

Table SI. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5164(1)	1395(1)	6757(1)	48(1)
Cu(2)	6824(1)	240(1)	7994(1)	47(1)
Cu(3)	7224(1)	2163(1)	7925(1)	50(1)
S(5)	3263(2)	1204(2)	8553(2)	70(1)
O(51)	4031(6)	1620(6)	8063(6)	109(3)
O(52)	3244(7)	1399(6)	9572(5)	127(4)
O(53)	3148(9)	457(5)	8291(10)	174(5)
C(51)	2167(11)	1667(10)	8066(11)	102(4)
F(51)	2047(9)	2355(6)	8265(8)	202(6)
F(52)	1999(6)	1502(5)	7144(5)	129(3)
F(53)	1337(7)	1315(8)	8477(7)	174(5)
S(6)	8150(2)	3793(2)	10737(2)	84(1)
O(61)	8007(5)	4153(4)	9828(5)	77(2)
O(62)	7992(9)	2940(8)	10714(10)	187(6)
O(63)	7709(10)	4169(11)	11457(7)	232(8)
C(61)	9470(11)	3853(9)	11030(14)	109(5)
F(61)	9728(6)	3524(8)	11842(7)	192(5)
F(62)	9820(9)	4522(7)	10987(11)	228(7)
F(63)	9956(6)	3468(7)	10375(9)	169(4)
O(6)	5908(6)	162(5)	9378(6)	102(3)
O(4)	6200(4)	1294(3)	7831(4)	45(2)
O(7)	6411(4)	2633(3)	9223(5)	62(2)
N(11)	5109(5)	295(4)	6663(5)	45(2)
N(12)	5751(5)	-210(4)	7141(5)	46(2)
N(13)	4574(5)	-899(4)	6316(6)	56(2)
N(14)	3623(5)	171(4)	5615(5)	54(2)
C(11)	4416(6)	-151(5)	6175(6)	44(2)
C(12)	5416(6)	-917(5)	6905(7)	57(3)
C(13)	3462(7)	935(6)	5450(7)	53(2)
C(14)	2549(7)	1128(6)	4818(8)	74(3)
O(11)	4042(5)	1445(3)	5767(4)	58(2)
N(21)	7980(5)	704(4)	8650(5)	43(2)
N(22)	8160(5)	1492(3)	8694(5)	49(2)
N(23)	9394(5)	887(4)	9558(6)	59(2)
N(24)	8832(5)	-414(3)	9256(5)	49(2)
C(21)	8730(6)	382(4)	9159(6)	41(2)
C(22)	9002(6)	1578(5)	9245(7)	63(3)
C(23)	8244(6)	-932(4)	8784(6)	45(2)
C(24)	8535(8)	-1764(5)	8949(7)	67(3)
O(21)	7517(5)	-785(3)	8226(4)	57(2)
N(31)	6377(5)	2748(4)	7033(5)	50(2)
N(32)	5487(5)	2478(4)	6573(5)	48(2)
N(33)	5788(6)	3662(4)	6012(6)	65(2)
N(34)	7360(6)	3898(4)	6941(6)	56(2)
C(31)	6518(6)	3444(5)	6673(7)	51(2)
C(32)	5190(7)	3043(5)	5978(7)	65(3)
C(33)	8172(6)	3654(5)	7490(7)	54(2)
C(34)	9011(7)	4246(6)	7644(8)	75(3)
O(31)	8268(4)	3005(3)	7827(5)	56(2)

Table SII. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	4401(1)	387(1)	3050(1)	31(1)
Cu(2)	3094(1)	-855(1)	1478(1)	28(1)
Cu(3)	672(1)	1941(1)	2580(1)	28(1)
N(11)	5740(4)	-1190(4)	2401(2)	29(1)
N(12)	5244(4)	-1812(4)	1803(2)	29(1)
N(13)	7713(4)	-3233(4)	2068(2)	35(1)
N(14)	8101(3)	-1802(4)	3120(2)	30(1)
C(11)	7200(4)	-2068(4)	2537(3)	28(1)
C(12)	6456(5)	-3021(5)	1631(3)	36(1)
C(13)	7583(5)	-672(5)	3640(3)	31(1)
C(14)	8739(5)	-531(6)	4195(3)	46(1)
O(11)	6238(3)	221(3)	3676(2)	42(1)
N(21)	919(3)	-197(3)	1415(2)	26(1)
N(22)	-129(4)	968(4)	1824(2)	29(1)
N(23)	-1386(4)	-81(4)	1172(2)	30(1)
N(24)	790(4)	-2020(4)	584(2)	31(1)
C(21)	135(4)	-789(4)	1049(2)	26(1)
C(22)	-1469(4)	990(4)	1663(3)	29(1)
C(23)	2302(5)	-2795(4)	480(3)	31(1)
C(24)	2780(5)	-4078(5)	-77(3)	42(1)
O(21)	3296(3)	-2523(3)	802(2)	38(1)
N(31)	1495(4)	2521(4)	3511(2)	30(1)
N(32)	3028(4)	2002(4)	3697(2)	32(1)
N(33)	1735(4)	3608(4)	4651(2)	36(1)
N(34)	-786(4)	4217(4)	4117(2)	33(1)
C(31)	792(4)	3468(4)	4089(3)	28(1)
C(32)	3115(5)	2677(5)	4371(3)	36(1)
C(33)	-1776(4)	3955(4)	3645(3)	29(1)
C(34)	-3444(5)	4827(5)	3810(3)	39(1)
O(31)	-1369(3)	3017(3)	3099(2)	36(1)
O(4)	2782(3)	905(3)	2107(2)	26(1)
O(6)	3449(4)	361(4)	90(2)	39(1)
O(7)	289(4)	4206(4)	1664(2)	43(1)
O(1W)	1082(4)	3222(4)	32(2)	48(1)
N(51)	3129(5)	-1753(5)	3964(3)	48(1)
O(51)	4126(4)	-1341(4)	4114(2)	60(1)
O(52)	2317(5)	-1178(5)	3299(3)	82(1)
O(53)	2905(6)	-2701(5)	4434(3)	86(2)
O(2W)	1163(5)	-3433(7)	3103(5)	114(2)
N(61)	4184(5)	3649(5)	1845(3)	51(1)
O(61)	2833(4)	4541(5)	1991(3)	80(1)
O(62)	4412(5)	2519(5)	1495(3)	79(1)
O(63)	5204(5)	3986(5)	2017(4)	90(2)

