

Supporting Information

For

Polymorphism, Composition and Structural Variability in Topology in 1D, 2D and 3D Copper Phosphonocarboxylate Materials

By

**Seema Lodhia, Adele Turner, Maria Papadaki,
Konstantinos D. Demadis, Gary B. Hix**

Single Crystal Data

α -Cu_{1.5}(O₃PCH₂CO₂).H₂O (1)

Table 1. Crystal data and structure refinement for α -Cu_{1.5}(O₃PCH₂CO₂).H₂O(1).

Identification code	CuCP-1
Empirical formula	C2 H4 Cu1.50 O6 P
Formula weight	250.33
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 4.6512(5) Å alpha = 108.3430(10) ° b = 7.9368(8) Å beta = 100.3880(10) ° c = 8.0583(8) Å gamma = 92.2010(10) °
Volume	276.29(5) Å ³
Z, Calculated density	2, 3.009 Mg/m ³
Absorption coefficient	6.081 mm ⁻¹
F(000)	245
Crystal size	0.20 x 0.15 x 0.03 mm
Theta range for data collection	4.43 to 27.46 deg.
Limiting indices	-5<=h<=5, -10<=k<=10, -10<=l<=10
Reflections collected / unique	3830 / 1229 [R(int) = 0.0936]
Completeness to theta = 27.46	97.5 %
Absorption correction	None
Max. and min. transmission	0.8386 and 0.3760
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1229 / 0 / 103
Goodness-of-fit on F ²	1.025
Final R indices [I>2sigma(I)]	R1 = 0.0420, wR2 = 0.1036
R indices (all data)	R1 = 0.0521, wR2 = 0.1107
Largest diff. peak and hole	0.776 and -1.136 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for α -Cu_{1.5}(O₃PCH₂CO₂).H₂O(1). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5000	5000	5000	14(1)
Cu(2)	3938(1)	3572(1)	676(1)	14(1)
P(1)	-558(2)	6305(2)	3023(1)	13(1)
O(3)	-2710(6)	5369(4)	1217(4)	14(1)
O(2)	2187(7)	5336(4)	3039(4)	16(1)
O(1)	-1978(7)	6493(4)	4597(4)	16(1)
C(1)	409(10)	8519(6)	2996(6)	16(1)
O(4)	4020(7)	9015(4)	1424(4)	19(1)
C(2)	1402(10)	8516(6)	1312(6)	15(1)
O(6)	-425(7)	7982(4)	-166(4)	15(1)
O(5)	6057(8)	2458(5)	2395(5)	18(1)

Table 3. Bond lengths [Å] and angles [deg] for α -Cu_{1.5}(O₃PCH₂CO₂)·H₂O(1).

Cu(1)-O(1)#1	1.940(3)
Cu(1)-O(1)#2	1.940(3)
Cu(1)-O(2)	1.956(3)
Cu(1)-O(2)#3	1.956(3)
Cu(2)-O(6)#4	1.909(3)
Cu(2)-O(3)#2	1.961(3)
Cu(2)-O(3)#4	1.972(3)
Cu(2)-O(5)	2.004(3)
Cu(2)-O(2)	2.284(3)
Cu(2)-Cu(2)#5	3.0120(10)
P(1)-O(1)	1.503(3)
P(1)-O(2)	1.516(3)
P(1)-O(3)	1.552(3)
P(1)-C(1)	1.805(4)
O(3)-Cu(2)#6	1.961(3)
O(3)-Cu(2)#4	1.972(3)
O(1)-Cu(1)#6	1.940(3)
C(1)-C(2)	1.510(6)
O(4)-C(2)	1.244(6)
C(2)-O(6)	1.269(5)
O(6)-Cu(2)#4	1.909(3)
O(1)#1-Cu(1)-O(1)#2	180.00(15)
O(1)#1-Cu(1)-O(2)	89.62(13)
O(1)#2-Cu(1)-O(2)	90.38(13)
O(1)#1-Cu(1)-O(2)#3	90.38(13)
O(1)#2-Cu(1)-O(2)#3	89.62(13)
O(2)-Cu(1)-O(2)#3	180.000(1)
O(6)#4-Cu(2)-O(3)#2	174.13(12)
O(6)#4-Cu(2)-O(3)#4	96.49(13)
O(3)#2-Cu(2)-O(3)#4	80.06(14)
O(6)#4-Cu(2)-O(5)	92.90(14)
O(3)#2-Cu(2)-O(5)	91.30(14)
O(3)#4-Cu(2)-O(5)	166.72(13)
O(6)#4-Cu(2)-O(2)	86.17(12)
O(3)#2-Cu(2)-O(2)	90.03(12)
O(3)#4-Cu(2)-O(2)	103.69(12)
O(5)-Cu(2)-O(2)	86.24(12)
O(6)#4-Cu(2)-Cu(2)#5	136.20(9)
O(3)#2-Cu(2)-Cu(2)#5	40.16(8)
O(3)#4-Cu(2)-Cu(2)#5	39.89(9)
O(5)-Cu(2)-Cu(2)#5	130.70(11)
O(2)-Cu(2)-Cu(2)#5	98.94(8)
O(1)-P(1)-O(2)	114.71(17)
O(1)-P(1)-O(3)	112.39(19)
O(2)-P(1)-O(3)	108.10(17)
O(1)-P(1)-C(1)	107.71(19)
O(2)-P(1)-C(1)	108.3(2)
O(3)-P(1)-C(1)	105.11(18)
P(1)-O(3)-Cu(2)#6	128.91(17)
P(1)-O(3)-Cu(2)#4	125.70(18)
Cu(2)#6-O(3)-Cu(2)#4	99.94(14)
P(1)-O(2)-Cu(1)	131.51(18)
P(1)-O(2)-Cu(2)	128.71(17)

