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Table S1 Fractional coordinates and equivalent isotropic temperature factors of non-H atoms with e.s.d.'s in parentheses.

Atom	x	y	z	B_{eq}(Å)
CU1	0.11440(8)	0.05335(6)	0.47614(8)	5.09(2)
CU2	0.29091(8)	0.01186(6)	0.60931(8)	5.63(3)
CL	0.2446(2)	0.4631(2)	0.6703(2)	8.61(8)
O1	0.2012(4)	0.1069(3)	0.5753(4)	4.9(1)
O2	0.2139(4)	-0.0314(3)	0.5056(4)	5.4(1)
O3	0.0330(4)	-0.0150(3)	0.3957(4)	5.9(1)
O4	0.3592(5)	-0.0905(4)	0.6333(5)	7.2(2)
O5	0.4519(6)	0.0772(5)	0.4781(5)	11.2(2)
N1	0.0531(4)	0.1632(4)	0.4384(4)	4.1(1)
N2	0.3570(5)	0.0784(4)	0.7138(5)	4.7(2)
C1	-0.0076(6)	0.0165(5)	0.3152(6)	5.2(2)
C2	-0.0071(6)	-0.0340(5)	0.2316(7)	5.9(2)
C3	-0.0567(6)	-0.0058(6)	0.1485(6)	6.5(2)
C4	-0.1016(7)	0.0712(6)	0.1399(6)	6.4(2)
C5	-0.0968(6)	0.1212(6)	0.2224(7)	5.9(2)
C6	-0.0504(6)	0.0953(5)	0.3076(6)	5.1(2)
C7	-0.0508(6)	0.1508(5)	0.3948(6)	4.9(2)
C8	0.0373(6)	0.2158(5)	0.5228(6)	4.6(2)
C9	0.1341(6)	0.2448(5)	0.5720(5)	4.2(2)
C10	0.1464(6)	0.3293(5)	0.5937(6)	4.7(2)
C11	0.2312(6)	0.3567(5)	0.6411(6)	4.8(2)
C12	0.3042(6)	0.3023(5)	0.6707(5)	4.7(2)
C13	0.2969(6)	0.2173(5)	0.6496(5)	4.1(2)
C14	0.2113(6)	0.1885(5)	0.5994(6)	4.3(2)
C15	0.3835(6)	0.1606(5)	0.6757(6)	4.9(2)
C16	0.4530(6)	0.0330(6)	0.7428(7)	5.9(2)
C17	0.4364(6)	-0.0527(5)	0.7823(7)	5.9(2)
C18	0.4678(7)	-0.0754(6)	0.8723(7)	6.9(3)
C19	0.4541(9)	-0.1527(6)	0.9085(8)	8.9(3)
C20	0.4051(8)	-0.2110(6)	0.8527(8)	8.3(3)
C21	0.3706(7)	-0.1922(6)	0.7594(8)	7.2(3)
C22	0.3882(6)	-0.1106(5)	0.7207(7)	6.3(2)
C23	0.0444(9)	-0.1159(7)	0.2325(8)	8.9(3)
C24	-0.1594(7)	0.0984(6)	0.0500(6)	6.1(2)
C25	0.1176(6)	0.2069(6)	0.3710(6)	5.5(2)
C26	0.2937(6)	0.0873(6)	0.7971(7)	6.3(2)
C27	0.496(1)	-0.1794(8)	1.0062(8)	13.4(5)
C28	0.3219(8)	-0.2574(6)	0.6995(9)	10.1(4)
C29	0.2475(7)	-0.0955(5)	0.4452(7)	6.8(3)
C30	0.3906(8)	0.1164(7)	0.4087(7)	8.5(3)

Anisotropically refined atoms are given in the form of the isotropic equivalent displacement parameter defined as: (4/3) * [a2*B(1,1) + b2*B(2,2) + c2*B(3,3) + ab(cos gamma)*B(1,2) + ac(cos beta)*B(1,3) + bc(cos alpha)*B(2,3)]

