207	1	0.83766	-0.31040	0.31483	1.00000	0.68069
H208	3	0.80454	-0.31089	0.31463	1.00000	0.81683
H209	3	0.84778	-0.31636	0.33007	1.00000	0.81683
C210	1	0.85292	-0.34344	0.30143	1.00000	0.68069
H211	3	0.84242	-0.37276	0.30691	1.00000	0.81683
H212	3	0.88599	-0.34357	0.30108	1.00000	0.81683
H213	3	0.84140	-0.33911	0.28632	1.00000	0.81683
C214	1	0.64542	0.06435	0.06125	1.00000	0.41469
H215	3	0.64573	0.08033	0.04699	1.00000	0.49763
H216	3	0.64648	0.08608	0.07354	1.00000	0.49763
C217	1	0.60688	0.04042	0.06295	1.00000	0.41628
H218	3	0.60691	0.02448	0.07724	1.00000	0.49954
H219	3	0.60598	0.01799	0.05096	1.00000	0.49954
C220	1	0.56993	0.06723	0.06175	1.00000	1.53974
H221	3	0.57080	0.08953	0.07380	1.00000	1.84769
H222	3	0.57003	0.08335	0.04751	1.00000	1.84769
C223	1	0.53167	0.04243	0.06349	1.00000	0.68069
H224	3	0.53181	0.01886	0.05203	1.00000	0.81683
H225	3	0.53083	0.02776	0.07810	1.00000	0.81683
C226	1	0.49435	0.06833	0.06095	1.00000	0.68069
H227	3	0.49556	0.08333	0.04643	1.00000	0.81683
H228	3	0.49366	0.09158	0.07255	1.00000	0.81683
C229	1	0.45636	0.04296	0.06224	1.00000	0.68069

H230	3	0.45372	0.03036	0.07725	1.00000	0.81683
H231	3	0.45850	0.01786	0.05165	1.00000	0.81683
C232	1	0.41911	0.06765	0.05748	1.00000	0.68069
H233	3	0.41670	0.09282	0.06799	1.00000	0.81683
H234	3	0.42206	0.08008	0.04244	1.00000	0.81683
C235	1	0.38122	0.04210	0.05869	1.00000	0.68069
H236	3	0.37599	0.03336	0.07418	1.00000	0.81683
H237	3	0.38528	0.01455	0.04985	1.00000	0.81683
C238	1	0.34477	0.06481	0.05096	1.00000	0.68069
H239	3	0.34129	0.09293	0.05937	1.00000	0.81683
H240	3	0.34974	0.07239	0.03529	1.00000	0.81683
C241	1	0.30665	0.03972	0.05294	1.00000	0.68069
H242	3	0.29878	0.03638	0.06869	1.00000	0.81683
H243	3	0.31220	0.00940	0.04695	1.00000	0.81683
C244	1	0.27124	0.05755	0.04166	1.00000	0.68069
H245	3	0.27930	0.06179	0.02600	1.00000	0.81683
H246	3	0.24614	0.03603	0.04220	1.00000	0.81683
C247	1	0.25696	0.09707	0.05025	1.00000	0.68069
H248	3	0.22891	0.10624	0.04290	1.00000	0.81683
H249	3	0.27950	0.12073	0.04781	1.00000	0.81683
H250	3	0.25110	0.09397	0.06617	1.00000	0.81683
C251	1	0.62132	0.29442	0.21378	1.00000	0.12010
H252	3	0.63298	0.31515	0.22504	1.00000	0.14412
H253	3	0.63118	0.26375	0.21719	1.00000	0.14412
C254	1	0.57588	0.29456	0.21407	1.00000	0.19739
H255	3	0.56505	0.29537	0.22947	1.00000	0.23687
H256	3	0.56525	0.32210	0.20677	1.00000	0.23687
C257	1	0.55901	0.25805	0.20324	1.00000	0.56497
H258	3	0.57911	0.24930	0.19100	1.00000	0.67796
H259	3	0.53021	0.26629	0.19649	1.00000	0.67796
C260	1	0.55242	0.22262	0.21714	1.00000	0.68069
H261	3	0.52704	0.22932	0.22701	1.00000	0.81683
H262	3	0.57913	0.21802	0.22646	1.00000	0.81683
C263	1	0.54421	0.18424	0.20570	1.00000	0.68069
H264	3	0.52330	0.19021	0.19346	1.00000	0.81683
H265	3	0.57277	0.17387	0.19939	1.00000	0.81683
C266	1	0.52704	0.15155	0.21896	1.00000	0.68069
H267	3	0.49740	0.16069	0.22462	1.00000	0.81683
H268	3	0.54639	0.14792	0.23192	1.00000	0.81683
C269	1	0.52402	0.11133	0.20828	1.00000	0.68069
H270	3	0.52289	0.08722	0.21943	1.00000	0.81683
H271	3	0.55089	0.10616	0.19909	1.00000	0.81683
C272	1	0.48628	0.10914	0.19572	1.00000	0.68069
H273	3	0.46004	0.11152	0.20559	1.00000	0.81683
H274	3	0.48582	0.13458	0.18534	1.00000	0.81683
C275	1	0.48391	0.07011	0.18403	1.00000	0.68069
H276	3	0.49336	0.04490	0.19353	1.00000	0.81683
H277	3	0.50453	0.07141	0.17129	1.00000	0.81683
C278	1	0.44129	0.06146	0.17704	1.00000	0.68069
H279	3	0.42117	0.06207	0.18991	1.00000	0.81683
H280	3	0.44027	0.03093	0.17074	1.00000	0.81683
C281	1	0.42652	0.09121	0.16159	1.00000	0.68069
H282	3	0.44329	0.08670	0.14773	1.00000	0.81683
H283	3	0.43110	0.12221	0.16672	1.00000	0.81683

