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Antiferromagnetically Coupled Dimeric Dodecacopper Supramolecular Architectures of Macrocyclic Ligands with a Symmetrical μ_6-BO_3^{3-} Central Moiety

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Table S6: Bond distances (Å) and angles (º) for **5**.

Table S7: Bond distances (Å) and angles (º) for **6**.

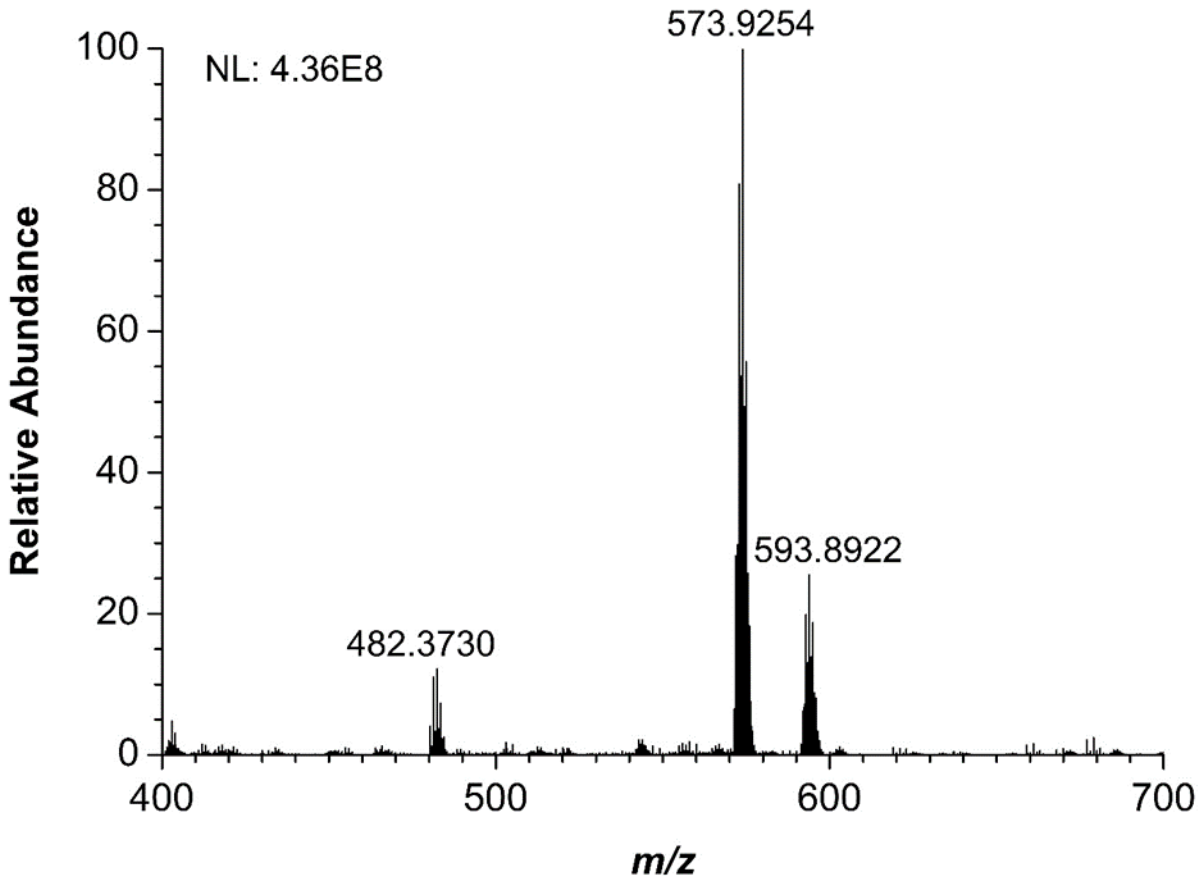

Figure S1. The full mass spectrum of complex **2**.

Preparation of complexes (3-5)

{[Cu_6(L5)(μ_6-BO_3)(μ-OH)(H_2O)$_3$(C_3H_7NO)][BF_4]$_2$·6C_3H_7NO·4C_2H_5OH·2H_2O}$_2$ (3)

Complex **3** was prepared by using exactly the same procedure as used for **1** by replacing DFMP with 2,6-diformy-4-tertiarybutylphenol (DFTBP). A mixture of DFTBP (0.41 g, 2.0 mmol), $Cu(BF_4)_2.6H_2O$ (1.3 g, 3.8 mmol), 1,3-DAP (0.18 g, 2.0 mmol), and TEA (0.42 g, 4.2 mmol) in 80 mL of methanol was stirred under reflux for ca. 36 hrs. A bluish green clear solution formed was reduced at rotary evaporator to ca. 10 mL and 30 mL of ethanol was added. The reaction mixture was stirred further under reflux for ca. 4 hrs. and left undisturbed at ambient temperature for a few days. A bluish green solid separated was filtered off, washed with ethanol (3 X 3 mL) and air dried. Crystals suitable for X-ray study were obtained by slow diffusion of

diethyl ether into a solution of **3** in a mixture of DMF:EtOH (1:1). (Yield: 0.73 g, 67% based on DFTBP). IR spectrum: υ(H_2O/C_2H_5OH), 3566, 3395 cm^{-1}, υC=N, 1653 cm^{-1}, υBF_4, 1051 cm^{-1}. UV-Vis spectrum: 595 nm and 310 nm. Elemental analysis (air dried sample): Found (%): C, 33.92; H, 4.86; N, 5.06. Calcd. (%) for $\{Cu_6(C_{45}H_{54}N_6O_6)(BO_3)(BF_4)_2(H_2O)_{10}\}_2$: C, 34.08; H, 4.77; N, 5.30.

$\{[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3OH)(CH_3OH)_2][ClO_4]_3\cdot 10H_2O\}_2$ (4)

4 was obtained by using exactly the same method as used for **2** by replacing DFMP with DFTBP under argon. (Yield: 0.44 g, 39% based on DFTBP). IR spectrum: υ(H_2O/CH_3OH), 3534, 3390 cm^{-1}, υC=N, 1653 cm^{-1}, υClO_4, 1098, 1046 cm^{-1}. UV-Vis spectrum: 595 nm and 308 nm. Elemental analysis (air dried sample): Found (%): C, 31.87; H, 4.58; N, 5.15. Calcd. (%) for $\{[Cu_6(C_{45}H_{54}N_6O_6)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3OH)(CH_3OH)_2][ClO_4]_3\cdot 10H_2O\}_2$: C, 32.21; H, 4.84; N, 4.70.

$\{[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3CO_2)(\mu\text{-}CH_3O)(CH_3OH)]BF_4\cdot 13CH_3OH\cdot 8H_2O\}_2$ (5)

To a suspension of **3** (0.20 g) in 30 mL of methanol was added a solution of $Co(CH_3CO_2)_2$ (0.400 g) in 20 mL of the same solvent and the reaction mixture was stirred under reflux with an intention to trans-metallate Cu with Co. After ca. 30 min. the solid dissolved completely forming a bluish green solution. A solution of NaN_3 (0.025 g) in 10 mL of hot methanol was added drop wise with stirring under reflux. The reaction mixture was refluxed further for 5 min. and filtered hot. The filtrate was left unperturbed at ambient temperature. After four weeks very nice dark green crystals suitable for X-ray study separated in dark green solution were filtered off and washed with methanol (2 X 2 mL). (Yield: 0.12 g, 60% based on DFMP). IR spectrum: υ(H_2O/CH_3OH), 3596, 3378 cm^{-1}, υC=N, 1652 cm^{-1}, υBF_4, 1042 cm^{-1}. UV-Vis spectrum: 600 nm and 310 nm. Elemental analysis (air dried sample): Found (%): C, 36.87; H, 5.15; N, 5.72. Calcd. (%) for **{**$[Cu_6(C_{45}H_{54}N_6O_6)(BO_3)(CH_3O)(CH_3CO_2)(CH_3OH)][BF_4]\cdot 10H_2O\}_2$**:** C, 36.69; H, 5.28; N, 5.24.

Structural Description

$\{[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}OH)(H_2O)_3(C_3H_7NO)][BF_4]_2\cdot 6C_3H_7NO\cdot 4C_2H_5OH\cdot 2H_2O\}_2$ (3)

The structures of hexacopper monomer and dimeric dodecacopper complex **3** are depicted in Figures S2 and S3-S4 respectively. The bond distances and angles relevant to the copper coordination spheres are given in Table S4**.** Figure S2 shows the hexanuclear cationic core $[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}OH)(H_2O)_3(C_3H_7NO)]^{2+}$ of **3** with a distorted hexagonal arrangement of six copper(II) centers as in **1** and **2**. The solid angles at the copper centers [359.08(10)-360.19(10)°] clearly reveal almost perfectly planar arrangements around these centers in the equatorial plane, which are bridged alternately by the μ-phenoxide and $\mu_{1,1}$-O(BO_3^{3-}) pair and the μ-alkoxide and $\mu_{1,3}$-O(BO_3^{3-}) pair exactly similar to **1**. In each hexacopper monomeric unit (Figure S2) longer axial interactions with $\mu_{1,1}$-O(11)(OH) [Cu(1) and Cu(6)], O(12)(OH_2) [Cu(4)], O(13)(H_2O) [Cu(3)], O(14)(H_2O) [Cu(4)], and $\mu_{1,1}$-O(10)(DMF) [Cu(1) and Cu(6)] give rise to slightly distorted square pyramidal stereochemical arrangements around Cu(1)-Cu(5) and a distorted octahedral geometry around Cu(6) ions respectively. $\mu_{1,1}$-OH and $\mu_{1,1}$-DMF provide unsymmetrical bridges between Cu(1), Cu(6) and Cu(5, Cu(6) respectively.

