

$K_5[H_3O]_2Fe_3[SO_4]_6O[OH]_2[H_2O]_6$	<i>hP98</i>	(176) $P6_3/m - i^6h^2f^2dba$
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$K_5Fe_3(SO_4)_6(OH)_2 \cdot 8-9H_2O$ [1], Maus' salt

Structural features: $Fe_3O(H_2O)_3(SO_4)_6$ units (a ring of three vertex-linked $Fe(O_5[OH_2])$ octahedra sharing vertices with three SO_4 tetrahedra on each side) arranged in layers separated by K and additional H_2O .

Giacovazzo C. et al. (1975) [1]

$Fe_3H_{20}K_5O_{35}S_6$

$a = 0.971$, $c = 1.896$ nm, $c/a = 1.953$, $V = 1.5481$ nm³, $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>i</i>	1	0.0884	0.2941	0.1764		single atom S
O2	12 <i>i</i>	1	0.2687	0.0477	0.0699		single atom S
O3	12 <i>i</i>	1	0.2992	0.1848	0.1775		single atom S
S4	12 <i>i</i>	1	0.3133	0.0609	0.1414		tetrahedron O ₄
M5	12 <i>i</i>	1	0.358	0.4274	0.0541		9-vertex polyhedron O ₆ (OH ₂) ₂ K
O6	12 <i>i</i>	1	0.4732	0.0954	0.1465		single atom S
Fe7	6 <i>h</i>	<i>m..</i>	0.1738	0.2157	$\frac{1}{4}$		octahedron O ₅ (OH ₂)
(OH ₂)8	6 <i>h</i>	<i>m..</i>	0.3677	0.4551	$\frac{1}{4}$		single atom Fe
(OH ₂)9	4 <i>f</i>	3.. <i></i>	$\frac{1}{3}$	$\frac{2}{3}$	0.1428		bicapped square prism K ₃ (OH ₂) ₄ O ₃
(OH ₂)10	4 <i>f</i>	3.. <i></i>	$\frac{1}{3}$	$\frac{2}{3}$	0.518		non-coplanar triangle K ₃
K11	2 <i>d</i>	-6.. <i></i>	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{4}$		trigonal prism O ₆
K12	2 <i>b</i>	-3.. <i></i>	0	0	0		octahedron O ₆
O13	2 <i>a</i>	-6.. <i></i>	0	0	$\frac{1}{4}$		coplanar triangle Fe ₃

$M5 = 0.5K + 0.5OH_2$

Experimental: single crystal, diffractometer, X-rays, R = 0.086

Remarks: The authors state that sites (OH₂)9 and (OH₂)10 may be occupied by $[H_3O]^+$ and $[OH]^-$, or vice versa. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Giacovazzo C., Scordari F., Menchetti S. (1975), Acta Crystallogr. B 31, 2171-2173.