Table S1. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for Cu(**1**)Cl_2. *U*(eq) is defined as one third of the trace of the orthogonalized **U**ij tensor.

	x	y	z	U(eq)
Cu(1)	1640.6(4)	2083.0(13)	3520.2(2)	16(1)
Cu(2)	900.3(4)	2919.5(12)	1038.3(2)	16(1)
Cl(11)	794.0(9)	3393(2)	2986.3(4)	28(1)
Cl(12)	591.4(9)	3255.1(19)	4014.7(4)	24(1)
N(11)	2399(5)	80(6)	3136(3)	18(2)
C(12)	1838(4)	-1737(8)	3217.2(16)	22(1)
C(13)	1669(4)	-2061(11)	3674(2)	21(2)
N(14)	2676(3)	-1982(8)	3893.1(15)	16(1)
C(15)	2539(5)	-2139(10)	4356(2)	28(2)
C(16)	2050(6)	-332(9)	4533(3)	25(2)
C(17)	2652(4)	1424(10)	4408.5(17)	22(2)
N(18)	2829(3)	1537(8)	3941.0(15)	16(1)
C(19)	3600(3)	3096(8)	3873.8(13)	20(1)
C(110)	3804(3)	3338(7)	3414.1(14)	21(1)
N(111)	4120(3)	1500(6)	3230.0(11)	18(1)
C(112)	4255(3)	1653(7)	2771.4(14)	24(1)
C(113)	3224(3)	1899(7)	2549.9(15)	26(1)
C(114)	2490(5)	319(9)	2682(3)	24(2)
C(115)	3462(5)	-132(8)	3337(3)	17(2)
C(116)	3299(5)	-324(9)	3803(3)	15(1)
Cl(21)	1748.3(9)	1607(2)	1573.8(4)	27(1)
Cl(22)	1948.9(8)	1751.2(19)	543.8(4)	23(1)
N(21)	144(4)	4956(5)	1414(2)	13(2)
C(22)	722(4)	6764(8)	1341.6(17)	22(1)
C(23)	851(4)	7074(11)	880(2)	21(2)
N(24)	-133(3)	6985(9)	652.0(18)	23(1)
C(25)	-5(5)	7134(10)	204(2)	28(2)
C(26)	478(6)	5314(9)	12(3)	26(2)
C(27)	-137(5)	3562(10)	154.7(18)	23(2)
N(28)	-297(3)	3462(8)	610.1(16)	16(1)
C(29)	-1064(3)	1894(7)	693.0(14)	18(1)
C(210)	-1269(3)	1693(7)	1152.0(14)	21(1)
N(211)	-1578(3)	3546(6)	1334.7(11)	18(1)
C(212)	-1703(3)	3382(8)	1791.0(14)	25(1)
C(213)	-665(3)	3165(8)	2014.7(15)	28(1)
C(214)	61(6)	4735(8)	1888(2)	21(2)
C(215)	-912(5)	5134(8)	1241(3)	16(2)
C(216)	-760(5)	5336(9)	769(3)	18(2)

Table S2. Bond lengths [A] and angles [deg] for $Cu(1)Cl_2$.

Cu(1)-N(18)	2.083(5)
Cu(1)-N(11)	2.099(6)
Cu(1)-Cl(11)	2.2248(13)
Cu(1)-Cl(12)	2.2404(13)
Cu(2)-N(21)	2.098(6)
Cu(2)-N(28)	2.107(4)
Cu(2)-Cl(21)	2.2303(14)
Cu(2)-Cl(22)	2.2388(13)
N(11)-C(114)	1.465(10)
N(11)-C(12)	1.478(7)
N(11)-C(115)	1.531(10)
C(12)-C(13)	1.495(8)
C(13)-N(14)	1.485(7)
N(14)-C(116)	1.434(8)
N(14)-C(15)	1.495(7)
C(15)-C(16)	1.514(9)
C(16)-C(17)	1.500(8)
C(17)-N(18)	1.515(7)
N(18)-C(19)	1.489(7)
N(18)-C(116)	1.493(8)
C(19)-C(110)	1.503(6)
C(110)-N(111)	1.462(6)
N(111)-C(115)	1.458(7)
N(111)-C(112)	1.481(5)
C(112)-C(113)	1.525(6)
C(113)-C(114)	1.512(8)
C(115)-C(116)	1.510(12)
N(21)-C(22)	1.478(7)
N(21)-C(215)	1.484(9)
N(21)-C(214)	1.526(9)
C(22)-C(23)	1.500(8)
C(23)-N(24)	1.474(7)
N(24)-C(25)	1.446(8)
N(24)-C(216)	1.452(8)
C(25)-C(26)	1.536(10)
C(26)-C(27)	1.523(9)
C(27)-N(28)	1.473(7)
N(28)-C(29)	1.498(6)
N(28)-C(216)	1.518(8)
C(29)-C(210)	1.499(6)
C(210)-N(211)	1.466(6)
N(211)-C(215)	1.430(7)
N(211)-C(212)	1.473(5)
C(212)-C(213)	1.533(6)
C(213)-C(214)	1.496(8)
C(215)-C(216)	1.530(12)
N(18)-Cu(1)-N(11)	84.8(2)
N(18)-Cu(1)-Cl(11)	159.48(15)
N(11)-Cu(1)-Cl(11)	93.0(2)
N(18)-Cu(1)-Cl(12)	93.47(14)
N(11)-Cu(1)-Cl(12)	159.80(17)
Cl(11)-Cu(1)-Cl(12)	95.36(5)
N(21)-Cu(2)-N(28)	84.6(2)

N(21)-Cu(2)-Cl(21)	93.8(2)
N(28)-Cu(2)-Cl(21)	159.53(14)
N(21)-Cu(2)-Cl(22)	158.90(15)
N(28)-Cu(2)-Cl(22)	93.13(15)
Cl(21)-Cu(2)-Cl(22)	95.44(5)
C(114)-N(11)-C(12)	108.0(5)
C(114)-N(11)-C(115)	110.8(6)
C(12)-N(11)-C(115)	106.8(5)
C(114)-N(11)-Cu(1)	122.9(4)
C(12)-N(11)-Cu(1)	103.2(4)
C(115)-N(11)-Cu(1)	103.9(5)
N(11)-C(12)-C(13)	111.8(6)
N(14)-C(13)-C(12)	109.0(4)
C(116)-N(14)-C(13)	115.6(5)
C(116)-N(14)-C(15)	109.0(5)
C(13)-N(14)-C(15)	111.0(4)
N(14)-C(15)-C(16)	111.2(6)
C(17)-C(16)-C(15)	110.6(6)
C(16)-C(17)-N(18)	112.6(6)
C(19)-N(18)-C(116)	108.0(4)
C(19)-N(18)-C(17)	106.4(4)
C(116)-N(18)-C(17)	108.0(5)
C(19)-N(18)-Cu(1)	105.9(3)
C(116)-N(18)-Cu(1)	105.6(4)
C(17)-N(18)-Cu(1)	122.3(3)
N(18)-C(19)-C(110)	109.9(4)
N(111)-C(110)-C(19)	110.2(4)
C(115)-N(111)-C(110)	114.5(4)
C(115)-N(111)-C(112)	111.0(5)
C(110)-N(111)-C(112)	111.7(4)
N(111)-C(112)-C(113)	111.4(3)
C(114)-C(113)-C(112)	110.1(5)
N(11)-C(114)-C(113)	114.2(5)
N(111)-C(115)-C(116)	112.5(6)
N(111)-C(115)-N(11)	110.8(5)
C(116)-C(115)-N(11)	107.2(6)
N(14)-C(116)-N(18)	113.7(6)
N(14)-C(116)-C(115)	110.4(6)
N(18)-C(116)-C(115)	105.8(6)
C(22)-N(21)-C(215)	109.9(5)
C(22)-N(21)-C(214)	106.0(5)
C(215)-N(21)-C(214)	108.2(6)
C(22)-N(21)-Cu(2)	104.0(4)
C(215)-N(21)-Cu(2)	106.0(5)
C(214)-N(21)-Cu(2)	122.3(4)
N(21)-C(22)-C(23)	109.4(6)
N(24)-C(23)-C(22)	112.6(5)
C(25)-N(24)-C(216)	112.1(6)
C(25)-N(24)-C(23)	112.9(5)
C(216)-N(24)-C(23)	113.1(6)
N(24)-C(25)-C(26)	112.6(6)
C(27)-C(26)-C(25)	108.7(6)
N(28)-C(27)-C(26)	114.0(6)
C(27)-N(28)-C(29)	107.6(5)
C(27)-N(28)-C(216)	110.3(5)
C(29)-N(28)-C(216)	107.3(4)
C(27)-N(28)-Cu(2)	123.2(4)

