

NaLi[CO ₃]	<i>hP</i> 21	(174) <i>P</i> -6 – k ² j ⁴ eda
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LiNaCO₃ γ [1]

Structural features: CO₃ trigonal units (perpendicular to [001], in part rotational disorder) in an ω Ti-type arrangement. Li₃(CO₃)₂ layers alternate with Na₃(CO₃) layers along [001].

Zhukov S.G. et al. (1999) [1]

CLiNaO₃

a = 0.83115, *c* = 0.33858 nm, *c/a* = 0.407, *V* = 0.2026 nm³, *Z* = 3

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	3 <i>k</i>	<i>m</i> ..	0.16067	0.53433	1/2		single atom C
Na2	3 <i>k</i>	<i>m</i> ..	0.31867	0.30633	1/2		5-vertex polyhedron O ₅
Li3	3 <i>j</i>	<i>m</i> ..	0.08267	0.32633	0		single atom O
O4	3 <i>j</i>	<i>m</i> ..	0.10567	0.17933	0	0.5	single atom O
O5	3 <i>j</i>	<i>m</i> ..	0.17967	0.10833	0	0.5	single atom O
O6	3 <i>j</i>	<i>m</i> ..	0.54967	0.15633	0		single atom C
C7	1 <i>e</i>	-6..	2/3	1/3	0		coplanar triangle O ₃
C8	1 <i>d</i>	-6..	1/3	2/3	1/2		coplanar triangle O ₃
C9	1 <i>a</i>	-6..	0	0	0		coplanar hexagon O ₆

Transformation from published data: *y,x,z*; origin shift 1/3 2/3 0

Experimental: powder, diffractometer, X-rays, *R*_p = 0.058, *T* = 713 K

Remarks: Phase stable at *T* > 623 K. Short interatomic distances: d(Li3-O4) = 0.133 nm. Short interatomic distances for partly occupied site(s).

References: [1] Zhukov S.G., Yatsenko A.V., Chernyshev V.V., D'yakov V.A., Le Loux R., Schenk H. (1999), *Z. Kristallogr.* 214, 255-258.