FOUNDATIONS
ADVANCES

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**Supporting information for article:**

# Bond topology of chain, ribbon and tube silicates. Part I. Graph-theory generation of infinite one-dimensional arrangements of $(TO4)^{n-}$ tetrahedra

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**Appendix D: Instructions for Appendices E, F and G**

For vertex connectivities (${}^{c}V_{r}$) in which $\sum r \leq 8$, all valid matrix-element combinations and their corresponding adjacency matrices are listed in Appendix E. All proto-graphs that correspond to each adjacency matrix in Appendix E are compiled in Appendix F. All non-isomorphic chain graphs are compiled in Appendix G. Clusters will only be included in Appendix G if they are non-isomorphic with the proto-graph (Appendix F) from which they were generated. In Appendices E, F and G, ${}^{c}V_{r}$ expressions are listed in accordance with the hierarchical ordering scheme given in Table 1 (section 7); note that ${}^{c}V_{r}$ where $e_A$ is odd cannot form graphs and are not listed in the Appendices. For certain ${}^{c}V_{r}$ where the number of edges ($e$) is relatively large, deriving all distinct matrices, the corresponding non-isomorphic proto-graphs and chain graphs is computationally intensive and results in an unmanageable number of graphs, these ${}^{c}V_{r}$ are indicated as NG (not generated). For some ${}^{c}V_{r}$ where $e$ is relatively large, all adjacency matrices and proto-graphs are generated but the corresponding chain graphs are not shown and indicated as NG in Appendix G.

For each ${}^{c}V_{r}$ (where $e_A$ is even) only valid matrix-element combinations are listed and are written in the format ($m_1$ x **1**, $m_2$ x **2**, $m_3$ x $\mathbf{2^1}$, $m_4$ x $\mathbf{2^2}$) where $m_i$ are the numbers of those matrix elements in the adjacency matrix of interest. In Appendix E, matrix-element combinations that correspond to more than one distinct matrix are listed as ($m_1$ x **1**, $m_2$ x **2**, $m_3$ x $\mathbf{2^1}$, $m_4$ x $\mathbf{2^2}$) **a,** ($m_1$ x **1**, $m_2$ x **2**, $m_3$ x $\mathbf{2^1}$, $m_4$ x $\mathbf{2^2}$) **b,** ($m_1$ x **1**, $m_2$ x **2**, $m_3$ x $\mathbf{2^1}$, $m_4$ x $\mathbf{2^2}$) **c**…etc. and the corresponding proto-graphs are labelled the same way in Appendix F. In Appendix G, matrix-element combinations that correspond to more than one non-isomorphic chain graph are listed as above or as ($m_1$ x **1**, $m_2$ x **2**, $m_3$ x $\mathbf{2^1}$, $m_4$ x $\mathbf{2^2}$) **a-1,** ($m_1$ x **1**, $m_2$ x **2**, $m_3$ x $\mathbf{2^1}$, $m_4$ x $\mathbf{2^2}$) **a-2,** ($m_1$ x **1**, $m_2$ x **2**, $m_3$ x $\mathbf{2^1}$, $m_4$ x $\mathbf{2^2}$) **a-3**…etc. Non-isomorphic directed proto-graphs are not listed in the appendices as the edge combinations (number and direction of wrapped edges) used to generate a given chain graph may be derived by simply constructing an adjacency matrix for any chain graph of interest (section 5).

**Example: ${}^{1}V_3{}^{3}V_3$**

Consider ${}^{1}V_3{}^{3}V_3$ as an example of how to use Appendices E, F and G. Here, there are eight valid matrix-element combinations that correspond to 15 distinct matrices, and the element combinations that correspond to more than one matrix are labelled as described above in Appendix E. One may then locate the proto-graph to which each of these 15 matrices corresponds in Appendix F, for example the matrix labelled (8 x **1**, 2 x $\mathbf{2^1}$) **b** corresponds to the proto-graph labelled (8 x **1**, 2 x $\mathbf{2^1}$) **b**. One may then locate all non-isomorphic chain graphs generated from a given proto-graph in Appendix G, for example the proto-graph labelled (8 x **1**, 2 x $\mathbf{2^1}$) **b** produces three chain graphs labelled (8 x **1**, 2 x $\mathbf{2^1}$) **b-1,** (8 x **1**, 2 x $\mathbf{2^1}$) **b-2** and (8 x **1**, 2 x $\mathbf{2^1}$) **b-3**.