Table SIII. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	6581(1)	3479(1)	98(1)	43(1)
Cu(2)	7755(1)	4718(1)	1902(1)	44(1)
Cu(3)	7734(1)	2700(1)	2405(1)	42(1)
Cl(5)	8367(3)	3478(2)	-2036(3)	66(1)
Cl(8)	5732(2)	3719(2)	3637(3)	63(1)
O(4)	7593(4)	3598(4)	1239(6)	35(2)
O(6)	9087(5)	4710(5)	809(7)	62(2)
O(7)	9174(5)	2424(4)	1571(6)	54(2)
O(11)	5685(5)	3412(5)	-1185(6)	57(2)
O(21)	7991(5)	5796(5)	2571(7)	57(2)
O(31)	7757(5)	1753(4)	3468(7)	51(2)
N(11)	6506(6)	4634(5)	6(8)	39(2)
N(21)	8410(6)	4266(5)	3164(7)	42(3)
N(31)	6919(5)	2057(5)	1448(7)	33(2)
N(12)	6927(6)	5175(6)	757(8)	41(3)
N(22)	8413(6)	3440(6)	3462(8)	44(3)
N(32)	6448(6)	2338(5)	515(8)	40(2)
N(13)	6104(6)	5896(5)	-530(8)	42(3)
N(23)	9391(7)	4114(6)	4618(8)	60(3)
N(33)	5986(6)	1065(6)	813(9)	51(3)
N(14)	5488(6)	4761(6)	-1624(8)	49(3)
N(24)	9125(6)	5448(5)	3879(7)	46(3)
N(34)	6946(6)	814(6)	2476(8)	52(3)
C(11)	6039(8)	5100(7)	-719(10)	43(3)
C(21)	8982(8)	4598(7)	3896(9)	38(3)
C(31)	6628(8)	1308(7)	1587(10)	40(3)
C(12)	6681(7)	5889(7)	360(9)	41(3)
C(22)	9009(8)	3371(8)	4307(9)	53(3)
C(32)	5887(7)	1743(7)	174(11)	54(4)
C(13)	5355(8)	3954(7)	-1780(10)	45(3)
C(23)	8607(8)	5978(7)	3282(10)	40(3)
C(33)	7488(8)	1052(7)	3382(10)	41(3)
C(14)	4792(8)	3781(7)	-2860(10)	70(4)
C(24)	8871(8)	6839(7)	3495(10)	62(4)
C(34)	7756(8)	409(7)	4224(10)	63(4)
O(51)	8142(9)	3045(8)	-1079(12)	163(5)
O(52)	7596(12)	3951(9)	-2269(14)	211(7)
O(53)	8450(8)	2947(7)	-2951(10)	132(4)
O(54)	9092(11)	4005(9)	-1969(12)	184(6)
O(81)	6039(10)	4181(9)	2738(14)	184(6)
O(82)	4831(9)	3926(7)	3795(11)	155(5)
O(83)	6277(10)	3830(8)	4564(13)	179(6)
O(84)	5841(9)	2915(8)	3397(11)	163(5)

Table SIV. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(6A)	6393	103	9934	152
H(6B)	5474	-282	9348	152
H(4)	5804	1358	8411	54
H(7A)	6076	3115	9046	93
H(7B)	6907	2731	9742	93
H(14)	3190	-147	5346	65
H(12)	5730	-1374	7123	68
H(14A)	2188	659	4645	111
H(14B)	2764	1381	4243	111
H(14C)	2106	1468	5158	111
H(24)	9307	-586	9647	59
H(22)	9293	2057	9400	76
H(24A)	9112	-1791	9400	100
H(24B)	8711	-1996	8347	100
H(24C)	7969	-2040	9206	100
H(34)	7364	4371	6742	68
H(32)	4609	3008	5570	78
H(34A)	8812	4724	7333	112
H(34B)	9627	4056	7373	112
H(34C)	9130	4334	8324	112

Table SV. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**.

	x	y	z	U(eq)
H(14)	9056	-2397	3153	36
H(12)	6436	-3667	1241	43
H(14A)	9729	-1305	4097	69
H(14B)	8472	-612	4803	69
H(14C)	8762	417	4043	69
H(24)	188	-2311	344	37
H(22)	-2385	1681	1869	35
H(24A)	1887	-4147	-282	63
H(24B)	3400	-4982	266	63
H(24C)	3357	-3920	-571	63
H(34)	-1164	4907	4466	39
H(32)	4032	2527	4628	43
H(34A)	-3570	5495	4245	59
H(34B)	-3896	4160	4015	59
H(34C)	-3937	5384	3274	59
H(4)	2932	1622	1671	31
H(6A)	3130 (8)	-50 (7)	-210 (4)	108
H(6B)	2800 (6)	1200 (3)	100 (5)	108
H(7A)	-380 (6)	4940 (5)	1840 (5)	108
H(7B)	1110 (5)	4240 (8)	1730 (5)	108
H(1W1)	890 (8)	4020 (4)	-240 (4)	108
H(2W1)	870 (8)	3390 (8)	530 (2)	108
H(1W2)	1650 (7)	-3270 (8)	3460 (4)	108
H(2W2)	1720 (7)	-3960 (7)	2740 (4)	108

Table SVI. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**.

	x	y	z	U(eq)
H(4)	8159	3534	776	42
H(6A)	9634	4657	1290	92
H(6B)	9130	5210	378	92
H(7A)	9134	1919	1137	80
H(7B)	9650	2367	2147	80
H(14)	5225	5091	-2099	58
H(24)	9580	5640	4285	55
H(34)	6785	309	2451	62
H(12)	6901	6370	690	49
H(22)	9160	2878	4659	64
H(32)	5469	1788	-439	64
H(14A)	5210	3621	-3462	105
H(14B)	4457	4263	-3086	105
H(14C)	4354	3348	-2717	105
H(24A)	8345	7186	3322	92
H(24B)	9390	6984	3017	92
H(24C)	9047	6905	4285	92
H(34A)	8410	281	4143	94
H(34B)	7388	-72	4086	94
H(34C)	7643	603	4986	94

Table SVII. Bond lengths [Å] and angles [deg] for 1.

Cu(1)-N(11)	1.897(6)
Cu(1)-N(32)	1.930(7)
Cu(1)-O(11)	1.967(5)
Cu(1)-O(4)	1.977(5)
Cu(1)-O(51)	2.416(8)
Cu(2)-N(21)	1.906(6)
Cu(2)-N(12)	1.955(6)
Cu(2)-O(4)	1.998(5)
Cu(2)-O(21)	2.002(5)
Cu(2)-O(6)	2.306(8)
Cu(3)-N(31)	1.912(6)
Cu(3)-N(22)	1.963(6)
Cu(3)-O(31)	1.999(6)
Cu(3)-O(4)	2.008(5)
Cu(3)-O(7)	2.274(7)
S(5)-O(53)	1.342(8)
S(5)-O(51)	1.427(8)
S(5)-O(52)	1.450(8)
S(5)-C(51)	1.751(14)
C(51)-F(51)	1.226(16)
C(51)-F(52)	1.317(15)
C(51)-F(53)	1.387(16)
S(6)-O(63)	1.338(11)
S(6)-O(61)	1.408(7)
S(6)-O(62)	1.483(13)
S(6)-C(61)	1.759(14)
C(61)-F(62)	1.241(17)
C(61)-F(61)	1.291(17)
C(61)-F(63)	1.307(18)
O(6)-H(6A)	0.982(8)
O(6)-H(6B)	0.952(9)
O(4)-H(4)	0.9800
O(7)-H(7A)	0.964(5)
O(7)-H(7B)	0.963(6)
N(11)-C(11)	1.347(9)
N(11)-N(12)	1.361(8)
N(12)-C(12)	1.328(10)
N(13)-C(11)	1.315(10)
N(13)-C(12)	1.344(10)
N(14)-C(13)	1.349(11)
N(14)-C(11)	1.385(10)
N(14)-H(14)	0.8600
C(12)-H(12)	0.9300
C(13)-O(11)	1.229(10)
C(13)-C(14)	1.488(11)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
N(21)-C(21)	1.306(9)
N(21)-N(22)	1.377(8)
N(22)-C(22)	1.321(9)
N(23)-C(21)	1.332(9)
N(23)-C(22)	1.359(10)
N(24)-C(23)	1.330(9)
N(24)-C(21)	1.381(9)
N(24)-H(24)	0.8600
C(22)-H(22)	0.9300
C(23)-O(21)	1.226(9)
C(23)-C(24)	1.498(11)

