Supporting Information

Diverse Self-Assembly from Pre-Designed Conformationally Flexible Pentanuclear Clusters Observed in a Ternary Cu^{II}-Triazolate-Sulfoisophthalate System: Synthesis, Structure, and Magnetism

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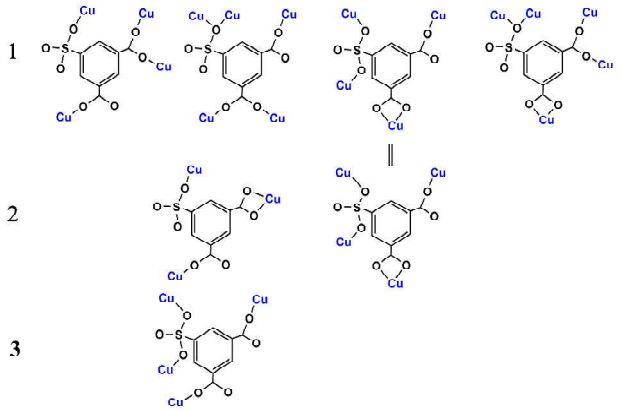

Figure S1. Binding modes of sip^{3-} ligand in **1–3**.

Table S1. Selected Bond Lengths (Å) and Angles (deg) for **1** [a]

Cu(1)–O(8)$^{\#1}$	1.978(4)	Cu(9)–O(34)	2.253(4)
Cu(1)–O(29)	2.009(4)	Cu(9)–N(54)	2.009(5)
Cu(1)–N(4)	2.022(5)	Cu(10)–O(22)	1.995(4)
Cu(1)–N(3)	2.030(5)	Cu(10)–N(24)$^{\#5}$	2.017(5)
Cu(1)–O(25)$^{\#2}$	2.183(4)	Cu(10)–N(46)	2.018(5)
Cu(2)–O(24)$^{\#2}$	1.943(4)	Cu(10)–O(34)	2.029(4)
Cu(2)–N(45)$^{\#3}$	1.994(5)	Cu(10)–O(11)$^{\#4}$	2.150(4)
Cu(2)–N(9)	2.010(5)	Cu(11)–O(31)	1.938(4)
Cu(2)–N(5)	2.029(5)	Cu(11)–N(19)	1.969(5)
Cu(2)–O(29)	2.252(4)	Cu(11)–N(14)	1.968(5)
Cu(3)–O(29)	1.909(4)	Cu(11)–N(12)	2.016(5)
Cu(3)–O(30)	1.941(4)	Cu(11)–O(37)	2.550(6)
Cu(3)–N(2)	1.983(5)	Cu(12)–O(4)$^{\#6}$	1.966(4)
Cu(3)–N(8)	2.053(5)	Cu(12)–N(16)	1.990(6)
Cu(4)–N(10)	1.979(5)	Cu(12)–O(31)	1.991(4)
Cu(4)–O(30)	1.994(4)	Cu(12)–N(15)	2.013(5)
Cu(4)–N(58)	1.999(5)	Cu(12)–O(18)$^{\#7}$	2.320(4)
Cu(4)–N(1)	2.022(5)	Cu(13)–O(32)	1.940(4)
Cu(4)–N(56)	2.295(5)	Cu(13)–O(31)	1.964(4)
Cu(5)–N(7)	1.984(5)	Cu(13)–N(17)	1.967(5)
Cu(5)–N(13)	2.000(5)	Cu(13)–N(20)	2.011(5)
Cu(5)–N(11)	2.021(5)	Cu(13)–O(38)	2.310(4)
Cu(5)–N(55)	2.028(5)	Cu(14)–N(22)	2.018(5)
Cu(5)–O(30)	2.283(4)	Cu(14)–N(28)	2.020(5)
Cu(6)–O(33)	1.972(4)	Cu(14)–N(26)	2.021(5)
Cu(6)–N(57)	1.980(5)	Cu(14)–N(21)	2.027(5)
Cu(6)–N(49)	2.000(5)	Cu(14)–O(32)	2.324(4)
Cu(6)–N(48)	2.036(6)	Cu(14)–O(26)	2.521(4)
Cu(6)–N(59)	2.360(5)	Cu(15)–O(32)	1.973(4)
Cu(7)–N(52)	1.979(5)	Cu(15)–N(31)	1.973(5)
Cu(7)–N(42)$^{\#1}$	2.003(5)	Cu(15)–N(25)	1.993(5)
Cu(7)–N(50)	2.007(5)	Cu(15)–N(18)	2.028(5)
Cu(7)–N(60)	2.029(5)	Cu(15)–N(29)	2.303(5)
Cu(7)–O(33)	2.251(4)	Cu(16)–O(35)	1.973(4)
Cu(8)–O(34)	1.918(4)	Cu(16)–N(43)	1.983(5)
Cu(8)–O(33)	1.940(4)	Cu(16)–N(30)	1.989(5)
Cu(8)–N(47)	1.968(5)	Cu(16)–N(34)	2.013(5)
Cu(8)–N(53)	2.031(5)	Cu(16)–N(32)	2.278(5)
Cu(8)–O(6)	2.400(4)	Cu(17)–N(6)$^{\#3}$	2.001(5)
Cu(9)–O(10)$^{\#4}$	1.942(4)	Cu(17)–N(37)	2.004(5)
Cu(9)–N(27)$^{\#5}$	1.997(5)	Cu(17)–N(33)	2.012(5)
Cu(9)–N(23)$^{\#5}$	2.006(5)	Cu(17)–N(44)	2.037(5)

