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ELECTRONIC SUPPLEMENTARY INFORMATION

Cu^{II}-PDC-bpe frameworks (PDC=2,5-pyridinedicarboxylate, bpe=1,2-di(4-pyridyl)ethylene): mapping of herringbone-type structures

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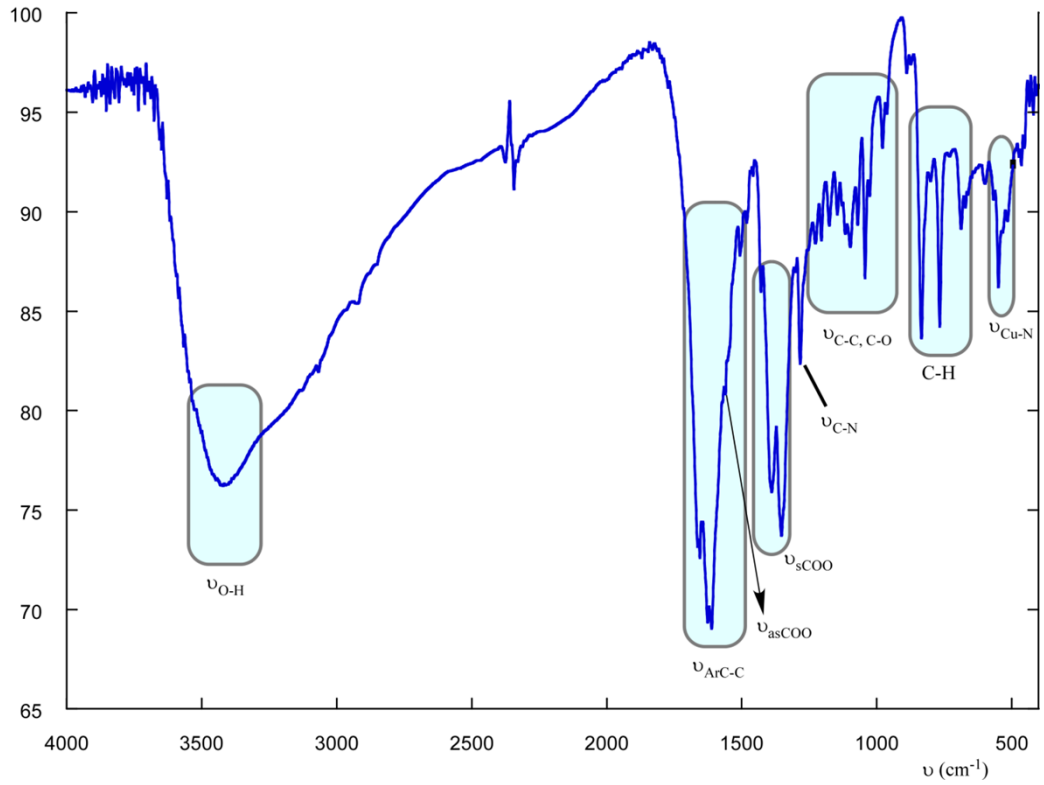


Fig. S1. IR spectra for compound **1**. The following bands (cm^{-1}) are marked: 3415 (OH), 1656 and 1608 (aroC-C), 1286 (C-N), 1561 (asCOO), 1428, 1387 and 1352 (sCOO), 833, 770 and 692 (C-H) and 550-534 (Cu-N).

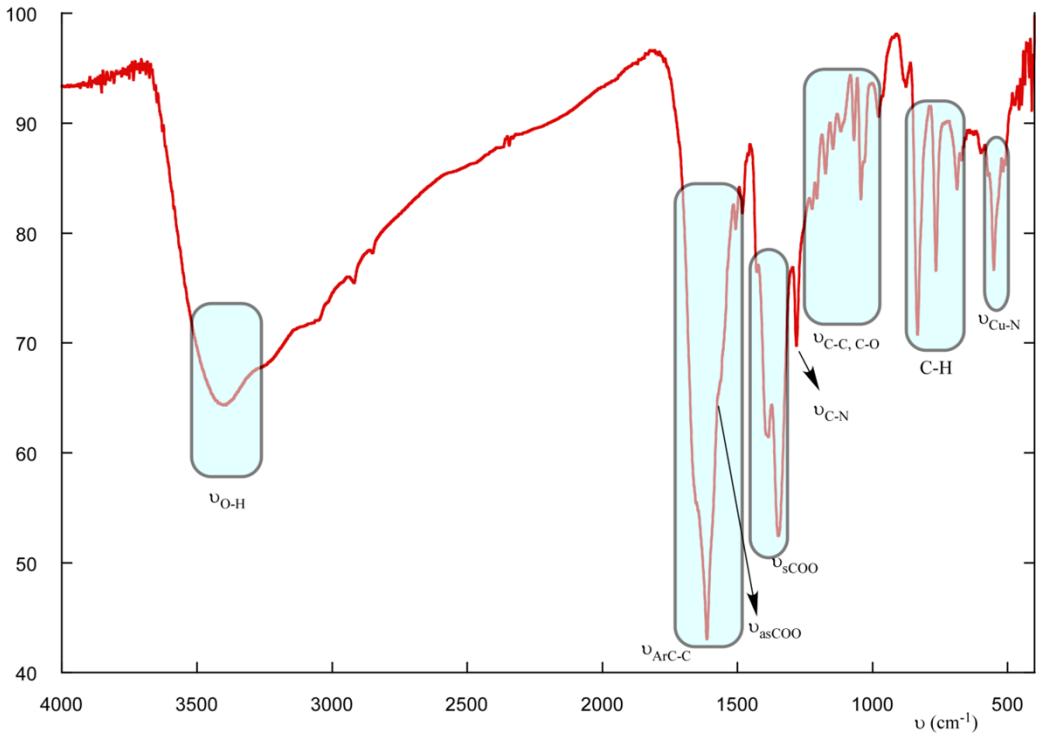


Fig. S2. IR spectra for compound **2**. The following bands (cm^{-1}) are marked: 3410 (OH), 1656 and 1617 (aroC-C), 1281 (C-N), 1569-1560 (asCOO), 1428, 1390 and 1348 (sCOO), 834, 765 and 687 (C-H) and 551-534 (Cu-N).