C(29)-N(28)-Cu(2)	104.3(3)
C(216)-N(28)-Cu(2)	103.1(4)
N(28)-C(29)-C(210)	111.0(4)
N(211)-C(210)-C(29)	111.0(4)
C(215)-N(211)-C(210)	115.1(4)
C(215)-N(211)-C(212)	109.5(5)
C(210)-N(211)-C(212)	111.0(4)
N(211)-C(212)-C(213)	111.9(4)
C(214)-C(213)-C(212)	110.9(5)
C(213)-C(214)-N(21)	112.8(5)
N(211)-C(215)-N(21)	114.6(5)
N(211)-C(215)-C(216)	110.8(6)
N(21)-C(215)-C(216)	104.8(6)
N(24)-C(216)-N(28)	111.4(6)
N(24)-C(216)-C(215)	113.5(6)
N(28)-C(216)-C(215)	107.7(6)

Table S3. Anisotropic displacement parameters (A^2 x 10^3) for $Cu(1)Cl_2$. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	14(1)	14(1)	19(1)	0(1)	-1(1)	2(1)
Cu(2)	14(1)	15(1)	18(1)	0(1)	0(1)	2(1)
Cl(11)	27(1)	30(1)	26(1)	0(1)	-8(1)	12(1)
Cl(12)	22(1)	23(1)	28(1)	0(1)	8(1)	5(1)
N(11)	12(3)	22(5)	21(4)	-1(2)	-2(3)	2(2)
C(12)	17(2)	20(4)	29(3)	-7(2)	-2(2)	-3(2)
C(13)	17(3)	8(4)	39(5)	1(3)	9(2)	-1(2)
N(14)	19(2)	10(3)	17(2)	2(2)	1(2)	-2(2)
C(15)	27(3)	28(5)	29(3)	12(3)	5(2)	0(3)
C(16)	34(4)	27(4)	14(3)	1(3)	2(3)	-3(3)
C(17)	23(2)	30(5)	11(2)	0(2)	0(2)	0(3)
N(18)	14(2)	15(3)	17(2)	-4(2)	5(2)	-2(2)
C(19)	19(2)	21(3)	20(2)	-2(2)	-3(2)	-4(2)
C(110)	20(2)	18(3)	25(2)	5(2)	0(2)	-5(2)
N(111)	13(2)	21(3)	20(2)	0(2)	2(2)	-4(2)
C(112)	19(2)	34(4)	19(2)	4(2)	1(2)	-2(2)
C(113)	24(2)	35(4)	19(2)	3(2)	2(2)	-4(2)
C(114)	17(3)	29(4)	26(4)	-8(3)	-3(2)	3(2)
C(115)	10(3)	17(5)	26(5)	1(2)	-7(3)	2(2)
C(116)	14(3)	14(3)	16(3)	5(3)	-4(2)	3(2)
Cl(21)	27(1)	30(1)	24(1)	1(1)	-6(1)	12(1)
Cl(22)	21(1)	22(1)	26(1)	-1(1)	5(1)	4(1)
N(21)	14(3)	10(5)	16(4)	-3(1)	-2(3)	1(1)
C(22)	20(2)	16(4)	30(3)	-7(2)	-3(2)	2(2)
C(23)	18(3)	13(4)	31(4)	3(3)	-4(2)	-4(2)
N(24)	20(2)	13(3)	35(3)	9(2)	5(2)	2(2)
C(25)	28(3)	23(5)	34(3)	11(3)	-1(2)	2(3)
C(26)	28(3)	27(4)	23(3)	14(3)	2(3)	0(3)
C(27)	29(3)	26(4)	15(2)	-2(3)	-3(2)	6(3)
N(28)	17(2)	14(3)	17(2)	5(2)	-3(2)	-5(2)
C(29)	18(2)	11(3)	26(2)	-5(2)	-2(2)	-3(2)
C(210)	18(2)	19(3)	26(2)	2(2)	-1(2)	-8(2)
N(211)	15(2)	20(2)	19(2)	2(2)	1(2)	-3(2)
C(212)	20(2)	36(4)	19(2)	3(2)	4(2)	-1(2)
C(213)	23(2)	44(4)	16(2)	5(2)	0(2)	1(2)
C(214)	26(3)	29(4)	9(3)	-2(2)	-2(2)	5(2)
C(215)	16(3)	15(5)	17(4)	-3(2)	2(2)	2(2)
C(216)	11(3)	15(3)	29(3)	-3(3)	0(2)	6(2)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for $Cu(1)Cl_2$.

	x	y	z	U(eq)
H(12A)	2234	-2833	3101	27
H(12B)	1163	-1695	3073	27
H(13A)	1205	-1054	3787	25
H(13B)	1343	-3335	3720	25
H(15A)	3217	-2348	4490	34
H(15B)	2098	-3267	4420	34
H(16A)	1335	-216	4430	30
H(16B)	2026	-423	4842	30
H(17A)	3326	1406	4553	26
H(17B)	2278	2593	4501	26
H(19A)	4249	2766	4020	24
H(19B)	3338	4323	3992	24
H(11A)	3173	3807	3273	25
H(11B)	4352	4311	3372	25
H(11C)	4599	474	2666	29
H(11D)	4702	2771	2707	29
H(11E)	2927	3174	2620	31
H(11F)	3327	1845	2243	31
H(11G)	1800	606	2567	29
H(11H)	2724	-917	2559	29
H(11I)	3789	-1343	3231	21
H(11J)	3983	-481	3942	18
H(22A)	1406	6682	1477	27
H(22B)	344	7865	1465	27
H(23A)	1172	8352	833	25
H(23B)	1323	6079	768	25
H(25A)	437	8260	140	34
H(25B)	-685	7361	74	34
H(26A)	468	5404	-297	31
H(26B)	1203	5190	104	31
H(27A)	-817	3583	15	28
H(27B)	226	2378	63	28
H(29A)	-799	657	582	22
H(29B)	-1716	2194	546	22
H(21A)	-1822	731	1197	25
H(21B)	-640	1221	1294	25
H(21C)	-2140	2249	1855	30
H(21D)	-2058	4547	1897	30
H(21E)	-774	3215	2321	33
H(21F)	-361	1895	1945	33
H(21G)	752	4452	2003	26
H(21H)	-176	5972	2010	26
H(21I)	-1231	6347	1351	19
H(21J)	-1453	5495	637	22

Table S5. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for Cu(**2**)Cl_2. *U*(eq) is defined as one third of the trace of the orthogonalized **U**ij tensor.

	x	y	z	U(eq)
Cu(1)	1491.3(3)	7032.0(2)	4995.0(2)	18(1)
Cl(1)	2771.0(6)	5876.4(4)	6174.6(4)	29(1)
Cl(2)	-169.6(6)	7713.9(5)	5961.9(4)	35(1)
N(1)	3140.8(18)	6746.1(13)	4068.4(11)	18(1)
C(2)	2812(2)	5585.1(16)	3663.1(15)	24(1)
C(3)	1071(2)	5432.4(16)	3344.4(15)	23(1)
N(4)	436.6(19)	6271.4(13)	2563.4(12)	22(1)
C(5)	-1264(2)	6423.7(17)	2542.3(15)	25(1)
C(6)	-1419(2)	7279.7(18)	3391.9(16)	26(1)
N(7)	194.1(18)	7746.7(13)	3690.9(12)	18(1)
C(8)	326(2)	8986.7(16)	3788.4(15)	23(1)
C(9)	2048(2)	9256.8(16)	4115.1(15)	23(1)
N(10)	3052.8(18)	8711.1(13)	3466.2(12)	20(1)
C(11)	4734(2)	8843.9(18)	3879.6(15)	26(1)
C(12)	5265(2)	8061.2(17)	4782.3(16)	26(1)
C(13)	4840(2)	6855.8(17)	4490.7(16)	25(1)
C(14)	2720(2)	7548.2(16)	3193.3(14)	19(1)
C(15)	1004(2)	7395.2(16)	2828.7(14)	18(1)

Table S6. Bond lengths [A] and angles [deg] for $Cu(2)Cl_2$.

