IMA 2022
MINERALOGY AND SPACE
Lyon, France • 18-22 July

On (IMA) mineral species

Ferdinando Bosi

Department of Earth Sciences, Sapienza Università di Roma, Italy

Frédéric Hatert

Laboratory of Mineralogy, University of Liège, Belgium

SAPIENZA
UNIVERSITÀ DI ROMA

PLAN OF THE TALK

Chapter 1. Definition of a mineral

Chapter 2. The formulae of minerals

Chapter 3. Unstable minerals

Chapter 4. Biominerals

Chapter 5. Exceptions to the CNMNC rules

All mineral pictures from Mindat

CHAPTER 1: DEFINITION OF MINERALS

MINERALS are the **SOLID** part of terrestrial and extra-terrestrial materials.

- It is important to realize what a mineral is.

MINERAL SPECIES ACCORDING TO THE IMA-CNMNC

(International Mineralogical Association's Commission on New Minerals, Nomenclature and Classification)

The concept of IMA mineral species is discussed in detail in Nickel (1995), and Nickel and Grice (1998).

The Canadian Mineralogist
Vol. 33, pp. 689-690 (1995)

THE DEFINITION OF A MINERAL

ERNEST H. NICKEL*

Division of Exploration & Mining, CSIRO, Wembley, WA 6014, Australia

The Canadian Mineralogist
Vol. 36, pp. x-xx (1998)

THE IMA COMMISSION ON NEW MINERALS AND MINERAL NAMES: PROCEDURES AND GUIDELINES ON MINERAL NOMENCLATURE, 1998

ERNEST H. NICKEL*

Division of Exploration and Mining, CSIRO, Private Bag, P.O. Wembley, W.A., 6014, Australia

JOEL D. GRICE**

Mineral Sciences Division, Canadian Museum of Nature, P.O. Box 3443A, Station "D", Ottawa, Ontario KIP 6P4

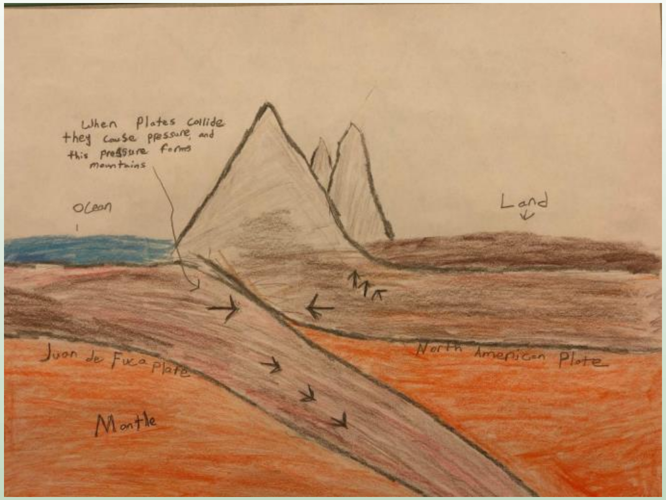
Summarizing Nickel (1995), and Nickel and Grice (1998):
A mineral species is a solid chemical substance that forms by geological processes.

This definition implies that:

- substances of biogenic origin that are transformed by the action of geological processes may be regarded as minerals;
- mineral structures can be crystalline, quasi-crystalline or non-crystalline.

The basic requirement for an inorganic/organic solid phase to be a mineral is *to have a **homogeneous atomic arrangement** proving its uniqueness.*

Non-homogeneous geological objects are called "rocks"…



Recognized mineral species with quasi-crystalline and non-crystalline structure

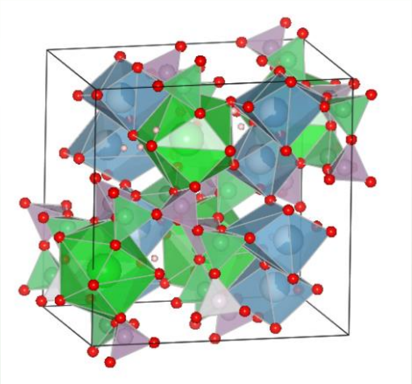
Amorphous minerals					
Allophane	$Al_2O_3(SiO_2)_{1.3\text{-}2.0} \cdot 2.5\text{-}3.0H_2O$	G	Metastibnite	Sb_2S_3	G
Angastonite	$CaMgAl_2(PO_4)_2(OH)_4 \cdot 7H_2O$	Rd	Meymacite	$WO_3 \cdot 2H_2O$	Rd
Cadwaladerite	$Al_2(H_2O)(OH)_4 \cdot n(Cl,OH,H_2O)$	Rd	Moluranite	$H_4U^{4+}(UO_2)_3(MoO_4)_7 \cdot 18H_2O$	G
Delvauxite	$CaFe^{3+}{}_4(PO_4)_2(OH)_8 \cdot 4\text{-}5H_2O$	G	Neotocite	$(Mn,Fe)SiO_3 \cdot H_2O$ (?)	G
Diadochite	$Fe^{3+}{}_2(PO_4)(SO_4)(OH) \cdot 6H_2O$	G	Opal	$SiO_2 \cdot nH_2O$	G
Evansite	$Al_3(PO_4)(OH)_6 \cdot 8H_2O$	G	Santabarbaraite	$Fe^{3+}{}_3(PO_4)_2(OH)_3 \cdot 5H_2O$	A
Georgeite	$Cu_2(CO_3)(OH)_2$	Rd	Thorosteenstrupine	$(Ca,Th,Mn)_3Si_4O_{11}F \cdot 6H_2O$	A
Gerasimovskite	$Mn^{2+}(Ti,Nb)_5O_{12} \cdot 9H_2O$ (?)	G	Umbozerite	$Na_3Sr_4ThSi_8(O,OH)_{24}$	A
Jordisite	MoS_2	G			
Quasicrystal minerals					
Icosahedrite	$Al_{63}Cu_{24}Fe_{13}$	A	Decagonite	$Al_{71}Ni_{24}Fe_5$	A

