Copper/zinc directed heterometallic uranyl-organic polycatenating frameworks: synthesis, characterization and anion-dependent structural regulation

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Supporting information

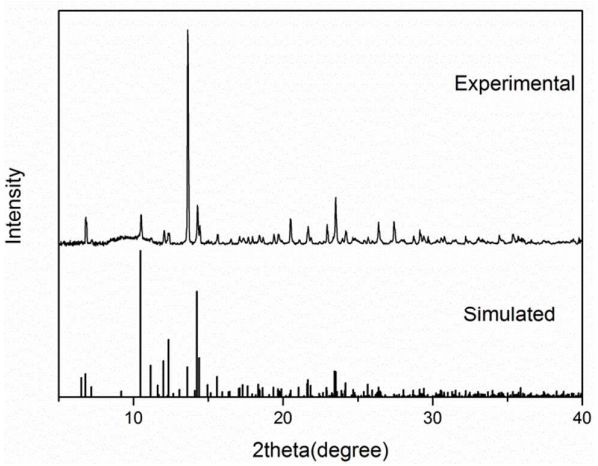

Figure S1. Powder patterns: an experimental PXRD for **1-Cu** and the simulated PXRD pattern calculated from single-crystal structure of **1-Cu**.

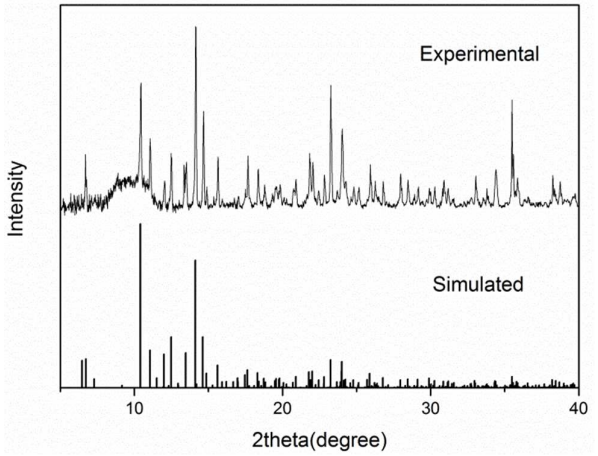

Figure S2. Powder patterns: an experimental PXRD for **1'-Zn** and the simulated PXRD pattern calculated from single-crystal structure of **1'-Zn**.

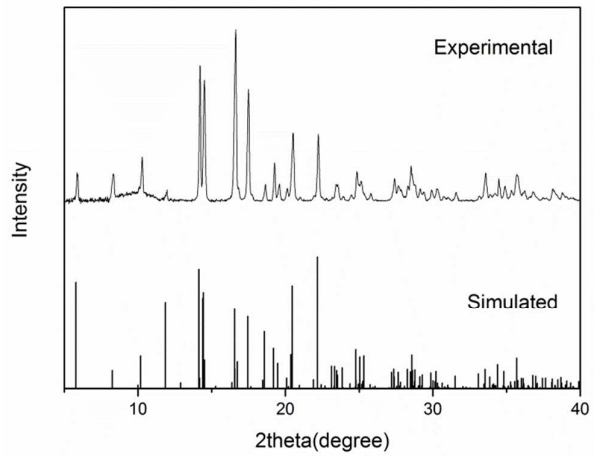

Figure S3. Powder patterns: an experimental PXRD for **2-Cu** and the simulated PXRD pattern calculated from single-crystal structure of **2-Cu.**

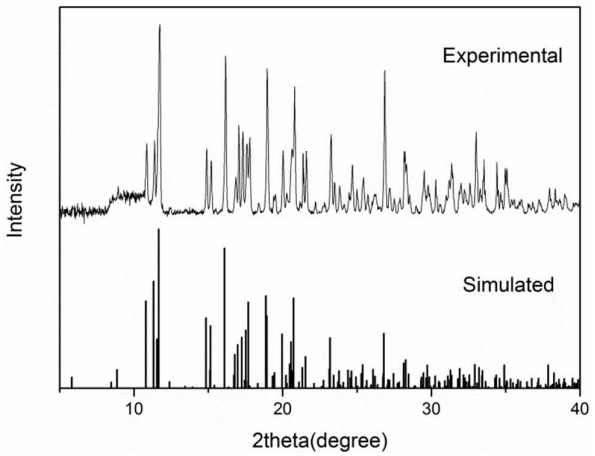

Figure S4. Powder patterns: an experimental PXRD for **3-Zn** and the simulated PXRD pattern calculated from single-crystal structure of **3-Zn.**

