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S 1

Table S1 Atomic Coordinates and Isotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$, 3

atom	x	y	z	B_{eq}
Cu(1)	0.2836(1)	0.06031(10)	0.87236(4)	4.89(3)
Cu(2)	0.3177(1)	0.08335(10)	0.58846(5)	5.20(4)
Cl(1)	0.4051(2)	0.2419(2)	0.97885(9)	6.17(7)
Cl(2)	-0.1147(2)	0.1729(2)	0.94589(10)	5.97(7)
Cl(3)	0.5186(3)	-0.1503(2)	0.7475(1)	7.53(9)
Cl(4)	0.9851(6)	0.1819(5)	0.6918(3)	10.5(2)
Cl(4')	0.9235(8)	0.1489(8)	0.6313(5)	12.5(3)
O(11)	0.5015(6)	0.2233(6)	0.9718(3)	8.9(2)
O(12)	0.4170(7)	0.2846(6)	1.0246(3)	9.2(2)
O(13)	0.3529(7)	0.1514(5)	0.9759(3)	9.1(3)
O(14)	0.3511(6)	0.3052(6)	0.9416(3)	9.0(2)
O(21)	-0.2020(6)	0.1897(6)	0.9622(3)	8.9(3)
O(22)	-0.0552(6)	0.2600(5)	0.9522(3)	8.5(2)
O(23)	-0.0585(6)	0.0931(5)	0.9704(3)	7.8(2)
O(24)	-0.1459(6)	0.1528(6)	0.8948(3)	8.4(2)
O(31)	0.5880(6)	-0.2275(6)	0.7533(2)	8.7(2)
O(32)	0.5332(9)	-0.0790(8)	0.7146(4)	15.5(4)
O(33)	0.4210(7)	-0.1863(7)	0.7279(3)	10.4(3)
O(34)	0.5216(8)	-0.1147(7)	0.7941(3)	11.1(3)
O(41)	0.969(1)	0.090(1)	0.6763(7)	23.2(7)
O(42)	0.9680(10)	0.2449(10)	0.6479(5)	15.5(4)
O(43)	0.955(2)	0.223(2)	0.7288(9)	17.5(8)
O(43')	0.817(2)	0.163(3)	0.628(1)	24(1)
O(44')	0.930(2)	0.134(3)	0.5801(7)	18(1)

Table S1 Atomic Coordinates and Isotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	x	y	z	B_{eq}
O(44)	1.090(2)	0.176(2)	0.7063(7)	14.1(6)
N(1)	0.2190(6)	-0.0303(5)	0.8091(2)	4.5(2)
N(1')	0.2420(6)	-0.0171(5)	0.6301(2)	5.0(2)
N(2)	0.1522(7)	0.0401(6)	0.8908(4)	6.9(2)
N(2')	0.3632(7)	-0.0443(6)	0.5625(3)	6.5(2)
N(3)	0.3202(6)	-0.0723(6)	0.9050(3)	5.9(2)
N(3')	0.1998(7)	0.0677(6)	0.5350(3)	6.6(2)
N(4)	0.2289(6)	0.1940(6)	0.8522(3)	5.4(2)
N(4')	0.4579(6)	0.0916(6)	0.6229(3)	5.4(2)
N(5)	0.4265(6)	0.0674(6)	0.8772(2)	5.0(1)
N(5')	0.2559(6)	0.2130(6)	0.5963(3)	5.5(2)
C(1)	0.1117(8)	-0.0138(10)	0.8050(4)	8.0(3)
C(1')	0.273(1)	-0.1184(7)	0.6208(3)	7.1(3)
C(2)	0.0840(9)	-0.004(1)	0.8512(5)	9.4(4)
C(2')	0.364(1)	-0.1199(7)	0.6022(4)	7.7(3)
C(3)	0.182(1)	-0.0264(10)	0.9376(5)	10.9(5)
C(3')	0.297(1)	-0.0723(9)	0.5171(4)	9.0(4)
C(4)	0.2468(10)	-0.101(1)	0.9332(5)	9.2(4)
C(4')	0.236(1)	0.0108(10)	0.4948(4)	9.5(4)
C(5)	0.324(1)	-0.1448(7)	0.8657(4)	8.2(3)
C(5')	0.1211(9)	0.0120(8)	0.5516(4)	7.3(3)
C(6)	0.2469(10)	-0.1323(8)	0.8220(4)	7.1(3)
C(6')	0.1406(8)	0.0027(9)	0.6063(4)	6.8(3)
C(7)	0.1218(9)	0.1401(8)	0.9042(4)	7.4(3)

Table S1 Atomic Coordinates and Isotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	x	y	z	B_{eq}
C(7')	0.4657(10)	-0.0207(8)	0.5590(4)	7.2(3)
C(8)	0.1476(8)	0.2154(8)	0.8696(4)	6.5(3)
C(8')	0.5198(9)	0.0353(8)	0.6029(4)	6.2(3)
C(9)	0.096(1)	0.302(1)	0.8585(5)	9.1(4)
C(9')	0.6184(10)	0.0294(9)	0.6190(5)	7.3(3)
C(10)	0.123(1)	0.368(1)	0.8271(6)	9.8(5)
C(10')	0.6623(9)	0.0817(10)	0.6604(6)	8.3(4)
C(11)	0.204(1)	0.3474(9)	0.8095(5)	8.6(4)
C(11')	0.6024(9)	0.1363(8)	0.6832(5)	7.5(3)
C(12)	0.2521(9)	0.2593(8)	0.8221(4)	6.5(3)
C(12')	0.5035(8)	0.1400(7)	0.6626(4)	6.0(3)
C(13)	0.4196(8)	-0.0576(7)	0.9358(3)	5.8(2)
C(13')	0.1615(9)	0.1670(8)	0.5165(4)	7.4(3)
C(14)	0.4794(8)	0.0031(7)	0.9093(3)	5.3(2)
C(14')	0.1819(8)	0.2377(8)	0.5599(4)	5.9(3)
C(15)	0.5797(9)	-0.0050(9)	0.9175(4)	7.0(3)
C(15')	0.1286(9)	0.3228(9)	0.5589(5)	7.4(3)
C(16)	0.6302(9)	0.0542(10)	0.8916(5)	7.7(4)
C(16')	0.1506(9)	0.3839(8)	0.5986(5)	7.5(4)
C(17)	0.5801(10)	0.1195(8)	0.8583(5)	7.3(3)
C(17')	0.2262(9)	0.3604(8)	0.6376(5)	7.3(3)
C(18)	0.4818(8)	0.1236(7)	0.8516(4)	6.1(3)
C(18')	0.2772(8)	0.2736(8)	0.6358(4)	6.0(3)
C(19)	0.2522(7)	0.0068(6)	0.7660(3)	4.8(2)

Table S1 Atomic Coordinates and Isotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	x	y	z	B_{eq}
C(19')	0.2676(7)	0.0119(6)	0.6818(3)	4.6(2)
C(20)	0.2136(7)	-0.0397(7)	0.7169(3)	5.1(2)
H(1a)	0.0932	0.0448	0.7867	9.5484
H(1b)	0.0768	-0.0683	0.7881	9.5484
H(1'a)	0.2834	-0.1547	0.6504	8.5562
H(1'b)	0.2214	-0.1485	0.5973	8.5562
H(2a)	0.0702	-0.0682	0.8613	11.2769
H(2b)	0.0255	0.0349	0.8457	11.2769
H(2'a)	0.4186	-0.1064	0.6285	9.2298
H(2'b)	0.3719	-0.1836	0.5894	9.2298
H(3a)	0.1236	-0.0554	0.9439	13.1297
H(3b)	0.2117	0.0144	0.9643	13.1297
H(3'a)	0.2548	-0.1237	0.5235	10.7778
H(3'b)	0.3347	-0.0953	0.4949	10.7778
H(4a)	0.2808	-0.1196	0.9650	11.0089
H(4b)	0.2101	-0.1551	0.9174	11.0089
H(4'a)	0.1805	-0.0132	0.4714	11.3455
H(4'b)	0.2738	0.0533	0.4792	11.3455
H(5a)	0.3177	-0.2092	0.8781	9.8286
H(5b)	0.3858	-0.1386	0.8569	9.8286
H(5'a)	0.0600	0.0454	0.5405	8.7238
H(5'b)	0.1169	-0.0523	0.5377	8.7238
H(6a)	0.2693	-0.1612	0.7955	8.5123
H(6b)	0.1898	-0.1663	0.8267	8.5123

Table S1 Atomic Coordinates and Isotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	x	y	z	B_{eq}
H(6'a)	0.1010	-0.0497	0.6139	8.1814
H(6'b)	0.1214	0.0628	0.6190	8.1814
H(7a)	0.0525	0.1410	0.9022	8.9129
H(7b)	0.1555	0.1555	0.9366	8.9129
H(7'a)	0.4638	0.0183	0.5306	8.6024
H(7'b)	0.5000	-0.0804	0.5564	8.6024
H(9)	0.0414	0.3168	0.8728	10.9224
H(9')	0.6571	-0.0100	0.6023	8.7457
H(10)	0.0863	0.4262	0.8177	11.7922
H(10')	0.7318	0.0798	0.6727	9.9047
H(11)	0.2274	0.3930	0.7888	10.3186
H(11')	0.6290	0.1709	0.7126	8.9659
H(12)	0.3066	0.2446	0.8078	7.7821
H(12')	0.4639	0.1807	0.6782	7.1944
H(13a)	0.4144	-0.0250	0.9651	6.9532
H(13b)	0.4506	-0.1199	0.9435	6.9532
H(13'a)	0.1944	0.1890	0.4922	8.8751
H(13'b)	0.0925	0.1634	0.5032	8.8751
H(15)	0.6141	-0.0509	0.9407	8.4244
H(15')	0.0777	0.3391	0.5315	8.8972
H(16)	0.7001	0.0495	0.8968	9.2984
H(16')	0.1137	0.4427	0.5992	9.0433
H(17)	0.6143	0.1611	0.8403	8.7494
H(17')	0.2429	0.4030	0.6650	8.7979

