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Esseneite from Xenoliths in Dacite Lavas: Crystal Structure and Genesis

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Abstract—Esseneite from ultramafic xenoliths in dacite flow of the Ten'-01 paleovolcano at the Lena–Vilyui watershed, East Yakutia has been studied. The empirical formula of the mineral has been obtained using electron microprobe analysis: $\text{Ca}_{0.99}\text{Fe}_{0.52}^{3+}\text{Mg}_{0.32}\text{Fe}_{0.06}^{2+}\text{Ti}_{0.05}\text{Mn}_{0.01}^{2+}\text{Al}_{0.71}\text{Si}_{1.34}\text{O}_6$. Its crystal structure has been refined on the basis of the single crystal X-ray diffraction data, ($R = 0.0152$). The resulting crystal chemical formula is: ${}^{\text{Ca}}\text{Ca}^{\text{M}}\left(\text{Fe}_{0.48}^{3+}\text{Mg}_{0.33}\text{Ti}_{0.05}\text{Al}_{0.14}\right)^{\text{T}}\left(\text{Si}_{1.28}\text{Al}_{0.68}\text{Fe}_{0.04}^{3+}\right)\text{O}_6$. The monoclinic unit-cell parameters are: $a = 9.7610(12)$, $b = 9.8223(8)$, $c = 5.3360(5)$ Å, $\beta = 105.92(1)$, $V = 441.89(8)$ Å³, $Z = 4$, space group $C2/c$. The distribution of atoms over positions in the crystal structures of the Ca–Fe–Al clinopyroxenes and coordination polyhedron distortions, which reflect the formation conditions of the minerals, have been analyzed. The Yakutia esseneite has been formed in a highly oxidizing environment at 1200–950°C and approximate pressure of 2 kbar.

Key words: esseneite, crystal structure, Ten'-01 paleovolcano, Yakutia

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INTRODUCTION

Esseneite, a rare pyroxene-group mineral, is both natural and technogenic. As a new mineral species with the idealized formula $\text{CaFe}^{3+}\text{AlSiO}_6$, it was described in 1987 as a pyrometamorphic compound that came from paralava that resulted from coal bed combustion in Durham Ranch, Wyoming, United States (Cosca and Peacor, 1987). That year, the data on the compositionally close Ca-clinopyroxene with the high Fe and Al content from the similar rock, buchite, from Buffalo and Wyoming were published (Foit et al., 1987). According to (Cosca and Peacor, 1987), pyroxene from fassaite–garnet–anorthite xenolith found in the Udachanya kimberlite pipe, Yakutia (Shatsky, 1983) should be considered as esseneite. Calcium pyroxenes with the high Fe^{3+} and Al content were documented in burnt dumps of the coal pits in the Chelyabinsk and Kizel coal basins in the Urals (Chesnokov and Shcherbakova, 1991). A detailed description of the Al- and Fe^{3+} -rich clinopyroxenes in the skarns of Ciclova and Magureaua Vatei, Carpathians, Romania is given in (Pascal et al., 2005)

During the study of rocks identified within the cone-shaped paleovolcanic construction Ten'-01 located at the Lena–Vilyui divide (Kostin et al., 2015; Kostin, 2017) in the Lunga and Tyugene headwaters

(tributaries of the Lena River), we found coarse-grained rock predominantly composed of Ca-pyroxene crystals with unusual high Fe and Al content. This rock is presented as xenoliths in dacitic flow.

On the basis of the chemical composition and powder X-ray diffraction data, the pyroxene was preliminary attributed to esseneite (Zayakina et al., 2016). In this study, the additional chemical data and refined crystal structure, as well as a crystal chemical comparison of esseneite with its synthetic analogue, and compositionally close clinopyroxenes, are given.

OCCURRENCE AND CHEMICAL COMPOSITION

The described mineral was identified in pyroxene (23 vol %)–anorthite (75 vol %) rock as dark-green to nearly black crystals up to 1 cm in size (Fig. 1). Spinel (magnesian ferrite and hercynite), garnets (pyrope, grossular, andradite, and almandine), fayalite, zircon, and baddeleyite are minor associated phases.

