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Solid solutions of triangle clinopyroxenes: synthesis and cell parameters refinement

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Clinopyroxenes are the minerals widespread in metamorphic and magmatic rocks. As a general rule clinopyroxenes are solid solutions of three or more minales. The study of alkaline clinopyroxene solid solutions represented by the diopside–hedenbergite–aegirine system was the purpose of our work. In previous papers the binary solid solutions aegirine–diopside [*Nolan, Edgar*, 1963], diopside–hedenbergite [*Nolan,* 1969], aegirine–hedenbergite [*Redhammer, et al.,* 1998] have been investigated. These studies show insignificant deviation of clinopyroxenes solid solutions from ideality. At the same time the Nolan`s results [*Nolan,* 1969] concerned with synthesis of clinopyroxenes in triangle system (*Di–Hed–Aeg*) demonstrate the existence of valuable deviations from ideality in spite of great data dispersion. To estimate the influence of aegirine intromission to the clinopyroxene solid solutions systematically it has been necessary to synthesize the triangle solid solutions with constant content of aegirine minal (20 mol.%). The synthesis of clinopyroxene triangle solid solutions (in the system diopside–hedenbergite–aegirine) was carried out at the temperature 750°C and pressure 1.5 kbar; experiment duration was 45 days. The initial materials were gel mixtures of corresponding compositions in mole proportions. Hedenbergite gel was previously deoxidizing in hydrogen flow at 600°C during 2 hours. We select mixtures with mole part of aegirine 0.2 in every one. Synthesis of clinopyroxene was carried out in solution of potassium fluoride which is good mineralizer. Herewith potassium doesn't penetrate into clinopyroxene composition. Oxygen potential was preseted by iron–wustite (or wustite–magnetite) buffer. The ratio test charge:fluid was 12÷15. Microanalysis shows correspondence of synthetic clinopyroxenes to theoretical formula. Aegirine content in synthetic clinopyroxenes is according to mole fraction X_{Aeg}^{CPx3}=0.22±0.03. Based on the x-ray study the cell parameters refinement has been produced. Estimation of cell parameters was realizing for c2/c space group (tabl. 1).

Table 1. Cell parameters of triangle solid solutions of clinopyroxenes (Di – Hed – Aeg system); average mole fraction of aegirine is 0.22±0.03

Mol.% Aeg	Mol.% Hed	Mol.% Di	X_{Mg}^{CPx} [1]	a, Å	b, Å	c, Å	β,°	V, Å^3	References[2]
20	80	0	0	9.821	8.984	5.253	105.17	447.3	1
20.6	57.5	21.9	0.276	9.777	8.957	5.265	105.66	443.9	2
33	46	21	0.31	9.767	8.933	5.266	105.84	442.0	1
25.4	47.3	27.3	0.366	9.764	8.937	5.262	105.81	441.7	2
22	41	37	0.47	9.763	8.925	5.270	105.96	441.5	1
20	40	40	0.50	9.758	8.926	.269	105.94	441.3	1
20	37.7	42.3	0.529	9.761	8.937	5.261	105.82	441.5	2
22	29	49	0.63	9.752	8.923	5.263	105.93	440.4	1
25	25	50	0.67	9.758	8.930	5.262	105.82	441.2	1
24.6	22.9	52.5	0.696	9.747	8.919	5.264	106.00	439.9	2
23	13	64	0.83	9.744	8.906	5.262	106.03	438.9	1
14.5	13.5	72	0.842	9.746	8.924	5.263	105.92	440.1	2
12	12	76	0.87	9.740	8.912	5.256	105.94	438.7	1
29	9	62	0.873	9.728	8.902	5.261	106.15	437.6	2
20	0	80	1	9.723	8.919	5.220	106.43	434.2	1

[1] X_{Mg}^{CPx}= Mg/(Mg+Fe^{2+})