Cu(17)–O(14)	2.506(4)	Cu(19)–O(15)	2.030(4)
Cu(17)–O(35)	2.296(4)	Cu(19)–O(36)	2.035(4)
Cu(18)–O(35)	1.921(4)	Cu(19)–O(1)$^{\#5}$	2.115(4)
Cu(18)–N(35)	1.988(5)	Cu(20)–O(2)$^{\#5}$	1.999(4)
Cu(18)–N(38)	2.064(5)	Cu(20)–N(39)	2.001(5)
Cu(18)–O(39)	2.263(5)	Cu(20)–N(41)	2.014(5)
Cu(18)–O(36)	1.916(2)	Cu(20)–N(51)$^{\#8}$	2.064(5)
Cu(19)–N(36)	2.003(5)	Cu(20)–O(36)	2.237(4)
Cu(19)–N(40)	2.016(5)		
O(8)$^{\#1}$–Cu(1)–O(29)	151.92(16)	N(13)–Cu(5)–N(11)	93.2(2)
O(8)$^{\#1}$–Cu(1)–N(4)	91.32(18)	N(7)–Cu(5)–N(55)	87.1(2)
O(29)–Cu(1)–N(4)	88.71(17)	N(13)–Cu(5)–N(55)	164.5(2)
O(8)$^{\#1}$–Cu(1)–N(3)	89.85(19)	N(11)–Cu(5)–N(55)	92.4(2)
O(29)–Cu(1)–N(3)	87.69(18)	N(7)–Cu(5)–O(30)	92.36(17)
N(4)–Cu(1)–N(3)	174.42(19)	N(13)–Cu(5)–O(30)	109.58(18)
O(8)$^{\#1}$–Cu(1)–O(25)$^{\#2}$	109.99(16)	N(11)–Cu(5)–O(30)	82.51(18)
O(29)–Cu(1)–O(25)$^{\#2}$	98.02(15)	N(55)–Cu(5)–O(30)	85.44(17)
N(4)–Cu(1)–O(25)$^{\#2}$	93.93(18)	O(33)–Cu(6)–N(49)	88.39(18)
O(24)$^{\#2}$–Cu(2)–N(9)	86.06(18)	N(57)–Cu(6)–N(49)	92.7(2)
N(45)$^{\#3}$–Cu(2)–N(9)	89.1(2)	O(33)–Cu(6)–N(48)	89.35(18)
O(24)$^{\#2}$–Cu(2)–N(5)	95.87(19)	N(57)–Cu(6)–N(48)	89.2(2)
N(45)$^{\#3}$–Cu(2)–N(5)	90.3(2)	O(33)–Cu(6)–N(59)	89.81(16)
O(24)$^{\#2}$–Cu(2)–O(29)	95.05(15)	N(57)–Cu(6)–N(59)	100.25(18)
N(45)$^{\#3}$–Cu(2)–O(29)	94.14(17)	N(49)–Cu(6)–N(59)	82.01(19)
N(9)–Cu(2)–O(29)	88.50(17)	N(48)–Cu(6)–N(59)	99.9(2)
O(29)–Cu(3)–N(2)	88.7(2)	N(52)–Cu(7)–N(42)$^{\#1}$	91.3(2)
O(30)–Cu(3)–N(2)	88.1(2)	N(42)$^{\#1}$–Cu(7)–N(50)	89.7(2)
O(29)–Cu(3)–N(8)	91.66(18)	N(52)–Cu(7)–N(60)	92.6(2)
O(30)–Cu(3)–N(8)	94.57(18)	N(50)–Cu(7)–O(33)	83.98(17)
N(2)–Cu(3)–N(8)	142.5(2)	N(50)–Cu(7)–N(60)	88.6(2)
N(10)–Cu(4)–O(30)	88.74(18)	N(52)–Cu(7)–O(33)	88.68(17)
N(10)–Cu(4)–N(58)	92.3(2)	N(42)$^{\#1}$–Cu(7)–O(33)	106.31(17)
O(30)–Cu(4)–N(1)	89.16(17)	N(60)–Cu(7)–O(33)	90.89(17)
N(58)–Cu(4)–N(1)	89.2(2)	O(34)–Cu(8)–N(47)	86.93(19)
N(10)–Cu(4)–N(56)	85.1(2)	O(33)–Cu(8)–N(47)	89.28(19)
O(30)–Cu(4)–N(56)	89.22(16)	O(34)–Cu(8)–N(53)	94.08(18)
N(58)–Cu(4)–N(56)	101.76(18)	O(33)–Cu(8)–N(53)	90.71(18)
N(1)–Cu(4)–N(56)	98.0(2)	N(47)–Cu(8)–N(53)	139.2(2)
N(7)–Cu(5)–N(13)	88.5(2)	O(34)–Cu(8)–O(6)	90.67(17)
N(7)–Cu(5)–N(11)	174.9(2)	O(33)–Cu(8)–O(6)	88.66(17)
N(47)–Cu(8)–O(6)	119.81(19)	O(31)–Cu(13)–N(17)	88.70(19)
N(53)–Cu(8)–O(6)	101.02(17)	O(32)–Cu(13)–N(20)	92.51(19)
O(10)$^{\#4}$–Cu(9)–N(23)$^{\#5}$	95.64(19)	O(31)–Cu(13)–N(20)	86.89(19)
N(27)$^{\#5}$–Cu(9)–N(23)$^{\#5}$	89.39(19)	O(32)–Cu(13)–O(38)	105.34(17)