The chemical composition was determined using a CAMEBAX-micro electron microprobe. A thin polished section of the mineral coated by carbon was examined. The measurement was performed at acceleration voltage 20 kV, current intensity 40 nA, and beam diameter 2 μm, (analyst N.V. Khristoforova).

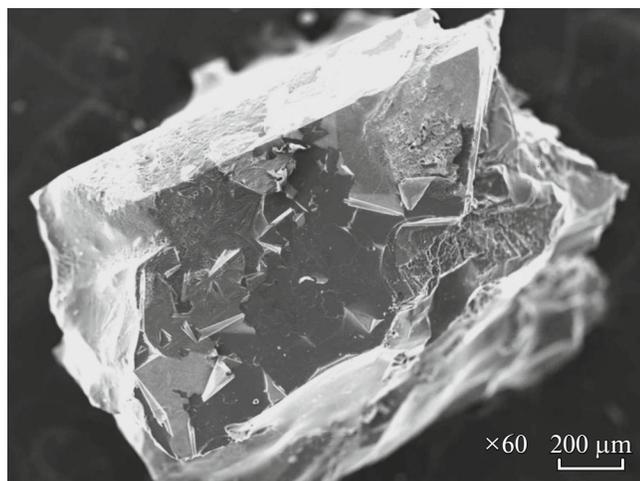


Fig. 1. Secondary electron image of esseneite crystal.

The following standards were used: garnet (IGEM) (Fe, Mn), blue diopside (Si, Mg, Ca), pyrope (O-145) (Al), albite (Na), ilmenite (IL-GF-55) (Ti). The results of five-point analyses are given in Table 1. The empirical formula of the examined pyroxene calculated on the basis of 4 cations with Fe^{2+} and Fe^{3+} contents calculated from charge balance constraints is $\text{Ca}_{0.99}\text{Fe}_{0.52}^{3+}\text{Mg}_{0.32}\text{Fe}_{0.06}^{2+}\text{Ti}_{0.05}\text{Mn}_{0.01}^{2+}\text{Al}_{0.71}\text{Si}_{1.34}\text{O}_6$.

X-RAY DIFFRACTION AND CRYSTAL STRUCTURE REFINEMENT

A single crystal pyroxene fragment of $0.04 \times 0.10 \times 0.14$ mm in size for the X-ray structure analysis was picked up under an optical microscope equipped with the universal table. The X-ray diffraction data were collected in a full sphere of reciprocal space using an Xcalibur S single crystal diffractometer equipped with a CCD detector. The Crys Alis RED (Oxford Diffraction Ltd) software package was used for processing of the reflection intensities, including corrections for the Lorentz factor and polarization, and refinement of the unit-cell parameters. The empirical absorption correction was introduced during the shape modelling of the crystal studied. The winGX (Farrugia, 2012) software was used to determine and refine the structure. Curves of atomic scattering and anomalous dispersion corrections taken from (*International ...*, 2004) were used. The structure was resolved by the direct methods in the $C2/c$ space group usual for monoclinic clinopyroxenes and was refined in anisotropic approximation of atom vibrations using the SHELX software package (Sheldrick, 2015a, 2015b). Initially, the cation distribution was refined on the basis of the chemical composition of the mineral in the following approximation: Fe + Mg (as predominant in octahedra) at site $M1$, site $M2$ in the eight-fold polyhedron is completely occupied by the Ca atoms, and fixed occupation of tet-