C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
N(31)-C(31)	1.312(10)
N(31)-N(32)	1.384(8)
N(32)-C(32)	1.321(10)
N(33)-C(32)	1.321(11)
N(33)-C(31)	1.348(10)
N(34)-C(33)	1.346(11)
N(34)-C(31)	1.388(10)
N(34)-H(34)	0.8600
C(32)-H(32)	0.9300
C(33)-O(31)	1.214(10)
C(33)-C(34)	1.506(12)
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
N(11)-Cu(1)-N(32)	164.0(3)
N(11)-Cu(1)-O(11)	88.3(2)
N(32)-Cu(1)-O(11)	91.5(2)
N(11)-Cu(1)-O(4)	89.3(2)
N(32)-Cu(1)-O(4)	92.1(2)
O(11)-Cu(1)-O(4)	174.6(2)
N(11)-Cu(1)-O(51)	100.9(3)
N(32)-Cu(1)-O(51)	95.1(3)
O(11)-Cu(1)-O(51)	92.9(3)
O(4)-Cu(1)-O(51)	82.8(3)
N(21)-Cu(2)-N(12)	171.3(3)
N(21)-Cu(2)-O(4)	89.2(2)
N(12)-Cu(2)-O(4)	90.7(2)
N(21)-Cu(2)-O(21)	87.0(2)
N(12)-Cu(2)-O(21)	93.2(2)
O(4)-Cu(2)-O(21)	176.1(2)
N(21)-Cu(2)-O(6)	93.3(3)
N(12)-Cu(2)-O(6)	95.4(3)
O(4)-Cu(2)-O(6)	85.5(3)
O(21)-Cu(2)-O(6)	93.6(3)
N(31)-Cu(3)-N(22)	172.6(3)
N(31)-Cu(3)-O(31)	87.3(3)
N(22)-Cu(3)-O(31)	92.9(2)
N(31)-Cu(3)-O(4)	89.0(2)
N(22)-Cu(3)-O(4)	89.8(2)
O(31)-Cu(3)-O(4)	172.2(3)
N(31)-Cu(3)-O(7)	92.6(3)
N(22)-Cu(3)-O(7)	94.7(3)
O(31)-Cu(3)-O(7)	98.0(3)
O(4)-Cu(3)-O(7)	89.0(2)
O(53)-S(5)-O(51)	115.1(8)
O(53)-S(5)-O(52)	118.5(7)
O(51)-S(5)-O(52)	112.8(5)
O(53)-S(5)-C(51)	104.5(7)
O(51)-S(5)-C(51)	99.8(7)
O(52)-S(5)-C(51)	102.9(7)
S(5)-O(51)-Cu(1)	137.8(6)
F(51)-C(51)-F(52)	114.2(14)
F(51)-C(51)-F(53)	102.7(14)
F(52)-C(51)-F(53)	101.6(12)
F(51)-C(51)-S(5)	117.6(11)
F(52)-C(51)-S(5)	112.1(11)
F(53)-C(51)-S(5)	106.6(10)
O(63)-S(6)-O(61)	114.1(7)
O(63)-S(6)-O(62)	115.5(10)
O(61)-S(6)-O(62)	113.7(6)

O(63)-S(6)-C(61)	104.5(9)
O(61)-S(6)-C(61)	105.8(7)
O(62)-S(6)-C(61)	101.3(7)
F(62)-C(61)-F(61)	111.3(16)
F(62)-C(61)-F(63)	104.2(16)
F(61)-C(61)-F(63)	105.4(13)
F(62)-C(61)-S(6)	113.8(11)
F(61)-C(61)-S(6)	113.2(12)
F(63)-C(61)-S(6)	108.2(12)
Cu(2)-O(6)-H(6A)	108.4(6)
Cu(2)-O(6)-H(6B)	109.9(6)
H(6A)-O(6)-H(6B)	108.4(8)
Cu(1)-O(4)-Cu(2)	115.4(3)
Cu(1)-O(4)-Cu(3)	114.7(2)
Cu(2)-O(4)-Cu(3)	113.6(2)
Cu(1)-O(4)-H(4)	103.7
Cu(2)-O(4)-H(4)	103.7
Cu(3)-O(4)-H(4)	103.7
Cu(3)-O(7)-H(7A)	109.1(5)
Cu(3)-O(7)-H(7B)	109.2(4)
H(7A)-O(7)-H(7B)	108.9(6)
C(11)-N(11)-N(12)	105.6(6)
C(11)-N(11)-Cu(1)	128.7(5)
N(12)-N(11)-Cu(1)	125.7(5)
C(12)-N(12)-N(11)	105.9(6)
C(12)-N(12)-Cu(2)	137.0(6)
N(11)-N(12)-Cu(2)	116.9(5)
C(11)-N(13)-C(12)	103.4(7)
C(13)-N(14)-C(11)	126.3(7)
C(13)-N(14)-H(14)	116.9
C(11)-N(14)-H(14)	116.9
N(13)-C(11)-N(11)	112.6(7)
N(13)-C(11)-N(14)	125.6(7)
N(11)-C(11)-N(14)	121.7(7)
N(12)-C(12)-N(13)	112.4(7)
N(12)-C(12)-H(12)	123.8
N(13)-C(12)-H(12)	123.8
O(11)-C(13)-N(14)	123.1(7)
O(11)-C(13)-C(14)	121.3(8)
N(14)-C(13)-C(14)	115.6(8)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-O(11)-Cu(1)	130.5(6)
C(21)-N(21)-N(22)	105.7(6)
C(21)-N(21)-Cu(2)	129.9(5)
N(22)-N(21)-Cu(2)	124.4(4)
C(22)-N(22)-N(21)	105.8(6)
C(22)-N(22)-Cu(3)	137.1(6)
N(21)-N(22)-Cu(3)	117.0(4)
C(21)-N(23)-C(22)	101.9(6)
C(23)-N(24)-C(21)	124.4(6)
C(23)-N(24)-H(24)	117.8
C(21)-N(24)-H(24)	117.8
N(21)-C(21)-N(23)	114.2(7)
N(21)-C(21)-N(24)	122.6(7)
N(23)-C(21)-N(24)	123.1(6)
N(22)-C(22)-N(23)	112.4(8)
N(22)-C(22)-H(22)	123.8
N(23)-C(22)-H(22)	123.8
O(21)-C(23)-N(24)	126.1(7)

O(21)-C(23)-C(24)	118.6(7)
N(24)-C(23)-C(24)	115.3(7)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-O(21)-Cu(2)	128.0(5)
C(31)-N(31)-N(32)	105.1(6)
C(31)-N(31)-Cu(3)	129.7(6)
N(32)-N(31)-Cu(3)	125.0(5)
C(32)-N(32)-N(31)	105.0(7)
C(32)-N(32)-Cu(1)	137.1(6)
N(31)-N(32)-Cu(1)	116.7(5)
C(32)-N(33)-C(31)	101.6(7)
C(33)-N(34)-C(31)	125.0(7)
C(33)-N(34)-H(34)	117.5
C(31)-N(34)-H(34)	117.5
N(31)-C(31)-N(33)	113.9(8)
N(31)-C(31)-N(34)	122.3(8)
N(33)-C(31)-N(34)	123.8(8)
N(33)-C(32)-N(32)	114.4(7)
N(33)-C(32)-H(32)	122.8
N(32)-C(32)-H(32)	122.8
O(31)-C(33)-N(34)	124.7(8)
O(31)-C(33)-C(34)	120.3(8)
N(34)-C(33)-C(34)	115.0(8)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-O(31)-Cu(3)	129.2(6)

Table SVIII. Bond lengths [Å] and angles [deg] for **2**.