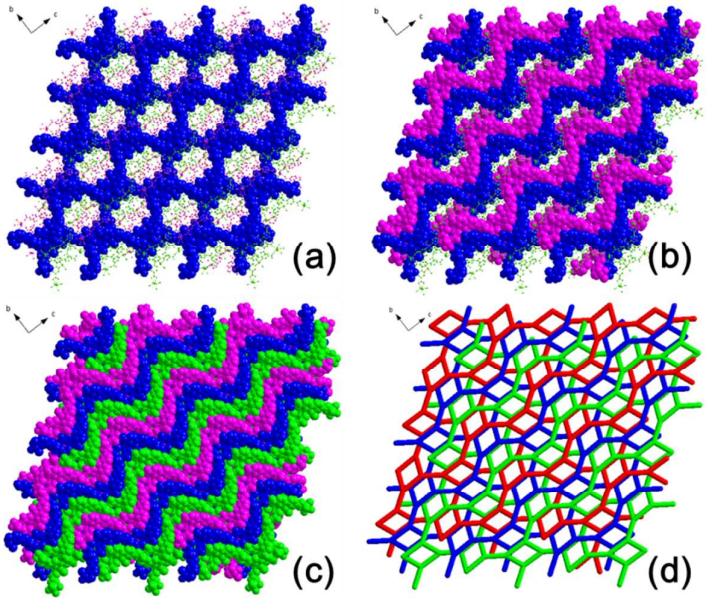

Figure S5. The three-fold interpenetration of 2D networks in **2-Cu**.

