

CLASSIFICATION OF PHYLLOSILICATES ACCORDING TO THE SYMMETRY OF THEIR OCTAHEDRAL SHEETS

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A system of additional prefixes homo-, meso-, hetero- extends the current nomenclature of phyllosilicates based on the occupation of octahedral positions in their crystal structures (tri-, dioctahedral) so as to characterize also the symmetry proper of octahedral sheets.

INTRODUCTION

Refinements of the crystal structures of various phyllosilicates revealed that the current classification into the tri- or dioctahedral classes according to the occupation of octahedral positions should be improved. If a structure is trioctahedral, then the three octahedral positions per unit structure can either be occupied by three atoms of the same kind, or two positions, or even all three may be occupied differently in an ordered way. A similar situation can be encountered in dioctahedral species. Such facts are usually described by additional comments (*e. g.* a trioctahedral structure with octahedral ordering, refinement of a mica structure in subgroup symmetry), which *de facto* indicate the symmetry of the corresponding octahedral sheet.

The symmetry of the octahedral sheet is indispensable for a theoretical investigation of polytypism of phyllosilicates, mainly for the calculation of the number of possible positions in the stacking of individual layers, for the systematic derivation of standard, regular, or MDO (Maximum Degree of Order) polytypes, and for the analysis of the symmetry of entire polytypes. The distribution of distinct crystallochemical entities (including voids) over the three octahedral positions is irrelevant in such cases and it is only the symmetry which counts.

It is thus desirable to modify the current classification system so as to express both the occupancy and the symmetry of octahedral sheets. It should be flexible enough to allow either one and/or the other aspect to be stressed or ignored at will.

To achieve this goal, we started using a system of prefixes indicating the symmetry of octahedral sheets [1-5]. It is the aim of this paper to explain this system more thoroughly and illustrate it by examples.

THE NEW PREFIXES

The prefixes which indicate the symmetry proper of an octahedral sheet are as follows:

- | | |
|---------|--|
| homo- | all three octahedral sites are occupied by the same kind of crystallochemical entity, <i>i. e.</i> by the same kind of ion or by a statistical average of different kinds of ions including voids; ideal symmetry of the octahedral sheet is $H(3)m$ or $H(\bar{3})12/m$, |
| meso- | two octahedral sites are occupied by the same kind of crystallochemical entity, the third by a different one in an ordered way; ideal symmetry of the octahedral sheet is $P(3)m$ or $P(\bar{3})12/m$, |
| hetero- | each of the three octahedral sites is occupied by a different crystallochemical entity in an ordered way; ideal symmetry of the octahedral sheet is $P(3)$ or $P(3)2^1$. |

These prefixes can either be combined with the current prefixes di-, tri-, perhaps also mon- for cases when there is only one octahedral cation per the three sites, omitted if irrelevant or if the available information on the structure (which depends on the resolving power of the experimental method used) does not warrant their use, or used without the second prefix tri-, di-, mon-, if only the symmetry is relevant to the given problem. Either of the two kinds of prefixes or their combination refers also to the mineral itself.

DISCUSSION

The combinations of prefixes together with schemes showing the occupation of the three octahedral sites are given in Table I and refer to one unit cell or to a strictly periodic structure. For such cases no other combinations (empty windows in Table I) are possible. However, average structures can be conceived, with incomplete occupancies of octahedral sites, such as the structure of heat-treated muscovite which has been supposed [6] to contain two Al atoms randomly distributed over the three octahedral sites². Such

¹The symbols of polar and non-polar layer groups refer to the structures of the serpentine-kaolinite group and to those containing 2:1 layers, respectively. *H* denotes a hexagonally centred cell.

²This structural model, however, was later discredited [7,8].

Table I
Possible combinations of prefixes characterizing an octahedral sheet

		Crystal chemistry		
		trioctahedral	dioctahedral	monooctahedral
Symmetry	homo-	homo-trioctahedral ● ● ●	—	—
	meso-	meso-trioctahedral ● △ △	meso-dioctahedral □ ● ●	meso-monooctahedral ● □ □
	hetero-	hetero-trioctahedral ● △ ○	hetero-dioctahedral □ △ ○	—

□ - vacancy, ● ○ △ - different atoms

structure would then be labelled homo-dioctahedral.

Some examples are given in Table II.

Different occupancies of octahedral positions influence shapes and sizes of the corresponding octahedra. This also should be kept in mind when deciding about the classification. For example, cronstedtite-3T [15] has all three octahedra completely occupied by Fe atoms, but one of these octahedra is significantly different than the other two. Accordingly, this polytype is meso-trioctahedral.

It should be pointed out that in our earlier papers [16, 17], we assigned symmetry to terms "trioctahedral", "dioctahedral" and "monooctahedral" rather than just occupancy. This created undesirable confusion and, ultimately, prompted the creation of the system of prefixes presented in this paper.