rahedra by the Si and Al atoms in ratio of 1.3 : 0.7. As a result the Fe : Mg ratio is 0.49 : 0.51. The excessive Mg content is caused by the presence of Al, which has close scattering capacity. During further refinement of the structure, we varied the Fe, Mg, Al, and Ti contents at the octahedral site, which were the closest to those determined with an electron microprobe and controlled by the residual factor and behavior of thermal vibration ellipsoids. The Si : Al ratio in tetrahedra that could not be refined on the basis of the X-ray diffraction data due to close scattering capability was taken according to the matter electroneutrality. The applied number of Si and Al atoms at the tetrahedral site is consistent with the polyhedron size: average distance $T\text{--}O = 1.677$ Å. The following step-by-step addition of small amounts of Fe^{3+} instead of Al at the tetrahedral site corresponded to the R factor value during the structure refinement. The following crystal chemical formula $\text{Ca}(\text{Fe}_{0.48}^{3+}\text{Mg}_{0.33}\text{Ti}_{0.05}\text{Al}_{0.14})(\text{Si}_{1.28}\text{Al}_{0.68}\text{Fe}_{0.04}^{3+})\text{O}_6$ corresponds to the minimal residual factor ($R = 0.0152$). This formula is consistent with that calculated from electron microprobe data: $\text{Ca}_{0.99}\text{Fe}_{0.52}^{3+}\text{Mg}_{0.32}\text{Fe}_{0.06}^{2+}\text{Ti}_{0.05}\text{Mn}_{0.01}^{2+}\text{Al}_{0.71}\text{Si}_{1.34}\text{O}_6$. The main differences between them are slightly lower Fe (0.52 against 0.58) and Si (1.28 against 1.34) and higher Al (0.82 against 0.71) in the crystal chemical formula. These differences are probably caused by the real composition of the crystal studied deviated from the average mineral composition and are generally within the uncertainty of the used methods.

The crystallographic characteristics, conditions of the X-ray diffraction experiment, and the data of the structure refinement are given in Table 2; atom coordinates and interatomic distances are given in Tables 3 and 4, respectively. The main fragments forming crystal structure are octahedra MO_6 isomorphically occupied by Fe, Mg, Al, and Ti; tetrahedra TO_4 containing minor Fe^{3+} in addition to the major constituents Si and Al; and the Ca atoms in the center of the oxygen eight-fold polyhedra (Fig. 2). Ellipsoids of thermal atom vibrations (small size and closeness to the spherical shape)¹ presented with the 90% probability indicate a high reliability of the structure information obtained.

The powder X-ray diffraction pattern of esseneite was obtained using a D2 PHASER diffractometer operated at $\text{CuK}\alpha$ radiation. It is consistent with that calculated from the structure data (Table 5) that also supports the reliability of the latter.

¹ Ellipsoids determine the space, in which the center of electron density can be localized with a specific probability. The higher probability percentage of ellipsoids is used, the more reliable structural information is obtained.

Table 1. Chemical composition of Ca–Fe³⁺–Al clinopyroxenes, wt %

Component	Range of content (<i>n</i> = 5)	Average content (<i>n</i> = 5)	2	3	4
	1				
SiO ₂	33.38–34.11	33.88	29.51	34.40	36.99
TiO ₂	1.47–1.61	1.54	0.99	2.19	0.59
Al ₂ O ₃	14.67–15.94	15.31	17.95	19.80	13.04
Cr ₂ O ₃	0.02–0.06	0.03	No data	No data	0.02
Fe ₂ O ₃	19.66–19.85	17.64	23.89	11.50	17.39
FeO		1.93	0.69	3.65	0.03
MnO	0.13–0.16	0.15	0.11	No data	No data
MgO	5.06–5.93	5.50	2.68	4.93	7.70
CaO	23.35–23.59	23.45	23.40	23.70	24.19
Na ₂ O	0.00–0.02	0.00	0.14	0.07	0.03
Total	99.54–99.85	99.43	99.36	100.24	99.98
Formula coefficients					
Si	1.34	1.19	1.32	1.43	
Al	0.71	0.85	0.90	0.59	
Fe ³⁺	0.52	0.72	0.33	0.51	
Fe ²⁺	0.06	0.02	0.12	0.00	
Ti	0.05	0.03	0.06	0.02	
Mg	0.32	0.16	0.28	0.44	
Mn	0.01	0.00			
Na	0.00	0.01	0.01		
Ca	0.99	1.01	0.98	1.00	