Cu(1)-O(2)-Cu(2)	99.50(13)
P(1)-O(1)-Cu(1)#6	132.2(2)
C(2)-C(1)-P(1)	113.0(3)
O(4)-C(2)-O(6)	122.2(4)
O(4)-C(2)-C(1)	118.3(4)
O(6)-C(2)-C(1)	119.4(4)
C(2)-O(6)-Cu(2)#4	125.4(3)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for α - $\text{Cu}_{1.5}(\text{O}_3\text{PCH}_2\text{CO}_2) \cdot \text{H}_2\text{O}(1)$. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	11(1)	23(1)	11(1)	10(1)	3(1)	1(1)
Cu(2)	12(1)	22(1)	12(1)	10(1)	1(1)	-1(1)
P(1)	11(1)	20(1)	11(1)	9(1)	3(1)	1(1)
O(3)	11(2)	19(2)	13(1)	10(1)	2(1)	-2(1)
O(2)	13(2)	23(2)	12(1)	8(1)	3(1)	1(1)
O(1)	12(2)	24(2)	12(1)	6(1)	3(1)	-2(1)
C(1)	14(2)	19(2)	16(2)	6(2)	6(2)	-1(2)
O(4)	12(2)	27(2)	22(2)	12(1)	7(1)	2(1)
C(2)	18(2)	15(2)	17(2)	7(2)	7(2)	5(2)
O(6)	13(2)	19(2)	15(2)	9(1)	2(1)	-1(1)
O(5)	14(2)	21(2)	22(2)	10(1)	4(2)	0(2)

β -Cu_{1.5}(O₃PCH₂CO₂).H₂O (2)

Table 1. Crystal data and structure refinement for β -Cu_{1.5}(O₃PCH₂CO₂).H₂O (2)

Identification code	CuCP-2
Empirical formula	C ₂ H ₄ Cu _{1.50} O ₆ P
Formula weight	250.33
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P 1 21/c 1
Unit cell dimensions	a = 8.2713(2) Å alpha = 90 ° b = 7.5587(2) Å beta = 90.195(2) ° c = 9.0004(2) Å gamma = 90 °
Volume	562.70(2) Å ³
Z, Calculated density	4, 2.955 Mg/m ³
Absorption coefficient	5.972 mm ⁻¹
F(000)	490
Crystal size	0.26 x 0.26 x 0.24 mm
Theta range for data collection	3.52 to 27.49 deg.
Limiting indices	-10<=h<=9, -9<=k<=9, -11<=l<=10
Reflections collected / unique	5573 / 1295 [R(int) = 0.0582]
Completeness to theta = 27.49	99.6 %
Absorption correction	None
Max. and min. transmission	0.3283 and 0.3058
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1295 / 0 / 107
Goodness-of-fit on F ²	1.135
Final R indices [I>2sigma(I)]	R1 = 0.0277, wR2 = 0.0703
R indices (all data)	R1 = 0.0289, wR2 = 0.0709
Extinction coefficient	0.0230(15)
Largest diff. peak and hole	0.825 and -0.775 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\beta\text{-Cu}_{1.5}(\text{O}_3\text{PCH}_2\text{CO}_2)\cdot\text{H}_2\text{O}(2)$. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Cu(1)	0	5000	5000	4(1)
Cu(2)	3440(1)	4704(1)	3254(1)	5(1)
P(1)	2844(1)	6349(1)	6950(1)	3(1)
O(1)	4349(2)	5302(3)	7404(2)	7(1)
O(2)	2198(2)	5768(3)	5419(2)	6(1)
O(3)	3033(2)	8342(3)	6971(2)	8(1)
O(4)	-1000(2)	5825(3)	6833(2)	5(1)
O(5)	3863(2)	2578(3)	4430(2)	8(1)
O(6)	-1064(2)	7159(3)	9016(2)	7(1)
C(2)	-319(3)	6298(4)	8081(3)	6(1)
C(1)	1383(3)	5699(4)	8336(3)	5(1)

Table 3. Bond lengths [Å] and angles [deg] for β -Cu_{1.5}(O₃PCH₂CO₂)·H₂O(2)