C284	1	0.38217	0.08598	0.15763	1.00000	0.68069
H285	3	0.37263	0.10627	0.14568	1.00000	0.81683
H286	3	0.36482	0.09300	0.17103	1.00000	0.81683
H287	3	0.37566	0.05496	0.15318	1.00000	0.81683
C288	1	0.83237	0.31980	0.30836	1.00000	0.08851
H289	3	0.84980	0.29209	0.30581	1.00000	0.10621
H290	3	0.80036	0.31390	0.30543	1.00000	0.10621
C291	1	0.83735	0.33226	0.32982	1.00000	0.12492
H292	3	0.82199	0.36120	0.33220	1.00000	0.14990
H293	3	0.82297	0.30961	0.33933	1.00000	0.14990
C294	1	0.88158	0.33609	0.33529	1.00000	0.26048
H295	3	0.89519	0.35986	0.32615	1.00000	0.31258
H296	3	0.89675	0.30740	0.33213	1.00000	0.31258
C297	1	0.88743	0.34648	0.35701	1.00000	0.68069
H298	3	0.87799	0.32103	0.36632	1.00000	0.81683
H299	3	0.86823	0.37240	0.36072	1.00000	0.81683
C300	1	0.93082	0.35778	0.36176	1.00000	0.68069
H301	3	0.94124	0.38102	0.35133	1.00000	0.81683
H302	3	0.93146	0.37106	0.37669	1.00000	0.81683
C303	1	0.95936	0.32194	0.36132	1.00000	0.68069
H304	3	0.95893	0.30785	0.34660	1.00000	0.81683
H305	3	0.94961	0.29970	0.37235	1.00000	0.81683
C306	1	1.00212	0.33488	0.36605	1.00000	0.68069
H307	3	1.01148	0.35769	0.35522	1.00000	0.81683
H308	3	1.00297	0.34843	0.38090	1.00000	0.81683
C309	1	1.03119	0.29960	0.36520	1.00000	0.68069
H310	3	1.02158	0.27640	0.37577	1.00000	0.81683
H311	3	1.03090	0.28670	0.35018	1.00000	0.81683
C312	1	1.07362	0.31262	0.37053	1.00000	0.68069
H313	3	1.08231	0.33843	0.36138	1.00000	0.81683
H314	3	1.07434	0.32204	0.38613	1.00000	0.81683
C315	1	1.10379	0.27898	0.36722	1.00000	0.68069
H316	3	1.10402	0.27078	0.35142	1.00000	0.81683
H317	3	1.09493	0.25250	0.37593	1.00000	0.81683
C318	1	1.14564	0.29182	0.37358	1.00000	0.68069
H319	3	1.15364	0.32069	0.36667	1.00000	0.81683
H320	3	1.14601	0.29576	0.38969	1.00000	0.81683
C321	1	1.17685	0.26083	0.36801	1.00000	0.68069
H322	3	1.20655	0.27051	0.37337	1.00000	0.81683
H323	3	1.17822	0.25753	0.35185	1.00000	0.81683
H324	3	1.16956	0.23162	0.37471	1.00000	0.81683
O325	5	1.03235	0.11938	0.18631	1.00000	0.44139	0.08120 =
		0.05275	0.01452	-0.03113	0.07838		
N326	4	0.99483	0.15852	0.16668	1.00000	0.50976
C327	1	0.99932	0.13014	0.18103	1.00000	0.50976
H328	3	0.97338	0.11684	0.18782	1.00000	0.61171
C329	1	1.02902	0.17781	0.15719	1.00000	0.50976
H330	3	1.05794	0.16694	0.16300	1.00000	0.61171
H331	3	1.02756	0.21049	0.15961	1.00000	0.61171
H332	3	1.02828	0.17182	0.14119	1.00000	0.61171
C333	1	0.95492	0.17051	0.16034	1.00000	0.50976
H334	3	0.93124	0.15394	0.16829	1.00000	0.61171
H335	3	0.95143	0.16465	0.14442	1.00000	0.61171
H336	3	0.95070	0.20285	0.16306	1.00000	0.61171