The copper-copper distances lie in the range 2.801-3.380 Å. The shortest distance of 2.801 Å is observed for a triply bridged (two single-atom and a three-atom bridges) pair [Cu(5), Cu(6)] and the longest distance of 3.380 Å is observed for doubly bridged (a single atom alkoxy and three-atom borate bridges) pair [Cu(2), Cu(3)]. In **3** the bridging pattern of the macrocyclic ligand $L5^{6-}$ and the central species μ_6-(BO_3^{3-}) in the equatorial plane is exactly identical to **1** and **2**. The conformation of the macrocyclic ring is similar to that as found in **1**. The Cu-N (1.911(5)-1.961(6) A) and Cu-O (1.87694)-2.007(4) Å) distances are quite normal and are similar to those reported for other hexacopper complexes in this paper. The sums of the angles around alkoxide oxygen bridges are O(5) 356.9(3), O(7) 328.2(3), and O(9) 325.6(3)° indicative of a slight distortion from planarity at O(5) and a strong pyramidal distortions around O(7) and O(9). The sums of the angles around phenoxide oxygen bridges are O(4) 359.8(9), O(6) 358.3(9), and O(8) 343.2(9)°, indicate fairly planar arrangements around O(4) and O(6) oxygen bridges and much deviation from planarity around O(8) bridge. The sums of the angles around oxygen atoms of BO_3^{3-} species lie in the range 352.3(9)-356.8(9)° indicating slight distortions from the planarity around these atoms. The sum of the angles at B atom of the central species is 360.00 (6)° revealing a perfect planar arrangement around this atom. The bridge angles: Cu-O(alkoxy)-Cu 102.4(2)-129.7(2)°, Cu-O(phenoxy)-Cu 92.58(19)-99.87(19)°, and Cu-O(BO_3^{3-})-Cu 92.95(18)-

97.43(18)° in the equatorial plane suggest moderately strong interactions between Cu(II) ions in hexanuclear units.

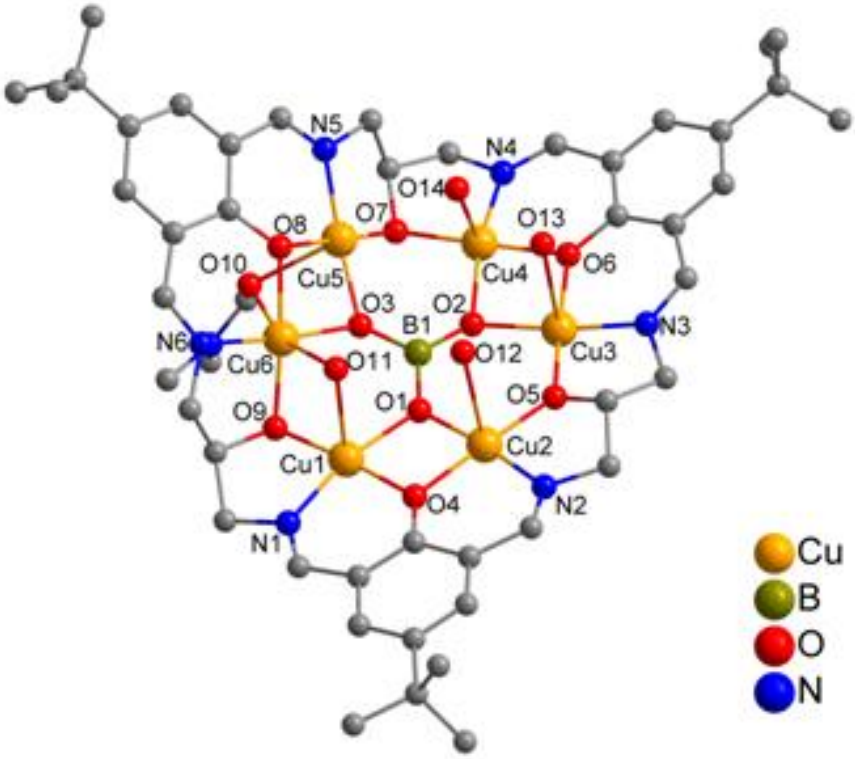

Figure S2. Structural view of hexacopper cation $\{[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}OH)(H_2O)_3(C_3H_7NO)]^{2+}$ (**3**).

Two of the three oxygen atoms [μ_3-O(1) and μ_3-O(2)] of the central (μ_6-BO_3^{3-}) species, in addition to providing bridges between copper pairs Cu(1), Cu(2) and Cu(3), Cu(4) within the same macrocyclic ring, also provide bridges to Cu(3) and Cu(2) on the other macrocyclic ring respectively generating a dimeric complex (Figures S3 & S4) in which two macrocycle rings are held together through convex surfaces as in **1**. The inter-hexacopper bridging also involves the symmetry related atoms so that the two macrocycle rings are held together by four long axial oxygen-copper inter-hexacopper [O(1)-Cu(3), 2.8359(3) Å and O(2)-Cu(2), 2.9865(13) bridges leading to distorted octahedral geometry for Cu(2) and Cu(3) in dimeric cluster. This mode of inter-hexacopper bridging is different from that observed in **1** and **2** where two rings are held together by 2 and 6 axial bridges respectively.

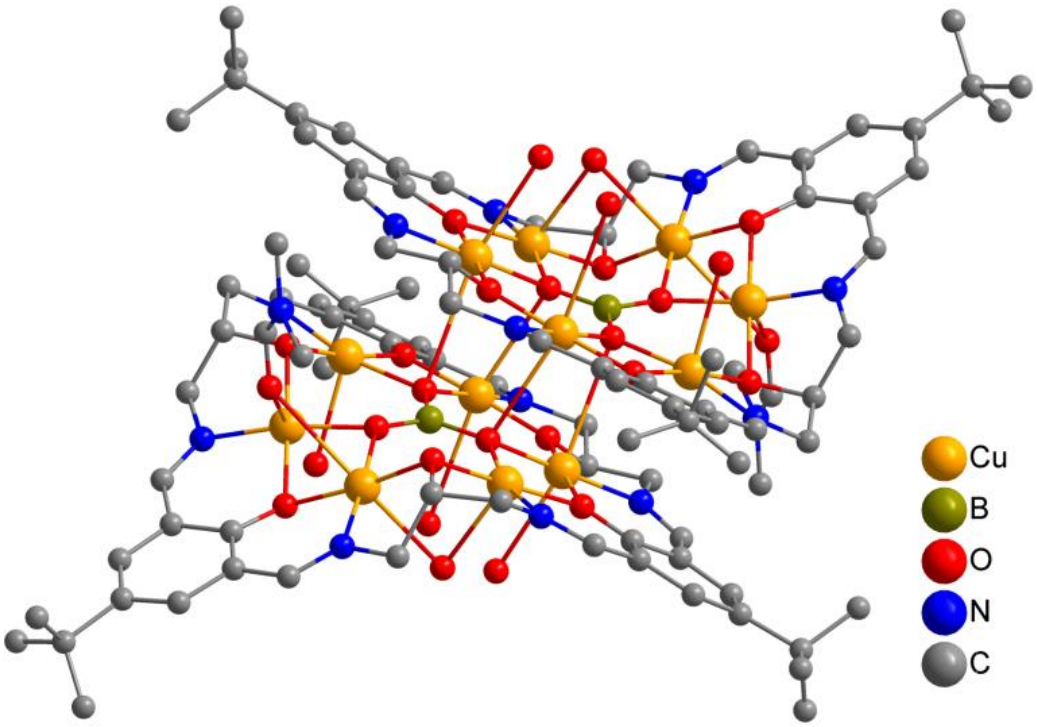

Figure S3. Structural view of dimeric cation $[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}OH)(H_2O)_3(C_3H_7NO)]^{2+}$ (**3**). (Hydrogen atoms are omitted for clarity)

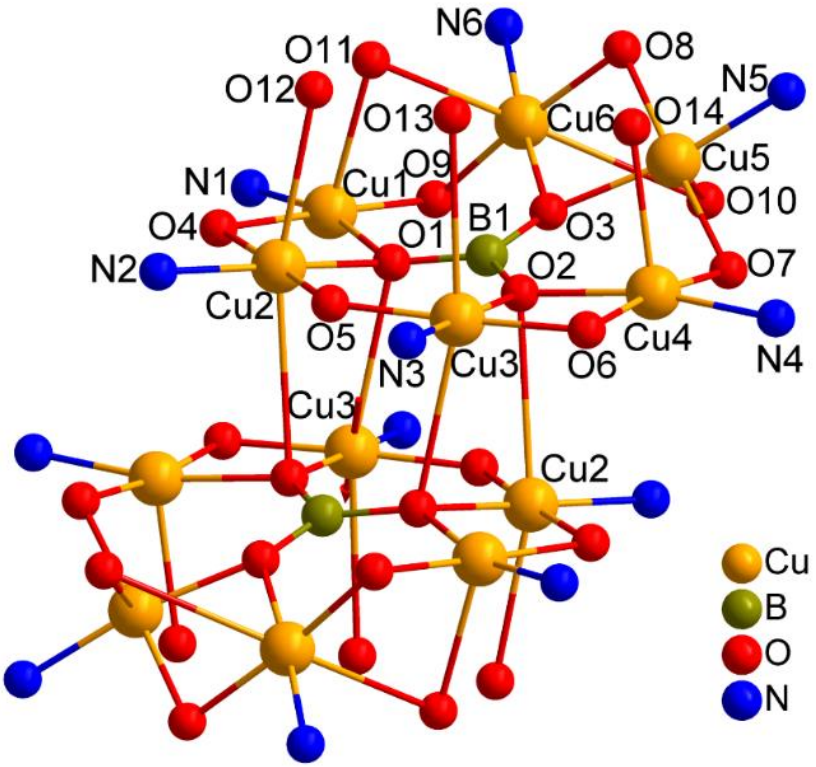

Figure S4. Structural view of dimeric cation $[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}OH)(H_2O)_3(C_3H_7NO)]_2^{4+}$ (**3**).

