

$\text{Na}_{0.42}(\text{Na}_{0.18}\text{Ca}_{0.06}\text{Y}_{0.64}\text{Er}_{0.12})\text{F}_3$	<i>hP12</i>	(176) <i>P6₃/m – hec</i>
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Na_{1.2}Ca_{0.12}Y_{1.28}R_{0.24}F₆ [1], gagarinite-(Y); Na_{1.5}Y_{1.5}F₆ hp [2]

Structural features: Infinite columns of base-linked (Y,Na,Er,Ca)F₆F₃ tricapped trigonal prisms share atoms to form a 3D-framework; additional Na in channels of hexagonal cross-section parallel to [001] (partial disorder). Filled-up derivative of UCl₃.

Kabalov Y.K. et al. (1993) [1]

Ca_{0.06}Er_{0.12}F₃Na_{0.60}Y_{0.65}

a = 0.59855, *c* = 0.35469 nm, *c/a* = 0.593, *V* = 0.1100 nm³, *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> ..	0.3879	0.0787	¹ / ₄		
Na2	4 <i>e</i>	3..	0	0	0.069	0.216	
M3	2 <i>c</i>	-6..	¹ / ₃	² / ₃	¹ / ₄		tricapped trigonal prism F ₉

M3 = 0.65Y + 0.17Na + 0.12Er + 0.06Ca

Transformation from published data: origin shift 0 0 ¹/₂

Experimental: powder, diffractometer, X-rays, R = 0.036

Remarks: Natural specimen from Araskan, Eastern Sayans, Mongolia. Composition Na_{1.40}Ca_{0.11}Y_{1.03}La_{0.01}Ce_{0.03}Pr_{0.01}Nd_{0.02}Sm_{0.01}Gd_{0.04}Tb_{0.02}Dy_{0.12}Ho_{0.02}Er_{0.10}Yb_{0.08})F₆ from electron microprobe analysis. We adjusted the charge balance in the chemical formula given in [1] by changing the Na index from 1.23 to 1.2 and assigned an approximate value to the Er/Y ratio of site M3 based on the nominal composition, Er representing the rare-earth elements. Short interatomic distances for partly occupied site(s). Supersedes a structure proposal in space group (147) *P*-3 in [3]. Different arrangements of Na atoms are proposed in [4] and [5]. In table 1 of [1] the Wyckoff position of former sites (Y,TR), Na and Ca is misprinted as 2*c* instead of 2*d*.

References: [1] Kabalov Y.K., Sokolova E.V., Grigor'ev A.P. (1993), Dokl. Akad. Nauk 330, 713-715. [2] Grzechnik A., Bouvier P., Mezouar M., Mathews M.D., Tyagi A.K., Köhler J. (2002), J. Solid State Chem. 165, 159-164. [3] Voronkov A.A., Shumyatskaya N.G., Pyatenko Y.A. (1962), J. Struct. Chem. 3, 665-669 (Zh. Strukt. Khim. 3, 691-696). [4] Frank Kamenetskaya O.V., Fundamenskii V.S., Tsytsenko A.K., Frank Kamenetskii V.A. (1994), Crystallogr. Rep. 39, 923-928 (Kristallografiya 39, 1009-1014). [5] Hughes J.M., Drexler J.W. (1994), Can. Mineral. 32, 563-565.