**Supplemental Data Table 1**

Crystallographic coordinates, occupancies, equivalent isotropic (Å2) and anisotropic displacement parameters of the study micas

 **Sample EJ20\_1**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9398(5)  | 0.0306  | 0.0322(2)  | 0.0331(2)  | 0.0264(1)  | 0 | 0.0046(1)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.8992(8)  | 0.0082  | 0.0064(1)  | 0.0073(1)  | 0.0111(1)  | 0 | 0.00201(7)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.1010(5)  | 0.0082  | 0.0064(1)  | 0.0073(1)  | 0.0111(1)  | 0 | 0.00201(7)  | 0 |
| **M2** | **Mg2+** | 0  | 0.33131(2)  | ½ | 0.9013(8)  | 0.0082  | 0.00641(8)  | 0.00704(8)  | 0.01116(9)  | 0 | 0.00193(5)  | 0 |
|  | **Fe2+** | 0  | 0.33131(2)  | ½ | 0.0987(6)  | 0.0082  | 0.00641(8)  | 0.00704(8)  | 0.01116(9)  | 0 | 0.00193(5)  | 0 |
| **T** | **Si, Si4+** | 0.07587(2)  | 0.16665(1)  | 0.22726(1)  | 0.9713(9) | 0.0083  | 0.00744(5)  | 0.00813(5)  | 0.00941(5)  | 0.00002(3)  | 0.00174(3)  | 0.00001(3)  |
| **O1** | **O, O2-** | 0.32945(8)  | 0.22718(5)  | 0.16969(4)  | 0.9995(8) | 0.0176  | 0.0161(1)  | 0.0230(2)  | 0.0141(1)  | -0.0027(1)  | 0.0039(1)  | -0.0062(1)  |
| **O2** | **O, O2-** | 0.0112(1)  | 0  | 0.16960(6)  | 0.9997(8) | 0.0176  | 0.0243(2)  | 0.0130(2)  | 0.0142(2)  | 0  | -0.0005(2)  | 0  |
| **O3** | **O, O2-** | 0.13078(6)  | 0.16660(3)  | 0.39143(3)  | 0.9973(8) | 0.0101  | 0.0094(1)  | 0.0103(1)  | 0.0108(1)  | -0.00015(8)  | 0.00213(8)  | 0.00004(7)  |
| **O4** | **O, O2-** | 0.13246(8)  | ½ | 0.39915(5)  | 1.0002(7) | 0.0102  | 0.0092(2)  | 0.0108(2)  | 0.0105(2)  | 0 | 0.0017(1)  | 0 |
|  | **H** | 0.12121(8)  | ½ | 0.32529(5)  | 0.296(1) | 0.0102  | 0.0092(2)  | 0.0108(2)  | 0.0105(2)  | 0 | 0.0017(1)  | 0 |

**Sample EJ20\_2**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9401(6)  | 0.0312  | 0.0327(2)  | 0.0334(2)  | 0.0276(2)  | 0 | 0.0051(2)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.8960(8)  | 0.0090  | 0.0072(2)  | 0.0074(1)  | 0.0126(2)  | 0 | 0.0026(1)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.1038(5)  | 0.0090  | 0.0072(2)  | 0.0074(1)  | 0.0126(2)  | 0 | 0.0026(1)  | 0 |
| **M2** | **Mg2+** | 0  | 0.33129(3)  | ½ | 0.8992(8)  | 0.0088  | 0.0070(1)  | 0.0071(1)  | 0.0126(1)  | 0 | 0.00233(8)  | 0 |
|  | **Fe2+** | 0  | 0.33129(3)  | ½ | 0.1009(6)  | 0.0088  | 0.0070(1)  | 0.0071(1)  | 0.0126(1)  | 0 | 0.00233(8)  | 0 |
| **T** | **Si, Si4+** | 0.07589(3)  | 0.16666(2)  | 0.22730(2)  | 0.9730(9) | 0.0090  | 0.00807(7)  | 0.00814(7)  | 0.01097(8)  | 0.00000(4)  | 0.00225(5)  | 0.00002(4)  |
| **O1** | **O, O2-** | 0.3296(1)  | 0.22708(7)  | 0.16973(6)  | 0.9995(8) | 0.0182  | 0.0167(2)  | 0.0231(2)  | 0.0156(2)  | -0.0026(2)  | 0.0046(2)  | -0.0063(2)  |
| **O2** | **O, O2-** | 0.0109(2)  | 0  | 0.16969(8)  | 0.9993(8) | 0.0182  | 0.0248(3)  | 0.0133(3)  | 0.0153(3)  | 0  | 0.0002(2)  | 0  |
| **O3** | **O, O2-** | 0.13059(9)  | 0.16657(4)  | 0.39142(5)  | 0.9988(8) | 0.0107  | 0.0099(2)  | 0.0097(2)  | 0.0126(2)  | -0.0002(1)  | 0.0025(1)  | 0.0001(1)  |
| **O4** | **O, O2-** | 0.1325(1)  | ½ | 0.39918(7)  | 1.0001(7) | 0.0107  | 0.0096(2)  | 0.0107(2)  | 0.0119(2)  | 0 | 0.0023(2)  | 0 |
|  | **H** | 0.1056(1)  | ½ | 0.32037(7)  | 0.413(1) | 0.0107  | 0.0096(2)  | 0.0107(2)  | 0.0119(2)  | 0 | 0.0023(2)  | 0 |

**Sample EJ20\_3**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
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| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9463(6)  | 0.0310  | 0.0323(2)  | 0.0333(2)  | 0.0271(2)  | 0  | 0.0044(1)  | 0  |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.8996(8)  | 0.0082  | 0.0063(2)  | 0.0069(2)  | 0.0117(2)  | 0  | 0.0018(1)  | 0  |
|  | **Fe2+** | 0 | 0 | ½ | 0.1003(5)  | 0.0082  | 0.0063(2)  | 0.0069(2)  | 0.0117(2)  | 0  | 0.0018(1)  | 0  |
| **M2** | **Mg2+** | 0 | 0.33132(2)  | ½ | 0.8954(8)  | 0.0084  | 0.0064(1)  | 0.0070(1)  | 0.0118(1)  | 0  | 0.00155(8)  | 0  |
|  | **Fe2+** | 0  | 0.33132(2)  | ½ | 0.1045(6)  | 0.0084  | 0.0064(1)  | 0.0070(1)  | 0.0118(1)  | 0  | 0.00155(8)  | 0  |
| **T** | **Si, Si4+** | 0.07591(3)  | 0.16664(2)  | 0.22727(2)  | 0.9746(9) | 0.0086  | 0.00742(8)  | 0.00809(8)  | 0.01021(8)  | -0.00010(4)  | 0.00152(5)  | 0.00000(4)  |
| **O1** | **O, O2-** | 0.32958(9)  | 0.22730(6)  | 0.16974(5)  | 0.9996(8) | 0.0177  | 0.0159(2)  | 0.0228(2)  | 0.0147(2)  | -0.0029(2)  | 0.0039(1)  | -0.0061(2)  |
| **O2** | **O, O2-** | 0.0111(1)  | 0  | 0.16966(7)  | 0.9999(8) | 0.0176 | 0.0235(3)  | 0.0132(2)  | 0.0147(3)  | 0  | -0.0007(2)  | 0  |
| **O3** | **O, O2-** | 0.13068(8)  | 0.16660(4)  | 0.39131(4)  | 0.9988(8) | 0.0102  | 0.0094(2)  | 0.0097(2)  | 0.0114(2)  | -0.0002(1)  | 0.0018(1)  | 0.0003(1)  |
| **O4** | **O, O2-** | 0.1324(1)  | ½ | 0.39946(6)  | 1.0000(7) | 0.0102  | 0.0092(2)  | 0.0110(2)  | 0.0101(2)  | 0  | 0.0011(2)  | 0  |
|  | **H** | 0.1119(1)  | ½ | 0.34101(6)  | 0.922(1) | 0.0102  | 0.0092(2)  | 0.0110(2)  | 0.0101(2)  | 0  | 0.0011(2)  | 0  |

**Sample EJ25\_2**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9628(9)  | 0.0271  | 0.0260(8)  | 0.0282(8)  | 0.0269(8)  | 0  | 0.0035(6)  | 0  |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9701(8)  | 0.0068  | 0.0023(7)  | 0.0039(7)  | 0.0143(9)  | 0  | 0.0018(6)  | 0  |
|  | **Fe2+** | 0 | 0 | ½ | 0.0299(7)  | 0.0068  | 0.0023(7)  | 0.0039(7)  | 0.0143(9)  | 0  | 0.0018(6)  | 0  |
| **M2** | **Mg2+** | 0 | 0.3311(1)  | ½ | 0.9548(8)  | 0.0072  | 0.0029(5)  | 0.0049(5)  | 0.0137(6)  | 0  | 0.0012(4)  | 0  |
|  | **Fe2+** | 0  | 0.3311(1)  | ½ | 0.0451(8)  | 0.0072  | 0.0029(5)  | 0.0049(5)  | 0.0137(6)  | 0  | 0.0012(4)  | 0  |
| **T** | **Si, Si4+** | 0.0755(1)  | 0.16669(7)  | 0.22698(8)  | 0.980(1) | 0.0070  | 0.0048(3)  | 0.0062(3)  | 0.0102(4)  | -0.0002(3)  | 0.0014(2)  | -0.0003(2)  |
| **O1** | **O, O2-** | 0.3309(4)  | 0.2250(2)  | 0.1696(2)  | 1.0000(8) | 0.0166  | 0.0137(9)  | 0.020(1)  | 0.016(1)  | -0.0024(9)  | 0.0031(8)  | -0.0049(8)  |
| **O2** | **O, O2-** | 0.0070(6)  | 0 | 0.1699(3)  | 1.0001(8) | 0.0159  | 0.020(1)  | 0.013(1)  | 0.014(2)  | 0 | -0.002(1)  | 0 |
| **O3** | **O, O2-** | 0.1303(3)  | 0.1668(2)  | 0.3924(2)  | 1.0000(8) | 0.0086  | 0.0069(8)  | 0.0056(7)  | 0.013(1)  | 0.0006(7)  | 0.0017(7)  | 0.0000(6)  |
| **O4** | **O, O2-** | 0.1334(4)  | ½ | 0.4006(3)  | 1.0009(8) | 0.0058  | 0.004(1)  | 0.009(1)  | 0.005(1)  | 0  | 0.0004(9)  | 0  |
|  | **H** | 0.1289(4) | ½ | 0.3220(3) | 0.977(1) | 0.0058 | 0.004(1)  | 0.009(1)  | 0.005(1)  | 0  | 0.0004(9)  | 0  |

