

Ba _{1.1} Bi ₂ S ₄	<i>hP</i> 86	(176) <i>P</i> 6 ₃ / <i>m</i> – h ¹⁴ a
--	--------------	--

BaBi₂S₄ (Z=12) [1]; Eu_{1.1}Bi₂S₄ [2]

Structural features: Infinite ribbons of edge-linked distorted BiS₆ octahedra (8 octahedra in the cross-section) share vertices to form a 3D-framework.

Aurivillius B. (1983) [1]

Ba_{1.08}Bi₂S₄

a = 2.5272, *c* = 0.41852 nm, *c/a* = 0.166, *V* = 2.3149 nm³, *Z* = 12

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
S1	6 <i>h</i>	<i>m</i> ..	0.0017	0.3673	¹ / ₄		octahedron Bi ₅ Ba
Bi2	6 <i>h</i>	<i>m</i> ..	0.0236	0.1787	¹ / ₄		octahedron S ₆
Bi3	6 <i>h</i>	<i>m</i> ..	0.05	0.5904	¹ / ₄		square pyramid S ₅
S4	6 <i>h</i>	<i>m</i> ..	0.1151	0.3069	¹ / ₄		non-coplanar triangle Bi ₃
S5	6 <i>h</i>	<i>m</i> ..	0.1351	0.0728	¹ / ₄		tetrahedron Bi ₃ Ba
Bi6	6 <i>h</i>	<i>m</i> ..	0.1448	0.496	¹ / ₄		octahedron S ₆
S7	6 <i>h</i>	<i>m</i> ..	0.215	0.2474	¹ / ₄		non-coplanar triangle Bi ₃
S8	6 <i>h</i>	<i>m</i> ..	0.2495	0.5929	¹ / ₄		single atom Bi
S9	6 <i>h</i>	<i>m</i> ..	0.3046	0.4529	¹ / ₄		square pyramid BiBa ₄
Bi10	6 <i>h</i>	<i>m</i> ..	0.3329	0.2743	¹ / ₄		octahedron S ₆
Ba11	6 <i>h</i>	<i>m</i> ..	0.3495	0.1216	¹ / ₄		square antiprism S ₈
S12	6 <i>h</i>	<i>m</i> ..	0.449	0.272	¹ / ₄		trigonal bipyramid Bi ₃ Ba ₂
S13	6 <i>h</i>	<i>m</i> ..	0.5461	0.094	¹ / ₄		octahedron Bi ₅ Ba
Ba14	6 <i>h</i>	<i>m</i> ..	0.5546	0.232	¹ / ₄		square antiprism S ₈
Ba15	2 <i>a</i>	-6..	0	0	¹ / ₄	0.5	

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.108

Remarks: The author assumes that Wyckoff position 2*a* is occupied by 50% Ba and suggests that, to achieve charge neutrality, some of the Bi sites are only partly occupied. The authors of [2] state that for Eu_{1.1}Bi₂S₄ (metallic) all the Bi sites are fully occupied.

References: [1] Aurivillius B. (1983), Acta Chem. Scand. A 37, 399-407. [2] Lemoine P., Carré D., Guittard M. (1986), Acta Crystallogr. C 42, 259-261.