

Ta <sub>9</sub> Fe <sub>2</sub> S <sub>6</sub>	<i>hP</i> 34	(189) <i>P</i> -62 <i>m</i> – kji <sup>2</sup> hgf
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**Fe<sub>2</sub>Ta<sub>9</sub>S<sub>6</sub>** [1]; Co<sub>2</sub>Ta<sub>9</sub>S<sub>6</sub> [1]

Structural features: Infinite columns of base-linked FeTa<sub>6</sub>Ta<sub>3</sub> tricapped trigonal prisms share the capping atoms to form a 3D-framework; S in large channels parallel to [001]. Deformation derivative of Ta<sub>9</sub>Ni<sub>2</sub>S<sub>6</sub> with distortions towards the formation of Fe<sub>2</sub> dumbbells.

Harbrecht B. (1986) [1]

Fe<sub>2</sub>S<sub>6</sub>Ta<sub>9</sub>

*a* = 1.0266, *c* = 0.6583 nm, *c/a* = 0.641, *V* = 0.6008 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Ta1	6 <i>k</i>	<i>m</i> ..	0.2583	0.4707	<sup>1</sup> / <sub>2</sub>		square pyramid S <sub>3</sub> Fe <sub>2</sub>
Ta2	6 <i>j</i>	<i>m</i> ..	0.2643	0.4531	0		square pyramid S <sub>3</sub> Fe <sub>2</sub>
Ta3	6 <i>i</i>	.. <i>m</i>	0.4578	0	0.2537		coplanar triangle S <sub>3</sub>
S4	6 <i>i</i>	.. <i>m</i>	0.7042	0	0.267		5-vertex polyhedron Ta <sub>5</sub>
Fe5	4 <i>h</i>	3.. <sup>1</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.2188		trigonal prism Ta <sub>6</sub>
S6	3 <i>g</i>	<i>m</i> 2 <i>m</i>	0.272	0	<sup>1</sup> / <sub>2</sub>		4-vertex polyhedron Ta <sub>4</sub>
S7	3 <i>f</i>	<i>m</i> 2 <i>m</i>	0.274	0	0		4-vertex polyhedron Ta <sub>4</sub>

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

Experimental: single crystal, diffractometer, X-rays, R = 0.045

Remarks: Supersedes a report on Fe<sub>2</sub>Ta<sub>9</sub>S<sub>6</sub> with half cell volume (Ni<sub>2</sub>Ta<sub>9</sub>S<sub>6</sub> type) in [2].

References: [1] Harbrecht B. (1986), J. Less-Common Met. 124, 125-134. [2] Harbrecht B., Franzen H.F. (1986), J. Less-Common Met. 115, 177-189.