



hP60

(176) $P6_3/m - i^2h^4\text{g}ec$

Ca₄Mn₃(BO₃)₃(CO₃)O₃ [1], gaudefroyite

Structural features: Infinite chains of edge-linked MnO₆ octahedra share vertices with BO₃ trigonal units to form a 3D-framework; CO₃ trigonal units (partial disorder) and Ca in large channels parallel to [001], additional Ca in other channels.

Hoffmann C. et al. (1997) [1]

B₃CCa₄Mn₃O₁₅

$a = 1.0589$ nm, $c/a = 0.556$, $V = 0.5720$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.14	0.0534	0.0738	0.5	single atom C
O2	12 <i>i</i>	1	0.4722	0.1692	0.0439		single atom B
O3	6 <i>h</i>	<i>m</i> ..	0.0926	0.4727	¹ / ₄		non-colinear Mn ₂
Ca4	6 <i>h</i>	<i>m</i> ..	0.16788	0.29957	¹ / ₄		octahedron O ₆
O5	6 <i>h</i>	<i>m</i> ..	0.4009	0.3169	¹ / ₄		single atom B
B6	6 <i>h</i>	<i>m</i> ..	0.4494	0.2179	¹ / ₄		coplanar triangle O ₃
Mn7	6 <i>g</i>	-1	¹ / ₂	0	0		octahedron O ₆
C8	4 <i>e</i>	3..	0	0	0.0699	0.5	single atom C
Ca9	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		tricapped trigonal prism O ₉

Experimental: single crystal, diffractometer, X-rays, R = 0.017, T = 301 K

Remarks: Natural specimen from the N'chwaning II mine, Kalahari, South Africa. Space group (173) $P6_3$, used in earlier refinements ([2], [3]), was tested and rejected (R = 0.017). Short interatomic distances for partly occupied site(s).

References: [1] Hoffmann C., Armbruster T., Kunz M. (1997), Eur. J. Mineral. 9, 7-19. [2] Granger M.M., Protas J. (1965), C. R. Hebd. Seances Acad. Sci. 260, 4553-4555. [3] Yakubovich O.V., Simonov M.A., Belov N.V. (1975), Sov. Phys. Crystallogr. 20, 87-88 (Kristallografiya 20, 152-155).