Supplementary Materials

The Crystal Structure of Apatite and Copper-Doped Apatite

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It can be observed from Figures S1 and S2 that the XRD peaks of the intermediates $Pb_2(SO_4)O$ and Cu_3P closely match those of their respective Powder Diffraction File (PDF) cards. This consistency confirms that the intermediates are indeed $Pb_2(SO_4)O$ and Cu_3P, thereby establishing a foundation for the final synthesis of copium-doped lead apatite.

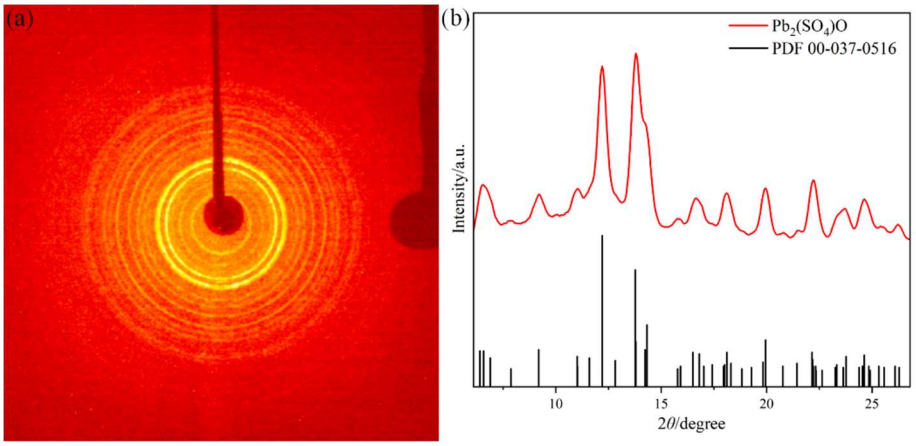

Figure S1 (a) The Phi360 diffraction pattern of the intermediate $Pb_2(SO_4)O$, (b) the powder diffraction pattern obtained by integrating the Phi360 diffraction pattern.

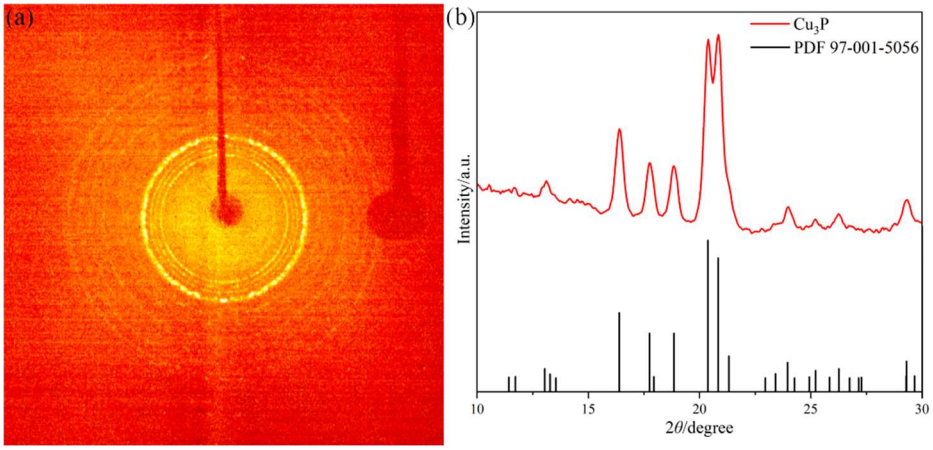

Figure S2 (a) The Phi360 diffraction pattern of the intermediate Cu_3P, (b) the powder diffraction pattern obtained by integrating the Phi360 diffraction pattern.

In order to determine the natural fluorapatite sample (A1) purchased from Shi-kong-dui-wang mineral morphology and the proportion of elements, Hitachi S-3400 field emission scanning electron microscope (SEM) was used to observe the morphology of single crystal sample, the elements in the sample were analyzed by energy dispersive X-ray spectroscopy (EDX), which was used in electron microscopy, the types and corresponding contents of the elements were analyzed. Concerning the selected fragment of the single crystal sample, EDX analysis was carried out and the corresponding results are listed in Table S1. It should be noted that although the element Cu is detected by Spot5, the detection position of Spot5 is the impurity on the surface of the sample, not the sample itself.

It can be seen from Table S1 that the sample is indeed fluorapatite; However, due to the conductive adhesives, small amount of glue attached to the surface, and the uneven surface of the sample, the proportion of elements may fluctuate. This explanation also applies to the SEM/EDX test results of the several samples presented below.

