

Co₃Bi[CO]₉*hP44*(186) *P6₃mc – c⁷b***BiCo₃(CO)₉** [2]

Structural features: BiCo₃(CO)₉ clusters (a central Co₃ triangle capped by a Bi atom; one CO beyond each edge, two additional CO bonded to each Co) in a Mg-type (h.c.p.) arrangement.

Martinengo S., Ciani G. (1987) [1]

BiC₉Co₃O₉

$a = 1.1094$, $c = 0.7301$ nm, $c/a = 0.658$, $V = 0.7782$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>c</i>	. <i>m</i> .	0.13	0.87	0.095		single atom C
C2	6 <i>c</i>	. <i>m</i> .	0.183	0.817	0.167		single atom O
Co3	6 <i>c</i>	. <i>m</i> .	0.2568	0.7432	0.3092		tetrahedron C ₄
C4	6 <i>c</i>	. <i>m</i> .	0.449	0.551	0.332		single atom O
O5	6 <i>c</i>	. <i>m</i> .	0.5088	0.4912	0.342		single atom C
C6	6 <i>c</i>	. <i>m</i> .	0.78	0.22	0.023		single atom O
O7	6 <i>c</i>	. <i>m</i> .	0.806	0.194	0.173		single atom C
Bi8	2 <i>b</i>	3 <i>m</i> .	$\frac{1}{3}$	$\frac{2}{3}$	0.0		non-coplanar triangle Co ₃

Transformation from published data: origin shift 0 0 0.5

Experimental: single crystal, diffractometer, X-rays, R = 0.025

References: [1] Martinengo S., Ciani G. (1987), J. Chem. Soc., Chem. Commun. 1987, 1589-1591. [2] Whitmire K.H., Leigh J.S., Gross M.E. (1987), J. Chem. Soc., Chem. Commun. 1987, 926-927.