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Unusual silicate mineralization in fumarolic sublimates of the Tolbachik volcano, Kamchatka, Russia – Part 2: Tectosilicates

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Table S1. Powder X-ray diffraction data for kalsilite from the Arsenatnaya fumarole and earlier studied sample of kalsilite

Sample	**Kalsilite by Perrotta et al. (1965)**		**Kalsilite from the Arsenatnaya fum.**		**Kalsilite from the Arsenatnaya fum.**	
Type of X-ray diffraction pattern	Calculated		Experimental		Calculated	
Sp. gr.	$P6_3$		$P6_3$		$P6_3$	
	d (Å)	*I*(%)	*d* (Å)	*I* (%)	*d* (Å)	*I* (%)
Reflections with	4.47	1			4.465	1
I ≥ 1	4.347	14	4.36	55	4.344	14
	3.975	55	3.97	73	3.972	54
	3.116	100	3.11	100	3.114	100
	2.581	53	2.58	61	2.578	61
	*2.474	17	2.47	26	2.472	18
	2.431	11	2.43	17	2.43	11
	2.235	3	2.22	30	2.233	3
	2.219	8			2.217	13
	2.173	14	2.17	16	2.172	17
	2.164	8			2.162	9
	1.988	7	1.99	8	1.986	6
	1.955	3	1.95	9	1.953	3
	*1.927	5	1.92	9	1.926	7
	1.77	5	1.77	8	1.768	4
	1.689	1				
	1.662	4	1.66	17	1.661	5
	1.658	7			1.657	4
	1.62	10	1.62	8	1.62	12
	1.575	14	1.58	16	1.573	9
	1.558	5	1.56	19	1.557	7
	1.49	15	1.49	20	1.489	22
	1.459	6	1.46	6	1.458	3
	1.449	1	1.45	6	1.448	1
	*1.442	1	1.44	5	1.441	2
	1.409	1	1.4	12	1.408	1

*The pointed reflections are forbidden for space group *P*-31*c*.

Table S2. Atomic coordinates and equivalent displacement parameters atoms (U_{eq}, Å^2) in the crystal structure of kalsilite from the Arsenatnaya fumarole.

Site	***x/a***	***y/b***	***z/c***	U_{eq}
K	0	0	0.2439(8)	0.0261(6)
Al	0.3333	0.6667	0.0489(6)	0.0104(12)
Si	0.3333	0.6667	0.4309(7)	0.0189(13)
O1	0.3333	0.6667	0.245(3)	0.022(2)
O2	0.3919(8)	1.0011(10)	0.4885(14)	0.0259(18)

Table S3. Selected interatomic distances in crystal structure of kalsilite from the Arsenatnaya fumarole

K	O2	2.930(1) × 3
	O1	2.976(2) × 3
	O2	2.999(1) × 3
Al	O2	1.670(1) × 3
	O1	1.703(1)
Si	O1	1.615(1)
	O2	1.671(2) × 3

Table S4. Powder X-ray diffraction data for samples of sodalite and haüyne from the Arsenatnaya fumarole

Mineral	Sodalite		Sodalite		Haüyne		Haüyne	
Sp. gr.	*P*-43*n*		*P*-43*n*		*P*-43*n*		*P*-43*n*	
***a* (Å)**	8.870(2)		8.880(2)		9.113(2)		9.118(5)	
***V* (Å^3)**	700.3(3)		700.4(2)		756.8(4)		758.1(7)	
Reflections with I ≥ 1	experimental		experimental		experimental		experimental	
	d (Å)	*I* (%)	*d* (Å)	*I* (%)	*d* (Å)	*I* (%)	*d* (Å)	*I* (%)
	6.27	32	6.28	30	6.42	21	6.46	21
	4.44	8	4.45	6	4.02	2	4.02	2
	3.97	1	3.97	4	3.71	100	3.72	100
	3.63	100	3.63	100	3.25	5	3.21	10
	2.82	15	2.81	10	2.89	42	2.89	43
	2.57	20	2.57	18	2.63	32	2.63	32
	2.38	17	2.38	16	2.43	11	2.44	11
	2.22	2	2.23	2	2.28	7	2.28	11
	2.1	24	2.1	27	2.15	18	2.15	18
	1.99	3	1.99	4	1.94	6	1.94	6
	1.9	3	1.9	3	1.86	5	1.82	4
	1.81	4	1.82	4	1.79	8	1.79	8
	1.74	3	1.75	3	1.66	3	1.66	3
	1.62	3	1.63	3	1.61	5	1.66	3
	1.57	8	1.58	7	1.56	3	1.56	3
	1.53	4	1.53	4	1.52	5	1.52	5
	1.5	1	1.51	1	1.48	3	1.48	3
	1.48	6	1.49	6				
	1.44	7	1.45	6				
	this proposal		**this proposal**		**this proposal**		**this proposal**	

Table S5. Chemical composition of sanidine (Snd), anorthoclase (Anrth), leucite (Lc), and haüyne (Hau) from ancient fumarole fields of Mountain 1004.

Component	Snd	Snd	Anrth	Lc	Hau
	wt. %				
SiO_2	64.13	64.32	61.75	55.69	32.42
Al_2O_3	20.05	20.41	19.81	22.75	26.69
Fe_2O_3	0.60	0.47	1.76	-	1.46
CuO	-	-	0.33	-	-
MgO	-	-	0.53	-	-
CaO	0.39	0.74	1.93	-	7.88
Na_2O	0.75	2.12	2.44	-	15.15
K_2O	15.75	13.96	11.38	21.04	3.05
SO_3	-	-	-	-	12.15
Total	101.67	102.02	99.93	99.48	98.80
	empirical formulae				
Si	2.92	2.91	2.85	2.02	5.99
Al	1.08	1.09	1.08	0.97	5.81
Fe^{3+}	0.02	0.02	0.06	-	0.20
Cu	-	-	0.01	-	-
Mg	-	-	0.04	-	-
Ca	0.02	0.04	0.10	-	1.56
Na	0.07	0.19	0.22	-	5.43
K	0.92	0.80	0.67	0.98	0.72
S^{6+}	-	-	-	-	2.10
$\Sigma T+A$	5.02	5.04	5.02	3.98	19.71
BoFC	8 O	8 O	8 O	6 O	*

Note. Dash means the content below the detection limit $\Sigma T+A$ = sum of all atoms except of oxygen BoFC is a basis of formula calculation, * BoFC = 12 framework-forming tetrahedrally coordinated [Si+Al+Fe+Cu] *apfu*.