

Pr₆₂Fe₂₁M₁₆C₃₂ vs. Pr₂₁Fe₈M'₇C₁₂ (M = Si, P; M' = Si, Ge, Sn): Competing intermetallic carbides grown from Pr/Ni flux

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Supporting Information

Table S1. Atom positions and thermal parameters for Pr₆₂Fe₂₁Si₁₆C₃₂.

atom	Wyckoff	x	y	z	sof	U_{eq}
Pr(1)	16u	0.12239(2)	0.35922(2)	0.16524(3)	1	0.00737(8)
Pr(2)	8s	0.15500(3)	0	0.21416(4)	1	0.0087(1)
Pr(3)	8r	0.35897(2)	0.35897(2)	0.23380(4)	1	0.0067(1)
Pr(4)	8q	0.16865(3)	0.35412(3)	½	1	0.0057(1)
Pr(5)	4o	0.35314(5)	½	½	1	0.0115(1)
Pr(6)	4n	0.27249(4)	½	0	1	0.0074(1)
Pr(7)	4k	0.12607(3)	0.12607(3)	½	1	0.0052(1)
Pr(8)	4j	0.15688(3)	0.15688(3)	0	1	0.0103(1)
Pr(9)	4i	0	½	0.35094(5)	1	0.0059(1)
Pr(10)	2f	0	½	0	0.498(6)	0.0166(7)
Pr(11)	1c	½	½	0	1	0.0069(3)
Fe(1)	8s	0.29531(7)	0	0.3851(1)	1	0.0043(2)
Fe(2)	8r	0.19858(5)	0.19858(5)	0.2705(1)	1	0.0042(2)
Fe(3)	4j	0.29166(7)	0.29166(7)	0	1	0.0046(3)
Fe(4)	2g	0	0	0.3912(3)	0.36(2)	0.006(1)
Si(4)	2g	0	0	0.3912(3)	0.64(2)	0.006(1)
Si(1)	8t	0.2160(2)	½	0.2989(2)	1	0.0078(4)
Si(2)	4l	0.2778(3)	0	0	1	0.0146(7)
Si(3)	2h	½	½	0.3111(4)	1	0.0092(9)
Si(5)	1a	0	0	0	1	0.010(1)
C(1)	16u	0.1028(4)	0.2507(4)	0.3366(5)	1	0.006(1)
C(2)	8r	0.2500(4)	0.2500(4)	0.1406(7)	1	0.007(2)
C(3)	4m	0.3873(7)	0	½	1	0.005(2)
C(4)	4j	0.3799(6)	0.3799(6)	0	1	0.010(2)

Table S2. Atom positions and thermal parameters for Pr₂₁Fe₈Si₇C₁₂.

atom	Wyckoff	x	y	z	U_{eq}
Pr(1)	48 <i>h</i>	0	0.16544(2)	0.16544(2)	0.0052(2)
Pr(2)	32 <i>f</i>	0.36835(2)	0.36835(2)	0.36835(2)	0.0043(2)
Pr(3)	4 <i>b</i>	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0.0195(4)
Fe	32 <i>f</i>	0.19311(5)	0.19311(5)	0.19311(5)	0.0041(3)
Si(1)	24 <i>e</i>	0.2910(2)	0	0	0.0060(6)
Si(2)	4 <i>a</i>	0	0	0	0.011(2)
C	48 <i>g</i>	0.1045(5)	$\frac{1}{4}$	$\frac{1}{4}$	0.007(1)