Cu(1)-N(1)	2.0683(16)
Cu(1)-N(7)	2.0903(15)
Cu(1)-Cl(2)	2.2394(6)
Cu(1)-Cl(1)	2.2407(5)
N(1)-C(13)	1.490(2)
N(1)-C(2)	1.494(2)
N(1)-C(14)	1.507(2)
C(2)-C(3)	1.507(3)
C(3)-N(4)	1.482(2)
N(4)-C(15)	1.448(2)
N(4)-C(5)	1.478(3)
C(5)-C(6)	1.548(3)
C(6)-N(7)	1.494(2)
N(7)-C(8)	1.484(2)
N(7)-C(15)	1.505(2)
C(8)-C(9)	1.515(3)
C(9)-N(10)	1.477(2)
N(10)-C(14)	1.448(2)
N(10)-C(11)	1.476(2)
C(11)-C(12)	1.533(3)
C(12)-C(13)	1.516(3)
C(14)-C(15)	1.495(3)
N(1)-Cu(1)-N(7)	84.03(6)
N(1)-Cu(1)-Cl(2)	168.19(5)
N(7)-Cu(1)-Cl(2)	91.52(5)
N(1)-Cu(1)-Cl(1)	90.62(4)
N(7)-Cu(1)-Cl(1)	165.96(5)
Cl(2)-Cu(1)-Cl(1)	96.08(2)
C(13)-N(1)-C(2)	109.55(15)
C(13)-N(1)-C(14)	109.51(14)
C(2)-N(1)-C(14)	107.32(14)
C(13)-N(1)-Cu(1)	119.66(12)
C(2)-N(1)-Cu(1)	105.09(12)
C(14)-N(1)-Cu(1)	105.02(11)
N(1)-C(2)-C(3)	109.59(15)
N(4)-C(3)-C(2)	110.69(16)
C(15)-N(4)-C(5)	100.79(15)
C(15)-N(4)-C(3)	112.27(14)
C(5)-N(4)-C(3)	110.28(15)
N(4)-C(5)-C(6)	105.94(15)
N(7)-C(6)-C(5)	104.45(15)
C(8)-N(7)-C(6)	116.64(15)
C(8)-N(7)-C(15)	107.74(14)
C(6)-N(7)-C(15)	103.04(14)
C(8)-N(7)-Cu(1)	107.97(11)
C(6)-N(7)-Cu(1)	114.82(12)
C(15)-N(7)-Cu(1)	105.76(11)
N(7)-C(8)-C(9)	107.09(15)
N(10)-C(9)-C(8)	112.61(15)
C(14)-N(10)-C(11)	109.80(15)
C(14)-N(10)-C(9)	117.14(15)
C(11)-N(10)-C(9)	111.93(15)
N(10)-C(11)-C(12)	112.14(16)

C(13)-C(12)-C(11)	110.17(17)
N(1)-C(13)-C(12)	111.24(15)
N(10)-C(14)-C(15)	110.10(15)
N(10)-C(14)-N(1)	113.45(15)
C(15)-C(14)-N(1)	105.91(15)
N(4)-C(15)-C(14)	118.04(16)
N(4)-C(15)-N(7)	105.19(15)
C(14)-C(15)-N(7)	106.32(15)

Table S7. Anisotropic displacement parameters (A^2 x 10^3) for Cu(2)Cl_2.
The anisotropic displacement factor exponent takes the form:
-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	19(1)	21(1)	15(1)	2(1)	4(1)	1(1)
Cl(1)	34(1)	29(1)	22(1)	8(1)	0(1)	-1(1)
Cl(2)	32(1)	51(1)	24(1)	0(1)	14(1)	9(1)
N(1)	17(1)	19(1)	18(1)	1(1)	3(1)	3(1)
C(2)	30(1)	19(1)	24(1)	-2(1)	4(1)	7(1)
C(3)	30(1)	17(1)	22(1)	-2(1)	3(1)	-1(1)
N(4)	23(1)	21(1)	19(1)	0(1)	1(1)	-2(1)
C(5)	22(1)	27(1)	25(1)	3(1)	-1(1)	-5(1)
C(6)	16(1)	35(1)	26(1)	2(1)	3(1)	-1(1)
N(7)	16(1)	21(1)	18(1)	2(1)	5(1)	1(1)
C(8)	24(1)	21(1)	24(1)	1(1)	5(1)	6(1)
C(9)	23(1)	18(1)	26(1)	-1(1)	3(1)	3(1)
N(10)	17(1)	22(1)	22(1)	2(1)	4(1)	-2(1)
C(11)	19(1)	30(1)	30(1)	4(1)	4(1)	-3(1)
C(12)	17(1)	33(1)	26(1)	2(1)	2(1)	-2(1)
C(13)	16(1)	29(1)	30(1)	5(1)	4(1)	6(1)
C(14)	20(1)	21(1)	16(1)	3(1)	6(1)	2(1)
C(15)	21(1)	20(1)	15(1)	2(1)	5(1)	0(1)

Table S8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Cu(**2**)Cl_2.

	x	y	z	U(eq)
H(2A)	3215	5027	4192	29
H(2B)	3350	5463	3074	29
H(3A)	855	4666	3069	28
H(3B)	543	5517	3943	28
H(5A)	-1762	5701	2671	30
H(5B)	-1771	6715	1874	30
H(6A)	-2173	7881	3137	31
H(6B)	-1774	6904	3974	31
H(8A)	-289	9262	4300	27
H(8B)	-77	9351	3131	27
H(9A)	2195	10081	4093	27
H(9B)	2379	9008	4825	27
H(11A)	4939	9633	4098	31
H(11B)	5357	8682	3339	31
H(12A)	6413	8125	4997	31
H(12B)	4753	8286	5361	31
H(13A)	5468	6599	3979	30
H(13B)	5098	6369	5096	30
H(14A)	3307	7333	2638	22
H(15A)	669	7905	2238	22

Table S9. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for Cu(3)Cl_2. *U*(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	407.8(3)	50.3(2)	2943.9(2)	18(1)
Cl(1)	3115.6(8)	246.3(7)	3044.5(6)	44(1)
Cl(2)	343.1(8)	-55.5(6)	1266.1(4)	26(1)
N(1)	-2121(2)	147.1(15)	3002.3(14)	16(1)
C(2)	-2726(3)	-1016(2)	2732(2)	22(1)
C(3)	-1715(3)	-1885(2)	3330.6(19)	22(1)
N(4)	-1706(3)	-1651.7(16)	4425.5(16)	21(1)
C(5)	-208(3)	-2129(2)	4913(2)	26(1)
C(6)	1073(4)	-1138(2)	4940(2)	27(1)
N(7)	192(2)	-142.4(17)	4489.5(14)	18(1)
C(8)	511(4)	1008(2)	4931(2)	25(1)
C(9)	-492(4)	1882(2)	4324(2)	26(1)
N(10)	-2241(3)	1576.6(17)	4245.8(17)	23(1)
C(11)	-3013(4)	2084(2)	3331(2)	27(1)
C(12)	-2847(3)	1173(2)	2482.3(19)	22(1)
C(13)	-2572(3)	364(2)	4075.1(18)	19(1)
C(14)	-1550(3)	-442(2)	4689.0(19)	19(1)

Table S10. Bond lengths [A] and angles [deg] for $Cu(3)Cl_2$.

