

TABLE 1. Data and experimental details for the selected steinhardtite crystal

| Crystal data | |
|---|--|
| Formula | Al _{0.38} Ni _{0.32} Fe _{0.30} |
| Crystal size (mm) | 0.008 × 0.009 × 0.010 |
| Form | block |
| Color | black |
| Crystal system | cubic |
| Space group | $Im\bar{3}m$ (no. 229) |
| <i>a</i> (Å) | 3.0214(8) |
| <i>V</i> (Å ³) | 27.58(2) |
| <i>Z</i> | 2 |
| Data collection | |
| Instrument | Oxford Diffraction Xcalibur 3 |
| Radiation type | MoK α (λ = 0.71073) |
| Temperature (K) | 298(3) |
| Detector to sample distance (cm) | 5 |
| Number of frames | 115 |
| Measuring time (s) | 350 |
| Maximum covered 2 θ (°) | 70.37 |
| Absorption correction | multi-scan (ABSPACK; Oxford Diffraction 2006) |
| Collected reflections | 465 |
| Unique reflections | 12 |
| Reflections with $F_o > 4\sigma(F_o)$ | 11 |
| R_{int} | 0.0285 |
| Range of <i>h</i> , <i>k</i> , <i>l</i> | $0 \leq h \leq 4, 0 \leq k \leq 4, 0 \leq l \leq 4$ |
| Refinement | |
| Refinement | Full-matrix least squares on F^2 |
| Final R_1 [$F_o > 4\sigma(F_o)$] | 0.0209 |
| Final R_1 (all data) | 0.0254 |
| Number of least-squares parameters | 3 |
| $\Delta\rho_{max}$ (e Å ⁻³) | 0.22 |
| $\Delta\rho_{min}$ (e Å ⁻³) | -0.38 |
| Note: $R_{int} = (n/n - 1)^{1/2} [F_o^2 - F_o(\text{mean})^2] / \Sigma F_o^2$; $R_1 = \Sigma F_o - F_c / \Sigma F_o $. | |

