

NaCu<sub>5</sub>S<sub>3</sub>*hP*18(182) *P*6<sub>3</sub>22 – hgfb**NaCu<sub>5</sub>S<sub>3</sub>** [1]

Structural features: Close-packed S layers in h stacking; Na in octahedral, Cu in linear and trigonal voids. Infinite layers of vertex-linked CuS<sub>3</sub> trigonal units are interconnected via S-Cu-S linear units (infinite zigzag chains parallel to [001]) to form a 3D-framework.

Effenberger H., Pertlik F. (1985) [1]

Cu<sub>5</sub>NaS<sub>3</sub>*a* = 0.6978, *c* = 0.7209 nm, *c/a* = 1.033, *V* = 0.3040 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Cu1	6 <i>h</i>	..2	0.51369	0.02738	<sup>1</sup> / <sub>4</sub>		non-colinear S <sub>2</sub>
S2	6 <i>g</i>	.2.	0.32424	0	0		non-coplanar square Cu <sub>4</sub>
Cu3	4 <i>f</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.02363		non-coplanar triangle S <sub>3</sub>
Na4	2 <i>b</i>	3.2	0	0	<sup>1</sup> / <sub>4</sub>		octahedron S <sub>6</sub>

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays, wR = 0.017, T = 295 K

References: [1] Effenberger H., Pertlik F. (1985), Monatsh. Chem. 116, 921-926.