$Ba_{0.5}SrY_3O_6$	*hP*24	(176) $P6_3/m$ – h^3dba

$BaSr_2Y_6O_{12}$ [1]
Structural features: Double infinite chains of edge-linked YO_6 octahedra share vertices to form a 3D-framework; Sr in trigonal prismatic voids, Ba in channels of hexagonal cross-section parallel to [001] (partial disorder). Variant of $Sr_{0.5}CaSc_3O_6$. See Fig. IV.57.

Schulze A.R., Müller Buschbaum H. (1981) [1]
$Ba_{0.50}O_6SrY_3$
a = 1.0299, c = 0.3409 nm, c/a = 0.331, V = 0.3131 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Y1	6*h*	*m*..	0.0016	0.3478	$^1/_4$		octahedron O_6
O2	6*h*	*m*..	0.132	0.603	$^1/_4$		square pyramid Y_3Sr_2
O3	6*h*	*m*..	0.301	0.191	$^1/_4$		non-coplanar triangle Y_3
Sr4	2*d*	-6..	$^2/_3$	$^1/_3$	$^1/_4$		trigonal prism O_6
Ba5	2*b*	-3..	0	0	0	0.25	
Ba6	2*a*	-6..	0	0	$^1/_4$	0.25	

Experimental: single crystal, diffractometer, X-rays, R = 0.080

Remarks: Short interatomic distances for partly occupied site(s). In table I of [1] the *z*-coordinates of former O1 and O2 are misprinted as $^1/_4$ instead of $^3/_4$ (checked on interatomic distances).

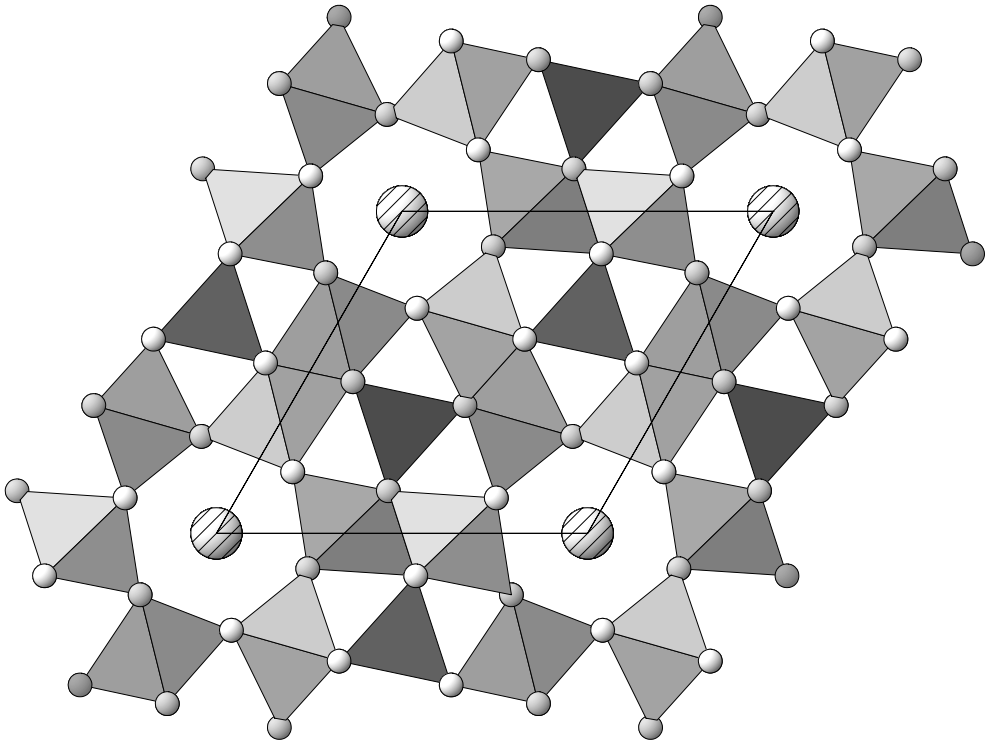

Fig. IV.57. **$BaSr_2Y_6O_{12}$**

Arrangement of SrO_6 trigonal prisms (dark), YO_6 octahedra (light) (O atoms small) and Ba atoms (large; partly occupied sites) viewed along [001].

References: [1] Schulze A.R., Müller Buschbaum H. (1981), Z. Naturforsch. B 36, 837-839.