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TOWARDS A REVISITATION OF VESUVIANITE-GROUP NOMENCLATURE: THE CRYSTAL STRUCTURE OF Ti-RICH VESUVIANITE FROM ALCHURI, SHIGAR VALLEY, PAKISTAN

Sergey M. Aksenov, Nikita V. Chukanov, Vyacheslav S. Rusakov, Taras L. Panikorovskii, Ramiza K. Rastsvetaeva, Ramil R. Gainov, Farit G. Vagizov, Konstantin A. Lyssenko and Dmitry I. Belakovskiy

Table S1 Powder X-ray diffraction data for Ti-rich vesuvianite.

I_{meas}	d_{meas}, Å	I_{calc}	d_{calc}, Å	*hkl*
7	5.91	12	5.91	002
3	5.50	2	5.50	220
3	4.706	3	4.710	202
4	4.507	0.8	4.508	212
2	4.054	2	4.056	321
14	4.031	14	4.030	222
8	3.892	3	3.891	400
1	3.670	0.5	3.669	330
15	3.481	10	3.481	420
9	3.252	11	3.251	402
4	3.079	4	3.078	313
11	3.054	8	3.052	510
13	3.010	7	3.010	501
42	2.959	45	2.958	004
4	2.913	5	2.911	323
4	2.856	3	2.856	114
100	2.754	100	2.755	432
4	2.668	2	2.669	530
26	2.606	38	2.605	224
58	2.598	32	2.597	522
6	2.535	3	2.535	314
3	2.500	2	2.501	611
34	2.462	33	2.461	620
9	2.445	9	2.443	503
9	2.375	5	2.375	602
10	2.355	7	2.355	404
13	2.328	10	2.328	414
3	2.303	4	2.302	334
6	2.277	3	2.277	631
2	2.253	1	2.254	424

I_{meas}	d_{meas}, Å	I_{calc}	d_{calc}, Å	*hkl*
3	2.154	2	2.153	305
4	2.145	3	2.144	434
12	2.133	12	2.132	315
10	2.124	9	2.124	514
3	2.103	0.5	2.104	721
8	2.088	4	2.088	623
6	2.069	4	2.069	543
4	2.064	3	2.063	712
13	2.044	6	2.043	730
5	2.028	2	2.027	642
8	2.014	4	2.014	731
8	2.000	6	1.999	633
7	1.9655	4	1.9650	651
8	1.9309	6	1.9310	732
4	1.9226	3	1.9220	713
3	1.9121	4	1.9110	206
4	1.9062	3	1.9050	741
3	1.8981	2	1.8970	216
7	1.8888	6	1.8880	652
3	1.8839	2	1.8840	505
3	1.8709	2	1.8700	515
12	1.7979	7	1.7980	822
8	1.7657	4	1.7660	714
3	1.7187	6	1.7180	910
9	1.6811	2	1.6810	734
16	1.6659	9	1.6660	436
12	1.6294	21	1.6290	526
26	1.6238	12	1.6230	922
6	1.5722	5	1.5720	770
6	1.5620	10	1.5620	616

4	2.240	2	2.240	215
4	2.211	4	2.210	533
8	2.202	6	2.201	710
4	2.185	3	2.185	701

5	1.5589	4	1.5590	664
3	1.5265	2	1.5260	1020
3	1.5121	2	1.5110	950
6	1.4995	5	1.4990	844
4	1.4789	3	1.4790	008

Table S2 Fractional coordinates, site multiplicities, equivalent atomic displacement parameters (U_{eq}, Å^2) and site composition in the structure of Ti-rich vesuvianite.

