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Computerized crystal-chemical classification of silicates and related materials with CRYSTANA and formula notation for classified structures

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ABSTRACT

The computer program CRYSTANA is described which implements a method for the crystal-chemical classification of silicates and related materials. This method is mainly based upon the topological structure of the connected units of a compound and can be applied when the units are built from tetrahedra as coordination polyhedra. The classification parameters and the rules which have to be applied for their determination are summarized and a formalization of the method is provided based upon a finite graph representation of the units. A description of how CRYSTANA can be used and which kind of output it produces is included. From this output crystal-chemical formulas can be derived, which differ slightly from an existing notation in order to meet recommendations of the International Union of Crystallography.

1. Introduction

Silicates form one of the largest classes of inorganic chemical compounds. The more than 1243 natural silicates that have been approved as of May 2007 by the International Mineralogical Association (IMA) as minerals [1], comprise more than 90 vol% of the earth's crust and mantle. In addition to the silicate minerals a large number of synthetic silicates have been reported, many of which are of great technical importance. It is obvious that classifications are needed to handle this large number of silicates.

In addition, many other inorganic compounds follow very similar structural principles. Therefore, a classification of silicates should be applicable to other compounds as well, in particular to compounds that contain units of corner-sharing tetrahedra.

The well-known silicate classification of Bragg [2] and Náray-Szabó [3] is based on the atomic structures of the silicate anions. It has been extended considerably [4] by selecting a number of classification parameters, the application of which reveals correlations between structures, chemical compositions, and stability of the silicates under varying thermodynamic conditions. This classification, which is sometimes called 'Liebau classification', is now widely used.

Free-hand classification of more complicated silicate structures by using only the information given in [4] may be troublesome and has sometimes led to miss-assignments. Therefore, the program system CRYSTANA has been developed which allows to automatically classify silicates according to the rules of the method. CRYSTANA has been tested intensively and may now be considered as the reference implementation of the classification. In addition, a formula notation is proposed which differs slightly from that used in [4], in order to be in accordance with recommendations of the International Union of Crystallography (IUCr) [5].

In Section 2 the classification parameters are defined and rules for their application are given. In Section 3 the classification method is described on a more formal basis using notions from graph theory. A description of how to use the program system and how to interpret the results is given in Section 4. In the last section an extended notation of crystal-chemical formulas is introduced.

2. Classification parameters and classification rules

The composition of a silicate can be given as $(\mathbf{A}_i)_{m_i}\mathrm{Si}_n\mathrm{O}_p(\mathbf{Y}_j)_{q_j}(\mathbf{Z}_k)_{r_k}(\mathbf{M}_l)_{s_l}$. Such a silicate contains, in addition to silicon atoms Si, cations **A**,[1] oxygen anions O and additional anions **Y**, **Z**, and molecules **M** which are not bonded to Si. If there are

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[1] Following a recommendation [6], distinction is made between usual *element symbols* such as Si, Al, O, ..., given as normal-face Latin letters, and *structure site symbols*, given as bold-face Latin letters such as **T**, **G**, **A** ... for cations with tetrahedral coordination, octahedral coordination and without regard to their coordination, respectively, and **X**, **Y** for monoatomic anions, **Z** for polyatomic anions, and **M** for molecules such as H_2O, CO_2, etc.

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more than one kind of atoms **A**, **Y**, **Z**, and **M** they are indicated by their running indices *i, j, k,* and *l*, respectively. The subindices m, n, q, r, and s designate the number of corresponding atoms per formula unit. As an example, the compositional formula of the mineral roeblingite is given as $Pb_2Ca_6MnSi_6O_{18}(OH)_2(SO_4)_2(H_2O)_4$ with $\mathbf{A} = Pb, Ca, Mn$; $\mathbf{Y} = OH$; $\mathbf{Z} = SO_4$; $\mathbf{M} = H_2O$ [7].

