Thorium Copper Phosphides: More Diverse Metal–Phosphorus and Phosphorus–Phosphorus Interactions than U analogues

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Supplementary Information

Figure S1. Powder X-ray diffraction patterns of black products from Th/Cu/P/CuI reactions. a). ThCuP$_2$ synthesized at 923 K; b). β-ThCu$_2$P$_2$ and ThCu$_5$P$_3$ synthesized at 923 K; c). ThCu$_5$P$_3$ synthesized at 1073 K; d) and e) Reaction of Th, Cu, and P in a molar ratio of 1:2:2 without CuI at 923 K for 8 days.
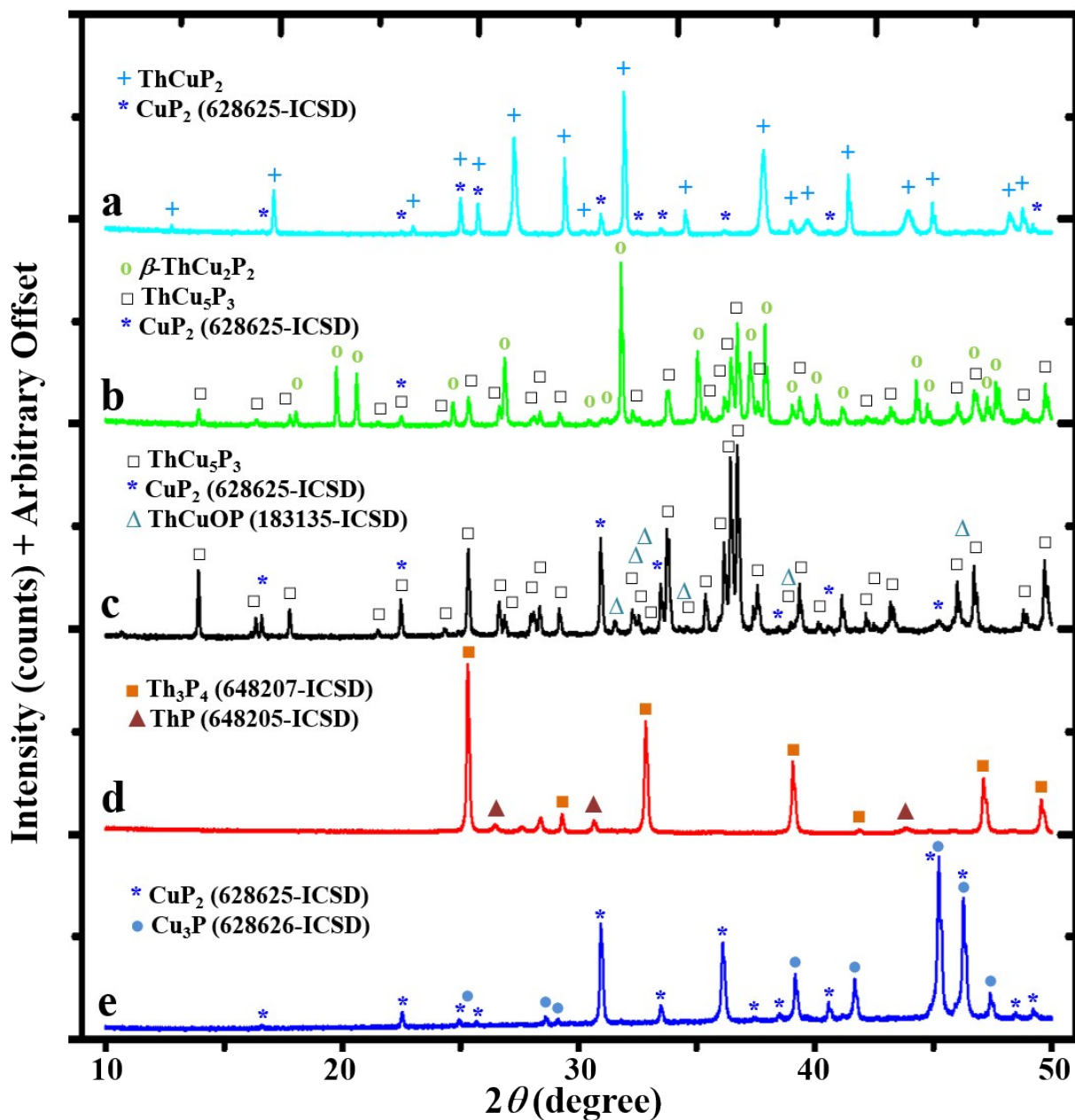
Figure S2. Synthesized *hk1* precession images in APEX2 from diffraction frames of a crystal of ThCuP$_2$.
