

$\text{K}_{0.31}\text{Na}_{0.64}\text{Ba}_{0.71}\text{Mg}_{0.29}\text{Fe}_{10.55}\text{O}_{17.30}$ 

hP80

(174)  $P-6 - 1^6k^2; 2^4h^4g^7ed$  $\text{K}_{0.31}\text{Na}_{0.64}\text{Ba}_{0.71}\text{Mg}_{0.29}\text{Fe}_{10.55}\text{O}_{17.30}$  [1], magnetoplumbite familyStructural features: Intergrowth of M-type ferrite and  $\beta$ -alumina type structures in the ratio 2:1.

Stergiou A.C. et al. (1998) [1]

 $\text{Ba}_{0.71}\text{Fe}_{10.56}\text{K}_{0.26}\text{Mg}_{0.27}\text{Na}_{0.61}\text{O}_{17.29}$  $a = 0.591$ ,  $c = 2.3203$  nm,  $c/a = 3.926$ ,  $V = 0.7019$  nm<sup>3</sup>,  $Z = 2$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	6l	1	0.0052	0.4882	0.0959	0.91	trigonal bipyramid Fe <sub>4</sub> O
O2	6l	1	0.0057	0.5	0.4009	0.91	trigonal bipyramid Fe <sub>4</sub> O
O3	6l	1	0.1553	0.301	0.1979	0.86	trigonal bipyramid Fe <sub>4</sub> O
M4	6l	1	0.1655	0.3349	0.3594	0.873	8-vertex polyhedron O <sub>7</sub> Fe
O5	6l	1	0.3182	0.1638	0.3022	0.86	trigonal bipyramid Fe <sub>4</sub> O
M6	6l	1	0.339	0.167	0.1435	0.873	8-vertex polyhedron O <sub>7</sub> Fe
O7	3k	<i>m</i> ..	0.0165	0.5104	1/2	0.107	coplanar triangle O <sub>2</sub> Ba
O8	3k	<i>m</i> ..	0.3696	0.1666	1/2	0.9	
O9	3j	<i>m</i> ..	0.157	0.3517	0	0.9	
O10	3j	<i>m</i> ..	0.5253	0.0405	0	0.107	coplanar triangle BaO <sub>2</sub>
Fe11	2i	3..	2/3	1/3	0.1084	0.11	7-vertex polyhedron O <sub>4</sub> Fe <sub>3</sub>
M12	2i	3..	2/3	1/3	0.1925		trigonal bipyramid Fe <sub>5</sub>
M13	2i	3..	2/3	1/3	0.2786	0.943	tetrahedron O <sub>4</sub>
M14	2i	3..	2/3	1/3	0.4418	0.913	9-vertex polyhedron O <sub>9</sub>
M15	2h	3..	1/3	2/3	0.0638	0.913	9-vertex polyhedron O <sub>9</sub>
M16	2h	3..	1/3	2/3	0.2236	0.943	tetrahedron O <sub>4</sub>
M17	2h	3..	1/3	2/3	0.303		trigonal bipyramid Fe <sub>5</sub>
Fe18	2h	3..	1/3	2/3	0.381	0.11	7-vertex polyhedron O <sub>4</sub> Fe <sub>3</sub>
M19	2g	3..	0	0	0.0117	0.387	
M20	2g	3..	0	0	0.0995	0.904	
O21	2g	3..	0	0	0.1389	0.21	
M22	2g	3..	0	0	0.2521		7-vertex polyhedron O <sub>7</sub>
O23	2g	3..	0	0	0.3471	0.21	single atom O
M24	2g	3..	0	0	0.4043	0.904	single atom O
M25	2g	3..	0	0	0.4927	0.387	
M26	1e	-6..	2/3	1/3	0	0.896	
M27	1d	-6..	1/3	2/3	1/2	0.896	

M4 = 0.973Fe + 0.027Mg; M6 = 0.973Fe + 0.027Mg; M12 = 0.94O + 0.04K + 0.02Na; M13 = 0.975Fe + 0.025Mg; M14 = 0.974Fe + 0.026Mg; M15 = 0.974Fe + 0.026Mg; M16 = 0.975Fe + 0.025Mg; M17 = 0.94O + 0.04K + 0.02Na; M19 = 0.835Fe + 0.09Ba + 0.052Na + 0.023Mg; M20 = 0.745O + 0.155Na + 0.10K; M22 = 0.98Fe + 0.02Mg; M24 = 0.745O + 0.155Na + 0.10K; M25 = 0.835Fe + 0.09Ba + 0.052Na + 0.023Mg; M26 = 0.72Ba + 0.28Na; M27 = 0.72Ba + 0.28Na

Transformation from published data: -*x*, -*y*, -*z*; origin shift 0 0 1/2

Experimental: single crystal, diffractometer, X-rays, wR = 0.032

Remarks: Phase referred to as (Na,K)- $\beta$ "-ferrite. The total occupancies of sites M12 and M17 were set to unity, published value 1.023. In table 2 of [1] the Wyckoff position of former O(30) is misprinted as 3j instead of 3k. Short interatomic distances for partly occupied site(s).

References: [1] Stergiou A.C., Litsardakis G., Samaras D. (1998), Solid State Ionics 109, 55-64.