(1) Volcanic structure Ten'-01, (2) paralava, Wyoming, US (Cosca and Peacor, 1987), (3) xenolith from the Udachnaya kimberlite pipe (Shatsky, 1983), (4) pyrometamorphic rock from burnt coal dump, Chelyabinsk coal basin, South Urals (Chesnokov and Shcherbakova, 1991). The Fe₂O₃ and FeO contents are calculated from charge balance constraints in the formula calculated on the basis of 4 cations.

DUSCUSSION

In the structure of esseneite studied here, the interatomic distances *M*–O in octahedra range from 1.973(1) to 2.110(1) Å. The range of the similar cation–oxygen distances in the structures of pyroxenes with high Fe³⁺ and Al (Table 6) shows that octahedron distortions in our case are very close to those in esseneite from fritted sedimentary rocks in the vicinity of the Gillette town, Wyoming, United States. The highly distorted Al,Si–O tetrahedra have average *T*–O bond length of 1.677 Å, which follows the trend of the *T*–O distances as a function of the Al : (Al + Si) ratio at the tetrahedral site of aluminosilicate pyroxenes (Hazen and Finger, 1977). The ranges of the cation–oxygen bond lengths in tetrahedron are also consistent with those in the structure of esseneite from Wyoming (Table 6). The mentioned correlations are regular and are caused by the specific features of the octahedron and tetrahedron chemistry: among described minerals, occupancies of the *M* and *T* structure sites in esseneite from paralava (Wyoming, United States) and

our esseneite are the closest. The Ca–O distances range from 2.390(1)–2.638(1) Å and are typical of the CaO₈ eight-fold polyhedra.

The review of the studied crystal structures of the Ca–Fe³⁺–Al clinopyroxenes indicates variable distribution of Fe³⁺ between the *M* and *T* sites. Ferric iron occupies not only the octahedral site, but also the tetrahedral one in the structure of synthetic analogue of esseneite, pyroxene from the burnt dumps in the Chelyabinsk coal basin and our mineral from Yakutia. According to (Ghose et al., 1986; Cosca and Peacor, 1987), distribution of the Fe³⁺ cations at sites *M* and *T* reflects the formation conditions of the mineral and is caused by the cooling rate of the crystallization system. The synthetic sample with the composition close to ideal CaFe³⁺AlSiO₆ was synthesized by rapid crystallization (48 h) in the high-pressure reaction vessel at 1375°C and 20 kbar from mixture of synthetic anorthite, gehlenite, wollastonite, and hematite (Ohashi and Hariya, 1975) as a result of the reaction

Table 2. Crystallographic characteristics of esseneite, X-ray diffraction data, and parameters of its structure refinement

Structural formula	$\text{Ca}(\text{Fe}_{0.48}^{3+}\text{Mg}_{0.33}\text{Ti}_{0.05}\text{Al}_{0.14})\text{(Si}_{1.28}\text{Al}_{0.68}\text{Fe}_{0.04}^{3+})\text{O}_6$
Symmetry, space group, Z	Monoclinic, $C2/c$, 4
a , Å	9.7610(12)
b , Å, β , degree	8.8223(8), 105.918(13)
c , Å	5.3360(5)
V , Å ³	441.89(8)
D_x , g/cm ³	3.512
Radiation, λ , Å	$\text{MoK}\alpha$; 0.71073
Crystal size, mm	$0.04 \times 0.10 \times 0.15$
μ , mm ⁻¹	3.650
Diffraction method	Xcalibur-S-CCD
Scanning mode	ω
Absorption correction	Empirical
T_{\min} , T_{\max}	0.611, 0.868
θ_{\max} , degree	29.982
Ranges of h , k , l	$-13 \leq h \leq 13$, $-12 \leq k \leq 12$, $-7 \leq l \leq 7$
Number of reflections: observed/unique (N_1)/with $I > 2\sigma(I)$ (N_2)	3974/ 648/ 633
Refinement method	by F^2
Number of refined parameters	48
Extinction coefficient	0.0057(8)
R_{inner} , R_{σ}	0.0257, 0.0154
$R/\omega R_2$ by N_1	0.0160/0.0418
$R1/\omega R_2$ by N_2	0.0152/0.0414
S	1.265
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$, e/Å ³	0.267, -0.258