Usually, the Si atoms are tetrahedrally coordinated by four, sometimes by six, very seldom by five or more than six O atoms. $[SiO_4]$ tetrahedra can directly be connected with other $[SiO_4]$ tetrahedra by sharing corners. Edge-sharing of $[SiO_4]$ tetrahedra, although topologically possible, has not been observed. A group of directly connected tetrahedra is called a *connected silicate unit*. In chemical formulas it is set within square brackets. Five-, six-, and higher coordinated Si atoms are considered as cations which, together with the other **A** cations, compensate for the valences of both the connected silicate units and the **Y** anions.

The classification of silicates is mainly based on the topological structure of their connected silicate units. The majority of crystalline silicates contain only one type of connected silicate units. There is, however, a smaller number of silicates, called *mixed silicate– anion silicates* such as synthetic $Y_4[SiO_4][Si_3O_{10}]$ [8] and the mineral okenite, $Ca_{10}[Si_6O_{16}][Si_6O_{15}](H_2O)_{18}$ [9], which contain more than one type of connected silicate units.

If a silicate contains tetrahedrally coordinated cations **T** other than Si, such as Li^{I}, Zn^{II}, Al^{III}, Ge^{IV}, P^{V}, etc., they may optionally be considered as part of the connected unit. In a similar way, oxygen atoms of a $[\mathbf{T}O_4]$ tetrahedron may, fully or partially, be replaced by other anions, such as F^{-I}, S^{-II}, or N^{-III}, to give $[\mathbf{TX}_4]$ tetrahedra and $[\mathbf{T}_x\mathbf{X}_y]$ as composition of a more general connected unit. In this sense, the general composition of a connected unit may be written as $[\mathbf{T}_x\mathbf{X}_y]$ and its topological structure describes the way the $[\mathbf{TX}_4]$ tetrahedra are connected. Therefore, the presented crystal-chemical classification works not only for silicates, but also for any compound with connected units built from $[\mathbf{TX}_4]$ tetrahedra, such as aluminates, germanates, phosphates, chromates, etc.

To characterize the topological structure of a connected unit, the following classification parameters are used, which are described in more detail in [4, p. 52ff], and [10, p. 30ff]. The symbols of these classification parameters are given as bold-face italic letters.

- The *linkedness* ***L*** of a $[\mathbf{TX}_4]$ tetrahedron is the number of **X** anions that it has in common with a neighboring $[\mathbf{TX}_4]$ tetrahedron. $\boldsymbol{L} = 0, 1, 2$, and 3 stands for isolated, corner-, edge-, and face-sharing $[\mathbf{TX}_4]$ tetrahedra, respectively (Fig. 1). So far, no oxosilicate anion $[Si_xO_y]$ with $\boldsymbol{L} > 1$ has been observed. However, $[\mathbf{TX}_4]$ tetrahedra with $\mathbf{T} \neq Si$ and with $\boldsymbol{L} > 1$ are quite common.
- The *connectedness* ***s*** of a $[\mathbf{TX}_4]$ tetrahedron is the number of other $[\mathbf{TX}_4]$ tetrahedra that are linked to it via common **X** atoms, independent of the value of ***L***. In oxosilicates so far only values $\boldsymbol{s} = 0, 1, 2, 3$, and 4 have been observed, although higher ***s*** values are theoretically possible (Fig. 2).
- *Branchedness* ***B***: Multiple tetrahedra, single rings, and single chains are called *unbranched* (***uB***) if they contain only $[\mathbf{TX}_4]$ tetrahedra with $\boldsymbol{s} \leqslant 2$; when they contain tetrahedra with $\boldsymbol{s} > 2$ they are termed *branched* (***B***) anions. If each branch is linked to the non-branch part (stem) of the anion by only one common element (corner, edge, or face), the anion is called *open-branched* (***oB***). If there are two such common elements for each branch, the anion is called *loop-branched* (***lB***). If a multiple tetrahedron, single ring, or single chain has both kinds of branches, the term *mixed-branched* (***olB***) is used (Fig. 3).