**Sample EJ25\_3**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9601(8)  | 0.0331  | 0.0321(4)  | 0.0329(5)  | 0.0346(4)  | 0  | 0.0063(3)  | 0  |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9171(8)  | 0.0128  | 0.0089(3)  | 0.0102(4)  | 0.0199(4)  | 0  | 0.0041(3)  | 0  |
|  | **Fe2+** | 0 | 0 | ½ | 0.0832(6)  | 0.0128  | 0.0089(3)  | 0.0102(4)  | 0.0199(4)  | 0  | 0.0041(3)  | 0  |
| **M2** | **Mg2+** | 0 | 0.33118(7)  | ½ | 0.9282(8)  | 0.0123  | 0.0084(2)  | 0.0098(3)  | 0.0191(3)  | 0  | 0.0036(2)  | 0  |
|  | **Fe2+** | 0  | 0.33118(7)  | ½ | 0.0718(7)  | 0.0123  | 0.0084(2)  | 0.0098(3)  | 0.0191(3)  | 0  | 0.0036(2)  | 0  |
| **T** | **Si, Si4+** | 0.07581(7)  | 0.16665(4)  | 0.22714(4)  | 0.978(1) | 0.0118  | 0.0095(2)  | 0.0099(2)  | 0.0163(2)  | -0.0001(1)  | 0.0031(1)  | 0.0001(1)  |
| **O1** | **O, O2-** | 0.3312(2)  | 0.2255(1)  | 0.1696(1)  | 0.9999(8) | 0.0209  | 0.0181(4)  | 0.0232(5)  | 0.0224(5)  | -0.0029(4)  | 0.0059(4)  | -0.0055(4)  |
| **O2** | **O, O2-** | 0.0081(4)  | 0  | 0.1696(2)  | 1.0001(8) | 0.0212  | 0.0252(8)  | 0.0159(7)  | 0.0211(7)  | 0 | 0.0002(6)  | 0 |
| **O3** | **O, O2-** | 0.1307(2)  | 0.1668(1)  | 0.3918(1)  | 0.9999(8) | 0.0136  | 0.0111(4)  | 0.0114(4)  | 0.0187(4)  | -0.0002(3)  | 0.0038(3)  | 0.0005(3)  |
| **O4** | **O, O2-** | 0.1328(3)  | ½ | 0.4008(2)  | 1.0000(7) | 0.0125  | 0.0108(5)  | 0.0120(5)  | 0.0148(6)  | 0  | 0.0027(4)  | 0  |
|  | **H** | 0.1003(3)  | ½ | 0.3440(2)  | 0.984(1) | 0.0125 | 0.0108(5)  | 0.0120(5)  | 0.0148(6)  | 0  | 0.0027(4)  | 0  |

**Sample EJ42\_2**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9824(5)  | 0.0305  | 0.0339(1)  | 0.0338(1)  | 0.0235(1)  | 0  | 0.00402(8)  | 0  |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9779(8)  | 0.0083  | 0.0072(1)  | 0.0069(1)  | 0.0110(1)  | 0  | 0.00208(8)  | 0  |
|  | **Fe2+** | 0 | 0 | ½ | 0.0221(5)  | 0.0083  | 0.0072(1)  | 0.0069(1)  | 0.0110(1)  | 0  | 0.00208(8)  | 0  |
| **M2** | **Mg2+** | 0 | 0.33164(2)  | ½ | 0.9755(8)  | 0.0085  | 0.0073(1)  | 0.0070(1)  | 0.0113(1)  | 0  | 0.00200(6)  | 0  |
|  | **Fe2+** | 0  | 0.33164(2)  | ½ | 0.0248(6)  | 0.0085  | 0.0073(1)  | 0.0070(1)  | 0.0113(1)  | 0  | 0.00200(6)  | 0  |
| **T** | **Si, Si4+** | 0.07618(2)  | 0.16668(1)  | 0.22831(1)  | 0.9759(9) | 0.0085  | 0.00810(6)  | 0.00787(6)  | 0.00955(6)  | -0.00005(2)  | 0.00169(4)  | 0.00001(2)  |
| **O1** | **O, O2-** | 0.33082(6)  | 0.22610(4)  | 0.17048(3)  | 0.9991(8) | 0.0175  | 0.0167(1)  | 0.0224(2)  | 0.0140(1)  | -0.0028(1)  | 0.00404(9)  | -0.0060(1)  |
| **O2** | **O, O2-** | 0.0088(1)  | 0  | 0.17047(4)  | 0.9991(8) | 0.0175  | 0.0244(2)  | 0.0128(2)  | 0.0140(2)  | 0 | -0.0004(1)  | 0 |
| **O3** | **O, O2-** | 0.13054(6)  | 0.16668(3)  | 0.39164(3)  | 0.9989(8) | 0.0097  | 0.0094(10)  | 0.0094(1)  | 0.0105(1)  | -0.00013(7)  | 0.00183(9)  | 0.00012(7)  |
| **O4** | **O, O2-** | 0.13272(7)  | ½ | 0.39894(4)  | 1.0001(8)  | 0.0100  | 0.0096(1)  | 0.0099(1)  | 0.0104(1)  | 0  | 0.0015(1)  | 0  |
|  | **H** | 0.11250(7)  | ½ | 0.32092(4)  | 0.392(1) | 0.0100  | 0.0096(1)  | 0.0099(1)  | 0.0104(1)  | 0  | 0.0015(1)  | 0  |

**Sample EJ42\_3**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
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| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9686(6)  | 0.0309  | 0.0341(2)  | 0.0346(2)  | 0.0238(1)  | 0  | 0.0042(1)  | 0  |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9225(8)  | 0.0083  | 0.0068(1)  | 0.0071(1)  | 0.0112(1)  | 0  | 0.00204(8)  | 0  |
|  | **Fe2+** | 0 | 0 | ½ | 0.0774(5)  | 0.0083  | 0.0068(1)  | 0.0071(1)  | 0.0112(1)  | 0  | 0.00204(8)  | 0  |
| **M2** | **Mg2+** | 0  | 0.33199(2)  | ½ | 0.9238(8)  | 0.0084  | 0.00658(9)  | 0.00762(9)  | 0.0109(1)  | 0  | 0.00174(6)  | 0  |
|  | **Fe2+** | 0  | 0.33199(2)  | ½ | 0.0763(6)  | 0.0084  | 0.00658(9)  | 0.00762(9)  | 0.0109(1)  | 0  | 0.00174(6)  | 0  |
| **T** | **Si, Si4+** | 0.07612(2)  | 0.16668(1)  | 0.22815(1)  | 0.9767(9) | 0.0081  | 0.00729(6)  | 0.00784(5)  | 0.00920(6)  | -0.00008(3)  | 0.00163(3)  | 0.00007(3)  |
| **O1** | **O, O2-** | 0.32959(8)  | 0.22729(5)  | 0.17028(4)  | 0.9996(8) | 0.0174  | 0.0163(2)  | 0.0228(2)  | 0.0137(1)  | -0.0029(1)  | 0.0040(1)  | -0.0062(1)  |
| **O2** | **O, O2-** | 0.0113(1)  | 0  | 0.17047(5)  | 0.9998(8) | 0.0174  | 0.0243(2)  | 0.0132(2)  | 0.0132(2)  | 0  | -0.0005(2)  | 0.0000  |
| **O3** | **O, O2-** | 0.13047(6)  | 0.16668(3)  | 0.39144(3)  | 0.9992(8) | 0.0094  | 0.0090(1)  | 0.0091(1)  | 0.0100(1)  | -0.00024(7)  | 0.00175(9)  | 0.00004(7)  |
| **O4** | **O, O2-** | 0.13241(9)  | ½ | 0.39853(5)  | 1.0001(7) | 0.0098  | 0.0092(1)  | 0.0100(1)  | 0.0103(2)  | 0  | 0.0017(1)  | 0  |
|  | **H** | 0.10560(9)  | ½ | 0.30556(5)  | 0.431(1) | 0.0098  | 0.0092(1)  | 0.0100(1)  | 0.0103(2)  | 0  | 0.0017(1)  | 0  |

