$Ba_7[SiO_4][BO_3]_3[CN]$	*hP*56	(186) $P6_3mc$ – $d^2c^4b^3a$

$Ba_7(SiO_4)(BO_3)_3CN$ [1]
Structural features: BO_3 trigonal units and SiO_4 tetrahedra in a Mg_3Cd-type (h.c.p.) arrangement; Ba atoms and CN dumbbells (orientational disorder) in voids.

Schmid S. et al. (2003) [1]
$B_3Ba_7CNO_{13}Si$
a = 1.1299, c = 0.7334 nm, c/a = 0.649, V = 0.8109 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*d*	1	0.186	0.563	0.163	0.5	
O2	12*d*	1	0.3964	0.093	0.0522		single atom B
Ba3	6*c*	.*m*.	0.14442	0.85558	0.19303		10-vertex polyhedron O_9CN
Ba4	6*c*	.*m*.	0.52535	0.47465	0.3505		
B5	6*c*	.*m*.	0.8162	0.1838	0.136		coplanar triangle O_3
O6	6*c*	.*m*.	0.8445	0.1555	0.308		single atom B
Si7	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.0832		
Ba8	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.492		
O9	2*b*	3*m*.	$^1/_3$	$^2/_3$	0.86		single atom Si
CN10	2*a*	3*m*.	0	0	0.0		trigonal prism Ba_3O_3

Experimental: single crystal, diffractometer, X-rays, R = 0.033

Remarks: The coordinates of site (CN)10 correspond to the centers of CN dumbbells. Short interatomic distances for partly occupied site(s).

References: [1] Schmid S., Senker J., Schnick W. (2003), J. Solid State Chem. 174, 221-228.