  The ensemble of multiple tetrahedra, single rings, and single chains, irrespective of whether they are branched or unbranched, forms the group of *fundamental anions*. Non-linear condensation of fundamental anions leads to *complex anions*. The branchedness of a complex anion is defined as follows:
  - ○ If all fundamental anions have the same kind of branchedness then this is also the branchedness of the complex anion.
  - ○ If among the fundamental anions there are open-branched and loop-branched chains but no unbranched chains then the complex anion has the branchedness *mixed-branched*.
  - ○ In all other cases the branchedness is *hybrid* (***hB***) (Fig. 3).
- The *periodicity* ***P*** is the number of tetrahedra in the repeat unit of the non-branch part of a fundamental anion, in particular of a single ring ($\boldsymbol{P}^{\mathbf{R}}$) or single chain ($\boldsymbol{P}^{\mathbf{C}}$).
- The *dimensionality* ***D*** is the number of dimensions of infinite extension of an anion.
- The *multiplicity* ***M*** is the number of single tetrahedra, rings, chains, or layers which are linked to a complex anion of the same dimensionality.

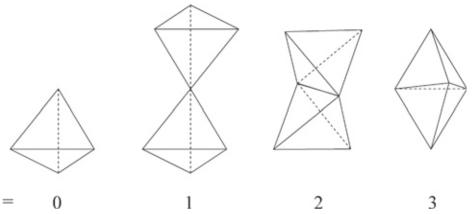

Fig. 1. $[\mathbf{TX}_4]$ tetrahedra with different values of linkedness ***L***.

In general, there are several possibilities for choosing fundamental chains in complex silicate anions of infinite extension. Hence appropriate rules have to be fixed in order to get an unambiguous classification. An intention of the classification is to give preference to silicate anions that are most common, assuming that they are the most stable ones. This is accomplished when the following rules are applied in the given order:

Rule 1: The fundamental chains are chosen as chains of lowest periodicity which run parallel to the shortest identity period within the anion, regardless of their branchedness, and from which the anion can be generated by successive linkage.

Rule 2: If more than one chain is derived in agreement with Rule 1 the fundamental chains are chosen in the order of preference: unbranched (***uB***) > loop-branched (***lB***) > open-branched (***oB***) > mixed-branched (***olB***) > hybrid (***hB***).

Rule 3: If more than one chain is derived in agreement with Rules 1 and 2, the fundamental chains are chosen such that their number is lowest.

With respect to the order of these rules there is a difference to the order given in [4]: Rule 2 and Rule 3 have been interchanged. The reason for this modification is that minimizing the number of fundamental chains before determining the branchedness would result in selecting sets of fundamental chains with as many tetrahedra assigned to branches as possible. This is not in accordance with the preference stated above. An example will be provided in the next section.

3. Graph-based formalization of the classification method

The application of graph theory is common for the analysis of the bonding of chemical compounds at different levels of detail [11]. Graphs allow to provide definitions of properties in a formal setting and constitute a suitable basis for the specification and realization of algorithms. At the level of atoms and bonds, the

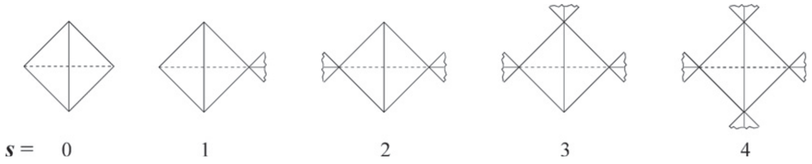

Fig. 2. [$\mathbf{TX}_4$] tetrahedra with different values of connectedness ***s***.