**Sample EJ42\_4**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9758(6)  | 0.0315  | 0.0339(2)  | 0.0350(2)  | 0.0253(2)  | 0  | 0.0043(1)  | 0  |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9465(8)  | 0.0090  | 0.0069(2)  | 0.0075(2)  | 0.0128(2)  | 0  | 0.0024(1)  | 0  |
|  | **Fe2+** | 0 | 0 | ½ | 0.0534(5)  | 0.0090  | 0.0069(2)  | 0.0075(2)  | 0.0128(2)  | 0  | 0.0024(1)  | 0  |
| **M2** | **Mg2+** | 0 | 0.33179(3)  | ½ | 0.9486(8)  | 0.0090  | 0.0067(1)  | 0.0078(1)  | 0.0126(1)  | 0  | 0.00204(9)  | 0  |
|  | **Fe2+** | 0  | 0.33179(3)  | ½ | 0.0515(6)  | 0.0090  | 0.0067(1)  | 0.0078(1)  | 0.0126(1)  | 0  | 0.00204(9)  | 0  |
| **T** | **Si, Si4+** | 0.07611(3)  | 0.16669(2)  | 0.22822(2)  | 0.9815(9) | 0.0089  | 0.00774(8)  | 0.00831(8)  | 0.01085(8)  | -0.00009(4)  | 0.00194(5)  | -0.00003(4)  |
| **O1** | **O, O2-** | 0.3294(1)  | 0.22743(6)  | 0.17021(5)  | 0.9996(8) | 0.0180  | 0.0163(2)  | 0.0229(2)  | 0.0153(2)  | -0.0027(2)  | 0.0044(2)  | -0.0061(2)  |
| **O2** | **O, O2-** | 0.0118(2)  | 0  | 0.17033(7)  | 1.0005(8) | 0.0181  | 0.0242(3)  | 0.0138(3)  | 0.0150(3)  | 0 | -0.0002(2)  | 0 |
| **O3** | **O, O2-** | 0.13042(8)  | 0.16666(4)  | 0.39134(5)  | 0.9994(8) | 0.0099  | 0.0087(2)  | 0.0092(2)  | 0.0119(2)  | -0.0002(1)  | 0.0023(1)  | 0.0001(1)  |
| **O4** | **O, O2-** | 0.1327(1)  | ½ | 0.39878(6)  | 1.0000(7) | 0.0100  | 0.0088(2)  | 0.0099(2)  | 0.0115(2)  | 0  | 0.0019(2)  | 0  |
|  | **H** | 0.1053(1)  | ½ | 0.31745(6)  | 0.432(1) | 0.0100  | 0.0088(2)  | 0.0099(2)  | 0.0115(2)  | 0  | 0.0019(2)  | 0  |

**Sample EJ47\_2**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9900(4)  | 0.0274  | 0.0297(1)  | 0.0301(1)  | 0.02233(9)  | 0  | 0.00388(7)  | 0  |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9399(8)  | 0.0080  | 0.0069(1)  | 0.0065(1)  | 0.0110(1)  | 0  | 0.00255(7)  | 0  |
|  | **Fe2+** | 0 | 0 | ½ | 0.0611(5)  | 0.0080  | 0.0069(1)  | 0.0065(1)  | 0.0110(1)  | 0  | 0.00255(7)  | 0  |
| **M2** | **Mg2+** | 0  | 0.33221(1)  | ½ | 0.9338(8)  | 0.0082  | 0.00637(8)  | 0.00766(9)  | 0.01065(8)  | 0  | 0.00161(5)  | 0  |
|  | **Fe2+** | 0  | 0.33221(1)  | ½ | 0.0668(5)  | 0.0082  | 0.00637(8)  | 0.00766(9)  | 0.01065(8)  | 0  | 0.00161(5)  | 0  |
| **T** | **Si, Si4+** | 0.07607(2)  | 0.166712(9)  | 0.22798(1)  | 0.9754(9) | 0.0082  | 0.00779(5)  | 0.00778(5)  | 0.00904(5)  | -0.00005(2)  | 0.00157(3)  | -0.00001(2)  |
| **O1** | **O, O2-** | 0.33444(6)  | 0.22255(3)  | 0.17091(3)  | 0.9991(8) | 0.0170  | 0.0159(1)  | 0.0216(1)  | 0.0141(1)  | -0.00335(9)  | 0.00431(8)  | -0.00570(9)  |
| **O2** | **O, O2-** | 0.00212(9)  | 0  | 0.17121(4)  | 1.0021(8)  | 0.0171  | 0.0234(2)  | 0.0123(2)  | 0.0140(2)  | 0 | -0.0011(1)  | 0  |
| **O3** | **O, O2-** | 0.13091(5)  | 0.16686(2)  | 0.39251(3)  | 0.9983(8)  | 0.0104  | 0.0105(1)  | 0.0103(1)  | 0.0103(1)  | -0.00008(6)  | 0.00182(8)  | 0.00013(6)  |
| **O4** | **O, O2-** | 0.13283(7)  | ½ | 0.39989(4)  | 1.0001(8) | 0.0109  | 0.0106(1)  | 0.0121(1)  | 0.0100(1)  | 0 | 0.0015(1)  | 0 |
|  | **H** | 0.10375(7)  | ½ | 0.31499(4)  | 0.307(1) | 0.0109  | 0.0106(1)  | 0.0121(1)  | 0.0100(1)  | 0 | 0.0015(1)  | 0 |

**Sample EJ4\_2**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.963(3)  | 0.0324  | 0.036(2)  | 0.028(2)  | 0.034(2)  | 0 | 0.009(1)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.984(4)  | 0.0132  | 0.014(2)  | 0.005(1)  | 0.022(2)  | 0 | 0.004(1)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.016(3)  | 0.0132 | 0.014(2)  | 0.005(1)  | 0.022(2)  | 0 | 0.004(1)  | 0 |
| **M2** | **Mg2+** | 0  | 0.3321(2)  | ½ | 0.962(4)  | 0.0142  | 0.012(1)  | 0.007(1)  | 0.024(1)  | 0 | 0.0060(9)  | 0 |
|  | **Fe2+** | 0  | 0.3321(2)  | ½ | 0.038(4)  | 0.0142 | 0.012(1)  | 0.007(9)  | 0.024(1)  | 0 | 0.0060(9)  | 0 |
| **T** | **Si, Si4+** | 0.0750(3)  | 0.1668(1)  | 0.2251(2)  | 0.990(8) | 0.0117  | 0.0113(7)  | 0.0054(5)  | 0.0186(6)  | -0.0001(6)  | 0.0034(5)  | 0.0000(5)  |
| **O1** | **O, O2-** | 0.3217(7)  | 0.2344(4)  | 0.1672(4)  | 1.000(7) | 0.0214  | 0.024(2)  | 0.019(2)  | 0.023(2)  | -0.000(2)  | 0.008(2)  | -0.004(1)  |
| **O2** | **O, O2-** | 0.026(1)  | 0  | 0.1674(6)  | 1.000(7) | 0.0219  | 0.033(3)  | 0.009(2)  | 0.023(3)  | 0  | 0.005(2)  | 0  |
| **O3** | **O, O2-** | 0.1310(6)  | 0.1670(3)  | 0.3909(3)  | 1.000(7) | 0.0109  | 0.011(2)  | 0.003(1)  | 0.019(2)  | -0.000(1)  | 0.004(1)  | 0.001(1)  |
| **O4** | **F-** | 0.1311(9)  | ½ | 0.4017(4)  | 1.000(1) | 0.0164  | 0.020(2)  | 0.011(2)  | 0.018(2)  | 0  | 0.004(2)  | 0  |

 **Sample EJ6\_1**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9418(9)  | 0.0356  | 0.0309(8)  | 0.0338(9)  | 0.042(1)  | 0 | 0.0050(7)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9887(8)  | 0.0142  | 0.0084(7)  | 0.0105(8)  | 0.024(1)  | 0 | 0.0029(7)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.0112(7)  | 0.0142  | 0.0084(7)  | 0.0105(8)  | 0.024(1)  | 0 | 0.0029(7)  | 0 |
| **M2** | **Mg2+** | 0  | 0.3324(1)  | ½ | 0.9609(8)  | 0.0154  | 0.0093(5)  | 0.0137(6)  | 0.0233(7)  | 0 | 0.0032(4)  | 0 |
|  | **Fe2+** | 0  | 0.3324(1)  | ½ | 0.0391(8)  | 0.0154  | 0.0093(5)  | 0.0137(6)  | 0.0233(7)  | 0 | 0.0032(4)  | 0 |
| **T** | **Si, Si4+** | 0.0754(1)  | 0.16661(8)  | 0.22525(9)  | 0.995(1) | 0.0137  | 0.0094(3)  | 0.0118(3)  | 0.0199(4)  | 0.0001(3)  | 0.0020(2)  | -0.0003(2)  |
| **O1** | **O, O2-** | 0.3196(4)  | 0.2357(3)  | 0.1667(2)  | 0.9999(8) | 0.0224  | 0.0175(9)  | 0.025(1)  | 0.025(1)  | -0.0008(9)  | 0.0036(8)  | -0.0063(8)  |
| **O2** | **O, O2-** | 0.0269(6)  | 0  | 0.1665(3)  | 0.9998(8) | 0.0215  | 0.027(2)  | 0.015(1)  | 0.022(2)  | 0  | -0.001(1)  | 0  |
| **O3** | **O, O2-** | 0.1307(3)  | 0.1670(2)  | 0.3910(2)  | 1.0002(8) | 0.0133  | 0.0080(7)  | 0.0106(7)  | 0.0211(9)  | 0.0007(7)  | 0.0018(6)  | 0.0001(6)  |
| **O4** | **F-** | 0.1330(4)  | ½ | 0.4017(3)  | 0.9998(7) | 0.0179  | 0.013(1)  | 0.015(1)  | 0.025(1)  | 0  | 0.0035(9)  | 0  |

