

$\text{Ba}_3\text{Fe}(\text{Fe}_{0.5}\text{Te}_{0.5})_2\text{O}_9$	<i>hP30</i>	(182) <i>P6<sub>3</sub>22</i> – <i>ihf<sup>2</sup>ba</i>
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**Ba<sub>3</sub>Fe<sub>2</sub>TeO<sub>9</sub>** [1], perovskite 6H

Structural features: Close-packed BaO<sub>3</sub> layers in hc<sub>2</sub> stacking; Fe and (Fe,Te) in octahedral (O<sub>6</sub>) voids. Pairs of face-linked (Fe,Te)O<sub>6</sub> octahedra ((Fe,Te)<sub>2</sub> dumbbells) share vertices with single FeO<sub>6</sub> octahedra to form a 3D-framework.

Gagulin V.V. et al. (1978) [1]

Ba<sub>3</sub>Fe<sub>2</sub>O<sub>9</sub>Te

*a* = 0.5804, *c* = 1.413 nm, *c/a* = 2.435, *V* = 0.4122 nm<sup>3</sup>, *Z* = 2

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.343	0.159	0.081		non-colinear Fe <sub>2</sub>
O2	6 <i>h</i>	..2	0.514	0.028	1/4		non-colinear Fe <sub>2</sub>
Ba3	4 <i>f</i>	3..	1/3	2/3	0.093		cuboctahedron O <sub>12</sub>
M4	4 <i>f</i>	3..	1/3	2/3	0.649		octahedron O <sub>6</sub>
Ba5	2 <i>b</i>	3.2	0	0	1/4		anticuboctahedron O <sub>12</sub>
Fe6	2 <i>a</i>	32.	0	0	0		octahedron O <sub>6</sub>

M4 = 0.5Fe + 0.5Te

Transformation from published data: -*x*, -*y*, -*z*

Experimental: powder, diffractometer, neutrons, R<sub>B</sub> = 0.080

Remarks: The structure was also refined in space group (194) *P6<sub>3</sub>/mmc* (R = 0.089).

References: [1] Gagulin V.V., Fadeeva N.V., Belous A.G., Titov A.V., Mitrofanov K.P., Plotnikova M.V., Soloviev S.P., Venevtsev Y.N. (1978), Phys. Status Solidi A 48, 183-189.