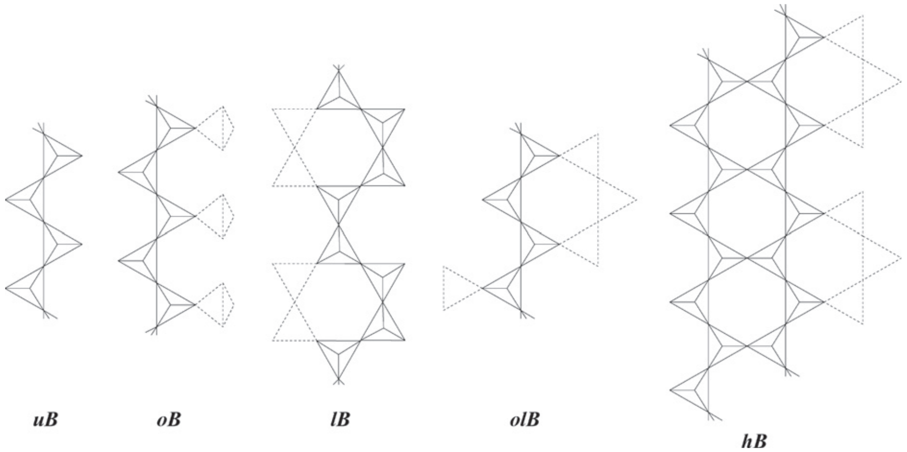

Fig. 3. Single chains with different kinds of branchedness ***B***. The branches are given with dotted lines.

nodes of a graph correspond to the atoms and its edges to the bonds. When local bonds are modeled by coordination polyhedra and when a single kind of polyhedron and a single kind of connection between polyhedra are considered, the same simple graph form can be used to represent the polyhedra and their connections. In both cases, the information content of a graph can be enriched, if necessary. Nodes, for example, can be labeled with geometric information such as coordinates of atoms and information about bond types can be added to the edges.

For the crystal-chemical classification, structures are considered here at the level of corner-sharing tetrahedra. Geometric information is used only for the determination of the shortest identity period, and symmetry information is needed for relating fundamental chains. Hence a simple graph having nodes labeled with the coordinates of the central **T** atoms of the corresponding tetrahedra is well-suited for representing a structure assuming that cell data and the space-group of the structure are given separately. Let us call such a graph *simple crystal graph*. For ideal crystals the graph of a structure is infinite. It may consist of a single or a finite number of infinite components (frameworks), an infinite number of infinite components (layers, chains), or an infinite number of finite components (rings, clusters). Taking translational symmetry into account it is, however, always possible to provide a finite representation by general graphs in which multiple edges as well as loops are allowed. The edges of these graphs are directed from a start node to an end node and are eventually labeled with a translation vector. For a single component such a graph can be constructed as follows (for a formal definition of this graph form see [12]):

Consider the unit cell of the structure with respect to a primitive basis and all tetrahedra of the component with their central atoms in this (primitive) unit cell. The set of nodes of the graph contains exactly one node for each of these tetrahedra. This means that a node represents a class of translationally equivalent tetrahedra and that the tetrahedron associated with the node is the representative of this class. To generate the directed edges of the graph, consider each node n and all connections of the associated tetrahedron t. Let t be linked to a tetrahedron t' and let n' be that node, which represents the equivalence class of t'. Then the link between t and t' is modeled by an edge e directed from n to n'. If the central atom of t' is located in the unit cell, e remains unlabeled; if it is located in a neighboring cell of the unit cell, e is labeled with the integral translation vector (xyz) identifying this cell. Because of translational symmetry every edge e from a node n to a node n' has an inverse from n' to n labeled with -t when t is the label of e. It is, therefore, convenient to use a single undirected edge instead of two directed edges for every pair of connected nodes and to label it appropriately.

The resulting graph is called *direction-labeled graph*.

Remark. This graph form is similar to the labeled quotient graph of [13] and the convoluted graph of [14]. When all symmetry operations of the space-group of the structure are taken into account, a similar construction based upon an asymmetric unit instead of the unit cell results in a so-called *symmetry-labeled graph* [15].