Structural description of $\{[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3OH)(CH_3OH)_2][ClO_4]_3\cdot 10H_2O\}_2$ (4)

Complex **4** is prepared by reacting 2,6-DFTBP and 1,3-DAP in the presence of $Cu(ClO4)_2/H_3BO_3$/TEA/Ar and the crystals suitable for x-ray analysis were obtained by layering solution of **4** in a degassed mixture of DMF:EtOH with ether in dry box. The structure of hexacopper monomer and dimeric dodecacopper metallocluster **4** are depicted in Figures S5 and S6 respectively. The bond distances and angles relevant to the copper coordination spheres are given in Table S5**.** Figure S5 shows the hexanuclear cationic core $[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3OH)(CH_3OH)_2]^{3+}$ of (**4**) with a distorted hexagonal arrangement of six copper(II) centers with $\mu_6\text{-}(BO_3^{3-})$ central species bonded to all copper centers as in **1-3** and **5**, clearly indicating that the central species is BO_3^{3-} from H_3BO_3. In each hexacopper monomeric unit (Figure S5) longer axial interactions with $\mu_{1,1}$-O(OCH_3) [Cu(3) and Cu(4)], O($HOCH_3$) [Cu(2)] and [Cu(5)], give rise to slightly distorted square pyramidal stereochemical arrangements around Cu(2)-Cu(5) and a distorted square planar arrangement around Cu(1) and Cu(6) ions respectively.

In **4** which is not very well refined, the bridging pattern of the macrocyclic ligand $L5^{6-}$ and the central species μ_6-(BO_3^{3-}) in the equatorial plane is exactly identical to **1-3** and **5**. The conformation of the macrocyclic ring is similar to that as found in **1, 3,** and **5**. Two of the three oxygen atoms [μ_3-O(1) and μ_3-O(2)] of the central (μ_6-BO_3^{3-}) species, in addition to providing intra-dinuclear bridge between copper pair within the same macrocyclic ring, also provide inter-metallocycle bridges to copper ion on the other macrocyclic ring generating a dimeric complex (Figure S6) in which two macrocycle rings are held together through convex surfaces as in **1, 3** and **5**. The inter-hexacopper bridging also involves the symmetry related atoms so that the two metallocycle rings are held together by four long axial oxygen-copper inter-hexacopper bridges. This mode of inter-hexacopper bridging is different from that observed in (**1 & 5)** and **2** where two rings are held together by 2 and 6 axial bridges respectively and is similar to complex **3**.

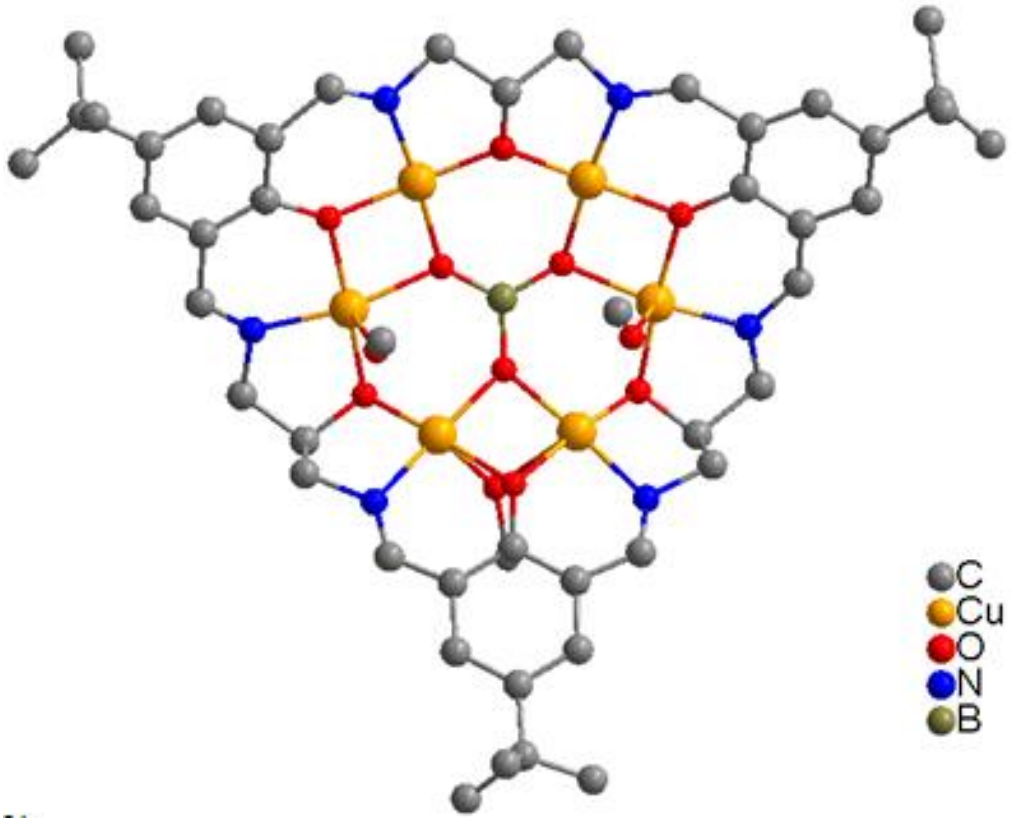

Figure S5. Structural view of hexacopper cation $[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3OH)(CH_3OH)_2]^{3+}$ (**4**) . (Hydrogen atoms are omitted for clarity)

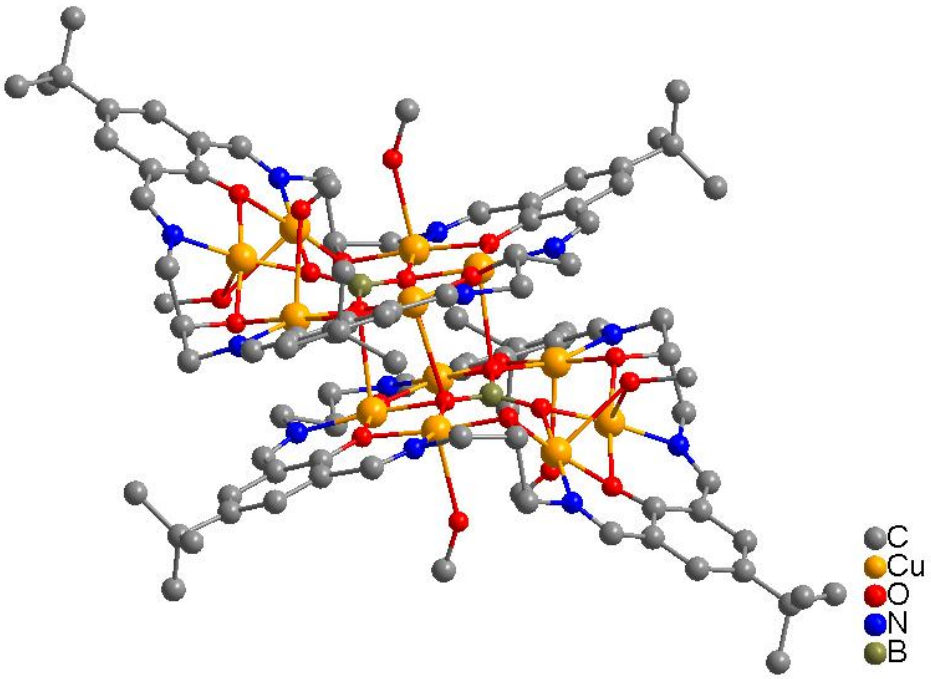

Figure S6. Structural view of dimeric dodecacopper cation $[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3OH)(CH_3OH)_2]_2^{6+}$ (**4**). (Hydrogen atoms are omitted for clarity)

$\{[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3CO_2)(\mu\text{-}CH_3O)(CH_3OH)]BF_4\cdot 13CH_3OH\cdot 8H_2O\}_2$ (5)

Dark green crystals of **5** suitable for X-ray analysis were obtained by keeping the reaction mixture at ambient temperature for four weeks. The molecular structure of hexacopper monomer and dimeric dodecacopper metallocluster **5** are shown in Figures S7 and S8-S9 respectively. The bond distances and angles relevant to the copper coordination spheres are given in Table S6**.** Compound **5** crystallizes in the monoclinic system space group *P*2(1)/*c*. In **5**, the coordination mode and the bridging pattern of the macrocyclic ligand in the basal plane and the presence of a central $\mu_6\text{-}BO_3^{3-}$ species bonded to all six copper centers providing three alternating one-atom ($\mu_{1,1}\text{-}O(BO_3^{3-})$) and three three-atom ($\mu_{1,3}\text{-}O(BO_3^{3-})$) bridges is same (Figure S7) as present in other similar complexes (**1-4**) reported in this paper. All copper centers except Cu(2) have distorted square pyramidal geometries $[NO_4]$ due to axial interactions with two unsymmetrical bridging bidentate $\mu\text{-}CH_3CO_2^-$ and $\mu\text{-}CH_3O^-$ anions which provide two-atom and a single atom bridges between Cu(3), Cu(4) and Cu(1), Cu(6) respectively causing an upward bending of the macrocyclic ring. A CH_3OH molecule

occupies axial position on Cu(5) in a distorted square pyramidal arrangement.

