Supplementary information to the paper

**The mineralogy of the historical Mochalin Log *REE* deposit, South Urals, Russia. Part IV. Alexkuznetsovite-(La), La2Mn(CO3)(Si2O7), alexkuznetsovite-(Ce), Ce2Mn(CO3)(Si2O7), and biraite-(La), La2Fe2+(CO3)(Si2O7), three new isostructural minerals and a definition of the biraite group**

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## Table S1. Powder X-ray diffraction data (d in Å) of alexkuznetsovite-(La).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *I*obs | *d*obs | *I*calc\* | *d*calc\*\* | *h k l* |
| **63** | **4.595** | 69 | 4.579 | 110 |
| **56** | **4.489** | 44 | 4.463 | 102 |
| **62** | **4.331** | 36 | 4.324 | –104 |
| **50** | **4.208** | 46 | 4.200 | 111 |
| 34 | 3.732 | 49 | 3.709 | 014 |
| 21 | 3.335 | 45 | 3.324 | 021 |
| **49** | **3.171** | 55 | 3.162 | 022 |
| **100** | **2.962** | 6, 100, 46 | 2.973, 2.956, 2.952 | 120, 006, –212 |
| 44 | 2.861 | 2, 1, 31 | 2.865, 2.861, 2.834 | 114, 121, –123 |
| **76** | **2.785** | 9, 45 | 2.803, 2.777 | –116, –214 |
| **59** | **2.692** | 18, 35, 67 | 2.697, 2.690, 2.678 | 122, 024, 202 |
| 27 | 2.465 | 13 | 2.449 | 025 |
| 13 | 2.332 | 4, 2 | 2.338, 2.328 | –108, –223 |
| 16 | 2.263 | 36 | 2.253 | 116 |
| 11 | 2.210 | 2, 7 | 2.210, 2.206 | –118, 221 |
| 17 | 1.946 | 7, 15 | 1.945, 1.942 | –316, –227 |
| 41 | 1.853 | 6, 4, 18 | 1.854, 1.852, 1.845 | 028, –231, –233 |
| 31 | 1.832 | 5, 10, 17 | 1.833, 1.832, 1.826 | 118, –322, 230 |
| 26 | 1.777 | 15 | 1.772 | –129 |
| 13 | 1.725 | 1, 12 | 1.726, 1.716 | 232, 0.1.10 |
| 12 | 1.640 | 4, 4 | 1.640, 1.637 | –404, –1.2.10 |
| 14 | 1.494 | 2, 7, 2 | 1.486, 1.486, 1.485 | 240, –239, –418 |

\*For the calculated pattern, only reflections with intensities ≥1 are given;

\*\*for the unit-cell parameters calculated from single-crystal data.

The strongest reflections are given in boldtype.

## Table S2. Powder X-ray diffraction data (d in Å) of alexkuznetsovite-(Ce).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *I*obs | *d*obs | *I*calc\* | *d*calc\*\* | *h k l* |
| **35** | **4.145** | 45 | 4.205 | 111 |
| 18 | 3.736 | 19, 47 | 3.731, 3.713 | 112, 014 |
| 16 | 3.585 | 19 | 3.648 | -114 |
| 17 | 3.273 | 43 | 3.324 | 021 |
| **26** | **3.177** | 16, 56 | 3.196, 3.162 | -115, 022 |
| **100** | **2.893** | 100, 44, 14, 10 | 2.960, 2.956, 2.938, 2.903 | 006, -212, 023, -213 |
| **36** | **2.797** | 30, 7, 9, 45 | 2.837, 2.830, 2.806, 2.781 | -123, 210, -116, -214 |
| 11 | 2.331 | 8, 3, 2 | 2.344, 2.342, 2.330 | -221, -108, -223 |
| 9 | 2.228 | 17, 3 | 2.238, 2.228 | 031, 026 |
| 10 | 2.129 | 4, 19, 4 | 2.134, 2.126. 2.123 | -131, 125, 214 |
| 15 | 2.074 | 7, 1, 2, 35 | 2.080, 2.077, 2.063, 2.062 | 131, 300, -314, -218 |
| **24** | **2.027** | 5, 15 | 2.030, 2.027 | 027, 117 |
| 14 | 1.949 | 2, 6, 15 | 1.954, 1.948, 1.944 | 126, -316, -227 |
| 7 | 1.929 | 5 | 1.926 | -128 |
| 15 | 1.900 | 5, 3 | 1.905, 1.898 | 035, -219 |
| **26** | **1.833** | 5, 9, 16 | 1.836, 1.835, 1.827 | 118, -322, 230 |
| **25** | **1.808** | 3, 6, 7, 3 | 1.814, 1.813, 1.811, 1.806 | -234, -2.0.10, -321, -1.1.10 |
| 8 | 1.779 | 14 | 1.774 | -129 |
| **20** | **1.686** | 5, 11, 2, 6, 5 | 1.705, 1.705, 1.686, 1.685, 1.684 | 029, -236, 037, 304, 041 |
| 5 | 1.640 | 3, 3 | 1.643, 1.639 | -404, -1.2.10 |
| 16 | 1.586 | 9, 4, 3 | 1.584, 1.583, 1.583 | 208, 142, 038 |
| 11 | 1.579 | 7, 2 | 1.580, 1.576 | -412, -144 |
| 7 | 1.520 | 4, 3 | 1.528, 1.518 | 045, 410 |

\*For the calculated pattern, only reflections with intensities ≥1 are given;

\*\*for the unit-cell parameters calculated from single-crystal data.

The strongest reflections are given in boldtype.

## Table S3. Powder X-ray diffraction data (d in Å) of biraite-(La).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *I*obs | *d*obs | *I*calc\* | *d*calc\*\* | *h k l* |
| **49** | **4.594** | 63 | 4.575 | 110 |
| **47** | **3.723** | 18, 45 | 3.717, 3.701 | 112, 014 |
| **100** | **3.055** | 63, 30 | 3.049, 3.007 | -204, -121 |
| **66** | **2.962** | 45, 100 | 2.953, 2.947 | -212, 006 |
| 15 | 2.895 | 10 | 2.901 | -213 |
| **35** | **2.787** | 49 | 2.780 | -214 |
| **38** | **2.690** | 18, 35 | 2.693, 2.687 | 122, 024 |
| 26 | 2.509 | 1, 11, 8 | 2.522, 2.501, 2.484 | 115, 123, 212 |
| 23 | 2.259 | 33 | 2.245 | 116 |
| 13 | 2.189 | 4, 24 | 2.186, 2.179 | 032, -302 |
| 21 | 2.127 | 3, 18, 18 | 2.133, 2.119, 2.115 | -131, 125, -132 |
| 18 | 2.029 | 4, 13 | 2.024, 2.017 | 027, 117 |
| **33** | **1.843** | 7, 14, 7, 3 | 1.851, 1.846, 1.838, 1.837 | 028, -233, -308, -323 |
| 24 | 1.585 | 4, 4, 3, 8 | 1.581, 1.580, 1.579, 1.577 | 142, 044, 038, -412 |
| 8 | 1.422 | 2, 4 | 1.419, 1.417 | 412, -4.0.10 |
| 13 | 1.349 | 6, 4 | 1.346, 1.343 | 244, 048 |

\*For the calculated pattern, only reflections with intensities ≥1 are given;

\*\*for the unit-cell parameters calculated from single-crystal data.

The strongest reflections are given in boldtype.