Table S2 Bond distances (Å) for non-H atoms with e.s.d.'s in parentheses

CU1-O1	1.979(5)	C2-C3	1.40(1)
CU1 -O2	1.922(5)	C2-C23	1.47(1)
CU1 -O3	1.888(6)	C3-C4	1.37(1)
CU1 -N1	1.992(6)	C4-C5	1.41(1)
CU2-O1	1.973(5)	C4-C24	1.53(1)
CU2-O2	1.892(6)	C5-C6	1.40(1)
CU2-O4	1.888(6)	C6-C7	1.52(1)
CU2-N2	1.999(6)	C8-C9	1.51(1)
CL -C11	1.750(8)	C9-C10	1.39(1)
O1-C14	1.349(9)	C9-C14	1.40(1)
O2-C29	1.41(1)	C10-C11	1.36(1)
O3-C1	1.34(1)	C11-C12	1.35(1)
O4-C22	1.32(1)	C12-C13	1.39(1)
O5-C30	1.40(1)	C13-C14	1.39(1)
N1-C7	1.50(1)	C13-C15	1.50(1)
N1-C8	1.48(1)	C16-C17	1.49(1)
N1-C25	1.47(1)	C17-C18	1.38(1)
N2-C15	1.46(1)	C17-C22	1.41(1)
N2-C16	1.51(1)	C18-C19	1.35(1)
N2-C26	1.47(1)	C19-C20	1.37(1)
C1-C2	1.43(1)	C19-C27	1.53(2)
C1-C6	1.38(1)	C20-C21	1.42(2)
C21-C22	1.43(1)	C21-C28	1.48(1)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S3 Bond angles(°) for non-H atoms with e.s.d.'s in parentheses

O1-Cu1-O2	76.6(2)	Cu1-N1-C25	110.5(5)
O1-Cu1-O3	169.6(2)	C7-N1-C8	104.9(6)
O1-Cu1-N1	92.0(2)	C7-N1-C25	109.6(6)
O2-Cu1-O3	95.8(2)	C8-N1-C25	110.6(6)
O2-Cu1-N1	160.8(2)	Cu2-N2-C15	107.8(5)
O3-Cu1-N1	97.1(2)	Cu2-N2-C16	107.1(5)
O1-Cu2-O2	77.5(2)	Cu2-N2-C26	113.4(5)
O1-Cu2-O4	170.4(2)	C15-N2-C16	108.6(6)
O1-Cu2-N2	91.3(2)	C15-N2-C26	110.9(6)
O2-Cu2-O4	94.0(2)	C16-N2-C26	108.8(6)
O2-Cu2-N2	168.7(2)	O3-C1-C2	118.8(7)
O4-Cu2-N2	97.3(3)	O3-C1-C6	123.9(8)
Cu1-O1-Cu2	100.1(2)	C2-C1-C6	117.3(8)
Cu1-O1-C14	130.2(5)	C1-C2-C3	120.0(8)
Cu2-O1-C14	128.4(5)	C1-C2-C23	120.2(8)
Cu1-O2-Cu2	105.2(2)	C3-C2-C23	119.7(8)
Cu1-O2-C29	127.0(5)	C2-C3-C4	123.6(8)
Cu2-O2-C29	124.2(5)	C3-C4-C5	115.0(8)
Cu1-O3-C1	120.2(5)	C3-C4-C24	122.3(8)
Cu2-O4-C22	120.1(5)	C5-C4-C24	122.6(8)
Cu1-N1-C7	110.8(4)	C4-C5-C6	123.7(8)
Cu1-N1-C8	110.3(4)	C1-C6-C5	120.2(8)
C1-C6-C7	118.5(7)	C9-C14-C13	120.3(7)
C5-C6-C7	121.2(7)	N2-C15-C13	116.1(6)
N1-C7-C6	112.7(6)	N2-C16-C17	114.1(7)
N1-C8-C9	114.0(6)	C16-C17-C18	122.9(8)
C8-C9-C10	119.3(7)	C16-C17-C22	115.7(8)
C8-C9-C14	122.2(7)	C18-C17-C22	121.4(8)
C10-C9-C14	118.5(7)	C17-C18-C19	123.5(9)
C9-C10-C11	120.6(7)	C18-C19-C20	118(1)
Cl-C11-C10	120.1(6)	C18-C19-C27	123(1)
Cl-C11-C12	118.7(6)	C20-C19-C27	119(1)
C10-C11-C12	121.1(7)	C19-C20-C21	121.9(9)
C11-C12-C13	120.9(7)	C20-C21-C22	119.8(9)
C12-C13-C14	118.6(7)	C20-C21-C28	120.6(9)
C12-C13-C15	119.1(7)	C22-C21-C28	119(1)
C14-C13-C15	122.1(7)	O4-C22-C17	122.3(8)
O1-C14-C9	118.5(7)	O4-C22-C21	122.2(8)
O1-C14-C13	121.2(7)	C17-C22-C21	115.6(9)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S4 Anisotropic displacement thermal parameter for all non-H atoms with e.s.d's are in parentheses

