

NaLi[CO ₃]	<i>hP</i> 54	(174) <i>P</i> -6 – k ^{7:10} J ^{eca}
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LiNaCO₃ β [1]

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

Yatsenko A.V. et al. (1995) [1]

CLiNaO₃

a = 1.4355, *c* = 0.3341 nm, *c/a* = 0.233, *V* = 0.5962 nm³, *Z* = 9

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Na1	3 <i>k</i>	<i>m</i> ..	0.19983	0.44197	¹ / ₂		square pyramid O ₅
Na2	3 <i>k</i>	<i>m</i> ..	0.21243	0.08787	¹ / ₂		5-vertex polyhedron O ₅
O3	3 <i>k</i>	<i>m</i> ..	0.24483	0.27727	¹ / ₂		single atom C
C4	3 <i>k</i>	<i>m</i> ..	0.34533	0.34627	¹ / ₂		coplanar triangle O ₃
O5	3 <i>k</i>	<i>m</i> ..	0.37633	0.44737	¹ / ₂		single atom C
O6	3 <i>k</i>	<i>m</i> ..	0.41473	0.31517	¹ / ₂		single atom C
Na7	3 <i>k</i>	<i>m</i> ..	0.52563	0.11437	¹ / ₂		square pyramid O ₅
O8	3 <i>j</i>	<i>m</i> ..	0.00763	0.41507	0		single atom C
O9	3 <i>j</i>	<i>m</i> ..	0.08053	0.31277	0		single atom C
O10	3 <i>j</i>	<i>m</i> ..	0.09213	0.08357	0		single atom C
Li11	3 <i>j</i>	<i>m</i> ..	0.10783	0.56757	0		tetrahedron O ₄
Li12	3 <i>j</i>	<i>m</i> ..	0.15223	0.23377	0		tetrahedron O ₄
O13	3 <i>j</i>	<i>m</i> ..	0.24653	0.57467	0		single atom C
C14	3 <i>j</i>	<i>m</i> ..	0.32453	0.00237	0		coplanar triangle O ₃
O15	3 <i>j</i>	<i>m</i> ..	0.33353	0.09477	0		single atom C
Li16	3 <i>j</i>	<i>m</i> ..	0.43953	0.24667	0		tetrahedron O ₄
O17	3 <i>j</i>	<i>m</i> ..	0.57493	0.24747	0		single atom C
C18	1 <i>e</i>	-6..	² / ₃	¹ / ₃	0		coplanar triangle O ₃
C19	1 <i>c</i>	-6..	¹ / ₃	² / ₃	0		coplanar triangle O ₃
C20	1 <i>a</i>	-6..	0	0	0		coplanar triangle O ₃

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

Experimental: single crystal, diffractometer, X-rays, *R* = 0.033, *T* = 503 K

Remarks: Phase stable at *T* > 448 K. In [1] the Hermann-Mauguin symbol for the space group is misprinted as *P*6 instead of *P*-6 (from the description of the structure).

References: [1] Yatsenko A.V., Zhukov S.G., D'yakov V.A., Etz A., Molleman W., Schenk H. (1995), Mater. Res. Bull. 30, 739-744.