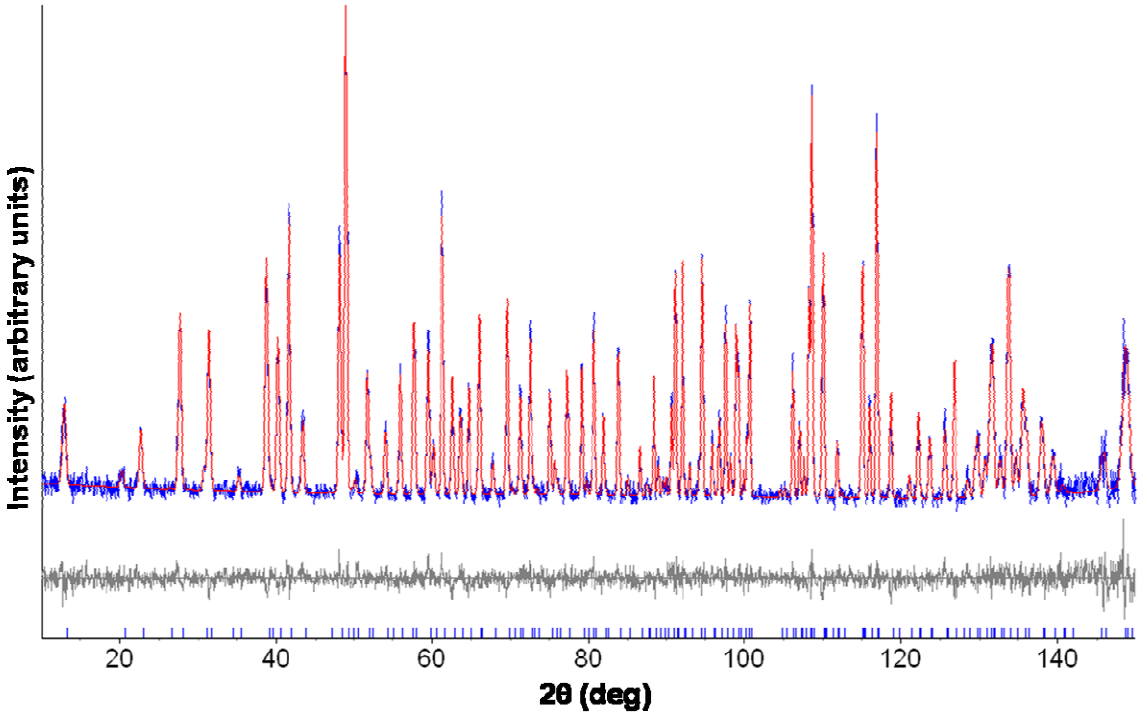
Refinement details

$Ca_{10}(PO_4)_6Cu_xO_yH_z$ $x = 0.2$



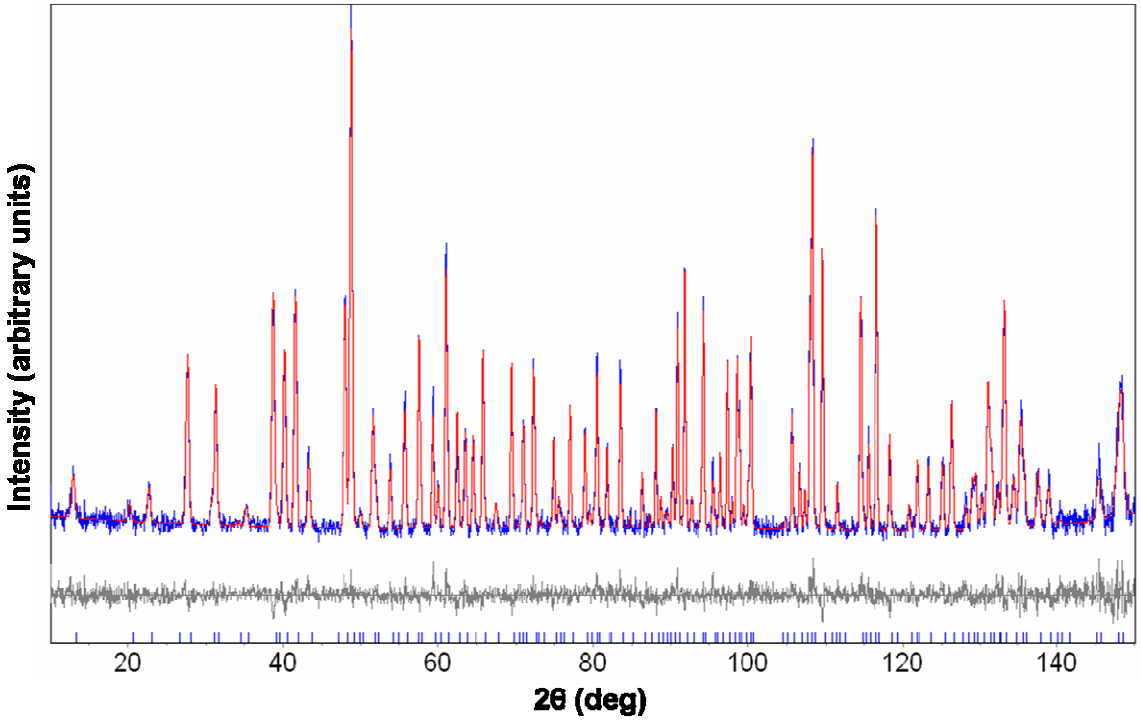
s.g	*P*6$_3$/*m*	*a* = 9.4145(1) Å	*c* = 6.8811(1) Å	R_{wp} = 6.85 %	R_{Bragg} = 2.12 %
Site	***x***	***y***	***z***	***B***	**Occ.**
Ca(1)	1/3	2/3	-0.0024(7)	0.68(9)	1
Ca(2)	0.2521(5)	0.0071(5)	¼	0.58(8)	1
P	0.3684(4)	0.3986(5)	¼	0.41(7)	1
O(1)	0.4846(4)	0.3281(4)	¼	0.52(7)	1
O(2)	0.4668(5)	0.5888(4)	¼	1.15(8)	1
O(3)	0.2584(3)	0.3441(3)	0.0708(3)	1.25(5)	1
O(4)	0.0000	0.0000	0.2016(4)	0.6(2)	0.46(1)
Cu	0.0000	0.0000	0.0000	0.6(2)	0.10(1)
H	0.0000	0.0000	-0.0539(3)	1	0.32(1)

Bond	**Distance (Å)**
Ca(1)-O(1)	2.400(5)
Ca(1)-O(2)	2.461(5)
Ca(1)-O(3)	2.799(3)
Ca(2)-O(1)	2.702(12)
Ca(2)-O(2)	2.354(7)

Ca(2)-O(3)	2.351(3), 2.511(5)
Ca(2)-O(4)	2.364(5)
Ca(2)-Cu	2.905(4)
Ca(2)-H	2.702(12)
P-O(1)	1.538(7)
P-O(2)	1.551(5)
P-O(3)	1.525(3)
Cu-O(4)	1.387(9), 2.054(9)
Cu-H	0.37(2)
O(4)-H	1.02(2)
O(4)-O(4)	0.67(2)

Angle	°
O(1)-P-O(3)	111.4(3)
O(1)-P-O(2)	110.8(2)
O(3)-P-O(3)	108.0(3)
O(3)-P-O(2)	107.6(3)

