Supplementary Table S1. Modeled fractional atomic coordinates for synthetic 2*M*1 K-dioctahedral micas (group 1) and for 1*M* mica samples Mal-4 and Mal-6. Cation compositions and unit-cell parameters for group 1 samples are given in Tables 1 and 2, and for samples Mal-4 and Mal-6, in Zviagina et al. (2015).

|  |  |  |  |
| --- | --- | --- | --- |
|  | *x* | *y* | *z* |
|  |  | P13-1 |  |
| K | 0 | 0.089(1) | 0.25 |
| M | 0.2448(7) | 0.0810(2) | 0.0000(1) |
| T1 | 0.9649(8) | 0.422(1) | 0.1361(2) |
| T2 | 0.458(1) | 0.253(1) | 0.1361(2) |
| O1 | 0.451(2) | -0.069(1) | 0.0553(3) |
| O2 | 0.406(2) | 0.2501(4) | 0.0553(2) |
| OH | 0.453(1) | 0.5675(9) | 0.0555(3) |
| O3 | 0.460(3) | 0.088(1) | 0.1696(2) |
| O4 | 0.728(2) | 0.331(2) | 0.1639(3) |
| O5 | 0.230(2) | 0.344(1) | 0.1696(3) |
|  |  | P13-1e\* |  |
| K | 0 | 0.090(1) | 0.25 |
| M | 0.2448(7) | 0.0810(2) | 0.0000(1) |
| T1 | 0.9638(8) | 0.422(1) | 0.1361(2) |
| T2 | 0.458(1) | 0.254(1) | 0.1361(2) |
| O1 | 0.452(2) | -0.069(1) | 0.0553(3) |
| O2 | 0.404(2) | 0.2501(4) | 0.0553(2) |
| OH | 0.454(1) | 0.5667(9) | 0.0554(3) |
| O3 | 0.471(3) | 0.089(1) | 0.1696(2) |
| O4 | 0.721(2) | 0.338(2) | 0.1640(3) |
| O5 | 0.223(2) | 0.339(1) | 0.1696(3) |
|  |  | P17 |  |
| K | 0 | 0.090(1) | 0.25 |
| M | 0.2450(7) | 0.0811(2) | 0.0000(1) |
| T1 | 0.9634(8) | 0.422(1) | 0.1358(2) |
| T2 | 0.456(1) | 0.253(1) | 0.1358(2) |
| O1 | 0.451(2) | -0.069(1) | 0.0552(3) |
| O2 | 0.404(2) | 0.2501(4) | 0.0552(2) |
| OH | 0.453(1) | 0.5674(9) | 0.0553(3) |
| O3 | 0.457(3) | 0.088(1) | 0.1694(2) |
| O4 | 0.728(2) | 0.330(2) | 0.1636(3) |
| O5 | 0.229(2) | 0.350(1) | 0.1694(3) |
|  |  | P17e\* |  |
| K | 0 | 0.092(1) | 0.25 |
| M | 0.2450(7) | 0.0811(2) | 0.0000(1) |
| T1 | 0.9624(8) | 0.423(1) | 0.1358(2) |
| T2 | 0.456(1) | 0.254(1) | 0.1358(2) |
| O1 | 0.452(2) | -0.068(1) | 0.0552(3) |
| O2 | 0.403(2) | 0.2501(4) | 0.0552(2) |
| OH | 0.454(1) | 0.5666(9) | 0.0553(3) |
| O3 | 0.470(3) | 0.089(1) | 0.1694(2) |
| O4 | 0.719(2) | 0.338(2) | 0.1637(3) |
| O5 | 0.221(2) | 0.339(1) | 0.1694(3) |
|  |  | P11-2 |  |
| K | 0 | 0.096(1) | 0.25 |
| M | 0.2457(7) | 0.0814(2) | 0.0000(1) |
| T1 | 0.965(8) | 0.423(1) | 0.1354(2) |
| T2 | 0.457(1) | 0.254(1) | 0.1354(2) |
| O1 | 0.453(2) | -0.067(1) | 0.0549(3) |
| O2 | 0.402(2) | 0.2503(4) | 0.0549(2) |
| OH | 0.454(1) | 0.5665(9) | 0.0545(3) |
| O3 | 0.451(3) | 0.089(1) | 0.1693(2) |
| O4 | 0.733(2) | 0.327(2) | 0.1628(3) |
| O5 | 0.235(2) | 0.349(1) | 0.1693(3) |
|  |  | P18-2 |  |
| K | 0 | 0.091(1) | 0.25 |
