

Table 1. Crystal data and structure refinement for Pristine-HK.

Identification code	Pristine-HK	
Empirical formula	$C_{144}H_96Cu_{24}O_{120}$	
Formula weight	5271.16	
Temperature	100(2) K	
Wavelength	0.610 Å	
Crystal system	Cubic	
Space group	<i>Fm-3m</i>	
Unit cell dimensions	a = 26.274(3) Å	$\alpha = 90^\circ$.
	b = 26.274(3) Å	$\beta = 90^\circ$.
	c = 26.274(3) Å	$\gamma = 90^\circ$.
Volume	18137(6) Å ³	
Z	2	
Density (calculated)	0.965 Mg/m ³	
Absorption coefficient	0.944 mm ⁻¹	
F(000)	5232	
Crystal size	0.315 x 0.305 x 0.298 mm ³	
Theta range for data collection	1.152 to 24.986°.	
Index ranges	-36 ≤ h ≤ 36, -36 ≤ k ≤ 36, -36 ≤ l ≤ 36	
Reflections collected	40493	
Independent reflections	1315 [R(int) = 0.0765]	
Completeness to theta = 21.469°	99.3 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.946	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	1315 / 2 / 39	
Goodness-of-fit on F ²	1.111	
Final R indices [I > 2σ(I)]	R1 = 0.0342, wR2 = 0.0977	
R indices (all data)	R1 = 0.0399, wR2 = 0.1000	
Extinction coefficient	0.00042(6)	
Largest diff. peak and hole	0.813 and -0.439 e.Å ⁻³	

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

	x	y	z	U(eq)
Cu(1)	5000	2853(1)	2853(1)	25(1)
O(1)	4476(1)	2434(1)	3170(1)	39(1)
O(2)	5000	3436(1)	3436(1)	109(2)
C(1)	4312(1)	2029(1)	2971(1)	33(1)
C(2)	3871(1)	1775(1)	3226(1)	33(1)
C(3)	3658(1)	1990(1)	3658(1)	33(1)

Table 3. Bond lengths [\AA] and angles [$^\circ$] for Pristine-HK.

Cu(1)-O(1)	1.9495(12)
Cu(1)-O(1)#1	1.9496(12)
Cu(1)-O(1)#2	1.9496(12)
Cu(1)-O(1)#3	1.9496(12)
Cu(1)-O(2)	2.166(3)
Cu(1)-Cu(1)#4	2.6212(7)
O(1)-C(1)	1.2626(16)
O(2)-H(1O2)	1.008(18)
O(2)-H(1O2)#2	1.008(18)
C(1)-C(2)	1.495(3)
C(2)-C(3)	1.3869(17)
C(2)-C(3)#5	1.3869(17)
C(3)-H(3)	0.9500
O(1)-Cu(1)-O(1)#1	89.05(8)
O(1)-Cu(1)-O(1)#2	168.99(7)
O(1)#1-Cu(1)-O(1)#2	89.89(8)
O(1)-Cu(1)-O(1)#3	89.90(8)
O(1)#1-Cu(1)-O(1)#3	168.99(7)
O(1)#2-Cu(1)-O(1)#3	89.05(8)
O(1)-Cu(1)-O(2)	95.51(4)
O(1)#1-Cu(1)-O(2)	95.51(4)
O(1)#2-Cu(1)-O(2)	95.51(4)
O(1)#3-Cu(1)-O(2)	95.51(4)
O(1)-Cu(1)-Cu(1)#4	84.49(4)
O(1)#1-Cu(1)-Cu(1)#4	84.49(4)
O(1)#2-Cu(1)-Cu(1)#4	84.49(4)
O(1)#3-Cu(1)-Cu(1)#4	84.49(4)
O(2)-Cu(1)-Cu(1)#4	180.00(8)
C(1)-O(1)-Cu(1)	122.59(13)
Cu(1)-O(2)-H(1O2)	134.1(17)
Cu(1)-O(2)-H(1O2)#2	134.1(17)
H(1O2)-O(2)-H(1O2)#2	92(3)

O(1)#6-C(1)-O(1)	125.7(2)
O(1)#6-C(1)-C(2)	117.11(11)
O(1)-C(1)-C(2)	117.11(11)
C(3)-C(2)-C(3)#5	120.2(2)
C(3)-C(2)-C(1)	119.83(12)
C(3)#5-C(2)-C(1)	119.83(12)
C(2)#7-C(3)-C(2)	119.8(2)
C(2)#7-C(3)-H(3)	120.1
C(2)-C(3)-H(3)	120.1

Symmetry transformations used to generate equivalent atoms:

#1 x, z, y #2 $-x+1, z, y$ #3 $-x+1, y, z$ #4 $-x+1, -y+1/2, -z+1/2$
#5 $z, -x+1/2, -y+1/2$ #6 $x, -z+1/2, -y+1/2$ #7 $-y+1/2, -z+1/2, x$

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Pristine-HK. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cu(1)	24(1)	25(1)	25(1)	-15(1)	0	0
O(1)	37(1)	41(1)	39(1)	-11(1)	8(1)	-8(1)
O(2)	189(5)	68(2)	68(2)	-55(2)	0	0
C(1)	28(1)	35(1)	35(1)	-2(1)	-1(1)	1(1)
C(2)	28(1)	35(1)	35(1)	1(1)	0(1)	0(1)
C(3)	32(1)	36(1)	32(1)	-1(1)	-4(1)	-1(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for Pristine-HK.

	x	y	z	U(eq)
H(1O2)	5000	3430(11)	3819(7)	163
H(3)	3807	2283	3807	40

Table 6. Torsion angles [°] for Pristine-HK.

Cu(1)-O(1)-C(1)-O(1)#6	3.9(4)
Cu(1)-O(1)-C(1)-C(2)	-173.64(14)
O(1)#6-C(1)-C(2)-C(3)	-176.8(2)
O(1)-C(1)-C(2)-C(3)	0.9(3)
O(1)#6-C(1)-C(2)-C(3)#5	-0.9(3)
O(1)-C(1)-C(2)-C(3)#5	176.8(2)
C(3)#5-C(2)-C(3)-C(2)#7	-0.8(5)
C(1)-C(2)-C(3)-C(2)#7	175.10(16)

Symmetry transformations used to generate equivalent atoms:

#1 x, z, y #2 $-x+1, z, y$ #3 $-x+1, y, z$ #4 $-x+1, -y+1/2, -z+1/2$

#5 $z, -x+1/2, -y+1/2$ #6 $x, -z+1/2, -y+1/2$ #7 $-y+1/2, -z+1/2, x$