Cu(1)-N(11)	1.908(3)
Cu(1)-N(32)	1.938(3)
Cu(1)-O(11)	1.986(3)
Cu(1)-O(4)	2.034(3)
Cu(1)-O(51)	2.340(4)
Cu(2)-N(21)	1.919(3)
Cu(2)-N(12)	1.943(3)
Cu(2)-O(21)	1.988(3)
Cu(2)-O(4)	1.997(2)
Cu(2)-O(6)	2.421(4)
Cu(3)-N(31)	1.910(3)
Cu(3)-N(22)	1.953(3)
Cu(3)-O(31)	1.981(3)
Cu(3)-O(4)	1.999(2)
Cu(3)-O(7)	2.430(4)
N(11)-C(11)	1.319(5)
N(11)-N(12)	1.363(4)
N(12)-C(12)	1.319(5)
N(13)-C(11)	1.331(5)
N(13)-C(12)	1.335(5)
N(14)-C(13)	1.354(5)
N(14)-C(11)	1.389(5)
N(14)-H(14)	0.8600
C(12)-H(12)	0.9300
C(13)-O(11)	1.229(5)
C(13)-C(14)	1.490(6)
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
N(21)-C(21)	1.310(5)
N(21)-N(22)	1.369(4)
N(22)-C(22)	1.317(5)
N(23)-C(22)	1.344(5)
N(23)-C(21)	1.348(5)
N(24)-C(23)	1.344(5)
N(24)-C(21)	1.380(5)
N(24)-H(24)	0.8600
C(22)-H(22)	0.9300
C(23)-O(21)	1.234(5)
C(23)-C(24)	1.508(5)
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
N(31)-C(31)	1.312(4)
N(31)-N(32)	1.376(4)
N(32)-C(32)	1.313(5)
N(33)-C(31)	1.337(5)
N(33)-C(32)	1.346(5)
N(34)-C(33)	1.345(5)
N(34)-C(31)	1.385(5)
N(34)-H(34)	0.8600
C(32)-H(32)	0.9300
C(33)-O(31)	1.248(4)
C(33)-C(34)	1.497(5)
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
O(4)-H(4)	0.9800
O(6)-H(6A)	0.80(2)
O(6)-H(6B)	0.81(2)

O(7)-H(7A)	0.81(2)
O(7)-H(7B)	0.82(2)
O(1W)-H(1W1)	0.81(2)
O(1W)-H(2W1)	0.80(2)
N(51)-O(53)	1.216(5)
N(51)-O(52)	1.243(5)
N(51)-O(51)	1.232(5)
O(2W)-H(1W2)	0.81(2)
O(2W)-H(2W2)	0.82(2)
N(61)-O(63)	1.213(6)
N(61)-O(62)	1.230(5)
N(61)-O(61)	1.257(5)
N(11)-Cu(1)-N(32)	179.35(15)
N(11)-Cu(1)-O(11)	87.43(12)
N(32)-Cu(1)-O(11)	93.02(12)
N(11)-Cu(1)-O(4)	88.64(12)
N(32)-Cu(1)-O(4)	90.79(12)
O(11)-Cu(1)-O(4)	161.44(13)
N(11)-Cu(1)-O(51)	90.02(14)
N(32)-Cu(1)-O(51)	90.46(15)
O(11)-Cu(1)-O(51)	89.85(14)
O(4)-Cu(1)-O(51)	108.30(12)
N(21)-Cu(2)-N(12)	165.65(15)
N(21)-Cu(2)-O(21)	87.61(12)
N(12)-Cu(2)-O(21)	91.80(12)
N(21)-Cu(2)-O(4)	89.67(11)
N(12)-Cu(2)-O(4)	91.43(12)
O(21)-Cu(2)-O(4)	176.39(11)
N(21)-Cu(2)-O(6)	98.38(13)
N(12)-Cu(2)-O(6)	95.89(13)
O(21)-Cu(2)-O(6)	86.35(12)
O(4)-Cu(2)-O(6)	91.71(11)
N(31)-Cu(3)-N(22)	166.86(15)
N(31)-Cu(3)-O(31)	87.17(12)
N(22)-Cu(3)-O(31)	91.87(12)
N(31)-Cu(3)-O(4)	89.47(12)
N(22)-Cu(3)-O(4)	91.51(12)
O(31)-Cu(3)-O(4)	176.60(11)
N(31)-Cu(3)-O(7)	91.61(13)
N(22)-Cu(3)-O(7)	101.47(13)
O(31)-Cu(3)-O(7)	88.53(12)
O(4)-Cu(3)-O(7)	91.09(11)
C(11)-N(11)-N(12)	106.1(3)
C(11)-N(11)-Cu(1)	129.2(3)
N(12)-N(11)-Cu(1)	123.5(2)
C(12)-N(12)-N(11)	104.9(3)
C(12)-N(12)-Cu(2)	137.3(3)
N(11)-N(12)-Cu(2)	117.7(2)
C(11)-N(13)-C(12)	101.7(3)
C(13)-N(14)-C(11)	124.7(3)
C(13)-N(14)-H(14)	117.7
C(11)-N(14)-H(14)	117.7
N(11)-C(11)-N(13)	113.4(4)
N(11)-C(11)-N(14)	122.9(3)
N(13)-C(11)-N(14)	123.7(3)
N(12)-C(12)-N(13)	114.0(4)
N(12)-C(12)-H(12)	123.0
N(13)-C(12)-H(12)	123.0
O(11)-C(13)-N(14)	123.9(4)
O(11)-C(13)-C(14)	119.3(4)
N(14)-C(13)-C(14)	116.8(4)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5

H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-O(11)-Cu(1)	130.8(3)
C(21)-N(21)-N(22)	106.1(3)
C(21)-N(21)-Cu(2)	129.1(3)
N(22)-N(21)-Cu(2)	124.7(2)
C(22)-N(22)-N(21)	105.5(3)
C(22)-N(22)-Cu(3)	136.8(3)
N(21)-N(22)-Cu(3)	117.0(2)
C(22)-N(23)-C(21)	101.4(3)
C(23)-N(24)-C(21)	124.7(3)
C(23)-N(24)-H(24)	117.6
C(21)-N(24)-H(24)	117.6
N(21)-C(21)-N(23)	113.4(3)
N(21)-C(21)-N(24)	123.7(3)
N(23)-C(21)-N(24)	122.8(3)
N(22)-C(22)-N(23)	113.6(3)
N(22)-C(22)-H(22)	123.2
N(23)-C(22)-H(22)	123.2
O(21)-C(23)-N(24)	124.6(4)
O(21)-C(23)-C(24)	119.1(4)
N(24)-C(23)-C(24)	116.3(4)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(23)-O(21)-Cu(2)	130.1(3)
C(31)-N(31)-N(32)	105.3(3)
C(31)-N(31)-Cu(3)	129.7(3)
N(32)-N(31)-Cu(3)	124.9(2)
C(32)-N(32)-N(31)	106.0(3)
C(32)-N(32)-Cu(1)	137.2(3)
N(31)-N(32)-Cu(1)	116.2(2)
C(31)-N(33)-C(32)	102.0(3)
C(33)-N(34)-C(31)	125.3(3)
C(33)-N(34)-H(34)	117.3
C(31)-N(34)-H(34)	117.3
N(31)-C(31)-N(33)	113.7(3)
N(31)-C(31)-N(34)	122.5(3)
N(33)-C(31)-N(34)	123.8(3)
N(32)-C(32)-N(33)	112.9(4)
N(32)-C(32)-H(32)	123.5
N(33)-C(32)-H(32)	123.5
O(31)-C(33)-N(34)	123.4(3)
O(31)-C(33)-C(34)	119.4(4)
N(34)-C(33)-C(34)	117.2(3)
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-O(31)-Cu(3)	129.7(3)
Cu(2)-O(4)-Cu(3)	114.17(13)
Cu(2)-O(4)-Cu(1)	111.52(11)
Cu(3)-O(4)-Cu(1)	111.63(12)
Cu(2)-O(4)-H(4)	106.3
Cu(3)-O(4)-H(4)	106.3
Cu(1)-O(4)-H(4)	106.3
Cu(2)-O(6)-H(6A)	97(5)

Cu(2)-O(6)-H(6B)	103(5)
H(6A)-O(6)-H(6B)	107(7)
Cu(3)-O(7)-H(7A)	114(5)
Cu(3)-O(7)-H(7B)	100(5)
H(7A)-O(7)-H(7B)	109(7)
H(1W1)-O(1W)-H(2W1)	106(7)
O(53)-N(51)-O(52)	118.4(5)
O(53)-N(51)-O(51)	123.2(5)
O(52)-N(51)-O(51)	118.5(5)
N(51)-O(51)-Cu(1)	115.7(3)
H(1W2)-O(2W)-H(2W2)	111(7)
O(63)-N(61)-O(62)	122.9(5)
O(63)-N(61)-O(61)	117.8(5)
O(62)-N(61)-O(61)	119.2(5)

Table SIX. Bond lengths [Å] and angles [deg] for **3**.

