$BaCoO_3$	*hP*10	(187) *P*-6*m*2 – kjhfa

$BaCoO_3$ distorted [1], perovskite 2H
Structural features: Close-packed BaO_3 layers in h stacking; Co in octahedral (O_6) voids. CoO_6 octahedra share faces to form infinite columns; linear -Co- chains with alternatively shorter and longer interatomic distances.

Felser C. et al. (1999) [1]
$BaCoO_3$
$a = 0.5645$, $c = 0.4752$ nm, $c/a = 0.842$, $V = 0.1311$ nm^3, $Z = 2$

site	Wyck.	sym.	*x*	*y*	*z*	occ.	atomic environment
O1	3*k*	*mm*2	0.18513	0.81487	$^1/_2$		non-colinear Co_2
O2	3*j*	*mm*2	0.48153	0.51847	0		non-colinear Co_2
Co3	2*h*	3*m*.	$^1/_3$	$^2/_3$	0.24406		octahedron O_6
Ba4	1*f*	-6*m*2	$^2/_3$	$^1/_3$	$^1/_2$		anticuboctahedron O_{12}
Ba5	1*a*	-6*m*2	0	0	0		anticuboctahedron O_{12}

Transformation from published data: -*x*,-*y*,-*z*; origin shift $^2/_3$ $^1/_3$ $^1/_2$

Remarks: Simulation of Peierls distortions; the authors exclude this model for $BaCoO_3$ based on band structure calculations. The structure was determined in space group (194) $P6_3/mmc$ in [2].

References: [1] Felser C., Yamaura K., Cava R.J. (1999), J. Solid State Chem. 146, 411-417. [2] Taguchi H., Takeda Y., Kanamaru F., Shimada M., Koizumi M. (1977), Acta Crystallogr. B 33, 1299-1301.