Supporting Information

Composition, structure, bonding and thermoelectric properties of "CuT_2P_3" and "CuT_4P_3", members of the $T_{1-x}(CuP_3)_x$ series with T being Si and Ge

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1. Refinement results for "$CuSi_2P_3$" and "$CuGe_2P_3$" from neutron powder diffraction data

Table 1. Neutron powder refinement data for the $CuSi_2P_3$ and $CuGe_2P_3$ samples.

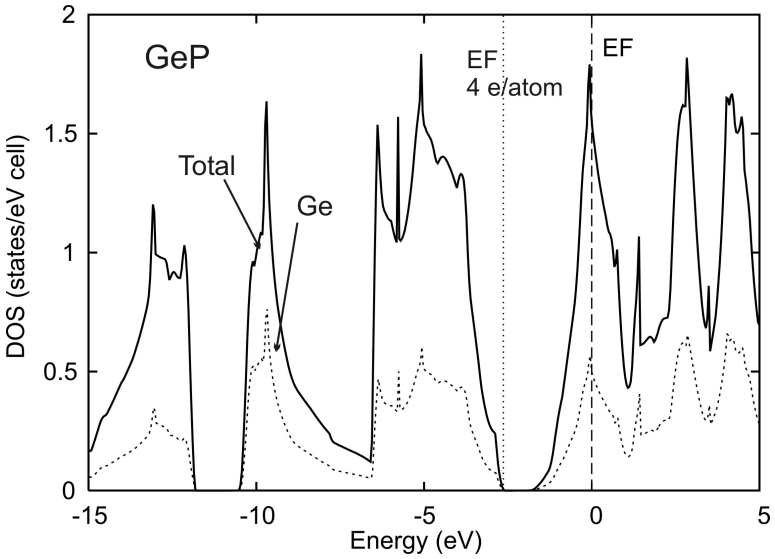
Loaded composition	$CuSi_2P_3$	$CuGe_2P_3$
Refined composition	$Cu_{1.0(4)}Si_{2.0(4)}P_3$	$Cu_{0.89}Ge_{2.6(2)}P_{2.5(2)}$
Lattice parameter, Å	a = 3.7110(1)	a = 5.3970(2)
	c = 5.1989(3)	
Volume, Å^3	71.595(5)	157.20(1)
Z	2/3	4/3
Reflections	31	16
Atomic param. refined	3	3
R_I	0.012	0.014
R_P	0.029	0.036
R_{wP}	0.038	0.045

$R_I = \Sigma |I_o - I_c| / \Sigma |I_o|$, $R_P = \Sigma |y_{oi} - y_{ci}| / \Sigma |y_{oi}|$, $R_{wP} = (\Sigma w_i (y_{oi} - y_{ci})^2 / \Sigma w_i (y_{oi})^2)^{1/2}$, $w_i = (y_{oi})^{-1/2}$.

Table 2. Atomic and isotropic temperature factor (*B*) parameters for the $CuSi_2P_3$ and $CuGe_2P_3$ samples from the neutron powder diffraction data.

Atom	Site	Occupancy	*x/a*	*y/b*	*z/c*	*B* (Å^2)
			$Cu_{1.0(4)}Si_{2.0(4)}P_3$			
Cu/Si(1)	4*a*	0.34/0.66(14)	0	0	0	0.4(2)
P(2)	4*c*	1.00	0	1/2	3/4	0.8(2)
			$Cu_{0.89}Ge_{2.6(2)}P_{2.5(2)}$			
Cu/Ge(1)	4*a*	0.295/0.705	0	0	0	0.77(6)
P/Ge(2)	4*c*	0.82/0.18(5)	1/4	1/4	1/4	0.86(10)

2. Density of states for the binary GeP with the zinc blende structure calculated using the TB-LMTO-ASA method:



3. Arrhenius plot for the $CuSi_2P_3$ sample.