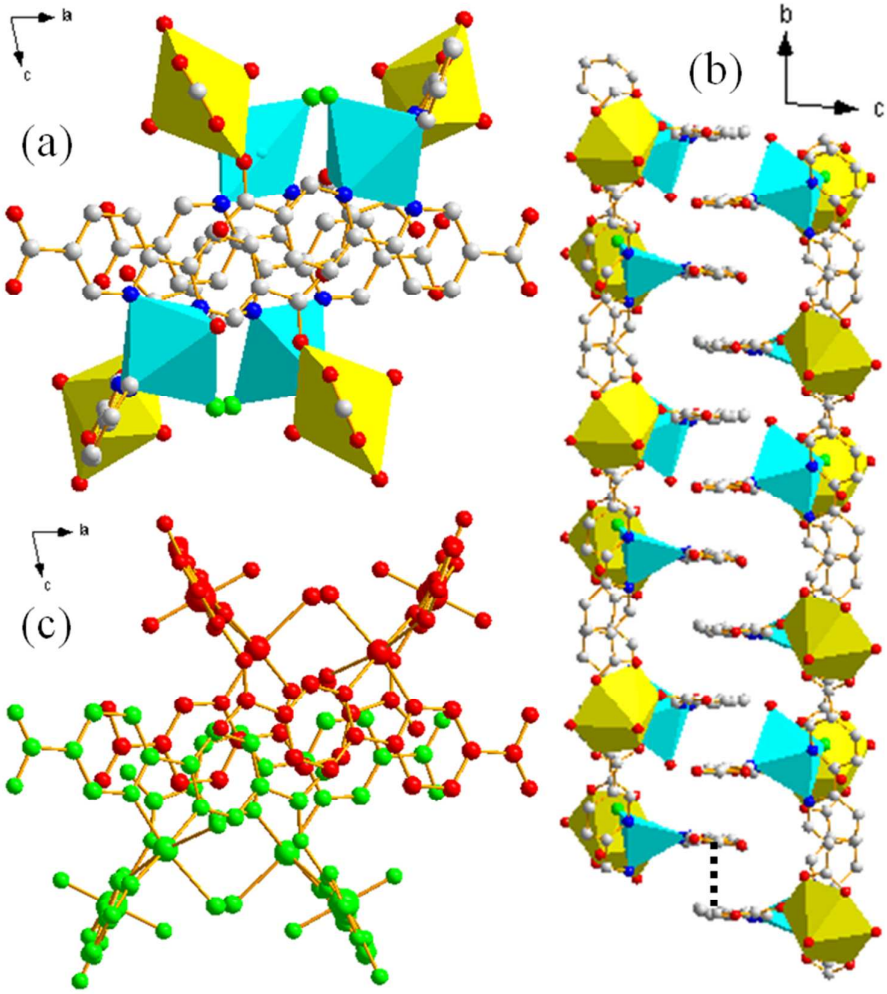

Figure S6. The assembling of the "ladder" through π-π stacking interaction in **2-Cu'**. The average distance between Hbpdc- "rungs" in (b) is about 3.5 Å (dotted line, as an example). Different colors in (c) representing different isolated "ladder".

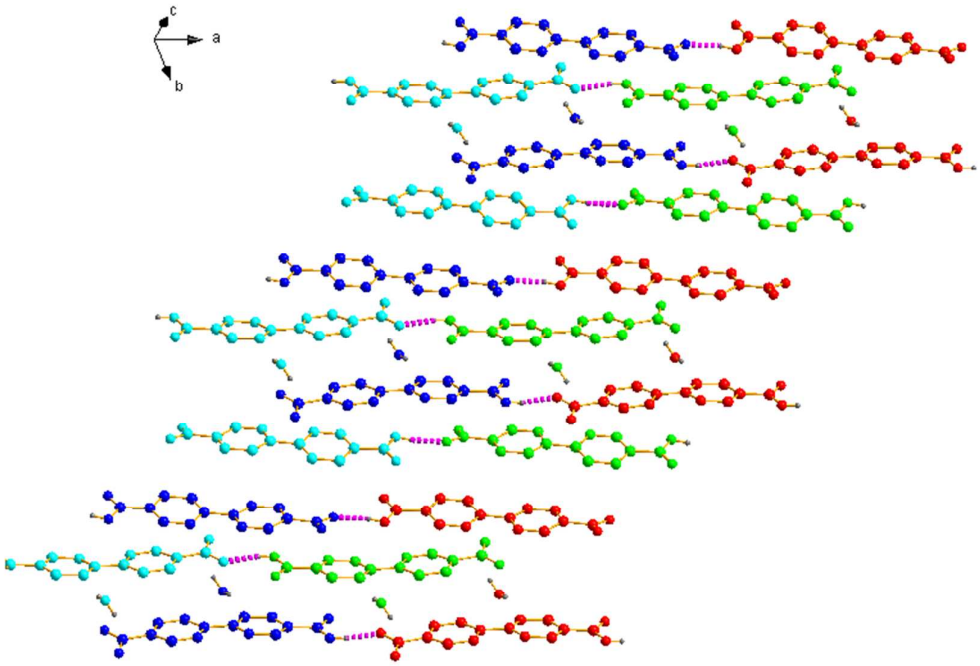

Figure S7. The presence of inter-ladder H-bonds in **2-Cu'** (dotted lines).

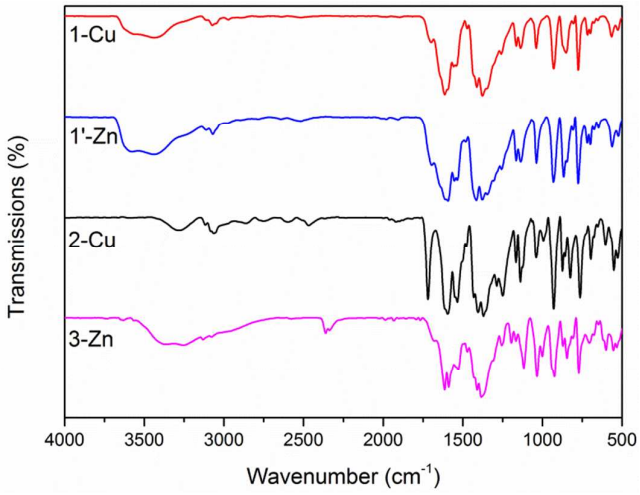

Figure S8. The IR spectrum of **1-Cu**, **1'-Zn**, **2-Cu**, and **3-Zn**.