**Sample EJ12\_3**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9332(1)  | 0.0295  | 0.0299(4)  | 0.0293(4)  | 0.0294(4)  | 0 | 0.0057(3)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9854(1)  | 0.0102  | 0.0100(4)  | 0.0070(4)  | 0.0142(4)  | 0 | 0.0039(3)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.0136(1)  | 0.0102  | 0.0100(4)  | 0.0070(4)  | 0.0142(4)  | 0 | 0.0039(3)  | 0 |
| **M2** | **Mg2+** | 0  | 0.33224(7)  | ½ | 0.9689(1)  | 0.0104  | 0.0080(2)  | 0.0091(3)  | 0.0144(3)  | 0 | 0.0026(2)  | 0 |
|  | **Fe2+** | 0  | 0.33224(7)  | ½ | 0.0307(1)  | 0.0104  | 0.0080(2)  | 0.0091(3)  | 0.0144(3)  | 0 | 0.0026(2)  | 0 |
| **T** | **Si, Si4+** | 0.07539(7)  | 0.16670(4)  | 0.22528(4)  | 0.9934(1) | 0.0087 | 0.0082(1)  | 0.0070(2)  | 0.0113(2)  | 0.0002(1)  | 0.0024(1)  | -0.0002(1)  |
| **O1** | **O, O2-** | 0.3194(2)  | 0.2363(2)  | 0.1667(1)  | 1.0001(1) | 0.0176  | 0.0160(4)  | 0.0220(5)  | 0.0152(5)  | -0.0007(4)  | 0.0042(4)  | -0.0067(4)  |
| **O2** | **O, O2-** | 0.0275(4)  | 0  | 0.1669(2)  | 1.0005(1) | 0.0177  | 0.0260(8)  | 0.0102(6)  | 0.0166(7)  | 0  | 0.0025(6)  | 0  |
| **O3** | **O, O2-** | 0.1304(2)  | 0.1669(1)  | 0.3906(1)  | 1.0003(1) | 0.0091  | 0.0083(3)  | 0.0085(4)  | 0.0108(4)  | -0.0002(3)  | 0.0021(3)  | 0.0007(3)  |
| **O4** | **F-** | 0.1331(2)  | ½ | 0.4020(1)  | 0.9992(1) | 0.0118  | 0.0104(5)  | 0.0105(5)  | 0.0143(5)  | 0  | 0.0020(4)  | 0  |

**Sample EJ13\_1**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9414(1)  | 0.0348  | 0.0336(4)  | 0.0343(5)  | 0.0364(5)  | 0 | 0.0063(3)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.9991(1)  | 0.0132  | 0.0100(4)  | 0.0100(4)  | 0.0199(4)  | 0 | 0.0035(3)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.0001(1)  | 0.0132  | 0.0100(4)  | 0.0100(4)  | 0.0199(4)  | 0 | 0.0035(3)  | 0 |
| **M2** | **Mg2+** | 0  | 0.33238(8)  | ½ | 0.9694(1)  | 0.0141  | 0.0100(3)  | 0.0124(3)  | 0.0200(3)  | 0 | 0.0031(2)  | 0 |
|  | **Fe2+** | 0  | 0.33238(8)  | ½ | 0.0308(1)  | 0.0141  | 0.0100(3)  | 0.0124(3)  | 0.0200(3)  | 0 | 0.0031(2)  | 0 |
| **T** | **Si, Si4+** | 0.07526(7)  | 0.16666(4)  | 0.22509(4)  | 0.9963(1) | 0.0132  | 0.0109(2)  | 0.0109(2)  | 0.0181(2)  | -0.0002(1)  | 0.0032(1)  | -0.0000(1)  |
| **O1** | **O, O2-** | 0.3199(2)  | 0.2357(2)  | 0.1666(1)  | 1.0002(1) | 0.0221  | 0.0186(5)  | 0.0253(6)  | 0.0227(5)  | -0.0015(4)  | 0.0046(4)  | -0.0062(4)  |
| **O2** | **O, O2-** | 0.0263(4)  | 0  | 0.1666(2)  | 1.0001(1) | 0.0220  | 0.0274(8)  | 0.0156(7)  | 0.0223(7)  | 0  | 0.0023(6)  | 0  |
| **O3** | **O, O2-** | 0.1304(2)  | 0.1667(1)  | 0.3906(1)  | 1.0004(1) | 0.0131  | 0.0107(4)  | 0.0110(4)  | 0.0178(4)  | 0.0000(3)  | 0.0030(3)  | 0.0003(3)  |
| **O4** | **F-** | 0.1332(2)  | ½ | 0.4023(1)  | 0.9976(1) | 0.0156  | 0.0126(5)  | 0.0134(5)  | 0.0210(6)  | 0  | 0.0033(4)  | 0  |

**Sample EJ72\_1**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9948(6) | 0.0315 | 0.0329(2)  | 0.0320(2)  | 0.0295(2)  | 0 | 0.0050(1)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.8114(8) | 0.0100 | 0.0091(2)  | 0.0075(2)  | 0.0138(2)  | 0  | 0.0032(1)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.1884(5) | 0.0100 | 0.0091(2)  | 0.0075(2)  | 0.0138(2)  | 0 | 0.0032(1)  | 0 |
| **M2** | **Mg2+** | 0 | 0.33462(3) | ½ | 0.8037(8) | 0.0109 | 0.0083(1)  | 0.0118(1)  | 0.0126(1)  | 0 | 0.00172(8)  | 0 |
|  | **Fe2+** | 0 | 0.33462(3) | ½ | 0.1964(6) | 0.0109 | 0.0083(1)  | 0.0118(1)  | 0.0126(1)  | 0 | 0.00172(8)  | 0  |
| **T** | **Si, Si4+** | 0.07554(3) | 0.16681(2) | 0.22679(2) | 0.9826(9) | 0.0097 | 0.00927(8)  | 0.00846(8)  | 0.01140(8)  | -0.00013(5)  | 0.00187(5)  | 0.00004(5)  |
| **O1** | **O, O2-** | 0.3296(1) | 0.22662(7) | 0.16935(5) | 0.9998(8) | 0.0188 | 0.0178(2)  | 0.0237(3)  | 0.0155(2)  | -0.0030(2)  | 0.0044(2)  | -0.0065(2)  |
| **O2** | **O, O2-** | 0.0095(2) | 0 | 0.17000(8) | 1.0002(8) | 0.0188 | 0.0262(4)  | 0.0129(3)  | 0.0160(3)  | 0  | -0.0003(3)  | 0  |
| **O3** | **O, O2-** | 0.1309(1) | 0.16735(5) | 0.39166(5) | 0.9997(8) | 0.0114 | 0.0117(2)  | 0.0107(2)  | 0.0117(2)  | -0.0001(1)  | 0.0022(1)  | 0.0002(1)  |
| **O4** | **O, O2-** | 0.1318(1) | ½ | 0.39890(7) | 1.0001(7) | 0.0121 | 0.0120(2)  | 0.0125(3)  | 0.0118(2)  | 0  | 0.0021(2)  | 0  |
|  | **H** | 0.1059(1) | ½ | 0.32195(7) | 0.569(1) | 0.0121 | 0.0120(2)  | 0.0125(3)  | 0.0118(2)  | 0  | 0.0021(2)  | 0  |

**Sample EJ72\_3**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9904(7)  | 0.0338  | 0.0347(4)  | 0.0333(4)  | 0.0336(4)  | 0 | 0.0066(3)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.8144(8)  | 0.0121  | 0.0107(3)  | 0.0081(2)  | 0.0183(3)  | 0 | 0.0046(2)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.1863(6)  | 0.0121  | 0.0107(3)  | 0.0081(2)  | 0.0183(3)  | 0 | 0.0046(2)  | 0 |
| **M2** | **Mg2+** | 0  | 0.33463(5)  | ½ | 0.8055(8)  | 0.0130  | 0.0097(2)  | 0.0127(2)  | 0.0169(2)  | 0 | 0.0032(1)  | 0 |
|  | **Fe2+** | 0  | 0.33463(5)  | ½ | 0.1948(7)  | 0.0130  | 0.0097(2)  | 0.0127(2)  | 0.0169(2)  | 0 | 0.0032(1)  | 0 |
| **T** | **Si, Si4+** | 0.07553(6)  | 0.16682(3)  | 0.22689(3)  | 0.9832(9)  | 0.0120  | 0.0112(1)  | 0.0095(1)  | 0.0156(1)  | -0.0000(1)  | 0.00333(9)  | -0.00003(9)  |
| **O1** | **O, O2-** | 0.3293(2)  | 0.2270(1)  | 0.1694(1)  | 1.0003(8)  | 0.0216  | 0.0200(4)  | 0.0250(4)  | 0.0206(4)  | -0.0030(3)  | 0.0056(3)  | -0.0065(3)  |
| **O2** | **O, O2-** | 0.0106(3)  | 0  | 0.1700(1)  | 0.9998(8)  | 0.0212  | 0.0282(7)  | 0.0139(5)  | 0.0202(6)  | 0  | 0.0009(5)  | 0  |
| **O3** | **O, O2-** | 0.1307(2)  | 0.16735(9)  | 0.39173(9)  | 0.9997(8)  | 0.0134  | 0.0130(3)  | 0.0114(3)  | 0.0161(3)  | -0.0001(3)  | 0.0035(2)  | 0.0000(2)  |
| **O4** | **O, O2-** | 0.1319(2)  | ½ | 0.3988(1)  | 1.0007(8)  | 0.0144  | 0.0141(5)  | 0.0137(4)  | 0.0156(5)  | 0 | 0.0034(4)  | 0 |
|  | **H** | 0.1162(2)  | ½ | 0.3204(1)  | 0.729(1)  | 0.0144  | 0.0141(5)  | 0.0137(4)  | 0.0156(5)  | 0 | 0.0034(4)  | 0 |

