Refinement of an Amesite-$2H_1$ Polytype from Postmasburg, South Africa

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Abstract: The crystal structure of amesite-$2H_1$ from the Postmasburg Mn ores of South Africa has been refined to R = 4.7% using Siemens P4 rotating-anode Mo$K\alpha$ X-ray data and SHELXL-93 software. Partial ordering of tetrahedral Si,Al and especially of octahedral Mg,Al has reduced the ideal $P6_3cm$ symmetry to triclinic $P1$ (refined as $C1$). Tetrahedral rotation of 15 ° moves the basal oxygens toward the octahedral cations in the same layer but away from the OH H-donors of the next layers. The ordering pattern of Al^{IV} and Al^{VI} is unique in that the locus of Al-rich sites consists of 2 intersecting sets of zigzag lines parallel to X_2 and X_3, plus 2 Al-rich octahedra in layer 2 instead of the usual 1 site.

Key Words: Amesite-$2H_1$ • Distortions • Ordering Patterns • Postmasburg • Refinement • South Africa • Twinning

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