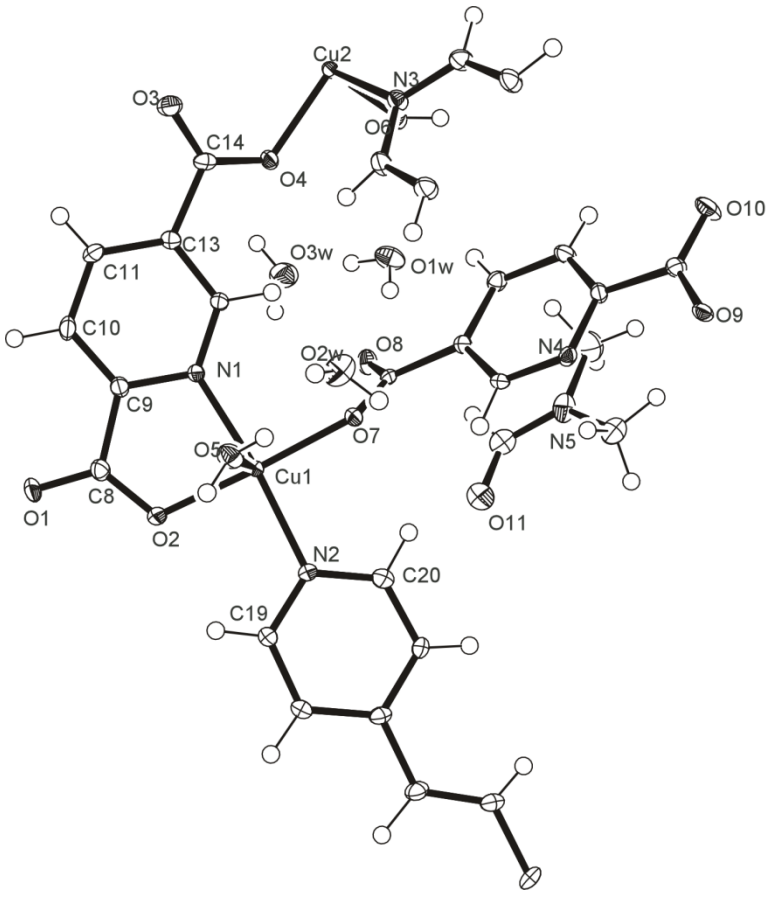


Fig. S3. Thermal ellipsoid plot (50% of probability) for compound **1.**

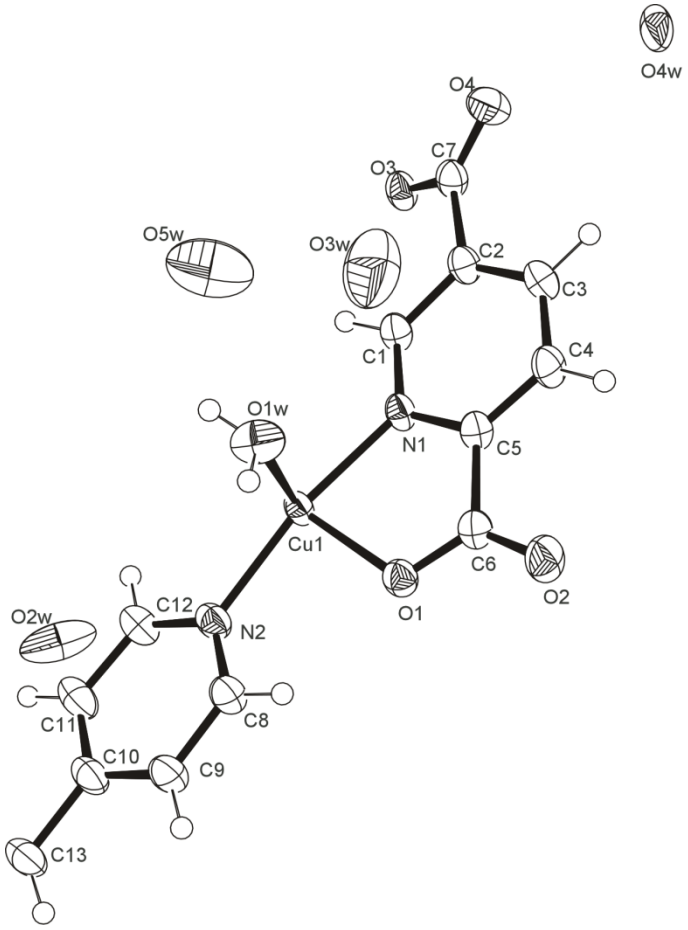


Fig. S4. Thermal ellipsoid plot (50% of probability) for compound **2**.

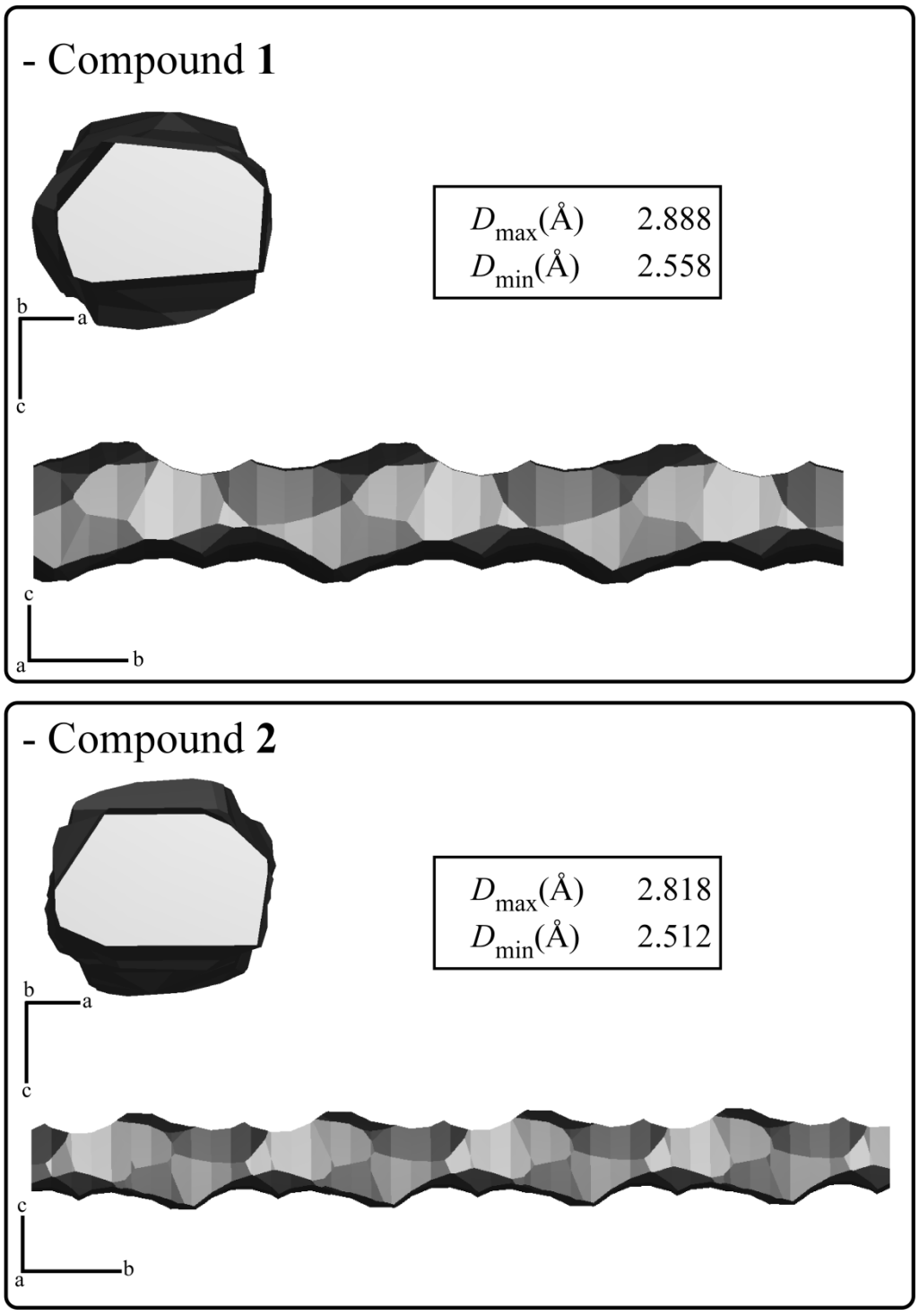
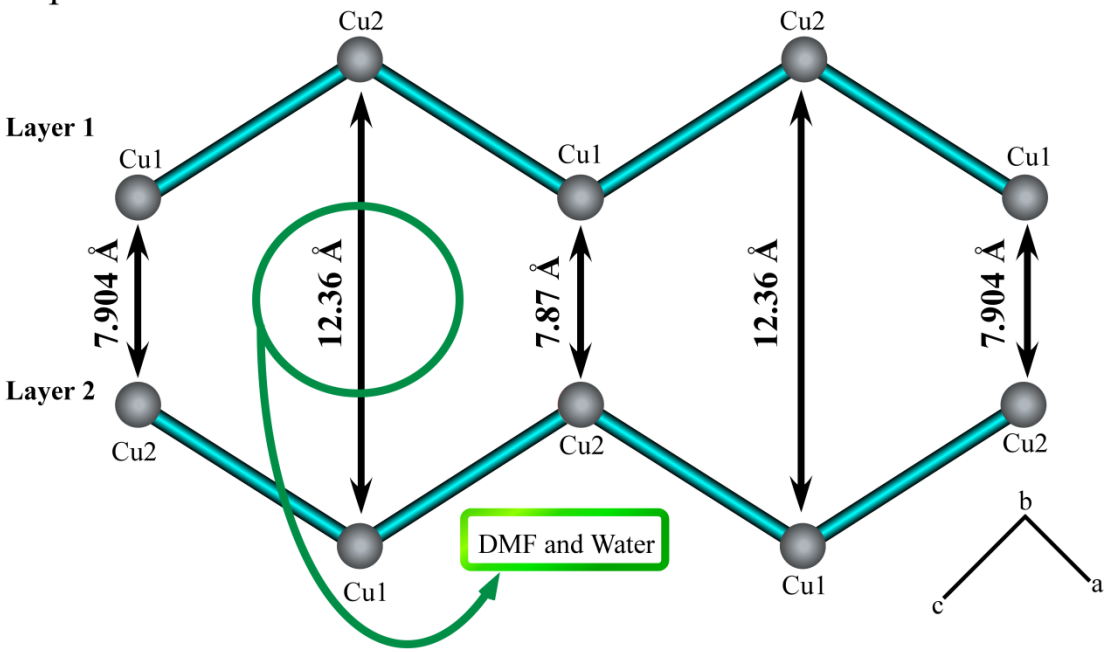