The bond distances [Cu-N 1.925(6)-1.950(5) Å and Cu-O 1.864(4)-1.987(4) Å] and bond angles at the bridging atoms O(1)-O(6) and O(10)-O(12) [Cu-O-Cu, 93.71(18)-128.4(2)°] for all copper centers in the equatorial plane are comparable to those found in other hexacopper clusters (**1**-**4**) reported in this paper. The solid angles at copper centers [Cu(1) 360.2(10), Cu(2) 360.01(18), Cu(3) 359.10(14), Cu(4) 358.4(10), Cu(5) 360.5(10), and Cu(6) 358.8(10)°] are indicative of fairly planar arrangements around these metal centers in the equatorial plane, providing effective pathways for magnetic exchange interactions between metal centers. The sums of the angles around bridging atoms in the equatorial plane [O(1) 329.2(5), O(2) 359.9(9), O(3) 355.3(3), O(4) 353.9(9), O(5) 329.8(3), O(6) 348.2(9), O(10) 354.0(9), O(11) 358.1(3), and O(12) 349.7(9)°] suggest slight to significant deviation from planarity around O(2)-O(4), O(6), O(10)-O(12) atoms and large pyramidal distortions around O(1) and (O(5) atoms respectively. The sum of the angles at B(2) is 360.0(6)° indicating planar arrangement at this atom. The bridge angles at Cu-O(alkoxy)-Cu 104.16(19)-128.4(2)°, Cu-O(phenoxy)-Cu 93.95(18)-100.34(19)°, and Cu-O(BO_3^{3-})-Cu 93.71(18)-97.5(2)° in the equatorial plane suggest moderate to strong ferromagnetic and antiferromagnetic spin interactions between Cu(II) ions in hexanuclear units.

One of the three oxygen atom (μ_3-O(12)) of central μ_6-BO_3^{3-} ion, in addition to bridging a copper pair (Cu(3), Cu(4) within the same hexacopper monomer, provides a longer axial inter-macrocycle bridge to Cu(2) on the other macrocyclic ring generating a dimeric assembly (Figures S8 & S9) in which two hexacopper rings are coupled from convex surfaces. As in **1**, the molecular symmetry dictates that this inter-hexacopper bridging also involves the symmetry related atoms and so the two rings are linked together by two axial O(12)-Cu(2) (2.8107(47) Å) bridges, thus leading to a chair like conformation for each macrocyclic ring and a double inverted chair like conformation for the dimeric complex.

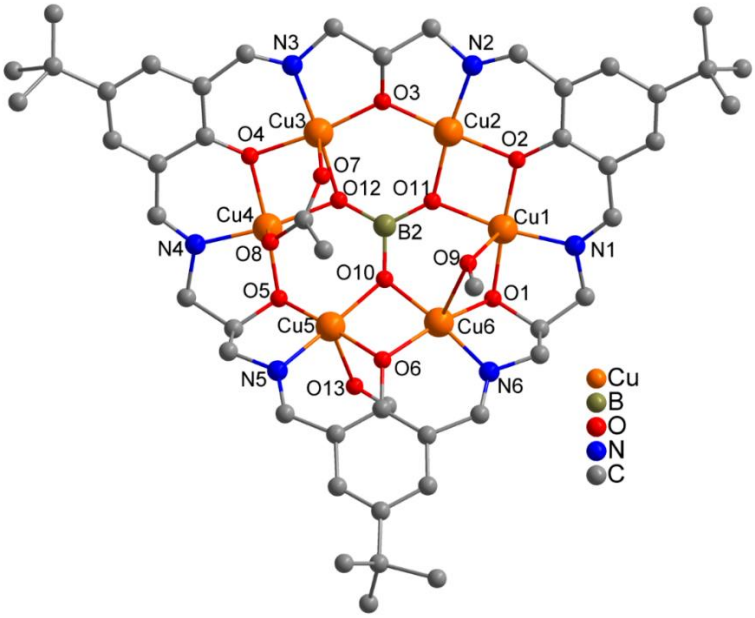

Figure S7. Structural representation of hexacopper monomeric cation $[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3CO_2)(\mu\text{-}CH_3O)(CH_3OH)]^+$ (**5**). (Hydrogen atoms are omitted).

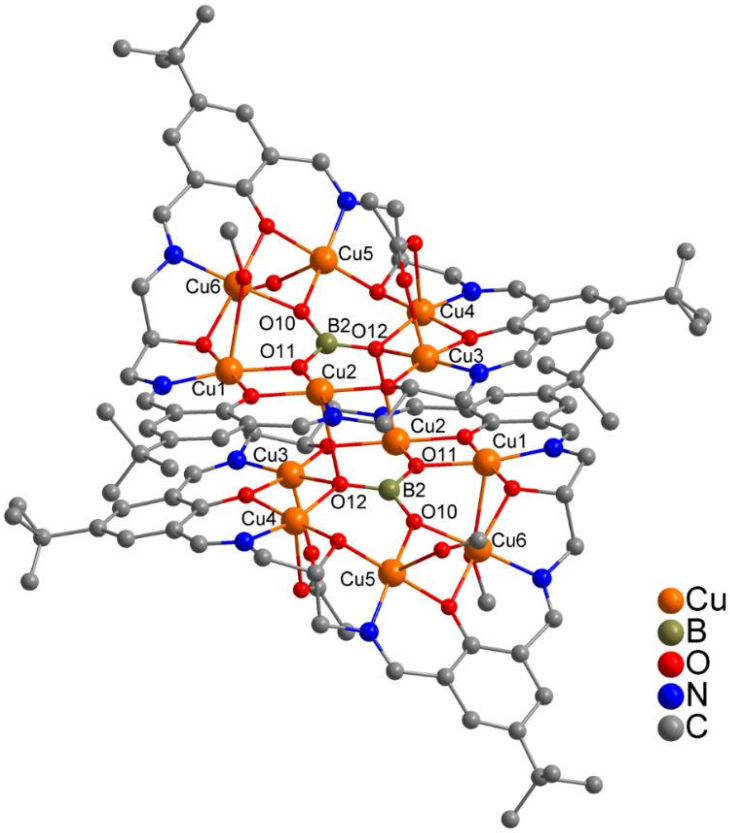

Figure S8. A view of dimeric dodecacopper cation $[Cu_6(L5)(\mu_6\text{-}BO_3)(\mu\text{-}CH_3CO_2)(\mu\text{-}CH_3O)(CH_3OH)]_2^{2+}$ (**5**).

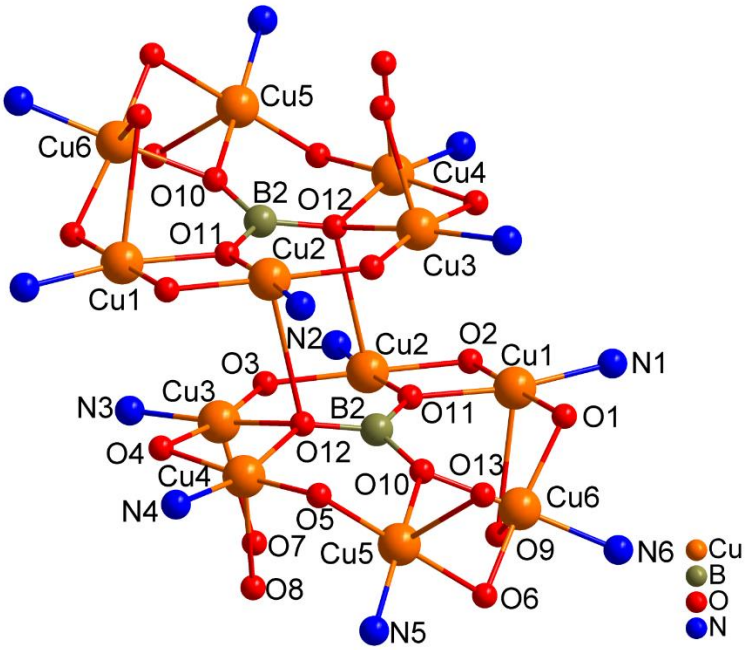

Figure S9. Structure of dimeric cation $[Cu_6(L)(BO_3)(OAc)(OCH_3)(HOCH_3)]^{2\,2+}$ (**5**) showing only coordination core.

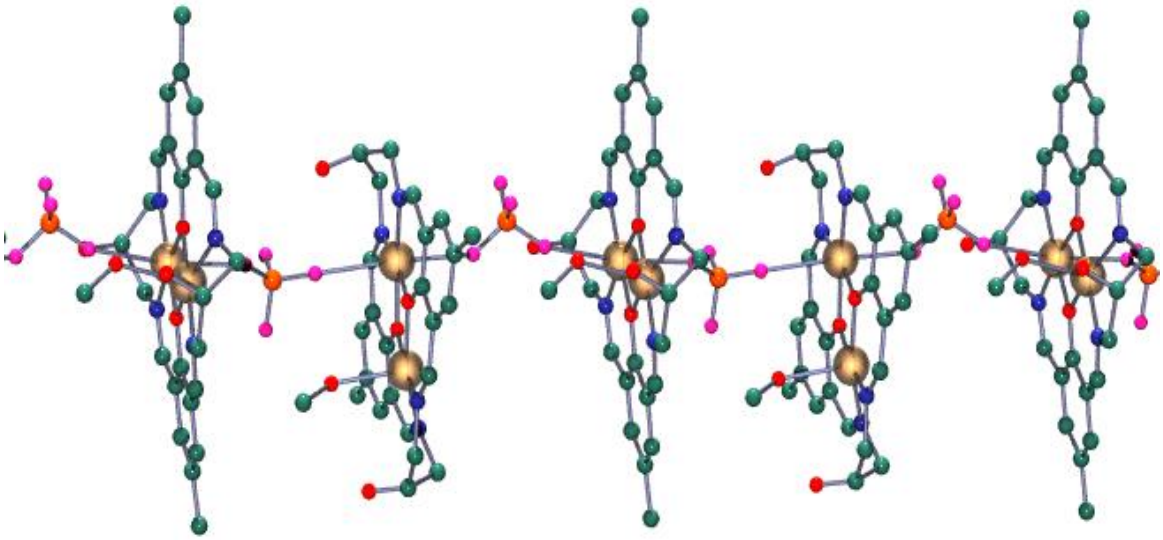

Figure S10. Molecular structure of 1D-single chain $\{[Cu_2(H_2M2)(CH_3OH)(BF_4)](BF_4)\}_n$ (**6**) along c-axis. Color Code: Brown (Cu), Blue (N), Green (C), Red (O), Orange (B), Rose (F).

