

LiAgC ₂	<i>hP4</i>	(187) <i>P-6m2</i> – gda
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LiAgC₂ [1]; LiAuC₂ [2]

Structural features: Ag atoms and C₂ dumbbells arranged in infinite chains parallel to [001]; Li in flattened trigonal prisms formed by three C₂ dumbbells.

Kockelmann W., Ruschewitz U. (1999) [1]

AgC₂Li

$a = 0.37882$, $c = 0.5328$ nm, $c/a = 1.406$, $V = 0.0662$ nm³, $Z = 1$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
C1	2 <i>g</i>	3 <i>m.</i>	0	0	0.38		single atom C
Li2	1 <i>d</i>	-6 <i>m2</i>	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		trigonal prism C ₆
Ag3	1 <i>a</i>	-6 <i>m2</i>	0	0	0		colinear C ₂

Experimental: powder, diffractometer, neutrons, R = 0.007

Remarks: Alternative models in space groups (191) *P6/mmm* and (194) *P6₃/mmc* (double *c*-parameter for the latter) were tested and rejected (R = 0.008 for both).

References: [1] Kockelmann W., Ruschewitz U. (1999), *Angew. Chem. Int. Ed.* 38, 3492-3495 (*Angew. Chem.* 111, 3697-3700). [2] Offermanns J., Ruschewitz U., Kneip C. (2000), *Z. Anorg. Allg. Chem.* 626, 649-654.