Cu(1)-N(11)	1.898(9)
Cu(1)-N(32)	1.941(9)
Cu(1)-O(11)	1.963(7)
Cu(1)-O(4)	1.963(6)
Cu(2)-N(21)	1.889(9)
Cu(2)-N(12)	1.928(9)
Cu(2)-O(21)	1.961(8)
Cu(2)-O(4)	2.004(6)
Cu(2)-O(6)	2.294(7)
Cu(3)-N(31)	1.920(8)
Cu(3)-N(22)	1.978(8)
Cu(3)-O(31)	1.987(8)
Cu(3)-O(4)	2.014(6)
Cu(3)-O(7)	2.322(7)
Cl(5)-O(54)	1.347(15)
Cl(5)-O(52)	1.369(15)
Cl(5)-O(51)	1.364(14)
Cl(5)-O(53)	1.384(12)
Cl(8)-O(82)	1.342(13)
Cl(8)-O(83)	1.340(14)
Cl(8)-O(84)	1.356(13)
Cl(8)-O(81)	1.368(15)
O(4)-H(4)	0.9800
O(6)-H(6A)	0.961(7)
O(6)-H(6B)	0.963(7)
O(7)-H(7A)	0.972(7)
O(7)-H(7B)	0.955(7)
O(11)-C(13)	1.220(12)
O(21)-C(23)	1.239(12)
O(31)-C(33)	1.214(12)
N(11)-C(11)	1.316(12)
N(11)-N(12)	1.381(10)
N(21)-C(21)	1.295(11)
N(21)-N(22)	1.397(11)
N(31)-C(31)	1.306(12)
N(31)-N(32)	1.355(10)
N(12)-C(12)	1.306(12)
N(22)-C(22)	1.301(12)
N(32)-C(32)	1.320(12)
N(13)-C(11)	1.328(12)
N(13)-C(12)	1.319(12)
N(23)-C(21)	1.293(12)
N(23)-C(22)	1.382(13)
N(33)-C(31)	1.342(12)
N(33)-C(32)	1.346(13)
N(14)-C(13)	1.349(12)
N(14)-C(11)	1.424(12)
N(14)-H(14)	0.8600
N(24)-C(23)	1.333(12)
N(24)-C(21)	1.409(12)
N(24)-H(24)	0.8600
N(34)-C(33)	1.362(13)
N(34)-C(31)	1.388(12)
N(34)-H(34)	0.8600
C(12)-H(12)	0.9300
C(22)-H(22)	0.9300
C(32)-H(32)	0.9300
C(13)-C(14)	1.516(14)
C(23)-C(24)	1.480(14)
C(33)-C(34)	1.489(13)

C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(34)-H(34A)	0.9600
C(34)-H(34B)	0.9600
C(34)-H(34C)	0.9600
N(11)-Cu(1)-N(32)	165.6(4)
N(11)-Cu(1)-O(11)	88.7(3)
N(32)-Cu(1)-O(11)	94.2(4)
N(11)-Cu(1)-O(4)	88.9(3)
N(32)-Cu(1)-O(4)	89.9(3)
O(11)-Cu(1)-O(4)	172.7(3)
N(21)-Cu(2)-N(12)	171.5(4)
N(21)-Cu(2)-O(21)	87.7(4)
N(12)-Cu(2)-O(21)	91.6(4)
N(21)-Cu(2)-O(4)	89.9(3)
N(12)-Cu(2)-O(4)	91.1(3)
O(21)-Cu(2)-O(4)	176.6(3)
N(21)-Cu(2)-O(6)	91.6(3)
N(12)-Cu(2)-O(6)	96.9(3)
O(21)-Cu(2)-O(6)	95.0(3)
O(4)-Cu(2)-O(6)	82.7(3)
N(31)-Cu(3)-N(22)	172.0(4)
N(31)-Cu(3)-O(31)	86.7(3)
N(22)-Cu(3)-O(31)	94.8(3)
N(31)-Cu(3)-O(4)	87.2(3)
N(22)-Cu(3)-O(4)	91.1(3)
O(31)-Cu(3)-O(4)	173.7(3)
N(31)-Cu(3)-O(7)	100.4(3)
N(22)-Cu(3)-O(7)	87.2(3)
O(31)-Cu(3)-O(7)	95.7(3)
O(4)-Cu(3)-O(7)	86.7(3)
O(54)-Cl(5)-O(52)	105.1(9)
O(54)-Cl(5)-O(51)	118.2(9)
O(52)-Cl(5)-O(51)	105.3(9)
O(54)-Cl(5)-O(53)	112.2(8)
O(52)-Cl(5)-O(53)	106.0(8)
O(51)-Cl(5)-O(53)	109.1(8)
O(82)-Cl(8)-O(83)	113.8(9)
O(82)-Cl(8)-O(84)	112.6(8)
O(83)-Cl(8)-O(84)	103.4(8)
O(82)-Cl(8)-O(81)	106.1(9)
O(83)-Cl(8)-O(81)	111.0(9)
O(84)-Cl(8)-O(81)	109.9(9)
Cu(1)-O(4)-Cu(2)	115.8(3)
Cu(1)-O(4)-Cu(3)	117.1(3)
Cu(2)-O(4)-Cu(3)	113.4(3)
Cu(1)-O(4)-H(4)	102.6
Cu(2)-O(4)-H(4)	102.6
Cu(3)-O(4)-H(4)	102.6
Cu(2)-O(6)-H(6A)	110.1(6)
Cu(2)-O(6)-H(6B)	110.0(5)
H(6A)-O(6)-H(6B)	109.2(7)
Cu(3)-O(7)-H(7A)	109.6(5)
Cu(3)-O(7)-H(7B)	110.4(5)
H(7A)-O(7)-H(7B)	108.9(7)
C(13)-O(11)-Cu(1)	129.7(8)
C(23)-O(21)-Cu(2)	127.0(8)
C(33)-O(31)-Cu(3)	133.1(8)
C(11)-N(11)-N(12)	104.5(9)