Fig. S5. Voronoi-Dirichlet representations for the channels observed for compounds **1** and **2**.

Compound **1**



Compound **2**

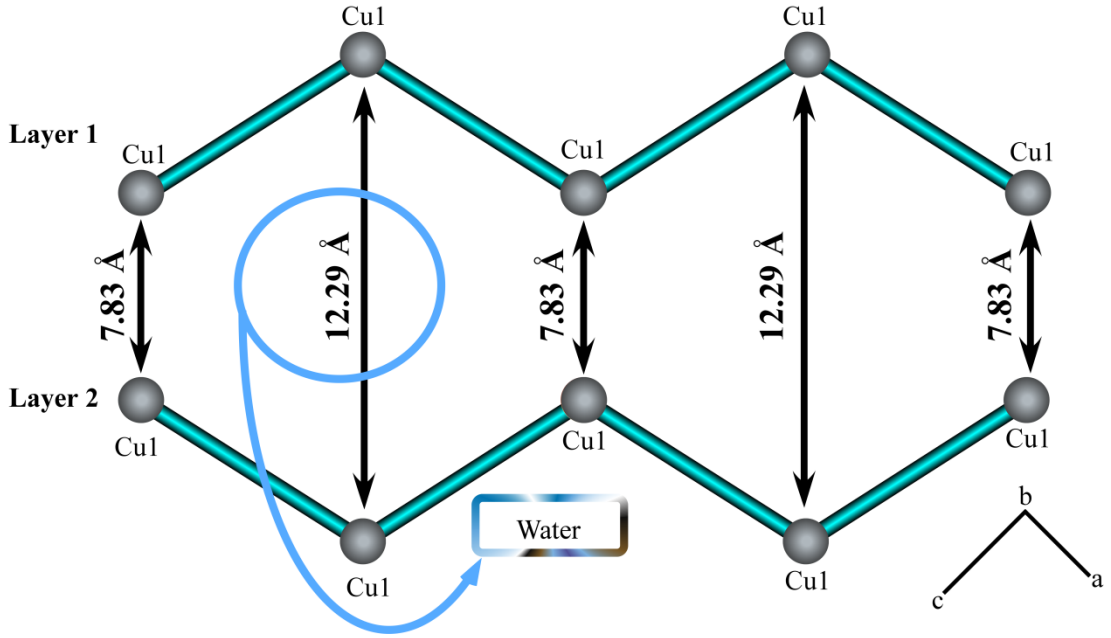


Fig. S6. Interlayer distances for compounds **1** and **2**.

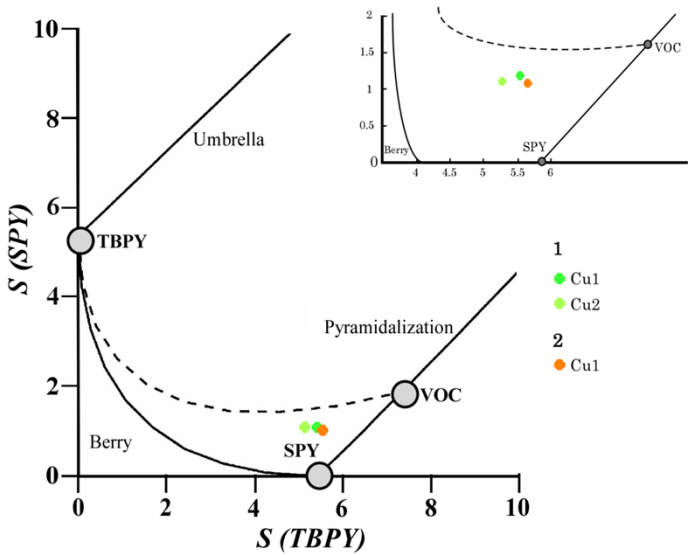


Fig. S7. Distortion modes diagram of a pyramidal based squared coordination environment. In the upper right is a zoom of the distortion for for compound **1** Cu1(green) and Cu2 (green light), and for compound **2** Cu1 (orange).