Table S1 Atomic Coordinates and Isotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	x	y	z	B_{eq}
H(18)	0.4474	0.1681	0.8277	7.2624
H(18')	0.3284	0.2557	0.6629	7.1664
H(19a)	0.2349	0.0748	0.7628	5.7079
H(19b)	0.3220	0.0003	0.7728	5.7079
H(19'a)	0.2550	0.0806	0.6833	5.5728
H(19'b)	0.3363	-0.0001	0.6933	5.5728
H(20a)	0.1443	-0.0298	0.7068	6.1430
H(20b)	0.2274	-0.1085	0.7182	6.1430

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

Table S2 Anisotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$, 3

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	0.089(1)	0.0518(8)	0.0516(7)	-0.0058(8)	0.0301(7)	-0.0018(7)
Cu(2)	0.097(1)	0.0541(8)	0.0473(7)	0.0066(8)	0.0187(7)	0.0074(7)
Cl(1)	0.112(2)	0.052(1)	0.070(1)	-0.007(2)	0.018(2)	-0.001(1)
Cl(2)	0.076(2)	0.075(2)	0.075(2)	-0.004(1)	0.014(1)	0.009(1)
Cl(3)	0.120(3)	0.093(2)	0.069(2)	0.025(2)	0.011(2)	0.009(1)
Cl(4)	0.159(7)	0.092(5)	0.169(5)	0.068(4)	0.079(5)	0.057(4)
Cl(4')	0.16(1)	0.128(9)	0.199(8)	-0.004(8)	0.063(7)	-0.014(8)
O(11)	0.119(5)	0.100(6)	0.132(7)	0.008(5)	0.056(6)	0.005(5)
O(12)	0.167(8)	0.113(7)	0.069(4)	-0.010(6)	0.022(5)	-0.027(4)
O(13)	0.183(9)	0.055(4)	0.116(6)	-0.048(4)	0.054(6)	-0.010(4)
O(14)	0.137(7)	0.090(6)	0.099(6)	0.016(5)	-0.006(5)	0.034(4)
O(21)	0.098(6)	0.129(7)	0.136(7)	0.019(5)	0.077(5)	0.036(6)
O(22)	0.105(6)	0.069(5)	0.146(7)	-0.017(4)	0.017(6)	-0.020(5)
O(23)	0.106(6)	0.085(5)	0.104(6)	0.026(4)	0.018(5)	0.032(4)
O(24)	0.120(7)	0.122(7)	0.074(3)	-0.020(6)	0.017(4)	-0.005(5)
O(31)	0.124(7)	0.141(7)	0.070(5)	0.072(5)	0.034(5)	0.022(5)
O(32)	0.25(1)	0.157(9)	0.20(1)	0.002(9)	0.092(9)	0.148(8)
O(33)	0.119(6)	0.140(8)	0.126(7)	0.008(6)	0.003(6)	0.021(6)
O(34)	0.212(10)	0.120(7)	0.082(4)	0.041(7)	0.020(6)	-0.028(5)
N(1)	0.070(4)	0.056(4)	0.049(3)	0.001(4)	0.022(3)	0.000(3)
N(1')	0.091(5)	0.056(4)	0.039(3)	-0.003(4)	0.004(3)	0.004(3)
N(2)	0.090(5)	0.065(5)	0.124(6)	-0.017(5)	0.062(5)	-0.018(4)
N(2')	0.140(7)	0.054(4)	0.060(4)	0.011(5)	0.039(5)	0.001(3)
N(3)	0.104(6)	0.057(4)	0.060(5)	-0.006(5)	0.011(3)	0.010(3)

Table S2 Anisotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
N(3')	0.108(6)	0.070(5)	0.063(5)	0.000(5)	0.000(3)	0.008(4)
N(4)	0.082(6)	0.058(4)	0.071(5)	0.001(4)	0.031(4)	0.003(3)
N(4')	0.091(3)	0.050(5)	0.073(5)	0.012(4)	0.034(3)	0.021(4)
N(5)	0.088(2)	0.052(5)	0.050(4)	0.000(4)	0.018(4)	-0.010(3)
N(5')	0.087(6)	0.053(4)	0.068(5)	0.007(4)	0.015(4)	0.019(3)
C(1)	0.061(5)	0.14(1)	0.095(7)	-0.018(7)	0.011(6)	0.021(8)
C(1')	0.18(1)	0.046(5)	0.057(6)	-0.003(6)	0.043(7)	0.008(5)
C(2)	0.096(9)	0.16(1)	0.127(9)	-0.045(9)	0.070(7)	-0.068(9)
C(2')	0.18(1)	0.041(6)	0.090(8)	0.026(7)	0.068(8)	0.021(5)
C(3)	0.24(2)	0.092(10)	0.14(1)	0.024(8)	0.16(1)	0.039(7)
C(3')	0.21(1)	0.089(8)	0.047(6)	-0.002(8)	0.029(6)	-0.012(6)
C(4)	0.12(1)	0.13(1)	0.115(10)	-0.014(7)	0.069(8)	0.052(9)
C(4')	0.22(2)	0.102(9)	0.036(6)	0.012(8)	0.016(7)	-0.004(5)
C(5)	0.17(1)	0.042(6)	0.080(7)	0.000(7)	-0.010(6)	-0.010(5)
C(5')	0.114(9)	0.085(8)	0.074(5)	-0.012(7)	0.013(7)	-0.002(6)
C(6)	0.16(1)	0.056(5)	0.054(6)	0.022(7)	0.034(5)	0.000(5)
C(6')	0.077(6)	0.106(9)	0.073(5)	-0.026(7)	0.010(5)	-0.006(6)
C(7)	0.107(9)	0.074(6)	0.121(9)	0.005(7)	0.069(8)	-0.014(6)
C(7')	0.141(8)	0.063(7)	0.083(7)	0.024(7)	0.056(7)	0.021(5)
C(8)	0.065(7)	0.080(7)	0.103(8)	-0.001(5)	0.019(6)	-0.014(5)
C(8')	0.102(7)	0.064(7)	0.081(7)	0.033(6)	0.048(5)	0.032(5)
C(9)	0.12(1)	0.097(10)	0.14(1)	0.055(8)	0.047(9)	0.005(7)
C(9')	0.099(7)	0.075(8)	0.122(9)	0.035(7)	0.066(7)	0.037(6)
C(10)	0.13(1)	0.089(10)	0.16(1)	0.035(9)	0.028(9)	0.022(8)

Table S2. Anisotropic Displacement Parameters for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(10')	0.082(9)	0.078(9)	0.16(1)	0.001(7)	0.040(8)	0.011(7)
C(11)	0.13(1)	0.063(7)	0.13(1)	0.018(7)	0.026(9)	0.025(7)
C(11')	0.079(6)	0.063(7)	0.14(1)	-0.005(6)	0.011(6)	0.007(7)
C(12)	0.112(10)	0.054(6)	0.080(7)	-0.007(5)	0.022(7)	0.017(5)
C(12')	0.080(6)	0.052(6)	0.093(7)	-0.001(6)	0.012(5)	0.013(5)
C(13)	0.103(6)	0.057(6)	0.058(6)	-0.002(6)	0.013(4)	0.002(5)
C(13')	0.13(1)	0.083(6)	0.062(6)	0.019(7)	0.003(7)	0.028(4)
C(14)	0.089(6)	0.058(6)	0.051(5)	0.002(5)	0.008(5)	-0.013(4)
C(14')	0.082(7)	0.069(6)	0.072(6)	0.006(5)	0.016(4)	0.026(4)
C(15)	0.090(6)	0.082(8)	0.088(8)	0.013(7)	0.004(6)	-0.033(6)
C(15')	0.099(9)	0.076(7)	0.113(9)	0.027(6)	0.037(8)	0.047(6)
C(16)	0.087(9)	0.078(9)	0.13(1)	0.000(6)	0.034(7)	-0.036(6)
C(16')	0.088(9)	0.060(8)	0.15(1)	0.022(7)	0.046(7)	0.016(6)
C(17)	0.091(7)	0.061(7)	0.14(1)	-0.012(6)	0.065(8)	-0.018(6)
C(17')	0.102(10)	0.058(6)	0.127(10)	0.002(6)	0.041(6)	-0.006(7)
C(18)	0.090(7)	0.056(6)	0.100(8)	-0.003(6)	0.055(7)	0.002(6)
C(18')	0.090(8)	0.059(6)	0.078(6)	0.001(5)	0.018(6)	0.003(4)
C(19)	0.088(7)	0.049(6)	0.044(4)	-0.003(5)	0.016(4)	0.000(4)
C(19')	0.081(7)	0.052(6)	0.041(3)	-0.007(5)	0.007(4)	-0.001(4)
C(20)	0.079(7)	0.078(7)	0.037(4)	-0.009(5)	0.012(4)	0.000(4)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table S3 Interatomic Distances (Å) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$

atom	atom	distance	atom	atom	distance
Cu(1)	N(1)	2.18(1)	Cu(1)	N(2)	2.02(1)
Cu(1)	N(3)	2.03(1)	Cu(1)	N(4)	2.00(1)
Cu(1)	N(5)	1.96(1)	Cu(2)	N(1')	2.20(1)
Cu(2)	N(2')	2.03(1)	Cu(2)	N(3')	1.97(1)
Cu(2)	N(4')	1.98(1)	Cu(2)	N(5')	1.99(1)
Cl(1)	O(11)	1.42(1)	Cl(1)	O(12)	1.38(1)
Cl(1)	O(13)	1.42(1)	Cl(1)	O(14)	1.43(1)
Cl(2)	O(21)	1.40(1)	Cl(2)	O(22)	1.43(1)
Cl(2)	O(23)	1.42(1)	Cl(2)	O(24)	1.43(1)
Cl(3)	O(31)	1.41(1)	Cl(3)	O(32)	1.38(1)
Cl(3)	O(33)	1.43(1)	Cl(3)	O(34)	1.39(1)
Cl(4)	Cl(4')	1.78(2)	Cl(4)	O(41)	1.32(3)
Cl(4)	O(42)	1.47(2)	Cl(4)	O(43)	1.32(4)
Cl(4)	O(44)	1.43(3)	Cl(4')	O(41)	1.51(3)
Cl(4')	O(42)	1.47(2)	Cl(4')	O(43')	1.47(3)
Cl(4')	O(44')	1.47(3)	N(1)	C(1)	1.48(2)
N(1)	C(6)	1.46(2)	N(1)	C(19)	1.47(2)
N(1')	C(1')	1.48(2)	N(1')	C(6')	1.44(2)
N(1')	C(19')	1.47(2)	N(2)	C(2)	1.42(2)
N(2)	C(3)	1.57(2)	N(2)	C(7)	1.49(2)
N(2')	C(2')	1.51(2)	N(2')	C(3')	1.45(2)
N(2')	C(7')	1.48(2)	N(3)	C(4)	1.47(2)
N(3)	C(5)	1.49(2)	N(3)	C(13)	1.47(2)
N(3')	C(4')	1.54(2)	N(3')	C(5')	1.48(2)

