# Kristalne strukture Cs2HoSi4O10F i Cs2TmSi4O10F

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# KRISTALNE STRUKTURE $Cs_2HoSi_4O_{10}F$ I $Cs_2TmSi_4O_{10}F$

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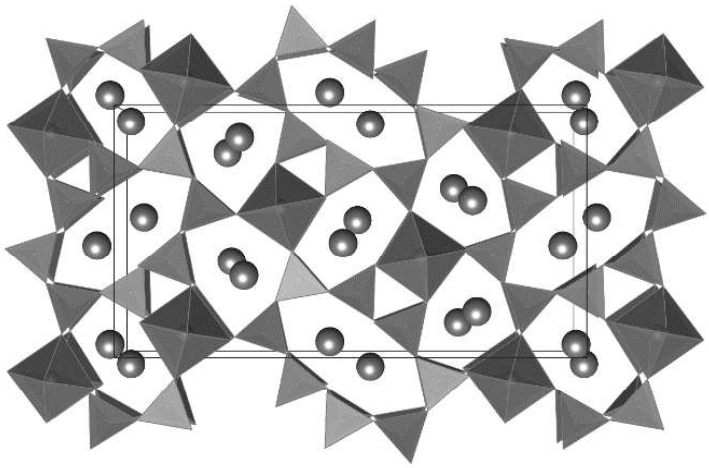
Tokom istraživanja fokusiranog na sintezu novih kalijumskih silikata elemenata retkih zemalja dobijena su dva jedinjenja do tada nepoznatog hemijskog sastava - $Cs_2HoSi_4O_{10}F$ i $Cs_2TmSi_4O_{10}F$, u obliku monokristala.

Jedinjenja su sintetisana metodom rasta kristala iz visokotemperaturnog rastvora ($T_{max}$ = 1373 K) koristeći $REE_2O_3$ (*REE* = Ho, Tm), $SiO_2$ i CsF kao polazne suptance. Kristalne strukture oba jedinjenja rešene su iz difrakcionih podataka prikupljenih na odabranim monokristalima. Dobijena jedinjenja su međusobno izostrukturna i kristališu u rombičnoj prostornoj grupi *Pnma* sa sledećim parametrima jediničnih ćelija: $a$ = 22,3809 (7), $b$ = 8,8686 (3), $c$ = 11,9827 (4) Å, $V$ = 2378,41 (14) Å$^3$, $Z$ = 8 (za jedinjenje $Cs_2HoSi_4O_{10}F$), $a$ = 22,3447 (5), $b$ = 8,8131 (2), $c$ = 11,9594 (3) Å, $V$ = 2355,12 (10) Å$^3$, $Z$ = 8 (za jedinjenje $Cs_2TmSi_4O_{10}F$). Ispitivana jedinjenja su izostrukturna sa $Cs_2YSi_4O_{10}F$ [1] i $Cs_2ErSi_4O_{10}F$ [2].

Kristalnu strukturu ovih jedinjenja čine višestruki lanci $SiO_4$-tetraedara koji su povezani beskonačnim jednodimenzionalnim lancima $REEO_4F_2$-oktaedara. U tunelima koji nastaju kondenzacijom tetraedarske mreže i oktaedarskih lanaca smešteni su katjoni cezijuma. $SiO_4$-tetraedri su međusobno povezani preko zajedničkih rogljeva i izgrađuju kolone, odnosno cevastu strukturu. $REEO_4F_2$-oktaedri međusobno su povezani preko zajedničkih anjona fluora, koji se nalaze u apikalnim rogljevima.



Slika 1. Projekcija strukture $Cs_2REESi_4O_{10}F$ paralelna sa pravcem [010] predstavljena poliedrima.

[1] M.C. Schäfer, T. Schleid, *Z. Naturforsch. B.*, **64** (2009) 1329–1338.
[2] P. Dabić, V. Kahlenberg, D. Schmidmair, A. Kremenović, P. Vulić, *Z. Krist.-Cryst. Mater.*, **231** (2016) 195–207.

# CRYSTAL STRUCTURES OF $Cs_2HoSi_4O_{10}F$ AND $Cs_2TmSi_4O_{10}F$

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During investigation focused on the synthesis of new potassium rare-earth elements silicates two compounds with a previously unknown chemical composition - $Cs_2HoSi_4O_{10}F$ and $Cs_2TmSi_4O_{10}F$ were obtained in form of single crystals.

The compounds were synthesized by the method of crystal growth from a high-temperature solution ($T_{max}$ = 1373 K) using $REE_2O_3$ (*REE* = Ho, Tm), $SiO_2$ and CsF as starting materials. The crystal structures of both compounds were determined by single-crystal X-ray diffraction analysis. They represent mutually isostructural compounds which crystallize in the orthorhombic space group *Pnma* with following unit cell parameters: $a$ = 22.3809 (7), $b$ = 8.8686 (3), $c$ = 11.9827 (4) Å, $V$ = 2378.41 (14) Å$^3$, $Z$ = 8 (for $Cs_2HoSi_4O_{10}F$ compound), $a$ = 22.3447 (5), $b$ = 8.8131 (2), $c$ = 11.9594 (3) Å, $V$ = 2355.12 (10) Å$^3$, $Z$ = 8 (for $Cs_2TmSi_4O_{10}F$ compound). The investigated compounds are isotypic to $Cs_2YSi_4O_{10}F$ [1] and $Cs_2ErSi_4O_{10}F$ [2].

The crystal structure of these compounds consists of multiple chains of $SiO_4$-tetrahedra connected by infinite one-dimensional chains of $REEO_4F_2$-octahedra. Cesium cations are located in tunnels formed by condensation of the tetrahedral network and octahedral chains. $SiO_4$-tetrahedra are interconnected through common vertices and form columns, i.e. a tubular structure. $REEO_4F_2$-octahedra are interconnected *via* common fluorine apical anions.

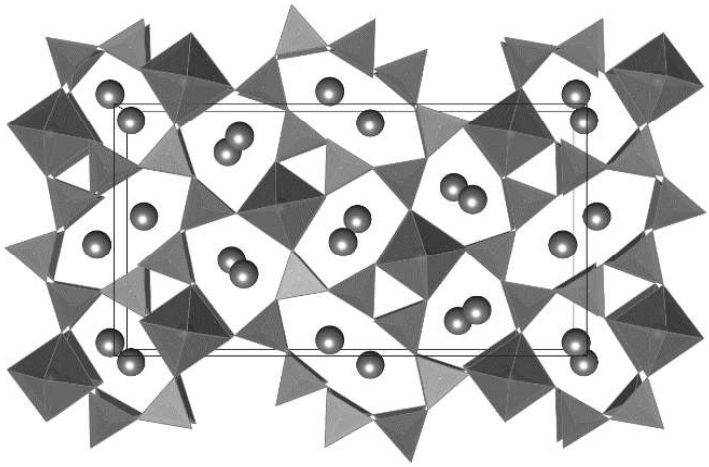

Figure 1. Projection of the structure of $Cs_2REESi_4O_{10}F$ parallel to the direction [010] represented by polyhedra.

[1] M.C. Schäfer, T. Schleid, *Z. Naturforsch. B.*, **64** (2009) 1329–1338.
[2] P. Dabić, V. Kahlenberg, D. Schmidmair, A. Kremenović, P. Vulić, *Z. Krist.-Cryst. Mater.*, **231** (2016) 195–207.