**Sample EJ72\_4**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9953(7)  | 0.0319  | 0.0318(3)  | 0.0322(3)  | 0.0314(3)  | 0 | 0.0050(2)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.8054(8)  | 0.0099  | 0.0078(2)  | 0.0071(2)  | 0.0151(2)  | 0 | 0.0030(1)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.1954(6)  | 0.0099  | 0.0078(2)  | 0.0071(2)  | 0.0151(2)  | 0 | 0.0030(1)  | 0 |
| **M2** | **Mg2+** | 0  | 0.33476(4)  | ½ | 0.7975(8)  | 0.0107  | 0.0068(1)  | 0.0116(1)  | 0.0136(2)  | 0 | 0.00136(9)  | 0 |
|  | **Fe2+** | 0  | 0.33476(4)  | ½ | 0.2028(7)  | 0.0107  | 0.0068(1)  | 0.0116(1)  | 0.0136(2)  | 0 | 0.00136(9)  | 0 |
| **T** | **Si, Si4+** | 0.07541(4)  | 0.16685(3)  | 0.22678(3)  | 0.9877(9)  | 0.0097  | 0.00839(9)  | 0.00818(9)  | 0.0126(1)  | -0.00014(8)  | 0.00172(7)  | -0.00013(8)  |
| **O1** | **O, O2-** | 0.3289(2)  | 0.2272(1)  | 0.16921(8)  | 0.9999(8)  | 0.0189  | 0.0169(3)  | 0.0234(4)  | 0.0170(3)  | -0.0027(3)  | 0.0043(2)  | -0.0062(3)  |
| **O2** | **O, O2-** | 0.0106(2)  | 0  | 0.1701(1)  | 1.0000(8)  | 0.0192  | 0.0259(5)  | 0.0129(4)  | 0.0173(4)  | 0  | 0.0000(4)  | 0  |
| **O3** | **O, O2-** | 0.1307(1)  | 0.16735(7)  | 0.39169(7)  | 0.9999(8)  | 0.0110  | 0.0099(2)  | 0.0102(2)  | 0.0129(2)  | -0.0001(2)  | 0.0021(2)  | 0.0001(2)  |
| **O4** | **O, O2-** | 0.1319(2)  | ½ | 0.3988(1)  | 1.0004(8)  | 0.0120  | 0.0105(3)  | 0.0124(3)  | 0.0130(4)  | 0 | 0.0018(3)  | 0 |
|  | **H** | 0.1068(2)  | ½ | 0.3205(1)  | 0.530(1)  | 0.0120  | 0.0105(3)  | 0.0124(3)  | 0.0130(4)  | 0 | 0.0018(3)  | 0 |

**Sample EJ72\_6**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Site** | **Atom** | **x/a** | **y/b** | **z/c** | **Occupancy** | **Uiso/equiv** | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| **K** | **K+** | 0 | ½ | 0 | 0.9873(8)  | 0.0326  | 0.0327(4)  | 0.0337(4)  | 0.0315(4)  | 0 | 0.0059(3)  | 0 |
| **M1** | **Mg2+** | 0 | 0 | ½ | 0.7941(8)  | 0.0110  | 0.0088(2)  | 0.0092(2)  | 0.0157(3)  | 0 | 0.0042(2)  | 0 |
|  | **Fe2+** | 0 | 0 | ½ | 0.2060(6)  | 0.0110  | 0.0088(2)  | 0.0092(2)  | 0.0157(3)  | 0 | 0.0042(2)  | 0 |
| **M2** | **Mg2+** | 0 | 0.33482(5)  | ½ | 0.7900(8)  | 0.0118  | 0.0076(2)  | 0.0136(2)  | 0.0142(2)  | 0 | 0.0022(1)  | 0 |
|  | **Fe2+** | 0  | 0.33482(5)  | ½ | 0.2101(7)  | 0.0118  | 0.0076(2)  | 0.0136(2)  | 0.0142(2)  | 0 | 0.0022(1)  | 0 |
| **T** | **Si, Si4+** | 0.07549(6)  | 0.16678(3)  | 0.22679(3)  | 0.9842(9)  | 0.0104  | 0.0086(1)  | 0.0101(1)  | 0.0126(1)  | -0.00020(9)  | 0.00252(9)  | -0.00015(9)  |
| **O1** | **O, O2-** | 0.3293(2)  | 0.2270(1)  | 0.1693(1)  | 1.0000(8) | 0.0199  | 0.0172(4)  | 0.0256(5)  | 0.0174(4)  | -0.0027(3)  | 0.0049(3)  | -0.0060(3)  |
| **O2** | **O, O2-** | 0.0107(3)  | 0  | 0.1700(1)  | 1.0000(8) | 0.0199  | 0.0266(6)  | 0.0151(5)  | 0.0166(5)  | 0  | 0.0000(4)  | 0  |
| **O3** | **O, O2-** | 0.1307(2)  | 0.16731(9)  | 0.39171(9)  | 1.0001(8) | 0.0119  | 0.0109(3)  | 0.0120(3)  | 0.0131(3)  | 0.0001(2)  | 0.0032(2)  | 0.0003(2)  |
| **O4** | **O, O2-** | 0.1322(2)  | ½ | 0.3988(1)  | 1.0005(8) | 0.0127  | 0.0114(4)  | 0.0139(4)  | 0.0130(4)  | 0 | 0.0026(3)  | 0 |
|  | **H** | 0.1126(2)  | ½ | 0.3283(1)  | 0.716(1) | 0.0127  | 0.0114(4)  | 0.0139(4)  | 0.0130(4)  | 0 | 0.0026(3)  | 0 |

**Supplemental Data Table 2**

Selected bond distances (Å) of the study micas

|  |  |
| --- | --- |
|  | **1631 Eruption**  |
|  | **EJ20\_1** | **EJ20\_2** | **EJ20\_3** | **EJ25\_2** | **EJ25\_3** | **EJ42\_2** | **EJ42\_3** | **EJ42\_4** | **EJ47\_2** |
| **T-O1**  | 1.6598(4) | 1.6596(6) | 1.6584(5) | 1.660(2) | 1.660(1) | 1.6617(3) | 1.6604(4) | 1.6605(5) | 1.6623(3) |
| **T-O1'** | 1.6597(4) | 1.6599(6) | 1.6600(5) | 1.657(2) | 1.661(1) | 1.6620(3) | 1.6611(4) | 1.6612(5) | 1.6623(3) |
| **T-O2** | 1.6597(2) | 1.6602(3) | 1.6594(3) | 1.657(1) | 1.6597(8) | 1.6622(2) | 1.6604(2) | 1.6605(3) | 1.6614(2) |
| **T-O3** | 1.6558(4) | 1.6549(5) | 1.6546(5) | 1.666(2) | 1.658(1) | 1.6528(3) | 1.6518(4) | 1.6503(5) | 1.6616(3) |
| **<T-O>** | 1.6590(7) | 1.659(1) | 1.6580(9) | 1.660(4) | 1.660(2) | 1.6600(6) | 1.6580(7) | 1.6580(9) | 1.6620(6) |
|  |  |  |  |  |  |  |  |  |  |
| **M1-O4(x2)** | 2.0466(4) | 2.0459(6) | 2.0453(6) | 2.032(2) | 2.037(1) | 2.0470(4) | 2.0503(5) | 2.0481(6) | 2.0397(4) |
| **M1-O3(x4)** | 2.0846(3) | 2.0843(4) | 2.0848(4) | 2.075(2) | 2.081(1) | 2.0839(3) | 2.0856(3) | 2.0858(4) | 2.0767(2) |
| **<M1-O>** | 2.0720(5) | 2.0720(7) | 2.0720(7) | 2.061(3) | 2.066(1) | 2.0720(5) | 2.0740(6) | 2.0730(7) | 2.0640(4) |
|  |  |  |  |  |  |  |  |  |  |
| **M2-O4(x2)** | 2.0573(3) | 2.0575(5) | 2.0551(4) | 2.049(2) | 2.047(1) | 2.0570(3) | 2.0570(3) | 2.0574(4) | 2.0439(3) |
| **M2-O3(x2)** | 2.0718(3) | 2.0717(5) | 2.0721(4) | 2.058(2) | 2.065(1) | 2.0722(3) | 2.0763(3) | 2.0755(5) | 2.0664(3) |
| **M2-O3'(x2)** | 2.0823(3) | 2.0826(5) | 2.0830(4) | 2.076(2) | 2.079(1) | 2.0838(3) | 2.0853(3) | 2.0858(5) | 2.0752(3) |
| **<M2-O>** | 2.0700(5) | 2.0710(9) | 2.0700(7) | 2.061(3) | 2.064(2) | 2.0710(5) | 2.0730(5) | 2.0730(8) | 2.0620(5) |
|  |  |  |  |  |  |  |  |  |  |
| **<M-O>** | 2.0710(7) | 2.071(1) | 2.071(1) | 2.061(4) | 2.065(2) | 2.0710(7) | 2.0730(8) | 2.073(1) | 2.0630(7) |
|  |  |  |  |  |  |  |  |  |  |
| **K-O1(x4)** | 2.9619(4) | 2.9614(6) | 2.9623(5) | 2.938(2) | 2.943(1) | 2.9587(3) | 2.9685(4) | 2.9691(5) | 2.9251(3) |
| **K-O1'(x4)** | 3.3695(5) | 3.3707(6) | 3.3689(5) | 3.379(2) | 3.380(1) | 3.3848(4) | 3.3739(5) | 3.3720(6) | 3.4127(3) |
| **K-O2 (x2)** | 2.9616(6) | 2.9598(9) | 2.9611(7) | 2.937(3) | 2.945(2) | 2.9577(5) | 2.9691(6) | 2.9705(8) | 2.9271(4) |
| **K-O2'(x2)** | 3.3686(6) | 3.3703(9) | 3.3688(8) | 3.384(3) | 3.379(2) | 3.3858(5) | 3.3752(7) | 3.3718(8) | 3.4156(5) |
| **<K-O>inner** | 2.9620(7) | 2.961(1) | 2.9620(9) | 2.938(4) | 2.944(2) | 2.9580(6) | 2.9690(7) | 2.9700(9) | 2.9260(5) |
| **<K-O>outer** | 3.3690(8) | 3.371(1) | 3.3690(9) | 3.381(4) | 3.380(2) | 3.3850(6) | 3.3740(9) | 3.372(1) | 3.4140(6) |
| **<K-O>** | 3.166(1) | 3.166(2) | 3.166(1) | 3.160(5) | 3.162(3) | 3.1720(9) | 3.172(1) | 3.171(1) | 3.1700(8) |