Cu(1)-O(2)	1.9443(18)
Cu(1)-O(2)#1	1.9443(18)
Cu(1)-O(4)#1	1.9508(18)
Cu(1)-O(4)	1.9508(18)
Cu(2)-O(3)#2	1.904(2)
Cu(2)-O(1)#3	1.9244(19)
Cu(2)-O(5)	1.955(2)
Cu(2)-O(4)#1	2.0580(19)
Cu(2)-O(2)	2.3484(19)
P(1)-O(3)	1.514(2)
P(1)-O(1)	1.530(2)
P(1)-O(2)	1.5396(19)
P(1)-C(1)	1.808(3)
O(1)-Cu(2)#3	1.9244(19)
O(3)-Cu(2)#4	1.9045(19)
O(4)-C(2)	1.305(3)
O(4)-Cu(2)#1	2.0580(19)
O(6)-C(2)	1.231(3)
C(2)-C(1)	1.495(4)
O(2)-Cu(1)-O(2)#1	180.0
O(2)-Cu(1)-O(4)#1	81.99(8)
O(2)#1-Cu(1)-O(4)#1	98.01(8)
O(2)-Cu(1)-O(4)	98.01(8)
O(2)#1-Cu(1)-O(4)	81.99(8)
O(4)#1-Cu(1)-O(4)	180.0
O(3)#2-Cu(2)-O(1)#3	88.93(8)
O(3)#2-Cu(2)-O(5)	175.45(9)
O(1)#3-Cu(2)-O(5)	89.78(8)
O(3)#2-Cu(2)-O(4)#1	87.49(8)
O(1)#3-Cu(2)-O(4)#1	157.00(8)
O(5)-Cu(2)-O(4)#1	92.00(8)
O(3)#2-Cu(2)-O(2)	99.22(8)
O(1)#3-Cu(2)-O(2)	132.45(8)
O(5)-Cu(2)-O(2)	84.85(8)
O(4)#1-Cu(2)-O(2)	70.53(7)
O(3)-P(1)-O(1)	115.27(12)
O(3)-P(1)-O(2)	109.29(11)
O(1)-P(1)-O(2)	111.79(11)
O(3)-P(1)-C(1)	109.33(12)
O(1)-P(1)-C(1)	102.72(12)
O(2)-P(1)-C(1)	108.03(12)
P(1)-O(1)-Cu(2)#3	133.82(12)
P(1)-O(2)-Cu(1)	125.45(11)
P(1)-O(2)-Cu(2)	133.55(11)
Cu(1)-O(2)-Cu(2)	98.50(8)
P(1)-O(3)-Cu(2)#4	142.88(13)
C(2)-O(4)-Cu(1)	129.21(17)
C(2)-O(4)-Cu(2)#1	120.45(16)
Cu(1)-O(4)-Cu(2)#1	108.93(9)
O(6)-C(2)-O(4)	121.2(2)
O(6)-C(2)-C(1)	121.9(2)
O(4)-C(2)-C(1)	116.9(2)
C(2)-C(1)-P(1)	116.26(19)

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for β - $\text{Cu}_{1.5}(\text{O}_3\text{PCH}_2\text{CO}_2) \cdot \text{H}_2\text{O}(2)$. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	3(1)	5(1)	3(1)	-2(1)	0(1)	-1(1)
Cu(2)	4(1)	4(1)	8(1)	3(1)	1(1)	1(1)
P(1)	3(1)	3(1)	4(1)	0(1)	0(1)	0(1)
O(1)	5(1)	8(1)	7(1)	3(1)	1(1)	2(1)
O(2)	5(1)	6(1)	6(1)	-1(1)	-1(1)	-1(1)
O(3)	10(1)	6(1)	8(1)	-3(1)	1(1)	-2(1)
O(4)	5(1)	8(1)	3(1)	-1(1)	-1(1)	0(1)
O(5)	8(1)	5(1)	11(1)	2(1)	5(1)	2(1)
O(6)	7(1)	6(1)	7(1)	-2(1)	2(1)	1(1)
C(2)	7(1)	4(1)	7(1)	1(1)	0(1)	-4(1)
C(1)	5(1)	6(1)	4(1)	-1(1)	0(1)	0(1)

Cu(HO₃PCH₂CO₂).H₂O (3)

Table 1. Crystal data and structure refinement for Cu(HO₃PCH₂CO₂).H₂O (3)

Identification code	CuCP-3
Empirical formula	C2 H5 Cu O6 P
Formula weight	219.57
Temperature	120(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 6.0979(2)Å alpha = 73.766(2)° b = 6.3860(3)Å beta = 69.441(2)° c = 8.0968(3)Å gamma = 80.937(2)°
Volume	282.829(19) Å ³
Z, Calculated density	2, 2.578 Mg/m ³
Absorption coefficient	4.109 mm ⁻¹
F(000)	218
Crystal size	0.42 x 0.38 x 0.04 mm
Theta range for data collection	3.58 to 27.50 deg.
Limiting indices	-7<=h<=7, -8<=k<=8, -10<=l<=10
Reflections collected / unique	4840 / 1293 [R(int) = 0.0549]
Completeness to theta = 27.50	99.0 %
Absorption correction	None
Max. and min. transmission	0.8529 and 0.2772
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1293 / 0 / 97
Goodness-of-fit on F ²	1.106
Final R indices [I>2sigma(I)]	R1 = 0.0323, wR2 = 0.0890
R indices (all data)	R1 = 0.0336, wR2 = 0.0903
Largest diff. peak and hole	0.814 and -0.988 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cu}(\text{HO}_3\text{PCH}_2\text{CO}_2)\cdot\text{H}_2\text{O}$ (**3**). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	$U(\text{eq})$
Cu(1)	6293(1)	7289(1)	9374(1)	7(1)
P(1)	11640(1)	7704(1)	8342(1)	6(1)
O(3)	13326(3)	6545(3)	9363(3)	9(1)
O(5)	7671(3)	7317(3)	6811(3)	11(1)
O(1)	9143(3)	7920(3)	9573(3)	10(1)
O(4)	4724(4)	8100(4)	11705(3)	17(1)
O(6)	10422(3)	7621(3)	4138(3)	10(1)
O(2)	12587(3)	9980(3)	7169(3)	10(1)
C(2)	9789(5)	7106(4)	5860(4)	8(1)
C(1)	11645(5)	6184(4)	6764(3)	9(1)

Table 3. Bond lengths [Å] and angles [deg] for Cu(HO₃PCH₂CO₂).H₂O (**3**).