$Ca_{10}(PO_4)_6Cu_xO_yH_z$ $x = 0.6$

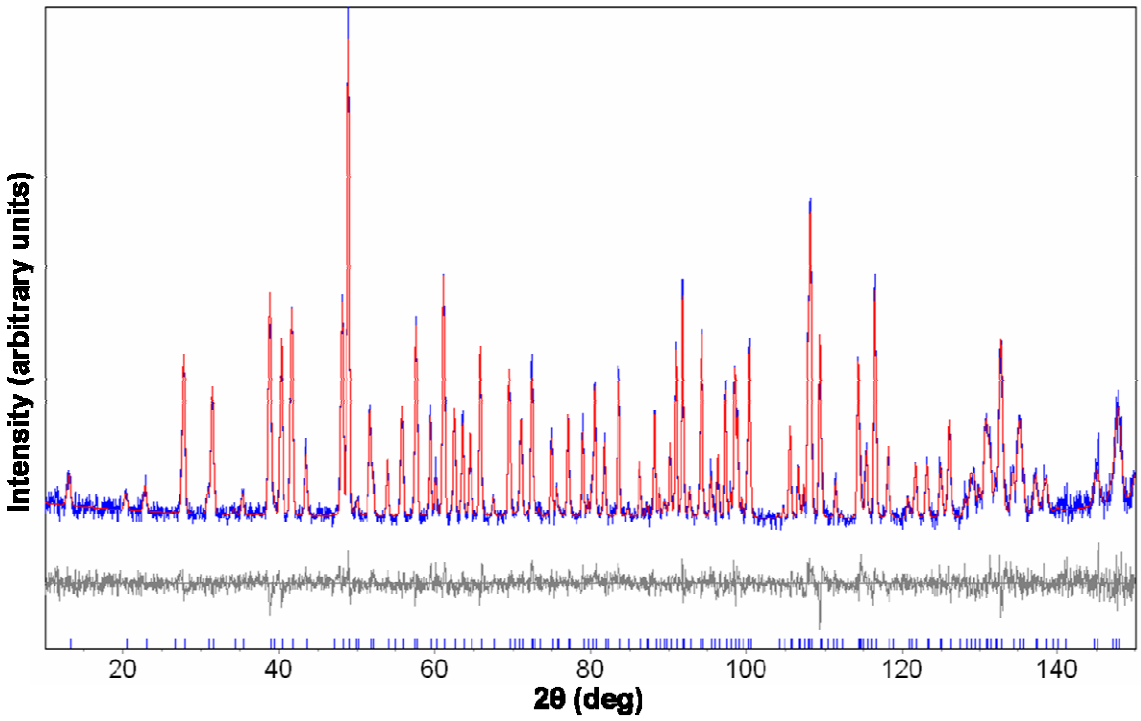


s.g	$P6_3/m$	a = 9.4262(1) Å	c = 6.9003(1) Å	R_{wp} = 6.90 %	R_{Bragg} = 2.32 %
Site	***x***	***y***	***z***	***B***	**Occ.**
Ca(1)	1/3	2/3	-0.0029(7)	1.02(9)	1
Ca(2)	0.2549(5)	0.0080(5)	1/4	0.64(8)	1
P	0.3696(4)	0.3999(5)	1/4	0.56(7)	1
O(1)	0.4846(4)	0.3292(4)	1/4	0.43(7)	1
O(2)	0.4667(5)	0.5890(4)	1/4	1.16(8)	1
O(3)	0.2589(3)	0.3455(3)	0.0712(3)	1.26(5)	1
O(4)	0.0000	0.0000	0.2058(12)	0.7(2)	0.50(1)
Cu	0.0000	0.0000	0.0000	0.7(2)	0.30(1)
H	0.0000	0.0000	-0.043(6)	1	0.20(1)

Bond	**Distance (Å)**
Ca(1)-O(1)	2.406(5)
Ca(1)-O(2)	2.467(5)
Ca(1)-O(3)	2.792(3)
Ca(2)-O(1)	2.702(5)
Ca(2)-O(2)	2.341(7)
Ca(2)-O(3)	2.358(5), 2.525(4)
Ca(2)-O(4)	2.385(5)
Ca(2)-Cu	2.928(4)
Ca(2)-H	2.76(2)
P-O(1)	1.531(7)
P-O(2)	1.543(5)
P-O(3)	1.529(3)
Cu-O(4)	1.420(8), 2.030(8)
Cu-H	0.30(3)
O(4)-H	1.12(4)
O(4)-O(4)	0.61(2)

Angle	**°**
O(1)-P-O(3)	111.5(3)
O(1)-P-O(2)	111.2(2)
O(3)-P-O(3)	107.5(3)
O(3)-P-O(2)	107.4(2)