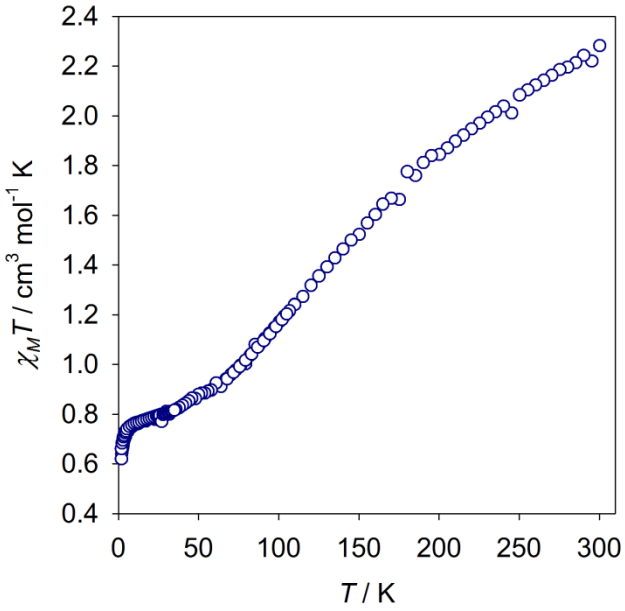

Figure S11. Temperature dependence of the χT product for compound **2**.

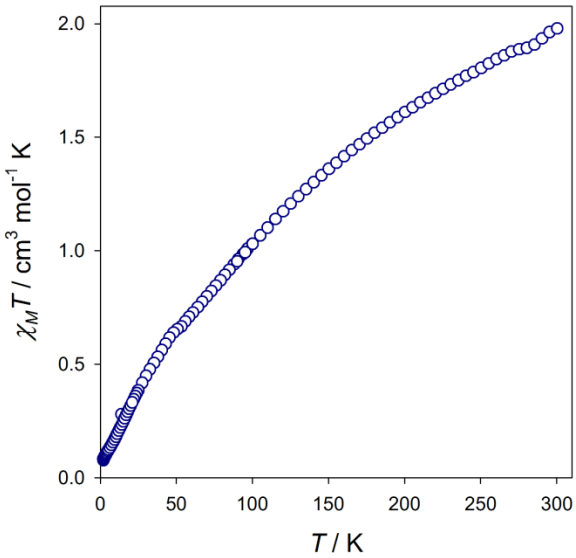

Figure S12. Temperature dependence of the χT product for compound **3**.

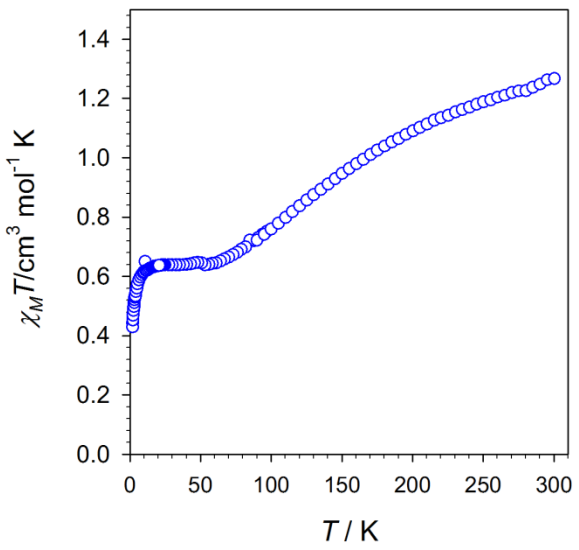

Figure S13. Temperature dependence of the χT product for compound **4**.

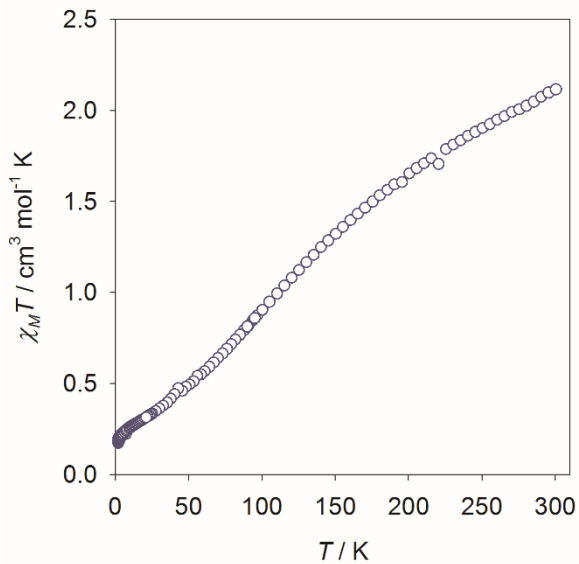

Figure S14. Temperature dependence of the χT product for compound **5**.

X-ray Crystal Structure Information

Each structure was determined using direct methods. This procedure yielded Cu along with a number of the B, C, N, F, and O atoms. Subsequent Fourier synthesis yielded the remaining atom positions. The hydrogen atoms were fixed in positions of ideal geometry and refined within the

XSHELL software. These idealized hydrogen atoms had their isotropic temperature factors fixed at 1.2 or 1.5 times the equivalent isotropic U of the C atoms to which they were bonded. The final refinement of each compound included anisotropic thermal parameters on all non-hydrogen atoms.

The crystal data for compounds **1-6** are given in Table S1.

Table S1 Summary of crystallographic data for compounds **1-6**

	1	**2**	**3**
Empirical formula	$C_{102}H_{146}B_8Cu_{12}F_{24}N_{22}O_{30}$	$C_{108}H_{156}B_2Cl_6Cu_{12}N_{24}O_{54}$	$C_{148}H_{269}B_6Cu_{12}F_{16}N_{26}O_{52}$
M	3465.36	3651.37	4376.22
Crystal System	monoclinic	hexagonal	monoclinic
Space group	*C*2/*c*	*R*-3	*C*2/*c*
a/Å	37.280(8)	26.976(3)	32.740(5)
b/Å	16.837(3)	26.976(3)	15.232(2)
c/ Å	21.5551(4)	16.5285(16)	33.008(4)
α/ °			
β/ °	92.9931(3		99.255(4)
γ/°		120	
V/A^3	13509(5)	10416(3)	16247(4)
ρ_{calcd}(g cm^{-3})	1.704	1.746	1.792
T/K	188	180	180
Z	4	3	4
μ/mm^{-1}	1.958	2.010	1.652
Crystal size (mm)	0.30 x 0.25 x 0.18	0.15 x 0.15 x 0.15	0.25 x 0.12 x 0.10
Reflections collected:			
Total	53334	28215	64065
Unique	11972	4111	14400
R_{int},	0.1194	0.0817	0.1117
Final R_1, wR_2	0.0674, 0.2036	0.0607, 0.2012	0.0618, 0.1838

Table S1 (Cont.) Summary of crystallographic data for compounds **1-6**

	4	**5**	**6**
Empirical formula	$C_{51}BCu_6F_4N_6O_{11}$	$C_{124}H_{264}B_4Cu_{12}F_8N_{12}O_{68}$	$C_{25}H_{30}B_2Cu_2F_8N_4O_5$
M	1340.62	3969.18	767.23
Crystal System	monoclinic	monoclinic	monoclinic
Space group	*P*2(1)/*c*	*P*2(1)/*c*	*P*2(1)/*c*
a/Å	14.459(11)	14.9843(18)	12.0563(12)
b/Å	14.846(10)	14.7739(18)	16.7837(17)
c/ Å	33.64(3)	33.108(4)	14.0937(14)
α/ °			
β/ °	100.718(17)	99.849(2)	92.807(2)

$\gamma/^{\circ}$			
V/A^3	7094(9)	7221.3(15)	2848.4(5)
ρ_{calcd}(g cm^{-3})		1.309	1.789
T/K	180	189	100
Z		2	4
μ/mm^{-1}		1.845	1.591
Crystal size (mm)	0.25 x 0.22 x 0.17	0.25 x 0.20 x 0.10	0.35 x 0.30 x 0.20
Reflections collected:			
Total		57289	22727
Unique		12777	5051
R_{int},		0.0663	0.0659
Final R_1, wR_2		0.0657, 0.1936	0.0450 0.1364

$R_1=\Sigma[|F_0| - |F_c|]/\Sigma|F_0|$, $wR_2=[\Sigma[w(|F_0|^2 - |F_c|^2)^2]/\Sigma[w(|F_0|^2)^2]]^{1/2}$
$R = \Sigma||Fo| - |Fc|| / \Sigma|Fo|$, $R_W = [\Sigma w (|Fo| - |Fc|)^2 / \Sigma w Fo^2]^{1/2}$

Table S2**.** Bond distances [Å] and angles [°] for **1**.