O337	5	0.89997	0.09713	0.12307	1.00000	0.08367	0.06387 =
		0.35472	-0.01109	0.02423	-0.03143		
O338	5	0.74876	0.18621	0.25479	1.00000	0.07212	0.07093 =
		0.04639	0.00931	0.02564	0.00548		
O339	5	0.87839	0.21315	0.18689	1.00000	0.11338	0.25817 =
		0.06699	0.02365	0.02631	-0.04929		
C340	1	0.75412	0.14811	0.26295	1.00000	0.15007	
H341	3	0.77994	0.14783	0.27323	1.00000	0.18008	
H342	3	0.75994	0.12668	0.25094	1.00000	0.18008	
C343	1	0.71623	0.13517	0.27366	1.00000	0.68069	
H344	3	0.69222	0.13113	0.26277	1.00000	0.81683	
H345	3	0.70687	0.15927	0.28384	1.00000	0.81683	
C346	1	0.72107	0.09656	0.28555	1.00000	0.68069	
H347	3	0.74204	0.10223	0.29785	1.00000	0.81683	
H348	3	0.69178	0.08890	0.29211	1.00000	0.81683	
C349	1	0.73637	0.06060	0.27377	1.00000	0.68069	
H350	3	0.73982	0.03528	0.28411	1.00000	0.81683	
H351	3	0.76630	0.06758	0.26784	1.00000	0.81683	
C352	1	0.70867	0.04814	0.25688	1.00000	0.68069	
H353	3	0.70577	0.07330	0.24642	1.00000	0.81683	
H354	3	0.67845	0.04142	0.26261	1.00000	0.81683	
C355	1	0.72566	0.01249	0.24535	1.00000	0.68069	
H356	3	0.71299	0.01240	0.23032	1.00000	0.81683	
H357	3	0.75835	0.01635	0.24355	1.00000	0.81683	
C358	1	0.71758	-0.02806	0.25506	1.00000	0.68069	
H359	3	0.72276	-0.02657	0.27110	1.00000	0.81683	
H360	3	0.73887	-0.05020	0.24896	1.00000	0.81683	
C361	1	0.67538	-0.04306	0.25104	1.00000	0.68069	
H362	3	0.67100	-0.07235	0.25830	1.00000	0.81683	
H363	3	0.67055	-0.04684	0.23505	1.00000	0.81683	
H364	3	0.65294	-0.02196	0.25687	1.00000	0.81683	
H365	3	0.75569	0.20535	0.26518	1.00000	0.00000	
H366	3	0.87195	0.23903	0.18070	1.00000	0.00000	
H367	3	0.90424	0.21782	0.19349	1.00000	0.00000	
H368	3	0.87964	0.11805	0.12089	1.00000	0.00000	
H369	3	0.90914	0.10142	0.13670	1.00000	0.00000	
O370	5	0.80510	0.43267	0.87464	1.00000	0.08120	0.44139 =
		0.05275	-0.03113	-0.01452	-0.07838		
N371	4	0.74801	0.39766	0.87008	1.00000	0.50976	
C372	1	0.76894	0.43252	0.87254	1.00000	0.50976	
H373	3	0.75330	0.46073	0.87246	1.00000	0.61171	
C374	1	0.76769	0.35887	0.86795	1.00000	0.50976	
H375	3	0.80058	0.36170	0.86693	1.00000	0.61171	
H376	3	0.76012	0.33963	0.88064	1.00000	0.61171	
H377	3	0.75712	0.34401	0.85438	1.00000	0.61171	
C378	1	0.70447	0.39870	0.86856	1.00000	0.50976	
H379	3	0.69118	0.37906	0.87990	1.00000	0.61171	
H380	3	0.69251	0.42926	0.87071	1.00000	0.61171	
H381	3	0.69511	0.38804	0.85386	1.00000	0.61171	
O382	5	0.43688	0.50941	0.24717	1.00000	0.08120	0.44139 =
		0.05275	-0.03113	-0.01452	-0.07838		
N383	4	0.42520	0.57274	0.23725	1.00000	0.50976	
C384	1	0.43187	0.54440	0.25141	1.00000	0.50976	
H385	3	0.43245	0.55290	0.26671	1.00000	0.61171	