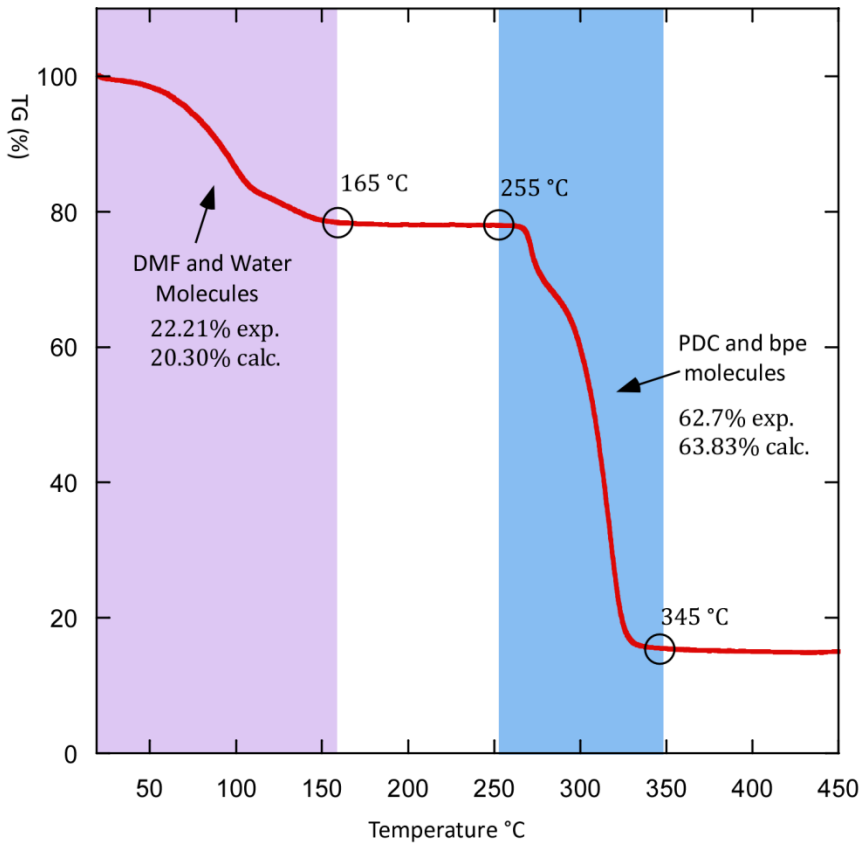


Fig. S8. Thermogravimetric analysis for compound **1**. Purple and blue ranges show the weight loss intervals.

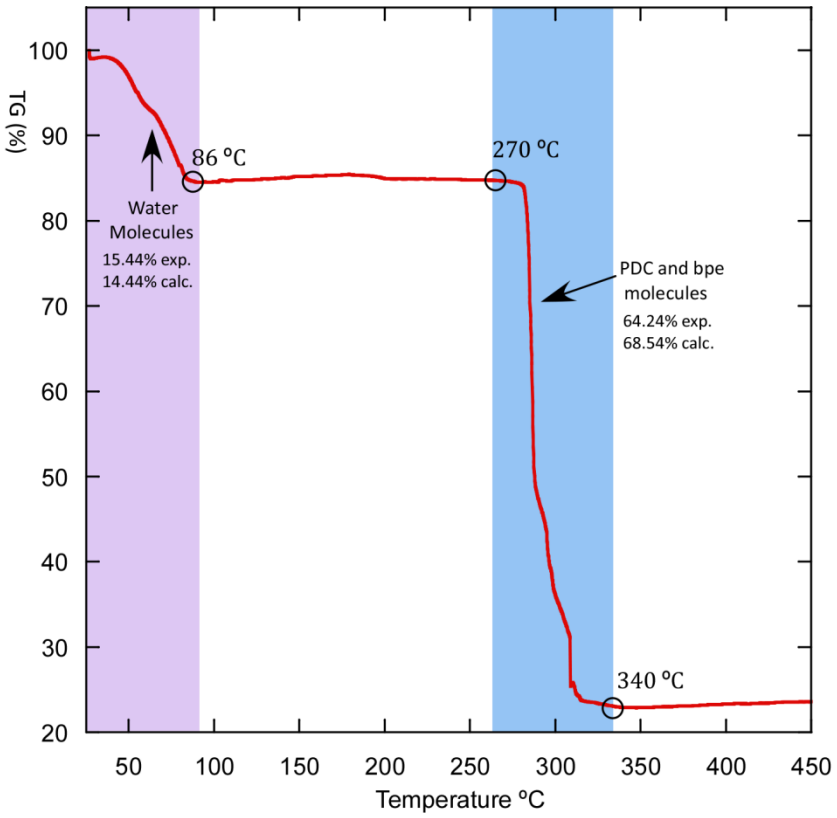


Fig. S9. Thermogravimetric analysis for compound **2**. Purple and blue ranges show the weight loss intervals.

Table S1. Selected bond angles (º) and distances (Å) for compound **1** (distances in bold).

Cu1	O2	O7	O5	N1	N2
N2	91.10(12)	91.38(12)	98.92(12)	170.03(14)	**2.030(3)**
N1	82.29(13)	95.26(12)	88.46(12)	**2.018(3)**	
O5	88.91(12)	90.66(11)	**2.259(3)**		
O7	177.53(12)	**1.947(3)**			
O2	**1.948(3)**				

Cu2	O4	$O9^{iii}$	O6	$N4^{iii}$	N3
N3	92.03(12)	92.04(12)	98.71(12)	169.05(14)	**2.034(3)**
$N4^{iii}$	94.16(12)	81.63(13)	89.95(12)	**2.024(3)**	
O6	93.33(11)	87.32(11)	**2.216(3)**		
$O9^{iii}$	175.74(12)	**1.970(3)**			
O4	**1.942(3)**				

iii) x,y-1,z

Table S2. Selected bond angles (º) and distances (Å) for compound **2** (distances in bold).

Cu1	O1	O1W	$O3^{i}$	N1	N2
N2	91.28(11)	98.73(11)	91.96(11)	170.25(11)	**2.027(3)**
N1	81.98(10)	88.17(11)	94.64(10)	**2.010(3)**	
$O3^{i}$	176.48(9)	92.45(11)	**1.943(2)**		
O1W	88.43(11)	**2.245(3)**			
O1	**1.960(2)**				

i) -x+1/2,y-1/2,-z+3/2

Table S3 Details of the crystal data, structural resolution in $P2_1/n$ space group and refinement procedure for compound **1**.

Compounds	**1**
Formula	$C_{14.5}H_{16.5}N_{2.5}O_7Cu$
FW, g·mol^{-1}	401.34
Crystal system	Monoclinic
S.G, (nº)	$P2_1/n$, (15)
a, Å	11.4682(2)
b, Å	8.8977(1)
c, Å	15.6872(2)
β, °	94.074(1)
V, Å^3,	1596.69(1)
Z, F(000)	4, 852
ρ_{obs}, ρ_{cal}, g·cm^{-3}	1.68(5), 1.66
μ, mm^{-1},	2.374
Crystal size, mm	0.096 x 0.064 x 0.035
Radiation, λ, Å	1.54184
Temperature, K	100(10)
Reflections collected, unique	11534, 3201 (R_{int} = 0.028)
Limiting indices	-14<=h<=12 -10<=k<=11 -17<=l<=19
Final R indices [I > 2σ(I)][a]	R1 = 0.1101, wR2 = 0.3149
R indices (all data)[a]	R1 = 0.1123, wR2 = 0.3160
Goodness of fit on F^2	1.206
Parameters /restraints	223 / 0
L. Diff. peak and hole (e Å^{-3})	1.149, -1.509

Table S4. Interlayer Hydrogen bounds for compound **1**.

O-H	**A(O)**	**O-H(Å)**	**H···A (Å)**	**O···A (Å)**	**O-H···A (°)**
O(1w)-H(34)	O(8)	0.83(4)	1.92(4)	2.739(4)	168(4)
O(1w)-H(35)	O(3w)	0.83(4)	1.81(4)	2.630(4)	166(5)
O(2w)-H(36)	O(1w)	0.82(4)	1.98(4)	2.799(4)	174(4)
O(2w)-H(37)	O(3)	0.82(3)	1.94(3)	2.756(3)	171(4)
O(3w)-H(39)	O(9)	0.82(4)	2.57(4)	3.25(3)	141(4)
O(3w)-H(39)	O(10)	0.82(4)	1.95(4)	2.740(4)	162(4)
O(5)-H(5w)	O(10)	0.82(3)	2.04(4)	2.845(3)	166(5)
C(28)-H(28)	O(2w)	0.99(3)	2.38(3)	3.292(5)	151(2)
O(3w)-H(38)	O(11)	0.830(17)	1.921(15)	2.749(4)	175(5)
C(20)-H(20)	O(11)	0.88(4)	2.72(4)	3.346(5)	121(3)
C(15)-H(15)	O(11)	0.94(3)	2.546(4)	3.198(5)	126(3)
C(18)-H(18)	O(11)	0.91(3)	2.745(3)	3.303(5)	120(2)

Table S5. Interlayer Hydrogen bounds for compound **2**.