O(10)$^{\#4}$–Cu(9)–N(54)	85.98(18)	O(31)–Cu(13)–O(38)	82.39(17)
N(27)$^{\#5}$–Cu(9)–N(54)	89.78(19)	N(17)–Cu(13)–O(38)	94.28(19)
O(10)$^{\#4}$–Cu(9)–O(34)	95.42(16)	N(20)–Cu(13)–O(38)	104.07(19)
N(27)$^{\#5}$–Cu(9)–O(34)	92.91(17)	N(22)–Cu(14)–N(26)	89.7(2)
N(23)$^{\#5}$–Cu(9)–O(34)	83.90(17)	N(28)–Cu(14)–N(26)	91.1(2)
N(54)–Cu(9)–O(34)	90.49(18)	N(22)–Cu(14)–N(21)	90.3(2)
O(22)–Cu(10)–N(24)$^{\#5}$	90.08(18)	N(28)–Cu(14)–N(21)	89.8(2)
O(22)–Cu(10)–N(46)	93.65(19)	N(22)–Cu(14)–O(32)	102.68(16)
O(22)–Cu(10)–O(34)	155.79(16)	N(28)–Cu(14)–O(32)	84.23(16)
N(24)$^{\#5}$–Cu(10)–O(34)	90.46(17)	N(26)–Cu(14)–O(32)	81.85(17)
N(46)–Cu(10)–O(34)	85.69(19)	N(21)–Cu(14)–O(32)	91.26(17)
O(22)–Cu(10)–O(11)$^{\#4}$	102.82(16)	N(22)–Cu(14)–O(26)	81.72(16)
N(24)$^{\#5}$–Cu(10)–O(11)$^{\#4}$	90.38(19)	N(28)–Cu(14)–O(26)	91.43(16)
N(46)–Cu(10)–O(11)$^{\#4}$	89.9(2)	N(26)–Cu(14)–O(26)	88.20(17)
O(34)–Cu(10)–O(11)$^{\#4}$	101.38(16)	N(21)–Cu(14)–O(26)	98.79(18)
O(31)–Cu(11)–N(19)	87.42(19)	O(32)–Cu(15)–N(25)	89.29(18)
O(31)–Cu(11)–N(14)	88.76(19)	N(25)–Cu(15)–N(29)	84.24(18)
O(31)–Cu(11)–N(12)	142.74(19)	N(31)–Cu(15)–N(25)	92.4(2)
N(19)–Cu(11)–N(12)	96.2(2)	O(32)–Cu(15)–N(18)	90.04(19)
N(14)–Cu(11)–N(12)	95.7(2)	N(31)–Cu(15)–N(18)	87.8(2)
O(31)–Cu(11)–O(37)	132.64(17)	N(18)–Cu(15)–N(29)	98.2(2)
N(19)–Cu(11)–O(37)	89.7(2)	O(32)–Cu(15)–N(29)	87.07(16)
N(14)–Cu(11)–O(37)	82.2(2)	N(31)–Cu(15)–N(29)	103.65(18)
N(12)–Cu(11)–O(37)	84.6(2)	N(30)–Cu(16)–N(32)	103.99(18)
O(4)$^{\#6}$–Cu(12)–N(16)	91.17(19)	O(35)–Cu(16)–N(43)	87.92(18)
N(16)–Cu(12)–O(31)	90.41(18)	N(43)–Cu(16)–N(32)	85.41(18)
O(4)$^{\#6}$–Cu(12)–N(15)	88.29(19)	N(43)–Cu(16)–N(30)	92.4(2)
N(16)–Cu(12)–N(15)	169.1(2)	O(35)–Cu(16)–N(34)	89.44(18)
O(31)–Cu(12)–N(15)	86.86(18)	N(30)–Cu(16)–N(34)	89.0(2)
O(4)$^{\#6}$–Cu(12)–O(18)$^{\#7}$	105.70(16)	N(34)–Cu(16)–N(32)	100.8(2)
N(16)–Cu(12)–O(18)$^{\#7}$	90.15(19)	O(35)–Cu(16)–N(32)	87.28(17)
O(31)–Cu(12)–O(18)$^{\#7}$	91.97(15)	N(33)–Cu(17)–O(35)	85.64(16)
N(15)–Cu(12)–O(18)$^{\#7}$	100.44(19)	N(37)–Cu(17)–O(35)	91.03(17)
O(32)–Cu(13)–N(17)	89.26(19)	N(38)–Cu(18)–O(39)	99.1(2)
N(6)$^{\#3}$–Cu(17)–N(44)	89.1(2)	N(35)–Cu(18)–O(39)	121.0(2)
N(37)–Cu(17)–N(33)	87.6(2)	O(15)–Cu(19)–O(36)	154.35(16)
N(33)–Cu(17)–N(44)	91.2(2)	N(36)–Cu(19)–O(15)	92.93(19)
N(6)$^{\#3}$–Cu(17)–O(35)	100.37(16)	N(40)–Cu(19)–O(15)	90.68(19)
N(6)$^{\#3}$–Cu(17)–N(37)	92.9(2)	N(36)–Cu(19)–O(36)	87.26(18)
N(44)–Cu(17)–O(14)	85.58(17)	N(40)–Cu(19)–O(36)	88.44(18)
N(44)–Cu(17)–O(35)	80.73(17)	N(36)–Cu(19)–O(1)$^{\#5}$	91.8(2)
N(6)$^{\#3}$–Cu(17)–O(14)	81.78(16)	N(40)–Cu(19)–O(1)$^{\#5}$	89.65(19)
N(37)–Cu(17)–O(14)	102.63(18)	O(15)–Cu(19)–O(1)$^{\#5}$	104.97(16)
N(33)–Cu(17)–O(14)	92.21(16)	O(36)–Cu(19)–O(1)$^{\#5}$	100.66(16)

