Bond Topology of Chain, Ribbon and Tube Silicates

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All chain, ribbon and tube arrangements of tetrahedra can be represented graphically by reducing (TO_4) tetrahedra to vertices and linkages between those tetrahedra to edges. In this graphical representation, only the connectivity of vertices (tetrahedra) are preserved and no geometrical properties. Using the expression $G_t = n_t$:(a-b-c-d), the topology of all chains may be described where G_t is the graphical representation of a specific chain, n_t is the topological repeat unit and a, b, c and d are the number of 1-, 2-, 3- and 4-connected vertices in n_t. The topological repeat unit (n_t) contains the minimum number of vertices required to generate a given graph through repetition operations. By sequentially inserting different values of a, b, c and d, all topologically distinct graphs are generated. Figure 1 shows examples of the tetrahedron and graphical representation of chains observed and not observed in inosilicates.

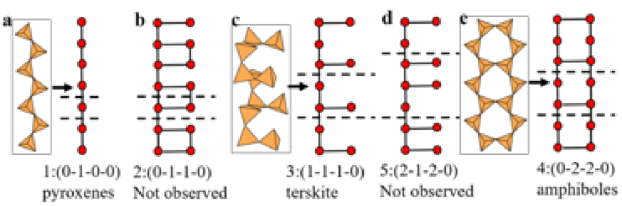

Figure 1. Tetrahedron and graphical representation of the chain in (a) pyroxenes; (b) the 2:(0-1-1-0) chain that is not observed; (c) terskite; (d) the 3:(2-1-2-0) chain that is not observed; (e) amphiboles. Dashed black lines outline the topological repeat unit (n_t) of each chain.

Each G_t expression corresponds to a set of topologically unique (non-isomorphic) graphs. This set can be generated by using modified adjacency matrices, where each row (or column) represents a vertex in n_t. The sums of all rows and columns can then be permuted, each permutation generates a topologically unique graph that corresponds to the respective G_t expression. By comparing all possible non-isomorphic graphs that correspond to chains, we have begun to identify topological characteristics that correspond to more abundant inosilicates and/or more stable chain arrangements. Thus far, it is apparent that 4-connected vertices are uncommon, and branches occur only as simple 1-connected vertices.