

$\text{Bi}_{6.33}\text{S}_9\text{I}$	$hP36$	$(176) P6_3/m - h^5ec$
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Bi(Bi₂S₃)₉I₃ [1]

Structural features: :BiS₃ ψ -tetrahedra share vertices to form infinite chains; additional Bi (partial disorder) and I between the chains.

Miehe G., Kupcik V. (1971) [1]

$\text{Bi}_{6.33}\text{IS}_9$

$a = 1.563$, $c = 0.402$ nm, $c/a = 0.257$, $V = 0.8505$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
S1	$6h$	$m..$	0.067	0.4546	$\frac{1}{4}$		square pyramid Bi ₅
S2	$6h$	$m..$	0.1847	0.0166	$\frac{1}{4}$		
S3	$6h$	$m..$	0.2635	0.3953	$\frac{1}{4}$		non-coplanar triangle Bi ₃
Bi4	$6h$	$m..$	0.2965	0.2407	$\frac{1}{4}$		square antiprism S ₈
Bi5	$6h$	$m..$	0.5115	0.1218	$\frac{1}{4}$		5-vertex polyhedron S ₅
Bi6	$4e$	$3..$	0	0	0.103	0.167	
I7	$2c$	$-6..$	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$		14-vertex polyhedron Bi ₆ S ₆ I ₂

Experimental: single crystal, diffractometer, X-rays, $R = 0.082$

Remarks: The cell parameters from [2] were confirmed. Short interatomic distances for partly occupied site(s). Space group (173) $P6_3$ could not be rejected ($R = 0.079$); according to [1] physical properties indicate the absence of an inversion center.

References: [1] Miehe G., Kupcik V. (1971), *Naturwissenschaften* 58, 219. [2] Otto H.H., Strunz H. (1968), *Neues Jahrb. Mineral., Abh.* 108, 1-19.