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Synthesis and Crystal Structure of the Zintl Phases NaSrSb, NaBaSb and NaEuSb

Yi Wang and Svilen Bobev *

Department of Chemistry and Biochemistry, University of Delaware, Newark, DE 19716, USA
* Correspondence: bobev@udel.edu

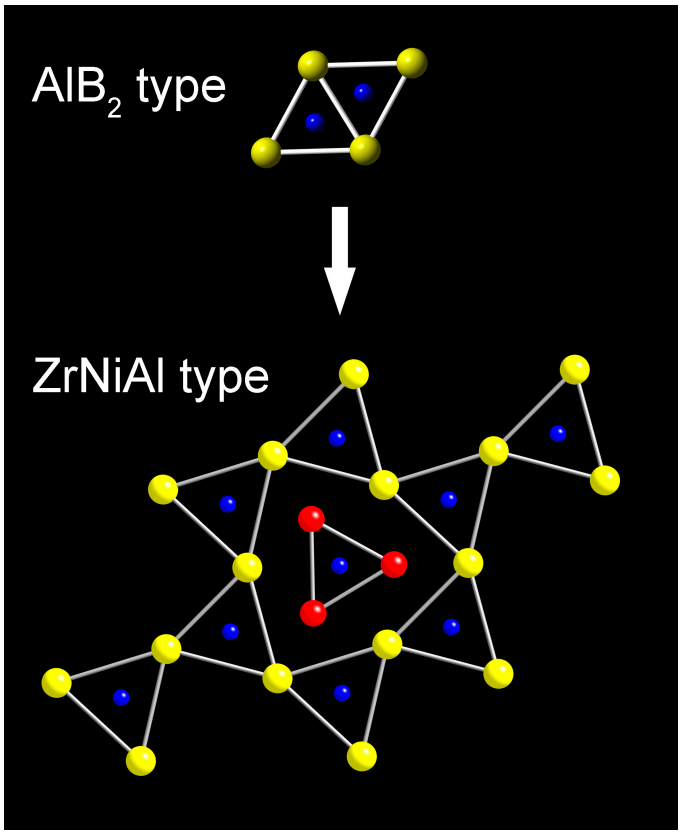

Figure S1. The hexagonal crystal structure of AlB_2, and the hexagonal crystal structure of ZrNiAl, both projected down the *c*-axis. The representation emphasizes the trigonal prisms having metal atoms at the corners and B atoms (AlB_2) and Al atoms ((ZrNiAl) at the center. The different three-dimensional connectivity of these prisms leads to the two structure types, respectively. For a comprehensive overview of the relationships between AlB_2-related intermetallic compounds, the reader is referred to the following review article: Hoffmann, R-D.; Pöttgen, R. AlB_2-related intermetallic compounds—a comprehensive view based on group-subgroup relations. *Z. Kristallogr.* **2001**, *216*, 127–145.

Table S1. Some known equiatomic compounds formed between the alkali metals (*A*), the alkaline-earth metals (*AE*), and the group 15 elements P, As, Sb, Bi, (*Pn*).

Compound	Structure Type	Space Group	Pearson Symbol	Ref.
LiBeP	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[1]
LiBeAs	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[2]
NaMgAs	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[3]
NaMgSb	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[3]
NaMgBi	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[4]
KMgP	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[5]
KMgAs	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[5]
KMgSb	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[5]
KMgBi	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[5]
KCaBi	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[6]
RbCaAs	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[7]
RbCaSb	PbClF (Cu_2Sb)	*P*4/*nmm*	*tP*6	[7]
LiMgP	LiAlSi (half-Heusler)	$F\bar{4}3m$	*cF*12	[1]
LiMgAs	LiAlSi (half-Heusler)	$F\bar{4}3m$	*cF*12	[8]
LiMgBi	LiAlSi (half-Heusler)	$F\bar{4}3m$	*cF*12	[8]
LiSrP *	LiBaSi	$P\bar{6}m2$	*hP*3	[9]
LiBaP *	LiBaSi	$P\bar{6}m2$	*hP*3	[9]
LiBaAs	LiBaSi	$P\bar{6}m2$	*hP*3	[9]
LiBeSb	LiGaGe	$P6_3mc$	*hP*6	[10]
NaBeAs	ZrBeSi (KZnP)	$P6_3/mmc$	*hP*6	[11]
NaBeSb	ZrBeSi (KZnP)	$P6_3/mmc$	*hP*6	[11]
LiSrP *	ZrBeSi (KZnP)	$P6_3/mmc$	*hP*6	[12]
LiBaP *	ZrBeSi (KZnP)	$P6_3/mmc$	*hP*6	[12]
LiBaSb	ZrBeSi (KZnP)	$P6_3/mmc$	*hP*6	[13]
CaLiAs	TiNiSi (SrMgSi)	*Pnma*	*oP*12	[14,15]
CaLiSb	TiNiSi (SrMgSi)	*Pnma*	*oP*12	[14,15]
CaLiBi	TiNiSi (SrMgSi)	*Pnma*	*oP*12	[14,15]
SrLiAs	TiNiSi (SrMgSi)	*Pnma*	*oP*12	[16]
SrLiSb	TiNiSi (SrMgSi)	*Pnma*	*oP*12	[14,17]
SrLiBi	TiNiSi (SrMgSi)	*Pnma*	*oP*12	[14]
NaSrP	ZrNiAl (Fe_2P)	$P\bar{6}2m$	*hP*9	[12]
NaSrAs	ZrNiAl (Fe_2P)	$P\bar{6}2m$	*hP*9	[18]
NaBaP	ZrNiAl (Fe_2P)	$P\bar{6}2m$	*hP*9	[19]
NaBaBi	ZrNiAl (Fe_2P)	$P\bar{6}2m$	*hP*9	[20]
$SrLi_{0.95}As_{0.98}$	-	$P6_3/mmc$	-	[16]

* contradicting structure determinations.

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