**Supplementary material -** Full details for Tables 3 and 4

**Uroxite and metauroxite, the first two uranyl-oxalate minerals**

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Table 3. Powder X-ray diffraction data (*d* in Å) for uroxite\*.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *I*obs | *I*calc | *d*obs | *d*calc | *hkl* |
| 38 | 38 | 10.05 | 10.0512 | 011 |
| 7 | 7 | 6.64 | 6.6322 | 021 |
| 9 | 9 | 6.11 | 6.1133 | 012 |
| 8 | 9 | 5.55 | 5.5561 | 100 |
| 100 | 51, 49 | 5.00 | 5.0256, 4.9750 | 022, -111 |
| 23 | 22 | 4.75 | 4.7604 | 031 |
| 51 | 14, 35 | 4.43 | 4.4943, 4.4240 | 120, -102 |
|  | 4 |  | 4.3340 | -121 |
| 9 | 2, 2 | 4.224 | 4.2696, 4.1879 | 013, 121 |
|  | 2 |  | 4.1292 | 102 |
| 13 | 4, 7 | 4.015 | 4.0493, 3.9863 | 032, 112 |
| 16 | 12 | 3.844 | 3.8435 | 023 |
| 8 | 7 | 3.739 | 3.7555 | 130 |
| 19 | 12, 8 | 3.649 | 3.6741, 3.6330 | 041, 122 |
| 33 | 31 | 3.567 | 3.5712 | 131 |
|  | 3 |  | 3.5011 | -113 |
| 29 | 17, 4, 5 | 3.341 | 3.3504, 3.3407, 3.3349 | 033, -132, 004 |
|  | 5 |  | 3.3161 | 042 |
| 20 | 12, 8 | 3.271 | 3.2806, 3.2583 | 113, 014 |
|  | 2 |  | 3.2082 | 132 |
| 12 | 10 | 3.070 | 3.0750 | 123 |
|  | 3 |  | 3.0378 | 141 |
| 5 | 6 | 2.975 | 2.9803 | 051 |
| 9 | 9 | 2.933 | 2.9385 | -133 |
|  | 3 |  | 2.8985 | -114 |
|  | 2 |  | 2.7794 | 052 |
|  | 2 |  | 2.7749 | 104 |
| 8 | 4 | 2.754 | 2.7538 | -124 |
|  | 4 |  | 2.7303 | 114 |
| 9 | 9 | 2.672 | 2.6787 | 150 |
|  | 6 |  | 2.6436 | -151 |
| 28 | 5, 7, 7, 10 | 2.623 | 2.6307, 2.6282, 2.6193, 2.6110 | -202, 015, -143, 220 |
| 10 | 4, 2, 5 | 2.515 | 2.5311, 2.5153, 2.5031 | 221, -152, 202 |
|  | 2 |  | 2.4702 | 212 |
| 12 | 6, 7 | 2.433 | 2.4370, 2.4259 | 134, -231 |
| 5 | 5, 2 | 2.385 | 2.4036, 2.3802 | -213, 062 |
|  | 3 |  | 2.3534 | -125 |
| 10 | 6 | 2.334 | 2.3376 | -232 |
|  | 2 |  | 2.3149 | 115 |
| 8 | 5, 2 | 2.253 | 2.2610, 2.2368 | 153, -241 |
| 16 | 8, 3, 6 | 2.201 | 2.2107, 2.2079, 2.1876 | 063, -162, 045 |
| 5 | 3, 2, 2 | 2.117 | 2.1248, 2.1159, 2.0959 | -224, -106, -116 |
| 12 | 4, 2, 2, 2 | 2.0516 | 2.0548, 2.0529, 2.0482, 2.0460 | 154, -243, -251, 214 |
| 13 | 5, 4, 6 | 2.0286 | 2.0378, 2.0300, 2.0160 | 036, 163, 106 |
| 20 | 4, 9, 2 | 1.9985 | 1.9987, 1.9968, 1.9932 | 116, 145, 224 |
| 10 | 8 | 1.9583 | 1.9614 | 243 |
| 11 | 8, 3 | 1.9216 | 1.9306, 1.9110 | 172, 080 |
| 5 | 3, 4 | 1.8919 | 1.9042, 1.8910 | -253, 017 |
| 13 | 3, 2, 5 | 1.8468 | 1.8580, 1.8520, 1.8474 | -235, 300, 261 |
|  | 2 |  | 1.8302 | -262 |
| 14 | 5, 4, 3, 4, 3 | 1.8075 | 1.8270, 1.8075, 1.8045, 1.7981, 1.7922 | 074, 225, 311, 056, -254 |
|  | 2 |  | 1.7860 | -216 |
| 12 | 5, 6 | 1.7764 | 1.7748, 1.7683 | -165, -322 |
| 10 | 3, 3, 2, 4 | 1.7494 | 1.7557, 1.7543, 1.7424, 1.7408 | -174, -182, -313, -331 |
| 4 | 2, 2 | 1.7174 | 1.7198, 1.7110 | 127, 254 |
| 7 | 4, 4, 2 | 1.6669 | 1.6695, 1.6598, 1.6589 | -304, -147, 313 |
| 7 | 3 | 1.6557 | 1.6576 | 018 |
|  | 2 |  | 1.6456 | 272 |
|  | 2 |  | 1.6411 | 341 |
| 4 | 3 | 1.6241 | 1.6165 | -191 |
| 3 | 2 | 1.5829 | 1.5858 | -192 |
| 4 | 2 | 1.5557 | 1.5564 | 281 |
|  | 2 |  | 1.5461 | -282 |
|  | 2 |  | 1.5352 | 128 |
| 6 | 3 | 1.5213 | 1.5209 | 352 |
| 3 | 2 | 1.4957 | 1.5025 | 265 |
| 10 | 2, 3, 2, 2 | 1.4532 | 1.4588, 1.4553, 1.4509, 1.4488 | 237, -345, 167, 194 |

\* The calculated intensities have been scaled such that the intensities of the adjacent 022 and -111 lines total 100. After scaling, only calculated lines with *I* ≥ 2 are included.