Table 3. Atom coordinates and equivalent isotropic displacement parameters (U_{eq} , Å²) in structure of esseneite

Atom position*	x/a	y/b	z/c	U_{eq}
M	0.5	0.90642(4)	0.75	0.00664(11)
Ca	0.0	0.80757(5)	0.75	0.01039(12)
T	0.28800(4)	0.59413(4)	0.72321(8)	0.00580(11)
O1	0.35359(12)	0.51998(14)	0.4877(2)	0.0120(2)
O2	0.36329(13)	0.75860(14)	0.8198(2)	0.0132(2)
O3	0.11090(13)	0.58665(13)	0.6336(2)	0.0117(2)

Composition of positions with mixed occupancy: $M(\text{Fe}_{0.48}^{3+}\text{Mg}_{0.33}\text{Ti}_{0.05}\text{Al}_{0.14})$ $T(\text{Si}_{1.28}\text{Al}_{0.68}\text{Fe}_{0.04}^{3+})$.

Table 4. Interatomic distances (Å) in esseneite crystal structure

M octahedron	Ca eight-fold polyhedron	T tetrahedron
M –O2 1.9726(12) × 2	Ca–O2 2.3895(11) × 2	T –O2 1.6444(12)
–O3 2.0371(12) × 2	–O3' 2.3926(11) × 2	–O3 1.6640(12)
–O3' 2.1103(12) × 2	–O1 2.5326(12) × 2	–O1 1.6906(12)
	–O1' 2.6384(11) × 2	–O1' 1.7088(12)
Average 2.040	Average 2.488	Average 1.677

Table 5. Observed and calculated powder X-ray diffraction data for esseneite

I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl	I_{obs}	d_{obs}	d_{calc}	I_{calc}	hkl	
5	4.691	4.693	9	200	2	1.858	1.857	2	331	
		4.437	9	11 $\bar{1}$	6	1.837	1.836	11	510	
11	4.414	4.411	18	020	14	1.736	1.734	9	150	
3	3.343	3.345	31	021	2	1.679	1.680	8	31 $\bar{3}$	
15	3.210	3.214	15	220	7	1.673	1.672	10	042	
100	2.989	2.988	100	22 $\bar{1}$	11	1.642	1.643	20	22 $\bar{3}$	
36	2.947	2.949	46	310	20	1.622	1.621	19	53 $\bar{1}$	
38	2.896	2.901	32	31 $\bar{1}$	7	1.607	1.607	11	440	
57	2.561	2.567 2.565	14	20 $\bar{2}$	11	1.537	1.537 1.536 1.535	6	350	
			39	002				7	60 $\bar{2}$	
29	2.554	2.552	23	13 $\bar{1}$				9	402	
46	2.518	2.519	46	221	5	1.517	1.517	20	13 $\bar{3}$	
3	2.385	2.381	11	131	4	1.471	1.470	7	060	
2	2.346	2.347	2	400	12	1.423	1.422	26	531	
15	2.311	2.312	16	311	10	1.405	1.405	7	223	
15	2.241	2.242	17	112	7	1.401	1.404	13	35 $\bar{2}$	
5	2.218	2.218	8	022	3	1.335	1.335	12	71 $\bar{2}$	
13	2.143	2.143	9	330	4	1.329	1.329	5	621	
26	2.124	2.124	14	33 $\bar{1}$	2	1.304	1.306 1.306	8	314	
20	2.107	2.106	7	42 $\bar{1}$				5	114	
39	2.028	2.031 2.029 2.026	9	40 $\bar{2}$	2	1.277	1.276 1.276	6	26 $\bar{2}$	
			5	202						
			24	041						
					4	1.247	1.247	9	062	
7	1.975	1.976	8	13 $\bar{2}$	2	1.068	1.068	6	750	
					5	1.058	1.057	5	57 $\bar{1}$	

The reflections with intensities ≥ 5 of the calculated X-ray diffraction pattern and two weaker reflections corresponding to observed reflection are given.