Bond lengths [Å]		**Bond angles [°]**	
Cu(1)-O(5)	1.915(6)	O(5)-Cu(1)-N(1)	86.5(3)
Cu(1)-N(1)	1.918(7)	O(5)-Cu(1)-O(1)	97.9(2)
Cu(1)-O(1)	1.919(6)	N(1)-Cu(1)-O(1)	169.7(3)
Cu(1)-O(4)	1.957(6)	O(5)-Cu(1)-O(4)	176.6(3)
Cu(1)-Cu(6)	2.7993(15)	N(1)-Cu(1)-O(4)	91.8(3)
Cu(2)-O(5)	1.917(6)	O(1)-Cu(1)-O(4)	84.2(2)
Cu(2)-O(6)	1.932(6)	O(5)-Cu(2)-O(6)	174.0(3)
Cu(2)-N(2)	1.956(7)	O(5)-Cu(2)-N(2)	84.0(3)
Cu(2)-O(2)	1.963(5)	O(6)-Cu(2)-N(2)	91.2(3)
Cu(2)-Cu(3)	2.9264(16)	O(5)-Cu(2)-O(2)	102.9(2)
Cu(3)-O(7)	1.880(5)	O(6)-Cu(2)-O(2)	81.6(2)
Cu(3)-O(2)	1.935(6)	N(2)-Cu(2)-O(2)	171.6(3)
Cu(3)-N(3)	1.941(7)	O(7)-Cu(3)-O(2)	101.3(2)
Cu(3)-O(6)	1.939(6)	O(7)-Cu(3)-N(3)	84.0(3)
Cu(4)-O(7)	1.875(6)	O(2)-Cu(3)-N(3)	174.5(3)
Cu(4)-N(4)	1.926(7)	O(7)-Cu(3)-O(6)	176.5(3)
Cu(4)-O(3)	1.930(6)	O(2)-Cu(3)-O(6)	82.1(2)
Cu(4)-O(8)	1.932(5)	N(3)-Cu(3)-O(6)	92.5(3)
Cu(4)-Cu(5)	2.9463(17)	O(7)-Cu(4)-N(4)	84.8(3)
Cu(5)-O(9)	1.910(6)	O(7)-Cu(4)-O(3)	100.1(2)
Cu(5)-N(5)	1.945(7)	N(4)-Cu(4)-O(3)	171.7(3)
Cu(5)-O(8)	1.945(6)	O(7)-Cu(4)-O(8)	176.1(3)
Cu(5)-O(3)	1.999(5)	N(4)-Cu(4)-O(8)	91.9(3)
Cu(5)-Cu(6)	3.0289(17)	O(3)-Cu(4)-O(8)	82.8(2)
Cu(6)-N(6)	1.907(7)	O(9)-Cu(5)-N(5)	84.9(3)
Cu(6)-O(1)	1.921(6)	O(9)-Cu(5)-O(8)	174.9(2)
Cu(6)-O(9)	1.929(6)	N(5)-Cu(5)-O(8)	90.9(3)
Cu(6)-O(4)	1.954(6)	O(9)-Cu(5)-O(3)	103.0(2)
B(1)-O(2)	1.392(12)	N(5)-Cu(5)-O(3)	167.7(3)

B(1)-O(3)	1.389(13)	O(8)-Cu(5)-O(3)	80.7(2)
B(1)-O(1)	1.375(12)	N(6)-Cu(6)-O(1)	175.8(3)
		N(6)-Cu(6)-O(9)	86.6(3)
		O(1)-Cu(6)-O(9)	97.5(2)
		N(6)-Cu(6)-O(4)	91.6(3)
		O(1)-Cu(6)-O(4)	84.3(2)
		O(9)-Cu(6)-O(4)	169.2(3)
		O(2)-B(1)-O(3)	122.2(9)
		O(2)-B(1)-O(1)	118.9(9)
		O(3)-B(1)-O(1)	118.8(9)
		B(1)-O(1)-Cu(6)	129.5(6)
		B(1)-O(1)-Cu(1)	132.1(6)
		Cu(6)-O(1)-Cu(1)	93.6(3)
		B(1)-O(2)-Cu(3)	129.9(6)
		B(1)-O(2)-Cu(2)	129.9(6)
		Cu(3)-O(2)-Cu(2)	97.3(2)
		B(1)-O(3)-Cu(4)	131.2(6)
		B(1)-O(3)-Cu(5)	128.4(6)
		Cu(4)-O(3)-Cu(5)	97.1(2)
		C(29)-O(4)-Cu(1)	122.1(6)
		C(29)-O(4)-Cu(6)	125.5(6)
		Cu(1)-O(4)-Cu(6)	91.4(3)
		C(2)-O(5)-Cu(1)	109.7(5)
		C(2)-O(5)-Cu(2)	113.3(5)
		Cu(1)-O(5)-Cu(2)	110.8(3)
		C(5)-O(6)-Cu(2)	128.7(6)
		C(5)-O(6)-Cu(3)	129.1(6)
		Cu(2)-O(6)-Cu(3)	98.2(3)
		C(14)-O(7)-Cu(4)	113.9(5)
		C(14)-O(7)-Cu(3)	115.4(5)
		Cu(4)-O(7)-Cu(3)	129.6(3)
		C(17)-O(8)-Cu(4)	129.8(6)
		C(17)-O(8)-Cu(5)	131.3(6)
		Cu(4)-O(8)-Cu(5)	98.9(3)
		C(26)-O(9)-Cu(5)	113.2(5)
		C(26)-O(9)-Cu(6)	110.5(5)
		Cu(5)-O(9)-Cu(6)	104.2(3)

Symmetry transformations used to generate equivalent atoms: #1 -x,y,-z+3/2

Table S3. Bond distances [Å] and angles [°] for **2.**

Bond lengths [Å]		**Bond angles [°] for 2**	
Cu(1)-O(4)	1.921(4)	O(4)-Cu(1)-N(1)	171.0(2)
Cu(1)-N(1)	1.928(5)	O(4)-Cu(1)-O(2)	103.10(18)

Cu(1)-O(2)	1.936(4)	N(1)-Cu(1)-O(2)	85.7(2)
Cu(1)-O(1)	1.940(5)	O(4)-Cu(1)-O(1)	80.19(18)
Cu(1)-Cu(2)	2.9204(11)	N(1)-Cu(1)-O(1)	91.1(2)
Cu(1)-Cu(2)#1	3.0600(12)	O(2)-Cu(1)-O(1)	176.34(19)
Cu(2)-O(4)	1.902(4)	O(4)-Cu(2)-N(2)	171.9(2)
Cu(2)-N(2)	1.925(6)	O(4)-Cu(2)-O(1)	80.67(18)
Cu(2)-O(1)	1.939(5)	N(2)-Cu(2)-O(1)	91.9(2)
Cu(2)-O(2)#2	1.948(4)	O(4)-Cu(2)-O(2)#2	102.28(18)
Cu(2)-O(3)	2.358(6)	N(2)-Cu(2)-O(2)#2	85.9(2)
Cu(2)-Cu(1)#2	3.0599(12)	O(1)-Cu(2)-O(2)#2	157.2(2)
B(1)-O(4)	1.378(4)	O(4)-Cu(2)-O(3)	92.22(18)
B(1)-O(4)#2	1.378(4)	N(2)-Cu(2)-O(3)	87.9(2)
B(1)-O(4)#1	1.378(4)	O(1)-Cu(2)-O(3)	115.0(2)
O(2)-Cu(2)#1	1.948(4)	O(2)#2-Cu(2)-O(3)	87.6(2)
		O(4)-B(1)-O(4)#2	119.97(4)
		O(4)-B(1)-O(4)#1	119.97(3)
		O(4)#2-B(1)-O(4)#1	119.97(4)
		Cu(2)-O(1)-Cu(1)	97.7(2)
		C(12)-O(2)-Cu(1)	112.6(4)
		C(12)-O(2)-Cu(2)#1	111.1(4)
		Cu(1)-O(2)-Cu(2)#1	104.0(2)
		C(13)-O(3)-Cu(2)	136.7(8)
		B(1)-O(4)-Cu(2)	127.1(3)
		B(1)-O(4)-Cu(1)	132.0(3)
		Cu(2)-O(4)-Cu(1)	99.62(19)

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

Table S4. Bond distances [Å] and angles [°] for **3.**

Bond lengths [Å]		**Bond angles [°] for 3**	
Cu(1)-O(9)	1.928(4)	O(9)-Cu(1)-O(4)	175.5(2)
Cu(1)-O(4)	1.931(4)	O(9)-Cu(1)-N(1)	85.4(2)
Cu(1)-N(1)	1.937(5)	O(4)-Cu(1)-N(1)	90.8(2)
Cu(1)-O(1)	2.007(4)	O(9)-Cu(1)-O(1)	102.95(17)
Cu(1)-O(11)	2.383(5)	O(4)-Cu(1)-O(1)	80.38(17)
Cu(2)-O(5)	1.867(4)	N(1)-Cu(1)-O(1)	166.5(2)
Cu(2)-O(1)	1.937(4)	O(9)-Cu(1)-O(11)	88.48(18)
Cu(2)-N(2)	1.942(5)	O(4)-Cu(1)-O(11)	94.9(2)
Cu(2)-O(4)	1.943(4)	N(1)-Cu(1)-O(11)	107.1(2)
Cu(3)-O(5)	1.867(4)	O(1)-Cu(1)-O(11)	83.98(18)
Cu(3)-O(6)	1.925(4)	O(5)-Cu(2)-O(1)	101.13(18)

