

Space group (209) *F*432209
*cF*104

KPF ₆	<i>cF</i> 104	(209) <i>F</i> 432 – jba
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KPF₆ α [1]Structural features: K atoms and PF₆ octahedra (orientational disorder) in a NaCl-type arrangement.

Mascarenhas Y.P., Pulcinelli S.H. (1981) [1]

F₆KP $a = 0.771 \text{ nm}$, $V = 0.4583 \text{ nm}^3$, $Z = 4$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
F1	96j	1	0.043	0.109	0.165	0.25	
P2	4b	432	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
K3	4a	432	0	0	0		

Transformation from published data: $-x, -y, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.093$ Remarks: Space groups (196) *F*23, (216) *F*-43*m*, and (225) *Fm*-3*m* were tested and rejected. Short interatomic distances for partly occupied site(s). In [1] one of the alternative space groups is misprinted as *F*-432 instead of *F*-43*m*.

References: [1] Mascarenhas Y.P., Pulcinelli S.H. (1981), Acta Crystallogr. A 37, C175d.

209
*cF*744

Na[NH ₄] ₇ Mo ₁₆ O ₄₀ [OH] ₁₂ [H ₂ O] ₄	<i>cF</i> 744	(209) <i>F</i> 432 – j ⁶ gf ² e ² c
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(NH₄)₇[NaMo₁₆(OH)₁₂O₄₀]·4H₂O [1]Structural features: NaMo₁₂O₂₈(OH)₁₂ Keggin units (twelve edge- and vertex-linked MoO₆ octahedra sharing vertices with a central NaO₄ tetrahedron) share vertices with four additional Mo(O,OH)₆ octahedra to form NaMo₁₆O₄₀(OH)₁₂ units; NH₄ and H₂O between the units.

Khan M.I. et al. (1996) [1]

H_{48.02}Mo₁₆N₇NaO_{56.01} $a = 2.6978 \text{ nm}$, $V = 19.6349 \text{ nm}^3$, $Z = 8$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
(OH ₂)1	96j	1	0.0	0.1558	0.3396	0.267	
O2	96j	1	0.0659	0.2886	0.2041		single atom Mo
O3	96j	1	0.112	0.1869	0.1191		single atom Mo
Mo4	96j	1	0.1274	0.2154	0.284		octahedron O ₄ (OH) ₂
(OH)5	96j	1	0.1373	0.1387	0.2864		non-colinear Mo ₂
O6	96j	1	0.1388	0.2085	0.2152		coplanar triangle Mo ₃
(NH ₄)7	48g	..2	0	0.1892	0.1892	0.778	non-colinear O ₂
Mo8	32f	.3.	0.1549	0.1549	0.1549		octahedron O ₆
O9	32f	.3.	0.2966	0.2966	0.2966		tetrahedron Mo ₃ Na
(OH ₂)10	24e	4..	0.0919	0	0	0.267	non-coplanar square (OH ₂) ₄
(NH ₄)11	24e	4..	0.303	0	0	0.778	coplanar square (OH ₂) ₄

Na12	8c	23.	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	tetrahedron O ₄
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Transformation from published data: $-x, -y, -z$

Experimental: single crystal, diffractometer, X-rays, R = 0.076, T = 213 K

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The partial site occupancies are omitted in [1], later communicated by the authors. In the abstract, table 1 and the supplementary material deposited for [1] the space group is misprinted as (216) $F\bar{4}3m$ instead of (209) $F432$ (checked on interatomic distances).

References: [1] Khan M.I., Chen Q., Salta J., O'Connor C.J., Zubieta J. (1996), Inorg. Chem. 35, 1880-1901.