$CaBe_2Ge_2$ Structure: A2BC2_tP10_129_ac_c_bc-001

This structure originally had the label `A2BC2_tP10_129_ac_c_bc`. Calls to that address will be redirected here.

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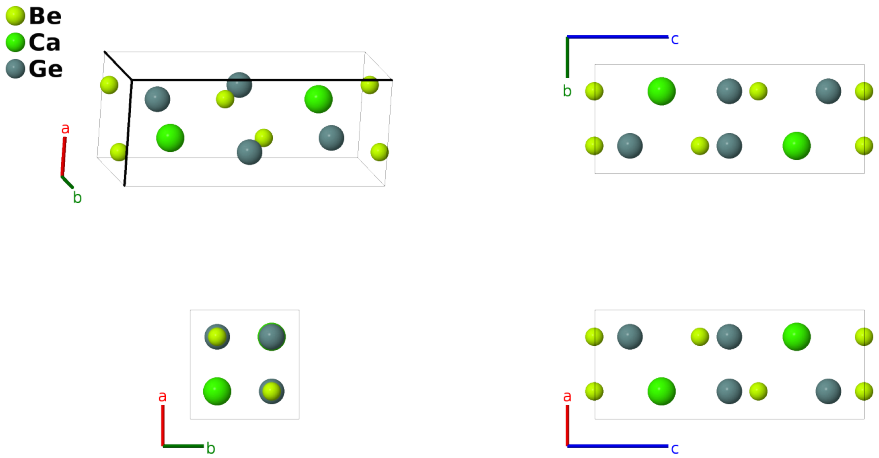
https://aflow.org/p/H0MM

https://aflow.org/p/A2BC2_tP10_129_ac_c_bc-001



Prototype	Be_2CaGe_2
AFLOW prototype label	A2BC2_tP10_129_ac_c_bc-001
ICSD	25337
Pearson symbol	tP10
Space group number	129
Space group symbol	$P4/nmm$
AFLOW prototype command	`aflow --proto=A2BC2_tP10_129_ac_c_bc-001 --params=`$a, c/a, z_3, z_4, z_5$

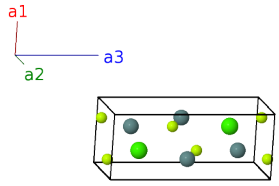
Other compounds with this structure

$BaAu_2Sn_2$, $BaMg_2Pb_2$, $BaPd_2Sb_2$, $BaZn_2Sn_2$, $CeCu_2Sn_2$, $CeRh_2As_2$, $CeRh_2P_2$, $EuAu_2Al_2$, $EuPd_2Sb_2$, $EuPt_2Ge_2$, $HoPt_2Si_2$, $LaCu_2Sn_2$, $LaPt_2Bi_2$, $LaPt_2Ge_2$, $LaPt_2Si_2$, $LaRh_2As_2$, $LaRh_2P_2$, $LiPd_2Bi_2$, $NdRh_2As_2$, $NdRh_2P_2$, $PrRh_2As_2$, $PrRh_2P_2$, $SrAu_2Sn_2$, $SrCu_2Sn_2$, $SrPd_2Sb_2$, $SrPt_2As_2$, $ThIr_2Si_2$, $ThPt_2Si_2$, UIr_2Si_2, UPt_2Si_2

- This is a ternary form of the $D1_3$ ($BaAl_4$) structure. The atomic positions are approximately the same as in the conventional cell of $BaAl_4$, but the distribution of the atoms on those sites and the resulting relaxation leads to a different structure.
- Space group $P4/nmm$ #129 has two settings, but both have the same z-axis origin, so either setting will do here. We chose our standard setting 2.

Simple Tetragonal primitive vectors

$$\mathbf{a_1} = a\,\hat{\mathbf{x}}$$
$$\mathbf{a_2} = a\,\hat{\mathbf{y}}$$
$$\mathbf{a_3} = c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}}$	(2a)	Be I
$\mathbf{B_2}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}}$	(2a)	Be I
$\mathbf{B_3}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ge I
$\mathbf{B_4}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(2b)	Ge I
$\mathbf{B_5}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_3\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_3\,\hat{\mathbf{z}}$	(2c)	Be II
$\mathbf{B_6}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_3\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_3\,\hat{\mathbf{z}}$	(2c)	Be II
$\mathbf{B_7}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_4\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_4\,\hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B_8}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_4\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_4\,\hat{\mathbf{z}}$	(2c)	Ca I
$\mathbf{B_9}$	=	$\frac{1}{4}\,\mathbf{a}_1 + \frac{1}{4}\,\mathbf{a}_2 + z_5\,\mathbf{a}_3$	=	$\frac{1}{4}a\,\hat{\mathbf{x}} + \frac{1}{4}a\,\hat{\mathbf{y}} + cz_5\,\hat{\mathbf{z}}$	(2c)	Ge II
$\mathbf{B_{10}}$	=	$\frac{3}{4}\,\mathbf{a}_1 + \frac{3}{4}\,\mathbf{a}_2 - z_5\,\mathbf{a}_3$	=	$\frac{3}{4}a\,\hat{\mathbf{x}} + \frac{3}{4}a\,\hat{\mathbf{y}} - cz_5\,\hat{\mathbf{z}}$	(2c)	Ge II

References

[1] B. Eisenmann, N. May, W. Müller, and H. Schäfer, *Eine neue strukturelle Variante des $BaAl_4$-Typs: Der $CaBe_2Ge_2$-Typ*, Z. Naturforsch. B **27** (1972), doi:10.1515/znb-1972-1008. 1155-1157.