O(36)–Cu(18)–O(35)	173.98(17)	O(2)$^{\#5}$–Cu(20)–N(39)	86.41(18)
O(36)–Cu(18)–N(35)	87.75(19)	O(2)$^{\#5}$–Cu(20)–N(41)	98.40(18)
O(35)–Cu(18)–N(35)	88.77(19)	N(39)–Cu(20)–N(51)$^{\#8}$	88.10(19)
O(36)–Cu(18)–N(38)	92.25(18)	N(41)–Cu(20)–N(51)$^{\#8}$	87.75(19)
O(35)–Cu(18)–N(38)	93.58(18)	O(2)$^{\#5}$–Cu(20)–O(36)	97.02(16)
N(35)–Cu(18)–N(38)	139.9(2)	N(39)–Cu(20)–O(36)	90.19(18)
O(36)–Cu(18)–O(39)	90.27(19)	N(41)–Cu(20)–O(36)	83.60(17)
O(35)–Cu(18)–O(39)	87.33(19)	N(51)$^{\#8}$–Cu(20)–O(36)	89.64(18)

[a] Symmetry codes: $^{\#1}$ $x-1, y-1, z-1$; $^{\#2}$ $-x, -y, 1-z$; $^{\#3}$ $-x, 1-y, 1-z$; $^{\#4}$ $1-x, 1-y, 1-z$; $^{\#5}$ $1-x, -y, 1-z$; $^{\#6}$ $x, 1+y, z$; $^{\#7}$ $1-x, 1-y, 2-z$; $^{\#8}$ $1+x, 1+y, 1+z$.