Cu(1)-O(1)	1.9136(19)
Cu(1)-O(5)	1.942(2)
Cu(1)-O(3)#1	1.945(2)
Cu(1)-O(4)	1.966(2)
Cu(1)-O(3)#2	2.3840(19)
P(1)-O(1)	1.509(2)
P(1)-O(3)	1.5176(19)
P(1)-O(2)	1.5668(19)
P(1)-C(1)	1.807(3)
O(3)-Cu(1)#3	1.9451(19)
O(3)-Cu(1)#2	2.3840(19)
O(5)-C(2)	1.258(3)
O(6)-C(2)	1.268(3)
C(2)-C(1)	1.515(3)
O(1)-Cu(1)-O(5)	94.03(8)
O(1)-Cu(1)-O(3)#1	175.76(7)
O(5)-Cu(1)-O(3)#1	89.81(8)
O(1)-Cu(1)-O(4)	85.96(9)
O(5)-Cu(1)-O(4)	164.58(10)
O(3)#1-Cu(1)-O(4)	90.83(9)
O(1)-Cu(1)-O(3)#2	95.43(8)
O(5)-Cu(1)-O(3)#2	99.14(8)
O(3)#1-Cu(1)-O(3)#2	82.14(8)
O(4)-Cu(1)-O(3)#2	96.21(9)
O(1)-P(1)-O(3)	113.13(11)
O(1)-P(1)-O(2)	111.94(11)
O(3)-P(1)-O(2)	108.17(11)
O(1)-P(1)-C(1)	107.39(12)
O(3)-P(1)-C(1)	109.46(12)
O(2)-P(1)-C(1)	106.52(11)
P(1)-O(3)-Cu(1)#3	133.13(12)
P(1)-O(3)-Cu(1)#2	126.10(11)
Cu(1)#3-O(3)-Cu(1)#2	97.86(8)
C(2)-O(5)-Cu(1)	130.03(18)
P(1)-O(1)-Cu(1)	129.81(12)
O(5)-C(2)-O(6)	121.4(2)
O(5)-C(2)-C(1)	120.2(2)
O(6)-C(2)-C(1)	118.4(2)
C(2)-C(1)-P(1)	112.09(19)

Symmetry transformations used to generate equivalent atoms:

#1 x-1,y,z #2 -x+2,-y+1,-z+2 #3 x+1,y,z

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cu}(\text{HO}_3\text{PCH}_2\text{CO}_2) \cdot \text{H}_2\text{O}$ (**3**). The anisotropic displacement factor exponent takes the form:

$$-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
Cu(1)	3(1)	12(1)	6(1)	-1(1)	-2(1)	-1(1)
P(1)	4(1)	9(1)	6(1)	0(1)	-2(1)	0(1)
O(3)	6(1)	11(1)	9(1)	0(1)	-4(1)	-1(1)
O(5)	6(1)	18(1)	8(1)	-2(1)	-3(1)	-1(1)
O(1)	5(1)	15(1)	10(1)	-4(1)	-3(1)	0(1)
O(4)	4(1)	34(1)	14(1)	-12(1)	2(1)	-6(1)
O(6)	9(1)	14(1)	7(1)	0(1)	-3(1)	-1(1)
O(2)	8(1)	11(1)	10(1)	1(1)	-5(1)	-1(1)
C(2)	8(1)	7(1)	9(1)	0(1)	-4(1)	-1(1)
C(1)	6(1)	12(1)	9(1)	-2(1)	-4(1)	1(1)

Cu(*R,S*-HO₃PCH(OH)CH₂CO₂)(H₂O)₂·H₂O (4).

Table 1. Crystal data and structure refinement for Cu(*R,S*-HO₃PCH(OH)CH₂CO₂)(H₂O)₂·H₂O (4).

Identification code	Cu-HPAA
Empirical formula	C2 H9 Cu O9 P
Formula weight	271.60
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, Pbca
Unit cell dimensions	a = 8.623(3) Å alpha = 90 deg. b = 9.893(3) Å beta = 90 deg. c = 18.924(5) Å gamma = 90 deg.
Volume	1614.3(8) Å ³
Z, Calculated density	8, 2.235 Mg/m ³
Absorption coefficient	2.929 mm ⁻¹
F(000)	1096
Crystal size	0.11 x 0.09 x 0.02 mm
Theta range for data collection	3.20 to 28.27 deg.
Limiting indices	-11<=h<=11, -12<=k<=13, -24<=l<=20
Reflections collected / unique	11181 / 1962 [R(int) = 0.0300]
Completeness to theta = 28.27	97.9 %
Absorption correction	None
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1962 / 0 / 138
Goodness-of-fit on F ²	1.087
Final R indices [I>2sigma(I)]	R1 = 0.0315, wR2 = 0.0646
R indices (all data)	R1 = 0.0413, wR2 = 0.0673
Largest diff. peak and hole	0.528 and -0.382 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cu}(\text{R}, \text{S-HO}_3\text{PCH}(\text{OH})\text{CH}_2\text{CO}_2)(\text{H}_2\text{O})_2 \cdot \text{H}_2\text{O}$ (4). $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	11294(1)	1479(1)	3515(1)	16(1)
P(1)	8037(1)	140(1)	3565(1)	17(1)
C(1)	8444(3)	260(2)	2617(1)	16(1)
C(2)	8910(3)	1697(2)	2425(1)	15(1)
O(1)	7118(2)	-107(2)	2218(1)	21(1)
O(2)	8141(2)	2308(2)	1951(1)	17(1)
O(3)	10009(2)	2247(2)	2749(1)	18(1)
O(4)	7400(2)	-1227(2)	3732(1)	25(1)
O(5)	6736(2)	1201(2)	3726(1)	27(1)
O(6)	9538(2)	507(2)	3942(1)	23(1)
O(7)	12581(2)	957(2)	4332(1)	25(1)
O(8)	717(3)	3583(2)	4153(1)	29(1)
O(9)	4438(3)	3040(2)	4742(1)	41(1)

