AUTOMATIC CRYSTAL CHEMICAL CLASSIFICATION OF SILICATES USING DIRECTION-LABELED GRAPHS

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1. INTRODUCTION

In crystallography several classification methods have been proposed to put crystals in an order suitable for specific purposes. The method we consider in this paper [Li1,Li2] has been developed for the classification of silicates in order to characterize the elements of this largest single group of minerals according to crystal chemical properties. The classification mainly refers to structures in the anion part of silicates which result from connections between $Si\text{-}O_n$ polyhedra via common oxygen atoms ('oxygen bridges'). Silicates are characterized by the shape of fundamental structures formed by the linked polyhedra and suited to compose their anion part by successive linkage.

Until now the classification of a silicate according to this method was performed 'by hand'. In close contact with colleagues from crystallography we have realized an algorithmic solution based on graphs which allows to classify silicates automatically.

After an informal presentation of the classification method we show how the anion part of silicates, considered as 'perfect crystals', can be represented by graphs. The vertices of these graphs represent the $Si\text{-}O_n$ polyhedra of the silicates; their edges are determined by oxygen bridges between polyhedra. Because of the regular structure of crystals such a graph can be characterized without loss of information by a finite directed graph. All classification parameters which cannot be computed from atomic coordinates in a direct way are defined by using this kind of graph.

After the definition of parameters we give algorithms for the determination of fundamental structures. The shape of these fundamental structures which may be finite combinations of polyhedra

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* Part of the work was done while this author was at the Rheinische Wilhelms-Universität Münster

or infinite chains of different types, yields the values of the parameters. Two subproblems turned out to be NP-complete.

2. THE CLASSIFICATION METHOD

Classification of crystals is usually based upon the idea of a 'perfect crystal'. Such an ideal structure can be understood as a 3-dimensional space composed of cells which are arranged in a strict grid-like manner and which are identical with respect to their atomic structure. In reality the extension of crystals is finite, of course, and there are often deviations from the ideal structure such as differences in the chemical composition as well as gaps or transpositions. Since all cells of a perfect crystal coincide in their atomic structure, the specification of a single specimen is sufficient for the complete description of the atomic structure of a perfect crystal. This specimen is called unit cell of the crystal; it is often specified in the form of a so-called asymmetric unit from which the respective unit cell can be generated by application of symmetry operators. To achieve a favourable form for the representation of a unit cell the axes of the coordination system, spanning the 3-dimensional space, are chosen different from the Cartesian system in most cases.

In general, Si-O bonds in silicates are stronger than other bonds. For this reason some classification methods for silicates consider only these bonds. Several elements, among them aluminium as the most important one, may replace silicon in a crystal structure. Under certain conditions these substitutes are identified with silicon. A silicon atom (or its substitute) is either coordinated by 4 oxygen atoms (Figure 1) or by 6 oxygen atoms forming a tetrahedron and an octahedron respectively with the silicon in the centre. In both cases an oxygen atom can be shared by two adjacent polyhedra. Complex structures can result from these connections.

By the method we consider, a silicate is classified by determining the values of several parameters for its anion. If the anion is composed of more than one part, each part is classified seperately. The first parameter, the coordination number, refers to the above mentioned number of oxygen atoms directly bonded to a silicon atom; its value is always 4 or 6, denoting $Si-O_4$ tetrahedra and $Si-O_6$ octahedra, resp. The next two parameters characterize the way polyhedra may be connected: linkedness (possible values: 0,1,2, or 3) specifies the maximal number of oxygen atoms which are shared by two adjacent polyhedra, i.e. whether two polyhedra are isolated, share a corner, an edge or a face (Figure 2). Connectedness specifies the number of different polyhedra a single polyhedron is connected with. The other parameters refer to the structures which result from the connections between polyhedra. These structures can be finite or they can extend to infinity into one, two or three dimensions forming infinite chains, infinite layers and infinite frameworks, resp. The parameter dimensionality gives the respective value (0,1,2 or 3). In the following we deal with structures of dimensionality greater than 0. Their classification is more difficult than the classification of finite structures.