C(11)-N(11)-Cu(1)	130.0(8)
N(12)-N(11)-Cu(1)	125.4(7)
C(21)-N(21)-N(22)	104.0(9)
C(21)-N(21)-Cu(2)	130.8(8)
N(22)-N(21)-Cu(2)	125.0(7)
C(31)-N(31)-N(32)	105.4(9)
C(31)-N(31)-Cu(3)	129.3(8)
N(32)-N(31)-Cu(3)	125.0(7)
C(12)-N(12)-N(11)	103.7(9)
C(12)-N(12)-Cu(2)	139.1(8)
N(11)-N(12)-Cu(2)	116.8(7)
C(22)-N(22)-N(21)	105.9(9)
C(22)-N(22)-Cu(3)	137.1(9)
N(21)-N(22)-Cu(3)	116.0(6)
C(32)-N(32)-N(31)	106.6(9)
C(32)-N(32)-Cu(1)	134.0(8)
N(31)-N(32)-Cu(1)	118.7(7)
C(11)-N(13)-C(12)	99.5(9)
C(21)-N(23)-C(22)	101.2(10)
C(31)-N(33)-C(32)	101.4(9)
C(13)-N(14)-C(11)	124.0(9)
C(13)-N(14)-H(14)	118.0
C(11)-N(14)-H(14)	118.0
C(23)-N(24)-C(21)	124.9(10)
C(23)-N(24)-H(24)	117.5
C(21)-N(24)-H(24)	117.5
C(33)-N(34)-C(31)	126.4(10)
C(33)-N(34)-H(34)	116.8
C(31)-N(34)-H(34)	116.8
N(11)-C(11)-N(13)	115.4(10)
N(11)-C(11)-N(14)	121.6(10)
N(13)-C(11)-N(14)	123.0(10)
N(21)-C(21)-N(23)	116.8(11)
N(21)-C(21)-N(24)	119.8(10)
N(23)-C(21)-N(24)	123.4(11)
N(31)-C(31)-N(33)	114.2(11)
N(31)-C(31)-N(34)	122.6(11)
N(33)-C(31)-N(34)	123.2(11)
N(12)-C(12)-N(13)	116.8(10)
N(12)-C(12)-H(12)	121.6
N(13)-C(12)-H(12)	121.6
C(11)-C(12)-H(12)	161.8
N(22)-C(22)-N(23)	112.1(11)
N(22)-C(22)-H(22)	124.0
N(23)-C(22)-H(22)	124.0
N(32)-C(32)-N(33)	112.5(10)
N(32)-C(32)-H(32)	123.8
N(33)-C(32)-H(32)	123.8
O(11)-C(13)-N(14)	125.7(11)
O(11)-C(13)-C(14)	122.5(10)
N(14)-C(13)-C(14)	111.7(11)
O(21)-C(23)-N(24)	125.4(11)
O(21)-C(23)-C(24)	121.3(11)
N(24)-C(23)-C(24)	113.3(10)
O(31)-C(33)-N(34)	120.7(11)
O(31)-C(33)-C(34)	122.4(11)
N(34)-C(33)-C(34)	116.8(10)
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(23)-C(24)-H(24A)	109.5

C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5

Table SX. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1**.
 The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	41(1)	42(1)	61(1)	6(1)	-23(1)	-3(1)
Cu(2)	40(1)	36(1)	64(1)	6(1)	-24(1)	-1(1)
Cu(3)	42(1)	32(1)	73(1)	3(1)	-26(1)	4(1)
S(5)	59(2)	60(2)	89(2)	6(2)	-22(2)	7(1)
O(51)	63(5)	153(8)	111(7)	-16(6)	7(5)	-27(6)
O(52)	102(7)	233(12)	42(5)	14(6)	-29(4)	-28(7)
O(53)	196(11)	43(5)	273(14)	-15(7)	-112(10)	-10(6)
C(51)	93(10)	110(11)	100(11)	0(9)	-25(8)	9(9)
F(51)	282(14)	124(8)	192(10)	-51(7)	-91(9)	142(9)
F(52)	106(6)	203(9)	74(5)	2(5)	-41(4)	-2(6)
F(53)	80(6)	301(16)	140(8)	6(8)	-23(6)	22(8)
S(6)	46(2)	147(3)	57(2)	17(2)	-11(1)	21(2)
O(61)	61(4)	105(6)	61(5)	6(4)	-18(3)	22(4)
O(62)	142(9)	197(12)	214(13)	127(11)	-84(9)	-79(9)
O(63)	170(11)	450(2)	74(7)	-5(11)	22(7)	176(14)
C(61)	62(8)	105(11)	159(14)	16(11)	-20(9)	9(8)
F(61)	90(6)	335(16)	146(8)	64(9)	-71(6)	25(8)
F(62)	181(10)	147(9)	343(17)	1(10)	-128(11)	-79(8)
F(63)	66(5)	200(10)	242(13)	44(9)	25(7)	39(6)
O(6)	85(6)	118(7)	102(6)	23(5)	15(5)	-1(5)
O(4)	30(3)	43(3)	60(4)	7(3)	-21(3)	-3(2)
O(7)	54(4)	60(4)	70(5)	11(3)	-17(3)	18(3)
N(11)	38(4)	41(4)	53(4)	4(3)	-19(3)	-5(3)
N(12)	32(3)	38(4)	68(5)	15(4)	-15(3)	-4(3)
N(13)	48(4)	39(4)	79(6)	4(4)	-19(4)	-10(3)
N(14)	34(4)	65(5)	63(5)	0(4)	-22(3)	-9(4)
C(11)	41(5)	45(5)	45(5)	1(4)	-19(4)	-13(4)
C(12)	50(5)	36(5)	82(7)	18(5)	-21(5)	-11(4)
C(13)	43(5)	60(6)	54(6)	3(5)	-18(4)	2(5)
C(14)	54(6)	80(7)	86(8)	-5(6)	-32(6)	18(5)
O(11)	55(4)	49(4)	67(4)	10(3)	-30(3)	-5(3)
N(21)	33(3)	36(4)	59(5)	7(3)	-20(3)	3(3)
N(22)	52(4)	22(3)	70(5)	-1(3)	-27(4)	0(3)
N(23)	50(4)	37(4)	85(6)	-8(4)	-42(4)	12(3)
N(24)	49(4)	29(3)	66(5)	10(3)	-35(4)	-2(3)
C(21)	36(4)	29(4)	56(5)	3(4)	-22(4)	-2(3)
C(22)	48(5)	49(5)	88(7)	-2(5)	-41(5)	0(4)
C(23)	52(5)	26(4)	56(6)	0(4)	-6(5)	-2(4)
C(24)	82(7)	32(5)	84(8)	-2(5)	-24(6)	2(5)
O(21)	62(4)	35(3)	70(4)	3(3)	-29(3)	3(3)
N(31)	45(4)	34(4)	69(5)	4(4)	-20(4)	4(3)
N(32)	32(4)	44(4)	66(5)	10(4)	-23(3)	0(3)
N(33)	74(6)	45(4)	75(6)	6(4)	-30(5)	-1(4)
N(34)	60(5)	33(4)	75(6)	1(4)	-14(4)	2(3)
C(31)	45(5)	34(5)	74(6)	-10(5)	-14(5)	12(4)
C(32)	74(6)	42(5)	74(7)	-1(5)	-48(5)	3(5)
C(33)	41(5)	50(6)	69(6)	-10(5)	-11(5)	1(4)
C(34)	59(6)	73(7)	92(8)	14(6)	-4(6)	-27(6)
O(31)	52(4)	33(3)	82(5)	2(3)	-24(3)	-1(3)

