LiGaGe Crystal Structure: ABC_hP6_186_b_b_a-003

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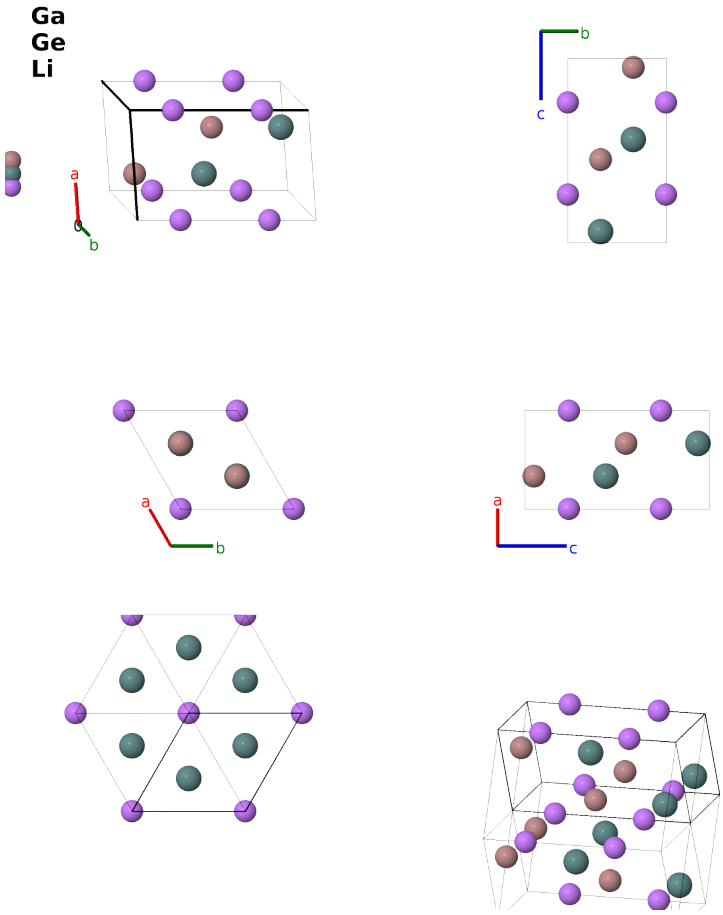
https://aflow.org/prototype-encyclopedia/ZZ7U

https://aflow.org/prototype-encyclopedia/ABC_hP6_186_b_b_a-003



Prototype	GaGeLi
AFLOW prototype label	ABC_hP6_186_b_b_a-003
ICSD	25310
CCDC	1601055
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=`$a, c/a, z_1, z_2, z_3$

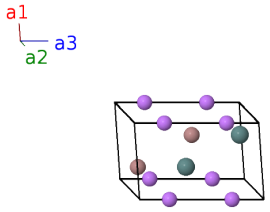
Other compounds with this structure

CaAgBi, CaAuBi, CaAuSb, CaHgSn, CaSnZn, CeAgGe, CeAgPb, CeAgSn, CeAuGe, CeAuSn, CeCuSn, DyAgPb, DyAgSn, DyAuGe, DyAuSn, DyCuGe, DyCuPb, DyCuSn, DyPbSb, ErAgSn, ErAuGe, ErCuGe, ErCuPb, ErGaZn, EuAuGe, EuCdPb, EuCdSn, EuHgPb, EuHgSn, GdAgPb, GdAgSn, GdAuGe, GdAuSn, GdCuGe, GdCuPb, GdCuSn, GdPbSb, HfCuSn, HoAgPb, HoAgSn, HoAuGe, HoAuSn, HoCuGe, HoCuPb, LaAgGe, LaAgPb, LaAgSn, LaAuGe, LaAuSn, LaCuSn, LiBiSb, LiBiZn, LiSbZn, LuAgSn, LuAuGe, LuCuPb, LuCuSn, NdAgPb, NdAgSn, NdAsPd, NdAuGe, NdAuSn, NdCuSn, NdPbSb, NdPtSb, PmAuGe, PrAgPb, PrAgSn, PrAuGe, PrAuSn, PrCuSn, PrPdSb, PrPtSb, ScAuGe, ScCuPb, ScCuSn, SmAgPb, SmAsPd, SmAuGe, SmAuSn, SmCuPb, SmCuSn, SrHgPb, SrHgSn, TbAgPb, TbAgSn, TbAuGe, TbAuSn, TbCuGe, TbCuPb, TiCuSn, TmAuGe, TmCuPb, UAuSn, UPdSn, YAgSn, YAuGe, YAuSi, YAuSn, YCuPb, YCuSb, YCuSn, YbAgBi, YbAuBi, YbAuGe, YbAuSb, YbBiCu, YbCuGe, YbHgSn, YbPbZn, YbSnZn

- 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).
- We have attempted to list the "other compounds" so that the (2a) atom is first, but do not guarantee that we are always correct.

Hexagonal primitive vectors

$$\mathbf{a_1} = \frac{1}{2}a\,\hat{\mathbf{x}} - \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_2} = \frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$z_1\,\mathbf{a}_3$	=	$cz_1\,\hat{\mathbf{z}}$	(2a)	Li 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)	Li 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.

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