Cu(1)-N(1)	2.070(2)
Cu(1)-N(7)	2.072(2)
Cu(1)-Cl(1)	2.2277(7)
Cu(1)-Cl(2)	2.2315(6)
N(1)-C(2)	1.481(3)
N(1)-C(13)	1.493(3)
N(1)-C(12)	1.498(3)
C(2)-C(3)	1.526(3)
C(3)-N(4)	1.479(3)
N(4)-C(14)	1.451(3)
N(4)-C(5)	1.491(3)
C(5)-C(6)	1.555(4)
C(6)-N(7)	1.486(3)
N(7)-C(8)	1.481(3)
N(7)-C(14)	1.488(3)
C(8)-C(9)	1.532(4)
C(9)-N(10)	1.476(4)
N(10)-C(13)	1.449(3)
N(10)-C(11)	1.490(3)
C(11)-C(12)	1.551(4)
C(13)-C(14)	1.496(3)
N(1)-Cu(1)-N(7)	83.33(8)
N(1)-Cu(1)-Cl(1)	169.43(6)
N(7)-Cu(1)-Cl(1)	92.07(6)
N(1)-Cu(1)-Cl(2)	90.96(5)
N(7)-Cu(1)-Cl(2)	168.76(6)
Cl(1)-Cu(1)-Cl(2)	95.11(3)
C(2)-N(1)-C(13)	107.6(2)
C(2)-N(1)-C(12)	118.6(2)
C(13)-N(1)-C(12)	102.0(2)
C(2)-N(1)-Cu(1)	105.94(14)
C(13)-N(1)-Cu(1)	106.95(14)
C(12)-N(1)-Cu(1)	114.9(2)
N(1)-C(2)-C(3)	107.1(2)
N(4)-C(3)-C(2)	113.2(2)
C(14)-N(4)-C(3)	114.5(2)
C(14)-N(4)-C(5)	100.5(2)
C(3)-N(4)-C(5)	111.2(2)
N(4)-C(5)-C(6)	106.7(2)
N(7)-C(6)-C(5)	103.8(2)
C(8)-N(7)-C(6)	117.1(2)
C(8)-N(7)-C(14)	108.0(2)
C(6)-N(7)-C(14)	102.1(2)
C(8)-N(7)-Cu(1)	106.3(2)
C(6)-N(7)-Cu(1)	116.2(2)
C(14)-N(7)-Cu(1)	106.43(14)
N(7)-C(8)-C(9)	107.1(2)
N(10)-C(9)-C(8)	113.3(2)
C(13)-N(10)-C(9)	115.1(2)
C(13)-N(10)-C(11)	100.2(2)
C(9)-N(10)-C(11)	111.9(2)
N(10)-C(11)-C(12)	106.6(2)
N(1)-C(12)-C(11)	103.9(2)

N(10)-C(13)-N(1)	105.5(2)
N(10)-C(13)-C(14)	114.6(2)
N(1)-C(13)-C(14)	106.1(2)
N(4)-C(14)-N(7)	105.5(2)
N(4)-C(14)-C(13)	115.1(2)
N(7)-C(14)-C(13)	106.9(2)

Table S11. Anisotropic displacement parameters (A^2 x 10^3) for $Cu(3)Cl_2$. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	14(1)	20(1)	20(1)	1(1)	2(1)	0(1)
Cl(1)	15(1)	71(1)	44(1)	11(1)	1(1)	-2(1)
Cl(2)	30(1)	27(1)	20(1)	-1(1)	5(1)	1(1)
N(1)	17(1)	17(1)	15(1)	-4(1)	2(1)	2(1)
C(2)	21(1)	21(1)	24(1)	-2(1)	-1(1)	-4(1)
C(3)	25(1)	14(1)	28(1)	-3(1)	0(1)	-1(1)
N(4)	23(1)	16(1)	24(1)	2(1)	1(1)	-2(1)
C(5)	30(2)	19(1)	29(2)	6(1)	-2(1)	0(1)
C(6)	26(2)	22(1)	33(2)	6(1)	-5(1)	1(1)
N(7)	17(1)	16(1)	19(1)	0(1)	-3(1)	-1(1)
C(8)	33(2)	20(1)	23(1)	-3(1)	-5(1)	-6(1)
C(9)	35(2)	17(1)	27(2)	-1(1)	-2(1)	-1(1)
N(10)	29(1)	17(1)	22(1)	-2(1)	3(1)	4(1)
C(11)	28(2)	23(1)	30(1)	-1(1)	1(1)	8(1)
C(12)	22(1)	23(1)	22(1)	5(1)	-1(1)	4(1)
C(13)	18(1)	21(1)	17(1)	0(1)	3(1)	1(1)
C(14)	23(2)	19(1)	15(1)	-1(1)	2(1)	-2(1)

Table S12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Cu(3)Cl_2.

	x	y	z	U(eq)
H(2A)	-2595	-1151	2008	26
H(2B)	-3888	-1090	2902	26
H(3A)	-2156	-2660	3214	27
H(3B)	-586	-1874	3082	27
H(5A)	213	-2784	4524	31
H(5B)	-457	-2393	5597	31
H(6A)	1409	-969	5633	32
H(6B)	2044	-1337	4542	32
H(8A)	1680	1193	4890	30
H(8B)	181	1022	5641	30
H(9A)	-396	2641	4644	32
H(9B)	-31	1941	3645	32
H(11A)	-2456	2800	3140	32
H(11B)	-4169	2257	3458	32
H(12A)	-3919	985	2193	26
H(12B)	-2126	1451	1945	26
H(13A)	-3749	201	4182	23
H(14A)	-1796	-335	5413	23

Table S13. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for Cu(**4**)Cl_2. *U*(eq) is defined as one third of the trace of the orthogonalized **U**ij tensor.

	x	y	z	U(eq)
Cu(1)	8191.0(5)	3168.2(3)	2729.6(3)	25(1)
Cl(1)	7382.7(10)	1591.6(6)	2813.8(6)	34(1)
Cl(2)	10439.8(10)	3082.9(6)	3990.0(7)	38(1)
N(1)	4413(3)	3795(2)	721(2)	29(1)
C(2)	3761(4)	3238(2)	1490(3)	33(1)
C(3)	3853(4)	3875(3)	2447(3)	33(1)
N(4)	5538(3)	4090.1(19)	2919(2)	26(1)
C(5)	5661(4)	4628(3)	3910(3)	32(1)
C(6)	7406(4)	4791(3)	4440(3)	36(1)
C(7)	8268(4)	5275(3)	3701(3)	36(1)
N(8)	7973(3)	4732.7(19)	2673.2(19)	27(1)
C(9)	8891(4)	5244(3)	1990(3)	38(1)
C(10)	9688(4)	4482(3)	1418(3)	39(1)
C(11)	8544(4)	3803(3)	665(2)	34(1)
N(12)	7237(3)	3415.4(19)	1128.5(19)	26(1)
C(13)	6332(4)	2611(3)	432(3)	33(1)
C(14)	4752(4)	3106(2)	-84(3)	35(1)
C(15)	5996(4)	4226(2)	1138(2)	28(1)
C(16)	6225(4)	4702(2)	2210(2)	26(1)

Table S14. Bond lengths [A] and angles [deg] for $Cu(4)Cl_2$.

Cu(1)-N(8)	2.095(3)
Cu(1)-N(12)	2.098(2)
Cu(1)-Cl(1)	2.2261(9)
Cu(1)-Cl(2)	2.2447(9)
N(1)-C(2)	1.467(4)
N(1)-C(15)	1.468(4)
N(1)-C(14)	1.480(4)
C(2)-C(3)	1.504(4)
C(3)-N(4)	1.473(4)
N(4)-C(16)	1.463(4)
N(4)-C(5)	1.468(4)
C(5)-C(6)	1.524(4)
C(6)-C(7)	1.499(5)
C(7)-N(8)	1.500(4)
N(8)-C(16)	1.493(4)
N(8)-C(9)	1.493(4)
C(9)-C(10)	1.519(5)
C(10)-C(11)	1.524(4)
C(11)-N(12)	1.495(4)
N(12)-C(13)	1.506(4)
N(12)-C(15)	1.525(4)
C(13)-C(14)	1.527(4)
C(15)-C(16)	1.515(4)
N(8)-Cu(1)-N(12)	78.28(9)
N(8)-Cu(1)-Cl(1)	156.30(8)
N(12)-Cu(1)-Cl(1)	98.22(7)
N(8)-Cu(1)-Cl(2)	97.58(7)
N(12)-Cu(1)-Cl(2)	144.94(8)
Cl(1)-Cu(1)-Cl(2)	98.27(3)
C(2)-N(1)-C(15)	114.5(2)
C(2)-N(1)-C(14)	110.4(3)
C(15)-N(1)-C(14)	100.8(3)
N(1)-C(2)-C(3)	109.6(3)
N(4)-C(3)-C(2)	108.5(3)
C(16)-N(4)-C(5)	109.5(2)
C(16)-N(4)-C(3)	110.4(2)
C(5)-N(4)-C(3)	109.2(3)
N(4)-C(5)-C(6)	109.6(3)
C(7)-C(6)-C(5)	110.7(3)
C(6)-C(7)-N(8)	111.6(3)
C(16)-N(8)-C(9)	113.4(2)
C(16)-N(8)-C(7)	109.0(2)
C(9)-N(8)-C(7)	108.5(2)
C(16)-N(8)-Cu(1)	93.5(2)
C(9)-N(8)-Cu(1)	114.8(2)
C(7)-N(8)-Cu(1)	116.9(2)
N(8)-C(9)-C(10)	110.9(3)
C(9)-C(10)-C(11)	114.7(3)
N(12)-C(11)-C(10)	112.3(3)
C(11)-N(12)-C(13)	109.5(2)
C(11)-N(12)-C(15)	111.0(2)
C(13)-N(12)-C(15)	104.0(2)
C(11)-N(12)-Cu(1)	107.7(2)