Table S1. The product of hydrothermal synthesis by choosing different transition metal salts

	NO_3^-	Cl^-	SO_4^{2-}
Cu	**1-Cu**	**2-Cu (2-Cu')**	**1-Cu**
Zn	**1'-Zn**	**1'-Zn**	**3-Zn**

Table S2. Selected Bond Lengths (Å) and Bond Angles (°) for **1-Cu**

Bond	Dist.	Bond	Dist.
U(1)-O(1)	1.738(9)	Cu(1)-O(9)iv	2.699(14)
U(1)-O(2)	1.746(8)	Cu(1)-O(10)iv	1.992(10)
U(1)-O(5)i	2.301(7)	Cu(1)-N(3)	1.995(8)
U(1)-O(3)	2.358(7)	Cu(1)-N(2)	2.021(8)
U(1)-O(4)ii	2.366(7)	Cu(1)-N(4)	2.054(10)
U(1)-O(8)iii	2.461(8)	Cu(1)-N(1)	2.119(9)
U(1)-O(7)iii	2.488(7)		
Angle	(°)	Angle	(°)
O(1)-U(1)-O(2)	178.4(4)	O(10)iv-Cu(1)-N(3)	94.0(4)
O(1)-U(1)-O(5)i	86.3(3)	O(10)iv-Cu(1)-N(2)	88.2(4)
O(2)-U(1)-O(5)i	95.1(4)	N(3)-Cu(1)-N(2)	177.4(3)
O(1)-U(1)-O(3)	89.2(3)	O(10)iv-Cu(1)-N(4)	128.4(4)
O(2)-U(1)-O(3)	89.2(3)	N(3)-Cu(1)-N(4)	80.2(4)
O(5)i-U(1)-O(3)	159.5(3)	N(2)-Cu(1)-N(4)	99.5(4)
O(1)-U(1)-O(4)ii	89.5(3)	O(10)iv-Cu(1)-N(1)	130.3(4)
O(2)-U(1)-O(4)ii	90.2(3)	N(3)-Cu(1)-N(1)	99.2(3)
O(5)i-U(1)-O(4)ii	77.1(3)	N(2)-Cu(1)-N(1)	78.4(3)
O(3)-U(1)-O(4)ii	82.9(3)	N(4)-Cu(1)-N(1)	101.1(4)
O(1)-U(1)-O(8)iii	89.7(4)	N(3)-Cu(1)-O(9)iv	90.080(382)
O(2)-U(1)-O(8)iii	91.4(3)	N(2)-Cu(1)-O(9)iv	90.183(368)
O(5)i-U(1)-O(8)iii	72.5(3)	N(1)-Cu(1)-O(9)iv	78.706(369)
O(3)-U(1)-O(8)iii	127.6(3)	N(4)-Cu(1)-O(9)iv	170.123(362)
O(4)ii-U(1)-O(8)iii	149.5(2)	O(10)iv-Cu(1)-O(9)iv	53.443(345)
O(1)-U(1)-O(7)iii	88.5(4)		
O(2)-U(1)-O(7)iii	91.2(3)		
O(5)i-U(1)-O(7)iii	125.1(3)		
O(3)-U(1)-O(7)iii	74.7(3)		
O(4)ii-U(1)-O(7)iii	157.5(2)		
O(8)iii-U(1)-O(7)iii	52.8(2)		

Symmetry transformation: (i): -0.5+*x*, 0.5+*y*, *z*; (ii): 1.5–*x*, 1.5-*y*, 1–*z*; (iii): *x*, 1–*y*, 0.5+*z*; (iv): *x*, 1–*y*, -0.5+*z*.