**Supplemental Data Table 2**

continuation

|  |  |  |
| --- | --- | --- |
|  | **1872 Eruption** | **1944 Eruption** |
|  | **EJ4\_2** | **EJ6\_1** | **EJ12\_3** | **EJ13\_1** | **EJ72\_1** | **EJ72\_3** | **EJ72\_4** | **EJ72\_6** |
| **T-O1** | 1.644(4) | 1.651(2) | 1.646(1) | 1.647(1) | 1.6619(6) | 1.661(1) | 1.6603(8) | 1.661(1) |
| **T-O1'** | 1.649(4) | 1.646(2) | 1.647(1) | 1.648(1) | 1.6615(6) | 1.660(1) | 1.6610(8) | 1.662(1) |
| **T-O2** | 1.647(2) | 1.648(2) | 1.6468(7) | 1.6479(8) | 1.6614(3) | 1.6603(6) | 1.6600(5) | 1.6597(6) |
| **T-O3** | 1.656(4) | 1.656(2) | 1.651(1) | 1.652(1) | 1.6630(5) | 1.6633(9) | 1.6632(7) | 1.6620(9) |
| **<T-O>** | 1.649(7) | 1.650(4) | 1.648(2) | 1.649(2) | 1.662(1) | 1.661(2) | 1.661(1) | 1.661(2) |
|  |  |  |  |  |  |  |  |  |
| **M1-O4(x2)** | 2.035(4) | 2.029(2) | 2.026(1) | 2.025(1) | 2.0531(7) | 2.052(1) | 2.0517(9) | 2.051(1) |
| **M1-O3(x4)** | 2.083(3) | 2.082(2) | 2.082(1) | 2.081(1) | 2.0908(5) | 2.0892(8) | 2.0900(7) | 2.0893(8) |
| **<M1-O>** | 2.067(5) | 2.064(3) | 2.063(1) | 2.062(1) | 2.0780(9) | 2.077(1) | 2.077(1) | 2.077(1) |
|  |  |  |  |  |  |  |  |  |
| **M2-O4(x2)** | 2.027(3) | 2.029(2) | 2.028(1) | 2.026(1) | 2.0364(5) | 2.0364(9) | 2.0365(7) | 2.0358(9) |
| **M2-O3(x2)** | 2.070(4) | 2.071(2) | 2.071(1) | 2.074(1) | 2.0836(5) | 2.0831(8) | 2.0831(6) | 2.0836(9) |
| **M2-O3'(x2)** | 2.073(3) | 2.078(2) | 2.079(1) | 2.079(1) | 2.0902(5) | 2.0887(9) | 2.0903(7) | 2.0906(9) |
| **<M2-O>** | 2.057(6) | 2.059(3) | 2.059(2) | 2.060(2) | 2.0700(9) | 2.069(2) | 2.070(1) | 2.070(2) |
|  |  |  |  |  |  |  |  |  |
| **<M-O>** | 2.060(8) | 2.061(4) | 2.060(2) | 2.061(2) | 2.073(1) | 2.072(2) | 2.072(2) | 2.072(2) |
|  |  |  |  |  |  |  |  |  |
|  **K-O1(x4)** | 2.998(4) | 3.007(3) | 3.011(3) | 3.006(1) | 2.9584(6) | 2.961(1) | 2.9626(9) | 2.960(1) |
| **K-O1'(x4)** | 3.278(4) | 3.264(2) | 3.258(1) | 3.263(1) | 3.3762(6) | 3.372(1) | 3.3686(9) | 3.371(1) |
| **K-O2 (x2)** | 3.001(6) | 3.007(3) | 3.009(2) | 3.002(2) | 2.9598(8) | 2.963(2) | 2.963(1) | 2.964(2) |
| **K-O2'(x2)** | 3.276(6) | 3.264(3) | 3.263(2) | 3.266(2) | 3.3826(9) | 3.376(2) | 3.379(1) | 3.377(2) |
| **<K-O>inner** | 2.999(7) | 3.007(4) | 3.010(4) | 3.005(2) | 2.959(1) | 2.962(2) | 2.963(1) | 2.961(2) |
| **<K-O>outer** | 3.277(7) | 3.264(4) | 3.260(2) | 3.264(2) | 3.378(1) | 3.373(2) | 3.372(1) | 3.373(2) |
| **<K-O>** | 3.14(1) | 3.136(6) | 3.135(4) | 3.135(3) | 3.169(1) | 3.168(3) | 3.168(2) | 3.167(3) |

**Supplemental Data Table 3**

Selected distortion parameters derived from the structure refinements of the study micas

|  |
| --- |
| **Eruption 1631** |
|  | **EJ20\_1** | **EJ20\_2** | **EJ20\_3** | **EJ25\_2** | **EJ25\_3** | **EJ42\_2** | **EJ42\_3** | **EJ42\_4** | **EJ47\_2** |
| **t tet [Å]** | 2.236 | 2.235 | 2.235 | 2.243 | 2.238 | 2.237 | 2.236 | 2.236 | 2.237 |
| BLDT | 0.110 | 0.121 | 0.116 | 0.181 | 0.040 | 0.214 | 0.218 | 0.244 | 0.031 |
| **VolumeT [Å3]** | 2.341 | 2.341 | 2.338 | 2.346 | 2.346 | 2.344 | 2.339 | 2.338 | 2.355 |
| TQE | 1.0003 | 1.0003 | 1.0003 | 1.0003 | 1.0003 | 1.0004 | 1.0004 | 1.0004 | 1.0002 |
| TAV[°] | 1.497 | 1.452 | 1.489 | 1.211 | 1.297 | 1.783 | 1.847 | 1.988 | 0.977 |
| **τ [°]** | 110.50 | 110.48 | 110.50 | 110.37 | 110.41 | 110.61 | 110.63 | 110.68 | 110.26 |
| **α[°]** | 8.97 | 9.02 | 8.96 | 9.76 | 9.61 | 9.42 | 8.95 | 8.89 | 10.76 |
| **Δz [Å]** | -0.001 | 0.000 | 0.000 | 0.003 | 0.000 | 0.000 | 0.002 | 0.001 | 0.003 |
| **D.M. [Å]** | 0.542 | 0.544 | 0.542 | 0.584 | 0.577 | 0.545 | 0.529 | 0.528 | 0.604 |
| **ψM(1) [°]** | 58.94 | 58.94 | 58.94 | 59.16 | 59.16 | 58.83 | 58.81 | 58.79 | 59.09 |
| **ψM(2) [°]** | 58.91 | 58.92 | 58.91 | 59.16 | 59.11 | 58.82 | 58.76 | 58.78 | 59.04 |
| **BLDM(1)** | 0.829 | 0.839 | 0.852 | 0.930 | 0.943 | 0.792 | 0.792 | 0.821 | 0.797 |
| **ELDM(1)** | 5.052 | 5.054 | 5.054 | 5.311 | 5.306 | 4.927 | 4.897 | 4.880 | 5.222 |
| **BLDM(2)** | 0.431 | 0.425 | 0.486 | 0.479 | 0.540 | 0.441 | 0.497 | 0.505 | 0.581 |
| **ELDM(2)** | 5.018 | 5.029 | 5.014 | 5.305 | 5.245 | 4.910 | 4.843 | 4.864 | 5.164 |
| **ShiftM(2) [Å]** | -0.019 | -0.019 | -0.019 | -0.020 | -0.020 | -0.016 | -0.012 | -0.014 | -0.010 |
| **Volume M(1) [Å]** | 11.663 | 11.656 | 11.657 | 11.448 | 11.546 | 11.670 | 11.727 | 11.702 | 11.527 |
| **OQEM(1)** | 1.011 | 1.011 | 1.011 | 1.013 | 1.013 | 1.011 | 1.011 | 1.011 | 1.012 |
| **OAVM(1)[°]** | 37.034 | 37.022 | 37.093 | 40.736 | 40.882 | 35.096 | 34.625 | 34.463 | 39.380 |
| **Volume M(2) [Å3]** | 11.638 | 11.638 | 11.628 | 11.446 | 11.500 | 11.658 | 11.686 | 11.691 | 11.483 |
| **OQEM(2)** | 1.011 | 1.011 | 1.0113 | 1.013 | 1.012 | 1.011 | 1.010 | 1.011 | 1.012 |
| **OAVM(2)[°]** | 37.146 | 37.310 | 37.186 | 41.500 | 40.782 | 35.431 | 34.364 | 34.779 | 38.959 |
| **euM(1)/esM(1)** | 1.106 | 1.107 | 1.107 | 1.112 | 1.112 | 1.104 | 1.103 | 1.102 | 1.110 |
| **euM(2)/esM(2)** | 1.106 | 1.106 | 1.106 | 1.112 | 1.111 | 1.103 | 1.102 | 1.102 | 1.109 |
| **t oct [Å]** | 2.138 | 2.138 | 2.138 | 2.113 | 2.119 | 2.145 | 2.149 | 2.149 | 2.121 |
| **t int [Å]** | 3.422 | 3.422 | 3.423 | 3.419 | 3.416 | 3.451 | 3.447 | 3.444 | 3.454 |
| **ΔK-O [Å]** | 0.407 | 0.410 | 0.407 | 0.443 | 0.436 | 0.427 | 0.406 | 0.403 | 0.487 |
| **t K-O4 [Å]** | 3.965 | 3.964 | 3.968 | 3.971 | 3.974 | 3.976 | 3.971 | 3.974 | 3.978 |