C(13)-N(12)-Cu(1)	121.7(2)
C(15)-N(12)-Cu(1)	102.5(2)
N(12)-C(13)-C(14)	104.3(3)
N(1)-C(14)-C(13)	104.9(2)
N(1)-C(15)-C(16)	114.9(3)
N(1)-C(15)-N(12)	108.4(2)
C(16)-C(15)-N(12)	111.4(2)
N(4)-C(16)-N(8)	106.1(2)
N(4)-C(16)-C(15)	111.9(3)
N(8)-C(16)-C(15)	107.0(3)

Table S15. Anisotropic displacement parameters (A^2 x 10^3) for Cu(4)Cl_2. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	28(1)	23(1)	20(1)	2(1)	-5(1)	0(1)
Cl(1)	40(1)	24(1)	32(1)	5(1)	-3(1)	-1(1)
Cl(2)	31(1)	41(1)	31(1)	4(1)	-11(1)	2(1)
N(1)	28(2)	28(2)	24(1)	-1(1)	-9(1)	-4(1)
C(2)	31(2)	34(2)	31(2)	-2(2)	-1(2)	-9(2)
C(3)	23(2)	40(2)	35(2)	0(2)	3(2)	-1(2)
N(4)	21(1)	34(2)	21(1)	3(1)	0(1)	0(1)
C(5)	35(2)	33(2)	29(2)	-1(2)	7(2)	3(2)
C(6)	37(2)	39(2)	29(2)	-10(2)	1(2)	2(2)
C(7)	38(2)	32(2)	31(2)	-9(2)	-4(2)	-3(2)
N(8)	26(2)	26(2)	22(1)	0(1)	-6(1)	-6(1)
C(9)	38(2)	41(2)	31(2)	6(2)	2(2)	-15(2)
C(10)	30(2)	55(2)	29(2)	5(2)	4(2)	-13(2)
C(11)	37(2)	40(2)	24(2)	-1(2)	6(2)	-2(2)
N(12)	27(2)	28(2)	20(1)	-4(1)	-2(1)	1(1)
C(13)	41(2)	32(2)	23(2)	-6(1)	-1(2)	-1(2)
C(14)	40(2)	34(2)	24(2)	-2(2)	-5(2)	1(2)
C(15)	32(2)	23(2)	23(2)	4(1)	-4(1)	-1(1)
C(16)	27(2)	23(2)	24(2)	1(1)	-2(1)	4(1)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for Cu(**4**)Cl_2.

	x	y	z	U(eq)
H(2A)	4373	2612	1686	40
H(2B)	2640	3056	1181	40
H(3A)	3263	4510	2252	40
H(3B)	3368	3516	2956	40
H(5A)	5139	4235	4376	39
H(5B)	5113	5284	3774	39
H(6A)	7488	5223	5064	43
H(6B)	7908	4138	4677	43
H(7A)	9424	5279	4022	43
H(7B)	7913	5979	3580	43
H(9A)	9709	5682	2423	45
H(9B)	8165	5670	1473	45
H(10A)	10402	4058	1944	47
H(10B)	10355	4846	1020	47
H(11A)	8076	4182	18	41
H(11B)	9142	3229	469	41
H(13A)	6161	2019	847	40
H(13B)	6910	2398	-101	40
H(14A)	4843	3481	-719	42
H(14B)	3901	2598	-282	42
H(15A)	6159	4763	642	33
H(16A)	5766	5394	2152	31

Table S17. Atomic Coordinates (x 10^4) and Equivalent Isotropic Displacement Parameters ($Å^2$ x 10^3) for [Cu(3)(μ-OH)$_2$Cu(3)][PF_6]$_2$ · 2 CH_3CN. *U*(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu(1)	6142.5(5)	10.6(3)	6017.1(4)	23(1)
O(1)	5865(3)	-528.8(18)	4695(2)	29(1)
N(1)	6609(4)	706(2)	7323(3)	26(1)
C(2)	5110(5)	934(3)	7772(3)	38(1)
C(3)	5026(6)	279(3)	8596(4)	43(1)
N(4)	6377(4)	-298(2)	8515(3)	31(1)
C(5)	5746(5)	-937(3)	7760(4)	36(1)
C(6)	7135(5)	-1321(3)	7275(4)	34(1)
N(7)	8016(4)	-680(2)	6830(3)	24(1)
C(8)	9406(5)	-910(3)	6286(4)	34(1)
C(9)	10750(5)	-249(3)	6621(4)	39(1)
N(10)	10003(4)	323(2)	7261(3)	33(1)
C(11)	9097(5)	959(3)	6598(4)	37(1)
C(12)	7729(6)	1341(3)	7079(4)	35(1)
C(13)	7597(5)	221(3)	8181(3)	28(1)
C(14)	8908(5)	-189(3)	7727(3)	28(1)
P(1)	2764.2(13)	2870.7(7)	5722.3(9)	30(1)
F(1)	2733(6)	2948(3)	6900(3)	136(2)
F(2)	2805(5)	2789(3)	4535(2)	113(2)
F3Aa	4709(4)	2738(3)	6054(4)	96(2)
F4Aa	824(4)	2974(3)	5399(4)	94(2)
F5Aa	3025(9)	3764(2)	5660(4)	172(4)
F6Aa	2533(7)	1958(2)	5767(4)	114(2)
F3Bb	3870(3)	2117(10)	5930(9)	124(14)
F4Bb	1690(3)	3628(9)	5487(8)	66(8)
F5Bb	4391(19)	3378(13)	5848(9)	165(19)
F6Bb	1150(2)	2366(13)	5572(9)	180(2)
C(01)	6984(6)	2362(5)	4295(4)	51(2)
N(01)	6940(6)	1687(4)	4354(4)	63(1)
C(02)	7046(8)	3186(4)	4211(6)	71(2)

Table S18. Bond lengths [A] and angles [deg] for $[Cu(3)(\mu\text{-}OH)_2Cu(3)][PF_6]_2$ 2 CH_3CN.

Cu(1)-O(1)	1.923(3)
Cu(1)-O(1)#1	1.925(3)
Cu(1)-N(1)	2.044(3)
Cu(1)-N(7)	2.047(3)
Cu(1)-Cu(1)#1	2.9179(9)
O(1)-Cu(1)#1	1.925(3)
N(1)-C(13)	1.490(5)
N(1)-C(12)	1.487(5)
N(1)-C(2)	1.501(5)
C(2)-C(3)	1.557(7)
C(3)-N(4)	1.492(6)
N(4)-C(13)	1.457(6)
N(4)-C(5)	1.489(6)
C(5)-C(6)	1.541(6)
C(6)-N(7)	1.483(5)
N(7)-C(8)	1.496(5)
N(7)-C(14)	1.501(5)
C(8)-C(9)	1.570(6)
C(9)-N(10)	1.486(6)
N(10)-C(14)	1.460(5)
N(10)-C(11)	1.487(6)
C(11)-C(12)	1.523(6)
C(13)-C(14)	1.489(6)
P(1)-F(1)	1.542(3)
P(1)-F5Aa	1.542(4)
P(1)-F6Bb	1.548(8)
P(1)-F(2)	1.556(3)
P(1)-F4Aa	1.559(3)
P(1)-F4Bb	1.557(7)
P(1)-F3Bb	1.559(7)
P(1)-F5Bb	1.561(8)
P(1)-F3Aa	1.570(3)
P(1)-F6Aa	1.570(4)
C(01)-N(01)	1.155(8)
C(01)-C(02)	1.412(9)
O(1)-Cu(1)-O(1)#1	81.36(12)
O(1)-Cu(1)-N(1)	171.74(13)
O(1)#1-Cu(1)-N(1)	97.75(12)
O(1)-Cu(1)-N(7)	97.55(12)
O(1)#1-Cu(1)-N(7)	170.58(13)
N(1)-Cu(1)-N(7)	84.66(13)
O(1)-Cu(1)-Cu(1)#1	40.70(8)
O(1)#1-Cu(1)-Cu(1)#1	40.66(8)
N(1)-Cu(1)-Cu(1)#1	137.83(10)
N(7)-Cu(1)-Cu(1)#1	137.50(10)
Cu(1)-O(1)-Cu(1)#1	98.64(12)
C(13)-N(1)-C(12)	107.6(3)
C(13)-N(1)-C(2)	102.2(3)
C(12)-N(1)-C(2)	118.1(4)
C(13)-N(1)-Cu(1)	106.5(2)
C(12)-N(1)-Cu(1)	105.5(2)
C(2)-N(1)-Cu(1)	116.1(3)
N(1)-C(2)-C(3)	103.3(3)
N(4)-C(3)-C(2)	107.1(3)
C(13)-N(4)-C(5)	114.5(3)
C(13)-N(4)-C(3)	99.9(4)
C(5)-N(4)-C(3)	111.5(3)