Table S3 Interatomic Distances (Å) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	distance	atom	atom	distance
N(3')	C(13')	1.50(2)	N(4)	C(8)	1.35(2)
N(4)	C(12)	1.31(2)	N(4')	C(8')	1.36(2)
N(4')	C(12')	1.33(2)	N(5)	C(14)	1.35(2)
N(5)	C(18)	1.39(2)	N(5')	C(14')	1.32(2)
N(5')	C(18')	1.36(2)	C(1)	C(2)	1.44(2)
C(1')	C(2')	1.47(2)	C(3)	C(4)	1.37(3)
C(3')	C(4')	1.46(3)	C(5)	C(6)	1.45(2)
C(5')	C(6')	1.50(2)	C(7)	C(8)	1.50(2)
C(7')	C(8')	1.50(2)	C(8)	C(9)	1.38(2)
C(8')	C(9')	1.35(2)	C(9)	C(10)	1.36(3)
C(9')	C(10')	1.38(3)	C(10)	C(11)	1.35(3)
C(10')	C(11')	1.37(2)	C(11)	C(12)	1.37(2)
C(11')	C(12')	1.37(2)	C(13)	C(14)	1.48(2)
C(13')	C(14')	1.53(2)	C(14)	C(15)	1.36(2)
C(14')	C(15')	1.37(2)	C(15)	C(16)	1.37(2)
C(15')	C(16')	1.37(2)	C(16)	C(17)	1.36(3)
C(16')	C(17')	1.38(3)	C(17)	C(18)	1.34(2)
C(17')	C(18')	1.38(2)	C(19)	C(20)	1.50(2)
C(19')	C(20)	1.53(2)			

Table 4 Interatomic Distances (Å) Involving Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$

atom	atom	distance	atom	atom	distance
C(1)	H(1a)	0.95	C(1)	H(1b)	0.95
C(1')	H(1'a)	0.95	C(1')	H(1'b)	0.95
C(2)	H(2a)	0.95	C(2)	H(2b)	0.95
C(2')	H(2'a)	0.95	C(2')	H(2'b)	0.95
C(3)	H(3a)	0.95	C(3)	H(3b)	0.95
C(3')	H(3'a)	0.95	C(3')	H(3'b)	0.95
C(4)	H(4a)	0.95	C(4)	H(4b)	0.95
C(4')	H(4'a)	0.95	C(4')	H(4'b)	0.95
C(5)	H(5a)	0.95	C(5)	H(5b)	0.95
C(5')	H(5'a)	0.95	C(5')	H(5'b)	0.95
C(6)	H(6a)	0.95	C(6)	H(6b)	0.95
C(6')	H(6'a)	0.95	C(6')	H(6'b)	0.95
C(7)	H(7a)	0.95	C(7)	H(7b)	0.95
C(7')	H(7'a)	0.95	C(7')	H(7'b)	0.95
C(9)	H(9)	0.95	C(9')	H(9')	0.95
C(10)	H(10)	0.95	C(10')	H(10')	0.95
C(11)	H(11)	0.95	C(11')	H(11')	0.95
C(12)	H(12)	0.95	C(12')	H(12')	0.95
C(13)	H(13a)	0.95	C(13)	H(13b)	0.95
C(13')	H(13'a	0.95	C(13')	H(13'b	0.95
C(15)	H(15)	0.95	C(15')	H(15')	0.95
C(16)	H(16)	0.95	C(16')	H(16')	0.95
C(17)	H(17)	0.95	C(17')	H(17')	0.95
C(18)	H(18)	0.95	C(18')	H(18')	0.95

Table 4 Interatomic Distances (Å) Involving Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ cont...)

atom	atom	distance	atom	atom	distance
C(19)	H(19a)	0.95	C(19)	H(19b)	0.95
C(19')	H(19'a	0.95	C(19')	H(19'b	0.95
C(20)	H(20a)	0.95	C(20)	H(20b)	0.95

Table 5S Interatomic Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Cu(1)	N(2)	84.2(5)	N(1)	Cu(1)	N(3)	83.5(4)
N(1)	Cu(1)	N(4)	102.5(5)	N(1)	Cu(1)	N(5)	108.2(4)
N(2)	Cu(1)	N(3)	85.1(6)	N(2)	Cu(1)	N(4)	83.6(5)
N(2)	Cu(1)	N(5)	160.9(6)	N(3)	Cu(1)	N(4)	166.5(5)
N(3)	Cu(1)	N(5)	82.1(5)	N(4)	Cu(1)	N(5)	106.9(5)
N(1')	Cu(2)	N(2')	83.4(5)	N(1')	Cu(2)	N(3')	85.7(5)
N(1')	Cu(2)	N(4')	107.9(4)	N(1')	Cu(2)	N(5')	102.7(5)
N(2')	Cu(2)	N(3')	84.6(6)	N(2')	Cu(2)	N(4')	82.8(6)
N(2')	Cu(2)	N(5')	165.5(5)	N(3')	Cu(2)	N(4')	160.1(5)
N(3')	Cu(2)	N(5')	82.8(5)	N(4')	Cu(2)	N(5')	107.3(5)
O(11)	Cl(1)	O(12)	106.2(9)	O(11)	Cl(1)	O(13)	108.8(8)
O(11)	Cl(1)	O(14)	111.3(8)	O(12)	Cl(1)	O(13)	111.7(8)
O(12)	Cl(1)	O(14)	111.4(8)	O(13)	Cl(1)	O(14)	107.3(8)
O(21)	Cl(2)	O(22)	110.0(8)	O(21)	Cl(2)	O(23)	112.7(7)
O(21)	Cl(2)	O(24)	105.3(8)	O(22)	Cl(2)	O(23)	109.2(7)
O(22)	Cl(2)	O(24)	108.7(8)	O(23)	Cl(2)	O(24)	110.8(8)
O(31)	Cl(3)	O(32)	113.6(10)	O(31)	Cl(3)	O(33)	110.9(9)
O(31)	Cl(3)	O(34)	105.7(8)	O(32)	Cl(3)	O(33)	104(1)
O(32)	Cl(3)	O(34)	114(1)	O(33)	Cl(3)	O(34)	108.1(10)
Cl(4')	Cl(4)	O(41)	55(1)	Cl(4')	Cl(4)	O(42)	52.7(9)
Cl(4')	Cl(4)	O(43)	133(1)	Cl(4')	Cl(4)	O(44)	120(1)
O(41)	Cl(4)	O(42)	106(1)	O(41)	Cl(4)	O(43)	126(2)
O(41)	Cl(4)	O(44)	98(1)	O(42)	Cl(4)	O(43)	112(1)
O(42)	Cl(4)	O(44)	103(1)	O(43)	Cl(4)	O(44)	105(2)

Table 5. Interatomic Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(4)	Cl(4')	O(41)	46(1)	Cl(4)	Cl(4')	O(42)	52.8(10)
Cl(4)	Cl(4')	O(43')	107(2)	Cl(4)	Cl(4')	O(44')	147(2)
O(41)	Cl(4')	O(42)	97(1)	O(41)	Cl(4')	O(43')	110(2)
O(41)	Cl(4')	O(44')	130(2)	O(42)	Cl(4')	O(43')	104(3)
O(42)	Cl(4')	O(44')	108(2)	O(43')	Cl(4')	O(44')	103(2)
Cl(4)	O(41)	Cl(4')	77(1)	Cl(4)	O(42)	Cl(4')	74(1)
Cu(1)	N(1)	C(1)	101.8(10)	Cu(1)	N(1)	C(6)	106.9(9)
Cu(1)	N(1)	C(19)	109.3(8)	C(1)	N(1)	C(6)	111(1)
C(1)	N(1)	C(19)	111(1)	C(6)	N(1)	C(19)	114(1)
Cu(2)	N(1')	C(1')	106.8(9)	Cu(2)	N(1')	C(6')	99.7(9)
Cu(2)	N(1')	C(19')	108.5(8)	C(1')	N(1')	C(6')	112(1)
C(1')	N(1')	C(19')	114(1)	C(6')	N(1')	C(19')	114(1)
Cu(1)	N(2)	C(2)	109(1)	Cu(1)	N(2)	C(3)	101(1)
Cu(1)	N(2)	C(7)	105.2(10)	C(2)	N(2)	C(3)	114(1)
C(2)	N(2)	C(7)	113(1)	C(3)	N(2)	C(7)	110(1)
Cu(2)	N(2')	C(2')	105.4(9)	Cu(2)	N(2')	C(3')	110(1)
Cu(2)	N(2')	C(7')	102.6(10)	C(2')	N(2')	C(3')	111(1)
C(2')	N(2')	C(7')	109(1)	C(3')	N(2')	C(7')	115(1)
Cu(1)	N(3)	C(4)	109(1)	Cu(1)	N(3)	C(5)	107.1(9)
Cu(1)	N(3)	C(13)	104.8(9)	C(4)	N(3)	C(5)	111(1)
C(4)	N(3)	C(13)	112(1)	C(5)	N(3)	C(13)	110(1)
Cu(2)	N(3')	C(4')	105(1)	Cu(2)	N(3')	C(5')	111.1(10)
Cu(2)	N(3')	C(13')	109(1)	C(4')	N(3')	C(5')	110(1)
C(4')	N(3')	C(13')	110(1)	C(5')	N(3')	C(13')	109(1)

