

$\text{K}_{0.5}(\text{Ca}_{0.5}\text{Nd}_{0.5})[\text{PO}_4]$  $hP21$ (180)  $P6_222 - kdca$ **KCaNd(PO<sub>4</sub>)<sub>2</sub>** [1]

Structural features: Distorted (Ca,Nd)O<sub>8</sub> square antiprisms are interconnected via common edges and PO<sub>4</sub> tetrahedra to form a 3D-framework; K in channels parallel to [001]. Filled-up derivative of hexagonal CePO<sub>4</sub>.

Vlasse M. et al. (1982) [1]

 $\text{Ca}_{0.50}\text{K}_{0.50}\text{Nd}_{0.50}\text{O}_4\text{P}$  $a = 0.7033$ ,  $c = 0.6397$  nm,  $c/a = 0.910$ ,  $V = 0.2740$  nm<sup>3</sup>,  $Z = 3$ 

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
O1	12 <i>k</i>	1	0.3013	0.4397	0.18683		single atom P
M2	3 <i>d</i>	222	$\frac{1}{2}$	0	$\frac{1}{2}$		8-vertex polyhedron O <sub>8</sub>
P3	3 <i>c</i>	222	$\frac{1}{2}$	0	0		tetrahedron O <sub>4</sub>
K4	3 <i>a</i>	222	0	0	0	0.5	colinear K <sub>2</sub>

 $\text{M2} = 0.5\text{Ca} + 0.5\text{Nd}$ Transformation from published data: origin shift 0 0  $\frac{1}{2}$ 

Experimental: single crystal, diffractometer, X-rays, R = 0.042

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Vlasse M., Bochu P., Parent C., Chaminade J.P., Daoudi A., Le Flem G., Hagenmuller P. (1982), Acta Crystallogr. B 38, 2328-2331.