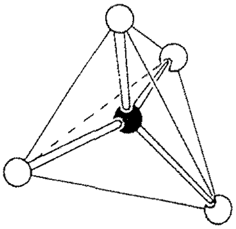


FIGURE 1

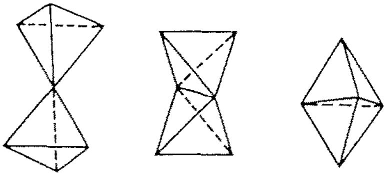


FIGURE 2

The main idea of the method is to build up structures with dimensionality greater than 0 by single chains, so-called fundamental chains. A chain is either a linear sequence of connected polyhedra or such a sequence together with so-called branches. Branches are finite sequences of connected polyhedra which stick out of the linear part of a chain. They may be bound back to the linear part of the chain (loop branch) or not (open branch). A chain without branches is called unbranched chain; chains which have only loop branches or only open branches are called loop branched and open branched, resp. If a chain has both kinds of branches it is called mixed branched. In Figure 3 examples for each of the four possible types of chains are shown. In general, there are several sets of chains which allow to compose the anion part of a silicate. Therefore several criteria are fixed for the selection of sets of fundamental chains. The first criterion determines that only those chains are considered which run into the direction of shortest repetition. This direction is defined by the minimal Euclidean distance between two repeating polyhedra of any chain. Because of the regular structure of crystals each chain has a structural motif which repeats after several polyhedra of its linear part. The number of polyhedra in the linear part of the structural motif is called periodicity of the chain.

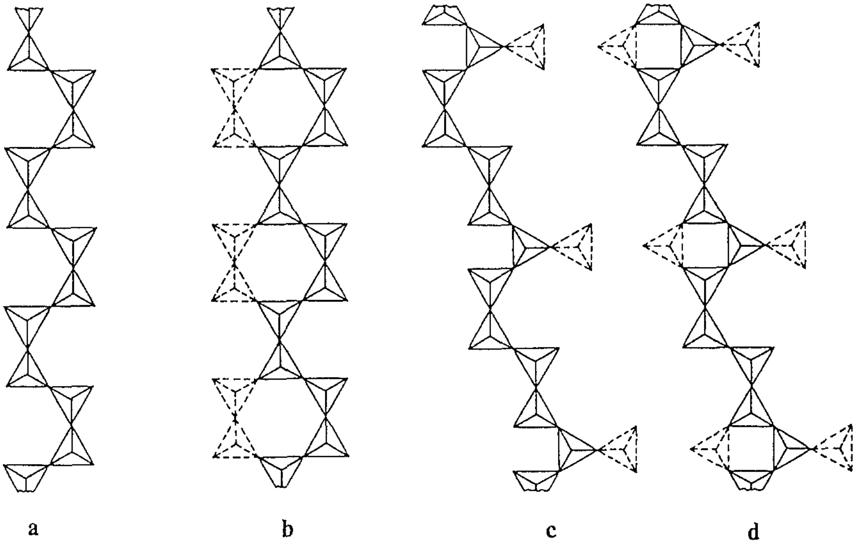
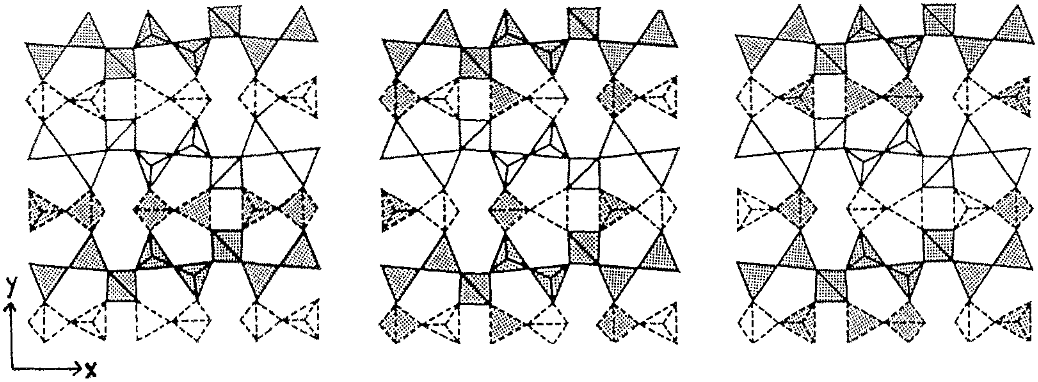


FIGURE 3

a) unbranched chain with periodicity 4 b) loop branched chain with periodicity 4 c) open branched chain with periodicity 5 d) mixed branched chain with periodicity 5

Fundamental chains have to be chosen in such a way that their periodicity is minimal. If there is more than one set of chains fulfilling equally good the criteria mentioned so far, only those sets with lowest number of chains are considered further. For silicates with dimensionality 1 this number is called <u>multiplicity</u> of the silicate. If dimensionality is 2 this parameter is determined by the number of layers which have to be linked to form the anion part of the silicate. In case of dimensionality 3 multiplicity is always 1.