Table 5. Interatomic Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	angle	atom	atom	atom	angle
Cu(1)	N(4)	C(8)	112(1)	Cu(1)	N(4)	C(12)	131(1)
C(8)	N(4)	C(12)	115(1)	Cu(2)	N(4')	C(8')	114(1)
Cu(2)	N(4')	C(12')	132(1)	C(8')	N(4')	C(12')	113(1)
Cu(1)	N(5)	C(14)	114(1)	Cu(1)	N(5)	C(18)	131(1)
C(14)	N(5)	C(18)	114(1)	Cu(2)	N(5')	C(14')	114(1)
Cu(2)	N(5')	C(18')	127(1)	C(14')	N(5')	C(18')	118(1)
N(1)	C(1)	C(2)	113(1)	N(1')	C(1')	C(2')	112(1)
N(2)	C(2)	C(1)	118(1)	N(2')	C(2')	C(1')	112(1)
N(2)	C(3)	C(4)	113(1)	N(2')	C(3')	C(4')	111(1)
N(3)	C(4)	C(3)	113(1)	N(3')	C(4')	C(3')	108(1)
N(3)	C(5)	C(6)	114(1)	N(3')	C(5')	C(6')	112(1)
N(1)	C(6)	C(5)	115(1)	N(1')	C(6')	C(5')	115(1)
N(2)	C(7)	C(8)	109(1)	N(2')	C(7')	C(8')	111(1)
N(4)	C(8)	C(7)	114(1)	N(4)	C(8)	C(9)	122(1)
C(7)	C(8)	C(9)	122(1)	N(4')	C(8')	C(7')	112(1)
N(4')	C(8')	C(9')	125(1)	C(7')	C(8')	C(9')	122(1)
C(8)	C(9)	C(10)	119(1)	C(8')	C(9')	C(10')	118(1)
C(9)	C(10)	C(11)	118(2)	C(9')	C(10')	C(11')	117(1)
C(10)	C(11)	C(12)	118(1)	C(10')	C(11')	C(12')	118(1)
N(4)	C(12)	C(11)	125(1)	N(4')	C(12')	C(11')	125(1)
N(3)	C(13)	C(14)	109(1)	N(3')	C(13')	C(14')	107(1)
N(5)	C(14)	C(13)	114(1)	N(5)	C(14)	C(15)	123(1)
C(13)	C(14)	C(15)	122(1)	N(5')	C(14')	C(13')	115(1)
N(5')	C(14')	C(15')	123(1)	C(13')	C(14')	C(15')	120(1)

Table S5 Interatomic Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	C(15)	C(16)	118(1)	C(14')	C(15')	C(16')	118(1)
C(15)	C(16)	C(17)	120(1)	C(15')	C(16')	C(17')	120(1)
C(16)	C(17)	C(18)	118(1)	C(16')	C(17')	C(18')	118(1)
N(5)	C(18)	C(17)	124(1)	N(5')	C(18')	C(17')	121(1)
N(1)	C(19)	C(20)	119(1)	N(1')	C(19')	C(20)	117(1)
C(19)	C(20)	C(19')	105(1)				

Table S6 Interatomic Angles(°) Involving Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	C(1)	H(1a)	108.3	N(1)	C(1)	H(1b)	108.3
C(2)	C(1)	H(1a)	108.3	C(2)	C(1)	H(1b)	108.3
H(1a)	C(1)	H(1b)	109.5	N(1')	C(1')	H(1'a)	108.8
N(1')	C(1')	H(1'b)	108.8	C(2')	C(1')	H(1'a)	108.7
C(2')	C(1')	H(1'b)	108.8	H(1'a)	C(1')	H(1'b)	109.5
N(2)	C(2)	H(2a)	107.1	N(2)	C(2)	H(2b)	107.1
C(1)	C(2)	H(2a)	107.1	C(1)	C(2)	H(2b)	107.1
H(2a)	C(2)	H(2b)	109.4	N(2')	C(2')	H(2'a)	108.7
N(2')	C(2')	H(2'b)	108.7	C(1')	C(2')	H(2'a)	108.7
C(1')	C(2')	H(2'b)	108.7	H(2'a)	C(2')	H(2'b)	109.5
N(2)	C(3)	H(3a)	108.4	N(2)	C(3)	H(3b)	108.4
C(4)	C(3)	H(3a)	108.4	C(4)	C(3)	H(3b)	108.4
H(3a)	C(3)	H(3b)	109.5	N(2')	C(3')	H(3'a)	108.9
N(2')	C(3')	H(3'b)	108.9	C(4')	C(3')	H(3'a)	108.9
C(4')	C(3')	H(3'b)	108.9	H(3'a)	C(3')	H(3'b)	109.5
N(3)	C(4)	H(4a)	108.4	N(3)	C(4)	H(4b)	108.4
C(3)	C(4)	H(4a)	108.4	C(3)	C(4)	H(4b)	108.4
H(4a)	C(4)	H(4b)	109.5	N(3')	C(4')	H(4'a)	109.6
N(3')	C(4')	H(4'b)	109.6	C(3')	C(4')	H(4'a)	109.6
C(3')	C(4')	H(4'b)	109.6	H(4'a)	C(4')	H(4'b)	109.5
N(3)	C(5)	H(5a)	108.2	N(3)	C(5)	H(5b)	108.2
C(6)	C(5)	H(5a)	108.2	C(6)	C(5)	H(5b)	108.2
H(5a)	C(5)	H(5b)	109.4	N(3')	C(5')	H(5'a)	108.7
N(3')	C(5')	H(5'b)	108.7	C(6')	C(5')	H(5'a)	108.7

Table S6 Interatomic Angles(°) Involving Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	angle	atom	atom	atom	angle
C(6')	C(5')	H(5'b)	108.7	H(5'a)	C(5')	H(5'b)	109.5
N(1)	C(6)	H(6a)	108.0	N(1)	C(6)	H(6b)	108.0
C(5)	C(6)	H(6a)	108.0	C(5)	C(6)	H(6b)	108.0
H(6a)	C(6)	H(6b)	109.5	N(1')	C(6')	H(6'a)	108.0
N(1')	C(6')	H(6'b)	108.0	C(5')	C(6')	H(6'a)	108.0
C(5')	C(6')	H(6'b)	108.0	H(6'a)	C(6')	H(6'b)	109.4
N(2)	C(7)	H(7a)	109.5	N(2)	C(7)	H(7b)	109.5
C(8)	C(7)	H(7a)	109.5	C(8)	C(7)	H(7b)	109.5
H(7a)	C(7)	H(7b)	109.5	N(2')	C(7')	H(7'a)	108.9
N(2')	C(7')	H(7'b)	108.9	C(8')	C(7')	H(7'a)	108.9
C(8')	C(7')	H(7'b)	108.9	H(7'a)	C(7')	H(7'b)	109.5
C(8)	C(9)	H(9)	120.1	C(10)	C(9)	H(9)	120.1
C(8')	C(9')	H(9')	120.6	C(10')	C(9')	H(9')	120.6
C(9)	C(10)	H(10)	120.7	C(11)	C(10)	H(10)	120.8
C(9')	C(10')	H(10')	121.1	C(11')	C(10')	H(10')	121.1
C(10)	C(11)	H(11)	120.8	C(12)	C(11)	H(11)	120.8
C(10')	C(11')	H(11')	120.7	C(12')	C(11')	H(11')	120.7
N(4)	C(12)	H(12)	117.3	C(11)	C(12)	H(12)	117.3
N(4')	C(12')	H(12')	117.1	C(11')	C(12')	H(12')	117.1
N(3)	C(13)	H(13a)	109.4	N(3)	C(13)	H(13b)	109.4
C(14)	C(13)	H(13a)	109.4	C(14)	C(13)	H(13b)	109.4
H(13a)	C(13)	H(13b)	109.5	N(3')	C(13')	H(13'a	110.0
N(3')	C(13')	H(13'b	110.0	C(14')	C(13')	H(13'a	110.0
C(14')	C(13')	H(13'b	110.0	H(13'a	C(13')	H(13'b	109.5

Table 6. Interatomic Angles(°) Involving Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	angle	atom	atom	atom	angle
C(14)	C(15)	H(15)	120.5	C(16)	C(15)	H(15)	120.5
C(14')	C(15')	H(15')	120.9	C(16')	C(15')	H(15')	120.9
C(15)	C(16)	H(16)	120.0	C(17)	C(16)	H(16)	120.0
C(15')	C(16')	H(16')	119.9	C(17')	C(16')	H(16')	119.9
C(16)	C(17)	H(17)	120.8	C(18)	C(17)	H(17)	120.8
C(16')	C(17')	H(17')	120.8	C(18')	C(17')	H(17')	120.8
N(5)	C(18)	H(18)	117.7	C(17)	C(18)	H(18)	117.7
N(5')	C(18')	H(18')	119.2	C(17')	C(18')	H(18')	119.2
N(1)	C(19)	H(19a)	106.8	N(1)	C(19)	H(19b)	106.9
C(20)	C(19)	H(19a)	106.9	C(20)	C(19)	H(19b)	106.9
H(19a)	C(19)	H(19b)	109.5	N(1')	C(19')	H(19'a	107.3
N(1')	C(19')	H(19'b	107.3	C(20)	C(19')	H(19'a	107.3
C(20)	C(19')	H(19'b	107.4	H(19'a	C(19')	H(19'b	109.5
C(19)	C(20)	H(20a)	110.4	C(19)	C(20)	H(20b)	110.4
C(19')	C(20)	H(20a)	110.4	C(19')	C(20)	H(20b)	110.4
H(20a)	C(20)	H(20b)	109.4				