Example 1. Fig. 4 shows part of the infinite tetrahedra framework of low-temperature cristobalite [16] (SiO_2, space-group $P4_12_12$, $a = 4.9226$, $b = 4.9226$, $c = 6.8173$ Å) and the corresponding direction-labeled graph. The tetrahedra with central atom in the unit cell are marked 1–4.

In the following, we provide definitions of the classification parameters referring to the representation of connected (silicate) units by direction-labeled graphs. The parameters *coordination number* $(CN)_{\mathbf{T}}$ and *linkedness* $\boldsymbol{L}$ are fixed to 4 and 1, respectively, since we only consider corner-sharing of tetrahedra.

- *Connectedness* ***s***: The connectedness of a tetrahedron is the outdegree of the corresponding node in the graph, i.e. it is the number of edges leaving the node. From the construction of the graph follows that the outdegree of a node is always identical to its indegree, i.e. to the number of edges entering the node.

  In Example 1, the outdegree of all nodes is 4; hence the connectedness ***s*** is 4 for all tetrahedra.

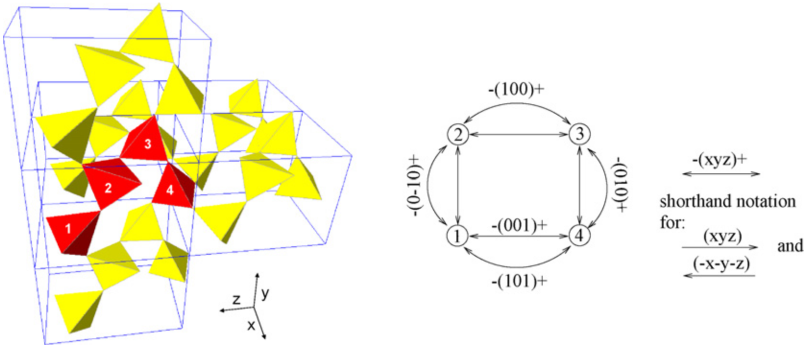

Fig. 4. Part of the tetrahedra framework and the direction-labeled graph of low-temperature cristobalite.

- *Direction of shortest repetition*: Two translationally equivalent tetrahedra are represented by the same node in the direction-labeled graph. It follows that paths between translationally equivalent nodes in the simple crystal graph correspond (are mapped) to closed directed walks in the direction-labeled graph. The sum of all vectors found as labels of the edges of such a walk determines a direction of repetition. For determining the shortest identity period it is sufficient to consider all directed cycles in the graph, i.e. closed walks with no repetition of nodes up to the start and the end node. The Euclidean distance associated with the direction of repetition of a cycle is an identity period. A direction of shortest repetition is a direction having the shortest identity period. In Fig. 4 the cycle ② $\xrightarrow{(100)}$ ③ $\longrightarrow$ ② has the shortest identity period (4.9226 Å); its direction of repetition is [100] (in the usual crystallographic notation). Due to the tetragonal symmetry of low-temperature cristobalite, the cycle ③ $\xrightarrow{(010)}$ ④ $\longrightarrow$ ③ has the same shortest identity period of 4.9226 Å with direction of repetition [010].
- *Dimensionality **D***: The set of directions of repetition is closed under addition since the direction-labeled graph represents a connected unit. It is closed under negation as well since every edge has an inverse. Hence it forms a submodule of the module $\mathbb{Z}^3$, the set of all integer triplets. The dimension of this submodule, i.e. the size of a basis, defines the dimensionality of the connected silicate unit.

  In Fig. 4 three linear independent directions of repetition are [100], [010], and [001]. Therefore, $\boldsymbol{D} = 3$.
- *Periodicity **P***: The non-branch part of a chain corresponds to a cycle in the direction-labeled graph with the following properties: its labels sum up to a direction of shortest repetition and there is no shorter cycle having this property. The periodicity of a connected silicate unit is the number of nodes of these cycles. The same holds for rings.