O-H	**A(O)**	**O-H(Å)**	**H···A (Å)**	**O···A (Å)**	**O-H···A (°)**
O(1w)-H(1A)	O(4w) x,-1+y,z	0.81(4)	1.97(4)	2.751(9)	160(4)
O(1w)-H(1A)	O(5w)	0.81(4)	2.38(5)	2.74(1)	109(4)
O(1w)-H(1B)	O(2) -1/2-x,-1/2+y,3/2-z	0.82(3)	1.91(4)	2.715(4)	171(5)

Table S6. Bond distances (Å) and angles (°) for compound **1**

Distances

C(1)-O(8)	1.230(5)
C(1)-O(7)	1.271(5)
C(1)-C(2)	1.520(5)
C(2)-C(4)	1.397(6)
C(2)-C(3)	1.404(5)
C(3)-N(4)	1.326(5)
C(4)-C(5)	1.390(6)
C(5)-C(6)	1.383(5)
C(6)-N(4)	1.335(5)
C(6)-C(7)	1.525(5)
C(7)-O(10)	1.227(5)
C(7)-O(9)	1.279(5)
C(8)-O(1)	1.235(5)
C(8)-O(2)	1.283(5)
C(8)-C(9)	1.499(5)
C(9)-N(1)	1.369(5)
C(9)-C(10)	1.382(5)
C(10)-C(11)	1.393(6)
C(11)-C(13)	1.383(6)
C(12)-N(1)	1.332(5)
C(12)-C(13)	1.384(5)
C(13)-C(14)	1.511(5)
C(14)-O(3)	1.243(5)
C(14)-O(4)	1.269(5)
C(15)-N(3)	1.346(5)
C(15)-C(18)	1.376(5)
C(16)-N(3)	1.355(5)
C(16)-C(17)	1.367(6)
C(17)-C(26)^{i}	1.393(6)
C(18)-C(26)^{i}	1.394(6)
C(19)-N(2)	1.335(5)
C(19)-C(22)	1.395(5)
C(20)-N(2)	1.336(5)
C(20)-C(21)	1.384(6)
C(21)-C(23)	1.386(6)
C(22)-C(23)	1.395(6)
C(23)-C(24)	1.464(5)
C(24)-C(25)	1.335(4)
C(25)-C(26)	1.476(5)
C(26)-C(17)^{ii}	1.393(6)
C(26)-C(18)^{ii}	1.394(6)
C(27)-O(11)	1.232(5)
C(27)-N(5)	1.323(5)
C(28)-N(5)	1.449(5)
C(29)-N(5)	1.450(5)
Cu(1)-O(7)	1.947(3)
Cu(1)-O(2)	1.948(3)
Cu(1)-N(1)	2.018(3)
Cu(1)-N(2)	2.030(3)
Cu(1)-O(5)	2.259(3)
Cu(2)-O(4)	1.942(3)
Cu(2)-O(9)^{iii}	1.970(3)
Cu(2)-N(4)^{iii}	2.024(3)
Cu(2)-N(3)	2.034(3)
Cu(2)-O(6)	2.216(3)
N(4)-Cu(2)^{iv}	2.024(3)
O(9)-Cu(2)^{iv}	1.970(3)

Angles

O(8)-C(1)-O(7)	126.9(4)
O(8)-C(1)-C(2)	120.5(3)
O(7)-C(1)-C(2)	112.6(3)
C(4)-C(2)-C(3)	118.5(3)
C(4)-C(2)-C(1)	123.1(3)
C(3)-C(2)-C(1)	118.3(3)
N(4)-C(3)-C(2)	121.6(4)
C(5)-C(4)-C(2)	119.1(3)
C(6)-C(5)-C(4)	118.2(4)
N(4)-C(6)-C(5)	123.0(4)
N(4)-C(6)-C(7)	114.3(3)
C(5)-C(6)-C(7)	122.7(4)
O(10)-C(7)-O(9)	125.7(4)
O(10)-C(7)-C(6)	119.6(3)
O(9)-C(7)-C(6)	114.7(3)
O(1)-C(8)-O(2)	124.4(4)
O(1)-C(8)-C(9)	119.5(4)
O(2)-C(8)-C(9)	116.1(3)
N(1)-C(9)-C(10)	121.3(4)
N(1)-C(9)-C(8)	113.3(3)
C(10)-C(9)-C(8)	125.4(4)
C(9)-C(10)-C(11)	119.2(4)
C(13)-C(11)-C(10)	119.3(4)
N(1)-C(12)-C(13)	123.3(4)
C(11)-C(13)-C(12)	118.3(4)
C(11)-C(13)-C(14)	123.6(4)
C(12)-C(13)-C(14)	118.1(3)
O(3)-C(14)-O(4)	126.3(4)
O(3)-C(14)-C(13)	119.2(4)
O(4)-C(14)-C(13)	114.4(3)
N(3)-C(15)-C(18)	122.8(4)
N(3)-C(16)-C(17)	124.0(4)
C(16)-C(17)-C(26)^{i}	119.3(4)
C(15)-C(18)-C(26)^{i}	120.2(4)
N(2)-C(19)-C(22)	122.7(4)
N(2)-C(20)-C(21)	123.1(4)
C(20)-C(21)-C(23)	120.0(4)
C(19)-C(22)-C(23)	119.7(4)
C(21)-C(23)-C(22)	116.8(4)
C(21)-C(23)-C(24)	122.7(4)
C(22)-C(23)-C(24)	120.4(4)
C(25)-C(24)-C(23)	124.5(3)
C(24)-C(25)-C(26)	125.3(4)
C(17)#2-C(26)-C(18^{ii}	117.1(4)
C(17)#2-C(26)-C(25)	123.4(4)
C(18)#2-C(26)-C(25)	119.5(4)
O(11)-C(27)-N(5)	122.5(4)
O(7)-Cu(1)-O(2)	177.53(12)
O(7)-Cu(1)-N(1)	95.26(12)
O(2)-Cu(1)-N(1)	82.29(13)
O(7)-Cu(1)-N(2)	91.38(12)
O(2)-Cu(1)-N(2)	91.10(12)
N(1)-Cu(1)-N(2)	170.03(14)
O(7)-Cu(1)-O(5)	90.66(11)
O(2)-Cu(1)-O(5)	88.91(12)
N(1)-Cu(1)-O(5)	88.46(12)
N(2)-Cu(1)-O(5)	98.92(12)
O(4)-Cu(2)-O(9)^{iii}	175.74(12)