Table 7. Torsion Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Cu(1)	N(1)	C(1)	C(2)	-35(1)	Cu(1)	N(1)	C(6)	C(5)	-13(1)
Cu(1)	N(1)	C(19)	C(20)	-176(1)	Cu(1)	N(2)	C(2)	C(1)	-8(2)
Cu(1)	N(2)	C(3)	C(4)	-43(2)	Cu(1)	N(2)	C(7)	C(8)	39(1)
Cu(1)	N(3)	C(4)	C(3)	-10(2)	Cu(1)	N(3)	C(5)	C(6)	-39(1)
Cu(1)	N(3)	C(13)	C(14)	-40(1)	Cu(1)	N(4)	C(8)	C(7)	5(1)
Cu(1)	N(4)	C(8)	C(9)	-177(1)	Cu(1)	N(4)	C(12)	C(11)	176(1)
Cu(1)	N(5)	C(14)	C(13)	-1(1)	Cu(1)	N(5)	C(14)	C(15)	178(1)
Cu(1)	N(5)	C(18)	C(17)	-178(1)	Cu(2)	N(1')	C(1')	C(2')	19(1)
Cu(2)	N(1')	C(6')	C(5')	41(1)	Cu(2)	N(1')	C(19')	C(20)	172(1)
Cu(2)	N(2')	C(2')	C(1')	47(1)	Cu(2)	N(2')	C(3')	C(4')	17(2)
Cu(2)	N(2')	C(7')	C(8')	42(1)	Cu(2)	N(3')	C(4')	C(3')	46(1)
Cu(2)	N(3')	C(5')	C(6')	13(1)	Cu(2)	N(3')	C(13')	C(14')	-32(1)
Cu(2)	N(4')	C(8')	C(7')	0(1)	Cu(2)	N(4')	C(8')	C(9')	178(1)
Cu(2)	N(4')	C(12')	C(11')	178(1)	Cu(2)	N(5')	C(14')	C(13')	-4(1)
Cu(2)	N(5')	C(14')	C(15')	178(1)	Cu(2)	N(5')	C(18')	C(17')	-177(1)
Cl(4)	O(41)	Cl(4')	O(42)	14(1)	Cl(4)	O(41)	Cl(4')	O(43')	-94(3)
Cl(4)	O(41)	Cl(4')	O(44')	136(3)	Cl(4)	O(42)	Cl(4')	O(41)	-12(1)
Cl(4)	O(42)	Cl(4')	O(43')	100(2)	Cl(4)	O(42)	Cl(4')	O(44')	-149(2)
Cl(4')	O(41)	Cl(4)	O(42)	-14(1)	Cl(4')	O(41)	Cl(4)	O(43)	122(2)
Cl(4')	O(41)	Cl(4)	O(44)	-121(1)	Cl(4')	O(42)	Cl(4)	O(41)	15(1)
Cl(4')	O(42)	Cl(4)	O(43)	-128(2)	Cl(4')	O(42)	Cl(4)	O(44)	118(1)
O(41)	Cl(4)	Cl(4')	O(42)	-162(2)	O(41)	Cl(4)	Cl(4')	O(43')	102(3)
O(41)	Cl(4)	Cl(4')	O(44')	-99(4)	O(41)	Cl(4')	Cl(4)	O(42)	162(2)
O(41)	Cl(4')	Cl(4)	O(43)	-110(3)	O(41)	Cl(4')	Cl(4)	O(44)	78(2)

Table 7 Torsion Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
O(42)	Cl(4)	Cl(4')	O(43')	-95(3)	O(42)	Cl(4)	Cl(4')	O(44')	63(4)
O(42)	Cl(4')	Cl(4)	O(43)	87(2)	O(42)	Cl(4')	Cl(4)	O(44)	-84(2)
O(43)	Cl(4)	Cl(4')	O(43')	-7(4)	O(43)	Cl(4)	Cl(4')	O(44')	150(4)
O(43')	Cl(4')	Cl(4)	O(44)	-179(3)	O(44')	Cl(4')	Cl(4)	O(44)	-20(5)
N(1)	Cu(1)	N(2)	C(2)	-10(1)	N(1)	Cu(1)	N(2)	C(3)	111(1)
N(1)	Cu(1)	N(2)	C(7)	-132(1)	N(1)	Cu(1)	N(3)	C(4)	-97(1)
N(1)	Cu(1)	N(3)	C(5)	23(1)	N(1)	Cu(1)	N(3)	C(13)	141.0(9)
N(1)	Cu(1)	N(4)	C(8)	96(1)	N(1)	Cu(1)	N(4)	C(12)	-76(1)
N(1)	Cu(1)	N(5)	C(14)	-98.0(9)	N(1)	Cu(1)	N(5)	C(18)	78(1)
N(1)	C(1)	C(2)	N(2)	32(2)	N(1)	C(6)	C(5)	N(3)	35(2)
N(1)	C(19)	C(20)	C(19')	-176(1)	N(1')	Cu(2)	N(2')	C(2')	-27(1)
N(1')	Cu(2)	N(2')	C(3')	93(1)	N(1')	Cu(2)	N(2')	C(7')	-142.5(10)
N(1')	Cu(2)	N(3')	C(4')	-112(1)	N(1')	Cu(2)	N(3')	C(5')	7(1)
N(1')	Cu(2)	N(3')	C(13')	128(1)	N(1')	Cu(2)	N(4')	C(8')	100.9(10)
N(1')	Cu(2)	N(4')	C(12')	-77(1)	N(1')	Cu(2)	N(5')	C(14')	-96(1)
N(1')	Cu(2)	N(5')	C(18')	79(1)	N(1')	C(1')	C(2')	N(2')	-45(1)
N(1')	C(6')	C(5')	N(3')	-40(2)	N(1')	C(19')	C(20)	C(19)	-178(1)
N(2)	Cu(1)	N(1)	C(1)	24.6(10)	N(2)	Cu(1)	N(1)	C(6)	-92(1)
N(2)	Cu(1)	N(1)	C(19)	143.1(10)	N(2)	Cu(1)	N(3)	C(4)	-12(1)
N(2)	Cu(1)	N(3)	C(5)	108(1)	N(2)	Cu(1)	N(3)	C(13)	-134.3(10)
N(2)	Cu(1)	N(4)	C(8)	14(1)	N(2)	Cu(1)	N(4)	C(12)	-158(1)
N(2)	Cu(1)	N(5)	C(14)	30(2)	N(2)	Cu(1)	N(5)	C(18)	-152(1)
N(2)	C(3)	C(4)	N(3)	36(2)	N(2)	C(7)	C(8)	N(4)	-31(2)
N(2)	C(7)	C(8)	C(9)	152(1)	N(2')	Cu(2)	N(1')	C(1')	5(1)

Table 7 Torsion Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(2')	Cu(2)	N(1')	C(6')	-111.5(10)	N(2')	Cu(2)	N(1')	C(19')	128.9(10)
N(2')	Cu(2)	N(3')	C(4')	-28(1)	N(2')	Cu(2)	N(3')	C(5')	91(1)
N(2')	Cu(2)	N(3')	C(13')	-147(1)	N(2')	Cu(2)	N(4')	C(8')	20.2(10)
N(2')	Cu(2)	N(4')	C(12')	-157(1)	N(2')	Cu(2)	N(5')	C(14')	17(2)
N(2')	Cu(2)	N(5')	C(18')	-167(1)	N(2')	C(3')	C(4')	N(3')	-42(2)
N(2')	C(7')	C(8')	N(4')	-29(1)	N(2')	C(7')	C(8')	C(9')	150(1)
N(3)	Cu(1)	N(1)	C(1)	110.4(10)	N(3)	Cu(1)	N(1)	C(6)	-6(1)
N(3)	Cu(1)	N(1)	C(19)	-131.2(9)	N(3)	Cu(1)	N(2)	C(2)	-94(1)
N(3)	Cu(1)	N(2)	C(3)	27(1)	N(3)	Cu(1)	N(2)	C(7)	143(1)
N(3)	Cu(1)	N(4)	C(8)	-18(2)	N(3)	Cu(1)	N(4)	C(12)	168(1)
N(3)	Cu(1)	N(5)	C(14)	-17.5(9)	N(3)	Cu(1)	N(5)	C(18)	159(1)
N(3)	C(13)	C(14)	N(5)	29(1)	N(3)	C(13)	C(14)	C(15)	-151(1)
N(3')	Cu(2)	N(1')	C(1')	90(1)	N(3')	Cu(2)	N(1')	C(6')	-26.4(10)
N(3')	Cu(2)	N(1')	C(19')	-146.1(10)	N(3')	Cu(2)	N(2')	C(2')	-113(1)
N(3')	Cu(2)	N(2')	C(3')	7(1)	N(3')	Cu(2)	N(2')	C(7')	131(1)
N(3')	Cu(2)	N(4')	C(8')	-30(2)	N(3')	Cu(2)	N(4')	C(12')	151(1)
N(3')	Cu(2)	N(5')	C(14')	-12(1)	N(3')	Cu(2)	N(5')	C(18')	162(1)
N(3')	C(13')	C(14')	N(5')	24(2)	N(3')	C(13')	C(14')	C(15')	-158(1)
N(4)	Cu(1)	N(1)	C(1)	-57.4(10)	N(4)	Cu(1)	N(1)	C(6)	-174(1)
N(4)	Cu(1)	N(1)	C(19)	61.0(9)	N(4)	Cu(1)	N(2)	C(2)	93(1)
N(4)	Cu(1)	N(2)	C(3)	-144(1)	N(4)	Cu(1)	N(2)	C(7)	-29(1)
N(4)	Cu(1)	N(3)	C(4)	20(2)	N(4)	Cu(1)	N(3)	C(5)	141(2)
N(4)	Cu(1)	N(3)	C(13)	-101(2)	N(4)	Cu(1)	N(5)	C(14)	152.3(9)
N(4)	Cu(1)	N(5)	C(18)	-31(1)	N(4)	C(8)	C(9)	C(10)	3(3)

