LiGaGe Crystal Structure: ABC_hP6_186_b_b_a-003

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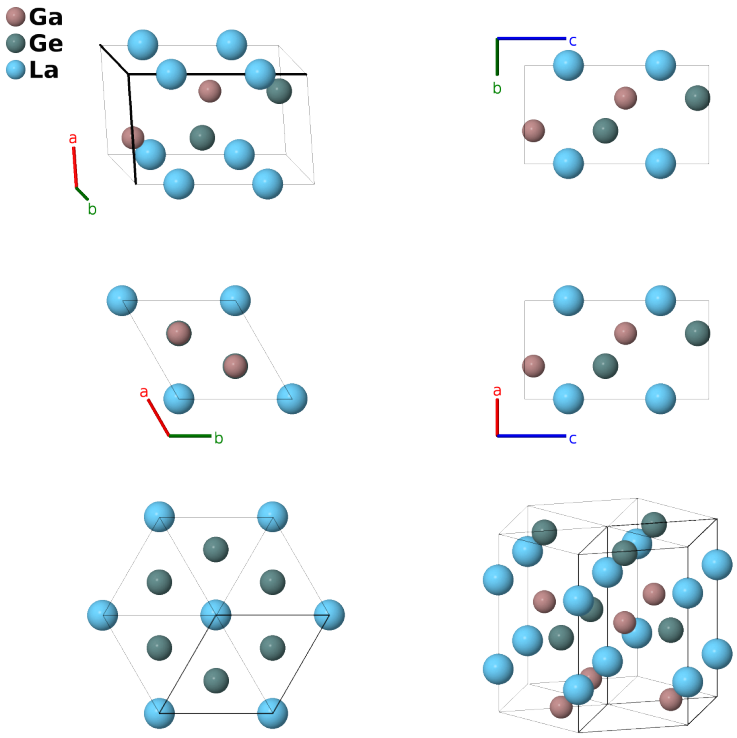
https://aflow.org/p/ZZ7U

https://aflow.org/p/ABC_hP6_186_b_b_a-003



Prototype	GaGeLi
AFLOW prototype label	ABC_hP6_186_b_b_a-003
ICSD	25310
Pearson symbol	hP6
Space group number	186
Space group symbol	$P6_3mc$
AFLOW prototype command	`aflow --proto=ABC_hP6_186_b_b_a-003 --params=`$a, c/a, z_1, z_2, z_3$

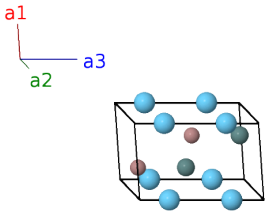
Other compounds with this structure
BeLiSb, CaAgBi, CeAuGe, DyAuGe, DyCuGe, ErAuGe, ErCuGe, EuAuGe, GdAuGe, HoAuGe, HoCuGe, LaAgSn, LaAuGe, LaAuSn, LaCuSn, LuAuGe, NdAgSn, NdAuGe, NdAuSn, NdCuSn, PmAuGe, PrAgSn, PrAuGe, PrAuSn, PrCuSn, SmAuGe, TbAuGe, TbCuGe, TiCuSn, TmAuGe, YAuGe, YCuPb, YbAuGe

- This is the ternary form of the $C27$ (CdI_2) structure.

- The choice of the origin of the z-axis in space group $P6_3mc$ #186 is arbitrary, we use the values given by (Bockelmann, 2012).

Hexagonal primitive vectors

$$\begin{aligned}
\mathbf{a_1} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_2} &= \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{\sqrt{3}}{2}a\,\hat{\mathbf{y}} \\
\mathbf{a_3} &= c\,\hat{\mathbf{z}}
\end{aligned}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	La I
$\mathbf{B_2}$	=	$\left(z_1+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$c\left(z_1+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2a)	La I
$\mathbf{B_3}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_2\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_2\,\hat{\mathbf{z}}$	(2b)	Ga I
$\mathbf{B_4}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_2+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_2+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ga I
$\mathbf{B_5}$	=	$\frac{1}{3}\,\mathbf{a}_1+\frac{2}{3}\,\mathbf{a}_2+z_3\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}+\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+cz_3\,\hat{\mathbf{z}}$	(2b)	Ge I
$\mathbf{B_6}$	=	$\frac{2}{3}\,\mathbf{a}_1+\frac{1}{3}\,\mathbf{a}_2+\left(z_3+\frac{1}{2}\right)\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}-\frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}}+c\left(z_3+\frac{1}{2}\right)\,\hat{\mathbf{z}}$	(2b)	Ge I

References

[1] W. Bockelmann and H.-U. Schuster, *Ternäre Phasen im Dreistoffsystem Lithium-Gallium-Germanium*, Z. Anorganische und Allgemeine Chemie **410**, 233–240 (1974), doi:10.1002/zaac.19744100303.