

Appendix TABLE S1. Miscellaneous information for magnesio-ferri-hornblende

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|---------------------------------|--|
| Chemical formula | K _{0.07} Na _{0.72} Ca _{1.82} Mg _{3.06} Fe _{1.94} Si _{6.94} Al _{1.06} O ₂₄ Cl _{0.11} |
| Formula weight | 888.41 g/mol |
| Temperature | 296(2) K |
| Crystal size | 0.058 × 0.078 × 0.110 mm |
| Crystal system | monoclinic |
| Space group | C2/m |
| Unit cell dimensions | $a = 9.8620(3)$ Å $b = 18.1060(5)$ Å $c = 5.30810(10)$ Å $\beta = 104.8480(10)$ ° |
| Volume | 916.17(4) Å ³ |
| Z | 2 |
| Density (calculated) | 3.213 g/cm ³ |
| Theta range for data collection | 2.25 to 40.25° |
| Index ranges | -17 ≤ <i>h</i> ≤ 17, -32 ≤ <i>k</i> ≤ 32, 0 ≤ <i>l</i> ≤ 9 |
| Independent reflections | 2953 ($R_{\text{int}} = 0.0726$) |
| Goodness-of-fit on F^2 | 1.058 |
| Final <i>R</i> indices | 2185 data: $I > 2\sigma(I)$, $R_1 = 0.0395$, $wR_2 = 0.0775$ all data: $R_1 = 0.0649$, $wR_2 = 0.0844$ |