Table 7. Torsion Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(4)	C(12)	C(11)	C(10)	-3(3)	N(4')	Cu(2)	N(1')	C(1')	-74(1)
N(4')	Cu(2)	N(1')	C(6')	168.3(9)	N(4')	Cu(2)	N(1')	C(19')	48(1)
N(4')	Cu(2)	N(2')	C(2')	81(1)	N(4')	Cu(2)	N(2')	C(3')	-157(1)
N(4')	Cu(2)	N(2')	C(7')	-33.4(9)	N(4')	Cu(2)	N(3')	C(4')	22(2)
N(4')	Cu(2)	N(3')	C(5')	142(1)	N(4')	Cu(2)	N(3')	C(13')	-96(1)
N(4')	Cu(2)	N(5')	C(14')	150(1)	N(4')	Cu(2)	N(5')	C(18')	-34(1)
N(4')	C(8')	C(9')	C(10')	2(2)	N(4')	C(12')	C(11')	C(10')	2(2)
N(5)	Cu(1)	N(1)	C(1)	-170.2(9)	N(5)	Cu(1)	N(1)	C(6)	72(1)
N(5)	Cu(1)	N(1)	C(19)	-51.7(10)	N(5)	Cu(1)	N(2)	C(2)	-142(1)
N(5)	Cu(1)	N(2)	C(3)	-19(2)	N(5)	Cu(1)	N(2)	C(7)	95(1)
N(5)	Cu(1)	N(3)	C(4)	153(1)	N(5)	Cu(1)	N(3)	C(5)	-85(1)
N(5)	Cu(1)	N(3)	C(13)	31.6(9)	N(5)	Cu(1)	N(4)	C(8)	-149(1)
N(5)	Cu(1)	N(4)	C(12)	37(1)	N(5)	C(14)	C(15)	C(16)	0(2)
N(5)	C(18)	C(17)	C(16)	1(2)	N(5')	Cu(2)	N(1')	C(1')	172(1)
N(5')	Cu(2)	N(1')	C(6')	55.2(10)	N(5')	Cu(2)	N(1')	C(19')	-64.5(10)
N(5')	Cu(2)	N(2')	C(2')	-143(2)	N(5')	Cu(2)	N(2')	C(3')	-22(2)
N(5')	Cu(2)	N(2')	C(7')	101(2)	N(5')	Cu(2)	N(3')	C(4')	144(1)
N(5')	Cu(2)	N(3')	C(5')	-95(1)	N(5')	Cu(2)	N(3')	C(13')	25(1)
N(5')	Cu(2)	N(4')	C(8')	-149.1(10)	N(5')	Cu(2)	N(4')	C(12')	32(1)
N(5')	C(14')	C(15')	C(16')	-2(2)	N(5')	C(18')	C(17')	C(16')	1(2)
C(1)	N(1)	C(6)	C(5)	-123(1)	C(1)	N(1)	C(19)	C(20)	-64(1)
C(1)	C(2)	N(2)	C(3)	-122(2)	C(1)	C(2)	N(2)	C(7)	109(2)
C(1')	N(1')	C(6')	C(5')	-71(1)	C(1')	N(1')	C(19')	C(20)	-68(1)
C(1')	C(2')	N(2')	C(3')	-72(1)	C(1')	C(2')	N(2')	C(7')	157(1)

Table 37 Torsion Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(2)	N(2)	C(3)	C(4)	75(2)	C(2)	N(2)	C(7)	C(8)	-80(1)
C(2)	C(1)	N(1)	C(6)	78(1)	C(2)	C(1)	N(1)	C(19)	-152(1)
C(2')	N(2')	C(3')	C(4')	134(1)	C(2')	N(2')	C(7')	C(8')	-69(1)
C(2')	C(1')	N(1')	C(6')	127(1)	C(2')	C(1')	N(1')	C(19')	-100(1)
C(3)	N(2)	C(7)	C(8)	148(1)	C(3)	C(4)	N(3)	C(5)	-128(2)
C(3)	C(4)	N(3)	C(13)	106(2)	C(3')	N(2')	C(7')	C(8')	163(1)
C(3')	C(4')	N(3')	C(5')	-74(2)	C(3')	C(4')	N(3')	C(13')	164(1)
C(4)	N(3)	C(5)	C(6)	80(1)	C(4)	N(3)	C(13)	C(14)	-159(1)
C(4)	C(3)	N(2)	C(7)	-154(1)	C(4')	N(3')	C(5')	C(6')	130(1)
C(4')	N(3')	C(13')	C(14')	-148(1)	C(4')	C(3')	N(2')	C(7')	-98(1)
C(5)	N(3)	C(13)	C(14)	74(1)	C(5)	C(6)	N(1)	C(19)	107(1)
C(5')	N(3')	C(13')	C(14')	89(1)	C(5')	C(6')	N(1')	C(19')	157(1)
C(6)	N(1)	C(19)	C(20)	63(1)	C(6)	C(5)	N(3)	C(13)	-152(1)
C(6')	N(1')	C(19')	C(20)	62(1)	C(6')	C(5')	N(3')	C(13')	-108(1)
C(7)	C(8)	N(4)	C(12)	-179(1)	C(7)	C(8)	C(9)	C(10)	179(2)
C(7')	C(8')	N(4')	C(12')	178(1)	C(7')	C(8')	C(9')	C(10')	-178(1)
C(8)	N(4)	C(12)	C(11)	3(2)	C(8)	C(9)	C(10)	C(11)	-3(3)
C(8')	N(4')	C(12')	C(11')	0(2)	C(8')	C(9')	C(10')	C(11')	0(2)
C(9)	C(8)	N(4)	C(12)	-3(2)	C(9)	C(10)	C(11)	C(12)	3(3)
C(9')	C(8')	N(4')	C(12')	-2(2)	C(9')	C(10')	C(11')	C(12')	-2(2)
C(13)	C(14)	N(5)	C(18)	-179(1)	C(13)	C(14)	C(15)	C(16)	-179(1)
C(13')	C(14')	N(5')	C(18')	179(1)	C(13')	C(14')	C(15')	C(16')	-179(1)
C(14)	N(5)	C(18)	C(17)	-2(2)	C(14)	C(15)	C(16)	C(17)	0(2)
C(14')	N(5')	C(18')	C(17')	-2(2)	C(14')	C(15')	C(16')	C(17')	1(2)

Table 7. Torsion Angles(°) Involving Non-Hydrogen Atoms for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
C(15)	C(14)	N(5)	C(18)	1(2)	C(15)	C(16)	C(17)	C(18)	0(2)
C(15')	C(14')	N(5')	C(18')	2(2)	C(15')	C(16')	C(17')	C(18')	-1(2)

Table S8 Non-bonded Contacts out to 3.60 Å for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$

atom	atom	distance	ADC	atom	atom	distance	ADC
Cu(1)	O(13)	3.11(1)	1	Cu(2)	O(12)	3.06(1)	55404
O(11)	N(5)	3.37(2)	1	O(11)	C(13)	3.42(2)	65703
O(11)	C(14)	3.44(2)	1	O(11)	C(18)	3.59(2)	1
O(12)	N(4')	3.17(2)	4	O(12)	N(5')	3.32(2)	4
O(12)	C(7')	3.37(2)	4	O(12)	C(8')	3.38(2)	4
O(12)	C(13')	3.56(2)	4	O(13)	C(13)	3.26(2)	1
O(13)	N(5)	3.35(2)	1	O(13)	C(3)	3.39(3)	1
O(13)	C(7)	3.39(2)	1	O(13)	C(14)	3.47(2)	1
O(13)	C(15)	3.54(2)	65703	O(13)	N(4)	3.57(2)	1
O(13)	N(2)	3.58(2)	1	O(13)	N(3)	3.60(2)	1
O(14)	N(4)	3.10(2)	1	O(14)	C(8)	3.32(2)	1
O(14)	C(12)	3.39(2)	1	O(14)	C(7')	3.47(2)	65602
O(14)	C(4')	3.47(2)	4	O(14)	C(9')	3.55(2)	65602
O(21)	C(16)	3.27(2)	45501	O(21)	C(4)	3.35(2)	55703
O(21)	C(1')	3.48(2)	55602	O(21)	C(3)	3.54(2)	55703
O(21)	C(3')	3.58(2)	55602	O(22)	C(13')	3.30(2)	4
O(22)	C(7)	3.45(2)	1	O(22)	C(5')	3.53(2)	55602
O(23)	O(23)	3.25(2)	55703	O(23)	C(15')	3.37(2)	4
O(23)	C(7)	3.48(2)	1	O(23)	C(16')	3.51(2)	54602
O(23)	C(3)	3.51(2)	55703	O(24)	C(16)	3.36(2)	45501
O(24)	C(1')	3.54(2)	55602	O(31)	C(18')	3.26(2)	64602
O(31)	C(12)	3.39(2)	64602	O(31)	C(12')	3.42(2)	64602
O(31)	C(18)	3.52(2)	64602	O(32)	C(11')	3.25(2)	1
O(32)	C(12')	3.29(2)	1	O(32)	C(10')	3.38(2)	1

Table 8. Non-bonded Contacts out to 3.60 Å for $C_{39}H_{54}Cl_4Cu_2N_{10}O_{16}$ (cont...)

atom	atom	distance	ADC	atom	atom	distance	ADC
O(32)	N(4')	3.45(2)	1	O(32)	C(8')	3.46(2)	1
O(32)	C(9')	3.48(2)	1	O(32)	C(2')	3.54(3)	1
O(33)	C(1')	3.38(2)	1	O(33)	C(20)	3.45(2)	1
O(33)	C(19')	3.49(2)	1	O(33)	C(11')	3.53(2)	64602
O(33)	C(2')	3.56(2)	1	O(33)	C(17)	3.57(2)	64602
O(34)	C(18')	3.40(2)	64602	O(34)	C(12')	3.58(2)	64602
O(41)	C(10)	3.27(4)	64602	O(42)	C(2)	3.48(3)	65602
O(43)	C(6)	3.46(4)	65602	O(43')	C(10')	2.74(5)	1
O(43')	C(9')	3.26(6)	1	O(43')	C(5)	3.28(5)	65602
O(43')	C(6)	3.31(6)	65602	O(44')	C(6')	3.37(5)	65501
O(44')	C(5')	3.37(5)	65501	O(44')	C(4')	3.38(5)	65603
O(44)	C(20)	3.37(4)	65501	O(44)	C(19)	3.39(4)	65501
O(44)	C(19')	3.50(4)	65501	C(5)	C(11')	3.51(2)	64602
C(16)	C(17')	3.50(2)	64602				