Cu(3)-N(3)	1.930(5)	O(5)-Cu(2)-N(2)	84.6(2)
Cu(3)-O(2)	1.945(4)	O(1)-Cu(2)-N(2)	173.7(2)
Cu(4)-O(7)	1.926(4)	O(5)-Cu(2)-O(4)	176.97(18)
Cu(4)-O(6)	1.955(4)	O(1)-Cu(2)-O(4)	81.87(17)
Cu(4)-N(4)	1.961(6)	N(2)-Cu(2)-O(4)	92.4(2)
Cu(4)-O(2)	2.001(4)	O(5)-Cu(3)-O(6)	175.6(2)
Cu(4)-O(12)	2.403(6)	O(5)-Cu(3)-N(3)	84.9(2)
Cu(5)-O(7)	1.913(4)	O(6)-Cu(3)-N(3)	91.7(2)
Cu(5)-N(5)	1.923(6)	O(5)-Cu(3)-O(2)	100.28(18)
Cu(5)-O(3)	1.933(4)	O(6)-Cu(3)-O(2)	83.02(18)
Cu(5)-O(8)	1.942(5)	N(3)-Cu(3)-O(2)	174.2(2)
Cu(5)-O(10)	2.412(5)	O(7)-Cu(4)-O(6)	172.7(2)
Cu(6)-O(9)	1.910(4)	O(7)-Cu(4)-N(4)	84.5(2)
Cu(6)-N(6)	1.911(5)	O(6)-Cu(4)-N(4)	90.8(2)
Cu(6)-O(3)	1.930(4)	O(7)-Cu(4)-O(2)	102.97(18)
Cu(6)-O(8)	1.933(5)	O(6)-Cu(4)-O(2)	80.81(17)
O(1)-B(1)	1.401(8)	N(4)-Cu(4)-O(2)	167.5(2)
O(2)-B(1)	1.372(8)	O(7)-Cu(4)-O(12)	93.6(2)
O(3)-B(1)	1.352(8)	O(6)-Cu(4)-O(12)	92.8(2)
		N(4)-Cu(4)-O(12)	102.6(2)
		O(2)-Cu(4)-O(12)	87.1(2)
		O(7)-Cu(5)-N(5)	87.4(2)
		O(7)-Cu(5)-O(3)	98.12(18)
		N(5)-Cu(5)-O(3)	168.9(2)
		O(7)-Cu(5)-O(8)	177.89(19)
		N(5)-Cu(5)-O(8)	91.4(2)
		O(3)-Cu(5)-O(8)	83.27(18)
		O(7)-Cu(5)-O(10)	99.3(2)
		N(5)-Cu(5)-O(10)	103.0(2)
		O(3)-Cu(5)-O(10)	85.62(18)
		O(8)-Cu(5)-O(10)	79.23(19)
		O(9)-Cu(6)-N(6)	86.8(2)
		O(9)-Cu(6)-O(3)	97.53(18)
		N(6)-Cu(6)-O(3)	175.6(2)
		O(9)-Cu(6)-O(8)	172.78(19)
		N(6)-Cu(6)-O(8)	92.0(2)
		O(3)-Cu(6)-O(8)	83.60(19)
		B(1)-O(1)-Cu(2)	129.3(4)
		B(1)-O(1)-Cu(1)	127.6(4)
		Cu(2)-O(1)-Cu(1)	97.43(18)
		B(1)-O(2)-Cu(3)	132.1(4)
		B(1)-O(2)-Cu(4)	128.0(4)
		Cu(3)-O(2)-Cu(4)	96.74(18)
		B(1)-O(3)-Cu(6)	129.6(4)
		B(1)-O(3)-Cu(5)	129.8(4)
		Cu(6)-O(3)-Cu(5)	92.95(18)

	C(11)-O(4)-Cu(1)	130.3(4)
	C(11)-O(4)-Cu(2)	129.6(4)
	Cu(1)-O(4)-Cu(2)	99.87(19)
	C(14)-O(5)-Cu(2)	113.6(4)
	C(14)-O(5)-Cu(3)	113.6(4)
	Cu(2)-O(5)-Cu(3)	129.7(2)
	C(26)-O(6)-Cu(3)	129.7(4)
	C(26)-O(6)-Cu(4)	129.6(4)
	Cu(3)-O(6)-Cu(4)	99.00(19)
	C(29)-O(7)-Cu(5)	110.0(4)
	C(29)-O(7)-Cu(4)	112.5(4)
	Cu(5)-O(7)-Cu(4)	105.7(2)
	C(41)-O(8)-Cu(6)	126.9(4)
	C(41)-O(8)-Cu(5)	123.7(4)
	Cu(6)-O(8)-Cu(5)	92.58(19)
	C(44)-O(9)-Cu(6)	111.0(4)
	C(44)-O(9)-Cu(1)	112.2(3)
	Cu(6)-O(9)-Cu(1)	102.4(2)
	C(46)-O(10)-Cu(5)	127.1(5)
	O(3)-B(1)-O(2)	120.3(6)
	O(3)-B(1)-O(1)	118.2(6)
	O(2)-B(1)-O(1)	121.5(6)

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

Table S5. Bond distances (Å) and angles (º) for **4**.

Bond lengths [Å]		**Bond angles [°] for 6**	
Cu(1)-O(9)	1.83(2)	O(9)-Cu(1)-O(4)	167.7(11)
Cu(1)-O(4)	1.88(2)	O(9)-Cu(1)-O(1)	99.8(10)
Cu(1)-O(1)	1.89(2)	O(4)-Cu(1)-O(1)	84.3(10)
Cu(1)-N(2)	1.96(3)	O(9)-Cu(1)-N(2)	84.0(11)
Cu(2)-O(5)	1.92(2)	O(4)-Cu(1)-N(2)	90.8(11)
Cu(2)-N(1)	1.94(3)	O(1)-Cu(1)-N(2)	173.1(10)
Cu(2)-O(4)	1.94(3)	O(5)-Cu(2)-N(1)	87.0(11)
Cu(2)-O(1)	1.98(2)	O(5)-Cu(2)-O(4)	173.6(10)
Cu(3)-O(5)	1.88(2)	N(1)-Cu(2)-O(4)	90.4(12)
Cu(3)-O(3)	1.88(2)	O(5)-Cu(2)-O(1)	101.1(9)
Cu(3)-N(6)	1.90(3)	N(1)-Cu(2)-O(1)	166.6(11)
Cu(3)-O(6)	1.98(3)	O(4)-Cu(2)-O(1)	80.3(9)
Cu(4)-O(7)	1.86(2)	O(5)-Cu(3)-O(3)	96.9(10)
Cu(4)-O(3)	1.89(2)	O(5)-Cu(3)-N(6)	87.4(12)
Cu(4)-N(5)	1.94(3)	O(3)-Cu(3)-N(6)	174.8(12)
Cu(4)-O(6)	1.95(2)	O(5)-Cu(3)-O(6)	174.8(10)
Cu(5)-O(7)	1.93(2)	O(3)-Cu(3)-O(6)	85.5(10)

Cu(5)-O(8)	1.92(2)	N(6)-Cu(3)-O(6)	90.6(12)
Cu(5)-N(4)	1.94(3)	O(7)-Cu(4)-O(3)	97.7(10)
Cu(5)-O(2)	1.98(2)	O(7)-Cu(4)-N(5)	88.7(13)
Cu(5)-O(10)	2.66(4)	O(3)-Cu(4)-N(5)	173.3(13)
Cu(6)-O(9)	1.85(2)	O(7)-Cu(4)-O(6)	172.4(11)
Cu(6)-O(2)	1.93(2)	O(3)-Cu(4)-O(6)	86.2(11)
Cu(6)-O(8)	1.97(2)	N(5)-Cu(4)-O(6)	87.7(14)
Cu(6)-N(3)	1.96(3)	O(7)-Cu(5)-O(8)	174.4(10)
O(2)-B(1)	1.36(5)	O(7)-Cu(5)-N(4)	80.4(15)
O(1)-B(1)	1.35(4)	O(8)-Cu(5)-N(4)	94.2(15)
O(3)-B(1)	1.40(5)	O(7)-Cu(5)-O(2)	101.7(10)
		O(8)-Cu(5)-O(2)	83.1(9)
		N(4)-Cu(5)-O(2)	164.8(11)
		O(7)-Cu(5)-O(10)	98.0(11)
		O(8)-Cu(5)-O(10)	85.4(11)
		N(4)-Cu(5)-O(10)	110.4(11)
		O(2)-Cu(5)-O(10)	84.3(10)
		O(9)-Cu(6)-O(2)	100.9(10)
		O(9)-Cu(6)-O(8)	170.6(11)
		O(2)-Cu(6)-O(8)	83.2(9)
		O(9)-Cu(6)-N(3)	83.1(13)
		O(2)-Cu(6)-N(3)	175.9(12)
		O(8)-Cu(6)-N(3)	92.6(13)
		C(34)-O(4)-Cu(1)	137(2)
		C(34)-O(4)-Cu(2)	123.7(19)
		Cu(1)-O(4)-Cu(2)	98.6(11)
		C(3)-O(6)-Cu(4)	126(2)
		C(3)-O(6)-Cu(3)	122(2)
		Cu(4)-O(6)-Cu(3)	88.3(12)
		C(13)-N(4)-Cu(5)	120(3)
		C(19)-N(4)-Cu(5)	116(3)
		C(38)-O(8)-Cu(5)	131(2)
		C(38)-O(8)-Cu(6)	132(2)
		Cu(5)-O(8)-Cu(6)	96.9(11)
		C(29)-O(9)-Cu(1)	116(2)
		C(29)-O(9)-Cu(6)	114(2)
		Cu(1)-O(9)-Cu(6)	129.8(14)
		C(12)-O(7)-Cu(4)	109(2)
		C(12)-O(7)-Cu(5)	116(2)
		Cu(4)-O(7)-Cu(5)	103.0(10)
		C(71)-O(10)-Cu(5)	132(7)
		C(93)-O(5)-Cu(3)	111(2)
		C(93)-O(5)-Cu(2)	114.8(19)
		Cu(3)-O(5)-Cu(2)	104.6(10)
		B(1)-O(1)-Cu(1)	131(3)
		B(1)-O(1)-Cu(2)	128(3)