N(4)-C(5)-C(6)	113.3(3)
N(7)-C(6)-C(5)	107.1(4)
C(6)-N(7)-C(8)	117.2(3)
C(6)-N(7)-C(14)	107.7(3)
C(8)-N(7)-C(14)	102.7(3)
C(6)-N(7)-Cu(1)	105.0(2)
C(8)-N(7)-Cu(1)	117.3(2)
C(14)-N(7)-Cu(1)	106.1(2)
N(7)-C(8)-C(9)	103.2(3)
N(10)-C(9)-C(8)	106.8(3)
C(14)-N(10)-C(11)	113.8(3)
C(14)-N(10)-C(9)	100.8(4)
C(11)-N(10)-C(9)	111.3(4)
N(10)-C(11)-C(12)	113.1(4)
N(1)-C(12)-C(11)	107.5(4)
N(4)-C(13)-N(1)	105.2(3)
N(4)-C(13)-C(14)	114.3(4)
N(1)-C(13)-C(14)	106.6(3)
N(10)-C(14)-C(13)	115.0(4)
N(10)-C(14)-N(7)	104.6(3)
C(13)-C(14)-N(7)	107.2(3)
F(1)-P(1)-F5Aa	89.8(3)
F(1)-P(1)-F6Bb	89.7(4)
F(1)-P(1)-F(2)	179.6(2)
F5Aa-P(1)-F(2)	90.4(3)
F6Bb-P(1)-F(2)	90.4(4)
F(1)-P(1)-F4Aa	92.6(2)
F5Aa-P(1)-F4Aa	90.9(3)
F(2)-P(1)-F4Aa	87.6(2)
F(1)-P(1)-F4Bb	90.4(4)
F6Bb-P(1)-F4Bb	90.4(5)
F(2)-P(1)-F4Bb	90.0(4)
F(1)-P(1)-F3Bb	91.1(4)
F6Bb-P(1)-F3Bb	90.4(5)
F(2)-P(1)-F3Bb	88.6(4)
F4Bb-P(1)-F3Bb	178.4(6)
F(1)-P(1)-F5Bb	91.5(4)
F6Bb-P(1)-F5Bb	178.8(6)
F(2)-P(1)-F5Bb	88.4(4)
F4Bb-P(1)-F5Bb	89.6(5)
F3Bb-P(1)-F5Bb	89.6(5)
F(1)-P(1)-F3Aa	87.2(2)
F5Aa-P(1)-F3Aa	90.9(3)
F(2)-P(1)-F3Aa	92.6(2)
F4Aa-P(1)-F3Aa	178.2(3)
F(1)-P(1)-F6Aa	91.3(3)
F5Aa-P(1)-F6Aa	178.5(3)
F(2)-P(1)-F6Aa	88.5(2)
F4Aa-P(1)-F6Aa	90.0(3)
F3Aa-P(1)-F6Aa	88.2(2)
N(01)-C(01)-C(02)	179.3(6)

Table S19. Anisotropic displacement parameters (A^2 x 10^3) for [Cu(3)(μ-OH)$_2$Cu(3)][PF$_6$]$_2$ 2 CH$_3$CN. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Cu(1)	19(1)	27(1)	20(1)	-2(1)	-1(1)	4(1)
O(1)	25(1)	38(2)	21(1)	-5(1)	-2(1)	10(1)
N(1)	29(2)	27(2)	21(2)	-1(2)	1(1)	3(2)
C(2)	33(2)	50(3)	32(3)	-7(2)	8(2)	10(2)
C(3)	31(2)	62(4)	38(3)	-3(2)	10(2)	2(2)
N(4)	30(2)	36(2)	28(2)	2(2)	7(2)	-3(2)
C(5)	35(2)	37(3)	38(3)	1(2)	11(2)	-10(2)
C(6)	32(2)	29(3)	37(3)	-1(2)	1(2)	-4(2)
N(7)	19(2)	25(2)	26(2)	-1(2)	2(1)	5(1)
C(8)	22(2)	40(3)	37(3)	-2(2)	3(2)	7(2)
C(9)	27(2)	52(3)	36(3)	0(2)	4(2)	-3(2)
N(10)	24(2)	37(2)	35(2)	-1(2)	4(2)	-6(2)
C(11)	38(2)	36(3)	37(3)	2(2)	9(2)	-11(2)
C(12)	47(3)	22(3)	34(3)	-2(2)	2(2)	-2(2)
C(13)	29(2)	33(3)	20(2)	-1(2)	-1(2)	4(2)
C(14)	26(2)	29(3)	26(2)	2(2)	-5(2)	-2(2)
P(1)	27(1)	29(1)	32(1)	-4(1)	1(1)	2(1)
F(1)	162(4)	208(6)	36(2)	-8(3)	13(3)	75(4)
F(2)	140(4)	164(5)	43(2)	-1(2)	33(2)	18(3)
F3Aa	27(2)	124(5)	128(4)	-2(3)	-5(2)	5(2)
F4Aa	34(2)	125(5)	115(4)	-35(3)	-4(2)	22(2)
F5Aa	222(8)	40(3)	184(6)	37(4)	-131(6)	-58(4)
F6Aa	122(5)	41(3)	147(5)	9(3)	-51(3)	-17(3)
C(01)	29(2)	94(6)	31(3)	13(3)	8(2)	2(3)
N(01)	69(3)	59(4)	56(3)	2(3)	2(3)	3(3)
C(02)	51(3)	78(5)	82(5)	30(4)	10(3)	-12(4)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for $[Cu(3)(\mu\text{-}OH)_2Cu(3)][PF_6]_2$ 2 CH_3CN.

	x	y	z	U(eq)
H(2A)	4076	941	7223	46
H(2B)	5268	1456	8110	46
H(3A)	5206	505	9310	52
H(3B)	3914	20	8447	52
H(5A)	4876	-721	7189	43
H(5B)	5209	-1344	8125	43
H(6A)	7931	-1609	7818	40
H(6B)	6639	-1694	6717	40
H(8A)	9015	-919	5515	40
H(8B)	9864	-1431	6523	40
H(9A)	11794	-474	7038	47
H(9B)	11022	11	5994	47
H(11A)	8584	739	5904	44
H(11B)	9915	1365	6486	44
H(12A)	8235	1626	7728	42
H(12B)	7082	1719	6579	42
H(13A)	8134	564	8777	34
H(14A)	9598	-532	8271	34
H(02A)	6053	3416	4419	360(9)
H(02B)	7065	3332	3484	100(2)
H(02C)	8062	3384	4673	120(3)