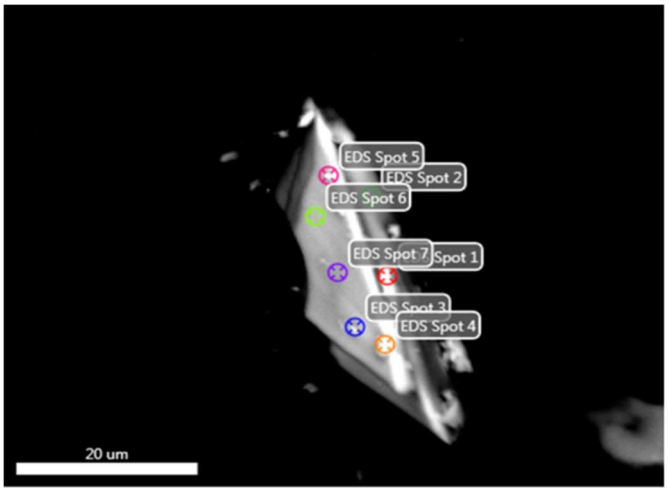

Figure S3 Scanning electron microscope (SEM) micrographs of single crystal sample of natural fluorapatite sample (A1) purchased from Shi-kong-dui-wang mineral. EDX analysis was performed for various locations as indicated in Table S1.

Table S1 The EDX results conducted at every scanning location in the natural fluorapatite sample (A1).

	Element	Atomic(%)	Error(%)
Spot1	O	60.45	9.87
	F	11.28	11.06
	Si	0.96	5.58
	P	10.08	3.26
	Ca	17.24	1.78
Spot2	O	58.89	10.03
	F	9.53	11.22
	Si	1.03	5.52
	P	11.05	3.23
	Ca	19.50	1.78
Spot3	C	41.39	9.02
	O	36.21	10.21
	F	5.32	11.31
	Si	0.33	6.35
	P	5.79	2.85
	Ca	10.96	1.56
Spot4	O	59.30	9.99
	F	11.16	11.14
	Si	0.92	5.69
	P	10.15	3.28

	Ca	18.46	1.79
Spot5	C	31.36	10.19
	O	33.93	10.57
	F	5.97	11.52
	P	9.17	3.23
	Ca	19.57	1.76
	Cu	1.81	4.89
Spot6	C	28.88	10.11
	O	39.29	10.43
	F	6.11	11.54
	P	8.91	2.89
	Ca	16.81	1.66
Spot7	C	39.36	9.35
	O	34.01	10.43
	F	5.65	11.41
	P	7.16	2.80
	Ca	13.82	1.59

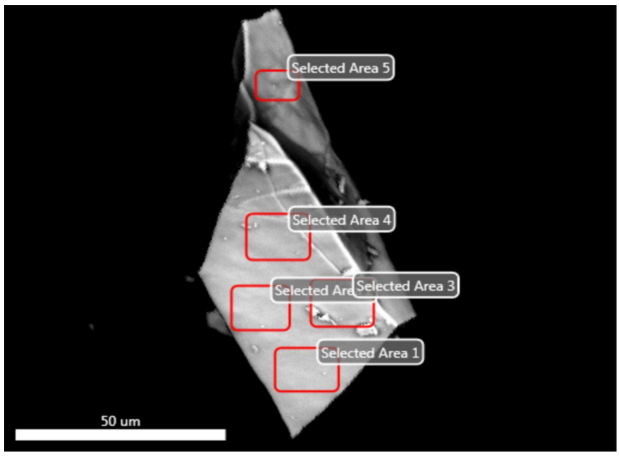

Figure S4 Scanning electron microscope (SEM) micrographs of single crystal sample of natural hydroxyapatite sample (A2) purchased from SNQP-yu-he mineral. EDX analysis was performed for various locations as indicated in Table S2.

Table S2 The EDX results conducted at every scanning location in the natural hydroxyapatite sample (A2).

