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Connectivity and formula-generating functions for sheet-silicate minerals

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Silicate sheets may be described by two-dimensional nets in which the vertices of the net are occupied by tetrahedra, and the edges of the net represent linkages between tetrahedra. A plane net must contain 3-connected vertices, but not all vertices need to be 3-connected. Simple silicate structures may thus be generated from simple 3-connected plane nets (e.g. 6^3, 4.8^2, 4.6.8, $(4.6.8)_2(6.8^2)_1$, etc.). More complicated silicate nets may be generated by various "building operations": (1) Insertion: insertion of 2- and 4-connected vertices into 3-connected plane nets; (2) Repetition: generation of double (or triple) nets by topological symmetry operations that retain transitivity at the junction between the repeated elements. Diversity is also introduced within the sheets of tetrahedra by [1] adjacent apical tetrahedron vertices pointing in the same or different directions, and [2] by folding of the sheets. For simple structures, net type strongly affects the stoichiometry of the resultant structure as the unit cells of the various nets are of different sizes (and shapes), although the stoichiometry may also be affected by non-tetrahedral components. Building operations strongly affect the stoichiometry of the resultant sheet, and this effect may be quantified. We define a formula-generating function F(k,l,…) that generates the formula of a sheet with specific topological features denoted by the indices k,l,… . A simple 3-connected net results in sheets of the form $(T_2O_5)n$ where n denotes the number of $(T_2O_5)n$ in the unit cell of the underlying net (for 6^3, n = 1; for 4.8^2, n = 2; for $(4.6.8)_2(6.8^2)_1$, n = 3, etc). Plane nets with k 3-connected vertices and l inserted 2-connected vertices result in sheets of the form [T(k+l) O(2.5k+3l)], where (…) are subscripted. Single- and double-sheet structures may be generated from the function F(k,l) = T(N{k+l}) O(N{3k+2.5l}-n{N-1}) where N = 1 and 2 for single- and double-sheets, respectively, and (…) are subscripted.

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