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Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy

atom	x	y	z	B_{eq}	occ
Cu(1)	0.74635(4)	0.23891(4)	0.22647(4)	2.766(8)	
Cl(1)	0.31212(8)	0.13515(8)	0.15557(9)	4.46(2)	
Cl(2)	0.92211(9)	0.34709(8)	-0.12692(9)	4.79(2)	
O(1)	1.0250(3)	0.7702(3)	-0.5386(2)	7.01(8)	
O(2)	0.6072(6)	0.4810(9)	0.6029(6)	13.0(2)	1/2
O(2')	0.4280(5)	0.3965(5)	0.6467(5)	7.5(1)	1/2
O(11)	0.3972(3)	0.1303(3)	0.0623(2)	7.13(8)	
O(12)	0.2560(3)	0.2533(3)	0.1201(3)	10.2(1)	
O(13)	0.2294(2)	0.0534(2)	0.1954(3)	7.48(8)	
O(14)	0.3712(3)	0.1057(3)	0.2483(3)	9.7(1)	
O(21)	1.0335(3)	0.3235(3)	-0.0988(3)	11.2(1)	
O(22)	0.9109(4)	0.4442(3)	-0.2320(3)	12.8(1)	
O(23)	0.8935(3)	0.2470(2)	-0.1273(3)	9.20(9)	
O(24)	0.8412(3)	0.3713(3)	-0.0409(3)	10.4(1)	
N(1)	0.6839(2)	0.1858(2)	0.4174(2)	3.06(5)	
N(2)	0.8125(2)	0.3765(2)	0.2225(2)	2.99(5)	
N(3)	0.8982(2)	0.1408(2)	0.2799(2)	3.29(6)	
N(4)	0.6105(2)	0.3636(2)	0.1721(2)	2.76(5)	
N(5)	0.7495(2)	0.1192(2)	0.1669(2)	2.98(5)	
N(6)	0.8686(4)	0.6904(5)	-0.5349(4)	18.2(2)	
N(7)	0.5835(4)	0.2909(4)	0.7130(3)	11.2(1)	
C(1)	0.6726(3)	0.3049(3)	0.4154(3)	3.50(7)	
C(2)	0.7778(3)	0.3759(3)	0.3395(3)	3.39(7)	
C(3)	0.9423(3)	0.3499(3)	0.1928(3)	3.94(7)	

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Table 7. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
C(4)	0.9787(3)	0.2202(3)	0.2745(3)	3.85(7)	
C(5)	0.8617(3)	0.0486(3)	0.4008(3)	3.61(7)	
C(6)	0.7832(3)	0.1013(3)	0.4769(3)	3.57(7)	
C(7)	0.7608(3)	0.4876(3)	0.1297(3)	3.66(7)	
C(8)	0.6342(3)	0.4776(3)	0.1353(3)	3.22(6)	
C(9)	0.5481(3)	0.5743(3)	0.1061(3)	3.81(7)	
C(10)	0.4348(3)	0.5551(3)	0.1145(3)	4.19(7)	
C(11)	0.4099(3)	0.4400(3)	0.1529(3)	3.72(7)	
C(12)	0.4991(3)	0.3465(3)	0.1816(3)	3.18(7)	
C(13)	0.9494(3)	0.0839(3)	0.2014(3)	3.80(8)	
C(14)	0.8554(3)	0.0532(3)	0.1656(3)	3.44(7)	
C(15)	0.8760(3)	-0.0338(3)	0.1266(3)	4.53(8)	
C(16)	0.7885(4)	-0.0514(3)	0.0861(3)	5.33(9)	
C(17)	0.6825(3)	0.0187(3)	0.0854(3)	4.70(8)	
C(18)	0.6653(3)	0.1018(3)	0.1266(3)	3.84(8)	
C(19)	0.5688(3)	0.1361(3)	0.4756(3)	3.39(7)	
C(20)	0.5602(3)	0.0217(3)	0.4709(3)	3.50(7)	
C(21)	0.9702(5)	0.7209(4)	-0.5767(3)	7.4(1)	
C(22)	0.8236(7)	0.6380(7)	-0.5904(6)	26.8(2)	
C(23)	0.8034(4)	0.7028(4)	-0.4367(5)	8.8(1)	
C(24)	0.5398(5)	0.3883(4)	0.6528(5)	11.1(2)	
C(25)	0.6889(4)	0.2561(6)	0.7335(5)	14.6(2)	
C(26)	0.4967(6)	0.1915(6)	0.7753(7)	28.6(3)	
H(1a)	0.6664	0.2933	0.4933	4.1802	

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Table V. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H(1b)	0.6028	0.3515	0.3853	4.1802	
H(2a)	0.8431	0.3405	0.3800	4.0670	
H(2b)	0.7576	0.4570	0.3276	4.0670	
H(3a)	0.9614	0.3621	0.1139	4.6756	
H(3b)	0.9815	0.4022	0.2015	4.6756	
H(4a)	1.0571	0.1976	0.2463	4.6268	
H(4b)	0.9741	0.2129	0.3503	4.6268	
H(5a)	0.9304	0.0058	0.4350	4.3205	
H(5b)	0.8206	-0.0063	0.3976	4.3205	
H(6a)	0.8280	0.1436	0.4932	4.2869	
H(6b)	0.7518	0.0378	0.5487	4.2869	
H(7a)	0.8040	0.4977	0.0556	4.3793	
H(7b)	0.7648	0.5547	0.1411	4.3793	
H(9)	0.5667	0.6529	0.0804	4.5678	
H(10)	0.3743	0.6209	0.0942	5.0076	
H(11)	0.3319	0.4253	0.1597	4.4702	
H(12)	0.4814	0.2672	0.2091	3.8146	
H(13a)	0.9947	0.1387	0.1330	4.5365	
H(13b)	0.9982	0.0126	0.2408	4.5365	
H(15)	0.9499	-0.0817	0.1289	5.4061	
H(16)	0.8006	-0.1102	0.0589	6.3458	
H(17)	0.6207	0.0096	0.0564	5.6413	
H(18)	0.5911	0.1487	0.1265	4.5870	
H(19a)	0.5083	0.1953	0.4383	4.0561	

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Table 1. Atomic coordinates and B_{iso}/B_{eq} and occupancy (continued)

atom	x	y	z	B_{eq}	occ
H(19b)	0.5569	0.1192	0.5555	4.0561	
H(20a)	0.5735	0.0368	0.3913	4.1656	
H(20b)	0.6187	-0.0393	0.5102	4.1656	

$$B_{eq} = \frac{8}{3}\pi^2(U_{11}(aa^*)^2 + U_{22}(bb^*)^2 + U_{33}(cc^*)^2 + 2U_{12}aa^*bb^*\cos\gamma + 2U_{13}aa^*cc^*\cos\beta + 2U_{23}bb^*cc^*\cos\alpha)$$

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Table 8. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu(1)	0.0300(2)	0.0368(2)	0.0416(2)	-0.0043(2)	-0.0058(2)	-0.0202(1)
Cl(1)	0.0428(5)	0.0534(5)	0.0660(6)	-0.0115(4)	-0.0029(4)	-0.0217(4)
Cl(2)	0.0661(6)	0.0525(5)	0.0652(6)	-0.0017(5)	-0.0166(5)	-0.0274(4)
O(1)	0.080(2)	0.102(2)	0.091(2)	-0.010(2)	-0.016(2)	-0.048(2)
O(2)	0.155(6)	0.299(6)	0.123(4)	-0.174(4)	0.077(4)	-0.147(4)
O(2')	0.097(4)	0.145(4)	0.078(3)	-0.058(3)	0.030(3)	-0.080(3)
O(11)	0.072(2)	0.108(2)	0.083(2)	-0.013(2)	0.020(1)	-0.051(2)
O(12)	0.090(3)	0.057(2)	0.163(3)	0.005(2)	0.029(2)	-0.015(2)
O(13)	0.056(2)	0.082(2)	0.147(3)	-0.033(1)	-0.005(2)	-0.048(2)
O(14)	0.141(3)	0.167(3)	0.066(2)	-0.076(2)	-0.037(2)	-0.023(2)
O(21)	0.062(2)	0.177(3)	0.214(3)	0.009(2)	-0.055(2)	-0.106(2)
O(22)	0.252(5)	0.092(3)	0.089(2)	-0.039(3)	-0.052(3)	0.019(2)
O(23)	0.144(3)	0.080(2)	0.165(2)	-0.036(2)	-0.009(2)	-0.084(1)
O(24)	0.113(3)	0.189(3)	0.133(2)	0.016(2)	0.014(2)	-0.133(2)
N(1)	0.035(1)	0.042(1)	0.041(1)	-0.008(1)	-0.004(1)	-0.019(1)
N(2)	0.037(1)	0.038(1)	0.043(1)	-0.012(1)	-0.005(1)	-0.020(1)
N(3)	0.030(1)	0.045(1)	0.050(1)	-0.002(1)	-0.008(1)	-0.022(1)
N(4)	0.037(1)	0.035(1)	0.034(1)	-0.001(1)	-0.009(1)	-0.016(1)
N(5)	0.036(1)	0.037(1)	0.043(1)	-0.004(1)	-0.002(1)	-0.023(1)
N(6)	0.128(4)	0.188(5)	0.120(4)	0.032(3)	0.095(3)	0.058(3)
N(7)	0.128(3)	0.231(3)	0.111(2)	0.101(2)	-0.067(2)	-0.141(2)
C(1)	0.051(2)	0.049(2)	0.039(2)	-0.009(2)	0.001(1)	-0.027(1)
C(2)	0.049(2)	0.041(2)	0.046(2)	-0.010(1)	-0.008(1)	-0.024(1)
C(3)	0.037(2)	0.059(2)	0.062(2)	-0.021(1)	0.002(2)	-0.033(1)