Table 3. Bond lengths [Å] and angles [deg] for Cu(*R,S*-HO₃PCH(OH)CH₂CO₂)(H₂O)₂]·H₂O (4).

Cu(1)-O(6)	1.9687(18)
Cu(1)-O(7)	1.9719(19)
Cu(1)-O(3)	1.9762(17)
Cu(1)-O(2)#1	1.9963(17)
Cu(1)-O(1)#1	2.2116(17)
Cu(1)-O(8)	2.457
P(1)-O(4)	1.4931(18)
P(1)-O(6)	1.5212(18)
P(1)-O(5)	1.5664(19)
P(1)-C(1)	1.833(3)
C(1)-O(1)	1.417(3)
C(1)-C(2)	1.521(3)
C(1)-H(1A)	0.9800
C(2)-O(3)	1.253(3)
C(2)-O(2)	1.268(3)
O(1)-Cu(1)#2	2.2116(17)
O(1)-H(1B)	0.8200
O(2)-Cu(1)#2	1.9963(17)
O(5)-H(5A)	0.8200
O(7)-H(7A)	0.8200
O(7)-H(7B)	0.72(4)
O(8)-H(8B)	0.77(4)
O(8)-H(8A)	0.72(4)
O(9)-H(9A)	0.80(4)
O(9)-H(9B)	0.73(5)
O(6)-Cu(1)-O(7)	88.98(8)
O(6)-Cu(1)-O(3)	93.32(7)
O(7)-Cu(1)-O(3)	172.43(8)
O(6)-Cu(1)-O(2)#1	174.92(7)
O(7)-Cu(1)-O(2)#1	90.29(8)
O(3)-Cu(1)-O(2)#1	88.04(7)
O(6)-Cu(1)-O(1)#1	99.09(7)
O(7)-Cu(1)-O(1)#1	97.16(8)
O(3)-Cu(1)-O(1)#1	89.60(7)
O(2)#1-Cu(1)-O(1)#1	76.02(6)
O(4)-P(1)-O(6)	115.46(11)
O(4)-P(1)-O(5)	107.57(11)
O(6)-P(1)-O(5)	111.01(11)
O(4)-P(1)-C(1)	109.64(11)
O(6)-P(1)-C(1)	106.33(10)
O(5)-P(1)-C(1)	106.48(11)
O(1)-C(1)-C(2)	109.00(19)
O(1)-C(1)-P(1)	110.50(16)
C(2)-C(1)-P(1)	110.22(16)
O(1)-C(1)-H(1A)	109.0
C(2)-C(1)-H(1A)	109.0
P(1)-C(1)-H(1A)	109.0
O(3)-C(2)-O(2)	122.3(2)
O(3)-C(2)-C(1)	119.3(2)
O(2)-C(2)-C(1)	118.5(2)
C(1)-O(1)-Cu(1)#2	114.25(13)
C(1)-O(1)-H(1B)	109.5

Cu(1)#2-O(1)-H(1B)	127.6
C(2)-O(2)-Cu(1)#2	122.22(14)
C(2)-O(3)-Cu(1)	128.03(15)
P(1)-O(5)-H(5A)	109.5
P(1)-O(6)-Cu(1)	125.31(11)
Cu(1)-O(7)-H(7A)	109.5
Cu(1)-O(7)-H(7B)	116(3)
H(7A)-O(7)-H(7B)	110.9
H(8B)-O(8)-H(8A)	97(4)
H(9A)-O(9)-H(9B)	105(4)

Symmetry transformations used to generate equivalent atoms:

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

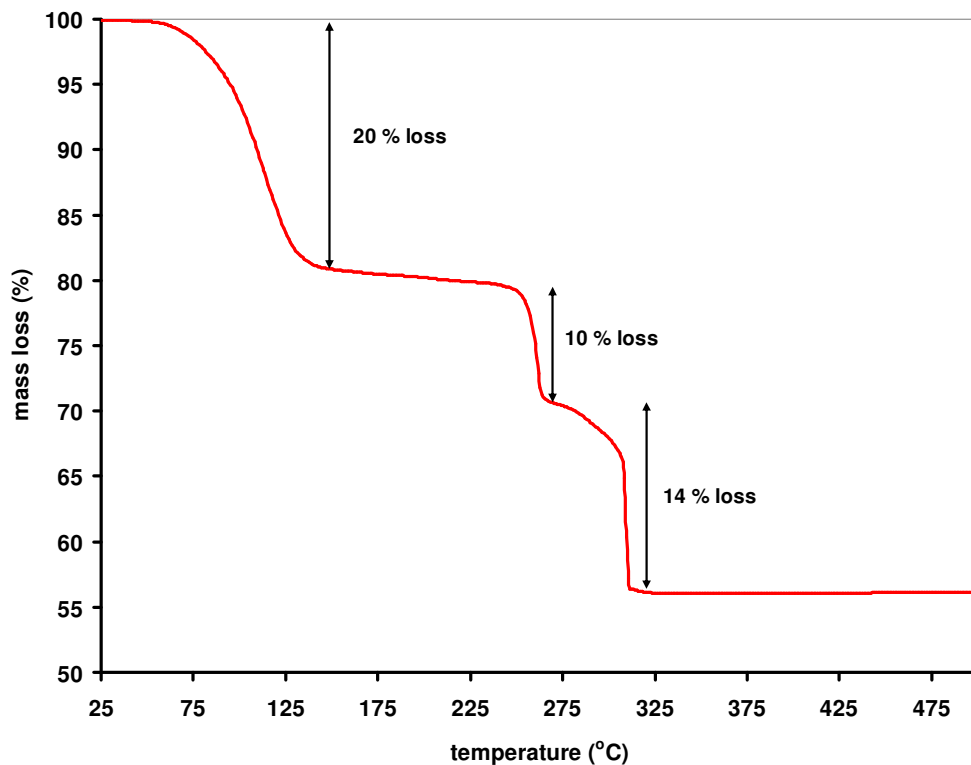
Table 4. Anisotropic displacement parameters ($\text{Å}^2 \times 10^3$) for $\text{Cu}(R,S\text{-HO}_3\text{PCH(OH)CH}_2\text{CO}_2)(\text{H}_2\text{O})_2 \cdot \text{H}_2\text{O}$ (4). The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	13(1)	16(1)	17(1)	1(1)	0(1)	-1(1)
P(1)	16(1)	14(1)	21(1)	2(1)	1(1)	-2(1)
C(1)	15(1)	12(1)	20(1)	-1(1)	-3(1)	0(1)
C(2)	16(1)	13(1)	17(1)	-1(1)	4(1)	0(1)
O(1)	23(1)	12(1)	29(1)	-1(1)	-9(1)	-2(1)
O(2)	17(1)	13(1)	23(1)	2(1)	-3(1)	-1(1)
O(3)	17(1)	15(1)	23(1)	2(1)	-3(1)	-2(1)
O(4)	26(1)	16(1)	31(1)	4(1)	2(1)	-5(1)
O(5)	22(1)	19(1)	41(1)	-1(1)	7(1)	1(1)
O(6)	19(1)	31(1)	20(1)	3(1)	-1(1)	-8(1)
O(7)	24(1)	24(1)	26(1)	1(1)	-7(1)	1(1)
O(8)	23(1)	31(1)	34(1)	3(1)	0(1)	2(1)
O(9)	60(2)	35(1)	28(1)	-1(1)	0(1)	-16(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{Cu}(R,S\text{-HO}_3\text{PCH(OH)CH}_2\text{CO}_2)(\text{H}_2\text{O})_2 \cdot \text{H}_2\text{O}$ (4).

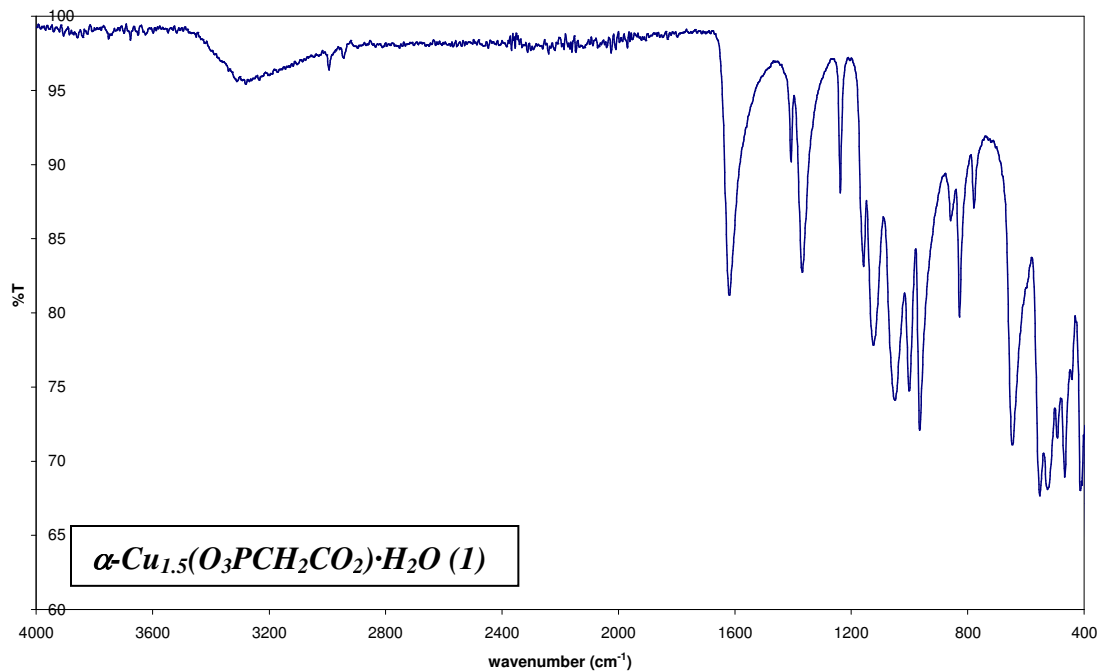
	x	y	z	U(eq)
H(1A)	9298	-353	2499	19
H(1B)	7116	-927	2155	32
H(5A)	7106	1964	3717	41
H(7A)	13129	1596	4448	37
H(8B)	-110(50)	3750(40)	4030(20)	42(11)
H(9A)	4320(50)	3510(40)	5080(20)	50(12)
H(8A)	510(40)	3340(40)	4500(20)	35(11)
H(7B)	13040(40)	350(40)	4290(20)	40(11)
H(9B)	4780(60)	3490(40)	4480(20)	62(15)