$CaAl_2Si_2O_8 + Ca_2Al_2SiO_7 + CaSiO_3 + 2Fe_2O_3 = 4CaFeAlSiO_6$. According to (Cosca and Peacor, 1987), its crystal structure is characterized by the highest Fe^{3+} content in tetrahedra (Table 6). The high cooling rate facilitates the Fe^{3+} disordered distribution between tetrahedra and octahedra. The lower Fe content in natural samples is evidently caused by lower cooling in the geological system. Kabalov et al. (1997) suggested the following formation parameters for the Chelyabinsk Si-rich diopside with minor Fe and Al in tetrahedra: high initial temperature ($\geq 1000^\circ C$) and cooling down to $300\text{--}500^\circ C$ in during the period of a few days to a few weeks under high oxygen fugacity. The mineral studied here appears to be formed also in the similar near-surface environment. Previously, we showed that pyroxene (“fassaite”) anorthosite, in which esseneite studied here was identified, crystallized at $1200\text{--}950^\circ C$ and 2 kbar (Kostin et al., 2017); here, temperature is consistent with that of the pyroxene formation in the burnt coal dump, but pressure is dramatically different.

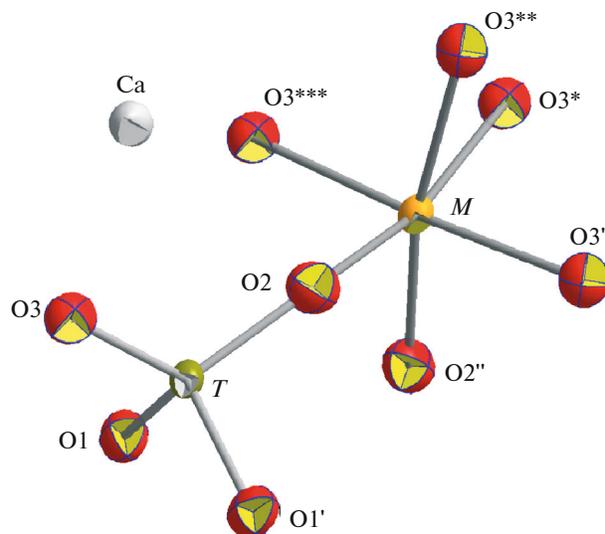


Fig. 2. Basic unites of esseneite crystal structure: octahedron MO_6 ($M = Fe_{0.48}^{3+}Mg_{0.33}Ti_{0.05}Al_{0.14}$) and tetrahedron TO_4 ($T = Si_{1.28}Al_{0.68}Fe_{0.04}^{3+}$). Atoms are shown as ellipsoids of the thermal vibration (with probability 90%).

Table 6. Crystallographic and some crystal chemical data for Ca-clinopyroxenes enriched in Fe³⁺ and Al (space group CD2/c, Z = 4)