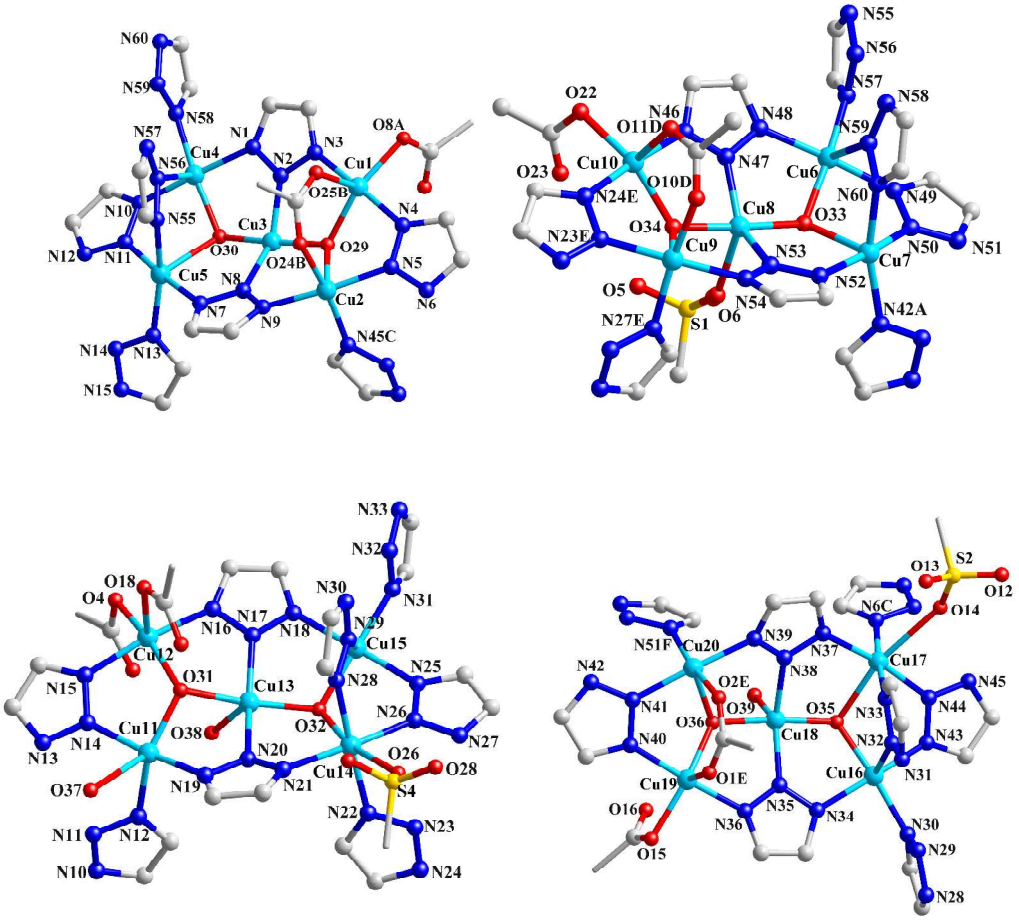

Figure S2. Local coordination environment of Cu^{II} atoms in each Cu^{II}_5 SBUs of **1** (H atoms and part of phenyl moiety of sip^{3-} were omitted for clarity, symmetry codes: A = $x - 1$, $y - 1$, $z - 1$; B = $-x$, $-y$, $1 - z$; C = $-x$, $1-y$, $1 - z$; D = $1 - x$, $1 - y$, $1 - z$; E = $1 - x$, $-y$, $1 - z$; F = $1 + x$, $1 + y$, $1 + z$).

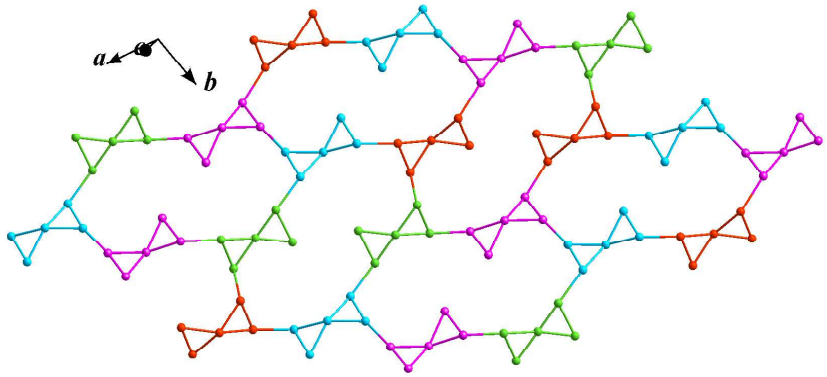

Figure S3. Metallic skeleton in the 2D sublayer of **1**.

