Ca₆Cu₂Sn₇: Novel 3D open framework with unusual Sn₄ tetramers

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Supporting Information

Table S1. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Ca₆Cu₂Sn₇.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ca(1)	15(1)	4(1)	13(1)	0	0(1)	0
Ca(2)	16(1)	5(1)	11(1)	0	2(1)	0
Ca(3)	16(1)	6(1)	14(1)	0	0(1)	0
Cu(1)	19(1)	9(1)	13(1)	0	3(1)	0
Sn(1)	13(1)	6(1)	9(1)	0	2(1)	0
Sn(2)	13(1)	6(1)	10(1)	0	2(1)	0
Sn(3)	17(1)	5(1)	10(1)	0	3(1)	0
Sn(4)	20(1)	5(1)	17(1)	0	-6(1)	0

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12} \dots]$

Table S2. Selected Bond Distances ($\text{\AA}$) and Mulliken Overlap Populations (MOP) for Ca₆Cu₂Sn₇.

Bond	bond length	MOP	Bond	bond length	MOP
Cu(1)-Sn(1)	2.633(2)	0.544	Cu(1)-Sn(4)	2.696(1)	0.274
Cu(1)-Sn(3)	2.766(2)	0.303	Cu(1)-Sn(3)	2.787(1)	0.286
Sn(1)-Sn(2)	2.881(2)	0.665	Sn(2)-Sn(2)	2.917(2)	0.644
Sn(3)-Sn(4)	3.241(1)	0.289	Sn(3)...Sn(3)	3.451(1)	0.124

Figure S1. Experimental and simulated XRD powder patterns for $\text{Ca}_6\text{Cu}_2\text{Sn}_7$.

Figure S2. Coordination geometries around Ca and Cu atoms in $\text{Ca}_6\text{Cu}_2\text{Sn}_7$.

Figure S3. The coordination geometries around the Sn atoms in $\text{Ca}_6\text{Cu}_2\text{Sn}_7$.