Supplementary information to the paper

**Kainotropite, Cu4Fe3+O2(V2O7)(VO4), a new mineral with complex vanadate anion from fumarolic exhalations of the Tolbachik volcano, Kamchatka, Russia**

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Table S1. The reflectance data of kainotropite

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| λ (nm) | *R*max, % | *R*min, % | λ (nm) | *R*max, % | *R*min, % |
| 400 | 19.4 | 18.2 | 560 | 17.2 | 16.1 |
| 420 | 19.1 | 17.9 | 580 | 17.0 | 15.8 |
| 440 | 18.8 | 17.6 | **589** | **16.9** | **15.7** |
| 460 | 18.4 | 17.4 | 600 | 16.8 | 15.6 |
| **470** | **18.3** | **17.3** | 620 | 16.6 | 15.3 |
| 480 | 18.1 | 17.1 | 640 | 16.4 | 15.2 |
| 500 | 17.8 | 16.7 | **650** | **16.3** | **15.1** |
| 520 | 17.6 | 16.5 | 660 | 16.1 | 15.0 |
| 540 | 17.4 | 16.2 | 680 | 15.9 | 14.9 |
| **546** | **17.3** | **16.3** | 700 | 15.7 | 14.7 |

The values for wavenumbers (λ) recommended by the IMA Commission on Ore Mineralogy are given in boldtype.

Table S2. Anisotropic displacement parameters (in Å2) for kainotropite

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Site | *U*11 | *U*22 | *U*33 | *U*23 | *U*13 | *U*12 |
| Cu(1) | 0.0239(17) | 0.0120(15) | 0.0188(16) | 0.000 | 0.0050(14) | 0.000 |
| Cu(2) | 0.0203(10) | 0.0083(9) | 0.0262(10) | 0.0007(8) | 0.0046(9) | 0.0024(8) |
| Cu(3) | 0.0212(16) | 0.0148(16) | 0.0172(15) | 0.000 | 0.0056(13) | 0.000 |
| Fe | 0.021(2) | 0.0088(17) | 0.0157(19) | 0.000 | -0.0005(17) | 0.000 |
| V(1) | 0.020(2) | 0.010(2) | 0.009(2) | 0.000 | 0.0018(17) | 0.000 |
| V(2) | 0.015(2) | 0.013(2) | 0.014(2) | 0.000 | -0.0006(16) | 0.000 |
| V(3) | 0.014(2) | 0.0112(18) | 0.0136(19) | 0.000 | 0.0019(17) | 0.000 |
| O(1) | 0.024(9) | 0.023(9) | 0.017(9) | 0.000 | 0.013(7) | 0.000 |
| O(2) | 0.007(7) | 0.017(8) | 0.008(8) | 0.000 | 0.002(6) | 0.000 |
| O(3) | 0.019(9) | 0.017(9) | 0.013(8) | 0.000 | 0.013(7) | 0.000 |
| O(4) | 0.040(12) | 0.028(11) | 0.011(9) | 0.000 | -0.008(8) | 0.000 |
| O(5) | 0.018(9) | 0.009(8) | 0.019(8) | 0.000 | 0.010(7) | 0.000 |
| O(6) | 0.019(6) | 0.018(6) | 0.016(6) | -0.008(5) | 0.000(5) | 0.003(5) |
| O(7) | 0.019(5) | 0.006(5) | 0.015(5) | 0.002(4) | -0.001(5) | -0.001(5) |
| O(8) | 0.004(6) | 0.013(6) | 0.013(6) | 0.000 | 0.007(5) | 0.000 |
| O(9) | 0.008(5) | 0.011(6) | 0.021(6) | -0.002(4) | 0.003(4) | 0.001(5) |
| O(10) | 0.036(11) | 0.014(9) | 0.021(10) | 0.000 | 0.005(8) | 0.000 |

Table S3. Bond valence calculations for kainotropite

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Cu(1) | Cu(2) | Cu(3) | Fe | V(1) | V(2) | V(3) | Σ |
| O(1) |  |  |  |  | 1.17 | 0.98 |  | 2.15 |
| O(2) |  | 0.59 x2→ | 0.52 | 0.51 |  |  |  | 2.21 |
| O(3) |  |  | 0.20 | 0.46 | 1.30 |  |  | 1.96 |
| O(4) |  |  | 0.50 |  |  |  | 1.52 | 2.02 |
| O(5) | 0.58 |  |  |  |  |  | 1.52 | 2.10 |
| O(6) |  | 0.32  0.07 |  | 0.52 x2↓ |  |  | 1.11 x2↓ | 2.02 |
| O(7) | 0.40x2↓ | 0.38 |  |  | 1.20 x2↓ |  |  | 1.98 |
| O(8) | 0.48 x2→ | 0.61 |  | 0.47 |  |  |  | 2.04 |
| O(9) |  | 0.15 | 0.36 x2↓ |  |  | 1.39 x2↓ |  | 1.90 |
| O(10) | 0.21 |  |  | 0.58 |  | 1.31 |  | 2.10 |
| Σ | 2.07 | 2.12 | 1.94 | 3.06 | 4.87 | 5.07 | 5.26\* |  |

Parameters are taken from Gagné & Hawthorne (2015). \*Could be slightly decreased if admixed As should be taken into cosideration in the V(3) site.