If there is still more than one set left, a choice is made in dependence upon the <u>branchedness</u> of the chains to respect the chemical stability of fundamental chains. The following priorities are fixed: unbranched > loop branched > open branched > mixed branched > hybrid branched. In the first three cases all chains of a set have to be of the same type. A set of fundamental chains is called hybrid branched if it contains open, loop or mixed branched chains together with at least one unbranched chain; in all other cases it is called mixed branched. Figure 4 shows three different ways to describe the single layer found in semenovite. In each case the represented set of candidates for fundamental chains consists of 2 chains with periodicity 6 running parallel to the x-axis. a) shows the correct classification because the represented set of chains is loop branched whereas in b) and c) it is open branched and mixed branched respectively.



a b c

FIGURE 4

3. FORMALIZATION OF THE METHOD

3.1. REPRESENTATION OF SILICATE ANIONS BY GRAPHS

The algorithmic realization of the classification method is restricted to silicate anions with coordination number 4 and linkedness 1. The values for both parameters as well as for the parameter connectedness can be determined in straightforward manner by considering distances between the positions of silicon atoms and oxygen atoms calculated from data of the unit cell. The other parameters refer to the structure formed by the connected $Si-O_n$ polyhedra. For each silicate anion this structure can be represented by an infinite undirected graph.

Definition: Let S be the anion part of a silicate with coordination number 4 and linkedness 1; the tetrahedra graph $G_S^T = (V_S^T, E_S^T)$ of S is derived from S by identifying the tetrahedra of S with the vertices of G_S^T and the connections via oxygen bridges between tetrahedra in S with the edges of G_S^T.

The regular composition of crystals allows to represent tetrahedra graphs by finite digraphs without loss of information. For the construction of this finite graph we adopt the following view of perfect crystals: the natural system spanned by the three linear independent vectors of the unit cell is considered to be the reference system for the position data of all atoms. Thus, each cell can be identified with an element of $\mathbb{Z}^3$, and the coordinates of atoms in the unit cell are elements of $Z_0 := \{(y_1,y_2,y_3) \in \mathbb{R}^3 \, / \, 0 \leq y_1,y_2,y_3 < 1\}$. Let $(y_1,y_2,y_3) \in \mathbb{R}^3$ be the coordinates of an arbitrary atom A of a

perfect crystal. Then its corresponding cell is given by the function
$z \mid \mathbb{R}^3 \rightarrow \mathbb{Z}^3, \quad z(y_1,y_2,y_3) := (\lfloor y_1\rfloor, \lfloor y_2\rfloor, \lfloor y_3\rfloor)$.

Let $t(A)$ be the atom in the unit cell which is translationally equivalent to A; the coordinates of $t(A)$ are given by
$(y_1 - \lfloor y_1\rfloor, y_2 - \lfloor y_2\rfloor, y_3 - \lfloor y_3\rfloor)$.

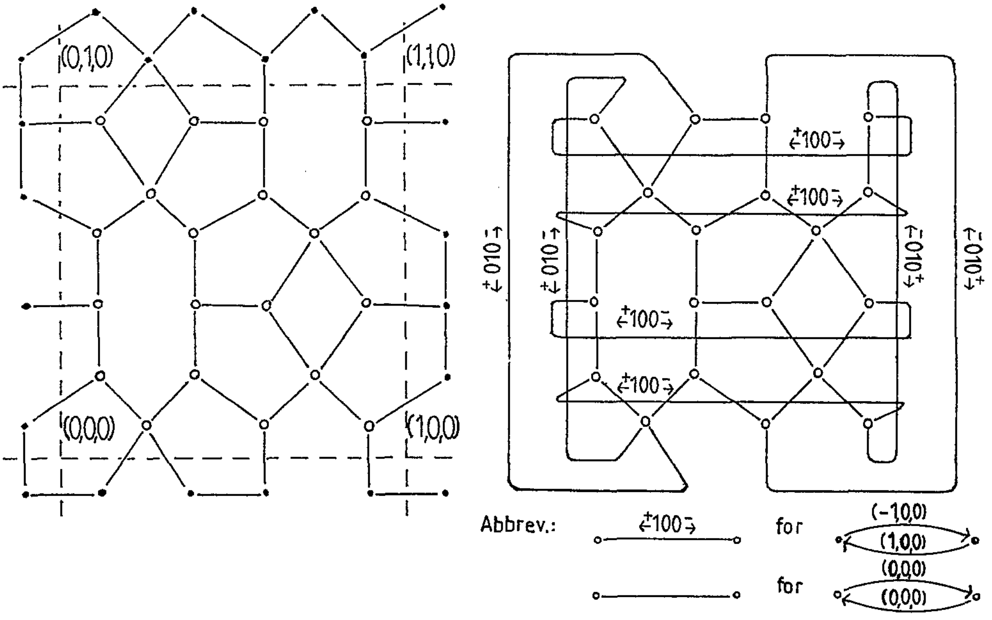
To each vertex v of a tetrahedra graph of a silicate anion S let be associated pos(v), the coordinates of the corresponding silicon atom in S.