Table S2. Selected Bond Lengths (Å) and Angles (deg) for **2** [a]

Cu(1)–O(10)$^{\#1}$	1.946(4)	Cu(4)–N(8)	1.914(4)
Cu(1)–N(10)	1.966(5)	Cu(4)–N(2)	1.918(4)
Cu(1)–N(1)	1.969(5)	Cu(4)–O(16)	1.950(4)
Cu(1)–O(15)	2.012(4)	Cu(4)–O(15)	1.971(4)
Cu(1)–O(5)	2.496(5)	Cu(4)–O(12)	2.444(5)
Cu(1)–O(11)	2.675(4)	Cu(5)–N(4)	1.973(5)
Cu(2)–N(6)$^{\#2}$	1.980(5)	Cu(5)–O(2)	1.981(4)
Cu(2)–O(15)	1.996(4)	Cu(5)–N(7)	2.001(5)
Cu(2)–N(11)	2.009(5)	Cu(5)–O(16)	2.039(4)
Cu(2)–N(9)	2.025(5)	Cu(5)–O(19W)	2.232(4)
Cu(2)–O(18W)	2.317(5)	Cu(5)–O(1)	2.668(4)
Cu(2)–O(14)	2.791(4)	Cu(6)–O(3)	1.936(4)
Cu(3)–N(5)	1.946(5)	Cu(6)–O(8)	1.952(4)
Cu(3)–N(12)$^{\#3}$	1.983(5)	Cu(6)–O(22W)	1.967(5)
Cu(3)–N(3)	1.991(5)	Cu(6)–O(20W)	1.999(6)
Cu(3)–O(16)	2.004(4)	Cu(6)–O(21W)	2.206(5)
Cu(3)–O(17W)	2.267(5)	N(8)–Cu(4)–O(16)	91.52(17)
O(10)$^{\#1}$–Cu(1)–N(10)	91.48(18)	N(2)–Cu(4)–O(16)	90.13(17)
O(10)$^{\#1}$–Cu(1)–N(1)	90.21(18)	N(8)–Cu(4)–O(15)	88.51(17)
N(10)–Cu(1)–O(15)	87.46(17)	N(2)–Cu(4)–O(15)	89.89(17)
N(1)–Cu(1)–O(15)	90.38(17)	N(4)–Cu(5)–O(2)	90.97(18)
N(6)$^{\#2}$–Cu(2)–N(11)	95.39(19)	O(16)–Cu(5)–O(19W)	94.09(17)
O(15)–Cu(2)–N(11)	84.95(16)	O(2)–Cu(5)–N(7)	95.32(18)
N(6)$^{\#2}$–Cu(2)–N(9)	93.01(19)	N(4)–Cu(5)–O(16)	83.08(17)
O(15)–Cu(2)–N(9)	87.55(17)	N(7)–Cu(5)–O(16)	90.31(17)
N(6)$^{\#2}$–Cu(2)–O(18W)	91.7(2)	N(4)–Cu(5)–O(19W)	93.62(19)
O(15)–Cu(2)–O(18W)	103.34(18)	O(2)–Cu(5)–O(19W)	103.49(17)
N(11)–Cu(2)–O(18W)	82.7(2)	N(7)–Cu(5)–O(19W)	86.87(19)
N(9)–Cu(2)–O(18W)	94.7(2)	O(20W)–Cu(6)–O(21W)	89.4(3)
N(5)–Cu(3)–N(12)$^{\#3}$	94.2(2)	O(3)–Cu(6)–O(22W)	91.2(2)
N(12)$^{\#3}$–Cu(3)–N(3)	94.1(2)	O(8)–Cu(6)–O(22W)	88.20(19)
N(5)–Cu(3)–O(16)	83.97(17)	O(3)–Cu(6)–O(20W)	86.7(2)
N(3)–Cu(3)–O(16)	90.20(18)	O(8)–Cu(6)–O(20W)	92.8(2)
N(5)–Cu(3)–O(17W)	107.6(2)	O(3)–Cu(6)–O(21W)	95.07(19)
N(12)$^{\#3}$–Cu(3)–O(17W)	90.8(2)	O(8)–Cu(6)–O(21W)	91.59(19)
N(3)–Cu(3)–O(17W)	88.9(2)	O(22W)–Cu(6)–O(21W)	100.0(2)
O(16)–Cu(3)–O(17W)	81.6(2)		

[a] Symmetry codes: $^{\#1}$ 3/2 + x, 1/2 – y, z – 1/2; $^{\#2}$ x – 1/2, 1/2 – y, z – 1/2; $^{\#3}$ x + 1/2, 1/2 – y, z + 1/2.

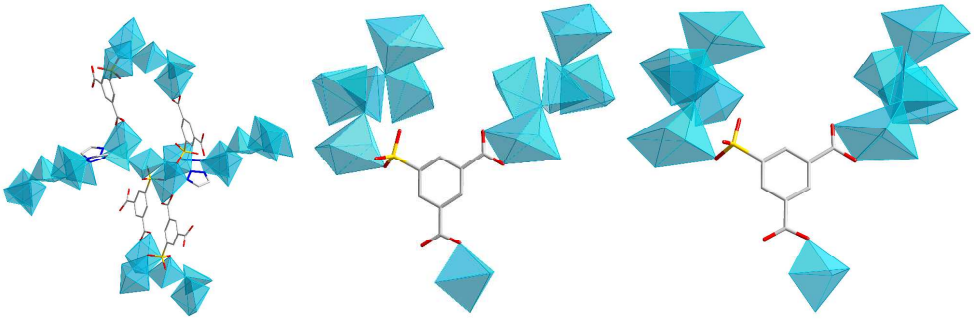

Figure S4. Linkages of Cu^{II}_5 cluster, Cu^{II}_1 ion, and sip^{3-} connector in **2**.