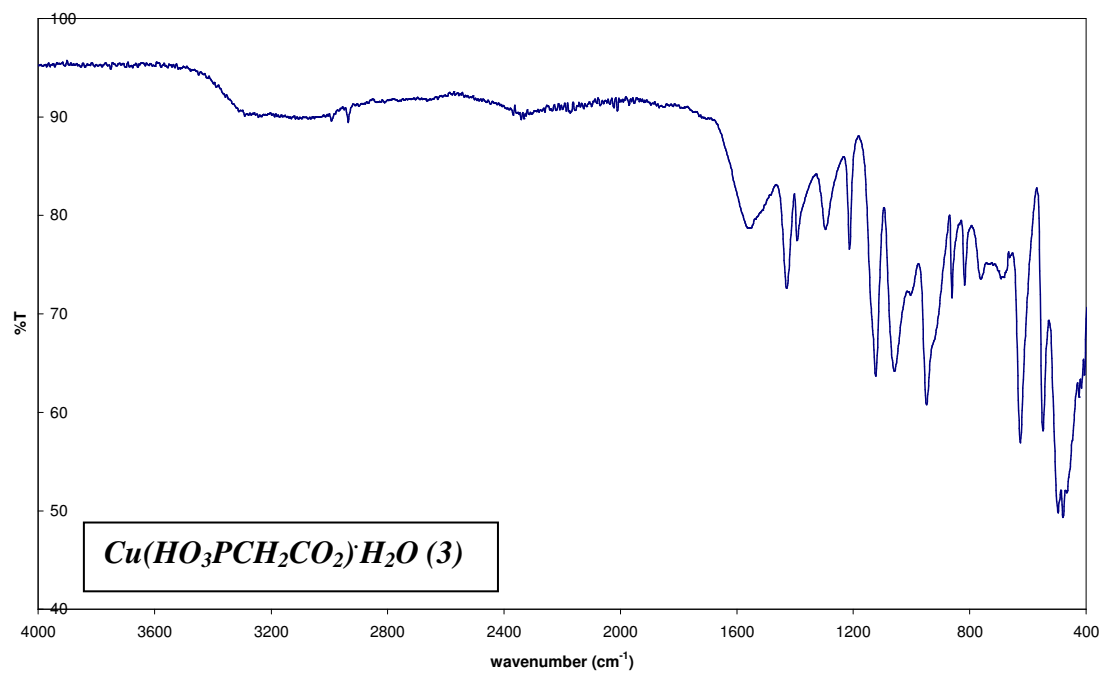
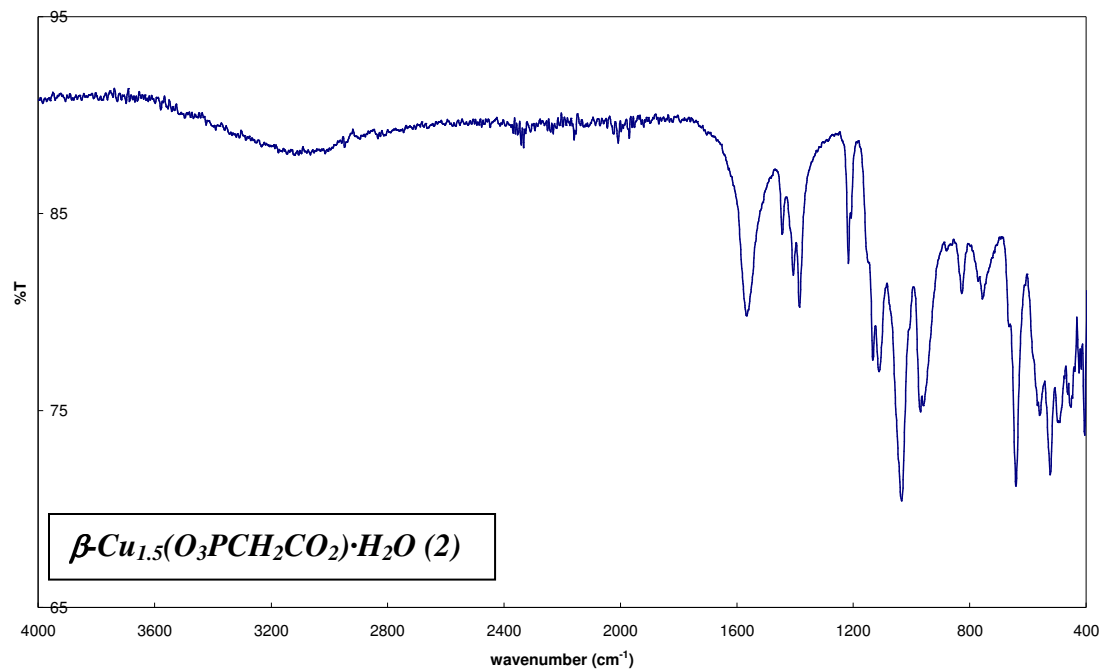
Thermogravimetric Studies