| M | 0.2458(7) | 0.0814(2) | 0.0000(1) |
| T1 | 0.9642(8) | 0.424(1) | 0.1352(2) |
| T2 | 0.456(1) | 0.255(1) | 0.1352(2) |
| O1 | 0.453(2) | -0.067(1) | 0.0548(3) |
| O2 | 0.402(2) | 0.2504(4) | 0.0548(2) |
| OH | 0.454(1) | 0.5664(9) | 0.0543(3) |
| O3 | 0.455(3) | 0.089(1) | 0.1692(2) |
| O4 | 0.730(2) | 0.329(2) | 0.1625(3) |
| O5 | 0.231(3) | 0.348(1) | 0.1692(3) |
|  |  | P12-1 |  |
| K | 0 | 0.093(1) | 0.25 |
| M | 0.2467(7) | 0.0818(2) | 0.0000(1) |
| T1 | 0.9642(8) | 0.425(1) | 0.1350(2) |
| T2 | 0.454(1) | 0.255(1) | 0.1350(2) |
| O1 | 0.455(2) | -0.065(1) | 0.0544(3) |
| O2 | 0.398(2) | 0.2506(4) | 0.0544(2) |
| OH | 0.455(1) | 0.5654(9) | 0.0534(3) |
| O3 | 0.446(3) | 0.090(1) | 0.1692(2) |
| O4 | 0.734(2) | 0.326(2) | 0.1617(3) |
| O5 | 0.235(2) | 0.353(1) | 0.1692(3) |
|  |  | P15 |  |
| K | 0 | 0.093(1) | 0.25 |
| M | 0.2467(7) | 0.0819(2) | 0.0000(1) |
| T1 | 0.9646(8) | 0.425(1) | 0.1350(2) |
| T2 | 0.455(1) | 0.255(1) | 0.1350(2) |
| O1 | 0.455(2) | -0.065(1) | 0.0544(3) |
| O2 | 0.398(2) | 0.2506(4) | 0.0544(2) |
| OH | 0.455(1) | 0.5653(9) | 0.0533(3) |
| O3 | 0.445(3) | 0.090(1) | 0.1692(2) |
| O4 | 0.735(2) | 0.325(2) | 0.1616(3) |
| O5 | 0.236(2) | 0.353(1) | 0.1692(3) |
|  |  | P28 |  |
| K | 0 | 0.096(1) | 0.25 |
| M | 0.2482(7) | 0.0825(2) | 0.0000(1) |
| T1 | 0.9649(8) | 0.428(1) | 0.1351(2) |
| T2 | 0.453(1) | 0.257(1) | 0.1351(2) |
| O1 | 0.457(2) | -0.062(1) | 0.0539(3) |
| O2 | 0.392(2) | 0.2510(4) | 0.0539(2) |
| OH | 0.456(1) | 0.5635(9) | 0.0519(3) |
| O3 | 0.436(3) | 0.092(1) | 0.1688(2) |
| O4 | 0.740(2) | 0.321(2) | 0.1598(3) |
| O5 | 0.240(2) | 0.360(1) | 0.1688(3) |
|  |  | P25 |  |
| K | 0 | 0.095(1) | 0.25 |
| M | 0.2480(7) | 0.0824(2) | 0.0000(1) |
| T1 | 0.9658(8) | 0.427(1) | 0.1352(2) |
| T2 | 0.454(1) | 0.257(1) | 0.1352(2) |
| O1 | 0.458(2) | -0.061(1) | 0.0538(3) |
| O2 | 0.393(2) | 0.2509(4) | 0.0538(2) |
| OH | 0.456(1) | 0.5638(9) | 0.0520(3) |
| O3 | 0.434(3) | 0.092(1) | 0.1686(2) |
| O4 | 0.742(2) | 0.319(2) | 0.1597(3) |
| O5 | 0.243(2) | 0.361(1) | 0.1686(3) |
|  |  | P33 |  |
| K | 0 | 0.097(1) | 0.25 |
| M | 0.2488(7) | 0.0828(2) | 0.0000(1) |
| T1 | 0.9648(8) | 0.429(1) | 0.1354(2) |
| T2 | 0.452(1) | 0.258(1) | 0.1354(2) |
| O1 | 0.459(2) | -0.059(1) | 0.0536(3) |
| O2 | 0.389(2) | 0.2512(4) | 0.0536(2) |
| OH | 0.457(1) | 0.5627(9) | 0.0512(3) |
| O3 | 0.423(3) | 0.093(1) | 0.1684(3) |
| O4 | 0.744(2) | 0.317(2) | 0.1587(3) |
| O5 | 0.244(2) | 0.364(1) | 0.1684(3) |
|  |  | P30 |  |
| K | 0 | 0.098(1) | 0.25 |