Definition: Let $G_S^T = (V_S^T, E_S^T)$ be the tetrahedra graph of a silicate anion S. The direction-labeled graph of S (dl-graph) is the finite digraph $G_S = (V_S, E_S)$ uniquely determined by G_S^T as follows:

$$V_S := V_S^T \cap \{v / pos(v) \in Z_0\}$$

$$E_S := \{e \;/\; e \text{ uniquely determined by: } \alpha(e) \in V_S,\ \omega(e) \in V_S,\ \delta(e) \in \mathbb{Z}^3$$
$$\wedge\ ((\exists\{\check{v}_1,\check{v}_2\} \in E_S^T)(\alpha(e) = \check{v}_1 \wedge \omega(e) = t(\check{v}_2) \wedge t(\check{v}_2) \neq \check{v}_2$$
$$\wedge\ \delta(e) = z(pos(\check{v}_2))) \vee (\{\alpha(e), \omega(e)\} \in E_S^T \wedge \delta(e) = (0,0,0)))\}$$

where α, ω and δ are as follows: an edge $e \in E_S$ is directed from vertex $\alpha(e)$ to vertex $\omega(e)$ and labeled with $\delta(e)$.



Part of the tetrahedra graph of semenovite (Figure 4) and the corresponding dl-graph

FIGURE 5

Lemma 1: There is an epimorphism h between the set of walks in G_S^T and the set of walks in G_S such that the following holds:
let $w = v_1, e_1, v_2, \dots, e_{n-1}, v_n$, $n > 1$, be a walk in G_S^T and let
$h(w) = \tilde{v}_1, \tilde{e}_1, \tilde{v}_2, \dots, \tilde{e}_{m-1}, \tilde{v}_m$;
1) $m = n$
2) $\tilde{v}_i = t(v_i)$, $i = 1, \dots, n$
3) $z(pos(v_j)) - z(pos(v_1)) = \Sigma_{i=1}^{j-1} \delta(\tilde{e}_i)$, $j = 2, \dots, n$.
$\Sigma_{i=1}^{n-1} \delta(\tilde{e}_i)$, the direction of a walk $\tilde{w} = \tilde{v}_1, \tilde{e}_1, \tilde{v}_2, \dots, \tilde{e}_{n-1}, \tilde{v}_n$ in G_S, is denoted by $\triangle(\tilde{w})$.

Corollary: There is a walk $w = v_1, e_1, v_2, \dots, e_{n-1}, v_n$ in G_S^T with $t(v_1) \neq t(v_i), t(v_i) \neq t(v_j)$, for $i \neq j$, $1 < i,j < n$ and $t(v_1) = t(v_n)$ $\Leftrightarrow$ $h(w)$ is a cycle in G_S.

Remarks: To each edge e of G_S there is an inverse edge $\bar{e}$ in G_S with $\alpha(\bar{e}) = \omega(e)$, $\omega(\bar{e}) = \alpha(e)$ and $\delta(\bar{e}) = -\delta(e)$. This redundancy is useful for the formulation of algorithms. In [CHK] a type of graph was introduced which corresponds to a dl-graph with respect to the represented information.

In the following, cycles are considered as sets of edges; a set $\{e, \bar{e}\}$ of inverse edges shall not be a cycle. For an arbitrary set E of edges, V(E) denotes the set of vertices incident with an edge of E; $\bar{E}$ denotes the set of edges being inverse to an edge of E.

