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Geometric crystal chemical models for structural analysis of micas and their stacking polytypes

PATRICK H.J. MERCIER,† R. JAMES EVANS, AND DENIS G. RANCOURT*

Department of Physics, University of Ottawa, Ottawa, Ontario K1N 6N5, Canada

ABSTRACT

A sequence of progressively more realistic geometric crystal chemical models for TOT layers in mica is developed, starting from the usual main uniform distortions (octahedral flattening, tetrahedral rotation, octahedral counter-rotation) toward additional features as they are shown to be required. These additional features include tetrahedral basal flattening and apical bond adjustment, geometric meso-octahedral sheets (having unequal M1 and M2/M3 site bond lengths), and geometric hetero-octahedral sheets (having unequal M1, M2, and M3 site bond lengths). A crystal chemical model for the unit cell of a 1*M* polytype with *C*2/*m* space group is developed from geometric homo-octahedral sheets (having equal M1, M2, and M3 site bond lengths) and is described using a minimal number of independent crystal chemical parameters: octahedral, tetrahedral basal, tetrahedral apical, and interlayer metal-anion bond lengths, and flattening angles of octahedral and tetrahedral sheets. The monoclinic lattice parameters (a, b, c, and β) and the tetrahedral rotation angle (α) follow from these assumed parameters. These models are designed to allow analyses (that are reported elsewhere) of both structural and lattice-parameter refinement data in terms of deviations from various predictions based on specified sets of crystal chemical assumptions. Fractional atomic coordinates are derived in terms of the atomic positions for the 1*M* unit cell of *C*2/*m* symmetry for each known homogeneous mica polytype with highest space group symmetry (polytype, space group = $2M_1$, $C2/c$; $2M_2$, $C2/c$; $2O$, $Ccmm$; $3T$, $P3_112$). These coordinates allow a structural analysis of diffraction data for different stacking polytype structures using the same 1*M*-type TOT layer as a modular unit.