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Crystal chemistry of kimzeyite from Stromboli, Aeolian Islands, Italy

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Abstract

Kimzeyite, a zirconium-rich garnet, found in a shoshonitic basalt from Stromboli has been submitted to chemical and X-ray structure analysis. The cell edge, determined with single-crystal diffractometry, is 12.365A. Three points on the crystal used for the X-ray structure refinement were analyzed with the electron microprobe. The chemical formula assigned on the basis of the chemical analysis, the site occupancy refinement, and the known spectral data is: $(Ca_{2.94}Mg_{0.06})(Zr_{1.21}Ti_{0.47}Mg_{0.32})Si_{1.51}Al_{1.00}Fe^{3+}_{0.49})O_{12}$. The bond distances are: T–O 1.725, Y–O 2.055, X–O 2.472A.

Introduction

The name kimzeyite is applied to the calcium garnets with zirconium as dominant cation in the six-coordinated position and containing Al and Fe^{3+} as compensating ions in the tetrahedral position (Ito and Frondel, 1967). The only example of kimzeyite known till now is that from Magnet Cove, Arkansas (Milton *et al.*, 1961), since the calcium garnets high in zirconium described by Borodin and Bykova (1961; quoted from Ito and Frondel, 1967) and by Koritnig *et al.* (1978) can be considered as Zr-schorlomites, their kimzeyitic component being less than 50 percent.

Previous works (Ito and Frondel, 1967; Dowty, 1971; Huggins *et al.*, 1977a,b) have utilized Mössbauer, optical and infrared spectroscopy, but no crystal-chemical study on natural Zr,Ti-bearing garnets based on X-ray structural determination is available at present. We aim to fill this gap with the determination of the crystal structure of kimzeyite found in a lava sample from Stromboli, Aeolian Islands.

Description of the sample and chemical analysis

A mineralogical and petrographic study was carried out on lava flow and scoria samples collected from the last effusive activity (November 1975) of Stromboli Island. The analyzed samples are shoshonitic basalts (Capaldi *et al.*, 1979). Minerals were separated from the lava sample with heavy liquids. The light fraction contains zoned plagioclase and some grains of saccharoidal azure quartz. The heavy fraction contains dark green salitic pyroxene, olivine, dark green spinel, monticellite, and some brown garnets with a cell edge (a = 12.365A) similar to that of kimzeyite. The unit cell of the Stromboli garnet is also similar to that of some Zr and Ti garnets synthesized in the ternary system $Ca_3Fe_2Si_3O_{12}$ (andradite)–$Ca_3Zr_2Fe_2SiO_{12}$ (kimzeyite)–$Ca_3Ti_2Fe_2SiO_{12}$ (schorlomite) (Ito and Frondel, 1967).

The same crystal was used for the electron microprobe analysis and for the X-ray data collection. In Table 1 the microprobe chemical analyses of three points in a crystal of the Stromboli kimzeyite are compared with the analysis of the Magnet Cove kimzeyite. The analyses were carried out in the wavelength dispersive mode on a fully automated ARL-SEMQ instrument operated at 15 kV, 0.2μA beam current and a defocused beam. On-line data reduction was based on the Ziebold and Ogilvie (1964) method by the use of Albee and Ray (1970) correction factors. The following standard were used: hornblende, Wilberforce, Ontario, for Fe; $Di_{85}Jd_{15}$ pyroxene for Ca; A 128 ilmenite for Ti and Mg; zircon for Zr and Si; Amelia albite for Al.

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Table 4. Observed and calculated structure factors of kimzeyite. The reflections marked by an asterisk were considered as unobserved.