Crystal chemical formula, mineral	Unit cell parameters (a, b, c, Å, β, V, Å ³), ρ, g/cm ³	Range of M–O distances, Å in octahedron	Range and average T–O distances, Å in tetrahedron	Reference
Ca(Fe _{0.48} ³⁺ Mg _{0.33} Ti _{0.05} Al _{0.14}) · (Si _{1.28} Al _{0.68} Fe _{0.04} ³⁺)O ₆ , esseneite	9.761(1) 8.822(1) 5.336(1) 105.92(1) 441.9, 3.51	1.973–2.110 (2.040)	1.644–1.709 (1.677)	This study
(Ca _{1.01} Na _{0.01})(Fe _{0.72} ³⁺ Fe _{0.02} ²⁺) · Mg _{0.16} Ti _{0.03} Al _{0.04} (Si _{1.19} Al _{0.81})O ₆ , esseneite	9.79(1) 8.822(9) 5.37(1) 105.81(9) 446.2, 3.51	1.971–2.125 (2.050)	1.646–1.714 (1.676)	Cosca & Peacor, 1987
Ca(Fe _{0.82} ³⁺ Al _{0.18}) · (Si _{1.00} Al _{0.82} Fe _{0.18} ³⁺)O ₆ , synthetic analogue of esseneite	9.780(2) 8.782(1) 5.369(1) 105.78(1) 443.7, 3.70	1.936–2.108 (2.024)	1.671–1.722 (1.698)	Ghose et al., 1986
Ca(Mg _{0.45} Fe _{0.35} ³⁺ Ti _{0.02} Al _{0.08}) · (Si _{1.42} Al _{0.42} Fe _{0.16} ³⁺)O ₆ , * Fe ³⁺ -Al-diopside	9.786(2) 8.860(1) 5.338(1) 105.87(1) 445.2, 3.45	2.030–2.100 (2.07)	1.652–1.742 (1.7)	Kabalov et al., 1997
(Ca _{0.98} Na _{0.01})(Fe _{0.33} ³⁺ Mg _{0.28} ²⁺) · Fe _{0.12} Ti _{0.06} Al _{0.22} (Si _{1.32} Al _{0.68})O ₆ , ** esseneite	9.733(6) 8.818(7) 5.326(3) 105.88(5)	No data	No data	Shatsky, 1983

*The structure was refined by the Rietveld method using the powder X-ray diffraction data.

**Calculated from the electron microprobe data.

CONCLUSIONS

A comprehensive study of rare Si-depleted clinopyroxene esseneite from xenoliths in dacite flow of the cone-shaped volcanic structure Ten'-10 on the Lena-Vilui watershed in East Yakutia has been carried out. The average empirical formula of the mineral calculated from the electron microprobe data is

Ca_{0.99}Fe_{0.52}³⁺Mg_{0.32}Fe_{0.06}²⁺Ti_{0.05}Mn_{0.01}²⁺Al_{0.71}Si_{1.34}O₆. The crystal chemical of the sample with full X-ray diffraction study is

$${}^{Ca}Ca^M(\text{Fe}_{0.48}^{3+}\text{Mg}_{0.33}\text{Ti}_{0.05}\text{Al}_{0.14})^T(\text{Si}_{1.28}\text{Al}_{0.68}\text{Fe}_{0.04}^{3+})\text{O}_6.$$

The mineral studied is formed under oxidative conditions at high temperature (1200–950°C) and approximate pressure of 2 kbar. Ferric iron cations at tetrahedral site may indicate rapid melt cooling during crystallization of the mineral.

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REFERENCES

- Chesnokov, B.V. and Shcherbakova, E.P., *Mineralogiya gorelykh otvalov Chelyabinskogo ugol'nogo basseina (opyt mineralogii tekhnogeneza)* (Mineralogy of Burnt Dumps of the Chelyabinsk Coal Basin (Experience of Mineralogy of Technogenesis), Moscow: Nauka, 1991.
- Cosca, M.A. and Peacor, D.R., Chemistry and structure of esseneite (CaFe³⁺AlSiO₆), a new pyroxene produced by pyrometamorphism, *Am. Mineral.*, 1987, vol. 72, pp. 148–156.
- Farrugia, L.J., WinGX and ORTEP for Windows: an update, *J. Appl. Cryst.*, 2012, vol. 45, pp. 849–854.
- Foit, F.F.Jr., Hooper, R.L., and Rosenberg, P.E., An unusual pyroxene, melilite, and iron oxide mineral assemblage in coal fire buchite from Buffalo, Wyoming, *Am. Mineral.*, 1987, vol. 72, pp. 137–142.
- Ghose, S., Okamura, F.P., and Ohashi, H., The crystal structure of CaFe³⁺SiAlO₆ and the crystal chemistry of Fe³⁺ → Al³⁺ substitution in calcium Tschermak's pyroxene, *Contrib. Mineral. Petrol.*, 1986, vol. 92, pp. 530–535.
- Hazen, R.M. and Finger, L.W., *Compressibility and crystal structure of Angra dos Reis fassaite to 52 kbar*, *Carnegie Inst. Wash. Year Book*, 1977, pp. 512–515.
- International Tables for Crystallography*, Prince, E., Ed., Dordrecht: Kluwer, 2004, Tables 4.2.6.8 and 6.1.14.