C386	1	0.42585	0.56341	0.21626	1.00000	0.50976
H387	3	0.43435	0.53200	0.21341	1.00000	0.61171
H388	3	0.39595	0.56896	0.20987	1.00000	0.61171
H389	3	0.44784	0.58279	0.20871	1.00000	0.61171
C390	1	0.41681	0.61394	0.24297	1.00000	0.50976
H391	3	0.41766	0.61793	0.25914	1.00000	0.61171
H392	3	0.43924	0.63417	0.23633	1.00000	0.61171
H393	3	0.38670	0.62253	0.23775	1.00000	0.61171

END

Powder X-ray Diffraction.

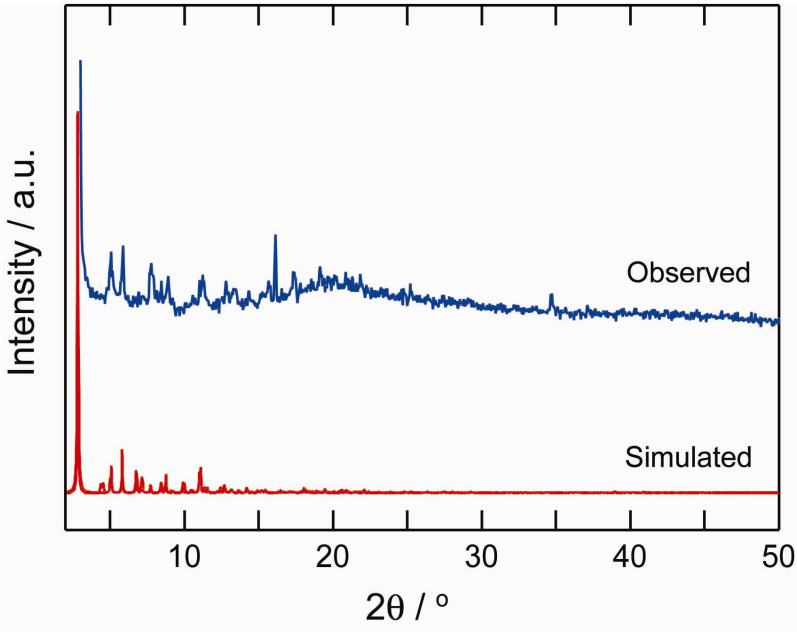

Figure S6. Simulated and Experimental PXRD Patterns of MOP-18.

Thermogravimetric Analysis.

The first weigh loss until 280 °C was due to the coordinating ligands and guest molecules. The coordinating ligands are 12 DMF, 4 octanol, and 8 H_2O molecules. The guest molecules were regarded as 20 DMF, 4 octanol, and 8 H_2O molecules. The observed weight loss was 25%, and the calculated was 27%. The weigh loss from 280 to 420 °C was due to the decomposition of the organic links in the MOP-18 framework. The observed value was 60%, and the calculated was 62%.