Table S3. Selected Bond Lengths (Å) and Angles (deg) for **3** [a]

Cu(1)–N(2)	1.930(4)	Cu(3)–N(4)$^{\#1}$	1.962(4)
Cu(1)–O(9)	1.983(3)	Cu(3)–O(4)$^{\#2}$	1.963(3)
Cu(1)–O(6)	2.484(2)	Cu(3)–N(1)	1.993(4)
Cu(2)–O(8)	1.915(3)	Cu(3)–O(9)	2.019(3)
Cu(2)–N(5)	1.959(4)	Cu(4)–O(8)	1.899(3)
Cu(2)–N(3)	1.987(4)	Cu(4)–O(2)$^{\#3}$	1.933(3)
Cu(2)–O(9)$^{\#1}$	2.024(3)	Cu(4)–O(10W)	1.943(4)
Cu(2)–O(5)	2.372(8)	Cu(4)–N(6)	1.981(4)
N(2)–Cu(1)–O(9)	89.77(13)	N(3)–Cu(2)–O(5)	88.3(2)
N(2)$^{\#1}$–Cu(1)–O(9)	90.23(13)	O(9)$^{\#1}$–Cu(2)–O(5)	89.4(3)
N(2)–Cu(1)–O(9)$^{\#1}$	90.23(13)	N(4)$^{\#1}$–Cu(3)–O(4)$^{\#2}$	89.99(15)
N(2)$^{\#1}$–Cu(1)–O(9)$^{\#1}$	89.77(13)	O(4)$^{\#2}$–Cu(3)–N(1)	92.23(14)
O(8)–Cu(2)–N(5)	85.83(14)	N(4)$^{\#1}$–Cu(3)–O(9)	88.72(13)
O(8)–Cu(2)–N(3)	96.05(14)	N(1)–Cu(3)–O(9)	90.07(13)
N(5)–Cu(2)–O(5)	106.4(2)	O(8)–Cu(4)–O(10W)	93.49(15)
N(5)–Cu(2)–O(9)$^{\#1}$	86.50(13)	O(2)$^{\#3}$–Cu(4)–O(10W)	92.34(16)
N(3)–Cu(2)–O(9)$^{\#1}$	91.25(13)	O(8)–Cu(4)–N(6)	87.24(15)
O(8)–Cu(2)–O(5)	93.2(3)	O(2)$^{\#3}$–Cu(4)–N(6)	87.80(16)

[a] Symmetry codes: $^{\#1}$ $2 - x, 2 - y, 2 - z$; $^{\#2}$ $1 - x, y + 1/2, 3/2 - z$; $^{\#3}$ $1 - x, 1 - y, 2 - z$.

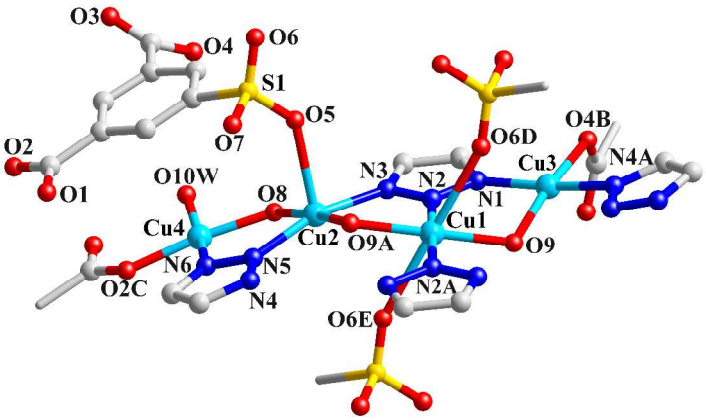

Figure S5. Local coordination environment of Cu^{II} atoms in **3** (H atoms and part of phenyl moiety of sip^{3-} were omitted for clarity, symmetry codes: A = 2 – *x*, 2 – *y*, 2 – *z*; B = 1 – *x*, *y* + 1/2, 3/2 – *z*; C = 1 – *x*, 1 – *y*, 2 – *z*; D = 1 – *x*, 2 – *y*, 2 – *z*; E = 1 + *x*, *y*, *z*).