H	K	L	/FO/	/FC/
4	0	0	614.2	617.1
8	0	0	615.3	615.1
12	0	0	226.3	223.5
16	0	0	303.7	299.9
2	2	0	201.2	186.6
4	2	0	385.3	-393.6
6	2	0	248.3	242.5
8	2	0	42.1	43.7
10	2	0	17.8	9.4
12	2	0	207.2	-203.9
14	2	0	96.0	96.1
16	2	0*	18.5	-13.1
4	4	0	60.5	58.7
6	4	0	368.6	372.7
8	4	0	401.7	404.5
10	4	0	239.4	239.8
12	4	0	114.2	114.1
14	4	0	150.7	149.7
16	4	0	201.7	203.1
6	6	0	102.6	102.8
8	6	0*	6.2	-3.5
10	6	0	54.4	54.0
12	6	0	165.7	-165.6
14	6	0	60.8	61.7
16	6	0	25.8	20.6
8	8	0	538.2	544.8
10	8	0	17.2	-15.0
12	8	0	240.5	240.0
14	8	0	19.5	16.2
10	10	0	188.5	193.6
12	10	0	137.8	-138.8
14	10	0	96.2	96.8
12	12	0	45.5	47.3
2	1	1*	8.8	9.4
6	1	1	173.5	168.1
10	1	1	39.8	40.0
14	1	1	17.5	-8.0
3	2	1*	8.7	-8.5
5	2	1	116.1	-108.4
7	2	1*	11.2	7.0
9	2	1*	12.5	-10.9
11	2	1*	10.2	14.4
13	2	1	22.7	21.7
15	2	1	28.0	29.8
17	2	1*	10.5	4.4
4	3	1	120.0	116.0
6	3	1	19.9	-19.9
8	3	1	19.1	-16.4
10	3	1	18.3	-14.6
12	3	1	27.3	29.5
14	3	1	33.0	33.7
15	3	1*	16.0	-13.9
5	4	1	18.5	15.8
7	4	1	66.5	65.2
9	4	1	80.9	82.2
11	4	1	49.7	-50.1
13	4	1*	12.6	-3.0
15	4	1*	14.1	-9.6
6	5	1	21.9	22.9
8	5	1	64.5	67.3
10	5	1	22.3	-21.7
12	5	1*	1.1	-1.0
14	5	1	24.0	-19.1
15	5	1*	5.7	6.4
7	6	1	60.2	63.7
9	6	1	19.6	19.3
11	6	1*	3.5	1.7
13	6	1*	13.5	-5.7
15	6	1*	15.3	7.5
8	7	1	23.3	-17.3
10	7	1	39.1	-39.1
12	7	1*	8.1	0.8
14	7	1	27.8	32.3
9	8	1	34.1	35.4
11	8	1	28.4	-28.1
13	8	1*	14.7	14.0
15	8	1	30.6	31.1
10	9	1*	10.7	-7.3
12	9	1*	12.1	-8.2
14	9	1*	0.4	7.8
11	10	1*	14.1	9.2
13	10	1	19.1	-17.7
12	11	1	28.4	-26.3
4	2	2	399.0	404.7
8	2	2	158.0	158.8
12	2	2	354.0	356.9
16	2	2	40.4	36.7
3	3	2	141.2	-139.3
5	3	2	111.1	107.6
7	3	2	28.0	-28.5
9	3	2	30.5	30.0
11	3	2*	8.8	3.9
13	3	2	20.0	18.8
15	3	2	35.4	37.4
17	3	2*	17.3	-1.0
6	4	2	488.1	489.8
8	4	2	259.4	-256.3
10	4	2	350.0	346.4
12	4	2*	11.8	10.6
14	4	2	268.7	269.8
16	4	2	154.7	-154.2
5	5	2	53.8	-54.2
7	5	2	33.2	37.8
9	5	2*	2.1	7.2
11	5	2	23.2	19.1
13	5	2	43.3	41.0
15	5	2*	10.7	0.4
8	6	2	74.5	73.1
10	6	2	30.7	-28.1
12	6	2	234.9	232.6
14	6	2	18.0	11.8
16	6	2	53.1	54.2
7	7	2	42.4	43.2
9	7	2	19.8	-15.0
11	7	2	27.6	26.4
13	7	2	25.2	27.5
15	7	2*	10.8	6.9
10	8	2	102.2	103.3
12	8	2	170.6	170.3
14	8	2	57.6	54.3
9	9	2	28.4	-30.1
11	9	2*	14.8	-14.1
13	9	2*	0.7	-0.6
12	10	2	222.1	224.3
14	10	2*	10.5	-6.7
11	11	2*	5.7	9.4
13	11	2	28.0	24.3
6	3	3	45.0	-40.3
10	3	3	26.0	25.2
14	3	3	18.7	-15.5
5	4	3	29.0	-27.6
7	4	3	28.4	-30.5
9	4	3	48.5	-46.2
11	4	3*	13.1	-9.7
13	4	3*	7.8	-9.9
15	4	3	26.1	21.2
6	5	3	57.6	55.9
8	5	3	84.8	-85.8
10	5	3	21.9	21.5
12	5	3	46.0	35.0
14	5	3	24.8	-23.4
15	5	3	22.8	16.7
7	6	3*	5.3	-7.9
9	6	3	18.7	22.9
11	6	3	58.3	-61.5
13	6	3*	8.4	-8.8
15	6	3	22.3	-11.2
8	7	3	37.9	37.7
10	7	3*	3.1	13.9
12	7	3	45.5	-49.5