**Supplemental Data Table 3**

continuation

|  |  |  |
| --- | --- | --- |
|  | **1872 Eruption** | **1944 Eruption** |
|  | **EJ4\_2** | **EJ6\_1** | **EJ12\_3** | **EJ13\_1** | **EJ72\_1** | **EJ72\_3** | **EJ72\_4** | **EJ72\_6** |
| **t tet [Å]** | 2.234 | 2.242 | 2.236 | 2.236 | 2.240 | 2.241 | 2.241 | 2.239 |
| BLDT | 0.221 | 0.188 | 0.096 | 0.093 | 0.042 | 0.062 | 0.063 | 0.042 |
| **VolumeT [Å3]** | 2.299 | 2.304 | 2.295 | 2.298 | 2.355 | 2.350 | 2.351 | 2.351 |
| TQE | 1.0004 | 1.0006 | 1.0006 | 1.0005 | 1.0002 | 1.0003 | 1.0003 | 1.0002 |
| TAV[°] | 1.641 | 2.472 | 2.362 | 2.230 | 1.090 | 1.221 | 1.200 | 1.122 |
| **τ [°]** | 110.54 | 110.49 | 110.79 | 110.75 | 110.32 | 110.38 | 110.37 | 110.33 |
| **α[°]** | 6.10 | 5.64 | 5.48 | 5.70 | 9.22 | 9.05 | 8.99 | 9.04 |
| **Δz [Å]** | 0.002 | -0.002 | 0.002 | 0.000 | 0.006 | 0.006 | 0.009 | 0.007 |
| **D.M. [Å]** | 0.508 | 0.502 | 0.495 | 0.503 | 0.555 | 0.547 | 0.548 | 0.552 |
| **ψM(1) [°]** | 58.36 | 59.31 | 59.26 | 59.30 | 59.07 | 59.03 | 59.05 | 59.06 |
| **ψM(2) [°]** | 59.19 | 59.23 | 59.19 | 59.25 | 58.93 | 58.90 | 58.92 | 58.96 |
| **BLDM(1)** | 1.026 | 1.115 | 1.208 | 1.206 | 0.805 | 0.813 | 0.827 | 0.812 |
| **ELDM(1)** | 5.540 | 5.492 | 5.427 | 5.472 | 5.205 | 5.153 | 5.177 | 5.193 |
| **BLDM(2)** | 0.973 | 0.979 | 1.003 | 1.092 | 1.073 | 1.054 | 1.091 | 1.096 |
| **ELDM(2)** | 5.337 | 5.388 | 5.342 | 5.413 | 5.039 | 5.001 | 5.025 | 5.068 |
| **ShiftM(2) [Å]** | -0.011 | -0.009 | -0.010 | -0.009 | 0.012 | 0.012 | 0.013 | 0.014 |
| **VolumeM(1) [Å]** | 11.540 | 11.491 | 11.484 | 11.458 | 11.756 | 11.741 | 11.743 | 11.727 |
| **OQEM(1)** | 1.014 | 1.014 | 1.013 | 1.0137 | 1.012 | 1.012 | 1.012 | 1.012 |
| **OAVM(1)[°]** | 44.909 | 43.954 | 43.066 | 43.893 | 39.039 | 38.221 | 38.620 | 38.862 |
| **VolumeM(2) [Å3]** | 11.384 | 11.413 | 11.421 | 11.416 | 11.626 | 11.622 | 11.625 | 11.630 |
| **OQEM(2)** | 1.013 | 1.013 | 1.013 | 1.0135 | 1.011 | 1.011 | 1.011 | 1.011 |
| **OAVM(2)[°]** | 42.466 | 43.039 | 42.566 | 43.704 | 36.898 | 36.366 | 36.692 | 37.299 |
| **euM(1)/esM(1)** | 1.117 | 1.116 | 1.115 | 1.116 | 1.110 | 1.109 | 1.109 | 1.110 |
| **euM(2)/esM(2)** | 1.113 | 1.114 | 1.113 | 1.115 | 1.106 | 1.105 | 1.106 | 1.107 |
| **t oct [Å]** | 2.107 | 2.107 | 2.110 | 2.106 | 2.136 | 2.138 | 2.137 | 2.135 |
| **t int [Å]** | 3.341 | 3.330 | 3.331 | 3.325 | 3.421 | 3.423 | 3.419 | 3.417 |
| **ΔK-O [Å]** | 0.277 | 0.257 | 0.249 | 0.259 | 0.420 | 0.411 | 0.409 | 0.412 |
| **t K-O4 [Å]** | 3.949 | 3.953 | 3.954 | 3.953 | 3.962 | 3.963 | 3.960 | 3.958 |

Notes.ttet: tetrahedral sheet thickness calculated from z coordinates of basal and apical O atoms; TQE: tetrahedral quadratic elongation (Robinson et al. 1971); TAV: tetrahedral angle variance (Robinson et al. 1971); τ: tetrahedral flattening angle; α: tetrahedral rotation angle (Hazen and Burnham 1973); Δ*z*: departure from complanarity of the basal O atoms (Güven 1971); D.M.: dimensional misfit between tetrahedral and octahedral sheets (Toraya 1981); ψ: octahedral flattening angles (Donnay et al. 1964a, 1964b); BLD: bond-length distortions (Renner and Lehmann 1986); ELD: edge-length distortion (Renner and Lehmann 1986); ShiftM(2): off-center shift of the M2 cation defined as the distance between the refined position of cation and the geometrical center of M2 site (coordinates: x/a = 0.0, y/b = 0.8333, z/c = 0.5); OQE: octahedral quadratic elongation (Robinson et al.1971); OAV: octahedral angle variance (Robinson et al. 1971); eu, es: mean lengths of unshared and shared edges, respectively (Toraya 1981); toct: octahedral sheet thickness (Toraya 1981); tint calculated from the z coordinates of basal O atoms; ΔK-O = <K-O>outer-<K-O>inner; tK-O4: projection of K-O4 distance along c\*.

Errors on distortion parameters, estimated by varying the refined positional parameters within one standard deviation are in the following ranges: < 0.5% for volumes, thicknesses, projected bond lengths, shifts; 0.1-13% for angles, bond/edge lengths distortions, sheet corrugations, D.M., ΔK-O.

**Supplemental Data Table 4**

 Mean atomic numbers (electrons, e-) of cation sites, octahedral and tetrahedral mean distances (Å), as determined by structure refinements (X-ref) and chemical analyses (EPMA) of the study micas. Average error for mean atomic numbers is ± 0.5 e-

|  |  |
| --- | --- |
|  | **1631 Eruption**  |
|  | **EJ20\_1** | **EJ20\_2** | **EJ20\_3** | **EJ25\_2** | **EJ25\_3** | **EJ42\_2** | **EJ42\_3** | **EJ42\_4** | **EJ47\_2** |
| **e- (M1) X-ref** | 13.42 | 13.45 | 13.40 | 12.42 | 13.17 | 12.31 | 13.08 | 12.74 | 12.87 |
| **e- (M2) X-ref** | 13.38 | 13.41 | 13.46 | 12.63 | 13.01 | 12.35 | 13.07 | 12.72 | 12.94 |
|  |  |  |  |  |  |  |  |  |  |
| **e- (M1+2M2) X-ref** | 40.18 | 40.31 | 40.32 | 37.68 | 39.19 | 37.01 | 39.22 | 38.18 | 38.75 |
| **e- (M1+2M2) EPMA** | 41.30 | 40.76 | 41.18 | 37.87 | 38.59 | 37.85 | 40.79 | 39.13 | 39.48 |
|  |  |  |  |  |  |  |  |  |  |
| **K e- X-ref** | 17.86 | 17.86 | 17.98 | 18.29 | 18.24 | 18.67 | 18.40 | 18.54 | 18.81 |
| **K e- EPMA** | 18.33 | 18.44 | 18.25 | 19.16 | 18.33 | 18.95 | 18.19 | 18.38 | 19.24 |
|  |  |  |  |  |  |  |  |  |  |
| **T e- X-ref** | 13.60 | 13.62 | 13.64 | 13.72 | 13.69 | 13.66 | 13.67 | 13.74 | 13.66 |
| **T e- EPMA** | 13.71 | 13.72 | 13.72 | 13.70 | 13.70 | 13.73 | 13.72 | 13.70 | 13.68 |
|  |  |  |  |  |  |  |  |  |  |
| **Σ+  EPMA** | 22.11 | 22.15 | 22.16 | 22.14 | 22.14 | 22.10 | 22.20 | 22.12 | 22.21 |
| **Σ-  EPMA**  | 22.12 | 22.16 | 22.17 | 22.10 | 22.13 | 22.11 | 22.21 | 22.17 | 22.20 |
|  |  |  |  |  |  |  |  |  |  |
| **<M-O> X-ref** | 2.071 | 2.071 | 2.071 | 2.061 | 2.065 | 2.071 | 2.073 | 2.073 | 2.063 |
| **<M-O> EPMA** | 2.076 | 2.075 | 2.074 | 2.068 | 2.065 | 2.076 | 2.076 | 2.077 | 2.064 |
|  |  |  |  |  |  |  |  |  |  |
| **<T-O> X-ref** | 1.659 | 1.659 | 1.658 | 1.660 | 1.660 | 1.660 | 1.658 | 1.658 | 1.662 |
| **<T-O> EPMA** | 1.658 | 1.657 | 1.657 | 1.659 | 1.659 | 1.655 | 1.656 | 1.654 | 1.662 |