Table SXI. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **2**.
 The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	21(1)	35(1)	32(1)	-20(1)	-2(1)	-2(1)
Cu(2)	20(1)	29(1)	33(1)	-16(1)	-1(1)	-5(1)
Cu(3)	21(1)	33(1)	29(1)	-18(1)	1(1)	-7(1)
N(11)	23(2)	31(2)	31(2)	-15(1)	-2(1)	-6(1)
N(12)	23(2)	31(2)	32(2)	-16(1)	1(1)	-8(1)
N(13)	24(2)	31(2)	41(2)	-13(2)	0(2)	-2(1)
N(14)	18(2)	35(2)	34(2)	-12(2)	-3(1)	-5(1)
C(11)	21(2)	28(2)	29(2)	-9(2)	2(2)	-5(2)
C(12)	30(2)	33(2)	40(2)	-19(2)	-5(2)	-6(2)
C(13)	28(2)	36(2)	29(2)	-8(2)	-4(2)	-15(2)
C(14)	34(2)	58(3)	47(3)	-18(2)	-9(2)	-17(2)
O(11)	25(1)	51(2)	45(2)	-28(2)	-5(1)	-6(1)
N(21)	20(1)	30(2)	28(2)	-17(1)	0(1)	-7(1)
N(22)	24(2)	31(2)	30(2)	-15(1)	2(1)	-8(1)
N(23)	21(2)	36(2)	32(2)	-12(2)	-1(1)	-11(1)
N(24)	26(2)	36(2)	36(2)	-18(2)	2(1)	-14(2)
C(21)	23(2)	32(2)	25(2)	-12(2)	-1(2)	-11(2)
C(22)	23(2)	30(2)	32(2)	-11(2)	3(2)	-6(2)
C(23)	31(2)	30(2)	31(2)	-12(2)	0(2)	-11(2)
C(24)	35(2)	40(2)	49(3)	-26(2)	3(2)	-10(2)
O(21)	28(1)	38(2)	51(2)	-26(1)	-2(1)	-10(1)
N(31)	25(2)	29(2)	29(2)	-16(1)	-1(1)	-2(1)
N(32)	23(2)	38(2)	30(2)	-19(2)	-4(1)	-2(1)
N(33)	29(2)	40(2)	33(2)	-22(2)	-2(2)	-7(2)
N(34)	25(2)	35(2)	34(2)	-24(2)	1(1)	-4(1)
C(31)	24(2)	28(2)	27(2)	-12(2)	0(2)	-3(2)
C(32)	25(2)	42(2)	37(2)	-18(2)	-9(2)	-6(2)
C(33)	25(2)	31(2)	30(2)	-12(2)	3(2)	-8(2)
C(34)	26(2)	44(3)	41(3)	-19(2)	4(2)	-6(2)
O(31)	23(1)	44(2)	44(2)	-28(1)	6(1)	-10(1)
O(4)	22(1)	24(1)	28(1)	-10(1)	-2(1)	-3(1)
O(6)	31(2)	52(2)	36(2)	-13(2)	0(1)	-18(1)
O(7)	36(2)	42(2)	43(2)	-17(2)	-1(2)	-6(2)
O(1W)	45(2)	56(2)	49(2)	-18(2)	0(2)	-26(2)
N(51)	44(2)	52(3)	42(2)	-6(2)	0(2)	-15(2)
O(51)	59(2)	75(3)	53(2)	-11(2)	-2(2)	-32(2)
O(52)	78(3)	113(4)	66(3)	29(3)	-25(2)	-59(3)
O(53)	95(4)	86(3)	81(3)	36(3)	-13(3)	-51(3)
O(2W)	30(2)	121(4)	187(6)	-102(4)	-9(3)	-9(2)
N(61)	36(2)	52(3)	63(3)	-9(2)	4(2)	-18(2)
O(61)	42(2)	96(3)	106(4)	-45(3)	21(2)	-27(2)
O(62)	78(3)	67(3)	108(4)	-39(3)	35(3)	-42(2)
O(63)	47(2)	106(4)	127(4)	-41(3)	-3(3)	-35(2)

Table SXII. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **3**.
 The anisotropic displacement factor exponent takes the form:
 $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	43(1)	44(1)	43(1)	-2(1)	-1(1)	0(1)
Cu(2)	47(1)	40(1)	45(1)	0(1)	-6(1)	-3(1)
Cu(3)	44(1)	38(1)	43(1)	-1(1)	-5(1)	-3(1)
Cl(5)	77(3)	66(2)	56(2)	4(2)	13(2)	-6(2)
Cl(8)	49(2)	85(3)	57(2)	1(2)	0(2)	8(2)
O(4)	32(4)	29(4)	45(5)	0(4)	0(4)	-2(3)
O(6)	34(5)	81(6)	70(6)	26(5)	19(4)	2(5)
O(7)	47(5)	61(6)	53(5)	-10(5)	5(4)	-6(4)
O(11)	74(6)	47(5)	51(6)	-4(5)	-24(5)	12(5)
O(21)	57(6)	49(5)	64(6)	3(5)	-19(5)	-11(4)
O(31)	54(6)	40(5)	59(6)	-9(5)	-4(5)	-9(4)
N(11)	27(5)	52(7)	38(6)	-8(5)	-11(5)	11(5)
N(21)	48(6)	41(6)	37(6)	-6(5)	-3(5)	-3(5)
N(31)	31(5)	28(6)	42(6)	5(5)	-3(5)	-7(4)
N(12)	32(6)	44(7)	46(7)	2(5)	2(5)	-1(5)
N(22)	47(6)	47(6)	39(6)	2(6)	-9(5)	-18(5)
N(32)	23(5)	48(6)	50(6)	2(6)	0(5)	-14(5)
N(13)	43(6)	33(6)	49(6)	-3(5)	-9(5)	10(5)
N(23)	72(8)	47(7)	60(8)	2(6)	-21(6)	-4(6)
N(33)	43(6)	49(7)	59(7)	5(6)	-12(6)	-3(5)
N(14)	49(7)	53(7)	43(7)	13(6)	-15(5)	2(5)
N(24)	56(7)	40(7)	40(6)	-1(5)	-4(5)	4(5)
N(34)	64(7)	37(6)	54(7)	7(6)	-4(6)	-18(5)
C(11)	48(8)	31(7)	48(9)	8(6)	-2(7)	-10(6)
C(21)	44(8)	34(7)	35(7)	0(6)	-7(6)	0(6)
C(31)	31(7)	51(9)	40(8)	-2(6)	10(6)	-4(6)
C(12)	30(7)	51(8)	43(8)	10(7)	6(6)	-17(6)
C(22)	45(8)	83(10)	31(7)	4(8)	-3(6)	6(8)
C(32)	35(8)	58(9)	68(10)	-11(8)	-23(7)	4(7)
C(13)	52(9)	38(8)	47(9)	-15(7)	7(7)	-9(7)
C(23)	39(8)	42(8)	38(8)	-7(7)	27(6)	3(6)
C(33)	29(7)	51(9)	45(8)	7(7)	10(6)	-4(6)

Compound 1

Possible hydrogen bonds

Donor-H	Donor...Acceptor	H...Acceptor	Donor-H.....Acceptor
O4 -H4 0.980(.006) 0.938	O4 ...O51 (0) 2.923(.009)	H4 ...O51 (0) 2.392(.008) 2.409	O4 -H4 ...O51 (0) 113.42(0.35) 114.34 (**)
O4 -H4 0.980(.006) 0.938	O4 ...O6 (0) 2.931(.010)	H4 ...O6 (0) 2.454(.009) 2.469	O4 -H4 ...O6 (0) 109.48(0.36) 110.40 (**)
O4 -H4 0.980(.006) 0.938	O4 ...O7 (0) 3.008(.008)	H4 ...O7 (0) 2.575(.006) 2.587	O4 -H4 ...O7 (0) 106.82(0.33) 107.71 (**)
O7 -H7B 0.963(.006) 0.938	O7 ...O62 (0) 2.908(.014)	H7B ...O62 (0) 1.948(.012) 1.972	O7 -H7B ...O62 (0) 175.39(0.51) 175.44 (**)
N14 -H14 0.860(.007) 1.030	N14 ...O61 (3) 2.807(.010)	H14 ...O61 (3) 1.982(.007) 1.823	N14 -H14 ...O61 (3) 160.16(0.50) 158.35 (**)
O6 -H6B 0.951(.009) 0.938	O6 ...N33 (3) 3.431(.011)	H6B ...N33 (3) 2.491(.008) 2.504	O6 -H6B ...N33 (3) 169.52(0.54) 169.57 (**)
O7 -H7A 0.964(.006) 0.938	O7 ...N13 (4) 2.918(.009)	H7A ...N13 (4) 1.954(.007) 1.980	O7 -H7A ...N13 (4) 178.76(0.41) 178.78 (**)
N34 -H34 0.860(.007) 1.030	N34 ...O53 (4) 2.779(.011)	H34 ...O53 (4) 1.984(.009) 1.834	N34 -H34 ...O53 (4) 153.21(0.52) 150.82 (**)
N24 -H24 0.860(.006) 1.030	N24 ...N23 (7) 2.902(.009)	H24 ...N23 (7) 2.051(.007) 1.884	N24 -H24 ...N23 (7) 170.25(0.48) 169.37 (**)