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Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(4)	0.030(2)	0.064(2)	0.063(2)	-0.013(1)	-0.003(2)	-0.036(1)
C(5)	0.039(2)	0.040(2)	0.056(2)	0.003(1)	-0.019(1)	-0.018(1)
C(6)	0.041(2)	0.048(2)	0.042(2)	-0.011(1)	-0.013(1)	-0.012(1)
C(7)	0.058(2)	0.032(2)	0.045(2)	-0.012(2)	-0.008(2)	-0.012(1)
C(8)	0.053(2)	0.038(1)	0.029(2)	-0.009(1)	-0.006(2)	-0.012(1)
C(9)	0.066(2)	0.037(2)	0.038(2)	0.000(1)	-0.010(2)	-0.016(1)
C(10)	0.061(2)	0.050(2)	0.045(2)	0.016(2)	-0.014(2)	-0.025(1)
C(11)	0.042(2)	0.058(2)	0.046(2)	0.001(1)	-0.011(2)	-0.028(1)
C(12)	0.038(2)	0.046(2)	0.039(2)	-0.007(1)	-0.005(1)	-0.021(1)
C(13)	0.035(2)	0.056(2)	0.062(2)	-0.001(2)	-0.003(2)	-0.036(1)
C(14)	0.036(2)	0.044(2)	0.043(2)	-0.003(1)	0.000(2)	-0.017(1)
C(15)	0.049(2)	0.052(2)	0.079(2)	0.005(2)	0.000(2)	-0.045(1)
C(16)	0.063(2)	0.075(2)	0.092(2)	-0.008(2)	-0.013(2)	-0.059(2)
C(17)	0.062(2)	0.068(2)	0.075(2)	-0.007(2)	-0.016(2)	-0.051(1)
C(18)	0.042(2)	0.057(2)	0.057(2)	-0.008(2)	-0.015(2)	-0.029(1)
C(19)	0.038(2)	0.049(2)	0.037(2)	-0.009(1)	0.000(1)	-0.017(1)
C(20)	0.041(2)	0.044(2)	0.043(2)	-0.009(2)	-0.003(2)	-0.015(1)
C(21)	0.143(4)	0.095(3)	0.065(2)	0.010(3)	-0.033(2)	-0.055(2)
C(22)	0.376(7)	0.586(6)	0.282(5)	-0.317(4)	0.019(4)	-0.301(3)
C(23)	0.068(3)	0.085(4)	0.141(4)	-0.021(3)	-0.014(3)	-0.017(3)
C(24)	0.103(4)	0.209(4)	0.131(4)	-0.005(3)	-0.001(4)	-0.106(3)
C(25)	0.129(4)	0.299(6)	0.206(4)	0.107(4)	-0.104(4)	-0.193(4)
C(26)	0.421(8)	0.452(7)	0.321(9)	-0.391(5)	0.224(7)	-0.251(6)

The general temperature factor expression:

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$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

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Table 8. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
Cu(1)	N(1)	2.242(5)	Cu(1)	N(2)	2.039(5)
Cu(1)	N(3)	2.016(5)	Cu(1)	N(4)	1.992(5)
Cu(1)	N(5)	2.014(5)	Cl(1)	O(11)	1.405(5)
Cl(1)	O(12)	1.403(6)	Cl(1)	O(13)	1.403(5)
Cl(1)	O(14)	1.407(6)	Cl(2)	O(21)	1.381(6)
Cl(2)	O(22)	1.357(6)	Cl(2)	O(23)	1.389(6)
Cl(2)	O(24)	1.407(6)	O(1)	C(21)	1.30(1)
O(2)	C(24)	1.36(1)	O(2')	C(24)	1.32(1)
N(1)	C(1)	1.482(8)	N(1)	C(6)	1.495(7)
N(1)	C(19)	1.491(7)	N(2)	C(2)	1.496(8)
N(2)	C(3)	1.490(8)	N(2)	C(7)	1.483(7)
N(3)	C(4)	1.495(8)	N(3)	C(5)	1.480(7)
N(3)	C(13)	1.482(8)	N(4)	C(8)	1.360(7)
N(4)	C(12)	1.342(7)	N(5)	C(14)	1.348(7)
N(5)	C(18)	1.334(8)	N(6)	C(21)	1.25(1)
N(6)	C(22)	1.44(2)	N(6)	C(23)	1.40(1)
N(7)	C(24)	1.188(9)	N(7)	C(25)	1.27(1)
N(7)	C(26)	1.57(1)	C(1)	C(2)	1.536(8)
C(3)	C(4)	1.511(8)	C(5)	C(6)	1.500(9)
C(7)	C(8)	1.505(9)	C(8)	C(9)	1.375(8)
C(9)	C(10)	1.38(1)	C(10)	C(11)	1.374(9)
C(11)	C(12)	1.374(8)	C(13)	C(14)	1.490(9)
C(14)	C(15)	1.387(9)	C(15)	C(16)	1.37(1)
C(16)	C(17)	1.370(9)	C(17)	C(18)	1.367(9)

Table 4. Bond Lengths($\AA$) (continued)

atom	atom	distance	atom	atom	distance
C(19)	C(20)	1.514(9)	C(20)	C(20)	1.52(1)

Table S12. Bond Lengths(Å)

atom	atom	distance	atom	atom	distance
C(1)	H(1a)	0.95	C(1)	H(1b)	0.95
C(2)	H(2a)	0.95	C(2)	H(2b)	0.95
C(3)	H(3a)	0.95	C(3)	H(3b)	0.95
C(4)	H(4a)	0.95	C(4)	H(4b)	0.95
C(5)	H(5a)	0.95	C(5)	H(5b)	0.95
C(6)	H(6a)	0.95	C(6)	H(6b)	0.95
C(7)	H(7a)	0.95	C(7)	H(7b)	0.95
C(9)	H(9)	0.95	C(10)	H(10)	0.95
C(11)	H(11)	0.95	C(12)	H(12)	0.95
C(13)	H(13a)	0.95	C(13)	H(13b)	0.95
C(15)	H(15)	0.95	C(16)	H(16)	0.95
C(17)	H(17)	0.95	C(18)	H(18)	0.95
C(19)	H(19a)	0.95	C(19)	H(19b)	0.95
C(20)	H(20a)	0.95	C(20)	H(20b)	0.95

Table 5. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
N(1)	Cu(1)	N(2)	85.6(2)	N(1)	Cu(1)	N(3)	84.0(2)
N(1)	Cu(1)	N(4)	95.3(2)	N(1)	Cu(1)	N(5)	118.8(2)
N(2)	Cu(1)	N(3)	84.9(2)	N(2)	Cu(1)	N(4)	83.2(2)
N(2)	Cu(1)	N(5)	151.7(2)	N(3)	Cu(1)	N(4)	168.1(2)
N(3)	Cu(1)	N(5)	83.7(2)	N(4)	Cu(1)	N(5)	106.8(2)
O(11)	Cl(1)	O(12)	109.0(4)	O(11)	Cl(1)	O(13)	112.4(4)
O(11)	Cl(1)	O(14)	107.7(4)	O(12)	Cl(1)	O(13)	110.7(4)
O(12)	Cl(1)	O(14)	108.5(5)	O(13)	Cl(1)	O(14)	108.5(4)
O(21)	Cl(2)	O(22)	113.1(5)	O(21)	Cl(2)	O(23)	110.0(4)
O(21)	Cl(2)	O(24)	108.2(5)	O(22)	Cl(2)	O(23)	109.1(5)
O(22)	Cl(2)	O(24)	107.5(5)	O(23)	Cl(2)	O(24)	108.8(4)
Cu(1)	N(1)	C(1)	99.6(3)	Cu(1)	N(1)	C(6)	104.9(4)
Cu(1)	N(1)	C(19)	120.1(4)	C(1)	N(1)	C(6)	112.5(5)
C(1)	N(1)	C(19)	107.6(5)	C(6)	N(1)	C(19)	111.7(4)
Cu(1)	N(2)	C(2)	109.8(3)	Cu(1)	N(2)	C(3)	103.7(4)
Cu(1)	N(2)	C(7)	105.1(4)	C(2)	N(2)	C(3)	112.2(5)
C(2)	N(2)	C(7)	111.8(5)	C(3)	N(2)	C(7)	113.6(5)
Cu(1)	N(3)	C(4)	110.0(4)	Cu(1)	N(3)	C(5)	104.6(4)
Cu(1)	N(3)	C(13)	106.4(4)	C(4)	N(3)	C(5)	112.6(5)
C(4)	N(3)	C(13)	112.1(5)	C(5)	N(3)	C(13)	110.7(5)
Cu(1)	N(4)	C(8)	113.4(4)	Cu(1)	N(4)	C(12)	127.9(4)
C(8)	N(4)	C(12)	118.2(5)	Cu(1)	N(5)	C(14)	112.2(5)
Cu(1)	N(5)	C(18)	129.2(4)	C(14)	N(5)	C(18)	118.5(6)
C(21)	N(6)	C(22)	117(1)	C(21)	N(6)	C(23)	122(1)

Table 8. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
C(22)	N(6)	C(23)	122(1)	C(24)	N(7)	C(25)	130(1)
C(24)	N(7)	C(26)	114.1(9)	C(25)	N(7)	C(26)	116.2(8)
N(1)	C(1)	C(2)	113.0(5)	N(2)	C(2)	C(1)	113.2(5)
N(2)	C(3)	C(4)	108.5(5)	N(3)	C(4)	C(3)	109.7(5)
N(3)	C(5)	C(6)	113.0(5)	N(1)	C(6)	C(5)	110.7(5)
N(2)	C(7)	C(8)	109.9(5)	N(4)	C(8)	C(7)	114.4(5)
N(4)	C(8)	C(9)	121.9(6)	C(7)	C(8)	C(9)	123.7(6)
C(8)	C(9)	C(10)	119.0(6)	C(9)	C(10)	C(11)	119.4(6)
C(10)	C(11)	C(12)	119.2(6)	N(4)	C(12)	C(11)	122.3(6)
N(3)	C(13)	C(14)	111.2(5)	N(5)	C(14)	C(13)	116.3(6)
N(5)	C(14)	C(15)	121.2(7)	C(13)	C(14)	C(15)	122.4(6)
C(14)	C(15)	C(16)	119.7(7)	C(15)	C(16)	C(17)	118.3(7)
C(16)	C(17)	C(18)	120.0(7)	N(5)	C(18)	C(17)	122.3(6)
N(1)	C(19)	C(20)	114.3(5)	C(19)	C(20)	C(20)	111.3(7)
O(1)	C(21)	N(6)	125(1)	O(2)	C(24)	O(2')	126(1)
O(2)	C(24)	N(7)	117(1)	O(2')	C(24)	N(7)	116(1)