Site	*x*	*y*	*z*	Mult.	U_{eq}	Composition
*X*1	0.75	0.25	0.25	4	0.00382(4)	$Ca_{0.552(8)}Na_{0.448(6)}$
*X*2	0.810822(7)	0.044932(7)	0.379290(8)	16	0.004390(18)	Ca
*X*3	0.898955(8)	0.820364(8)	0.886577(13)	16	0.00817(2)	Ca
*X*4	0.75	0.75	0.14320(4)	4	0.00523(5)	$Ca_{0.5}$
*Y*1a	0.75	0.75	0.06618(12)	4	0.00405(12)	$Fe_{0.151(9)}Mg_{0.104(8)}$
*Y*1b	0.75	0.75	0.03388(6)	4	0.00165(6)	$Fe_{0.245(11)}$
*Y*2	0	0	0	8	0.00264(4)	$Al_{0.898(8)}Mg_{0.102(4)}$
*Y*3	-0.110507(10)	0.120294(10)	0.128290(11)	16	0.00635(2)	$Al_{0.503(6)}Ti_{0.274(7)}$ $Fe_{0.223(4)}$
*Z*1	0.75	0.25	0	4	0.00334(4)	Si
*Z*2	0.819234(12)	0.039105(12)	0.871641(14)	16	0.00334(3)	Si
*Z*3	0.916428(13)	0.849330(11)	0.364516(15)	16	0.00415(3)	Si
O1	0.71974(3)	0.32788(3)	0.08497(3)	16	0.00502(6)	O
O2	0.84042(3)	0.11539(3)	0.77938(4)	16	0.00565(6)	O
O3	0.72184(3)	0.04851(3)	0.92452(3)	16	0.00453(5)	O
O4	0.89344(3)	0.06089(3)	0.97016(3)	16	0.00473(5)	O
O5	1.01464(3)	0.82977(3)	0.32077(4)	16	0.00663(6)	O
O6	0.88118(4)	0.77158(3)	0.44152(4)	16	0.00887(8)	O
O7	0.82485(3)	-0.05745(3)	0.82244(4)	16	0.00579(6)	O
O8	0.90897(3)	0.93965(3)	0.43275(3)	16	0.00463(5)	O
O9	0.85490(3)	0.85490(3)	0.25	8	0.00628(6)	O
O10	0.75	0.75	-0.13402(13)	4	0.01226(18)	$F_{0.67}(OH)_{0.33}$
O11	0.00440(3)	-0.06290(3)	-0.13546(3)	16	0.00528(6)	$(OH)_{0.65}O_{0.35}$

Table S3 Anisotropic atomic displacement parameters of Ti-rich vesuvianite.

Site	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
*X*1	0.00617(8)	0.00309(7)	0.00219(6)	0	0	0
*X*2	0.00350(3)	0.00573(3)	0.00393(3)	0.0006(1)	-0.00042(2)	-0.00012(2)
*X*3	0.00586(4)	0.00541(3)	0.01324(4)	0.00195(2)	-0.00441(3)	-0.00317(3)
*X*4	0.00400(6)	0.00400(6)	0.00769(11)	0	0	0
*Y*1a	0.00053(13)	0.00053(13)	0.0111(3)	0	0	0
*Y*1b	0.00175(10)	0.00175(10)	0.00143(13)	0	0	0
Y2	0.00200(7)	0.00229(7)	0.00365(7)	0.00011(5)	0.00036(5)	0.00032(5)
Y3	0.00816(4)	0.00591(4)	0.00499(4)	-0.00189(3)	0.00175(3)	-0.00082(3)
Z1	0.00334(5)	0.00334(5)	0.00332(8)	0	0	0
Z2	0.00308(5)	0.00340(5)	0.00354(5)	-0.00007(3)	-0.00027(3)	0.00017(3)
Z3	0.00729(5)	0.00243(5)	0.00273(4)	0.00037(4)	0.00043(4)	0.00001(3)
O1	0.00675(11)	0.00373(9)	0.00459(9)	0.00035(7)	0.00028(8)	-0.00033(7)
O2	0.00566(10)	0.00594(11)	0.00534(10)	-0.00103(8)	-0.00017(8)	0.00181(8)
O3	0.00402(9)	0.00507(10)	0.00451(9)	-0.00032(7)	0.00055(7)	0.00004(7)
O4	0.00373(9)	0.00558(10)	0.00488(9)	0.00008(7)	-0.00073(7)	0.00069(8)
O5	0.00871(12)	0.00570(11)	0.00548(10)	0.00324(9)	0.00059(9)	-0.00056(8)
O6	0.01575(18)	0.00501(11)	0.00584(11)	-0.00219(11)	-0.00169(11)	0.00232(9)
O7	0.00683(11)	0.00400(10)	0.00653(10)	0.00069(8)	0.00045(8)	-0.00053(8)
O8	0.00465(10)	0.00381(9)	0.00544(9)	0.00064(7)	-0.00082(7)	-0.00157(7)
O9	0.00754(10)	0.00754(10)	0.00377(12)	-0.00195(13)	-0.00041(8)	0.00041(8)
O10	0.00631(16)	0.00631(16)	0.0242(5)	0	0	0
O11	0.00503(10)	0.00657(11)	0.00422(9)	-0.00049(8)	-0.00033(7)	-0.00092(8)