

Na(Na<sub>0.5</sub>Nd<sub>0.5</sub>)NdF<sub>6</sub>*hP*10(174) *P*-6 – kjida**NaNdF<sub>4</sub>** [1]

Structural features: Infinite columns of base-linked NdF<sub>6</sub>F<sub>3</sub> and (Na,Nd)F<sub>6</sub>F<sub>3</sub> trigonal prisms share atoms to form a 3D-framework; additional Na in channels of hexagonal cross-section parallel to [001] (partial disorder).

Burns J.H. (1965) [1]

F<sub>6</sub>Na<sub>1.50</sub>Nd<sub>1.50</sub>*a* = 0.61, *c* = 0.3711 nm, *c/a* = 0.608, *V* = 0.1196 nm<sup>3</sup>, *Z* = 1

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	3 <i>k</i>	<i>m</i> ..	0.29043	0.25747	<sup>1</sup> / <sub>2</sub>		square pyramid NdNa <sub>4</sub>
F2	3 <i>j</i>	<i>m</i> ..	0.06723	0.42157	0		square pyramid Na <sub>3</sub> Nd <sub>2</sub>
Na3	2 <i>i</i>	3..	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>3</sub>	0.156	0.5	
Nd4	1 <i>d</i>	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>2</sub>		tricapped trigonal prism F <sub>9</sub>
M5	1 <i>a</i>	-6..	0	0	0		tricapped trigonal prism F <sub>9</sub>

M5 = 0.5Na + 0.5Nd

Transformation from published data: origin shift <sup>2</sup>/<sub>3</sub> <sup>1</sup>/<sub>3</sub> <sup>1</sup>/<sub>2</sub>Experimental: single crystal, diffractometer, X-rays, *R* = 0.019

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

References: [1] Burns J.H. (1965), *Inorg. Chem.* 4, 881-886.