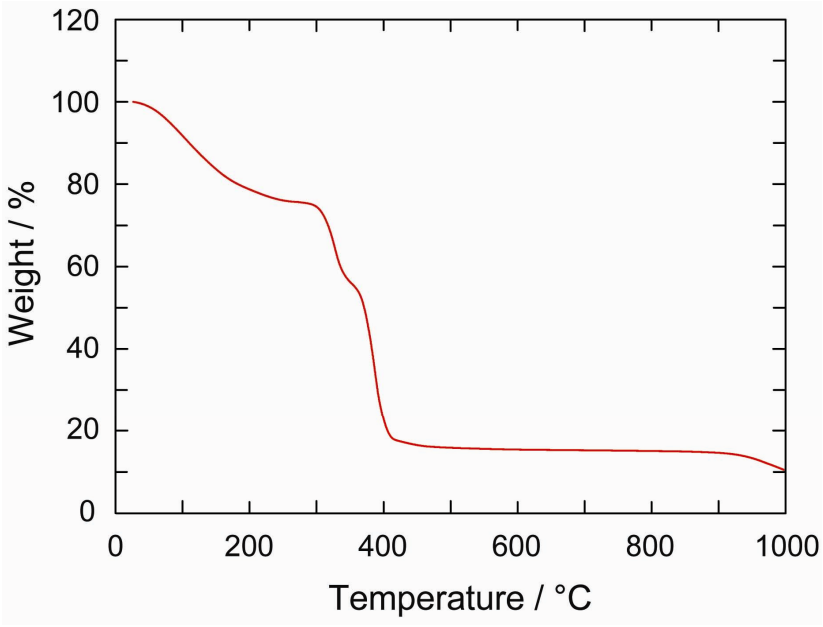

Figure S7. Thermogravimetric analysis (TGA) of as-synthesized MOP-18.

Scanning Tunneling Microscopy Studies.

A drop of 1-phenyloctane (Acros Organics) solution containing MOP-18 to be imaged was placed on freshly cleaved HOPG (SPI-1 grade, Structure Probe Inc.). The drop was allowed to evaporate over 5 days, then this thin film was imaged using a Nanoscope E STM (Digital Instruments). The degree of evaporation of solvent was critical to imaging. When STM imaging was attempted at shorter times (after several hours), no ordered self-assembly was observed due to the high mobility of MOPs on the surface. STM imaging at longer times (after one week) was not possible; the tip could not penetrate the thin film sufficiently to come within tunneling distance of the surface. The tips were fabricated from mechanically cut wire (Pt/Ir) 80/20%, California Fine Wire) and the quality of the tips was verified by scanning bare HOPG prior to imaging. STM imaging was performed under ambient conditions with typical settings of 400 pA of current and 1320 mV of bias voltage (sample positive) with a scan rate of 12.2 Hz.

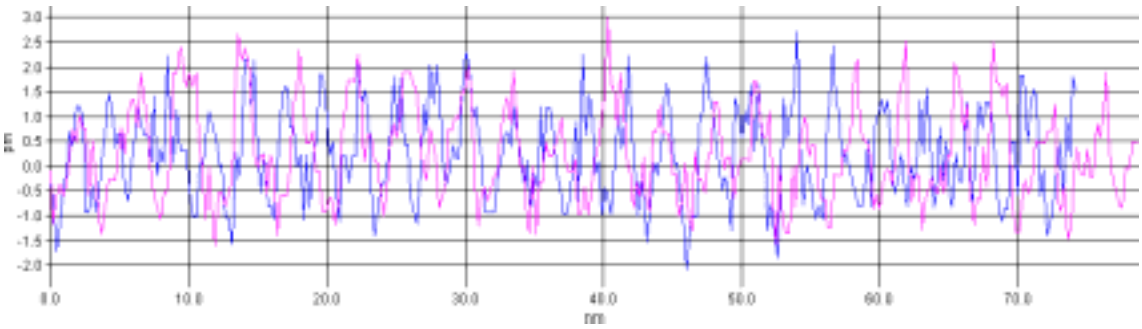

Figure S8. Line profiles of an STM images showing the measured height variation. Due to the packing and the quasi-constant height mode in which the images were collected, the magnitude of the height difference between MOPs is underestimated.