Santabarbaraite: Defined as amorphous mineral in 2000
Angastonite: Redefined as amorphous mineral in 2021

DIFFERENCES AMONG MINERAL SPECIES

Three criteria can be set up to distinguish the IMA-CNMNC mineral species:

1. **Compositional criterium**



2. **Structural criterium**

3. **Historical criterium**

1. Compositional criterium

- Since most of the mineral species (> 99%) have a crystalline structure, the so-called "50 % rule" was used in the past: "…at least one structural site in the potential new mineral should be dominated by a different chemical element than that present at an equivalent site in an existing mineral" (Nickel and Grice 2008).
- This rule was improved, leading to the the dominant-constituent rule and its extension: the dominant-valency rule (Hatert & Burke, 2008; Bosi et al., 2019).

$^{[8]}(Mg_{1.3}Fe^{2+}{}_{1.2}Ca_{0.5})_{\Sigma 3.00}{}^{[6]}Al_2(SiO_4)_3$ → $Mg_3Al_2(SiO_4)_3$ (pyrope)

($Mg > Fe^{2+} > Ca$)

(dominant-constituent rule)

$^{[8]}(Ca_{1.4}Fe^{2+}{}_{1.1}Mg_{0.5})_{\Sigma 3.00}{}^{[6]}Al_2(SiO_4)_3$ → $Ca_3Al_2(SiO_4)_3$ (grossular)

($Ca > Fe^{2+} > Mg$)

2. Structural criterium…for polymorphs

A mineral species is typically characterized by chemical composition and crystallographic properties.

The **IUCr online dictionary of crystallography** defines polymorphs as substances with the same chemical composition but exhibiting different crystal structures.

According to the **IMA-CNMNC guidelines** (Nickel and Grice 2008), the polymorphic forms of a mineral are regarded as different species **only if their structures are topologically different.**
(Bond topology: connectivity of chemical bonds in the structure)

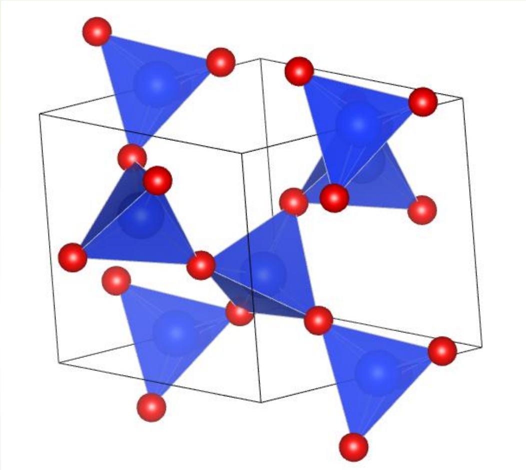
→ *Topologically similar polymorphs are not considered as separate species*

NOT ADDRESSED IN THIS TALK (for details, see Nickel & Grice 1998)

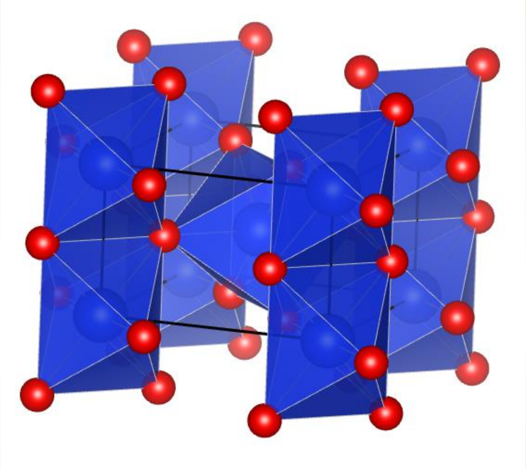
- ***Polytypes and polytypoids*** *are not regarded as separate species.*
- ***Modulated structures*** *are not regarded as separate species.*
- ***Polysomatic series****: may be regarded as separate species if they have specific properties.*
- ***Regular interstratifications:*** *a regular interstratification of talc and a trioctahedral smectite qualifies as a separate mineral species aliettite.*

