Table 5. Anisotropic displacement Parameters (Å2) for NON-HYDROGEN ATOMS IN postite§.

**(FOR DEPOSIT)**

|  | **U11** | **U22** | **U33** | **U23** | **U13** | **U12** |
| --- | --- | --- | --- | --- | --- | --- |
| V1 | 0.0166(7) | 0.0199(7) | 0.0126(7) | -0.0011(6) | -0.0021(6) | 0.0023(6) |
| V2 | 0.0180(7) | 0.0185(7) | 0.0189(7) | -0.0036(6) | -0.0002(6) | 0.0017(6) |
| V3 | 0.0250(7) | 0.0194(7) | 0.0214(7) | 0.0019(6) | -0.0034(7) | 0.0000(6) |
| V4 | 0.0166(7) | 0.0219(8) | 0.0143(7) | -0.0013(6) | 0.0015(6) | 0.0002(6) |
| V5 | 0.0173(7) | 0.0233(8) | 0.0187(7) | -0.0032(6) | -0.0006(6) | -0.0025(6) |
| Al1 | 0.0163(12) | 0.0258(13) | 0.0135(11) | -0.0006(11) | -0.0014(10) | -0.0022(10) |
| Mg1 | 0.032(2) | 0.089(4) | 0.029(2) | 0 | 0 | -0.016(2) |
| O1 | 0.017(2) | 0.022(3) | 0.013(2) | -0.003(2) | -0.003(2) | 0.005(2) |
| O2 | 0.019(3) | 0.017(3) | 0.015(3) | 0.001(2) | 0.003(2) | 0.001(2) |
| O3 | 0.018(3) | 0.021(3) | 0.018(3) | -0.003(2) | 0.000(2) | 0.001(2) |
| O4 | 0.017(3) | 0.018(3) | 0.021(3) | -0.001(2) | -0.001(2) | 0.000(2) |
| O5 | 0.020(3) | 0.020(3) | 0.018(3) | -0.002(2) | -0.001(2) | 0.002(2) |
| O6 | 0.022(3) | 0.023(3) | 0.017(3) | 0.001(2) | 0.002(2) | 0.000(2) |
| O7 | 0.019(3) | 0.024(3) | 0.015(3) | 0.000(2) | 0.002(2) | 0.001(2) |
| O8 | 0.024(3) | 0.016(3) | 0.022(3) | -0.002(2) | -0.001(2) | 0.006(2) |
| O9 | 0.014(2) | 0.027(3) | 0.018(3) | -0.005(2) | 0.002(2) | -0.002(2) |
| O10 | 0.022(3) | 0.026(3) | 0.031(3) | -0.010(2) | 0.008(2) | 0.006(2) |
| O11 | 0.019(3) | 0.032(3) | 0.027(3) | -0.009(3) | -0.004(2) | -0.001(2) |
| O12 | 0.042(3) | 0.024(3) | 0.027(3) | 0.007(2) | -0.006(3) | -0.002(3) |
| O13 | 0.017(3) | 0.031(3) | 0.021(3) | -0.004(2) | 0.003(2) | -0.001(2) |
| O14 | 0.015(2) | 0.022(3) | 0.014(2) | 0.000(2) | 0.003(2) | 0.001(2) |
| OH1 | 0.014(3) | 0.032(3) | 0.011(2) | 0.002(2) | -0.001(2) | -0.005(2) |
| OW1 | 0.025(3) | 0.032(3) | 0.018(3) | 0.003(3) | -0.002(2) | -0.008(2) |
| OW2 | 0.018(3) | 0.047(4) | 0.019(3) | -0.003(3) | -0.001(2) | -0.004(3) |
| OW3 | 0.026(3) | 0.029(3) | 0.022(3) | 0.001(3) | 0.012(2) | -0.003(3) |
| OW4 | 0.022(3) | 0.039(4) | 0.019(3) | -0.005(3) | 0.011(2) | 0.006(2) |
| OW5a | 0.054(12) | 0.069(17) | 0.034(14) | -0.006(9) | -0.014(11) | 0.042(12) |
| OW5b | 0.064(12) | 0.042(15) | 0.033(14) | -0.027(8) | -0.021(11) | 0.010(11) |
| OW6a | 0.060(8) | 0.049(9) | 0.048(9) | 0.012(8) | -0.008(6) | 0.001(8) |
| OW6b | 0.031(8) | 0.066(9) | 0.054(8) | -0.009(7) | 0.005(7) | 0.020(8) |
| OW7a | 0.035(8) | 0.050(9) | 0.062(10) | 0.001(8) | 0.030(8) | -0.008(7) |
| OW7b | 0.051(8) | 0.029(8) | 0.070(11) | 0.009(7) | -0.008(9) | -0.008(7) |
| OW8 | 0.027(3) | 0.044(4) | 0.039(4) | 0.002(3) | -0.001(3) | -0.003(3) |
| OW9 | 0.048(4) | 0.040(4) | 0.048(4) | 0.004(3) | -0.009(3) | -0.003(3) |
| OW10 | 0.051(4) | 0.026(3) | 0.052(4) | -0.012(3) | 0.005(3) | -0.001(3) |
| OW11 | 0.030(3) | 0.055(4) | 0.047(4) | -0.014(3) | -0.014(3) | 0.008(3) |
| OW12 | 0.073(7) | 0.089(7) | 0.237(13) | 0.061(7) | 0.049(6) | 0.035(5) |
| OW13 | 0.061(4) | 0.029(4) | 0.054(4) | -0.010(3) | -0.017(3) | 0.005(3) |
| OW14 | 0.073(6) | 0.023(5) | 0.040(5) | 0 | 0 | -0.018(5) |

§The anisotropic atomic displacement factor exponent takes the form: -2π2[ h2 a\*2 U11 + ... + 2 h k a\* b\* U12 ].