O(4)-Cu(2)-N(4)^{iii}	94.16(12)	**C(20)-N(2)-Cu(1)**	121.0(3)
O(9)#3-Cu(2)-N(4)^{iii}	81.63(13)	**C(15)-N(3)-C(16)**	116.5(3)
O(4)-Cu(2)-N(3)	92.03(12)	**C(15)-N(3)-Cu(2)**	122.1(3)
O(9)#3-Cu(2)-N(3)	92.04(12)	**C(16)-N(3)-Cu(2)**	121.3(3)
N(4)#3-Cu(2)-N(3)	169.05(14)	**C(3)-N(4)-C(6)**	119.6(3)
O(4)-Cu(2)-O(6)	93.33(11)	**C(3)-N(4)-Cu(2)^{iv}**	128.0(3)
O(9)#3-Cu(2)-O(6)	87.32(11)	**C(6)-N(4)-Cu(2)^{iv}**	111.7(3)
N(4)#3-Cu(2)-O(6)	89.95(12)	**C(27)-N(5)-C(28)**	121.3(3)
N(3)-Cu(2)-O(6)	98.71(12)	**C(27)-N(5)-C(29)**	123.8(3)
C(12)-N(1)-C(9)	118.4(3)	**C(28)-N(5)-C(29)**	114.9(3)
C(12)-N(1)-Cu(1)	129.6(3)	**C(8)-O(2)-Cu(1)**	115.0(3)
C(9)-N(1)-Cu(1)	110.6(3)	**C(14)-O(4)-Cu(2)**	123.6(3)
C(19)-N(2)-C(20)	117.7(3)	**C(1)-O(7)-Cu(1)**	128.9(3)
C(19)-N(2)-Cu(1)	121.3(3)	**C(7)-O(9)-Cu(2)^{iv}**	115.7(2)

Symmetry codes: i) x-1/2,-y+1,z+1/2; ii) x+1/2,-y+1,z-1/2; iii) x,y-1,z; iv) x,y+1,z

Table S7. Bond distances (Å) and angles (°) for compound **2.**

Distances	
Cu(1)-O(3)^{i}	1.943(2)
Cu(1)-O(1)	1.960(2)
Cu(1)-N(1)	2.010(3)
Cu(1)-N(2)	2.027(3)
Cu(1)-O(1W)	2.245(3)
C(1)-N(1)	1.326(4)
C(1)-C(2)	1.391(5)
C(1)-H(1)	0.9500
C(2)-C(3)	1.384(5)
C(2)-C(7)	1.508(5)
C(3)-C(4)	1.396(5)
C(3)-H(3)	0.9500
C(4)-C(5)	1.371(5)
C(4)-H(4)	0.9500
C(5)-N(1)	1.350(4)
C(5)-C(6)	1.509(5)
C(6)-O(2)	1.230(4)
C(6)-O(1)	1.279(4)
C(7)-O(4)	1.232(4)
C(7)-O(3)	1.275(4)
C(8)-N(2)	1.335(5)
C(8)-C(9)	1.390(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.403(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.390(6)
C(10)-C(13)	1.471(5)
C(11)-C(12)	1.377(5)
C(11)-H(11)	0.9500
C(12)-N(2)	1.353(5)
C(12)-H(12)	0.9500
C(13)-C(13)^{ii}	1.326(8)
C(13)-H(13)	0.9500
O(3)-Cu(1)^{iii}	1.943(2)
O(1W)-H(1B)	0.819(10)
O(1W)-H(1A)	0.816(10)

Angles			
O(3)^{i}-Cu(1)-O(1)	176.48(9)	**N(1)-C(5)-C(4)**	121.8(3)
O(3)^{i}-Cu(1)-N(1)	94.64(10)	**N(1)-C(5)-C(6)**	113.4(3)
O(1)-Cu(1)-N(1)	81.98(10)	**C(4)-C(5)-C(6)**	124.7(3)
O(3)^{i}-Cu(1)-N(2)	91.96(11)	**O(2)-C(6)-O(1)**	124.3(3)
O(1)-Cu(1)-N(2)	91.28(11)	**O(2)-C(6)-C(5)**	120.0(3)
N(1)-Cu(1)-N(2)	170.25(11)	**O(1)-C(6)-C(5)**	115.8(3)
O(3)^{i}-Cu(1)-O(1W)	92.45(11)	**O(4)-C(7)-O(3)**	126.2(3)
O(1)-Cu(1)-O(1W)	88.43(11)	**O(4)-C(7)-C(2)**	120.6(3)
N(1)-Cu(1)-O(1W)	88.17(11)	**O(3)-C(7)-C(2)**	113.3(3)
N(2)-Cu(1)-O(1W)	98.73(11)	**N(2)-C(8)-C(9)**	122.6(4)
N(1)-C(1)-C(2)	122.7(3)	**N(2)-C(8)-H(8)**	118.7
N(1)-C(1)-H(1)	118.6	**C(9)-C(8)-H(8)**	118.7
C(2)-C(1)-H(1)	118.6	**C(8)-C(9)-C(10)**	119.8(4)
C(3)-C(2)-C(1)	118.2(3)	**C(8)-C(9)-H(9)**	120.1
C(3)-C(2)-C(7)	123.2(3)	**C(10)-C(9)-H(9)**	120.1
C(1)-C(2)-C(7)	118.6(3)	**C(11)-C(10)-C(9)**	117.0(3)
C(2)-C(3)-C(4)	119.0(3)	**C(11)-C(10)-C(13)**	122.9(4)
C(2)-C(3)-H(3)	120.5	**C(9)-C(10)-C(13)**	120.2(4)
C(4)-C(3)-H(3)	120.5	**C(12)-C(11)-C(10)**	119.9(4)
C(5)-C(4)-C(3)	119.1(3)	**C(12)-C(11)-H(11)**	120.0
C(5)-C(4)-H(4)	120.4	**C(10)-C(11)-H(11)**	120.0
C(3)-C(4)-H(4)	120.4	**N(2)-C(12)-C(11)**	122.9(4)

N(2)-C(12)-H(12)	118.5	**C(8)-N(2)-C(12)**	117.8(3)
C(11)-C(12)-H(12)	118.5	**C(8)-N(2)-Cu(1)**	121.2(2)
C(13)^{ii}-C(13)-C(10)	124.8(5)	**C(12)-N(2)-Cu(1)**	121.0(2)
C(13)^{ii}-C(13)-H(13)	117.6	**C(6)-O(1)-Cu(1)**	115.1(2)
C(10)-C(13)-H(13)	117.6	**C(7)-O(3)-Cu(1)^{iii}**	127.3(2)
C(1)-N(1)-C(5)	119.1(3)	**Cu(1)-O(1W)-H(1B)**	114(4)
C(1)-N(1)-Cu(1)	128.5(2)	**Cu(1)-O(1W)-H(1A)**	107(4)
C(5)-N(1)-Cu(1)	111.7(2)	**H(1B)-O(1W)-H(1A)**	111(3)

Symmetry codes: i) -x+1/2,y-1/2,-z+3/2; ii) -x,-y,-z+2; iii) -x+1/2,y+1/2,-z+3/2

Table S8. Atomic coordinates (x·10^4) and equivalent isotropic displacement parameters of compound **1**.

