

$\text{Cu}_4\text{Zr}_3\text{Si}_2$	$hP9$	(189) $P\text{-}62m$ – gfd
-------------------------------------	-------	----------------------------

**Zr<sub>3</sub>Cu<sub>4</sub>Si<sub>2</sub>** [2]

Structural features: Infinite columns of base-linked  $\text{SiZr}_6$  trigonal prisms share edges to form a 3D-framework; single columns of base-linked  $\text{CuCu}_6$  trigonal prisms in channels parallel to [001] (capping atoms ignored). Ordering variant of  $\text{Fe}_2\text{P}$ .

Sprenger H. (1974) [1]

$\text{Cu}_4\text{Si}_2\text{Zr}_3$

$a = 0.6372$ ,  $c = 0.389$  nm,  $c/a = 0.610$ ,  $V = 0.1368$  nm<sup>3</sup>,  $Z = 1$

site	Wyck.	sym.	$x$	$y$	$z$	occ.	atomic environment
Cu1	3g	$m2m$	0.25	0	$\frac{1}{2}$		cuboctahedron $\text{Si}_2\text{Cu}_4\text{Zr}_6$
Zr2	3f	$m2m$	0.584	0	0		pseudo Frank-Kasper $\text{Cu}_8\text{Si}_4\text{Zr}_6$
Si3	2d	-6..	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{2}$		tricapped trigonal prism $\text{Cu}_3\text{Zr}_6$
Cu4	1a	$-62m$	0	0	0		tricapped trigonal prism $\text{Cu}_6\text{Zr}_3$

Transformation from published data: origin shift 0 0  $\frac{1}{2}$

Experimental: powder, film, X-rays

Remarks: The same data are reported in [2].

References: [1] Sprenger H. (1974), J. Less-Common Met. 34, 39-71. [2] Sprenger H., Nickl J.J. (1972), J. Less-Common Met. 27, 163-168.