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
CU1	0.0662(6)	0.0666(6)	0.0605(7)	0.0041(6)	-0.0000(5)	-0.0123(6)
CU2	0.0626(6)	0.0665(6)	0.0843(8)	0.0072(6)	-0.0049(6)	-0.0100(7)
CL	0.116(2)	0.073(2)	0.138(3)	0.005(2)	-0.005(2)	-0.026(2)
O1	0.066(3)	0.062(3)	0.059(4)	0.005(3)	-0.010(3)	-0.007(3)
O2	0.065(3)	0.062(3)	0.077(4)	0.005(3)	0.003(3)	-0.010(3)
O3	0.090(4)	0.072(3)	0.060(4)	0.002(3)	-0.015(3)	-0.012(3)
O4	0.094(4)	0.068(3)	0.111(5)	0.019(3)	-0.023(4)	-0.007(4)
O5	0.170(7)	0.155(6)	0.099(6)	0.075(5)	-0.001(6)	-0.017(5)
N1	0.050(4)	0.071(4)	0.036(4)	0.003(3)	0.014(3)	-0.010(4)
N2	0.046(4)	0.069(4)	0.064(5)	0.001(3)	0.013(4)	-0.006(4)
C1	0.057(5)	0.086(5)	0.055(6)	-0.008(5)	0.010(5)	-0.022(5)
C2	0.057(5)	0.081(6)	0.087(7)	-0.006(5)	0.013(5)	-0.021(5)
C3	0.062(5)	0.130(7)	0.053(6)	-0.029(5)	0.015(5)	-0.025(6)
C4	0.064(5)	0.113(7)	0.067(7)	-0.021(5)	0.023(5)	-0.021(6)
C5	0.059(5)	0.092(6)	0.075(7)	0.001(5)	0.016(5)	0.004(6)
C6	0.048(5)	0.082(5)	0.063(6)	0.003(5)	0.010(5)	-0.003(5)
C7	0.060(5)	0.078(5)	0.046(5)	0.001(5)	0.004(4)	-0.003(5)
C8	0.068(5)	0.065(5)	0.042(5)	0.010(4)	0.013(4)	-0.008(4)
C9	0.061(5)	0.061(5)	0.037(5)	0.000(4)	0.009(4)	-0.003(4)
C10	0.070(5)	0.063(5)	0.048(6)	0.008(4)	0.014(5)	-0.000(5)
C11	0.063(5)	0.062(5)	0.060(6)	0.004(4)	0.010(5)	-0.013(5)
C12	0.072(5)	0.068(5)	0.040(5)	-0.010(5)	0.013(5)	-0.020(4)
C13	0.050(4)	0.068(5)	0.037(5)	0.005(4)	0.009(4)	-0.004(4)
C14	0.065(5)	0.062(5)	0.038(5)	-0.002(4)	0.014(4)	-0.000(4)
C15	0.069(5)	0.073(5)	0.046(5)	-0.010(5)	-0.005(4)	-0.007(5)
C16	0.061(5)	0.100(7)	0.064(6)	-0.003(5)	0.004(5)	-0.013(5)
C17	0.055(5)	0.075(5)	0.095(7)	0.012(5)	0.015(5)	0.025(5)
C18	0.081(6)	0.105(7)	0.077(7)	0.025(6)	0.020(6)	0.018(6)
C19	0.125(8)	0.114(7)	0.101(8)	0.041(7)	0.050(7)	0.030(7)
C20	0.109(7)	0.082(6)	0.130(9)	0.025(6)	0.068(6)	0.041(6)
C21	0.070(6)	0.079(6)	0.128(9)	0.008(5)	0.041(6)	0.005(6)
C22	0.050(5)	0.083(6)	0.107(8)	0.004(5)	0.016(5)	0.014(6)
C23	0.119(8)	0.122(8)	0.097(8)	-0.024(7)	0.006(7)	-0.037(7)
C24	0.075(5)	0.131(7)	0.027(5)	-0.030(6)	-0.007(4)	0.012(5)
C25	0.061(5)	0.092(6)	0.054(6)	-0.007(5)	0.005(5)	0.003(5)
C26	0.060(5)	0.093(6)	0.088(7)	0.013(5)	0.015(5)	0.009(6)
C27	0.28(2)	0.15(1)	0.073(8)	0.06(1)	0.05(1)	0.056(7)
C28	0.096(8)	0.083(7)	0.21(1)	-0.004(6)	0.030(9)	-0.004(8)
C29	0.075(6)	0.076(6)	0.107(8)	0.010(5)	0.019(6)	-0.029(6)
C30	0.097(8)	0.150(9)	0.078(8)	0.019(7)	0.010(7)	0.009(7)

The form of the anisotropic displacement parameter is: $\exp[-2PI2\{h^2a^2U(1,1) + k^2b^2U(2,2)\ l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)\}]$ where a,b, and c are reciprocal lattice constants.