Table 4. Powder X-ray diffraction data (*d* in Å) for metauroxite.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| *I*obs | *I*calc | *d*obs | *d*calc | *hkl* |
| 9 | 10 | 7.90 | 7.8016 | 001 |
| 45 | 61 | 6.06 | 6.0432 | 010 |
| 33 | 38 | 5.52 | 5.5148 | 100 |
| 34 | 55 | 4.97 | 4.9665 | 011 |
| 100 | 24, 76 | 4.52 | 4.6087, 4.5031 | 0-11, 101 |
|  | 6 |  | 4.3724 | 110 |
| 80 | 44, 25, 34 | 3.888 | 3.9081, 3.9008, 3.8287 | 111, 002, -110 |
| 22 | 32 | 3.748 | 3.7267 | -1-11 |
|  | 5 |  | 3.5056 | -111 |
| 51 | 36, 20 | 3.180 | 3.1848, 3.1680 | -102, 0-12 |
| 7 | 4, 7 | 2.999 | 3.0216, 2.9948 | 020, 112 |
| 7 | 12 | 2.888 | 2.8938 | 021 |
|  | 2 |  | 2.8335 | -1-12 |
| 15 | 7, 12 | 2.796 | 2.8116, 2.8018 | 120, -112 |
| 14 | 19 | 2.746 | 2.7473 | 0-21 |
|  | 5 |  | 2.6680 | 1-12 |
|  | 7 |  | 2.6445 | 210 |
| 32 | 24, 8 | 2.604 | 2.5999, 2.5866 | -201, -1-21 |
|  | 5 |  | 2.5133 | -120 |
|  | 4 |  | 2.4832 | 022 |
|  | 4 |  | 2.4793 | -2-11 |
| 22 | 8, 16 | 2.455 | 2.4586, 2.4383 | 013, -121 |
|  | 3 |  | 2.3917 | -210 |
| 20 | 6, 6, 9 | 2.352 | 2.3626, 2.3520, 2.3486 | 122, 103, 1-21 |
|  | 3 |  | 2.3066 | -211 |
|  | 3 |  | 2.3043 | 0-22 |
| 13 | 5, 8 | 2.2611 | 2.2673, 2.2518 | 2-11, -202 |
| 27 | 18, 3, 9 | 2.2136 | 2.2239, 2.2071, 2.2019 | 212, -1-22, -113 |
| 11 | 4, 10, 3 | 2.1683 | 2.1862, 2.1823, 2.1555 | 220, -1-13, -2-12 |
|  | 3 |  | 2.1362 | 221 |
|  | 4 |  | 2.1039 | 1-13 |
| 16 | 10, 5 | 2.0664 | 2.0674, 2.0536 | -212, 1-22 |
| 8 | 10 | 2.0107 | 2.0144 | 030 |
|  | 4 |  | 1.9785 | 130 |
| 9 | 7, 2 | 1.9510 | 1.9534, 1.9504 | 131, 004 |
| 18 | 8, 7, 5 | 1.8994 | 1.9144, 1.9000, 1.8920 | -220, 0-23, -203 |
|  | 6, 5 |  | 1.8681, 1.8634 | -123, -2-22 |
| 22 | 5, 8, 8 | 1.8454 | 1.8489, 1.8444, 1.8389 | 032, -1-23, -104 |
| 21 | 5, 5, 6, 6, 4 | 1.8171 | 1.8274, 1.8238, 1.8193, 1.8157, 1.7967 | 310, -2-13, 114, 0-14, -131 |
|  | 4 |  | 1.7893 | -301 |
|  | 2 |  | 1.7885 | 311 |
| 17 | 3, 2, 5, 2, 4 | 1.7382 | 1.7528, 1.7454, 1.7423, 1.7361, 1.7342 | -222, -1-14, 1-31, 0-32, 2-13 |
| 13 | 4, 4, 5, 4, 2, 4 | 1.7073 | 1.7230, 1.7213, 1.7130, 1.6994, 1.6921, 1.6863 | 231, 223, -1-32, 024, -132, 2-22 |
| 16 | 3, 2, 3, 4, 2 | 1.6652 | 1.6749, 1.6698, 1.6659, 1.6628, 1.6592 | -2-31, 312, -311, 302, 124 |
|  | 4 |  | 1.6510 | 3-11 |
| 11 | 4, 3, 4 | 1.6401 | 1.6493, 1.6403, 1.6354 | 321, -3-12, 133 |
|  | 3 |  | 1.6208 | -3-21 |
|  | 2 |  | 1.5955 | 214 |
| 12 | 7, 2, 3 | 1.5885 | 1.5923, 1.5840, 1.5790 | 204, 0-24, -223 |
|  | 2 |  | 1.5603 | 005 |
| 8 | 2, 2, 2, 3 | 1.5399 | 1.5513, 1.5362, 1.5347, 1.5209 | -2-32, 0-33, -214, -231 |
| 16 | 3, 2, 3, 5, 2, 2 | 1.5012 | 1.5118, 1.5108, 1.5032, 1.5013, 1.4951, 1.4929 | 313, 040, 141, 105, 1-24, 233 |

\* The calculated intensities have been scaled such that the intensities of the adjacent 0-11 and 101 lines total 100. After scaling, only calculated lines with *I* ≥ 2 are included.