  In Fig. 4 there are two such cycles: ① $\xrightarrow{(101)}$ ④ $\xrightarrow{(00-1)}$ ① and ② $\xrightarrow{(100)}$ ③ $\longrightarrow$ ②, , which both have the periodicity $\boldsymbol{P} = 2$.
- *Branchedness **B***: Each fundamental chain corresponds to a connected subgraph of the simple crystal graph, i.e. for every pair of nodes of the subgraph there is a path connecting these nodes. Two fundamental chains do not share any node and the union of all nodes of the fundamental chains gives the complete set of nodes of the graph. This means that the set of fundamental chains has to provide a so-called node covering of the simple crystal graph.

  The edges of the graph are not represented completely in case of dimensionality different from 0 since 'successive linkage' of fundamental chains (Rule 1, see above) means connecting tetrahedra. Connections, however, are represented by edges.

  In the direction-labeled graph, possible branches are paths connected to a cycle *c* representing the non-branch part of a chain. The nodes of these paths have no direct connection to *c* up to the first node (open-branched) or up to the first and the last node (loop-branched). In order to determine the fundamental chains, cycles with distinct nodes have to be found and eventually completed by paths which represent branches.

  In Fig. 4 a node covering is obtained with unbranched chains of periodicity $\boldsymbol{P}^{\mathbf{C}} = 2$.
- *Multiplicity **M***: In case of oligosilicates and cyclosilicates, i.e. if dimensionality is 0, multiplicity is defined as the number of nodes of a maximal path in the direction-labeled graph and as the number of cycles representing fundamental anions, respectively. For dimensionality 1, the size of the set of fundamental chains determines the multiplicity. If dimensionality is 2, this parameter is defined as the number of partitions obtained by grouping fundamental chains into disjoint sets such that each set represents a layer. If the dimensionality of the connected unit is $\boldsymbol{D} = 3$, as in Example 1, the multiplicity is always 1.

Example 2. In order to demonstrate the possible effect of the interchange of the Rules 2 and 3 for selecting fundamental chains consider the two graphs in Fig. 5. They show part of the simple crystal graph of one sublayer of the double layer in naujakasite [17]. Two loop-branched chains A and B result if Rule 3 is applied before Rule 2, i.e. if the number of fundamental chains is minimized before the branchedness is considered (Fig. 5(a)). The intended classification, three unbranched fundamental chains A, B, and C, is obtained with the order Rule 2 before Rule 3, as given above (Fig. 5(b)).

In the current version of CRYSTANA, a method is used to determine the multiplicity of layers which might not be in accordance with the intuitive understanding of layers in some rare cases. This method works as follows: the set of fundamental chains is computed as described above and searched for a partition in two equal-sized subsets having the following property: for every fundamental chain in one of the subsets there is a chain in the other set such that both chains are directly connected. This proceeding is well suited for the majority of the double layers we analyzed but it may result in the classification of a silicate as a single layer when there are fundamental chains in the two 'layers' not being directly connected to the other 'layer' as in $Li_4[Si_6O_{14}]$ [18]. The system generates a warning message if such a situation cannot be excluded.

4. How to use the system

CRYSTANA [19] has been designed for direct (remote) use on the Internet. Structure data can be supplied by using a provided Web form or by specifying a link to a file in CIF format. In addition to the determination of fundamental chains it is possible to

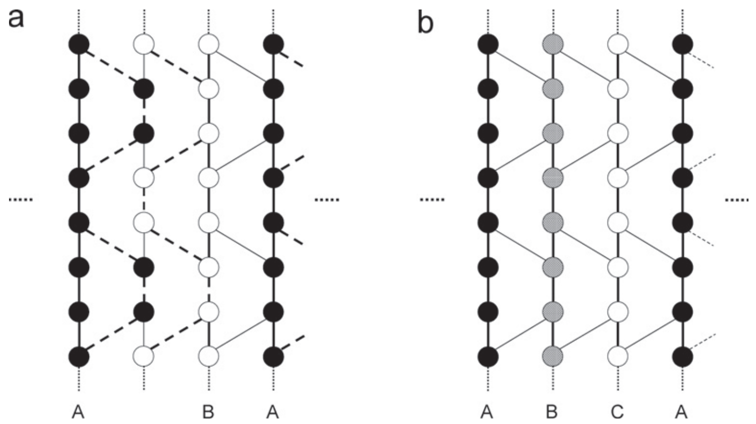

Fig. 5. Preference of (a) minimal number of chains and (b) ordering of branchedness for the connected unit of naujakasite.

compute rings and ring coverings and to compile some ring statistics. We do not comment on these facilities here, however.

