Ba_3FeS_5	*hP*56	(188) *P*-6*c*2 – $l^2k^2i^2hgca$

$Ba_9Fe_3S_{11}(S_2)_2$ [1]
Structural features: Infinite columns of face-sharing FeS_6 octahedra; additional single S and S_2 dumbbells arranged in chains parallel to [001].

Jenks J.M. et al. (1978) [1]
Ba_3FeS_5
a = 0.9218, c = 1.8042 nm, c/a = 1.957, V = 1.3277 nm^3, Z = 6

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Ba1	12*l*	1	0.0095	0.3841	0.0842		
S2	12*l*	1	0.2289	0.2206	0.0841		non-colinear Fe_2
S3	6*k*	*m*..	0.0054	0.2205	$^1/_4$		non-colinear Fe_2
Ba4	6*k*	*m*..	0.3897	0.3619	$^1/_4$		square antiprism S_8
S5	4*i*	3..	$^2/_3$	$^1/_3$	0.0179	0.5	
S6	4*i*	3..	$^2/_3$	$^1/_3$	0.1591		single atom S
S7	4*h*	3..	$^1/_3$	$^2/_3$	0.1936		single atom S
Fe8	4*g*	3..	0	0	0.1629		8-vertex polyhedron S_6Fe_2
S9	2*c*	3.2	$^1/_3$	$^2/_3$	0		square prism (cube) Ba_6S_2
Fe10	2*a*	3.2	0	0	0		8-vertex polyhedron S_6Fe_2

Experimental: single crystal, diffractometer, X-rays, R = 0.050

Remarks: High-pressure phase. Short interatomic distances for partly occupied site(s). Alternative models in space groups (185) $P6_3cm$ and (193) $P6_3/mcm$ were tested and rejected (R = 0.20 for the latter).

References: [1] Jenks J.M., Hoggins J.T., Rendon Diazmiron L.E., Cohen S., Steinfink H. (1978), Inorg. Chem. 17, 1773-1775.