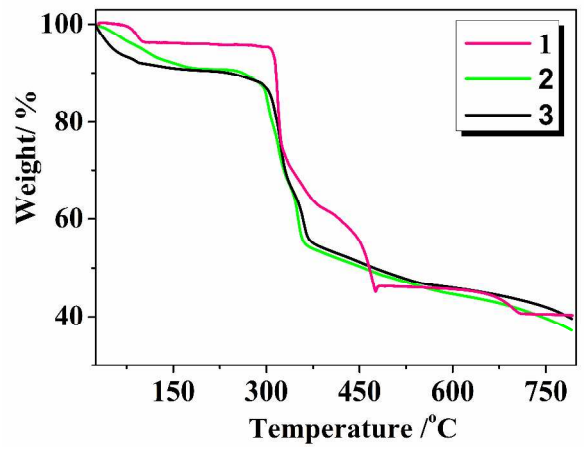

Figure S6. TG curves of **1** – **3**.

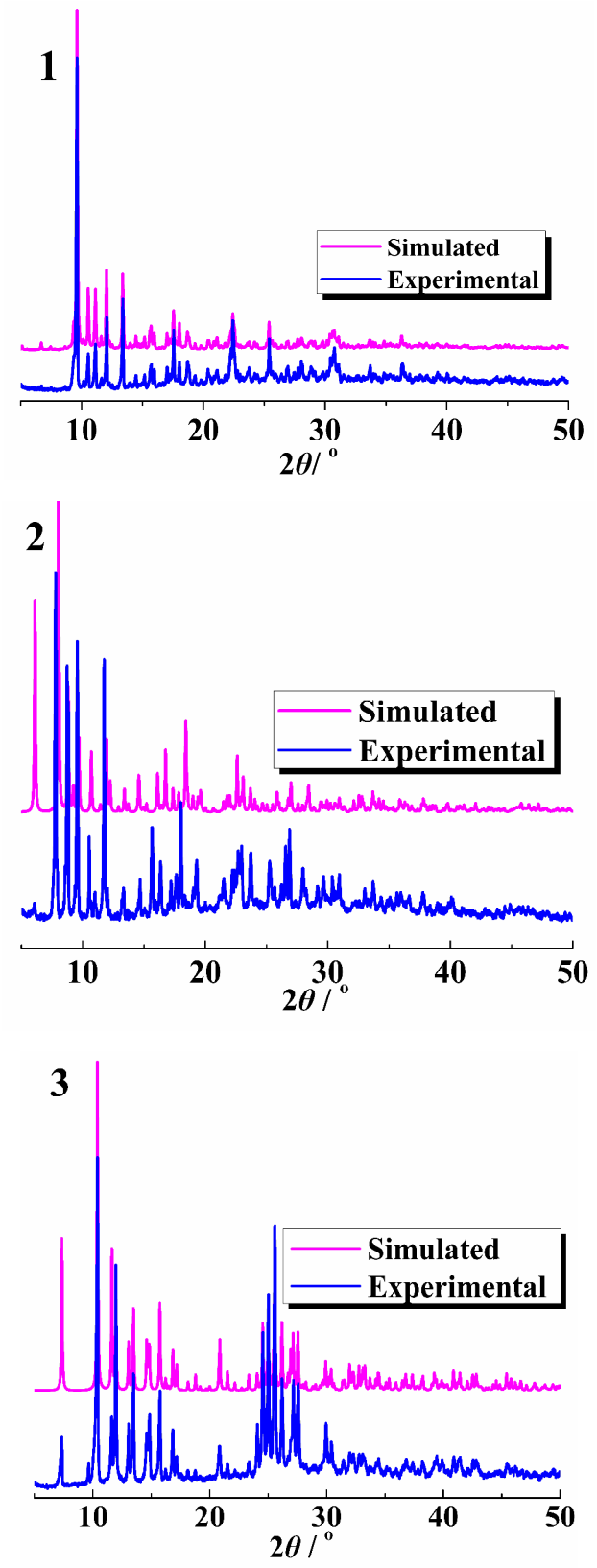

Figure S7. Simulated (purple) and experimental (blue) PXRD patterns for **1**–**3**.

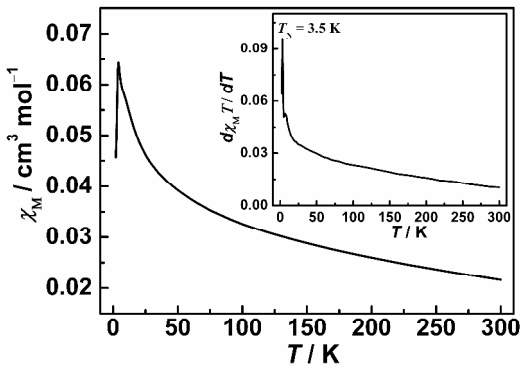

Figure S8. Plots of χ_M and d($\chi_M T$)/dT vs T for **1**.