

$\text{Na}_8\text{Ba}_{14}\text{CaN}_6$	<i>hP</i> 58	(176) $P6_3/m - i^3hf^2edb$
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$\text{Na}_8\text{Ba}_{14}\text{CaN}_6$ [1]

Structural features: $\text{CaN}_6\text{Ba}_{14}$ units consisting of six face-linked $\text{N}(\text{Ba}_5\text{Ca})$ octahedra (a central Ca atom surrounded by a N_6 octahedron, a Ba_8 cube and a large Ba_6 octahedron).

Vajenine G.V. et al. (1999) [1]

$\text{Ba}_{14}\text{CaN}_6\text{Na}_8$

$a = 1.14192$, $c = 2.1543$ nm, $c/a = 1.887$, $V = 2.4328$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ba1	12 <i>i</i>	1	0.03542	0.28913	0.04956		non-coplanar triangle N_3
N2	12 <i>i</i>	1	0.1945	0.1689	0.06864		octahedron Ba_5Ca
Ba3	12 <i>i</i>	1	0.37599	0.32832	0.1379		single atom N
Na4	6 <i>h</i>	<i>m</i> ..	0.0388	0.3532	$\frac{1}{4}$		13-vertex polyhedron $\text{Na}_3\text{Ba}_{10}$
Na5	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.1646		pentacapped trigonal prism Na_5Ba_6
Na6	4 <i>f</i>	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.5091		pseudo Frank-Kasper $\text{Na}_2\text{Ba}_{12}\text{N}_6$
Ba7	4 <i>e</i>	3..	0	0	0.15105		non-coplanar triangle N_3
Na8	2 <i>d</i>	-6..	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		tricapped trigonal prism Ba_6Na_3
Ca9	2 <i>b</i>	-3..	0	0	0		octahedron N_6

Transformation from published data: origin shift 0 0 $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.038$

References: [1] Vajenine G.V., Steinbrenner U., Simon A. (1999), C. R. Acad. Sci., Ser. IIc 2, 583-589.