3.2 DEFINITION OF CLASSIFICATION PARAMETERS

The dl-graph of a silicate anion splits up into several components if the anion is composed of several parts. Each part of an anion has to be analyzed seperately because there exist so-called mixed-anion silicates whose anion parts have different type. In the following we therefore suppose dl-graphs to be connected.

The parameter dimensionality specifies the number of linear independent directions of repetition in a crystal. In a tetrahedra graph G_S^T a direction of repetition can be found as the direction of a walk w from a node v_1 in the unit cell to a translationally equivalent node $\tilde{v}_1$ in a different cell. From Lemma 1 and its Corollary we know that the corresponding walk h(w) in G_S is a closed walk with direction $z(pos(\tilde{v}_1))$ and that $z(pos(\tilde{v}_1))$ can be obtained as the sum of directions of cycles in G_S.

Definition: Let $G_S = (V_S, E_S)$ be the dl-graph of a silicate anion S; for $U \leq \mathbb{Z}^3$ let <U> denote the closure of U under addition. An element of the set $DR_S := \langle\{\triangle(c) \mid c \text{ cycle in } G_S\}\rangle \cup \{(0,0,0)\}$ is called direction of repetition.

The existence of inverse edges implies that DR_S is closed under negation. By definition DR_S is closed under addition and thus under multiplication with natural numbers. Hence DR_S is a submodule of $\mathbb{Z}^3$ and we can define the parameter dimensionality as follows:

Definition: The dimensionality of a silicate anion S is the dimension of the set of directions of repetition in G_S.

The fundamental chains of a silicon anion S with dimensionality greater than 0 run parallel to the so-called direction of shortest repetition of S which can be defined in terms of the physical length of cycles in G_S.

Definition: Let S be a silicate anion with dimensionality greater than 0; let T be the real 3*3-matrix for the transformation of crystal coordinates as given in the unit cell into Cartesian coordinates and let $\| \ \|$ be the Euclidean norm. The set

$$\begin{aligned} DSR_S := \{ \triangle(c) \mid\ & c \text{ cycle with} \\ & \triangle(c) \neq (0,0,0) \text{ and for all cycles } c' \text{ with} \\ & \triangle(c') \neq (0,0,0) \text{ holds: } \| T * \triangle(c) \| \leq \| T * \triangle(c') \| \} \end{aligned}$$

is called set of directions of shortest repetition of S.

DSR_S is closed under negation. For most silicate anions the set DSR_S consists of an element $t \in \mathbb{Z}^3$ and its negation $-t$. There are a few silicate anions with linear independent elements in DSR_S; in these cases symmetry operators exist such that classification does not depend on the chosen element. For this reason, an arbitrary element of DSR_S can always be fixed as the direction of shortest repetition.
Fundamental chains have to be chosen among arbitrary chains defined as follows:

Definition: Let $G_S = (V_S, E_S)$ be the dl-graph of a silicate anion S with dimensionality greater than 0 and let dsr_S be the direction of shortest repetition of S. A pair ch = (L,B) with $L \subseteq E_S$, $B \subseteq 2^{E_S}$ is called a chain of S if the following holds:

1) L is a cycle in G_S with $\triangle(L) = dsr_S$ and there is no cycle L' in G with $\triangle(L') = dsr$ and $|L'| < |L|$; L is called linear part of the chain.
2) B is a -possibly empty- set of pairwise independent branches of L. Branches are either open branches or loop branches.

An *open branch* b of L is a non-empty set of edges forming a path $(e_1,\dots,e_n)$ with the following properties:

1) $\alpha(e_1) \in V(L)$
2) $\omega(e_i) \notin V(L)$, $i = 1,\dots,n$
3) for all edges $e \in E_S$ with $\alpha(e) \in V(b) \setminus V(L)$ the following holds: there is no cycle $c \neq L$ in $L \cup b \cup \{e\}$ with $\triangle(c) \in \langle\{dsr_S\}\rangle$.

A *loop branch* b of L is a non-empty set of edges forming a path $(e_1,\dots,e_n)$, $n \geq 2$, with the following properties:

1) $\alpha(e_1) \in V(L)$, $\omega(e_n) \in V(L)$
2) $\omega(e_i) \notin V(L)$, $i = 1,\dots,n-1$
3) for all edges $e \in E_S$ with $\alpha(e) \in V(b) \setminus V(L)$ the following holds: there is exactly one cycle $c \neq L$ in $L \cup b \cup \{e\}$ with $\triangle(c) \in \langle\{dsr_S\}\rangle$; this cycle is $b \cup L'$, where $L' = \{e_{n+1}\dots,e_{n+m}\}$ is the subset of edges of L which completes the path $(e_1,\dots,e_n)$ to a cycle.