	X	**Y**	**Z**	**U(eq)**
C(1)	2496(3)	698(4)	4919(3)	11(1)
C(2)	1434(3)	1389(4)	5295(2)	12(1)
C(3)	1553(3)	2811(4)	5679(2)	11(1)
C(4)	342(4)	687(4)	5264(3)	14(1)
C(5)	-576(3)	1396(4)	5635(3)	15(1)
C(6)	-373(3)	2795(4)	6000(2)	12(1)
C(7)	-1310(3)	3667(4)	6435(2)	13(1)
C(8)	6948(3)	-1194(4)	5131(2)	15(1)
C(9)	6006(3)	-2112(4)	5497(2)	13(1)
C(10)	6173(3)	-3471(4)	5914(3)	17(1)
C(11)	5220(4)	-4185(4)	6241(3)	14(1)
C(12)	4015(3)	-2203(4)	5670(2)	13(1)
C(13)	4121(3)	-3554(4)	6107(2)	11(1)
C(14)	3030(4)	-4240(4)	6430(3)	13(1)
C(15)	-633(3)	-1919(4)	7309(2)	16(1)
C(16)	1260(3)	-1327(4)	7050(3)	16(1)
C(17)	1198(4)	32(5)	7450(3)	18(1)
C(18)	-768(4)	-558(4)	7707(3)	18(1)
C(19)	6360(3)	3223(4)	4331(3)	18(1)
C(20)	4385(4)	3615(5)	4234(3)	20(1)
C(21)	4510(4)	5012(5)	3863(3)	18(1)
C(22)	6557(4)	4607(5)	3950(3)	21(1)
C(23)	5613(4)	5546(4)	3716(2)	14(1)
C(24)	5805(3)	7007(5)	3321(2)	16(1)
C(25)	4990(4)	8073(4)	3201(2)	15(1)
C(26)	5158(4)	9543(4)	2791(2)	14(1)
C(27)	1024(4)	1856(4)	3005(3)	26(1)
C(28)	-1026(4)	1401(5)	3166(3)	30(1)
C(29)	-113(3)	3687(4)	3762(3)	24(1)
Cu(1)	5046(1)	694(1)	5016(1)	11(1)
Cu(2)	544(1)	-4339(1)	6380(1)	10(1)
N(1)	4921(3)	-1470(4)	5385(2)	12(1)
N(2)	5290(3)	2721(4)	4462(2)	12(1)
N(3)	368(3)	-2329(4)	6974(2)	14(1)
N(4)	659(3)	3491(4)	6008(2)	12(1)
N(5)	30(3)	2287(4)	3308(2)	22(1)
O(1)	7957(2)	-1686(3)	5159(2)	24(1)
O(2)	6630(2)	77(3)	4806(2)	16(1)
O(1W)	738(2)	-2387(3)	3826(2)	24(1)
O(3)	3121(3)	-5110(3)	7051(2)	18(1)
O(2W)	4014(3)	2094(3)	7481(2)	28(1)
O(4)	2084(2)	-3808(3)	6035(2)	13(1)
O(3W)	1884(3)	-4317(3)	2929(2)	30(1)
O(5)	5683(2)	1275(3)	6372(2)	20(1)
O(6)	-332(2)	-3760(3)	5118(2)	18(1)
O(7)	3453(2)	1227(3)	5250(2)	14(1)
O(8)	2377(3)	-298(3)	4377(2)	17(1)
O(9)	-989(2)	4965(3)	6713(2)	14(1)
O(10)	-2280(2)	3109(3)	6486(2)	21(1)
O(11)	1926(3)	2608(3)	3099(2)	34(1)

Table S9. Anisotropic displacement parameters for compound **1**.

	U11	U22	U33	U23	U13	U12
C(1)	10(2)	6(2)	18(2)	2(1)	1(1)	0(1)
C(2)	12(2)	10(2)	15(2)	0(1)	4(1)	1(1)
C(3)	11(2)	10(2)	13(2)	1(1)	3(1)	-2(1)
C(4)	14(2)	11(2)	16(2)	-1(1)	0(1)	0(1)
C(5)	12(2)	15(2)	19(2)	-1(1)	4(1)	-3(1)
C(6)	9(2)	12(2)	14(2)	-1(1)	1(1)	2(1)
C(7)	15(2)	13(2)	12(2)	-1(1)	4(1)	0(1)
C(8)	12(2)	12(2)	20(2)	-2(1)	2(1)	0(1)
C(9)	11(2)	12(2)	17(2)	-1(1)	1(1)	0(1)
C(10)	12(2)	14(2)	24(2)	2(1)	-2(1)	4(1)
C(11)	17(2)	10(2)	15(2)	2(1)	0(1)	-1(1)
C(12)	10(2)	10(2)	20(2)	1(1)	1(1)	-1(1)
C(13)	11(2)	12(2)	11(2)	-2(1)	-1(1)	-2(1)
C(14)	17(2)	9(2)	13(2)	-3(1)	5(1)	-3(1)
C(15)	17(2)	13(2)	19(2)	-3(1)	4(1)	-4(1)
C(16)	12(2)	13(2)	24(2)	-5(1)	2(1)	-2(1)
C(17)	16(2)	14(2)	24(2)	-3(2)	4(1)	-3(1)
C(18)	16(2)	15(2)	24(2)	-5(1)	7(1)	-1(1)
C(19)	13(2)	15(2)	28(2)	5(2)	8(1)	2(1)
C(20)	13(2)	18(2)	29(2)	6(2)	2(2)	-2(1)
C(21)	12(2)	15(2)	26(2)	8(2)	0(1)	3(1)
C(22)	13(2)	19(2)	33(2)	8(2)	9(2)	1(1)
C(23)	17(2)	12(2)	12(2)	2(1)	4(1)	-2(1)
C(24)	20(2)	14(2)	15(2)	4(1)	5(1)	-1(1)
C(25)	19(2)	11(2)	14(2)	1(1)	4(1)	-3(1)
C(26)	22(2)	8(1)	12(2)	1(1)	-1(1)	2(1)
C(27)	26(2)	23(2)	28(2)	4(2)	2(2)	1(2)
C(28)	26(2)	33(2)	31(2)	-2(2)	-2(2)	0(2)
C(29)	27(2)	19(2)	24(2)	2(1)	1(2)	2(1)
Cu(1)	8(1)	8(1)	16(1)	2(1)	3(1)	1(1)
Cu(2)	9(1)	8(1)	14(1)	-2(1)	3(1)	-1(1)
N(1)	11(2)	10(1)	15(2)	1(1)	4(1)	1(1)
N(2)	12(1)	10(1)	15(1)	2(1)	2(1)	0(1)
N(3)	12(1)	14(2)	15(1)	-2(1)	2(1)	-1(1)
N(4)	11(2)	8(1)	16(2)	-1(1)	-1(1)	0(1)
N(5)	24(2)	23(2)	18(2)	-3(1)	-1(1)	6(1)
O(1)	11(1)	16(1)	47(2)	5(1)	7(1)	5(1)
O(2)	14(1)	11(1)	24(1)	4(1)	6(1)	1(1)
O(1W)	24(1)	29(1)	19(1)	-4(1)	5(1)	-7(1)
O(3)	19(1)	18(1)	18(1)	4(1)	1(1)	-3(1)
O(2W)	35(2)	23(1)	24(1)	1(1)	-1(1)	2(1)
O(4)	9(1)	11(1)	19(1)	-1(1)	2(1)	0(1)
O(3W)	34(2)	26(1)	31(2)	2(1)	13(1)	1(1)
O(5)	17(1)	20(1)	22(1)	-3(1)	0(1)	-4(1)
O(6)	17(1)	21(1)	16(1)	2(1)	5(1)	6(1)
O(7)	10(1)	11(1)	21(1)	1(1)	3(1)	0(1)
O(8)	17(1)	16(1)	18(1)	-4(1)	2(1)	4(1)
O(9)	11(1)	12(1)	20(1)	-2(1)	6(1)	-3(1)
O(10)	13(1)	21(1)	29(2)	-7(1)	9(1)	-6(1)
O(11)	27(2)	30(2)	47(2)	7(1)	13(1)	3(1)

Table S10. Atomic coordinates ($x \cdot 10^4$) and equivalent isotropic displacement parameters of compound **2**.