In the Web form the following structure data have to be supplied:

- a trivial name of the structure,
- space-group number (according to the International Tables for Crystallography),
- change of axes, if necessary,
- setting (0: normal setting, 1: monoclinic first setting, 2: rhombohedral setting),
- lattice centering $(P, A, B, \ldots)$,
- lengths of the basis vectors and interaxial angles of the unit cell (lattice constants),
- maximal bond distance $\mathrm{d}(\mathbf{T}-\mathbf{X})$ to consider for determining tetrahedra $[\mathbf{TX}_4]$,
- kind and coordinates of all atoms in the asymmetric unit,
- two lists of atoms: one with atoms to be regarded as cations (**T** atoms), the other with atoms to be regarded as anions (**X** atoms, usually O).

A description of the required format of these data is added to the input mask.

Results of the computerized classification are available in textual as well as in graphical form (using VRML and Java applets). Textual output data are given in the following order:

- input data,
- parameters and content of the primitive cell,
- distances between **T** atoms and adjacent **X** atoms.

For each **T** atom of the asymmetric unit:

- coordination number $(CN)_{\mathbf{T}}$.

For each **T** atom of the primitive cell:

- immediate neighbors (other **T** atoms sharing **X** atoms with the **T** atom considered).

For each connected unit:

- connectedness $\boldsymbol{s}$ and linkedness $\boldsymbol{L}$ of each **T** atom,
- all **T** atoms of the connected unit,
- type of anion (terminated, ring, chain, layer, and framework)
- dimensionality $\boldsymbol{D}$,
- chain and ring periodicity $\boldsymbol{P}^{\mathbf{R}}$ and $\boldsymbol{P}^{\mathbf{C}}$, respectively,
- multiplicity $\boldsymbol{M}$,
- branchedness $\boldsymbol{B}$,
- information on chains (direction and distance of shortest repetition, branchedness, atoms, symmetry relations to other chains),
- a warning when layers could be classified differently.

Fast algorithms are used to determine dimensionality and connected units; the determination of a set of fundamental chains, however, has been shown to be ‘computationally infeasible’ which means that runtime of the algorithm may be exponential in the size of the graph. Nevertheless, only for frameworks with large unit cells the computation of the classification may take more than a few seconds.

5. Crystal-chemical formula notation

From the values of the classification parameters, i.e. from the values of $\boldsymbol{B}, \boldsymbol{P}, \boldsymbol{M}, \boldsymbol{D}, (CN)_{\mathbf{T}}, \boldsymbol{s}$, and $\boldsymbol{L}$ given in the output, the crystal-chemical formula of the connected unit of a silicate is derived according to the notation

$$\{\boldsymbol{B}, \boldsymbol{P}, \boldsymbol{M}^{\boldsymbol{D}}_{\infty}\}[\mathbf{T}_t^{\lceil L;s \rfloor}\mathbf{T}'^{\lceil L;s \rfloor}_{t'} \cdots \mathbf{X}^{[1]}_{x_1}\mathbf{X}^{[2]}_{x_2}].$$

This notation follows the recommendation of IUCr [5]. It is, however, different from the one given in [4] where the periodicity $\boldsymbol{P}$ of the fundamental chain was written as preceding superscript to the corresponding silicate atoms. The order, in which the classification parameters are now given in the formula, are the same as that used in the spoken name of the connected unit.

In the new formula, information on the constitution of the connected unit as a whole is given within curly brackets, whereas information on the individual atoms forming the connected unit are included in the square brackets.