Two branches b_1, $b_2 \in B$ are called *independent*, if

1) $V(b_1) \cap V(b_2) \subseteq V(L)$
2) there is no edge $e \in E_S$ with $\alpha(e) \in V(b_1)\setminus V(L)$, $\omega(e) \in V(b_2)\setminus V(L)$ such that a cycle $c \subseteq L \cup b_1 \cup \overline{b}_1 \cup b_2 \cup \overline{b}_2 \cup \{e\}$ exists with $e \in c$ and $\triangle(c) \in \langle\{dsr_S\}\rangle$.

A chain ch = (L,B) is called

- unbranched, if $B = \emptyset$
- open branched, if $B \neq \emptyset$ and each $b \in B$ is an open branch
- loop branched, if $B \neq \emptyset$ and each $b \in B$ is a loop branch
- mixed branched, otherwise.

Definition: The *periodicity* of a chain ch = (L,B) is defined as the number of elements of its linear part L.

Some comments on these definitions are necessary. In the definition of chains we require of linear parts of chains to be minimal with respect to the total graph, i.e. all chains of a silicate anion must have the same periodicity in particular. For silicates known so far this condition has no influence on classification. Condition 3) for open branches guarantees that there is no direct link between an open branch in the corresponding tetrahedra graph and the linear part it sticks out. Links to translationally equivalent linear parts, however, are allowed. For loop branches a respective condition excludes direct links not being part of the loop and connecting inner loop nodes with the linear part the loop belongs to. In both cases, indirect links to the linear part are allowed because nodes of such links possibly can be assigned to another linear part. The independence condition is needed to ensure correct classification of branches as open or loop branches.

Fundamental chains for the composition of a silicate anion have to be chosen in such a way that their number is minimal and that the branchedness of the set of chosen chains is maximal with respect to the priorities given above.

Definition: A set $CH = \{ch_1, \dots, ch_n\}$ of chains of a dl-graph $G_S = (V_S, E_S)$ is called chain decomposition of G_S if $\{V(ch_1), \dots, V(ch_n)\}$ is a partition of V_S such that no chains exist in $G - V'$, where $V' \subseteq V_S$ is the set of nodes being part of the linear part of a chain in CH.

CH is called admissible chain decomposition if there is no chain decomposition of G_S with less elements than CH or with the same number of elements as CH and branchedness of higher priority than that of CH. An element of an admissible chain decomposition is called fundamental chain.

Obviously, the parameters multiplicity - in case of dimensionality 1 - and branchedness of a silicate anion S are uniquely determined by the specification of any admissible chain decomposition of G_S. In case of dimensionality 2, connections between fundamental chains have to be analyzed for the determination of multiplicity. This can be done with the help of direction-labeled graphs whose vertices represent fundamental chains and whose edges correspond to links between fundamental chains. Details can be found in [Go].

4. ALGORITHMS

We give a brief description of some of the algorithms for the determination of parameters with graph-based definition and consider two complexity problems connected with chain decomposition.

Following its definition, the parameter dimensionality of a silicate anion S can be determined by considering the directions of all cycles in G_S. This way can be quite inefficient because the number of cycles in a dl-graph can be very large. The following Lemma leads to a more favourable algorithm.

Lemma 2: Let $G_S = (V_S, E_S)$ be the dl-graph of a silicate anion S and let v_1 be an arbitrary but fixed vertex of V_S; for each $v_i \in V_S$ let be given an arbitrary but fixed walk w_{1i} from v_1 to v_i. Let $D_{v_1} = \{ \Delta(w_{1i}) + \Delta(e) - \Delta(w_{1j}) \; / \; e \in E_S, \; \alpha(e) = v_i, \; \omega(e) = v_j \}$. Then $DR_S = \langle D_{v_1} \rangle$.

