

$\text{Na}_{0.5}(\text{Ca}_{0.5}\text{Y}_{0.2}\text{Ce}_{0.15}\text{Nd}_{0.15})\text{F}_3$	$hP16$	$(176) P6_3/m - \text{he}^2c$
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**Na(Ca,R,Y)<sub>2</sub>F<sub>6</sub>** [1], gagarinite-(Y)

Structural features: Infinite columns of base-linked (RE,Ca)F<sub>6</sub>F<sub>3</sub> tricapped trigonal prisms share atoms to form a 3D-framework; Na (partial disorder) in channels of hexagonal cross-section parallel to [001]. Filled-up derivative of UCl<sub>3</sub>.

Frank Kamenetskaya O.V. et al. (1994) [1]

$\text{Ca}_{0.50}\text{Ce}_{0.15}\text{F}_3\text{Na}_{0.56}\text{Nd}_{0.15}\text{Y}_{0.20}$

$a = 0.60403$ ,  $c = 0.35899$  nm,  $c/a = 0.594$ ,  $V = 0.1134$  nm<sup>3</sup>,  $Z = 2$

site	Wyck.	sym.	<i>x</i>	<i>y</i>	<i>z</i>	occ.	atomic environment
F1	6 <i>h</i>	<i>m</i> ..	0.3932	0.0843	<sup>1</sup> / <sub>4</sub>		
Na2	4 <i>e</i>	3..	0	0	0.038	0.189	
Na3	4 <i>e</i>	3..	0	0	0.216	0.09	
M4	2 <i>c</i>	-6..	<sup>1</sup> / <sub>3</sub>	<sup>2</sup> / <sub>3</sub>	<sup>1</sup> / <sub>4</sub>		tricapped trigonal prism F <sub>9</sub>

$\text{M4} = 0.498\text{Ca} + 0.198\text{Y} + 0.152\text{Ce} + 0.152\text{Nd}$

Transformation from published data: origin shift 0 0 <sup>1</sup>/<sub>2</sub>

Experimental: single crystal, diffractometer, X-rays,  $R = 0.012$

Remarks: Natural specimen from eastern Siberia. Composition  $\text{Na}_{0.95}(\text{Sr}_{0.02}\text{Ca}_{0.94})(\text{Y}_{0.52}\text{La}_{0.04}\text{Ce}_{0.15}\text{Pr}_{0.02}\text{Nd}_{0.12}\text{Sm}_{0.04}\text{Gd}_{0.06}\text{Dy}_{0.07}\text{Ho}_{0.01}\text{Er}_{0.03}\text{Yb}_{0.02})\text{F}_6$  from X-ray spectroscopy. Refinement considering f(Eu) for the rare earths on site M4, refined partial occupancy 0.299(4). We replaced Eu by a mixture of Ce and Nd (majority rare-earth elements), assuming full occupation of site M4. Short interatomic distances for partly occupied site(s).

References: [1] Frank Kamenetskaya O.V., Fundamenskii V.S., Tsytsenko A.K., Frank Kamenetskii V.A. (1994), Crystallogr. Rep. 39, 923-928 (Kristallografiya 39, 1009-1014).