

SUPPORTING INFORMATION

Synthesis and crystal chemistry of new ternary pnictides containing lithium – adding structural complexity one step at a time

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Table S1. Selected interatomic distances (in Å) for $ALiPn$ ($M = Ca, Sr, Eu, Yb$; $Pn = As - Bi$).

atomic pair	CaLiAs	YbLiAs	EuLiAs	CaLiSb	YbLiSb
$A-Pn$	3.001(1)	2.995(1)	3.1270(7)	3.1965(8)	3.1875(7)
$A-Pn$ (2 \times)	3.065(1)	3.0666(8)	3.2013(5)	3.2619(5)	3.2590(5)
$A-Pn$ (2 \times)	3.101(1)	3.1001(8)	3.2156(5)	3.3067(6)	3.3047(5)
Li- Pn (2 \times)	2.614(4)	2.625(9)	2.651(5)	2.786(3)	2.764(7)
Li- Pn	2.737(6)	2.731(17)	2.815(11)	2.858(6)	2.853(12)
Li- Pn	2.766(7)	2.735(17)	2.885(11)	2.943(7)	2.955(14)

atomic pair	EuLiSb	CaLiBi	SrLiBi	YbLiBi	EuLiBi
$A-Pn$	3.3158(5)	3.245(2)	3.400(1)	3.251(1)	3.3667(8)
$A-Pn$ (2 \times)	3.3924(4)	3.310(1)	3.4702(9)	3.3189(8)	3.4380(6)
$A-Pn$ (2 \times)	3.3968(4)	3.356(2)	3.4758(9)	3.3648(8)	3.4471(6)
Li- Pn (2 \times)	2.825(4)	2.847(10)	2.874(10)	2.786(3)	2.836(12)
Li- Pn	2.897(4)	2.873(18)	3.002(21)	2.858(6)	2.976(21)
Li- Pn	3.080(8)	2.984(23)	3.150(23)	2.943(7)	3.178(28)

Table S2. Selected interatomic distances (in Å) for $A_3Li_4Pn_4$ ($A = Ba, Eu, Pn = As - Bi$).

atomic pair	$Eu_3Li_4As_4$	$Ba_3Li_4Sb_4$	$Eu_3Li_4Sb_4$	$Ba_3Li_4Bi_4$
$A1-Pn1$ (2×)	3.2419(7)	3.6011(4)	3.4206(6)	3.6176(6)
$A1-Pn2$ (4×)	3.2108(5)	3.5671(6)	3.4434(5)	3.6634(5)
$A2-Pn1$ (2×)	3.1413(9)	3.4979(7)	3.3338(7)	3.5562(6)
$A2-Pn2$ (4×)	3.1540(7)	3.4651(4)	3.2962(5)	3.4769(4)
$Pn2-Pn2$	2.496(2)	2.822(1)	2.833(1)	3.0546(9)
$Li-Pn1$ (2×)	2.668(5)	2.963(10)	2.835(6)	3.040(8)
$Li-Pn1$	2.679(10)	2.967(5)	2.872(11)	3.005(15)
$Li-Pn2$	2.767(10)	3.035(10)	2.877(11)	3.012(14)

Table S3. Selected interatomic distances (in Å) for $Eu_4Li_7Bi_6$.

atomic pair	d (in Å)	atomic pair	d (in Å)	atomic pair	d (in Å)
$Eu1-Bi3$ (2×)	3.3459(7)	$Li1-Bi3$ (2×)	2.822(15)	$Li1-Bi3$	2.820(25)
$Eu1-Bi1$ (2×)	3.3719(7)	$Li1-Bi1$	2.911(30)	$Li1-Bi3$	2.860(26)
$Eu1-Bi3$	3.383(1)	$Li1-Bi2$	2.928(29)	$Li1-Bi2$ (2×)	2.918(14)
$Eu1-Bi2$	3.416(1)				
		$Li2-Bi2$ (2×)	2.854(13)	$Li1-Bi2$ (2×)	3.2832(7)
$Eu2-Bi2$ (2×)	3.4614(7)	$Li2-Bi1$	2.894(26)	$Li1-Bi3$ (4×)	3.3427(5)
$Eu2-Bi1$ (2×)	3.4927(8)	$Li2-Bi2$	2.891(25)		
$Eu2-Bi1$ (2×)	3.5150(8)			$Bi1-Bi1$	3.046(1)

Figure S1. Representative results from the EDX analysis of the $\text{Eu}_4\text{Li}_7\text{Bi}_6$ single-crystals.

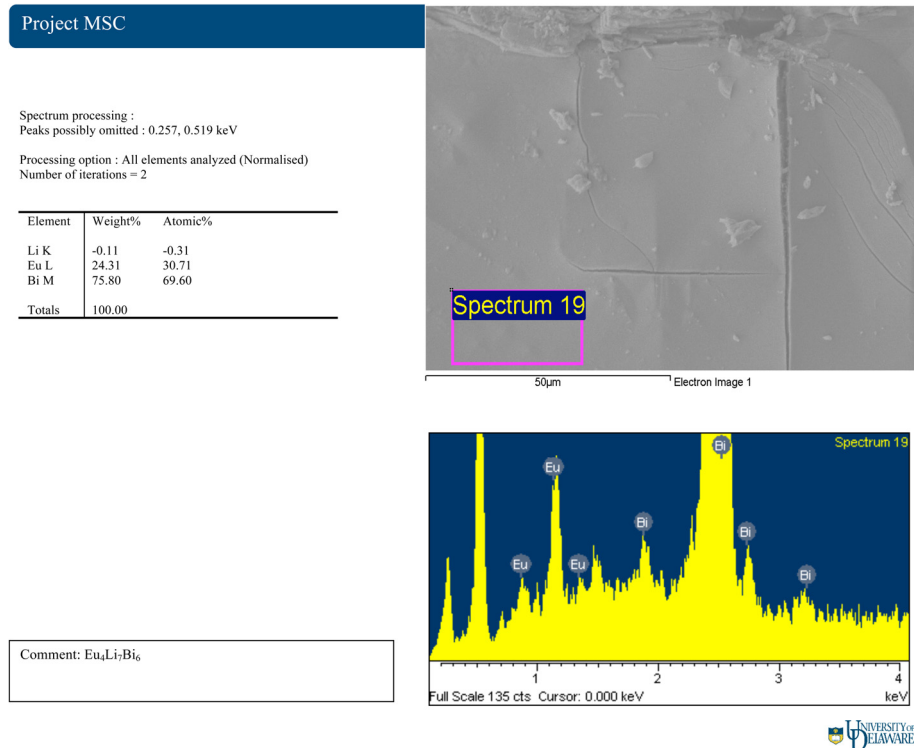


Figure S2. Results from the DSC/TG analysis of $\text{Eu}_3\text{Li}_4\text{Sb}_4$.