$Ca_{10}(PO_4)_6Cu_xO_yH_z$ *x* = 1.0



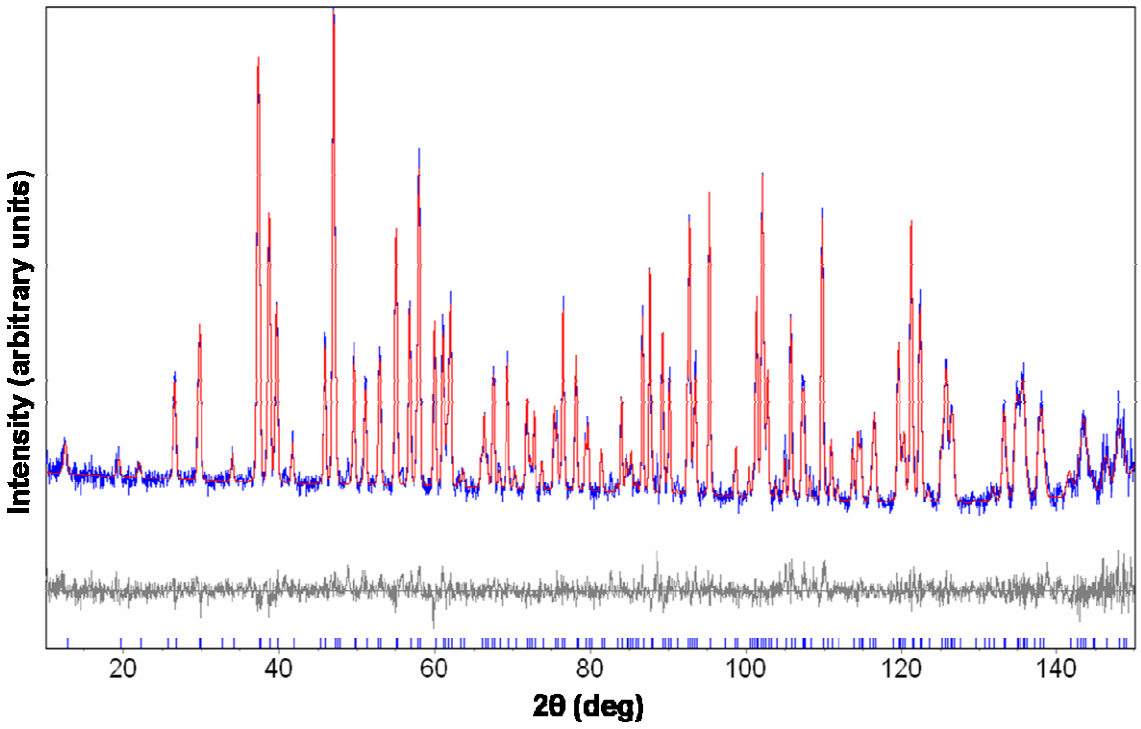
s.g	$P6_3/m$	a = 9.4392(2) Å	c = 6.9166(1) Å	R_{wp} = 7.37 %	R_{Bragg} = 2.30 %
Site	***x***	***y***	***z***	***B***	**Occ.**
Ca(1)	1/3	2/3	-0.0015(8)	0.9(1)	1
Ca(2)	0.2554(6)	0.0080(6)	1/4	0.6(1)	1
P	0.3697(5)	0.3994(5)	1/4	0.5(1)	1
O(1)	0.4850(5)	0.3293(4)	1/4	0.4(1)	1
O(2)	0.4661(5)	0.5891(5)	1/4	1.4(1)	1
O(3)	0.2589(4)	0.3463(4)	0.0704(3)	1.2(1)	1
O(4)	0.0000	0.0000	0.2111(16)	1.3 (2)	0.50(1)
Cu	0.0000	0.0000	0.0000	1.3(2)	0.36(1)
H	0.0000	0.0000	0.0472(7)	1	0.14(1)

Bond	**Distance (Å)**
Ca(1)-O(1)	2.415(3)
Ca(1)-O(2)	2.460(6)
Ca(1)-O(3)	2.786(4)
Ca(2)-O(1)	2.706(5)
Ca(2)-O(2)	2.345(8)
Ca(2)-O(3)	2.359(3), 2.532(5)
Ca(2)-O(4)	2.389(6)
Ca(2)-Cu	2.937(5)
Ca(2)-H	2.76(3)

P-O(1)	1.530(8)
P-O(2)	1.551(6)
P-O(3)	1.537(4)
Cu-O(4)	1.460(9), 1.998(9)
Cu-H	0.32(7)
O(4)-H	1.14(7)
O(4)-O(4)	0.54(2)

Angle	°
O(1)-P-O(3)	107.7(3)
O(1)-P-O(2)	106.7(3)
O(3)-P-O(3)	112.0(3)
O(3)-P-O(2)	106.7(3)

