Table S1. Anisotropic displacement parameters (in Å2) of atoms in the structure of natromelansonite.

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| **Site** | ***U*11** | ***U*22** | ***U*33** | ***U*23** | ***U*13** | ***U*12** |
| Zr1 | 0.00962(11) | 0.00827(10) | 0.01153(11) | -0.00018(8) | 0.00040(7) | -0.00072(7) |
| Si1 | 0.0101(2) | 0.0136(2) | 0.0104(2) | 0.00064(17) | -0.00005(16) | 0.00001(17) |
| Si2 | 0.0101(2) | 0.0133(2) | 0.0105(2) | -0.00006(17) | 0.00030(16) | 0.00066(17) |
| Si3 | 0.0066(2) | 0.0147(2) | 0.0139(2) | 0.00011(18) | 0.00012(16) | -0.00072(16) |
| Si4 | 0.0125(2) | 0.0096(2) | 0.0144(2) | -0.00025(18) | -0.00004(18) | 0.00019(18) |
| Na1 | 0.0247(7) | 0.0261(7) | 0.0168(6) | 0.0005(5) | 0.0016(5) | -0.0010(5) |
| Na2 | 0.0245(14) | 0.0210(13) | 0.0266(14) | -0.0007(9) | -0.0001(10) | 0.0054(9) |
| Na3 | 0.073(2) | 0.0297(12) | 0.0556(18) | 0 | -0.0280(18) | 0 |
| Na4 | 0.073(2) | 0.0297(12) | 0.0556(18) | 0 | -0.0280(18) | 0 |
| K5 | 0.073(2) | 0.0297(12) | 0.0556(18) | 0 | -0.0280(18) | 0 |
| O1 | 0.0226(8) | 0.0324(9) | 0.0098(6) | -0.0003(6) | 0.0007(5) | -0.0016(7) |
| O2 | 0.0343(10) | 0.0169(7) | 0.0237(8) | -0.0040(6) | -0.0014(7) | -0.0081(7) |
| O3 | 0.0353(10) | 0.0169(7) | 0.0219(8) | 0.0039(6) | -0.0071(7) | 0.0050(7) |
| O4 | 0.0144(7) | 0.0527(13) | 0.0178(7) | 0.0019(8) | 0.0056(6) | 0.0006(7) |
| O5 | 0.0370(10) | 0.0158(7) | 0.0248(8) | 0.0037(6) | 0.0023(7) | -0.0067(7) |
| O6 | 0.0335(10) | 0.0219(8) | 0.0215(8) | -0.0029(6) | 0.0049(7) | 0.0120(7) |
| O7 | 0.0154(7) | 0.0495(12) | 0.0190(8) | 0.0051(8) | -0.0064(6) | -0.0017(7) |
| O8 | 0.0308(10) | 0.0182(8) | 0.0339(10) | -0.0026(7) | -0.0014(8) | 0.0085(7) |
| O9 | 0.0222(8) | 0.0189(8) | 0.0398(11) | -0.0021(7) | 0.0003(7) | -0.0091(6) |
| O10 | 0.0189(11) | 0.0209(11) | 0.0286(12) | 0 | 0.0016(9) | 0 |
| O11= H2O | 0.045(3) | 0.027(3) | 0.70(3) | 0 | 0.081(8) | 0 |
| O12 = H2O | 0.090(10) | 0.086(10) | 0.169(15) | 0 | -0.043(10) | 0 |
| O13 = H2O | 0.0514(17) | 0.094(3) | 0.0398(14) | -0.0119(16) | -0.0088(12) | 0.0411(18) |
| O14 = H2O | 0.054(4) | 0.099(7) | 0.041(3) | -0.008(4) | 0.000(3) | -0.008(4) |