



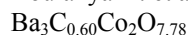
*hP56*

(174)  $P-6 - 1^4k^3j^4ih^2g^2e$

# **Ba<sub>3</sub>Co<sub>2</sub>O<sub>6</sub>(CO<sub>3</sub>)<sub>0.60</sub> [1]**

Structural features: Distorted close-packed BaO<sub>3</sub> layers in h stacking (partial vacancies ignored); Co in octahedral (O<sub>6</sub>), C in trigonal (O<sub>3</sub>) voids. Infinite columns of face-linked CoO<sub>6</sub> octahedra and columns of superposed CO<sub>3</sub> trigonal units (perpendicular to [001]).

Boulahya K. et al. (2000) [1]



$a = 0.9683$ ,  $c = 0.9518$  nm,  $c/a = 0.983$ ,  $V = 0.7729$  nm<sup>3</sup>,  $Z = 4$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6 <i>l</i>	1	0.152	0.153	0.25		non-colinear Co <sub>2</sub>
Ba2	6 <i>l</i>	1	0.335	0.008	0.244		pseudo Frank-Kasper O <sub>11</sub>
O3	6 <i>l</i>	1	0.336	0.52	0.248		non-colinear Co <sub>2</sub>
O4	6 <i>l</i>	1	0.529	0.326	0.313	0.8	single atom C
O5	3 <i>k</i>	<i>m</i> ..	0.154	0.001	$\frac{1}{2}$		non-colinear Co <sub>2</sub>
O6	3 <i>k</i>	<i>m</i> ..	0.173	0.516	$\frac{1}{2}$		non-colinear Co <sub>2</sub>
Ba7	3 <i>k</i>	<i>m</i> ..	0.323	0.335	$\frac{1}{2}$		10-vertex polyhedron O <sub>10</sub>
O8	3 <i>j</i>	<i>m</i> ..	0.001	0.153	0		non-colinear Co <sub>2</sub>
O9	3 <i>j</i>	<i>m</i> ..	0.176	0.516	0		non-colinear Co <sub>2</sub>
Ba10	3 <i>j</i>	<i>m</i> ..	0.31	0.314	0		10-vertex polyhedron O <sub>10</sub>
O11	3 <i>j</i>	<i>m</i> ..	0.523	0.201	0	0.78	single atom C
C12	2 <i>i</i>	3..	$\frac{2}{3}$	$\frac{1}{3}$	0.313	0.8	coplanar triangle O <sub>3</sub>
Co13	2 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.124		octahedron O <sub>6</sub>
Co14	2 <i>h</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.364		octahedron O <sub>6</sub>
Co15	2 <i>g</i>	3..	0	0	0.125		octahedron O <sub>6</sub>
Co16	2 <i>g</i>	3..	0	0	0.366		octahedron O <sub>6</sub>
C17	1 <i>e</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	0	0.78	coplanar triangle O <sub>3</sub>

Transformation from published data: -*x*,-*y*,-*z*; origin shift 0 0  $\frac{1}{2}$

Experimental: powder, diffractometer, neutrons, R<sub>p</sub> = 0.039

References: [1] Boulahya K., Amador U., Parras M., Gonzalez Calbet J.M. (2000), Chem. Mater. 12, 966-972.