	Element	**Atomic(%)**	**Error(%)**
Area 1	O	61.04	12.13
	P	7.12	4.67
	Ca	31.84	2.06
Area 2	O	46.29	11.99
	P	11.12	3.74
	Ca	42.60	1.81
Area 3	O	55.43	12.00
	P	6.46	4.53
	Ca	38.11	1.78
Area 4	O	45.91	12.18
	P	8.75	4.17
	Ca	45.34	1.75
Area 5	O	67.26	10.18
	P	11.66	3.10
	Ca	21.08	1.80

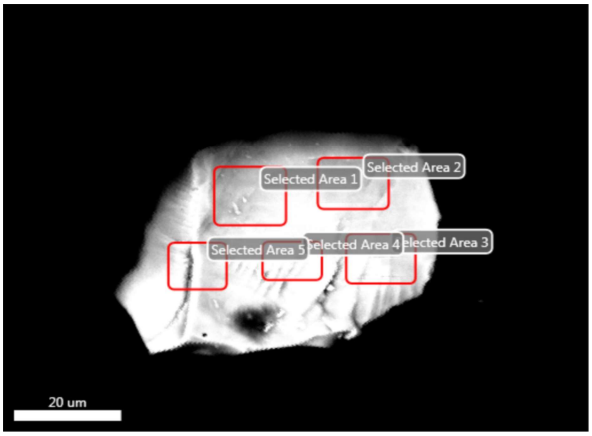

Figure S5 Scanning electron microscope (SEM) micrographs of single crystal sample of natural hydroxyapatite sample (A3) purchased from Jing-hua-shang-mao mineral. EDX analysis was performed for various locations as indicated in Table S3.

Table S3 The EDX results conducted at every scanning location in the natural hydroxyapatite sample (A3).

	Element	Atomic(%)	Error(%)
Area 1	O	34.53	12.75
	P	6.95	4.22
	Ca	58.52	1.64
Area 2	O	28.04	13.84
	P	5.65	6.26
	Ca	66.30	1.60
Area 3	O	27.85	13.81
	P	6.16	5.04
	Ca	65.99	1.60
Area 4	O	26.24	13.17
	P	9.89	3.87
	Ca	63.87	1.67
Area 5	O	25.80	13.11
	P	11.75	3.73
	Ca	62.45	1.71

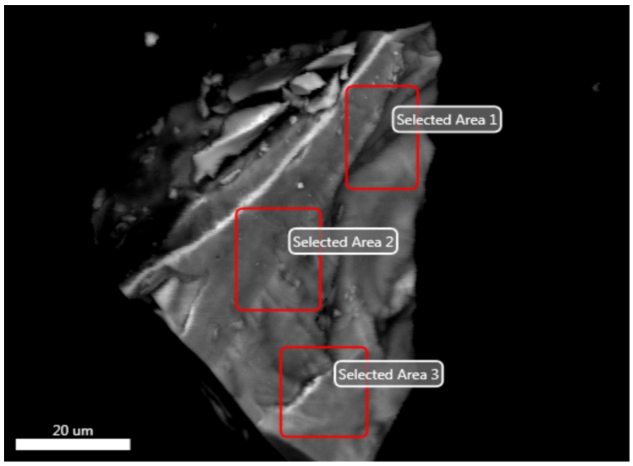

Figure S6 Scanning electron microscope (SEM) micrographs of single crystal sample of natural hydroxyapatite sample (A4) purchased from Xun-cheng-kuang-wu mineral. EDX analysis was performed for various locations as indicated in Table S4.

Table S4 The EDX results conducted at every scanning location in the natural hydroxyapatite sample (A4).

	Element	Atomic(%)	Error(%)
Area 1	C	61.43	7.36
	O	21.30	11.77
	P	2.11	3.88
	Ca	15.16	1.70
Area 2	C	58.19	7.70
	O	22.50	11.66
	P	2.73	3.66
	Ca	16.58	1.64
Area 3	C	74.91	5.12
	O	21.84	11.67
	Al	0.05	64.12
	P	0.14	17.82
	Ca	3.06	2.88

Table S5 Refined atomic coordinates of A1 (fluorapatite purchased from Shi-kong-dui-wang mineral) in the hexagonal $P6_3/m$ (No. 176) structure, extracted from single crystal XRD measurements. The obtained lattice constants are a, b = 9.3849(3) Å and c = 6.8814 (3) Å.