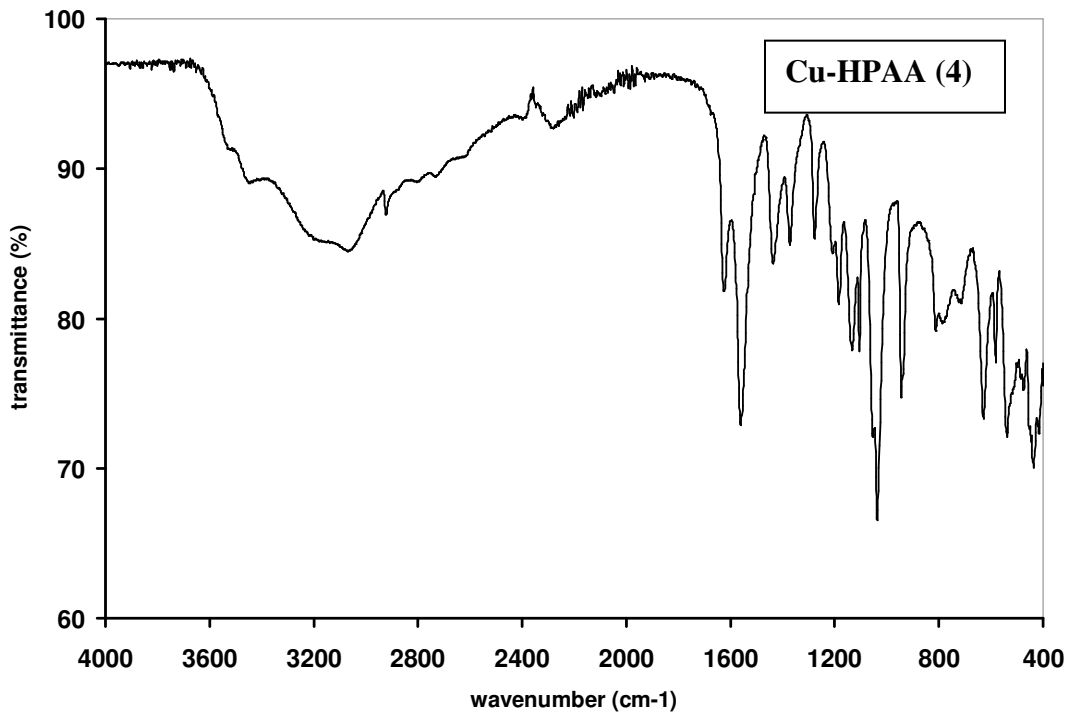
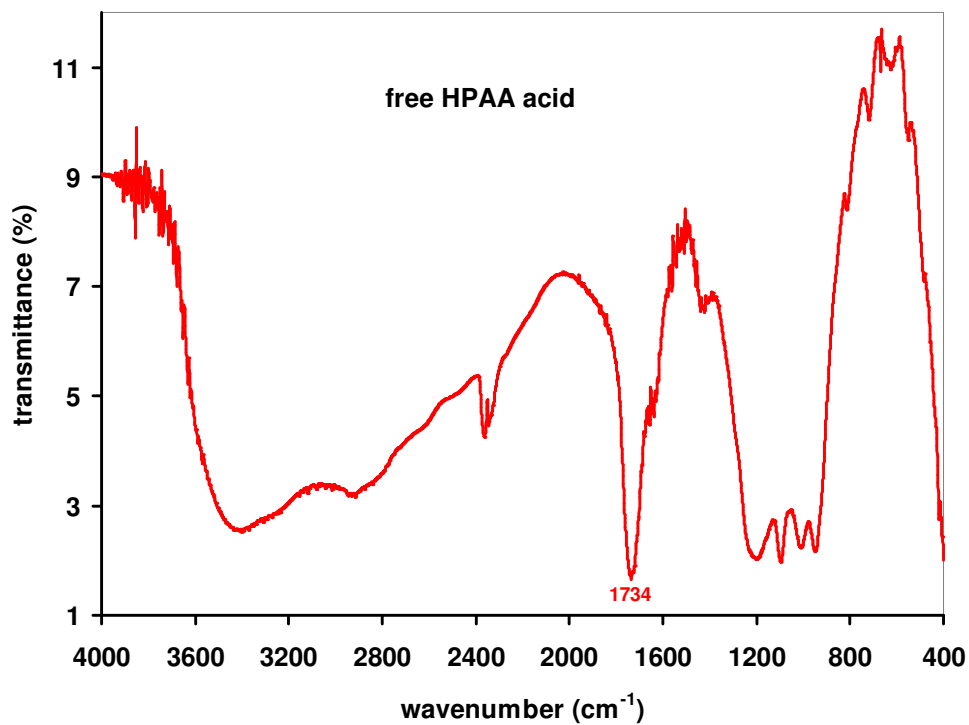


TGA of $[\text{Cu}(\text{R,S-HO}_3\text{PCH}(\text{OH})\text{CH}_2\text{CO}_2)(\text{H}_2\text{O})_2]\cdot\text{H}_2\text{O}$ (4)

FT-IR Spectroscopy







X-Ray Powder Patterns