$Sr_{10}(PO_4)_6Cu_xO_y$ $x = 1.0$



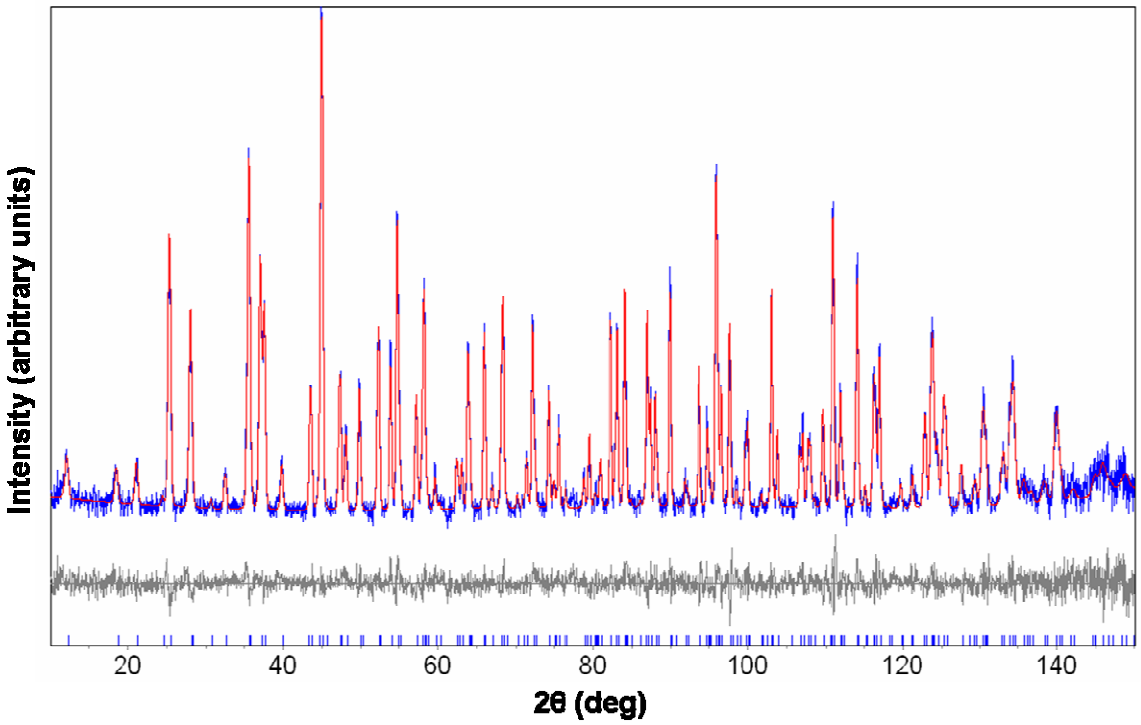
s.g	$P6_3/m$	$a = 9.7952(1)$ Å	$c = 7.2931(1)$ Å	$R_{wp} = 5.95$ %	$R_{Bragg} = 2.03$ %
Site	***x***	***y***	***z***	***B***	**Occ.**

Sr(1)	1/3	2/3	-0.0024(6)	0.51(8)	1
Sr(2)	0.2609(4)	0.0150(4)	1/4	0.67(7)	1
P	0.3675(5)	0.4008(5)	1/4	0.32 (9)	1
O(1)	0.4826(5)	0.3347(4)	1/4	0.82(8)	1
O(2)	0.4616(5)	0.5828(5)	1/4	1.09 (8)	1
O(3)	0.2624(4)	0.3482 (4)	0.0790(4)	1.03(7)	1
O(4)	0.0000	0.0000	0.2150(4)	1.8(2)	0.50(1)
Cu	0.0000	0.0000	0.0000	1.8(6)	0.44(1)
H	0.0000	0.0000	0.041(2)	1.0	0.06(1)

Bond	**Distance (Å)**
Sr(1)-O(1)	2.556(5)
Sr(1)-O(2)	2.583(5)
Sr(1)-O(3)	2.898(4)
Sr(2)-O(1)	2.779(4)
Sr(2)-O(2)	2.483(6)
Sr(2)-O(3)	2.525(3), 2.687(4)
Sr(2)-O(4)	2.499(4)
Sr(2)-Cu	3.083(3)
Sr(2)-H	2.92(7)
P-O(1)	1.556(8)
P-O(2)	1.545(6)
P-O(3)	1.533(4)
Cu-O(4)	1.57(14), 2.08(18)
O(4)-H	1.3(16)
O(4)-O(4)	0.51(3)

Angle	**°**
O(1)-P-O(3)	111.4(3)
O(1)-P-O(2)	110.0(1)
O(3)-P-O(3)	108.9(3)
O(3)-P-O(2)	107.5(3)

