$LiAgC_2$ Structure: AB2C_hP4_187_a_g_d-001

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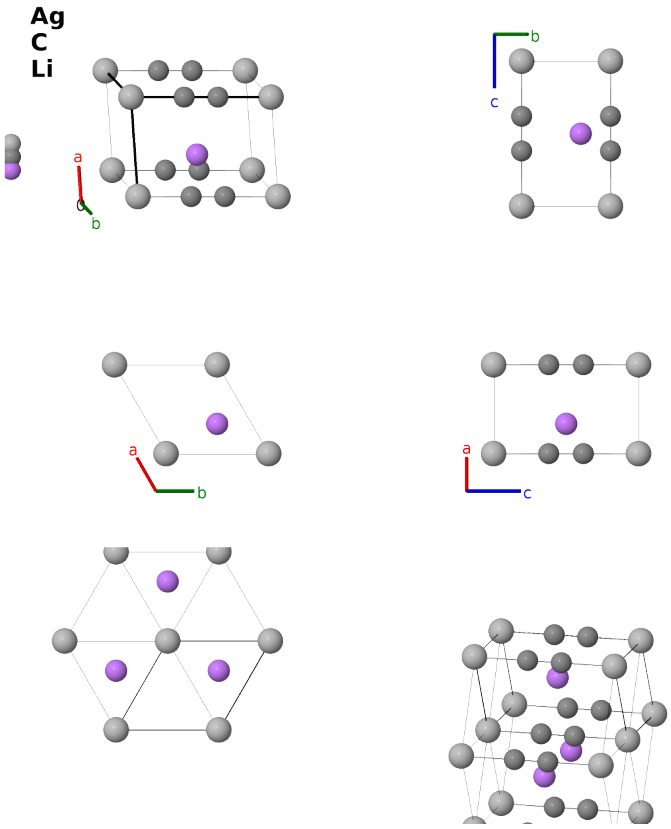
https://aflow.org/prototype-encyclopedia/ZZ9R

https://aflow.org/prototype-encyclopedia/AB2C_hP4_187_a_g_d-001



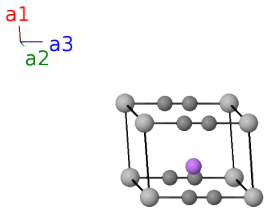
Prototype	AgC_2Li
AFLOW prototype label	AB2C_hP4_187_a_g_d-001
ICSD	410868
CCDC	1726615
Pearson symbol	hP4
Space group number	187
Space group symbol	$P\bar{6}m2$
AFLOW prototype command	`aflow --proto=AB2C_hP4_187_a_g_d-001 --params=`$a, c/a, z_3$

Other compounds with this structure
$CsAgC_2$, $KAgC_2$, $NaAgC_2$, $RbAgC_2$

- We do not use the lattice constants listed in Table 1 for (Kockelmann, 1999). Instead we follow the ICSD and infer the lattice constants and z_3 from the distances given in Figure 1.
- $LiAgC_2$ and $InTaS_2$ have the same AFLOW label, AB2C_hP4_187_a_g_d. They are generated by the same symmetry operations with different sets of parameters (`--params`) specified in their corresponding CIF files.

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
$\mathbf{B_1}$	=	0	=	0	(1a)	Ag I
$\mathbf{B_2}$	=	$\frac{1}{3}\,\mathbf{a}_1 + \frac{2}{3}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}} + \frac{\sqrt{3}}{6}a\,\hat{\mathbf{y}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(1d)	Li I
$\mathbf{B_3}$	=	$z_3\,\mathbf{a}_3$	=	$cz_3\,\hat{\mathbf{z}}$	(2g)	C I
$\mathbf{B_4}$	=	$-z_3\,\mathbf{a}_3$	=	$-cz_3\,\hat{\mathbf{z}}$	(2g)	C I

References

[1] W. Kockelmann and U. Ruschewitz, *Novel Ternary Alkali Metal Silver Acetylides $M^I AgC_2$ (M^I=Li, Na, K, Rb, Cs)*, Ange. Chem. Int. Ed. **38**, 3492–2495 (1999), doi:10.1002/(SICI)1521-3773(19991203)38:23%3C3492::AID-ANIE3492%3E3.0.CO;2-E.

Found in

[1] *AFLOW Database*, https://aflow.org. $LiAgC_2$, ICSD entry 410868.

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