

Tl<sub>3</sub>Ga<sub>9</sub>S<sub>13</sub>O<sub>2</sub>

*hP27*

(174) *P*-6 – 1<sup>2</sup>kj<sup>2</sup>hfeba

**Tl<sub>3</sub>Ga<sub>9</sub>O<sub>2</sub>S<sub>13</sub>** [1]

Structural features: Ga(OS<sub>3</sub>) and GaS<sub>4</sub> tetrahedra share vertices to form a 3D-framework; Tl in voids and in channels parallel to [001].

Jaulmes S. et al. (1986) [1]

Ga<sub>9</sub>O<sub>2</sub>S<sub>13</sub>Tl<sub>3</sub>

*a* = 0.9598, *c* = 0.7433 nm, *c/a* = 0.774, *V* = 0.5930 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ga1	6 <i>l</i>	1	0.10747	0.52743	0.2649		tetrahedron OS <sub>3</sub>
S2	6 <i>l</i>	1	0.35017	0.31023	0.2554		non-colinear Ga <sub>2</sub>
S3	3 <i>k</i>	<i>m</i> ..	0.02767	0.35833	<sup>1</sup> / <sub>2</sub>		non-colinear Ga <sub>2</sub>
S4	3 <i>j</i>	<i>m</i> ..	0.04967	0.37533	0		non-coplanar triangle Ga <sub>3</sub>
Ga5	3 <i>j</i>	<i>m</i> ..	0.20977	0.25973	0		tetrahedron S <sub>4</sub>
O6	2 <i>h</i>	3..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.261		non-coplanar triangle Ga <sub>3</sub>
Tl7	1 <i>f</i>	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>1</sup> / <sub>2</sub>		pseudo Frank-Kasper S <sub>9</sub> Tl <sub>2</sub>
Tl8	1 <i>e</i>	-6..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	0		tricapped trigonal prism S <sub>9</sub>
Tl9	1 <i>b</i>	-6..	0	0	<sup>1</sup> / <sub>2</sub>		pseudo Frank-Kasper S <sub>11</sub>
S10	1 <i>a</i>	-6..	0	0	0		coplanar triangle Ga <sub>3</sub>

Transformation from published data: -*y*, -*x*, -*z*; origin shift <sup>1</sup>/<sub>3</sub> <sup>2</sup>/<sub>3</sub> 0

Experimental: single crystal, diffractometer, X-rays, *R* = 0.050, *T* = 293 K

Remarks: Metastable phase.

References: [1] Jaulmes S., Julien Pouzol M., Dugue J., Laruelle P., Guittard M. (1986), Acta Crystallogr. C 42, 1111-1113.