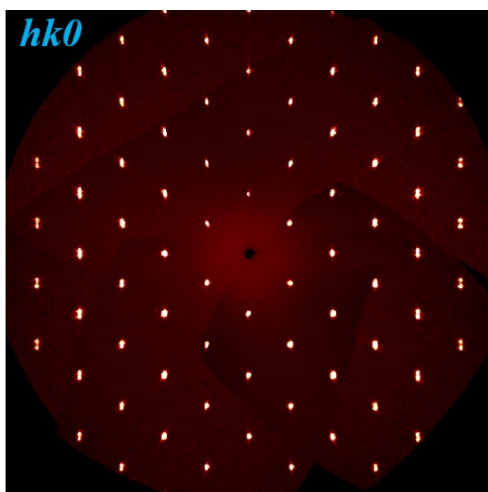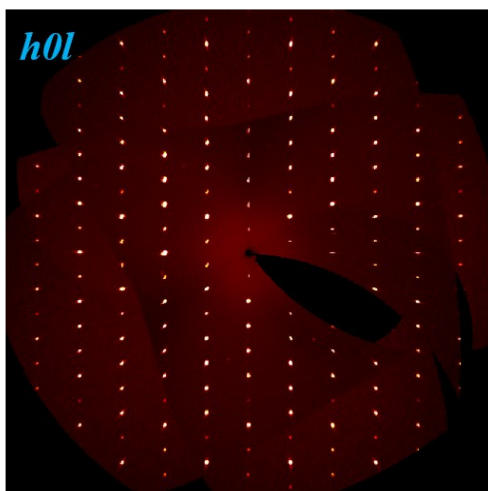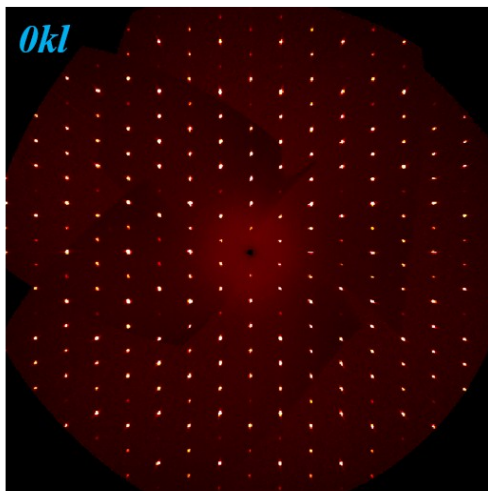
Figure S3. Synthesized *hk1* precession images simulated in APEX2 from diffraction frames of a crystal of ThCu$_5$P$_3$.
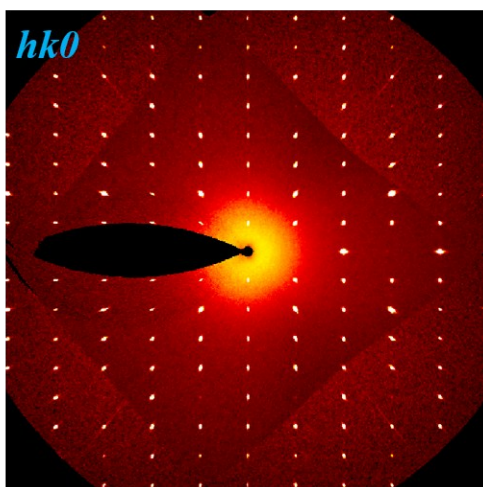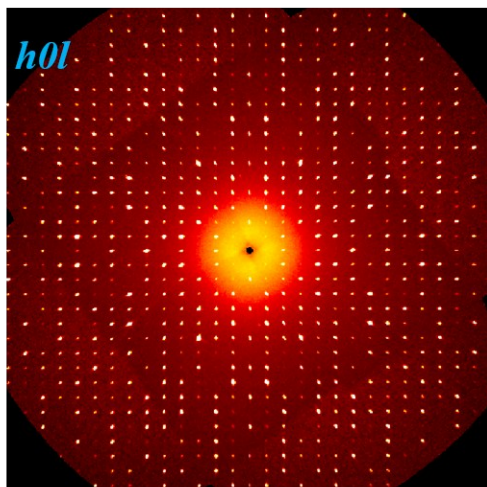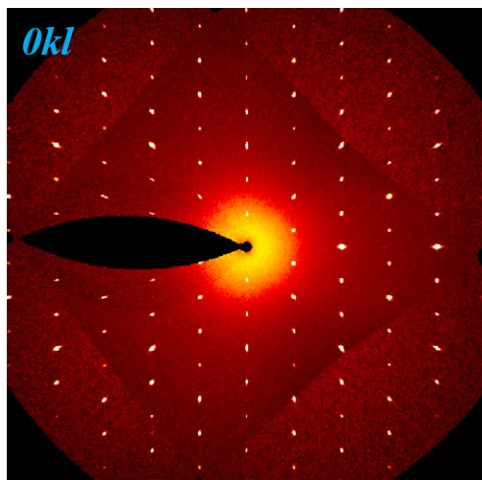
Figure S4. Solid products from reaction of Th, Cu, and P in a molar ratio of 1:2:2 at 923 K for 8 days.
