

$\text{Li}_8\text{CoO}_6$  $hP30$  $(185) P6_3cm - c^3b^2a^2$  **$\text{Li}_8\text{CoO}_6$**  [1]

Structural features: Close-packed O layers in hc stacking; Li and Co in tetrahedral voids. Single  $\text{CoO}_4$  tetrahedra.

Jansen M., Hoppe R. (1973) [1]

 $\text{CoLi}_8\text{O}_6$ 

$a = 0.544$ ,  $c = 1.087$  nm,  $c/a = 1.998$ ,  $V = 0.2786$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
O1	6c	$\bar{3}m$	0.288	0	0.203		trigonal bipyramid $\text{CoLi}_4$
Li2	6c	$\bar{3}m$	0.318	0	0.39		square pyramid $\text{O}_4\text{Li}$
Li3	6c	$\bar{3}m$	0.387	0	0.019		trigonal bipyramid $\text{O}_4\text{Li}$
Li4	4b	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.252		tetrahedron $\text{O}_4$
O5	4b	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.43		monocapped trigonal prism $\text{Li}_7$
O6	2a	3.m	0	0	0.0		7-vertex polyhedron $\text{CoLi}_6$
Co7	2a	3.m	0	0	0.153		tetrahedron $\text{O}_4$

Transformation from published data:  $-x, -y, -z$ ; origin shift 0 0 0.847

Experimental: single crystal, diffractometer, X-rays,  $R = 0.099$

References: [1] Jansen M., Hoppe R. (1973), Z. Anorg. Allg. Chem. 398, 54-62.