Equivalent positions:

- (0) x, y, z
- (1) -x+1, -y, -z+2
- (2) x, -y+1/2, +z+1/2
- (3) -x+1, +y-1/2, -z+1/2+1
- (4) -x+1, +y+1/2, -z+1/2+1
- (5) x, -y+1/2, +z-1/2
- (6) x-1, -y+1/2, +z-1/2
- (7) -x+2, -y, -z+2
- (8) -x+2, -y+1, -z+2

Compound 2

Possible hydrogen bonds

Donor-H	Donor...Acceptor	H...Acceptor	Donor-H.....Acceptor
O4 -H4 0.980(.003) 0.938	O4 ...O62 (0) 2.768(.006)	H4 ...O62 (0) 1.979(.005) 2.009	O4 -H4 ...O62 (0) 135.90(0.21) 136.73 (**)
O6 -H6B 0.811(.033) 0.938	O6 ...O1W (0) 2.800(.004)	H6B ...O1W (0) 1.992(.033) 1.865	O6 -H6B ...O1W (0) 174.47(3.39) 174.10 (**)
O7 -H7B 0.821(.059) 0.938	O7 ...O61 (0) 2.685(.006)	H7B ...O61 (0) 1.871(.066) 1.755	O7 -H7B ...O61 (0) 171.26(5.66) 170.68 (**)
O1W -H2W1 0.804(.035) 0.938	O1W ...O7 (0) 2.741(.005)	H2W1 ...O7 (0) 1.949(.042) 1.817	O1W -H2W1 ...O7 (0) 168.43(3.21) 167.58 (**)
O2W -H1W2 0.810(.078) 0.938	O2W ...O53 (0) 3.022(.009)	H1W2 ...O53 (0) 2.213(.079) 2.085	O2W -H1W2 ...O53 (0) 177.31(6.49) 177.15 (**)
N14 -H14 0.860(.003) 1.030	N14 ...O2W (1) 2.705(.005)	H14 ...O2W (1) 1.853(.004) 1.686	N14 -H14 ...O2W (1) 170.40(0.29) 169.44 (**)
N24 -H24 0.860(.004) 1.030	N24 ...O1W (2) 2.793(.006)	H24 ...O1W (2) 1.941(.005) 1.774	N24 -H24 ...O1W (2) 170.38(0.27) 169.47 (**)
O6 -H6A 0.798(.081) 0.938	O6 ...N23 (2) 2.943(.005)	H6A ...N23 (2) 2.229(.074) 2.111	O6 -H6A ...N23 (2) 149.18(6.56) 147.23 (**)
O2W -H2W2 0.817(.058) 0.938	O2W ...O61 (4) 2.707(.008)	H2W2 ...O61 (4) 1.903(.060) 1.785	O2W -H2W2 ...O61 (4) 167.72(6.24) 166.90 (**)
N34 -H34 0.860(.003) 1.030	N34 ...N33 (6) 2.852(.005)	H34 ...N33 (6) 1.999(.004) 1.831	N34 -H34 ...N33 (6) 171.67(0.24) 170.90 (**)
O7 -H7A 0.808(.047) 0.938	O7 ...N13 (8) 2.817(.004)	H7A ...N13 (8) 2.019(.043) 1.892	O7 -H7A ...N13 (8) 169.15(4.76) 168.41 (**)

(**) Values normalized following G.A.Jeffrey & L.Lewis, Carbohydr.Res. (1978).60,179; R.Taylor, O.Kennard, Acta Cryst.(1983).B39,133.

Equivalent positions:

- (0) x,y,z
- (1) x+1,+y,+z
- (2) -x,-y,-z
- (3) x-1,+y,+z
- (4) x,+y-1,+z
- (5) -x+1,-y,-z
- (6) -x,-y+1,-z+1
- (7) -x+1,-y,-z+1
- (8) x-1,+y+1,+z
- (9) -x,-y,-z+1
- (10) -x,-y+1,-z

Compound 3

Possible hydrogen bonds

Donor-H	Donor...Acceptor	H...Acceptor	Donor-H.....Acceptor
O4 -H4 0.980(.006) 0.938	O4 ...O6 (0) 2.849(.009)	H4 ...O6 (0) 2.337(.007) 2.352	O4 -H4 ...O6 (0) 111.75(0.38) 112.71 (**)
O4 -H4 0.980(.006) 0.938	O4 ...O7 (0) 2.985(.009)	H4 ...O7 (0) 2.499(.007) 2.514	O4 -H4 ...O7 (0) 110.38(0.38) 111.28 (**)
O4 -H4 0.980(.006) 0.938	O4 ...O51 (0) 2.965(.015)	H4 ...O51 (0) 2.310(.014) 2.333	O4 -H4 ...O51 (0) 123.49(0.50) 124.35 (**)
O7 -H7B 0.955(.007) 0.938	O7 ...O84 (1) 3.226(.015)	H7B ...O84 (1) 2.276(.013) 2.294	O7 -H7B ...O84 (1) 172.70(0.53) 172.75 (**)
O6 -H6A 0.961(.007) 0.938	O6 ...N33 (1) 2.988(.011)	H6A ...N33 (1) 2.331(.009) 2.344	O6 -H6A ...N33 (1) 124.97(0.47) 125.43 (**)
O6 -H6B 0.963(.008) 0.938	O6 ...N33 (3) 2.919(.012)	H6B ...N33 (3) 1.980(.010) 2.004	O6 -H6B ...N33 (3) 164.34(0.53) 164.53 (**)
O7 -H7A 0.972(.007) 0.938	O7 ...N13 (4) 2.810(.011)	H7A ...N13 (4) 1.850(.009) 1.883	O7 -H7A ...N13 (4) 168.79(0.49) 168.99 (**)
N34 -H34 0.860(.009) 1.030	N34 ...O52 (4) 3.132(.018)	H34 ...O52 (4) 2.403(.016) 2.270	N34 -H34 ...O52 (4) 142.85(0.71) 140.26 (**)
N34 -H34 0.860(.009) 1.030	N34 ...O54 (4) 3.363(.017)	H34 ...O54 (4) 2.536(.015) 2.375	N34 -H34 ...O54 (4) 161.75(0.69) 160.47 (**)
N14 -H14 0.860(.009) 1.030	N14 ...O81 (5) 3.064(.017)	H14 ...O81 (5) 2.280(.015) 2.131	N14 -H14 ...O81 (5) 151.70(0.69) 149.53 (**)
N24 -H24 0.860(.009) 1.030	N24 ...N23 (6) 2.828(.013)	H24 ...N23 (6) 1.979(.010) 1.812	N24 -H24 ...N23 (6) 169.19(0.65) 168.18 (**)

(**) Values normalized following G.A.Jeffrey & L.Lewis, Carbohydr.Res. (1978).60,179; R.Taylor, O.Kennard, Acta Cryst.(1983).B39,133.

Equivalent positions:

- (0) x, y, z
- (1) x+1/2, -y+1/2, +z
- (2) -x+2, -y+1, -z
- (3) -x+1/2+1, +y+1/2, -z
- (4) -x+1/2+1, +y-1/2, -z
- (5) -x+1, -y+1, -z
- (6) -x+2, -y+1, -z+1
- (7) x, +y, +z+1
- (8) x-1/2, -y+1/2, +z
- (9) x, +y, +z-1
- (10) -x+1/2+1, +y-1/2, -z+1