The crystal-chemical formula of a silicate that contains only one kind of connected unit follows the scheme

$$\mathbf{A}_a^{[(CN)_{\mathbf{A}}]}\mathbf{A}'^{[(CN)_{\mathbf{A}'}]}_{a'} \cdots \{\quad\}[\quad]\mathbf{Y}_y\mathbf{Y}'_{y'} \cdots \mathbf{Z}_z\mathbf{Z}'_{z'} \cdots \mathbf{M}_m\mathbf{M}'_{m'} \cdots,$$

where $\mathbf{A}, \mathbf{A}' \ldots, \mathbf{Y}, \mathbf{Y}' \ldots, \mathbf{Z}, \mathbf{Z}' \ldots$, and $\mathbf{M}, \mathbf{M}' \ldots$ are the cations, monoatomic and polyatomic anions, and molecules, respectively, that are not considered to be part of the connected unit (see Examples 3 and 4).

Example 3. For naujakasite [17] (compare Example 2) the crystal-chemical formula $\mathrm{Na}_4^{[5+3]}\mathrm{Na}_2^{[5+4]}\mathrm{Fe}^{[4+2]}\{\boldsymbol{uB}, 4, 2^2_{\infty}\}[(\mathrm{Al},\mathrm{Si})_8^{\lceil 1;3 \rfloor}(\mathrm{Al},\mathrm{Si})_4^{\lceil 1;4 \rfloor}\mathrm{O}_6^{[1]}\mathrm{O}_{20}^{[2]}]$ is derived, which can be shortened to $\mathrm{Na}_6\mathrm{Fe}\{\boldsymbol{uB}, 4, 2^2_{\infty}\}[(\mathrm{Al},\mathrm{Si})_{12}\mathrm{O}_{26}]$.

If a silicate contains more than one kind of connected unit, information on these units, written in their corresponding curly and square brackets, are arranged in the order of increasing values of dimensionality, ***D***, and multiplicity, ***M***.

Example 4. The crystal-chemical formula for the mineral okenite [9] is derived as $\mathrm{Ca}_{10}^{[6]}\{\boldsymbol{uB}, 3, 2_{\infty}^{1}\}[\mathrm{Si}_2^{\lceil 1;2 \rfloor}\mathrm{Si}_4^{\lceil 1;3 \rfloor}\mathrm{O}_8^{[1]}\mathrm{O}_8^{[2]}]\{\boldsymbol{uB}, 3, 1_{\infty}^{2}\}[\mathrm{Si}_6^{\lceil 1;3 \rfloor}\mathrm{O}_{15}^{[1]}](\mathrm{H_2O})_{18}$ or, shortened, $\mathrm{Ca}_{10}\{\boldsymbol{uB}, 3, 2_{\infty}^{1}\}[\mathrm{Si_6O_{16}}]\{\boldsymbol{uB}, 3, 1_{\infty}^{2}\}[\mathrm{Si_6O_{15}}](\mathrm{H_2O})_{18}$. These formulas indicate the co-existence of silicate double-chains and single-layers.

Following a recommendation by the International Union of Pure and Applied Chemistry (IUPAC) ([20]), the crystal chemical formulas of microporous materials with tetrahedral frameworks follow the general scheme

$$|\mathbf{A}_a\mathbf{A}'_{a'}\cdots\mathbf{X}_x\mathbf{X}'_{x'}\cdots\mathbf{Z}_z\mathbf{Z}'_{z'}\cdots\mathbf{M}_m\mathbf{M}'_{m'}|[\mathbf{T}_t\mathbf{T}'_{t'}\mathrm{O}_{x_1}^{[1]}\mathrm{O}_{x_2}^{[2]}].$$

Detailed crystal-chemical formulas for more complex silicates and for inorganic compounds with connected units built from other **T** cations than Si and Al, and other **X** anions than O, can be derived following the procedure described by Liebau [10].

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