$(Ti_{0.6}Fe_{0.4})_{13.89}O_{25}$	*hP*100	(182) $P6_322$ – $i^4h^4g^4ca$

$Fe_2Ti_3O_9$ [1], pseudorutile
Structural features: Close-packed O layers in h stacking; cations in octahedral voids (partial order).

Grey I.E., Reid A.F. (1975) [1]
$Fe_{5.93}O_{25}Ti_{8.89}$
a = 1.4375, c = 0.4615 nm, c/a = 0.321, V = 0.8259 nm^3, Z = 2

site	Wyck.	sym.	x	y	z	occ.	atomic environment
O1	12*i*	1	0.129	0.469	0.232		trigonal prism Ti_6
O2	12*i*	1	0.339	0.067	0.228		trigonal prism Ti_6
M3	12*i*	1	0.378	0.194	0.018	0.67	7-vertex polyhedron O_6Ti
M4	12*i*	1	0.619	0.224	0.017	0.68	bicapped square prism O_6Ti_4
O5	6*h*	..2	0.13	0.26	$^1/_4$		trigonal prism Ti_6
O6	6*h*	..2	0.533	0.066	$^1/_4$		trigonal prism Ti_6
O7	6*h*	..2	0.74	0.48	$^1/_4$		trigonal prism Ti_6
O8	6*h*	..2	0.934	0.868	$^1/_4$		trigonal prism Ti_6
M9	6*g*	.2.	0.191	0	0	0.81	octahedron O_6
M10	6*g*	.2.	0.409	0	0	0.98	octahedron O_6
M11	6*g*	.2.	0.6	0	0	0.02	octahedron O_6
M12	6*g*	.2.	0.794	0	0	0.18	octahedron O_6
O13	2*c*	3.2	$^1/_3$	$^2/_3$	$^1/_4$		trigonal prism Ti_6
M14	2*a*	32.	0	0	0	0.75	octahedron O_6

M3 = 0.6Ti + 0.4Fe; M4 = 0.6Ti + 0.4Fe; M9 = 0.6Ti + 0.4Fe; M10 = 0.6Ti + 0.4Fe; M11 = 0.6Ti + 0.4Fe; M12 = 0.6Ti + 0.4Fe; M14 = 0.6Ti + 0.4Fe
Transformation from published data: origin shift 0 0 $^1/_2$
Experimental: single crystal, Weissenberg photographs, X-rays, R = 0.069

Remarks: Natural specimen from Indonesia. Composition $Fe^{3+}_{1.34}Fe^{2+}_{0.26}Mn^{3+}_{0.15}Ti^{4+}_{3.25}O_9 \cdot 0.48H_2O$ from chemical analysis. When relevant, we changed the last digit of the atom coordinates to respect the symmetry conditions for special positions. Short interatomic distances: d(M3-M4) = 0.216 nm. Approximately 5-fold supercell; a = 0.2875/x nm, where x = 0.185-0.195, from Weissenberg and precession photographs. In table 2 of [1] the x-coordinate of former O_2 is misprinted as 0.666 instead of 0.066 (agreement with Wyckoff position 6*h*, closer to the ideal value).

References: [1] Grey I.E., Reid A.F. (1975), Am. Mineral. 60, 898-906.