Table S21. Atomic Coordinates and B_{iso}/B_{eq} for $[Cu(1)(\mu\text{-}OH)_2Cu(1)][PF_6]_2 CH_3CN$. $B_{eq} = 8/3p^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}(aa^*bb^*)\cos g + 2U_{13}(aa^*cc^*)\cos b + 2U_{23}(bb^*cc^*)\cos a)$

atom	x	y	z	B_{eq}
Cu(1)	0.96697(5)	0.10953(4)	0.50767(5)	1.75(1)
P(1)	0.5095(1)	0.30997(8)	0.7135(1)	2.66(2)
F(1)	0.4838(2)	0.2049(2)	0.5586(2)	3.65(5)
F(2)	0.3544(2)	0.2178(2)	0.7085(3)	5.36(6)
F(3)	0.5335(2)	0.4136(2)	0.8675(2)	5.05(6)
F(4)	0.6647(2)	0.4020(2)	0.7202(3)	5.04(6)
F(5)	0.4368(2)	0.3765(2)	0.5942(2)	4.16(5)
F(6)	0.5808(3)	0.2415(2)	0.8324(2)	5.53(7)
O(1)	1.0118(2)	0.0083(2)	0.3692(2)	2.07(5)
N(1)	0.8968(3)	0.1981(2)	0.6512(3)	1.70(6)
N(4)	0.7079(3)	0.1933(2)	0.3448(3)	1.89(6)
N(8)	0.9572(3)	0.2369(2)	0.3725(3)	1.58(6)
N(11)	1.0678(2)	0.4219(2)	0.6804(3)	1.70(6)
N(19)	0.1941(3)	0.1181(3)	0.1818(4)	3.48(8)
C(2)	0.7371(3)	0.1134(3)	0.5896(4)	2.09(8)
C(3)	0.6679(3)	0.0779(3)	0.4051(4)	2.54(8)
C(5)	0.6580(3)	0.1561(3)	0.1647(4)	2.54(8)
C(6)	0.7442(4)	0.0990(3)	0.1068(4)	2.64(9)
C(7)	0.9045(3)	0.1943(3)	0.1915(4)	2.19(8)
C(9)	1.1048(3)	0.3473(3)	0.4362(4)	2.07(8)
C(10)	1.1656(3)	0.3933(3)	0.6184(4)	2.30(8)
C(12)	1.1205(3)	0.4500(3)	0.8592(4)	2.63(9)
C(13)	1.1112(4)	0.3327(3)	0.9171(4)	2.78(9)
C(14)	0.9576(3)	0.2250(3)	0.8340(4)	2.19(8)
C(15)	0.9170(3)	0.3212(3)	0.6050(3)	1.57(8)
C(16)	0.8616(3)	0.2857(3)	0.4199(4)	1.57(8)
C(17)	0.4383(4)	0.3024(3)	0.2179(5)	3.7(1)
C(18)	0.3011(4)	0.1987(3)	0.1968(4)	2.53(9)
H(1)	1.0527	0.0376	0.2869	6(1)
H(2b)	0.6909	0.1703	0.6299	1.116
H(2a)	0.7216	0.0486	0.6299	0.285
H(3a)	0.5567	0.0332	0.3430	5.717
H(3b)	0.6945	0.0212	0.3676	1.000
H(5a)	0.5476	0.1038	0.1044	1.962
H(5b)	0.6652	0.2344	0.1263	0.467
H(6a)	0.7287	0.1011	-0.0057	2.477
H(6b)	0.7343	0.0165	0.1253	2.756
H(7b)	0.9743	0.1644	0.1627	1.274
H(7a)	0.9360	0.2890	0.1666	2.155
H(9b)	1.1754	0.3005	0.3856	2.901
H(9a)	1.1214	0.4347	0.3698	2.018
H(10b)	1.1864	0.3278	0.6412	3.019
H(10a)	1.2707	0.4873	0.6584	2.128
H(12b)	1.0646	0.4825	0.8969	1.000
H(12a)	1.2201	0.5156	0.9079	1.498
H(13b)	1.1400	0.3497	1.0413	2.612
H(13a)	1.1906	0.2980	0.9027	4.095
H(14b)	0.8651	0.2512	0.8620	4.345
H(14a)	0.9475	0.1336	0.8606	4.067
H(15)	0.8579	0.3681	0.6574	0.287
H(16)	0.8630	0.3600	0.3772	1.000
H(17b)	0.4405	0.3059	0.1135	5.430
H(17c)	0.4475	0.3822	0.2734	4.988
H(17a)		0.5154	0.2877	0.2812
	7.762			

Table S22. Bond Lengths [Å] and Angles [deg] for $[Cu(1)(\mu\text{-}OH)_2Cu(1)][PF_6]_2 \cdot CH_3CN$.

atom	atom	distance	atom	atom	distance
Cu(1)	O(1)	1.911(4)	Cu(1)	O(1)	1.907(4)
Cu(1)	N(1)	2.054(4)	Cu(1)	N(8)	2.047(4)
P(1)	F(1)	1.605(4)	P(1)	F(2)	1.592(4)
P(1)	F(3)	1.596(4)	P(1)	F(4)	1.587(4)
P(1)	F(5)	1.592(4)	P(1)	F(6)	1.600(4)
O(1)	H(1)	1.004(4)	N(1)	C(2)	1.492(7)
N(1)	C(14)	1.496(7)	N(1)	C(15)	1.501(6)
N(4)	C(3)	1.474(7)	N(4)	C(5)	1.472(7)
N(4)	C(16)	1.455(7)	N(8)	C(7)	1.479(7)
N(8)	C(9)	1.481(7)	N(8)	C(16)	1.510(7)
N(11)	C(10)	1.471(7)	N(11)	C(12)	1.462(7)
N(11)	C(15)	1.461(7)	N(19)	C(18)	1.130(7)
C(2)	C(3)	1.505(8)	C(2)	H(2b)	1.07
C(2)	H(2a)	0.86	C(3)	H(3a)	1.03
C(3)	H(3b)	0.89	C(5)	C(6)	1.521(8)
C(5)	H(5a)	1.02	C(5)	H(5b)	1.00
C(6)	C(7)	1.517(8)	C(6)	H(6a)	0.97
C(6)	H(6b)	0.97	C(7)	H(7b)	1.04
C(7)	H(7a)	1.10	C(9)	C(10)	1.485(8)
C(9)	H(9b)	1.26	C(9)	H(9a)	1.23
C(10)	H(10b)	0.91	C(10)	H(10a)	1.14
C(12)	C(13)	1.505(8)	C(12)	H(12b)	0.95
C(12)	H(12a)	0.96	C(13)	C(14)	1.508(8)
C(13)	H(13b)	1.02	C(13)	H(13a)	1.13
C(14)	H(14b)	1.25	C(14)	H(14a)	1.10
C(15)	C(16)	1.510(7)	C(15)	H(15)	1.16
C(16)	H(16)	0.99	C(17)	C(18)	1.446(9)
C(17)	H(17b)	0.95	C(17)	H(17c)	0.95
C(17)	H(17a)	0.95			

atom	atom	atom	angle	atom	atom	atom	angle
O(1)	Cu(1)	O(1)	80.1(2)	O(1)	Cu(1)	N(1)	173.1(2)
O(1)	Cu(1)	N(8)	96.8(2)	O(1)	Cu(1)	N(1)	96.7(2)
O(1)	Cu(1)	N(8)	175.8(2)	N(1)	Cu(1)	N(8)	86.7(2)
F(1)	P(1)	F(2)	90.1(2)	F(1)	P(1)	F(3)	179.4(2)
F(1)	P(1)	F(4)	90.2(2)	F(1)	P(1)	F(5)	90.6(2)
F(1)	P(1)	F(6)	89.1(2)	F(2)	P(1)	F(3)	89.3(2)
F(2)	P(1)	F(4)	179.5(3)	F(2)	P(1)	F(5)	89.7(2)
F(2)	P(1)	F(6)	89.7(2)	F(3)	P(1)	F(4)	90.3(2)
F(3)	P(1)	F(5)	89.4(2)	F(3)	P(1)	F(6)	90.9(2)
F(4)	P(1)	F(5)	90.7(2)	F(4)	P(1)	F(6)	89.9(2)
F(5)	P(1)	F(6)	179.3(2)	Cu(1)	O(1)	Cu(1)	99.9(2)
Cu(1)	O(1)	H(1)	124.8(3)	Cu(1)	O(1)	H(1)	130.6(3)
Cu(1)	N(1)	C(2)	105.3(3)	Cu(1)	N(1)	C(14)	121.6(3)
Cu(1)	N(1)	C(15)	104.6(3)	C(2)	N(1)	C(14)	107.2(4)
C(2)	N(1)	C(15)	107.0(4)	C(14)	N(1)	C(15)	110.3(4)
C(3)	N(4)	C(5)	110.9(4)	C(3)	N(4)	C(16)	115.1(4)
C(5)	N(4)	C(16)	110.0(4)	Cu(1)	N(8)	C(7)	120.5(3)
Cu(1)	N(8)	C(9)	107.3(3)	Cu(1)	N(8)	C(16)	103.3(3)
C(7)	N(8)	C(9)	107.8(4)	C(7)	N(8)	C(16)	109.9(4)
C(9)	N(8)	C(16)	107.3(4)	C(10)	N(11)	C(12)	111.7(4)
C(10)	N(11)	C(15)	114.1(4)	C(12)	N(11)	C(15)	109.8(4)
N(1)	C(2)	C(3)	110.6(5)	N(1)	C(2)	H(2b)	107.4
N(1)	C(2)	H(2a)	109.3	C(3)	C(2)	H(2b)	104.2
C(3)	C(2)	H(2a)	114.8	H(2b)	C(2)	H(2a)	110.1
N(4)	C(3)	C(2)	111.6(5)	N(4)	C(3)	H(3a)	100.5
N(4)	C(3)	H(3b)	113.5	C(2)	C(3)	H(3a)	121.1
C(2)	C(3)	H(3b)	106.4	H(3a)	C(3)	H(3b)	103.8