[2] References: 1 – our data; 2 – data of Nolan **[*Nolan,* 1969].**

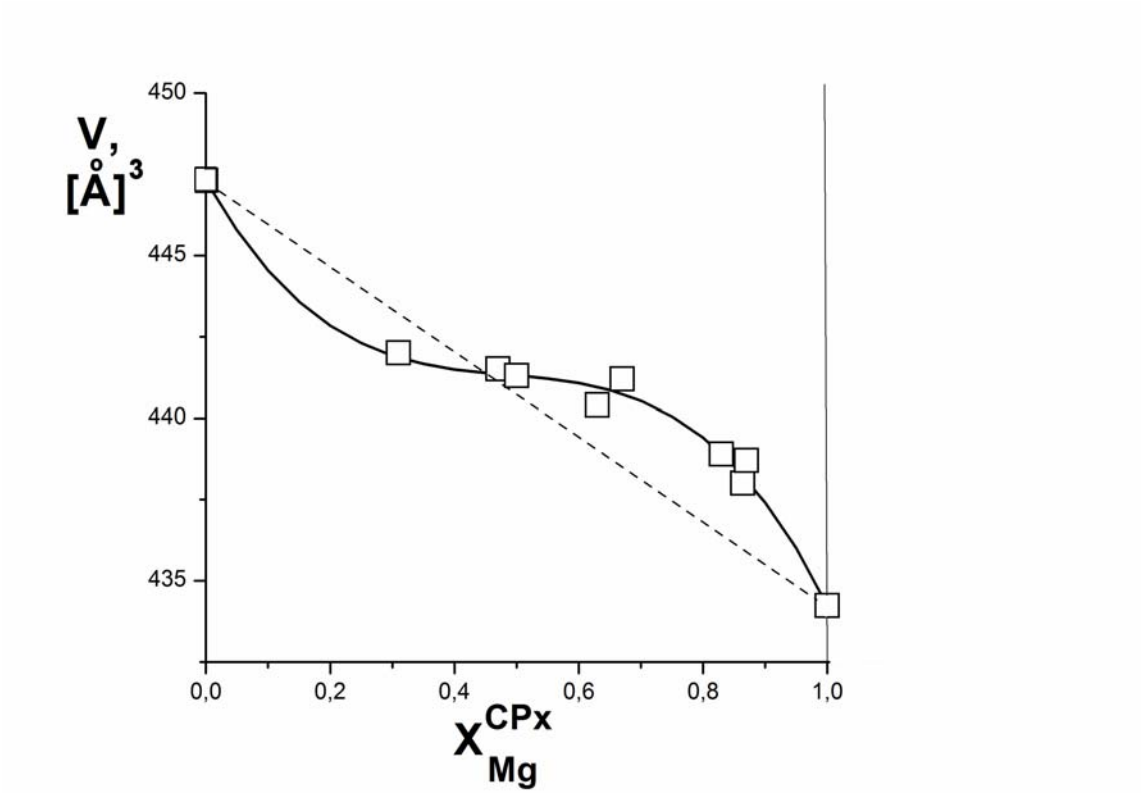

Fig. 1. The dependence of cell volume on the clinopyroxenes composition

For analytical description of clinopyroxene cell parameters it has been used the polynom as:

$$P = A_0 + A_1*x + A_2*(x^2) + A_3*(x^3) \quad (1)$$

where x is the mole fraction of magnesium in clinopyroxenes.

The values of coefficients of the equation (1) for the estimation of clinopyroxene cell parameters with aegirine mole fraction whose value is 0.2, are presented in the table 2.

The dependence of cell volume on the composition is shown at the fig. 1. It is observed that triangle solid solutions are characterized by alternating deviation from ideality. To describe the clinopyroxenes excess volumes of mixture the Margules approximation was used. For the triangle solid solutions of clinopyroxenes (aegirine – diopside – hedenbergite system) following values of Margules equation parameters were obtained: W1 = 3.59(±12); W2 = -2.66(±8) sm^3/mole. These parameters essentially exceed the values of analogical parameters for the binary hedenbergite-diopside solid solution: W1 = 0.34(±0.03); W2 = 0.71(±0.15) sm^3/mole. This evidences that nonideality of diopside-hedenbergite solid solution increase with entrance of aegirine minal.

Table 2. Polynom coefficients for the estimation of cell parameters of clinopyroxene triangle solid solutions (aegirine mole fraction is 0.2)

Parameters, (P)	A_0	A_1	A_2	A_3	S_x [1)]	E_x [2)]
a, Å	9.821	-0.27155	0.42079	-0.24709	0.005	0.002
b, Å	8.983	-0.15733	0.0979	-0.007406	0.007	0.003
c, Å	5.253	-0.012382	0.18647	-0.20505	0.007	0.003
β,°	105.16	4.10935	-7.95421	5.07771	0.08	0.04
V, $Å^3$	447.3	-30.1444	57.2286	-40.04632	0.57	0.31

[1)] S_x – root-mean-square deviation of experimental data approximation by polynom
[2)] E_x – approximation accuracy

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