*Mineralogical Magazine*

10.1180/minmag.2017.081.060

**From structure topology to chemical composition. XXIV. Revision of the crystal structure and chemical formula of vigrishinite, NaZnTi4(Si2O7)2O3(OH)(H2O)4,** **a seidozerite-supergroup mineral from the Lovozero alkaline massif, Kola peninsula, Russia**

Elena Sokolova\* and Frank C. Hawthorne

Department of Geological Sciences, University of Manitoba, 125 Dysart Road, Winnipeg, MB, R3T 2N2 Canada

\*E-mail: elena\_sokolova@umanitoba.ca

Table D. Anisotropic displacement parameters (Å2) for vigrishinite, space group *C*‾1.

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Atom | *U*11 | *U*22 | *U*33 | *U*23 | *U*13 | *U*12 | *U*eq |
| MH(1) | 0.0031(9) | 0.0098(12) | 0.0403(18) | 0.0031(10) | 0.0036(9) | 0.0013(7) | 0.0176(8) |
| MH(1) | 0.0031(9) | 0.0098(12) | 0.0403(18) | 0.0031(10) | 0.0036(9) | 0.0013(7) | 0.0176(8) |
| MO(1) | 0.0100(13) | 0.0200(15) | 0.0192(15) | 0.0018(10) | 0.0004(10) | –0.0003(9) | 0.0165(9) |
| MO(2) | 0.0149(14) | 0.0330(18) | 0.0216(16) | 0.0096(12) | 0.0016(10) | –0.0023(11) | 0.0229(10) |
| MO(3) | 0.018(4) | 0.016(4) | 0.032(5) | 0.006(3) | –0.009(3) | –0.002(3) | 0.023(3) |
| MO(4) | 0.018(4) | 0.016(4) | 0.032(5) | 0.006(3) | –0.009(3) | –0.002(3) | 0.023(3) |
| Si(1) | 0.0084(19) | 0.0108(19) | 0.016(2) | 0.0028(16) | 0.0015(15) | 0.0012(15) | 0.0117(9) |
| Si(2) | 0.0066(19) | 0.012(2) | 0.018(2) | 0.0008(16) | 0.0015(16) | 0.0031(15) | 0.0122(10) |
| Si(3) | 0.0083(19) | 0.013(2) | 0.019(2) | 0.0015(16) | 0.0027(16) | –0.0013(15) | 0.0130(10) |
| Si(4) | 0.0083(19) | 0.008(2) | 0.024(2) | 0.0020(16) | 0.0023(17) | 0.0016(15) | 0.0136(10) |
| A*P*(1) | 0.0048(10) | 0.0064(11) | 0.0283(14) | 0.0016(8) | 0.0016(8) | 0.0017(7) | 0.0132(7) |
| AI | 0.019(6) | 0.023(6) | 0.014(5) | 0.001(4) | –0.002(4) | 0.010(4) | 0.019(3) |
| O1 | 0.002(5) | 0.020(6) | 0.021(6) | –0.001(5) | –0.000(4) | 0.005(4) | 0.015(2) |
| O2 | 0.007(5) | 0.023(6) | 0.024(6) | –0.001(5) | 0.004(5) | –0.005(5) | 0.018(3) |
| O3 | 0.008(5) | 0.014(6) | 0.037(8) | –0.006(5) | 0.001(5) | 0.001(4) | 0.020(3) |
| O4 | 0.008(5) | 0.020(6) | 0.023(6) | –0.002(5) | –0.000(5) | 0.002(4) | 0.018(2) |
| O5 | 0.011(6) | 0.030(7) | 0.033(8) | 0.006(6) | 0.000(5) | 0.007(5) | 0.025(3) |
| O6 | 0.007(5) | 0.011(6) | 0.048(8) | 0.003(5) | 0.006(5) | 0.003(4) | 0.021(3) |
| O8 | 0.019(6) | 0.020(6) | 0.035(8) | –0.002(5) | 0.003(5) | 0.009(5) | 0.025(3) |
| O9 | 0.012(6) | 0.020(6) | 0.037(8) | 0.002(5) | 0.004(5) | 0.000(5) | 0.023(3) |
| O10 | 0.017(6) | 0.011(6) | 0.034(7) | 0.001(5) | 0.008(5) | –0.006(5) | 0.020(3) |
| O11 | 0.030(7) | 0.034(8) | 0.021(7) | 0.003(6) | –0.002(6) | –0.001(6) | 0.029(3) |
| O12 | 0.011(6) | 0.018(6) | 0.041(8) | 0.001(6) | 0.004(5) | –0.006(5) | 0.024(3) |
| O13 | 0.031(7) | 0.019(6) | 0.016(6) | –0.000(5) | 0.004(5) | 0.009(5) | 0.022(3) |
| O14 | 0.009(5) | 0.025(6) | 0.015(6) | 0.005(5) | –0.000(4) | –0.006(5) | 0.016(2) |
| (1) | 0.019(6) | 0.028(7) | 0.019(6) | –0.001(5) | 0.006(5) | –0.006(5) | 0.022(3) |
| (2) | 0.018(6) | 0.033(8) | 0.025(7) | 0.004(6) | 0.001(5) | 0.007(5) | 0.026(3) |
| (1) | 0.027(7) | 0.022(6) | 0.016(6) | –0.000(5) | –0.000(5) | 0.001(5) | 0.022(3) |
| (1) | 0.023(7) | 0.074(12) | 0.022(7) | 0.012(7) | –0.002(6) | –0.000(7) | 0.040(4) |
| (2) | 0.035(8) | 0.046(10) | 0.030(8) | 0.005(7) | 0.007(6) | 0.008(7) | 0.036(4) |
| (1) | 0.025(7) | 0.052(10) | 0.026(7) | 0.008(7) | 0.008(6) | –0.002(7) | 0.033(3) |
| (21) | 0.048(16) | 0.08(2) | 0.029(13) | 0.014(14) | –0.014(11) | –0.012(16) | 0.052(7) |
| (22) | 0.00(2) | 0.06(4) | 0.07(5) | –0.00(4) | 0.01(2) | 0.00(2) | 0.05(2) |
| Subsidiary peaks | | | | | | | |
| MH(1A) | 0.0031(9) | 0.0098(12) | 0.0403(18) | 0.0031(10) | 0.0036(9) | 0.0013(7) | 0.0176(8) |
| MH(2A) | 0.0031(9) | 0.0098(12) | 0.0403(18) | 0.0031(10) | 0.0036(9) | 0.0013(7) | 0.0176(8) |
| MH(2B) | 0.0031(9) | 0.0098(12) | 0.0403(18) | 0.0031(10) | 0.0036(9) | 0.0013(7) | 0.0176(8) |
| Si(1A) | 0.0084(19) | 0.0108(19) | 0.016(2) | 0.0028(16) | 0.0015(15) | 0.0012(15) | 0.0117(9) |
| Si(3A) | 0.0083(19) | 0.013(2) | 0.019(2) | 0.0015(16) | 0.0027(16) | –0.0013(15) | 0.0130(10) |
| Si(4A) | 0.0083(19) | 0.008(2) | 0.024(2) | 0.0020(16) | 0.0023(17) | 0.0016(15) | 0.0136(10) |