Label	Site	x	y	z	Occ.	U_{eq}
F1	2*a*	0.000000	0.000000	0.250000	1.000	0.0315(10)
Ca1	4*f*	0.666667	0.333333	0.00119(11)	1.000	0.01082(19)
Ca2	6*h*	-0.00749(8)	0.24145(8)	0.250000	1.000	0.00987(16)
P1	6*h*	0.36949(9)	0.39877(9)	0.250000	1.000	0.00759(18)
O1	6*h*	0.4844(3)	0.3266(3)	0.250000	1.000	0.0126(5)
O2	6*h*	0.4668(3)	0.5876(3)	0.250000	1.000	0.0150(5)
O3	12*i*	0.2578(2)	0.3422(2)	0.0707(3)	1.000	0.0184(4)

Table S6 Refined atomic coordinates of A2 (hydroxyapatite purchased from SNQP-yu-he mineral) in the hexagonal $P6_3/m$ (No. 176) structure, extracted from single crystal XRD measurements. The obtained lattice constants are a, b = 9.3654(4) Å and c = 6.8786 (3) Å.

Label	Site	x	y	z	Occ.	U_{eq}
Ca1	4*f*	0.666667	0.333333	0.00099(14)	1.000	0.0096(2)
Ca2	6*h*	-0.00735(9)	0.24181(9)	0.250000	1.000	0.0069(2)
P1	6*h*	0.36890(12)	0.39829(11)	0.250000	1.000	0.0059(2)
O1	6*h*	0.4848(3)	0.3269(3)	0.250000	1.000	0.0107(6)
O2	6*h*	0.4666(3)	0.5876(3)	0.250000	1.000	0.0128(6)
O3	12*i*	0.2571(2)	0.3415(3)	0.0705(3)	1.000	0.0145(5)
O4	4*e*	0.000000	0.000000	0.2709(15)	0.500	0.0017(10)
H1	4*e*	0.000000	0.000000	0.154(3)	0.500	0.00(3)

Table S7 Refined atomic coordinates of A3 (hydroxyapatite purchased from Jing-hua-shang-mao mineral) in the hexagonal $P6_3/m$ (No. 176) structure, extracted from single crystal XRD measurements. The obtained lattice constants are a, b = 9.3731(4) Å and c = 6.8769 (3) Å.

Label	Site	x	y	z	Occ.	U_{eq}
Ca1	4*f*	0.666667	0.333333	0.00112(11)	1.000	0.0094(2)
Ca2	6*h*	-0.00720(7)	0.24198(8)	0.250000	1.000	0.00777(17)
P1	6*h*	0.36889(9)	0.39830(9)	0.250000	1.000	0.00605(19)
O1	6*h*	0.4847(3)	0.3270(3)	0.250000	1.000	0.0107(5)
O2	6*h*	0.4668(3)	0.5876(3)	0.250000	1.000	0.0120(5)
O3	12*i*	0.25715(19)	0.3417(2)	0.0706(2)	1.000	0.0142(4)
O4	4*e*	0.000000	0.000000	0.2700(14)	0.500	0.0018(9)
H1	4*e*	0.000000	0.000000	0.155(3)	0.500	0.00(2)

Table S8 Refined atomic coordinates of A4 (hydroxyapatite purchased from Xun-cheng-kuang-wu mineral) in the hexagonal $P6_3/m$ (No. 176) structure, extracted from single crystal XRD measurements. The obtained lattice constants are a, b = 9.3801(3) Å and c = 6.8748 (3) Å.

Label	**Site**	***x***	***y***	***z***	**Occ.**	U_{eq}
Ca1	4*f*	0.666667	0.333333	0.00111(10)	1.000	0.00998(18)
Ca2	6*h*	-0.00719(7)	0.24222(7)	0.250000	1.000	0.00843(17)
P1	6*h*	0.36906(9)	0.39864(8)	0.250000	1.000	0.00646(18)
O1	6*h*	0.4849(2)	0.3274(3)	0.250000	1.000	0.0110(4)
O2	6*h*	0.4665(3)	0.5876(2)	0.250000	1.000	0.0134(5)
O3	12*i*	0.25741(17)	0.34203(19)	0.0705(2)	1.000	0.0159(3)
O4	4*e*	0.000000	0.000000	0.272(4)	0.500	0.008(4)
H1	4*e*	0.000000	0.000000	0.153(5)	0.500	0.009

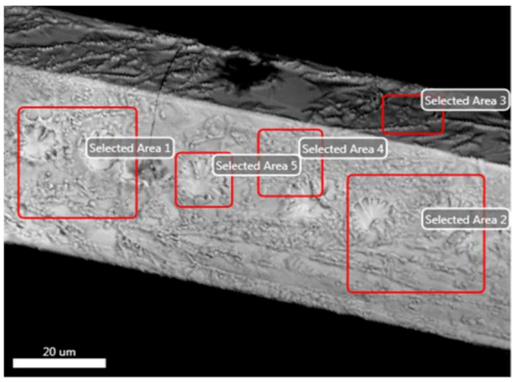

Figure S7 Scanning electron microscope (SEM) micrographs of single crystal sample of $Pb_{10-x}Cu_x(PO_4)_6O$-12h. EDX analysis was performed for various locations as indicated in Table S9.