Table S3. Selected Bond Lengths (Å) and Bond Angles (°) for **1'-Zn**

Bond	Dist.	Bond	Dist.
U(1)-O(3)	1.764(4)	Zn(1)-O(8)	2.080(4)
U(1)-O(4)	1.766(4)	Zn(1)-N(3)iv	2.092(4)
U(1)-O(5)i	2.333(3)	Zn(1)-N(2)	2.099(4)
U(1)-O(2)ii	2.352(3)	Zn(1)-N(4)iv	2.101(4)
U(1)-O(1)	2.367(3)	Zn(1)-N(1)	2.167(4)
U(1)-O(10)iii	2.460(4)	Zn(1)-O(7)	2.394(4)
U(1)-O(9)iii	2.469(3)		
Angle	(°)	Angle	(°)
O(3)-U(1)-O(4)	178.44(16)	O(8)-Zn(1)-N(3)iv	115.32(15)
O(3)-U(1)-O(5)i	84.81(15)	O(8)-Zn(1)-N(2)	139.16(14)
O(4)-U(1)-O(5)i	96.35(15)	N(3)iv-Zn(1)-N(2)	104.07(15)
O(3)-U(1)-O(2)ii	91.31(15)	O(8)-Zn(1)-N(4)iv	97.19(16)
O(4)-U(1)-O(2)ii	87.93(14)	N(3)iv-Zn(1)-N(4)iv	77.71(14)
O(5)i-U(1)-O(2)ii	78.14(12)	N(2)-Zn(1)-N(4)iv	101.40(15)
O(3)-U(1)-O(1)	88.44(15)	O(8)-Zn(1)-N(1)	85.89(15)
O(4)-U(1)-O(1)	90.12(14)	N(3)iv-Zn(1)-N(1)	100.38(15)
O(5)i-U(1)-O(1)	160.08(12)	N(2)-Zn(1)-N(1)	76.54(14)
O(2)ii-U(1)-O(1)	83.31(11)	N(4)iv-Zn(1)-N(1)	176.84(16)
O(3)-U(1)-O(10)iii	90.59(16)	O(8)-Zn(1)-O(7)	58.36(14)
O(4)-U(1)-O(10)iii	90.75(15)	N(3)iv-Zn(1)-O(7)	165.56(14)
O(5)i-U(1)-O(10)iii	72.87(12)	N(2)-Zn(1)-O(7)	85.50(14)
O(2)ii-U(1)-O(10)iii	150.65(11)	N(4)iv-Zn(1)-O(7)	89.90(14)
O(1)-U(1)-O(10)iii	126.02(11)	N(1)-Zn(1)-O(7)	92.30(14)
O(3)-U(1)-O(9)iii	90.16(16)		
O(4)-U(1)-O(9)iii	90.00(15)		
O(5)i-U(1)-O(9)iii	125.35(12)		
O(2)ii-U(1)-O(9)iii	156.49(11)		
O(1)-U(1)-O(9)iii	73.28(11)		
O(10)iii-U(1)-O(9)iii	52.76(11)		

Symmetry transformation: (i) -0.5+x, 0.5+y, z; (ii) 0.5-x, 1.5-y, 1-z; (iii) x, y, 1+z; (iv) x, 1-y, 0.5+z.