Table S5 Hydrogen coordinates and isotropic displacement parameters and Their estimated standard deviations in parentheses

Atom	x	y	z	B_{eq}(Å)
H3	-0.052(6)	-0.035(4)	0.088(5)	13(2)*
H5	-0.120(3)	0.171(2)	0.221(3)	4.5(9)*
H10	0.0960	0.3687	0.5767	6*
H12	0.3596	0.3224	0.7062	6*
H18	0.5035	-0.0323	0.9133	9*
H20	0.3931	-0.2683	0.8758	10*
H71	-0.087(4)	0.116(3)	0.450(4)	5(2)*
H72	-0.083(4)	0.208(3)	0.373(3)	4(1)*
H81	0.0057	0.1863	0.5692	6*
H82	-0.004(6)	0.271(4)	0.493(5)	8(2)*
H151	0.419(3)	0.182(2)	0.717(3)	5(1)*
H152	0.4179	0.1526	0.6149	6*
H161	0.477(4)	0.061(3)	0.783(3)	2(1)*
H162	0.4946	0.0258	0.6861	7*
H231	0.0325	-0.1421	0.1678	12*
H232	0.1099	-0.1137	0.2459	12*
H233	0.0082	-0.1543	0.2736	12*
H241	-0.1839	0.1526	0.0574	9*
H242	-0.1134	0.0967	-0.0016	9*
H243	-0.2126	0.0597	0.0369	9*
H251	0.1245	0.1729	0.3135	7*
H252	0.0823	0.2582	0.3480	7*
H253	0.1798	0.2210	0.3951	7*
H261	0.240(3)	0.106(3)	0.776(3)	2(1)*
H262	0.269(5)	0.030(4)	0.818(5)	6(2)*
H263	0.3281	0.1204	0.8477	8*
H271	0.4695	-0.2378	1.0139	17*
H272	0.5602	-0.1761	1.0108	17*
H273	0.4583	-0.1468	1.0516	17*
H281	0.3224	-0.3172	0.6779	12*
H282	0.3245	-0.2339	0.6334	12*
H283	0.2498	-0.2553	0.7125	12*
H291	0.2020	-0.0999	0.3897	8*
H292	0.2485	-0.1502	0.4740	8*
H293	0.3137	-0.0853	0.4211	8*

* Starred atoms were refined isotropically.

Table S6 Bond Distances (Å) for hydrogen atoms (e.s.d.'s are in parentheses)

C3	H3	0.98(8)	C24	H242	0.964(8)
C5	H5	0.85(4)	C24	H243	0.949(9)
C7	H71	1.08(6)	C25	H251	0.983(9)
C7	H72	1.04(5)	C25	H252	0.990(9)
C8	H81	0.917(8)	C25	H253	0.911(8)
C8	H82	1.11(7)	C26	H261	0.82(4)
C10	H10	0.941(8)	C26	H262	1.02(6)
C12	H12	0.935(8)	C26	H263	0.991(9)
C15	H151	0.81(4)	C27	H271	1.00(1)
C15	H152	0.991(8)	C27	H272	0.85(2)
C16	H161	0.78(5)	C27	H273	0.97(1)
C16	H162	0.991(9)	C28	H281	1.00(1)
C18	H18	1.007(9)	C28	H282	1.01(1)
C20	H20	0.982(9)	C28	H283	0.98(1)
C23	H231	1.01(1)	C29	H291	0.98(1)
C23	H232	0.88(1)	C29	H292	0.962(9)
C23	H233	0.98(1)	C29	H293	0.963(9)
C24	H241	0.929(9)			

Table S7. Least squares plane through various atoms

Plane 1 $0.654(4)x + 0.354(2)y - 0.669(1)z = -3.34(1)$

Atom	Deviation (Å)
O1	0.085(5)
Cu1	-0.003(2)
Cu2	-0.004(1)
O2	0.094(5)

Table S8 Inter and Intra molecular hydrogen bonding

Bond	D-H(Å)	D...A(Å)	H-A(Å)	D-H...A(°)
C15-H152...O5	0.99(8)	3.25(1)	2.33(7)	152.8(5)
C7-H71...O2	1.08(5)	3.23(1)	2.25(5)	148.9(4)