Experimental and theoretical investigations of the novel ternary compound Ca_4InGe_4

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SUPPORTING INFORMATION

Table S1. Important crystal data collection and structure refinement parameters for $Eu_{0.18}Ca_{3.82(1)}InGe_4$.

Empirical formula	$Eu_{0.18}Ca_{3.82(1)}InGe_4$
Formula weight, $Z = 4$	585.64
Crystal system	Monoclinic
Space group	$C2/c$ (No.15)
Temperature (K)	200
Unit cell dimensions	$a = 18.463(4)$ Å
	$b = 5.845(1)$ Å
	$c = 8.347(1)$ Å
	$\beta = 99.27(3)°$
Volume (Å^3)	888.9(3)
Density (calculated, g/cm^3)	4.376
Absorption coefficient (cm^{-1})	192.8
Data / restraints / parameters	1159 / 0 / 44
Final R[a] indices [I>2σ(I)]	$R_1 = 0.0482$
	$wR_2 = 0.0866$
R[a] indices (all data)	$R_1 = 0.0885$
	$wR_2 = 0.1029$
Goodness-of-fit on F^2	0.971
Largest diff. peak/ hole (e/Å^3)	1.728 / –1.355

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$; $wR_2 = [\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2}$, and $w = 1/[\sigma^2F_o^2 + (0.0159\cdot P)^2, P = (F_o^2 + 2F_c^2)/3$.

Table S2. Atomic coordinates and equivalent isotropic displacement parameters U_{eq} (Å^2) for $Eu_{0.18}Ca_{3.82(1)}InGe_4$.

Atom	Wyckoff site	*x*	*y*	*z*	U_{eq} [a]	Occupancy
Eu/Ca1	8*f*	0.0783(1)	0.1415(3)	0.1239(2)	0.0011(1)	0.917/0.083(1)
Eu/Ca2	8*f*	0.3057(1)	0.1324(3)	0.1993(2)	0.0010(1)	0.953/0.046(2)
In	4*e*	0	0.6547(2)	1/4	0.0012(1)	
Ge1	8*f*	0.0834(1)	0.3612(2)	0.4779(1)	0.0011(1)	
Ge2	8*f*	0.1944(1)	0.1269(2)	0.4415(1)	0.0012(1)	

[a] U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

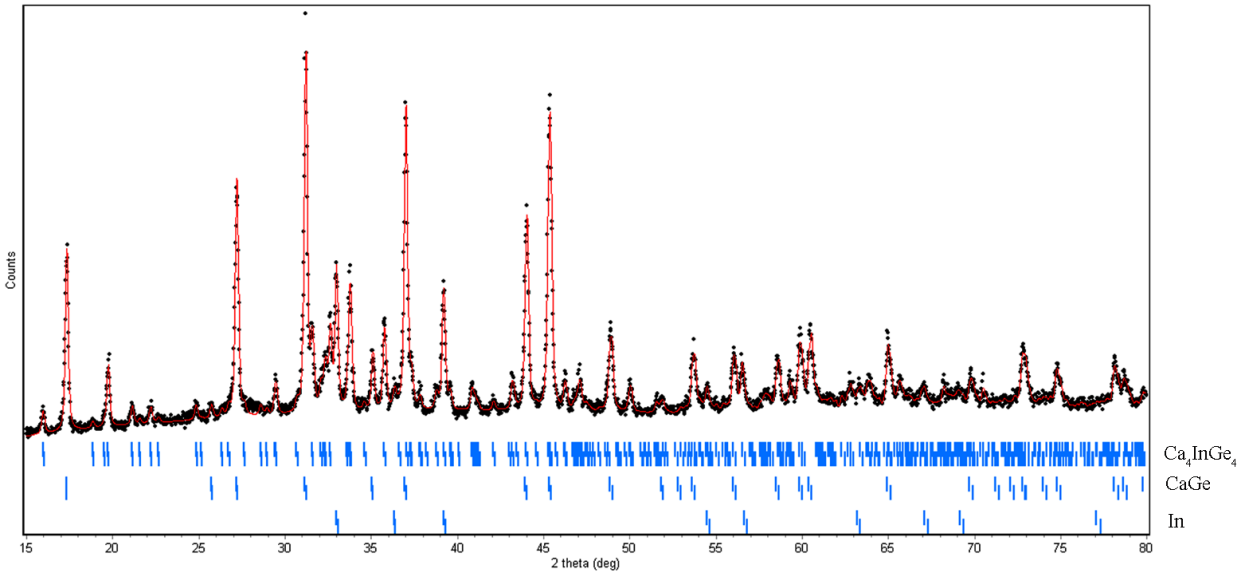

Figure S1. Measured and calculated powder X-ray diffraction pattern of Ca_4InGe_4. Peak positions are fitted using three phases: Ca_4InGe_4, CaGe, and elemental In.