Table S4. Selected Bond Lengths (Å) and Bond Angles (°) for **2-Cu**

Bond	Dist.	Bond	Dist.
U(1)-O(4)	2.277(3)	Cu(1)-N(2)ii	2.017(3)
U(1)-O(8)	2.492(3)	Cu(1)-N(1)ii	2.229(4)
U(1)-O(1)	1.751(4)	Cu(1)-Cl(1)	2.242(2)
U(1)-O(5)i	2.342(3)	Cu(1)-N(3)	2.031(3)
U(1)-O(1W)	2.463(3)	Cu(1)-N(4)	2.004(4)
U(1)-O(7)	2.445(3)		
U(1)-O(2)	1.754(3)		
Angle	(°)	Angle	(°)
O(4)-U(1)-O(8)	83.40(11)	N(2)ii-Cu(1)-N(3)	94.15(14)
O(4)-U(1)-O(5)i	85.10(12)	N(2)ii-Cu(1)-N(1)ii	77.17(13)
O(4)-U(1)-O(1)W	157.61(11)	N(2)ii-Cu(1)-Cl1	91.26(11)
O(4)-U(1)-O(7)	136.00(12)	N(4)-Cu(1)-N(2)ii	174.50(14)
O(1)-U(1)-O(4)	90.52(17)	N(4)-Cu(1)-N(3)	80.37(14)
O(1)-U(1)-O(8)	91.82(14)	N(4)-Cu(1)-N(1)ii	102.76(14)
O(1)-U(1)-O(5)i	91.25(15)	N(4)-Cu(1)-Cl(1)	93.69(11)
O(1)-U(1)-O(1)W	85.84(15)	N(3)-Cu(1)-N(1)ii	86.21(14)
O(1)-U(1)-O(7)	90.26(17)	N(3)-Cu(1)-Cl(1)	158.33(11)
O(1)-U(1)-O(2)	179.31(16)	N(1)ii-Cu(1)-Cl(1)	115.45(10)
O(5)i-U(1)-O(8)	168.12(10)		
O(5)i-U(1)-O(1)W	72.92(11)		
O(5)i-U(1)-O(7)	138.86(11)		
O(1)W-U(1)-O(8)	118.76(10)		
O(7)-U(1)-O(8)	52.61(10)		
O(7)-U(1)-O(1)W	66.20(11)		
O(2)-U(1)-O(4)	89.60(16)		
O(2)-U(1)-O(8)	88.87(13)		
O(2)-U(1)-O(5)i	88.09(14)		
O(2)-U(1)-O(1)W	93.79(13)		
O(2)-U(1)-O(7)	90.12(16)		

Symmetry transformation: (i): 1-x, 3-y, 1-z; (ii): x, 1.5-y, -0.5+z.