$Ba_{10}(PO_4)_6Cu_xO_y$ x = 1.0



s.g	$P6_3/m$	a = 10.2168(2) Å	c = 7.7347(2) Å	R_{wp} = 8.14 %	R_{Bragg} = 2.18 %
Site	***x***	***y***	***z***	***B***	**Occ.**
Ba(1)	1/3	2/3	0.0017(8)	0.7(1)	1
Ba(2)	0.2629(6)	0.0176(6)	1/4	0.9(1)	1
P	0.3689(5)	0.4026(6)	1/4	0.8(1)	1
O(1)	0.4796(5)	0.3412(5)	1/4	1.2(1)	1
O(2)	0.4578(5)	0.5774(5)	1/4	1.0(1)	1
O(3)	0.2670(4)	0.3478(4)	0.0886(4)	1.4(1)	1
O(4)	0.0000	0.0000	0.196(2)	3.4(4)	0.50(1)
Cu	0.0000	0.0000	0.0000	3.4(4)	0.45(1)
H	0.0000	0.0000	0.0002(4)	1.00	0.05(1)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(1)	0.016	0.021	0.020	0.014	0	0
O(2)	0.016	0.009	0.024	0.007	0	0
O(3)	0.017	0.033	0.017	0.016	-0.007	-0.009
O(4)	0.006	0.006	0.230	0.003	0	0
Cu	0.004	0.004	0.109	0.002	0	0

Bond	**Distance (Å)**

Ba(1)-O(1)	2.757(6)
Ba(1)-O(2)	2.702(6)
Ba(1)-O(3)	3.052(4)
Ba(2)-O(1)	2.918(6)
Ba(2)-O(2)	2.632(8)
Ba(2)-O(3)	2.733(3), 2.840(6)
Ba(2)-O(4)	2.632(6)
P-O(1)	1.544(9)
P-O(2)	1.543(7)
P-O(3)	1.540(4)
Cu-O(4)	1.52(14), 2.35(19)
O(4)-O(4)	0.84(4)

Angle	°
O(1)-P-O(3)	110.1(4)
O(1)-P-O(2)	108.6(4)
O(3)-P-O(3)	108.3(4)
O(3)-P-O(2)	108.6(4)

Oxygen O1s XPS spectra

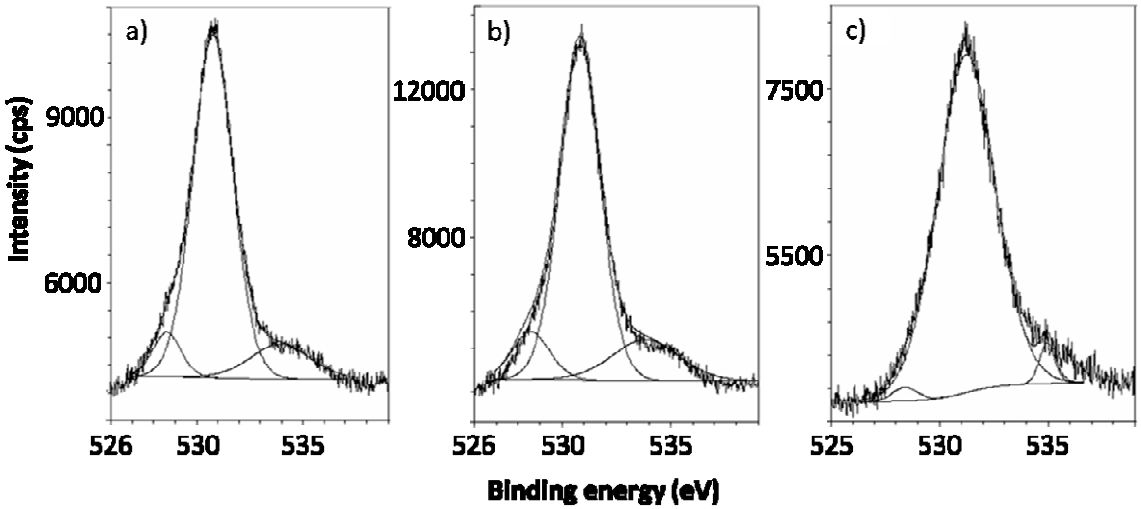


Figure S1. High resolution O1*s* spectra of Cu-apatite (x = 1.0 nominal) for a) Ca, b) Sr and c) Ba materials