Table S9 The EDX results conducted at every scanning location in the $Pb_{10-x}Cu_x(PO_4)_6O$-12h sample.

	Element	Atomic(%)	Error(%)
Area 1	O	52.92	10.62
	Si	3.46	9.14
	P	10.85	4.97
	S	16.89	4.49
	Pb	14.29	2.51
	Cu	1.60	23.23
Area 2	O	55.27	10.56
	Cu	0.23	67.21
	Si	2.42	10.03
	P	10.95	4.85
	S	17.00	4.41
	Pb	14.13	2.50
Area 3	O	71.37	9.80
	Cu	2.97	8.10
	Si	2.34	9.32
	P	8.58	5.16
	Pb	14.75	2.02
Area 4	O	60.04	10.61
	Si	2.65	10.35
	P	11.97	5.35
	Pb	23.29	1.93
	Cu	2.05	21.47
Area 5	O	55.26	10.49
	Cu	0.64	27.64

	Si	4.01	7.92
	P	11.27	4.91
	S	14.88	4.53
	Pb	13.94	2.32

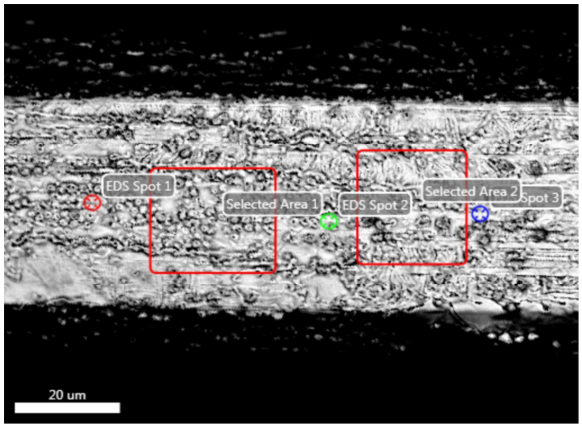

Figure S8 Scanning electron microscope (SEM) micrographs of single crystal sample of $Pb_{10-x}Cu_x(PO_4)_6O$-24h. EDX analysis was performed for various locations as indicated in Table S10.

Table S10 The EDX results conducted at every scanning location in the $Pb_{10-x}Cu_x(PO_4)_6O$-24h sample.

	Element	Atomic(%)	Error(%)
Spot 1	O	52.10	10.70
	P	11.47	4.83
	S	18.23	4.37
	Pb	18.20	2.28
Spot 2	O	51.44	10.72
	P	13.92	4.78
	S	15.99	4.52
	Pb	18.65	2.12
Spot 3	O	56.40	10.49
	P	10.45	4.79
	S	16.70	4.32
	Pb	16.44	2.36
Area 1	O	51.80	10.61
	P	8.63	5.16
	S	20.13	4.26
	Pb	16.78	2.35
	Cu	2.66	14.66
Area 5	O	52.31	10.62
	P	9.56	4.93
	S	19.22	4.30
	Pb	17.16	2.34
	Cu	1.75	20.72

Table S11 Refined atomic coordinates of $Pb_9Cu(PO_4)_6O$ in the hexagonal $P6_3/m$ (No. 176) structure, extracted from single crystal XRD measurements by Puphal *et al*. The obtained lattice constants are a, b = 9.7393 (19) Å and c = 7.3953 (12) Å.

Label	***x***	***y***	***z***	**Occ.**	**Uiso(Å²)**
Pb1	0.333333	0.666667	0.0040(3)	0.90(6)	0.0040(9)
Cu1	0.333333	0.666667	0.0040(3)	0.10(6)	0.0040(9)
Pb2	0.7531(2)	0.7546(3)	0.25	0.86(6)	0.0060(8)
Cu2	0.7531(2)	0.7546(3)	0.25	0.14(6)	0.0060(8)

P1	0.4026(16)	0.3724(14)	0.25	1	0.001(3)
O1	1	1	0.5	1	0.008(19)
O2	0.336(5)	0.490(4)	0.25	0.90(6)	0.002(8)
O3	0.587(4)	0.474(4)	0.25	0.86(6)	0.007(8)
O4	0.351(4)	0.266(4)	0.084(4)	1	0.023(8)