Table S5. Selected Bond Lengths (Å) and Bond Angles **(°)** for **2-Cu'**

Bond	Dist.	Bond	Dist.	Bond	Dist.
U(2)-O(8)	1.764(8)	U(1)-O(1)	1.769(8)	Cu(1)-N(1)	1.984(9)
U(2)-O(7)	1.783(8)	U(1)-O(2)	1.776(8)	Cu(1)-N(4)	1.985(9)
U(2)-O(13)	2.349(7)	U(1)-O(17)	2.343(7)	Cu(1)-N(3)	2.051(9)
U(2)-O(9)	2.464(8)	U(1)-O(5)	2.446(8)	Cu(1)-N(2)i	2.180(9)
U(2)-O(11)i	2.465(7)	U(1)-O(3)	2.482(7)	Cu(1)-Cl(2)	2.323(3)
U(2)-O(10)	2.522(7)	U(1)-O(1W)	2.517(7)	Cu(2)-N(5)	2.002(9)
U(2)-O(2W)	2.532(7)	U(1)-O(4)	2.530(8)	Cu(2)-N(8)	2.023(8)
U(2)-O(12)i	2.539(8)	U(1)-O(6)	2.585(8)	Cu(2)-N(6)	2.037(8)
				Cu(2)-N(7)	2.25(1)
				Cu(2)-Cl(1)	2.362(3)
				Cu(2)-O(3W)	2.606(10)
Angle	(°)	Angle	(°)	Angle	(°)
O(8)-U(2)-O(7)	179.0(4)	O(1)-U(1)-O(2)	179.2(3)	N(1)-Cu(1)-N(4)	173.2(4)
O(8)-U(2)-O(13)	94.4(3)	O(1)-U(1)-O(17)	95.7(3)	N(1)-Cu(1)-N(3)	93.9(4)
O(7)-U(2)-O(13)	85.4(3)	O(2)-U(1)-O(17)	84.2(3)	N(4)-Cu(1)-N(3)	81.0(3)
O(8)-U(2)-O(9)	90.4(3)	O(1)-U(1)-O(5)	92.7(3)	N(1)-Cu(1)-N(2)i	78.6(4)
O(7)-U(2)-O(9)	90.6(3)	O(2)-U(1)-O(5)	88.0(3)	N(4)-Cu(1)-N(2)i	106.8(3)
O(13)-U(2)-O(9)	118.1(3)	O(17)-U(1)-O(5)	117.6(3)	N(3)-Cu(1)-N(2)i	104.2(3)
O(8)-U(2)-O(11)i	89.4(3)	O(1)-U(1)-O(3)	90.2(3)	N(1)-Cu(1)-Cl(2)	88.1(3)
O(7)-U(2)-O(11)i	89.8(3)	O(2)-U(1)-O(3)	89.1(3)	N(4)-Cu(1)-Cl(2)	95.3(3)
O(13)-U(2)-O(11)i	119.4(3)	O(17)-U(1)-O(3)	120.3(3)	N(3)-Cu(1)-Cl(2)	160.9(3)
O(9)-U(2)-O(11)i	122.3(2)	O(5)-U(1)-O(3)	121.4(3)	N(2)i-Cu(1)-Cl(2)	94.9(3)
O(8)-U(2)-O(10)	86.0(3)	O(1)-U(1)-O(1W)	92.9(3)	N(5)-Cu(2)-N(8)	175.4(3)
O(7)-U(2)-O(10)	94.8(3)	O(2)-U(1)-O(1W)	87.1(3)	N(5)-Cu(2)-N(6)	80.7(3)
O(13)-U(2)-O(10)	66.7(3)	O(17)-U(1)-O(1W)	171.2(2)	N(8)-Cu(2)-N(6)	95.8(3)
O(9)-U(2)-O(10)	52.2(2)	O(5)-U(1)-O(1W)	60.2(3)	N(5)-Cu(2)-N(7)	106.4(3)
O(11)i-U(2)-O(10)	172.8(2)	O(3)-U(1)-O(1W)	61.2(3)	N(8)-Cu(2)-N(7)	77.0(3)
O(8)-U(2)-O(2W)	93.9(3)	O(1)-U(1)-O(4)	91.8(3)	N(6)-Cu(2)-N(7)	100.2(3)
O(7)-U(2)-O(2W)	86.3(3)	O(2)-U(1)-O(4)	87.4(3)	N(5)-Cu(2)-Cl(1)	94.5(2)
O(13)-U(2)-O(2W)	171.7(2)	O(17)-U(1)-O(4)	68.2(3)	N(8)-Cu(2)-Cl(1)	88.5(2)
O(9)-U(2)-O(2W)	61.7(2)	O(5)-U(1)-O(4)	172.2(3)	N(6)-Cu(2)-Cl(1)	169.4(3)
O(11)i-U(2)-O(2W)	60.8(2)	O(3)-U(1)-O(4)	52.2(2)	N(7)-Cu(2)-Cl(1)	90.1(2)
O(10)-U(2)-O(2W)	113.9(2)	O(1W)-U(1)-O(4)	113.2(3)		
O(8)-U(2)-O(12)i	91.9(3)	O(1)-U(1)-O(6)	87.5(3)		
O(7)-U(2)-O(12)i	87.0(3)	O(2)-U(1)-O(6)	93.2(3)		
O(13)-U(2)-O(12)i	67.4(2)	O(17)-U(1)-O(6)	67.1(3)		
O(9)-U(2)-O(12)i	173.8(2)	O(5)-U(1)-O(6)	51.6(2)		
O(11)i-U(2)-O(12)i	52.1(2)	O(3)-U(1)-O(6)	172.4(2)		
O(10)-U(2)-O(12)i	133.7(2)	O(1W)-U(1)-O(6)	111.7(3)		
O(2W)-U(2)-O(12)i	112.4(2)	O(4)-U(1)-O(6)	135.1(2)		

Symmetry transformation: (i): 1+ *x*, -1+*y*, *z*.