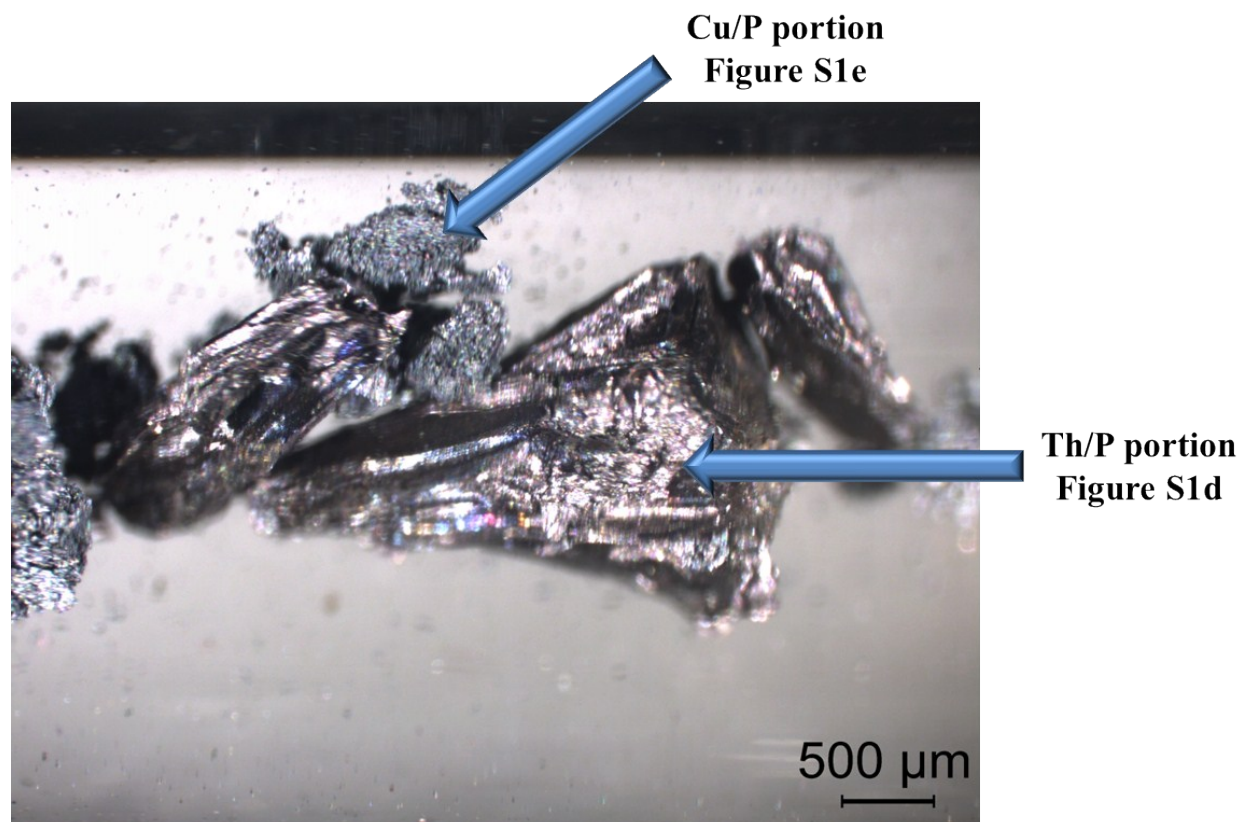
Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for ThCuP$_2$. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Th(1)	0	0	3526(1)	7(1)
Cu(1)	0	0	1180(1)	9(1)
P(1)	655(8)	3044(6)	0	8(1)
P(2)	5000	0	2034(2)	8(1)

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for β-ThCu$_2$P$_2$. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Th(1)	2503(1)	2500	3136(1)	6(1)
Cu(1)	563(1)	2500	5957(1)	7(1)
Cu(2)	696(1)	2500	476(1)	7(1)
P(1)	3243(1)	2500	248(1)	7(1)
P(2)	4750(1)	2500	6821(1)	7(1)

Table S3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for $ThCu_5P_3$. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
Th(1)	2910(1)	2500	764(1)	3(1)
Cu(1)	24(1)	2500	5937(1)	6(1)
Cu(2)	3136(1)	2500	3641(1)	6(1)
Cu(3)	3238(1)	2500	7826(1)	6(1)
Cu(4)	5604(1)	2500	5424(1)	5(1)
Cu(5A)	459(4)	2500	2000(4)	13(2)
Cu(5B)	260(20)	2500	2114(16)	63(4)
P(1)	1130(1)	2500	4030(1)	5(1)
P(2)	1326(1)	2500	7567(1)	4(1)
P(3)	3781(1)	2500	5735(1)	4(1)