

Dense sphere packing in the NaZn₁₃ structure type – supplementary information

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Table 2 - extended Parameters and properties of the globally optimal A₁₃B packing are compared to those of atomic structures (when the atomic sites are decorated with touching binary hard spheres).

Structure	r_A/r_B	ϕ	a/r_B	y	z
Globally optimal A ₁₃ B packing	0.578458	0.748431	5.39970	0.180551	0.115354
SbBe ₁₃ [Haase <i>et al.</i>]	0.5692	0.7393	5.360	0.1781(5)	0.1157(5)
BaBe ₁₃ [Klemm <i>et al.</i>]	0.5319	0.7178	5.168	0.1740	0.1100
CaBe ₁₃ [Baker <i>et al.</i>]	0.5518	0.7303	5.267	0.1769(2)	0.1123(2)
DyBe ₁₃ [Vigneron <i>et al.</i>]	0.5641	0.7360	5.334	0.1775(5)	0.1150(4)
MgBe ₁₃ [Baker <i>et al.</i>]	0.5713	0.7439	5.363	0.1789(10)	0.1143(8)
SrBe ₁₃ [Matyushenko <i>et al.</i>]	0.5360	0.7212	5.186	0.1750	0.1100
ThBe ₁₃ [Goldman <i>et al.</i>]	0.5440	0.7225	5.235	0.1745(1)	0.1129(1)
UBe ₁₃ [Goldman <i>et al.</i>]	0.5590	0.7315	5.311	0.1763(1)	0.1150(1)
UBe ₁₃ [McElfresh <i>et al.</i>]	0.5602	0.7324	5.317	0.1765(9)	0.1151(9)
CeBe ₁₃ [Wilson <i>et al.</i>]	0.5538	0.7292	5.283	0.1761(3)	0.1138(3)
LaCo ₁₃ [Zarechnyuk <i>et al.</i>]	0.5580	0.7038	5.373	0.1780	0.1220
BaCu ₁₃ [Braun <i>et al.</i>]	0.5633	0.7152	5.380	0.1806	0.1192
NaZn ₁₃ [Zintl <i>et al.</i>]	0.5580	0.7038	5.374	0.1780	0.1220
NaZn ₁₃ [Shoemaker <i>et al.</i>]	0.5631	0.7147	5.380	0.18063(25)	0.11924(28)
RbZn ₁₃ [Bruzzone <i>et al.</i>]	0.5654	0.7195	5.383	0.1800	0.1190

Table 4 - extended Parameters and properties of the optimal non-interstitial A₁₂BC packing in the NaZn₁₃ structure type are compared to those of atomic structures (when the atomic sites are decorated with touching ternary hard spheres)..

<i>Structure</i>	r_A/r_B	r_C/r_A	ϕ	a/r_B	y	z
Globally optimal A ₁₂ BC packing	0.59262	0.91796	0.77124	5.4169	0.17610	0.11408
SbBe ₁₃ [Haase <i>et al.</i>]	0.5821	0.9717	0.7533	5.404	0.1781(5)	0.1157(5)
BaBe ₁₃ [Klemm <i>et al.</i>]	0.5714	0.9098	0.7602	5.301	0.1740	0.1100
CaBe ₁₃ [Baker <i>et al.</i>]	0.5781	0.9414	0.7588	5.356	0.1769(2)	0.1123(2)
DyBe ₁₃ [Vigneron <i>et al.</i>]	0.5861	0.9519	0.7600	5.409	0.1775(5)	0.1150(4)
MgBe ₁₃ [Baker <i>et al.</i>]	0.5801	0.9722	0.7541	5.389	0.1789(10)	0.1143(8)
SrBe ₁₃ [Matyushenko <i>et al.</i>]	0.5743	0.9130	0.7626	5.315	0.1750	0.1100
ThBe ₁₃ [Goldman <i>et al.</i>]	0.5810	0.9176	0.7626	5.360	0.1745(1)	0.1129(1)
UBe ₁₃ [Goldman <i>et al.</i>]	0.5886	0.9354	0.7640	5.412	0.1763(1)	0.1150(1)
UBe ₁₃ [McElfresh <i>et al.</i>]	0.5878	0.9398	0.7626	5.411	0.1765(9)	0.1151(9)
CeBe ₁₃ [Wilson <i>et al.</i>]	0.5910	0.9191	0.7701	5.409	0.1761(3)	0.1138(3)
LaCo ₁₃ [Zarechnyuk <i>et al.</i>]	0.5580	1.0780	0.7133	5.373	0.1780	0.1220
BaCu ₁₃ [Braun <i>et al.</i>]	0.5633	1.0667	0.7234	5.380	0.1806	0.1192
NaZn ₁₃ [Zintl <i>et al.</i>]	0.5580	1.0780	0.7133	5.373	0.1780	0.1220
NaZn ₁₃ [Shoemaker <i>et al.</i>]	0.5631	1.0679	0.7231	5.380	0.18063(25)	0.11924(28)
RbZn ₁₃ [Bruzzone <i>et al.</i>]	0.5654	1.0545	0.7262	5.383	0.1800	0.1190

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