Table S6. Selected Bond Lengths (Å) and Bond Angles **(°)** for **3-Zn**

Bond	Dist.	Bond	Dist.	Bond	Dist.
U(1)-O(5)	2.482(3)	U(2)-O(11)	2.411(3)	Zn(1)-N(4)	2.135(4)
U(1)-O(6)	2.490(3)	U(2)-O(16)	2.359(3)	Zn(1)-N(3)	2.080(4)
U(1)-O(14)	2.341(3)	U(2)-O(12)	2.358(3)	Zn(1)-N(2)	2.068(3)
U(1)-O(3W)	2.400(3)	U(2)-O(7)	2.372(3)	Zn(1)-O(2W)	2.137(3)
U(1)-O(9)	2.321(3)	U(2)-O(1W)	2.445(4)	Zn(1)-O(13)	2.161(3)
U(1)-O(1)	1.765(3)	U(2)-O(4)	1.753(3)	Zn(1)-N(1)	2.132(4)
U(1)-O(2)	1.760(3)	U(2)-O(3)	1.767(4)		
Angle	(°)	Angle	(°)	Angle	(°)
O(5)-U(1)-O(6)	52.27(10)	O(11)-U(2)-O(1W)	146.60(12)	N(4)-Zn(1)-O(2W)	90.40(12)
O(14)-U(1)-O(5)	159.95(10)	O(16)-U(2)-O(11)	77.43(10)	N(4)-Zn(1)-O(13)	166.93(13)
O(14)-U(1)-O(6)	147.51(11)	O(16)-U(2)-O(7)	138.48(11)	N(3)-Zn(1)-N(4)	76.91(14)
O(14)-U(1)-O(3W)	76.85(11)	O(16)-U(2)-O(1W)	69.21(12)	N(3)-Zn(1)-O(2W)	91.92(13)
O(3W)-U(1)-O(5)	123.07(10)	O(12)-U(2)-O(11)	70.84(10)	N(3)-Zn(1)-O(13)	92.91(13)
O(3W)-U(1)-O(6)	70.8(1)	O(12)-U(2)-O(16)	147.65(10)	N(3)-Zn(1)-N(1)	97.87(14)
O(9)-U(1)-O(5)	84.65(10)	O(12)-U(2)-O(7)	73.83(10)	N(2)-Zn(1)-N(4)	99.38(13)
O(9)-U(1)-O(6)	136.85(10)	O(12)-U(2)-O(1W)	141.91(12)	N(2)-Zn(1)-N(3)	174.30(14)
O(9)-U(1)-O(14)	75.64(11)	O(7)-U(2)-O(11)	143.49(10)	N(2)-Zn(1)-O(2W)	92.43(13)
O(9)-U(1)-O(3W)	152.09(11)	O(7)-U(2)-O(1W)	69.81(12)	N(2)-Zn(1)-O(13)	91.35(13)
O(1)-U(1)-O(5)	92.53(13)	O(4)-U(2)-O(11)	87.76(14)	N(2)-Zn(1)-N(1)	78.48(13)
O(1)-U(1)-O(6)	90.19(13)	O(4)-U(2)-O(16)	90.26(14)	O(2W)-Zn(1)-O(13)	81.65(11)
O(1)-U(1)-O(14)	90.86(13)	O(4)-U(2)-O(12)	94.57(14)	N(1)-Zn(1)-N(4)	101.10(14)
O(1)-U(1)-O(3W)	86.54(13)	O(4)-U(2)-O(7)	86.12(15)	N(1)-Zn(1)-O(2W)	166.30(13)
O(1)-U(1)-O(9)	89.24(13)	O(4)-U(2)-O(1W)	93.9(2)	N(1)-Zn(1)-O(13)	88.28(13)
O(2)-U(1)-O(5)	87.10(13)	O(4)-U(2)-O(3)	178.90(17)		
O(2)-U(1)-O(6)	86.71(13)	O(3)-U(2)-O(11)	91.25(14)		
O(2)-U(1)-O(14)	90.72(13)	O(3)-U(2)-O(16)	89.06(14)		
O(2)-U(1)-O(3W)	90.62(14)	O(3)-U(2)-O(12)	85.55(14)		
O(2)-U(1)-O(9)	94.34(13)	O(3)-U(2)-O(7)	94.96(15)		
O(2)-U(1)-O(1)	176.35(15)	O(3)-U(2)-O(1W)	86.6(2)		