

BaBi ₂ S ₄	<i>hP</i> 64	(176) <i>P</i> 6 ₃ / <i>m</i> – h ¹⁰ ca
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BaBi₂S₄ (Z=9) [1]

Structural features: Infinite ribbons of edge-linked distorted BiS₆ octahedra (6 octahedra in the cross-section) share vertices to form a 3D-framework.

Aurivillius B. (1983) [1]

BaBi₂S₄

a = 2.1705, *c* = 0.4158 nm, *c/a* = 0.192, *V* = 1.6964 nm³, *Z* = 9

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Bi1	6 <i>h</i>	<i>m</i> ..	0.0304	0.3727	¹ / ₄		octahedron S ₆
S2	6 <i>h</i>	<i>m</i> ..	0.06101	0.1577	¹ / ₄		tetrahedron Bi ₃ Ba
S3	6 <i>h</i>	<i>m</i> ..	0.1715	0.5203	¹ / ₄		non-colinear Bi ₂
Bi4	6 <i>h</i>	<i>m</i> ..	0.2011	0.1933	¹ / ₄		octahedron S ₆
Ba5	6 <i>h</i>	<i>m</i> ..	0.2376	0.4161	¹ / ₄		square antiprism S ₈
S6	6 <i>h</i>	<i>m</i> ..	0.2995	0.0648	¹ / ₄		non-coplanar triangle Bi ₃
S7	6 <i>h</i>	<i>m</i> ..	0.3509	0.2464	¹ / ₄		non-coplanar triangle Bi ₃
S8	6 <i>h</i>	<i>m</i> ..	0.3944	0.4414	¹ / ₄		square pyramid Bi ₄ Ba
S9	6 <i>h</i>	<i>m</i> ..	0.5407	0.2262	¹ / ₄		single atom Bi
Bi10	6 <i>h</i>	<i>m</i> ..	0.5574	0.1179	¹ / ₄		square pyramid S ₅
Ba11	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		tricapped trigonal prism S ₉
Ba12	2 <i>a</i>	-6..	0	0	¹ / ₄	0.5	

Transformation from published data: *y*,*x*,*-z*

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.095

References: [1] Aurivillius B. (1983), Acta Chem. Scand. A 37, 399-407.