	Cu(1)-O(1)-Cu(2) 96.6(9) B(1)-O(3)-Cu(3) 130(2) B(1)-O(3)-Cu(4) 130(2) Cu(3)-O(3)-Cu(4) 93.1(10) O(3)-B(1)-O(1) 119(4) O(3)-B(1)-O(2) 117(4) O(1)-B(1)-O(2) 123(4)

Table S6. Bond distances [Å] and angles [°] for **5**

Bond lengths [Å]		**angles [°] for 5**	
Cu(1)-O(1)	1.889(4)	O(1)-Cu(1)-O(2)	176.39(18)
Cu(1)-O(2)	1.921(4)	O(1)-Cu(1)-N(1)	84.7(2)
Cu(1)-N(1)	1.927(5)	O(2)-Cu(1)-N(1)	92.2(2)
Cu(1)-O(11)	1.962(4)	O(1)-Cu(1)-O(11)	102.42(18)
Cu(2)-O(3)	1.889(4)	O(2)-Cu(1)-O(11)	80.88(17)
Cu(2)-O(2)	1.914(4)	N(1)-Cu(1)-O(11)	170.2(2)
Cu(2)-N(2)	1.929(5)	O(3)-Cu(2)-O(2)	176.59(18)
Cu(2)-O(11)	1.955(4)	O(3)-Cu(2)-N(2)	84.68(19)
Cu(3)-O(3)	1.864(4)	O(2)-Cu(2)-N(2)	92.34(19)
Cu(3)-O(4)	1.932(4)	O(3)-Cu(2)-O(11)	101.76(18)
Cu(3)-N(3)	1.950(5)	O(2)-Cu(2)-O(11)	81.23(18)
Cu(3)-O(12)	1.977(4)	N(2)-Cu(2)-O(11)	173.57(19)
Cu(3)-O(7)	2.326(5)	O(3)-Cu(3)-O(4)	170.99(19)
Cu(4)-O(5)	1.922(4)	O(3)-Cu(3)-N(3)	83.23(19)
Cu(4)-N(4)	1.941(6)	O(4)-Cu(3)-N(3)	91.0(2)
Cu(4)-O(4)	1.943(4)	O(3)-Cu(3)-O(12)	101.55(17)
Cu(4)-O(12)	1.987(4)	O(4)-Cu(3)-O(12)	83.32(18)
Cu(4)-O(8)	2.272(6)	N(3)-Cu(3)-O(12)	171.4(2)
Cu(5)-O(10)	1.904(4)	O(3)-Cu(3)-O(7)	93.56(19)
Cu(5)-O(5)	1.908(5)	O(4)-Cu(3)-O(7)	94.5(2)
Cu(5)-N(5)	1.925(6)	N(3)-Cu(3)-O(7)	102.4(2)
Cu(5)-O(6)	1.955(5)	O(12)-Cu(3)-O(7)	84.49(18)
Cu(6)-O(1)	1.911(4)	O(5)-Cu(4)-N(4)	83.8(2)
Cu(6)-O(6)	1.929(5)	O(5)-Cu(4)-O(4)	171.2(2)
Cu(6)-O(10)	1.934(4)	N(4)-Cu(4)-O(4)	90.4(2)
Cu(6)-N(6)	1.940(6)	O(5)-Cu(4)-O(12)	101.41(18)
Cu(6)-O(9)	2.430(6)	N(4)-Cu(4)-O(12)	166.1(2)
B(2)-O(12)	1.381(8)	O(4)-Cu(4)-O(12)	82.78(17)
B(2)-O(10)	1.389(7)	O(5)-Cu(4)-O(8)	96.6(2)
B(2)-O(11)	1.393(9)	N(4)-Cu(4)-O(8)	99.1(2)
		O(4)-Cu(4)-O(8)	90.8(2)
		O(12)-Cu(4)-O(8)	93.1(2)
		O(10)-Cu(5)-O(5)	98.95(19)

	O(10)-Cu(5)-N(5)	169.1(2)
	O(5)-Cu(5)-N(5)	87.1(2)
	O(10)-Cu(5)-O(6)	83.43(19)
	O(5)-Cu(5)-O(6)	176.25(19)
	N(5)-Cu(5)-O(6)	91.0(2)
	O(1)-Cu(6)-O(6)	164.89(19)
	O(1)-Cu(6)-O(10)	97.42(17)
	O(6)-Cu(6)-O(10)	83.34(19)
	O(1)-Cu(6)-N(6)	85.5(2)
	O(6)-Cu(6)-N(6)	92.5(2)
	O(10)-Cu(6)-N(6)	174.2(2)
	O(1)-Cu(6)-O(9)	89.5(2)
	O(6)-Cu(6)-O(9)	105.4(2)
	O(10)-Cu(6)-O(9)	96.68(19)
	N(6)-Cu(6)-O(9)	88.3(2)
	O(12)-B(2)-O(10)	118.9(6)
	O(12)-B(2)-O(11)	124.1(5)
	O(10)-B(2)-O(11)	117.0(6)
	C(1)-O(1)-Cu(1)	112.3(4)
	C(1)-O(1)-Cu(6)	112.7(3)
	Cu(1)-O(1)-Cu(6)	104.16(19)
	C(9)-O(2)-Cu(2)	130.1(4)
	C(9)-O(2)-Cu(1)	129.5(4)
	Cu(2)-O(2)-Cu(1)	100.34(19)
	C(16)-O(3)-Cu(3)	115.8(3)
	C(16)-O(3)-Cu(2)	111.1(3)
	Cu(3)-O(3)-Cu(2)	128.4(2)
	C(24)-O(4)-Cu(3)	129.3(4)
	C(24)-O(4)-Cu(4)	128.0(4)
	Cu(3)-O(4)-Cu(4)	96.55(19)
	C(31)-O(5)-Cu(5)	109.1(4)
	C(31)-O(5)-Cu(4)	112.7(4)
	Cu(5)-O(5)-Cu(4)	107.8(2)
	C(35)-O(6)-Cu(6)	128.0(5)
	C(35)-O(6)-Cu(5)	126.2(5)
	Cu(6)-O(6)-Cu(5)	93.95(18)
	C(46)-O(7)-Cu(3)	124.4(5)
	C(46)-O(8)-Cu(4)	120.2(5)
	C(48)-O(9)-Cu(6)	113.5(10)
	B(2)-O(10)-Cu(5)	131.6(4)
	B(2)-O(10)-Cu(6)	127.0(4)
	Cu(5)-O(10)-Cu(6)	95.42(18)
	B(2)-O(11)-Cu(2)	129.4(4)
	B(2)-O(11)-Cu(1)	131.2(4)
	Cu(2)-O(11)-Cu(1)	97.5(2)
	B(2)-O(12)-Cu(3)	127.0(4)

	B(2)-O(12)-Cu(4)	129.0(4)
	Cu(3)-O(12)-Cu(4)	93.71(18)

Table S7. Bond distances [Å] and angles [°] for **6.**

Bond lengths [Å]		**Bond angles [°] for 6**	
Cu(1)-N(1)	1.939(4)	N(1)-Cu(1)-O(2)	92.45(14)
Cu(1)-O(2)	1.958(3)	N(1)-Cu(1)-N(2)	95.89(16)
Cu(1)-N(2)	1.958(4)	O(2)-Cu(1)-N(2)	170.53(15)
Cu(1)-O(1)	1.964(3)	N(1)-Cu(1)-O(1)	161.36(14)
Cu(1)-O(3)	2.291(3)	O(2)-Cu(1)-O(1)	76.58(12)
Cu(2)-N(3)	1.953(4)	N(2)-Cu(1)-O(1)	94.19(15)
Cu(2)-O(1)	1.967(3)	N(1)-Cu(1)-O(3)	93.92(15)
Cu(2)-O(2)	1.972(3)	O(2)-Cu(1)-O(3)	87.78(13)
Cu(2)-N(4)	1.972(4)	N(2)-Cu(1)-O(3)	96.09(15)
Cu(2)-F(1)	2.394(3)	O(1)-Cu(1)-O(3)	100.57(13)
		N(3)-Cu(2)-O(1)	168.35(15)
		N(3)-Cu(2)-O(2)	92.72(14)
		O(1)-Cu(2)-O(2)	76.19(12)
		N(3)-Cu(2)-N(4)	98.21(16)
		O(1)-Cu(2)-N(4)	92.92(14)
		O(2)-Cu(2)-N(4)	169.06(14)
		N(3)-Cu(2)-F(1)	91.84(17)
		O(1)-Cu(2)-F(1)	91.73(16)
		O(2)-Cu(2)-F(1)	90.02(12)
		N(4)-Cu(2)-F(1)	89.30(14)
		C(1)-O(1)-Cu(1)	127.1(3)
		C(1)-O(1)-Cu(2)	128.3(3)
		Cu(1)-O(1)-Cu(2)	103.53(14)
		C(10)-O(2)-Cu(1)	126.5(3)
		C(10)-O(2)-Cu(2)	129.0(3)
		Cu(1)-O(2)-Cu(2)	103.61(14)
		C(25)-O(3)-Cu(1)	129.7(4)