**Supplemental Data Table 4**

continuation

|  |  |  |
| --- | --- | --- |
|  | **1872 Eruption** | **1944 Eruption** |
|  | **EJ4\_2** | **EJ6\_1** | **EJ12\_3** | **EJ13\_1** | **EJ72\_1** | **EJ72\_3** | **EJ72\_4** | **EJ72\_6** |
| **e- (M1) X-ref** | 12.22 | 12.16 | 12.18 | 11.99 | 14.64 | 14.62 | 14.75 | 14.89 |
| **e- (M2) X-ref** | 12.53 | 12.55 | 12.43 | 12.43 | 14.75 | 14.73 | 14.84 | 14.94 |
|  |  |  |  |  |  |  |  |  |
| **e- (M1+2M2) X-ref** | 37.28 | 37.26 | 37.04 | 36.85 | 44.14 | 44.08 | 44.43 | 44.77 |
| **e- (M1+2M2) EPMA** | 36.36 | 37.03 | 36.36 | 37.00 | 44.39 | 44.30 | 44.45 | 44.69 |
|  |  |  |  |  |  |  |  |  |
| **K e- X-ref** | 18.30 | 17.89 | 17.73 | 17.89 | 18.90 | 18.82 | 18.91 | 18.76 |
| **K e- EPMA** | 17.05 | 19.13 | 17.05 | 17.70 | 19.04 | 18.48 | 19.34 | 18.40 |
|  |  |  |  |  |  |  |  |  |
| **T e- X-ref** | 13.86 | 13.93 | 13.91 | 13.95 | 13.76 | 13.76 | 13.83 | 13.78 |
| **T e- EPMA** | 13.77 | 13.75 | 13.77 | 13.76 | 13.69 | 13.70 | 13.70 | 13.70 |
|  |  |  |  |  |  |  |  |  |
| **Σ+  EPMA** | 22.01 | 22.13 | 21.99 | 22.02 | 22.46 | 22.45 | 22.47 | 22.47 |
| **Σ-  EPMA**  | 22.00 | 22.14 | 22.00 | 22.04 | 22.44 | 22.46 | 22.48 | 22.46 |
|  |  |  |  |  |  |  |  |  |
| **<M-O> X-ref** | 2.060 | 2.061 | 2.060 | 2.061 | 2.073 | 2.072 | 2.072 | 2.072 |
| **<M-O> EPMA** | 2.070 | 2.065 | 2.069 | 2.066 | 2.069 | 2.068 | 2.067 | 2.069 |
|  |  |  |  |  |  |  |  |  |
| **<T-O> X-ref** | 1.649 | 1.650 | 1.648 | 1.649 | 1.662 | 1.661 | 1.661 | 1.661 |
| **<T-O> EPMA** | 1.650 | 1.653 | 1.650 | 1.651 | 1.660 | 1.659 | 1.659 | 1.659 |

*Notes:* Σ+ and Σ- are sum of positive andnegative charges, respectively

**Supplemental Data Table 5**

Structural formulas of the study micas

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Interlayer** | **Octahedral site** | **Tetrahedral site** | **Anionic site** |
| **1631 Eruption**  |  |  |  |  |
| **EJ20\_1** | **(K0.93Na0.06)Σ=0.99** | **(Mg2.49Al0.14Fe2+0.21Fe3+0.14Mn0.02)Σ=3.00** | **(Si2.84Al1.16)Σ=4.00** | **O10.12OH1.28F0.60** |
| **EJ20\_2** | **(K0.93Na0.07)Σ=1.00** | **(Mg2.51Al0.16Fe2+0.19Fe3+0.12Mn0.02)Σ=3.00** | **(Si2.87Al1.13)Σ=4.00** | **O10.16OH1.25F0.59** |
| **EJ20\_3** | **(K0.92Na0.07)Σ=0.99** | **(Mg2.48Al0.16Fe2+0.20Fe3+0.14Mn0.02)Σ=3.00** | **(Si2.87Al1.13)Σ=4.00** | **O10.17OH1.27F0.56** |
| **EJ25\_2** | **(K0.95Na0.05Ba0.01)Σ=1.01** | **(Mg2.65Al0.25Fe2+0.06Fe3+0.04Ti0.01)Σ=3.01** | **(Si2.79Al1.21)Σ=4.00** | **O10.10OH1.08F0.82** |
| **EJ25\_3** | **(K0.93Na0.06)Σ=0.99** | **(Mg2.57Al0.26Fe2+0.09Fe3+0.06Ti0.01Mn0.01)Σ=3.00** | **(Si2.81Al1.19)Σ=4.00** | **O10.13OH1.06F0.81** |
| **EJ42\_2** | **(K0.98Na0.03)Σ=1.01** | **(Mg2.76Al0.09Fe2+0.07Fe3+0.05Ti0.02)Σ=2.99** | **(Si2.93Al1.07)Σ=4.00** | **O10.11OH1.60F0.29** |
| **EJ42\_3** | **(K0.94Na0.03)Σ=0.97** | **(Mg2.50Al0.16Fe2+0.18Fe3+0.12Ti0.03Mn0.01)Σ=3.00** | **(Si2.89Al1.11)Σ=4.00** | **O10.21OH1.57F0.22** |
| **EJ42\_4** | **(K0.95Na0.03)Σ=0.98** | **(Mg2.65Al0.12Fe2+0.12Fe3+0.08Ti0.02)Σ=2.99** | **(Si2.92Al1.08)Σ=4.00** | **O10.17OH1.58F0.25** |
| **EJ47\_2** | **(K0.96Na0.04Ba0.01)Σ=1.01** | **(Mg2.42Al0.35Fe2+0.12Fe3+0.08 Ti0.02Mn0.01)Σ=3.00** | **(Si2.72Al1.28)Σ=4.00** | **O10.20OH1.57F0.23** |
|  |  |  |  |  |
| **1872 Eruption**  |  |  |  |  |
| **EJ4\_2** | **(K0.88Na0.03)Σ=0.91** | **(Mg2.83Fe3+0.05Ti0.05[ ]0.07)Σ=3.00** | **(Si3.09Al0.91)Σ=4.00** | **O10.00F1.82OH0.17Cl0.01** |
| **EJ6\_1** | **(K0.96Na0.03Ba0.01)Σ=1.00** | **(Mg2.81Al0.05Fe2+0.03 Fe3+0.03Ti0.05[ ]0.02)Σ=2.99** | **(Si3.00Al1.00)Σ=4.00** | **O10.14F1.85Cl0.01** |
| **EJ12\_3** | **(K0.88Na0.03)Σ=0.91** | **(Mg2.83Fe3+0.05Ti0.05[ ]0.07)Σ=3.00** | **(Si3.07Al0.93)Σ=4.00** | **O10.00F1.94OH0.05Cl0.01** |
| **EJ13\_1** | **(K0.92Na0.02)Σ=0.94** | **(Mg2.83Fe2+0.01Fe3+0.09Ti0.02[ ]0.04)Σ=2.99** | **(Si3.05Al0.95)Σ=4.00** | **O10.04F1.95Cl0.01** |
|  |  |  |  |  |
| **1944 Eruption**  |  |  |  |  |
| **EJ72\_1** | **(K0.92Na0.04Ba0.02)Σ=0.98** | **( Mg2.18Al0.19Fe2+0.28Fe3+0.19Ti0.15Cr0.01)Σ=3.00** | **(Si2.77****Al1.23)Σ=4.00** | **O10.44OH1.43F0.12Cl0.01** |
| **EJ72\_3** | **(K0.92Na0.04Ba0.01)Σ=0.97** | **(Mg2.18Al0.20Fe2+0.28Fe3+0.19Ti0.14Cr0.01)Σ=3.00** | **(Si2.79Al1.21)Σ=4.00** | **O10.46OH1.39F0.14Cl0.01** |
| **EJ72\_4** | **(K0.93Na0.05Ba0.02)Σ=1.00** | **(Mg2.16Al0.19Fe2+0.29Fe3+0.20Ti0.14Cr0.01)Σ=2.99** | **(Si2.79Al1.21)Σ=4.00** | **O10.48OH1.37F0.14Cl0.01** |
| **EJ72\_6** | **(K0.91Na0.05Ba0.01)Σ=0.97** | **(Mg2.16Al0.19Fe2+0.29Fe3+0.19Ti0.15Ni0.01Cr0.01)Σ=3.00** | **(Si2.80Al1.20)Σ=4.00** | **O10.46OH1.41F0.12Cl0.01** |