N(4)	C(5)	C(6)	112.5(5)	N(4)	C(5)	H(5a)	113.5
N(4)	C(5)	H(5b)	108.4	C(6)	C(5)	H(5a)	114.9
C(6)	C(5)	H(5b)	110.6	H(5a)	C(5)	H(5b)	95.6
C(5)	C(6)	C(7)	108.9(5)	C(5)	C(6)	H(6a)	109.0
C(5)	C(6)	H(6b)	117.1	C(7)	C(6)	H(6a)	99.5
C(7)	C(6)	H(6b)	106.9	H(6a)	C(6)	H(6b)	113.9
N(8)	C(7)	C(6)	113.5(5)	N(8)	C(7)	H(7b)	108.2
N(8)	C(7)	H(7a)	99.5	C(6)	C(7)	H(7b)	115.6
C(6)	C(7)	H(7a)	115.8	H(7b)	C(7)	H(7a)	102.5
N(8)	C(9)	C(10)	110.5(5)	N(8)	C(9)	H(9b)	103.3
N(8)	C(9)	H(9a)	117.2	C(10)	C(9)	H(9b)	112.0
C(10)	C(9)	H(9a)	113.8	H(9b)	C(9)	H(9a)	98.8
N(11)	C(10)	C(9)	112.6(5)	N(11)	C(10)	H(10b)	119.7
N(11)	C(10)	H(10a)	107.8	C(9)	C(10)	H(10b)	98.7
C(9)	C(10)	H(10a)	107.1	H(10b)	C(10)	H(10a)	110.1
N(11)	C(12)	C(13)	112.7(5)	N(11)	C(12)	H(12b)	109.4
N(11)	C(12)	H(12a)	109.3	C(13)	C(12)	H(12b)	108.6
C(13)	C(12)	H(12a)	108.7	H(12b)	C(12)	H(12a)	108.1
C(12)	C(13)	C(14)	109.8(5)	C(12)	C(13)	H(13b)	113.2
C(12)	C(13)	H(13a)	115.0	C(14)	C(13)	H(13b)	107.5
C(14)	C(13)	H(13a)	110.9	H(13b)	C(13)	H(13a)	100.0
N(1)	C(14)	C(13)	113.1(5)	N(1)	C(14)	H(14b)	98.5
N(1)	C(14)	H(14a)	107.2	C(13)	C(14)	H(14b)	114.6
C(13)	C(14)	H(14a)	112.7	H(14b)	C(14)	H(14a)	109.7
N(1)	C(15)	N(11)	113.0(4)	N(1)	C(15)	C(16)	106.4(4)
N(1)	C(15)	H(15)	110.3	N(11)	C(15)	C(16)	111.0(4)
N(11)	C(15)	H(15)	102.8	C(16)	C(15)	H(15)	113.6
N(4)	C(16)	N(8)	113.7(4)	N(4)	C(16)	C(15)	111.0(4)
N(4)	C(16)	H(16)	102.4	N(8)	C(16)	C(15)	107.0(4)
N(8)	C(16)	H(16)	110.6	C(15)	C(16)	H(16)	112.2
C(18)	C(17)	H(17b)	109.3	C(18)	C(17)	H(17c)	108.8
C(18)	C(17)	H(17a)	109.6	H(17b)	C(17)	H(17c)	109.5
H(17b)	C(17)	H(17a)	110.1	H(17c)	C(17)	H(17a)	109.5
N(19)	C(18)	C(17)	179.3(7)				

Table S23. Anisotropic Displacement Parameters for $[Cu(1)(\square\text{-}OH)_2Cu(1)][PF_6]_2 CH_3CN$. The general temperature factor expression: $exp(-2p2(a^*2U_{11}H^2 + b^*U_{22}K^2 + c^*U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	0.0298(3)	0.0211(3)	0.0228(3)	0.0152(2)	0.0132(2)	0.0103(2)
P(1)	0.0363(6)	0.0326(6)	0.0315(6)	0.0199(5)	0.0086(5)	0.0056(5)
F(1)	0.055(1)	0.047(1)	0.038(1)	0.032(1)	0.014(1)	0.002(1)
F(2)	0.065(2)	0.041(1)	0.114(2)	0.025(1)	0.054(1)	0.026(1)
F(3)	0.083(2)	0.063(2)	0.046(1)	0.044(1)	0.021(1)	-0.004(1)
F(4)	0.040(1)	0.052(1)	0.089(2)	0.016(1)	0.024(1)	0.002(1)
F(5)	0.064(1)	0.050(1)	0.053(1)	0.040(1)	0.015(1)	0.019(1)
F(6)	0.103(2)	0.090(2)	0.038(1)	0.071(2)	0.017(1)	0.021(1)
O(1)	0.043(1)	0.028(1)	0.029(1)	0.026(1)	0.024(1)	0.019(1)
N(1)	0.026(2)	0.022(2)	0.020(2)	0.013(1)	0.009(1)	0.008(1)
N(4)	0.026(2)	0.019(2)	0.024(2)	0.007(1)	0.011(1)	0.007(1)
N(8)	0.031(2)	0.019(1)	0.015(2)	0.014(1)	0.010(1)	0.009(1)
N(11)	0.025(2)	0.020(2)	0.012(2)	0.007(1)	0.004(1)	0.002(1)
N(19)	0.043(2)	0.043(2)	0.052(2)	0.018(2)	0.028(2)	0.018(2)
C(2)	0.037(2)	0.022(2)	0.033(2)	0.014(2)	0.024(2)	0.018(2)
C(3)	0.028(2)	0.032(2)	0.031(2)	0.015(2)	0.004(2)	0.005(2)
C(5)	0.028(2)	0.036(2)	0.018(2)	0.011(2)	-0.003(2)	0.007(2)
C(6)	0.044(2)	0.037(2)	0.022(2)	0.021(2)	0.014(2)	0.010(2)
C(7)	0.032(2)	0.031(2)	0.025(2)	0.015(2)	0.016(2)	0.011(2)
C(9)	0.023(2)	0.025(2)	0.028(2)	0.007(2)	0.011(2)	0.013(2)
C(10)	0.031(2)	0.021(2)	0.038(2)	0.012(2)	0.016(2)	0.011(2)
C(12)	0.033(2)	0.029(2)	0.029(2)	0.012(2)	0.008(2)	0.003(2)
C(13)	0.052(3)	0.035(2)	0.016(2)	0.021(2)	0.009(2)	0.008(2)
C(14)	0.042(2)	0.028(2)	0.018(2)	0.020(2)	0.011(2)	0.010(2)
C(15)	0.028(2)	0.013(2)	0.020(2)	0.011(2)	0.009(2)	0.005(1)
C(16)	0.026(2)	0.016(2)	0.025(2)	0.012(2)	0.013(2)	0.014(2)
C(17)	0.038(2)	0.039(2)	0.074(3)	0.021(2)	0.029(2)	0.022(2)
C(18)	0.046(3)	0.031(2)	0.031(2)	0.026(2)	0.018(2)	0.012(2)