| M | 0.2492(7) | 0.0829(2) | 0.0000(1) |
| T1 | 0.9648(8) | 0.429(1) | 0.1352(2) |
| T2 | 0.452(1) | 0.258(1) | 0.1352(2) |
| O1 | 0.460(2) | -0.058(1) | 0.0535(3) |
| O2 | 0.388(2) | 0.2512(4) | 0.0535(2) |
| OH | 0.457(1) | 0.5624(9) | 0.0509(3) |
| O3 | 0.424(3) | 0.093(1) | 0.1682(2) |
| O4 | 0.746(2) | 0.315(2) | 0.1581(3) |
| O5 | 0.246(2) | 0.366(1) | 0.1682(3) |
|  |  | P26 |  |
| K | 0 | 0.097(1) | 0.25 |
| M | 0.2489(7) | 0.0828(2) | 0.0000(1) |
| T1 | 0.9646(8) | 0.429(1) | 0.1355(2) |
| T2 | 0.452(1) | 0.258(1) | 0.1355(2) |
| O1 | 0.460(2) | -0.059(1) | 0.0535(3) |
| O2 | 0.387(2) | 0.2511(4) | 0.0535(2) |
| OH | 0.457(1) | 0.5627(9) | 0.0511(3) |
| O3 | 0.423(3) | 0.093(1) | 0.1682(2) |
| O4 | 0.746(2) | 0.315(2) | 0.1583(3) |
| O5 | 0.246(2) | 0.366(1) | 0.1682(3) |
|  |  | P31 |  |
| K | 0 | 0.099(1) | 0.25 |
| M | 0.2500(7) | 0.0833(2) | 0.0000(1) |
| T1 | 0.9651(8) | 0.430(1) | 0.1353(2) |
| T2 | 0.451(1) | 0.259(1) | 0.1353(2) |
| O1 | 0.461(2) | -0.056(1) | 0.0534(3) |
| O2 | 0.384(2) | 0.2514(4) | 0.0534(2) |
| OH | 0.458(1) | 0.5611(9) | 0.0503(3) |
| O3 | 0.417(3) | 0.093(1) | 0.1683(2) |
| O4 | 0.749(2) | 0.312(2) | 0.1573(3) |
| O5 | 0.249(2) | 0.370(1) | 0.1683(3) |
|  |  | P29 |  |
| K | 0 | 0.099(1) | 0.25 |
| M | 0.2500(7) | 0.0833(2) | 0.0000(1) |
| T1 | 0.9653(8) | 0.430(1) | 0.1352(2) |
| T2 | 0.451(1) | 0.259(1) | 0.1352(2) |
| O1 | 0.462(2) | -0.056(1) | 0.0534(3) |
| O2 | 0.384(2) | 0.2514(4) | 0.0534(2) |
| OH | 0.459(1) | 0.5609(9) | 0.0502(3) |
| O3 | 0.418(3) | 0.094(1) | 0.1682(2) |
| O4 | 0.750(2) | 0.312(2) | 0.1571(3) |
| O5 | 0.249(2) | 0.370(1) | 0.1682(3) |
|  |  | Mal-4\*\* |  |
| K | 0 | 0.5 | 0.5 |
| M | 0.5 | 0.1667 | 0 |
| T | 0.4166(8) | 0.329(1) | 0.2712(1) |
| O1 | 0.354(2) | 0.317(1) | 0.1090(2) |
| O2 | 0.464(2) | 0.5 | 0.3200(1) |
| O3 | 0.682(3) | 0.241(1) | 0.3363(2) |
| OH | 0.422(1) | 0 | 0.1061(2) |
|  |  | Mal-6\*\* |  |
| K | 0 | 0.5 | 0.5 |
| M | 0.5 | 0.1667 | 0 |
| T | 0.4174(8) | 0.329(1) | 0.2715(1) |
| O1 | 0.355(2) | 0.317(1) | 0.1093(2) |
| O2 | 0.470(2) | 0.5 | 0.3211(1) |
| O3 | 0.680(3) | 0.238(1) | 0.3368(2) |
| OH | 0.421(1) | 0 | 0.1067(2) |
|  |  |  |  |

\* Models P13-1e and P17e were obtained using extrapolated *a* and *b* parameters (P13-1e: *a*=5.217 Å, *b*=9.041 Å; P17e: *a*=5.217 Å, *b*=9.040 Å; *c* and *β* as in Table 2; see text for details).

\*\*Mal-4: *a*=5.227 Å, *b*=9.011 Å, *c*= 10.102 Å, *β*=101.2°; Mal-6: *a*=5.215 Å, *b*=9.013 Å, *c*=10.093 Å, *β*=101.1° (Zviagina *et al*., 2015).