- Kabalov, Y.K., Oeckerl, O., Sokolova, E.V., Mironov, A.B., and Chesnokov, B.V., Subsilicic ferrian aluminian diopside from the Chelyabinsk coal basin (Southern Urals)—an unusual clinopyroxene, *Eur. J. Mineral.*, 1997, vol. 9, no. 3, pp. 617–621.
- Kostin, A.V., A new geological object of volcanic origin on the Lena-Vilyui watershed (east of the Siberian Platform), *Usp. Sovremen. Estestvozn.*, 2017, no. 2, pp. 100–105.
- Kostin, A.V., Grinenko, B.C., Oleinikov, O.B., Zhelonkina, M.S., and Krivoshapkin, I.I., *The first data on the Upper Cretaceous volcanism of the transition zone Siberian Platform—Verkhoyansk—Kolyma folded region*, *Nauka Obrazov.*, 2015, no. 1, pp. 30–36.
- Kostin, A.V., Trinulina, B.A., and Grinenko, B.C., Geological model of the Tugeninsk field of volcanic rocks (east of the Siberian platform), *Geologiya i mineral'no-syr'evye resursy Severo-Vostoka Rossii. Mater. VII Vseross. Nauchn-Prakt. Conf.*, (Geology and Mineral Resources of the Northeast of Russia: Proc. VII Russian Sci. Pract. Conference), Yakutsk: SBFU Publishing house, 2017, vol. 2, pp. 219–221.
- Ohashi, H. and Hariya, Y., Phase relation of CaFeAlSiO_6 pyroxene at high pressures and temperatures. *J. Jap. Assoc. Mineral. Petrol. Econ. Geol.*, 1975, vol. 70, pp. 93–95.
- Pascal, M.-L., Katona, I., Fonteilles, M., and Verkaeren, J., Relics of high-temperature clinopyroxene on the join Di–CaTs with up to 72 mol % $\text{Ca}(\text{Al}, \text{Fe}^{3+})\text{AlSiO}_6$ in the skarns of Ciclova and MagureauaVatei, Carpathians, Romania. *Can. Mineral.*, 2005, vol. 43, pp. 857–881.
- Shatsky, V.S., Xenolith of fassaite–garnet–anorthite rock from the Udachnaya kimberlite pipe, (Yakutia), *Dokl. Akad. Nauk SSSR*, 1983, vol. 272, no. 1, pp. 188–192.
- Sheldrick, G.M., SHELXT—integrated space-group and crystal structure determination, *Acta Crystallogr.*, 2015a, A71, pp. 3–8.
- Sheldrick, G.M., Crystal structure refinement with SHELXL, *Acta Crystallogr.*, 2015b, C71, pp. 3–8.
- Zayakina, N.V., Oleinikov, O.B., Kostin, A.V., The discovery of rare pyroxene esseneite in Yakutia, *Geologiya i mineral'no-syr'evye resursy Severo-Vostoka Rossii. Mater. VI Vseross. Nauchn-Prakt. Conf.*, (Geology and Mineral Resources of the Northeast of Russia. Proc. VI Russian Sci. Pract. Conference), Yakutsk: 2016, pp. 219–221.

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