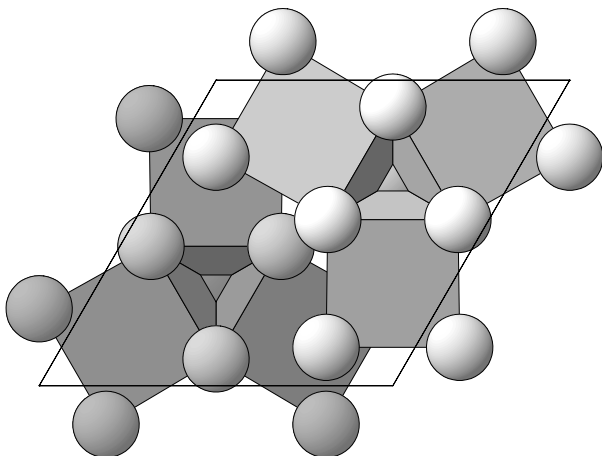


Th<sub>7</sub>Fe<sub>3</sub>*hP*20(186) *P*6<sub>3</sub>*mc* – c<sup>3</sup>b**Th<sub>7</sub>Fe<sub>3</sub>** [2], Strukturbericht notation D10<sub>2</sub>; Ru<sub>7</sub>B<sub>3</sub> [3]Structural features: FeTh<sub>6</sub>Th<sub>3</sub> tricapped trigonal prisms (non-parallel prism axes) share atoms to form a 3D-framework. See Fig. IV.23.Fig. IV.23. **Th<sub>7</sub>Fe<sub>3</sub>**Arrangement of FeTh<sub>6</sub> trigonal prisms viewed along [001]. Light and dark prisms are shifted by *c*/2.

Florio J.V. et al. (1956) [1]

Fe<sub>3</sub>Th<sub>7</sub>*a* = 0.985, *c* = 0.615 nm, *c/a* = 0.624, *V* = 0.5167 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
Fe1	6 <i>c</i>	. <i>m</i> .	0.185	0.815	0.25		tricapped trigonal prism Th <sub>9</sub>
Th2	6 <i>c</i>	. <i>m</i> .	0.544	0.456	0.03		15-vertex Frank-Kasper Fe <sub>4</sub> Th <sub>11</sub>
Th3	6 <i>c</i>	. <i>m</i> .	0.874	0.126	0.31		15-vertex Frank-Kasper Fe <sub>4</sub> Th <sub>11</sub>
Th4	2 <i>b</i>	3 <i>m</i> .	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	0.0		15-vertex Frank-Kasper Fe <sub>3</sub> Th <sub>12</sub>

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0.44000

Experimental: single crystal, oscillation photographs, X-rays

Remarks: In [1] and [2] the Th sites are interchanged in the lists of interatomic distances with respect to the lists of atom coordinates (see [4] and [5]).

References: [1] Florio J.V., Baenziger N.C., Rundle R.E. (1956), Acta Crystallogr. 9, 367-372. [2] Baenziger N.C. (1952), Iowa State Coll. J. Sci. 27, 126-128. [3] Aronsson B. (1959), Acta Chem. Scand. 13, 109-114. [4] (1969), Structure Reports 25, 356. [5] (1969), Structure Reports 25, 359.