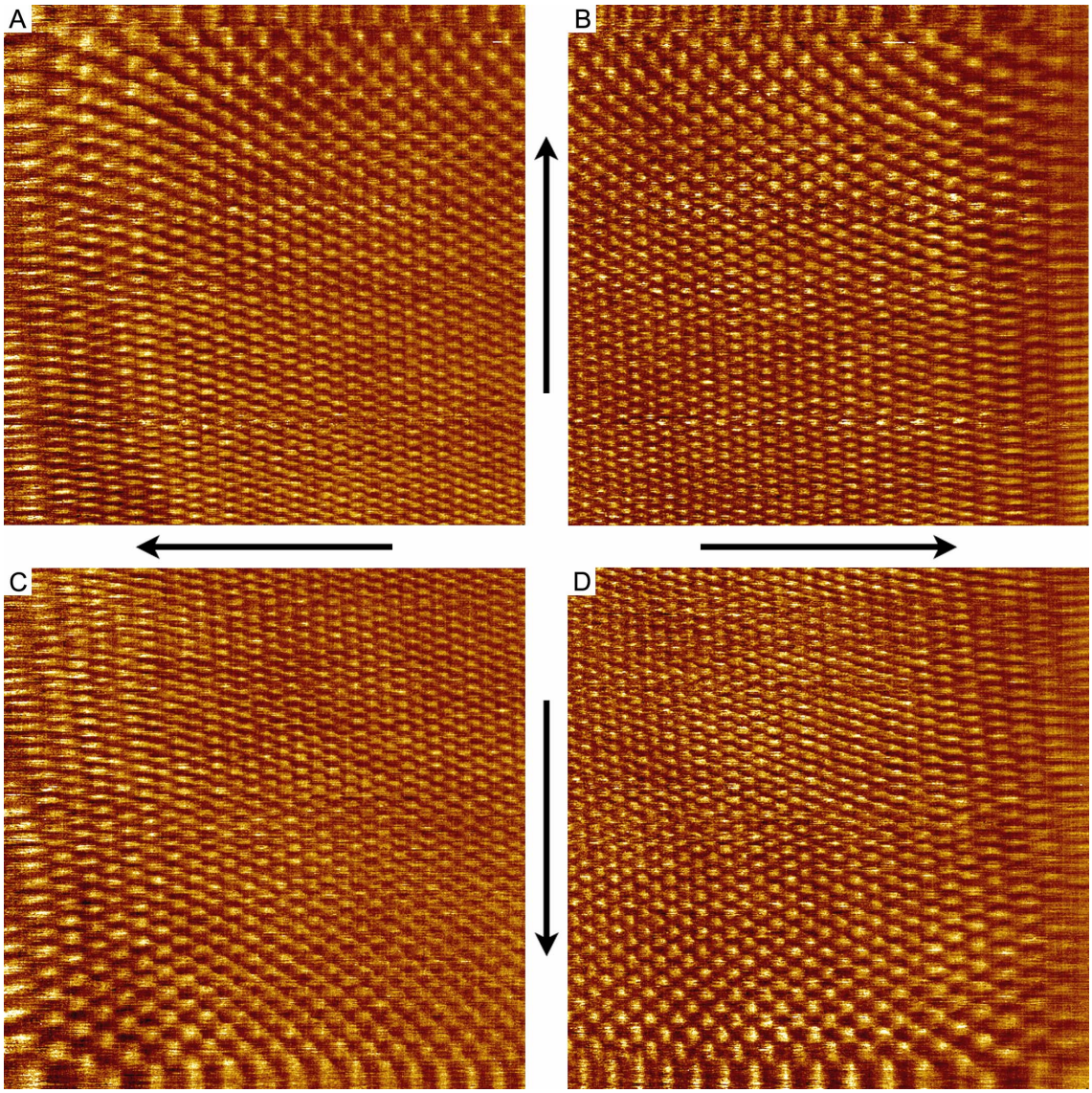

Figure S9. STM images (120 nm x 120 nm) collected with varying scanning directions, indicated by the arrows. These illustrate the significant image drift that was observed in all STM images of the MOPs. Note that the spacing observed between MOPs increases toward the end of the scan, in both the left-right and up-down directions. This indicates that the self-assembled MOPs are mobile, and that the motion of the STM tip is moving them as it scans.