The new prefixes imply nothing about the ordering of tetrahedral cations nor do they resolve the still open dispute concerning the exact limit³ between trioctahedral and dioctahedral species.

The described prefixed may appear complicated, especially for chlorites and vermiculites. But, is the situation not similar *e. g.* to that in the nomenclature of organic substances which also necessitate some-

times very complex system in order to specify exactly the substance with structure known in sufficient detail?

Finally, we believe that this system will cause no confusion among field geologists as expressed by our partners when working on this proposal. If they do not need it, they can simply ignore it. After all, even the prefixes tri-, di- are often left out when irrelevant, and the samples are simply called micas, chlorites, *etc.*

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³At present tacitly assumed at about 2.5 atoms per three octahedral sites, but nowhere stated explicitly.

Table II

Characteristics of some phyllosilicates relevant to their classification

Mineral [Ref] $\sum M_i$	Occupation of octahedra			Classification
	M1	M2	M3	
Lizardite-1T [9] 2.98	Mg _{2.82} Fe _{0.07} Al _{0.09} uniform distribution			homo- trioctahedral
Dickite [10] 2	□	Al	Al	meso- dioctahedral
Zinnwaldite-1M [11, 12] 2.72	Fe _{0.49} Mn _{0.03} Li _{0.34} □ 0.14	Al _{1.00}	Fe _{0.45} Mn _{0.03} Li _{0.33} □ 0.14 Al _{0.05}	hetero- trioctahedral
Protolithionite-1M [12] 2.94	Al _{0.11} Mg _{0.01} Fe _{0.72} Mn _{0.02} Li _{0.12} □ 0.02	Al _{0.18} Mg _{0.01} Fe _{0.66} Mn _{0.02} Li _{0.11} □ 0.02	Al _{0.18} Mg _{0.01} Fe _{0.66} Mn _{0.02} Li _{0.11} □ 0.02	meso- trioctahedral
Protolithionite-3T [12] 2.70	Fe _{0.62} Mn _{0.01} Li _{0.13} □ 0.24	Al _{0.77} Fe _{0.22} Mn _{0.01}	Fe _{0.67} Mn _{0.01} Li _{0.26} □ 0.06	hetero- trioctahedral
Mg-vermiculite [13] 3.00/0.41	Mg _{0.87} Fe _{0.13} Mg _{0.41}	Mg _{0.87} Fe _{0.13} □ in the interlayer	Mg _{0.87} Fe _{0.13} □	homo-tri, meso-mon- octahedral
Clinocllore IIb-2 [14] 3.00/3.00	Mg _{0.50} Al _{0.50} (M2 in [14])	Mg _{2.75} Fe _{0.25} uniform distribution in the 2:1 layer	Mg _{1.25} Al _{0.50} Fe _{0.25} uniform distribution in the interlayer	homo-tri, meso-tri- octahedral

 $\sum M_i$ – total number of atoms per three octahedral sites, □ – vacant position

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KLASIFIKÁCIA FYLOSILIKÁTOV PODĽA SYMETRIE ICH OKTAEDRICKÝCH SIETÍ

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Klasické delenie fylosilikátov na tri- a dioktaedricke nepostačuje v prípadoch, keď treba zohľadniť symetriu ich

oktaedrických sietí. Ak je napr. štruktúra trioktaedrická, potom tri oktaedrické polohy v jednotkovej štruktúre môžu byť obsadené buď tromi rovnakými atómami, alebo dva atómy sú rovnaké a tretí iný, alebo všetky tri atómy sú rôzne, ale rozmiestnené usporiadane: tieto skutočnosti podmieňujú symetriu príslušnej oktaedrickej siete.

Na odlíšenie týchto alternatív sa zaviedli osobitné predpony: homo-, ak sú všetky tri oktaedrické polohy obsadené rovnakými kryštalochemickými entitami, t.j. buď atómami rovnakého druhu, alebo štatistickým priemerom rôznych druhov včítane vakancií, mezo-, ak sú dve oktaedrické polohy obsadené rovnakými kryštalochemickými entitami a tretia je obsadená odlišne, hetero-, ak je každá z troch oktaedrických polôh obsadená odlišne, ale usporiadaným spôsobom.

Tieto predpony možno kombinovať s bežnými predponami tri-, di-, prípadne aj mon-, pre prípad jediného oktaedrického atómu pripadajúceho na tri polohy (Tabuľka I), a možno ich vynechať, ak sú nerelevantné alebo ak štruktúra nie je dostatočne známa. Možno ich však používať aj samotné, ak je dôležitá iba symetria.

Charakterizácia oktaedrickej siete pomocou jednotlivých predpón alebo ich kombinácií sa prenáša aj na samotný minerál (Tabuľka II).