$BaNiO_3$	*hP*10	(186) $P6_3mc$ – cba

$BaNiO_3$ [1]
Structural features: Close-packed BaO_3 layers in h stacking; Ni in octahedral (O_6) voids. NiO_6 octahedra share faces to form infinite columns (linear -Ni- chains).

Krischner H. et al. (1971) [1]
$BaNiO_3$
a = 0.5631, c = 0.4808 nm, c/a = 0.854, V = 0.1320 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	6*c*	.*m*.	0.85	0.15	0.2475		non-colinear Ni_2
Ba2	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.2225		anticuboctahedron O_{12}
Ni3	2*a*	3*m*.	0	0	0.0		octahedron O_6

Transformation from published data: origin shift 0 0 0.0275
Experimental: powder, film, X-rays, R = 0.084

Remarks: The description of $BaNiO_3$ in space group (186) $P6_3mc$ in [2] does not take into consideration all symmetry elements of the proposed structure, correct space group is (194) $P6_3/mmc$. The same is true for reports on $BaMnO_3$ ([3]; [4]), $BaTiS_3$ [5] and NH_4FeCl_3 [6]. The structure of $BaNiO_3$ was later refined in space group (194) $P6_3/mmc$ [7]. In table VI of [1] the x-coordinate of the O site is misprinted as 0.150 instead of -0.150 (better interatomic distances).

References: [1] Krischner H., Torkar K., Kolbesen B.O. (1971), J. Solid State Chem. 3, 349-357. [2] Lander J.J. (1951), Acta Crystallogr. 4, 148-156. [3] Hardy A. (1962), Acta Crystallogr. 15, 179-181. [4] Hardy A. (1962), Ann. Chim. (Paris) 7, 281-301. [5] Clearfield A. (1963), Acta Crystallogr. 16, 135-142. [6] Amit M., Zodkevitz A., Makovsky J. (1970), Isr. J. Chem. 8, 737-740. [7] Takeda Y., Kanamaru F., Shimada M., Koizumi M. (1976), Acta Crystallogr. B 32, 2464-2466.