| LiZnGe | *hP*10 | (187) *P*-6*m*2 – i$^2$hgda |
|---|---|---|

**LiZnGe** [1]
Structural features: 3D-framework of fused $ZnLi_6$ and $GeLi_6$ trigonal prisms; Zn and Ge are displaced from the prism centers (split Zn site) to form a tetrahedral framework with $Ge_2$ pairs. One $Ge_2$ dumbbell for one single Ge. Derivative of $CaIn_2$.

Belin C. et al. (1993) [1]
GeLiZn
$a$ = 0.42691, $c$ = 0.93461 nm, $c/a$ = 2.189, $V$ = 0.1475 nm$^3$, $Z$ = 3

| site | Wyck. | sym. | $x$ | $y$ | $z$ | occ. | atomic environment |
|---|---|---|---|---|---|---|---|
| Zn1 | 2*i* | 3*m*. | $^2/_3$ | $^1/_3$ | 0.0199 | 0.5 | |
| Ge2 | 2*i* | 3*m*. | $^2/_3$ | $^1/_3$ | 0.3635 | | tetrahedron $Zn_3Ge$ |
| Li3 | 2*h* | 3*m*. | $^1/_3$ | $^2/_3$ | 0.168 | | |
| Zn4 | 2*g* | 3*m*. | 0 | 0 | 0.2936 | | bicapped square prism $Ge_4Li_6$ |
| Li5 | 1*d* | -6*m*2 | $^1/_3$ | $^2/_3$ | $^1/_2$ | | rhombic dodecahedron $Ge_6Li_2Zn_6$ |
| Ge6 | 1*a* | -6*m*2 | 0 | 0 | 0 | | |

Experimental: single crystal, diffractometer, X-rays, R = 0.047

Remarks: The same data are also reported in [2]. Supersedes a structure proposal for so-called $Li_{1.25}ZnGe$ in space group (187) *P*-6*m*2 in [3] (original description in space group (143) *P*3). Short interatomic distances for partly occupied site(s).

References: [1] Belin C., Sportouch S., Tillard Charbonnel M. (1993), C. R. Acad. Sci., Ser. II 317, 769-773. [2] Sportouch S., Belin C., Tillard Charbonnel M., Rovira M.C., Canadell C. (1995), New J. Chem. 19, 243-251. [3] Schönemann H., Schuster H.U. (1977), Z. Anorg. Allg. Chem. 432, 87-94.