

AuScSi	<i>hP6</i>	(187) <i>P-6m2</i> – ihba
--------	------------	---------------------------

**ScAuSi** [1]

Structural features: Infinite columns of base-linked AuSc<sub>6</sub> and SiSc<sub>6</sub> trigonal prisms share rectangular faces to form a 3D-framework; Au and Si are displaced from the prism centers to form a tetrahedral framework with Au<sub>2</sub> and Si<sub>2</sub> pairs. Substitution derivative of CaIn<sub>2</sub>.

Fornasini M.L. et al. (1992) [1]

AuScSi

$a = 0.4212$ ,  $c = 0.6803$  nm,  $c/a = 1.615$ ,  $V = 0.1045$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Si1	<i>2i</i>	<i>3m.</i>	$\frac{2}{3}$	$\frac{1}{3}$	0.203		fourcapped trigonal prism Au <sub>3</sub> SiSc <sub>6</sub>
Au2	<i>2h</i>	<i>3m.</i>	$\frac{1}{3}$	$\frac{2}{3}$	0.2842		fourcapped trigonal prism Si <sub>3</sub> Sc <sub>6</sub> Au
Sc3	<i>1b</i>	<i>-6m2</i>	0	0	$\frac{1}{2}$		rhombic dodecahedron Au <sub>6</sub> Si <sub>6</sub> Sc <sub>2</sub>
Sc4	<i>1a</i>	<i>-6m2</i>	0	0	0		rhombic dodecahedron Si <sub>6</sub> Au <sub>6</sub> Sc <sub>2</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0  $\frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.030

References: [1] Fornasini M.L., Iandelli A., Pani M. (1992), J. Alloys Compd. 187, 243-247.