Table 4. continued

H	K	L	/FO/	/FC/
14	7	3*	15.2	-18.2
9	8	3	20.2	-13.0
11	8	3	23.4	-18.8
13	8	3	36.8	37.9
15	8	3	26.0	22.6
10	9	3	28.7	-3.0
12	9	3*	14.3	18.2
14	9	3*	3.9	-1.5
11	10	3	23.0	-14.1
13	10	3*	17.4	-8.3
12	11	3	17.5	-11.4
4	4	4	249.0	-251.5
8	4	4	155.1	154.4
12	4	4	64.2	-60.8
16	4	4	76.2	75.3
7	5	4	64.4	66.5
9	5	4	16.4	-18.4
11	5	4*	12.8	-0.4
13	5	4	22.0	23.3
15	5	4	25.6	-22.1
6	6	4	363.8	366.9
8	6	4	212.9	212.9
10	6	4	274.5	274.3
12	6	4*	13.3	-14.6
14	6	4	204.5	204.7
9	7	4	35.0	-33.5
11	7	4	48.5	-48.5
13	7	4	20.7	6.7
15	7	4*	10.3	-4.0
8	8	4	292.8	294.0
10	8	4	195.0	-195.7
12	8	4	51.6	51.5
14	8	4	136.0	-135.0
11	9	4*	14.1	-13.6
13	9	4*	5.3	7.7
10	10	4	253.1	255.6
12	10	4*	13.6	-1.7
6	5	5	35.3	34.5
10	5	5*	3.3	-8.3
14	5	5*	15.1	-10.7
7	6	5	50.1	-52.0
9	6	5*	12.4	12.0
11	6	5	18.9	-16.8
13	6	5*	20.1	22.1
15	6	5*	9.3	-1.6
8	7	5	27.5	26.7
10	7	5*	9.3	6.2
12	7	5*	17.5	0.3
14	7	5*	8.4	12.6
9	8	5	24.8	-21.3
11	8	5	41.9	42.9
13	8	5	34.7	-32.3
10	9	5*	13.3	1.3
12	9	5*	13.8	2.4
14	9	5*	16.6	24.3
11	10	5*	0.	-2.4
13	10	5*	10.3	-13.3
12	11	5*	1.0	0.1
8	6	6	90.0	87.9
12	6	6	248.5	248.1
7	7	6	31.8	32.4
9	7	6	50.4	-54.1
11	7	6*	11.6	-7.5
13	7	6*	5.4	-4.6
10	8	6	100.1	101.1
12	8	6	162.8	161.0
14	8	6	79.4	79.8
9	9	6	51.5	-52.5
11	9	6	30.3	-31.3
13	9	6*	5.6	12.7
12	10	6	225.2	228.3
11	11	6	30.9	16.8
10	7	7	16.7	2.9
14	7	7	28.0	-31.9
9	8	7	19.4	-14.2
11	8	7	19.2	12.4
13	8	7	23.4	19.3
10	9	7*	16.5	5.2
12	9	7	20.4	-19.7
11	10	7*	12.9	6.4
8	8	8	428.5	432.0
12	8	8	211.2	210.4
11	9	8*	8.3	1.1
10	10	8	46.4	46.1
10	9	9*	19.5	-22.9
11	10	9	36.5	37.3