	X	Y	Z	U(eq)
Cu(1)	233(1)	6851(1)	8200(1)	23(1)
C(1)	1231(3)	9711(4)	7485(2)	27(1)
C(2)	1121(3)	11110(3)	7088(2)	27(1)
C(3)	15(3)	11772(4)	7027(2)	30(1)
C(4)	-932(3)	11037(4)	7392(2)	31(1)
C(5)	-748(3)	9659(4)	7773(2)	26(1)
C(6)	-1684(3)	8753(4)	8203(2)	28(1)
C(7)	2204(3)	11821(3)	6729(2)	28(1)
C(8)	-1043(3)	4319(4)	8955(2)	34(1)
C(9)	-1216(4)	2927(4)	9337(3)	38(1)
C(10)	-243(4)	1996(4)	9543(2)	35(1)
C(11)	867(4)	2546(4)	9359(2)	38(1)
C(12)	970(3)	3949(4)	8996(2)	35(1)
C(13)	-419(4)	513(4)	9935(2)	39(1)
N(1)	324(2)	8995(3)	7808(2)	25(1)
N(2)	28(3)	4832(3)	8782(2)	29(1)
O(1)	-1353(2)	7475(3)	8505(2)	29(1)
O(2)	-2690(2)	9257(3)	8245(2)	42(1)
O(3)	3168(2)	11361(3)	7107(2)	30(1)
O(4)	2109(2)	12733(3)	6120(2)	39(1)
O(1W)	-520(3)	6282(3)	6842(2)	43(1)
O(4W)	988(10)	15304(8)	5600(4)	95(3)
O(3W)	-841(9)	8733(11)	5538(6)	93(3)
O(5W)	-245(10)	6538(12)	5061(7)	100(3)
O(2W)	3396(5)	3205(10)	10200(4)	70(2)

Table S11. Anisotropic displacement parameters for compound **2**.

	U11	U22	U33	U23	U13	U12
Cu(1)	22(1)	16(1)	31(1)	1(1)	0(1)	-1(1)
C(1)	21(1)	21(2)	37(2)	-1(1)	-1(1)	-1(1)
C(2)	26(2)	21(2)	32(2)	-2(1)	-3(1)	-1(1)
C(3)	33(2)	24(2)	34(2)	4(1)	-4(1)	2(1)
C(4)	23(2)	29(2)	40(2)	3(1)	-4(1)	6(1)
C(5)	22(2)	23(2)	31(2)	-2(1)	-2(1)	1(1)
C(6)	26(2)	25(2)	32(2)	-2(1)	0(1)	1(1)
C(7)	28(2)	21(2)	35(2)	-3(1)	1(1)	-1(1)
C(8)	41(2)	24(2)	36(2)	0(1)	5(1)	-2(1)
C(9)	50(2)	24(2)	40(2)	0(1)	10(2)	-7(2)
C(10)	59(2)	20(2)	26(2)	0(1)	3(2)	-4(2)
C(11)	54(2)	24(2)	35(2)	6(1)	-6(2)	0(2)
C(12)	40(2)	26(2)	38(2)	5(1)	-2(2)	-2(1)
C(13)	64(2)	23(2)	29(2)	2(1)	4(2)	-8(2)
N(1)	22(1)	18(1)	34(1)	-1(1)	-2(1)	0(1)
N(2)	39(2)	21(1)	28(1)	-1(1)	1(1)	-4(1)
O(1)	25(1)	24(1)	36(1)	0(1)	2(1)	-1(1)
O(2)	25(1)	37(1)	64(2)	4(1)	6(1)	5(1)
O(3)	25(1)	20(1)	44(1)	-1(1)	1(1)	-1(1)
O(4)	37(1)	38(1)	41(1)	11(1)	2(1)	-2(1)
O(1W)	43(2)	51(2)	36(1)	-6(1)	0(1)	-18(1)
O(4W)	197(10)	59(4)	33(3)	17(3)	47(4)	79(5)
O(3W)	103(7)	87(6)	87(6)	-29(5)	-1(5)	20(5)
O(5W)	105(7)	116(8)	78(6)	33(6)	-5(5)	-21(6)
O(2W)	22(3)	152(8)	36(3)	19(4)	-6(2)	-12(3)

Table S12. Fractional Atomic coordinates ($x10^4$) and isotropic thermal factors ($x10^3$) of hydrogen atoms for compound **1.**

	X	Y	Z	U(eq)
H(4)	228	-262	4992	16
H(10)	6928	-3912	5978	20
H(12)	3257	-1779	5569	16
H(22)	7330	4909	3849	26
H(28A)	-1668	1896	3436	45
H(28B)	-897	399	3414	45
H(28C)	-1227	1308	2550	45
H(29A)	-920	3768	3926	35
H(29B)	59	4533	3391	35
H(29C)	425	3707	4276	35
H(7W)	159	-3392	4805	27
H(3)	2240(50)	3310(60)	5660(40)	41
H(5)	-1270(50)	1010(60)	5640(40)	41
H(5W)	6330(20)	1670(60)	6440(30)	41
H(6W)	5220(30)	1650(60)	6690(30)	41
H(8W)	-820(50)	-3140(70)	5160(40)	41
H(11)	5350(50)	-5020(60)	6540(40)	41
H(15)	-1290(50)	-2620(60)	7260(40)	41
H(16)	1880(50)	-1470(60)	6740(40)	41
H(17)	1800(50)	640(70)	7470(40)	41
H(18)	-1470(50)	-380(60)	7950(40)	41
H(19)	6980(50)	2620(60)	4550(30)	41
H(20)	3640(50)	3210(60)	4310(30)	41
H(21)	3850(60)	5480(60)	3690(40)	41
H(24)	6620(50)	7230(60)	3220(40)	41
H(25)	4300(50)	7960(60)	3350(40)	41
H(34)	1160(40)	-1660(40)	3970(30)	41
H(35)	1180(40)	-3000(40)	3610(30)	41
H(36)	4480(40)	2200(50)	7900(20)	41
H(37)	3810(40)	2940(30)	7320(30)	41
H(38)	1900(50)	-5239(16)	3010(30)	41
H(39)	2230(40)	-4120(50)	2500(20)	41
H(27)	1020(50)	820(60)	2820(40)	41

Table S13. Fractional Atomic coordinates ($x10^4$) and isotropic thermal factors ($x10^3$) of hydrogen atoms for compound **2**.

	X	Y	Z	U(eq)
H(1)	1987	9248	7526	32
H(3)	-99	12712	6743	36
H(4)	-1693	11485	7376	37
H(8)	-1713	4929	8811	40
H(9)	-1991	2608	9458	45
H(11)	1552	1955	9485	46
H(12)	1738	4313	8890	42
H(13)	-1190	272	10109	46
H(1B)	-1100(30)	5740(40)	6840(40)	65
H(1A)	10(30)	5900(50)	6580(30)	65