Thus, dimensionality can be computed as follows: fix some vertex $v_1 \in V_S$; for each $v_i \in V_S$ determine a walk from v_1 to v_i and its direction; compute $\triangle(w_{1i}) + \triangle(e) - \triangle(w_{1j})$ for each $e \in E_S$ and find a basis for the resulting set of directions.
Because $\triangle(w_{1i}) + \triangle(e) - \triangle(w_{1j})$ and $\triangle(w_{1j}) + \triangle(\bar{e}) - \triangle(w_{1i})$ only differ in sign, the algorithm can be improved by considering only one element of each pair of inverse edges of E_S.

For silicate anions with dimensionality 1 the algorithm terminates with a basis consisting of a single element t which is identical to the direction of a cycle in the corresponding dl-graph. Furthermore, the physical length of this cycle is minimal with respect to the physical length of all nontrivial cycles. Thus, t may be chosen as direction of shortest repetition.

If the dimensionality of a silicate anion S is greater than 1, the computed basis consists of two or three elements which need not be directions of cycles in G_S (though that is rarely the case). Therefore we use a generate-and-test algorithm for the determination of the direction of shortest repetition in this case. This algorithm looks at the nonzero vectors of DR_S in ascending order of their length and tests whether there is a cycle in G_S the direction of which coincides with the vector under consideration. The first vector found by this proceeding gives the direction of shortest repetition.
To find admissible chain decompositions of a given G_S the linear parts of all chains are determined first. This is done by investigating all cycles in G_S in the order of increasing length. The first cycle c with direction dsr_S found in this way determines periodicity of S. All cycles with direction dsr_S having the same length as c are collected. The resulting set of cycles is searched for so-called admissible sets of linear parts suited to be completed to admissible chain decompositions.

Definition: Let $G_S = (V_S, E_S)$ be the dl-graph of a silicate anion S with dimensionality greater than 0, let C_S be the set of cycles in G_S with direction dsr_S having length equal to the periodicity of S. A set $LP_S \subseteq C_S$ is called admissible set of linear parts of chains if

1) for all L, L' $\in LP_S$ with $L \neq L'$, $V(L) \cap V(L') = \emptyset$ (independence)
2) for each linear part L'' $\in C_S$ there is some $L \in LP_S$ with $V(L) \cap V(L'') \neq \emptyset$ (completeness).

The number of chains and the number of admissible sets of linear parts of chains in G_S cannot be bound by polynomials in $|V_S|$ or $|E_S|$. We rather can state

<u>Lemma 3</u>: The problem 'given a dl-graph, is there an admissible set of linear parts of chains with cardinality k or less' is NP-complete in the number of linear parts of chains.

<u>Sketch of proof</u>: Admissible sets of linear parts of chains correspond one-to-one to dominating and independent sets of vertices in the simple graph G = (V,E), given as follows: For each linear part of a chain in the underlying dl-graph there is a vertex in V; two vertices are connected by an edge $e \in E$ if the corresponding linear parts have some vertex in common. The problem whether there exists some dominating and independent set with cardinality k or less is known to be NP-complete [GJ]∎

According to the definition of admissible chain decompositions, we have to look for those admissible sets of linear parts of chains which have lowest cardinality. If such a set doesn't cover all the vertices of G_S, it must be tried to connect the remaining vertices to the linear parts in form of loop branches and open branches. Should this not be possible, the next admissible set has to be considered. If there is no more such set, admissible sets with next higher cardinality are considered. A subproblem connected with the assignment of open branches turned out to be NP-complete.

<u>Lemma 4</u>: The problem 'given a dl-graph G_S and an admissible set of linear parts of chains, is there a chain decomposition of G_S in open branched chains with the given linear parts' is NP-complete.

<u>Sketch of proof</u>: The problem is in NP since a solution can be guessed and checked in nondeterministic polynomial time. The proof of completeness is based on a deterministic transformation of polynomial time-complexity from graph 3-colourability. The underlying idea is to extend a given instance of the graph 3-colourability problem in such a way that a dl-graph results which has a decomposition in open branched chains iff the given instance is 3-colourable∎

Although in theory determination of admissible chain decompositions is intractable, in practice such decompositions can mostly be found in reasonable time due to the preference of nature for simple shapes.

5. FINAL REMARKS

Based on the definitions and algorithms described in the previous sections an interactive system for the automatic classification of silicates was implemented on a SIEMENS 7760 computer. The system takes the atomic coordinates and the symmetry operators of asymmetric units or unit cells as input and computes all classification parameters (if possible). More than 300 of silicates have already been classified by the system. Some of these silicates could not be classified before because of their complexity.

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