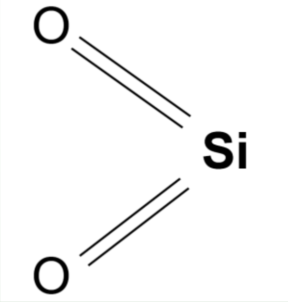
Quartz, [4]Si [2]O_2
$P3_221$

Stishovite, [6]Si [3]O_2
$P4_2/mnm$



Different structures

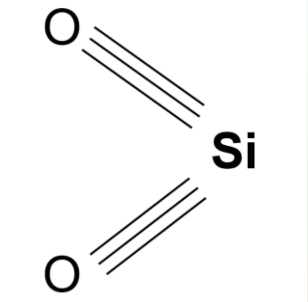




(bond graph)

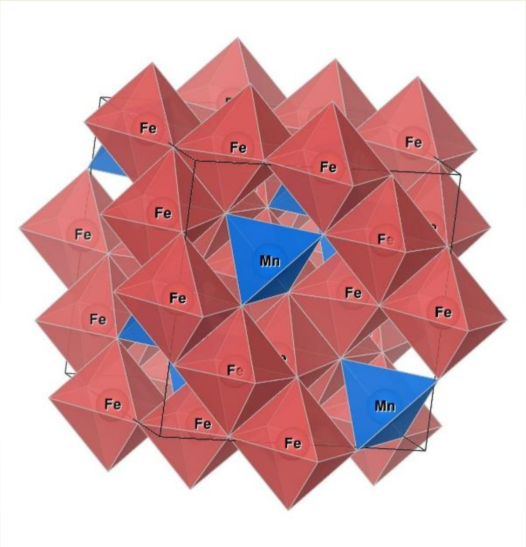
Different bond topology

DIFFERENT SPECIES



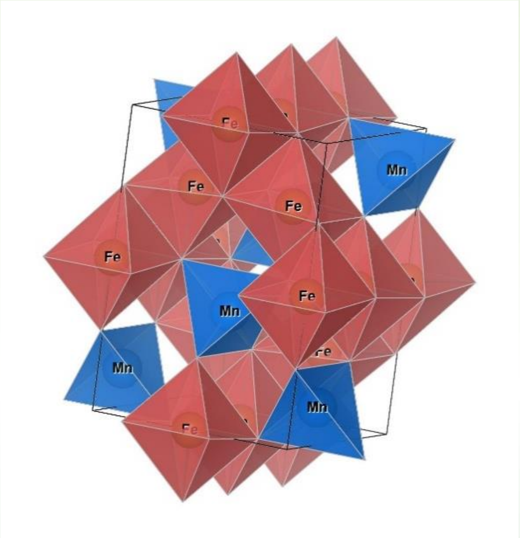
(bond graph)

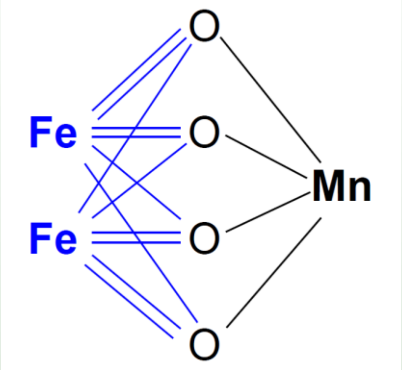
Jacobsite, $^{[4]}Mn\ ^{[6]}Fe_2\ O_4$ (***Fd-3m***)



“Different” structures

“Iwakiite”, $^{[4]}Mn\ ^{[6]}Fe_2\ O_4$ (***I4$_1$/amd***)



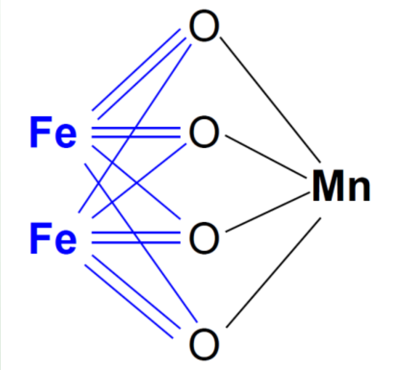


Same bond topology

SAME SPECIES

“Iwakiite” = Jacobsite-*Q*

(topologically similar polymorph of jacobsite)



Apparently odd with the IMA rules…

3. Historical criterium

Occasionally, mineral species with similar topologies and structures such as K-feldspars (monoclinic **sanidine,** triclinic **microcline** and **orthoclase**) are distinguished only by symmetry (space-group type) or atom ordering schemes.

Their names are retained in the mineral lexicon for *historical reasons*.

Some mineral species are so embedded in the scientific literature that their discreditation would have a negative effect on the scientific community.

Considerations of the historical criterion may therefore be overriding over the structural and chemical ones

<u>Historical criterium prevailing over compositional one</u>

Minerals may also be defined by a range of compositional variability in contrast to the dominant-constituent rule:

e.g., the tremolite – **actinolite** – ferro-actinolite join in amphiboles.

Maintained for "petrological" reasons

Tremolite

$\square Ca_2(Mg_5)Si_8O_{22}(OH)_2$

Ferro-actinolite

$\square Ca_2(Fe^{2+}_5)Si_8O_{22}(OH)_2$

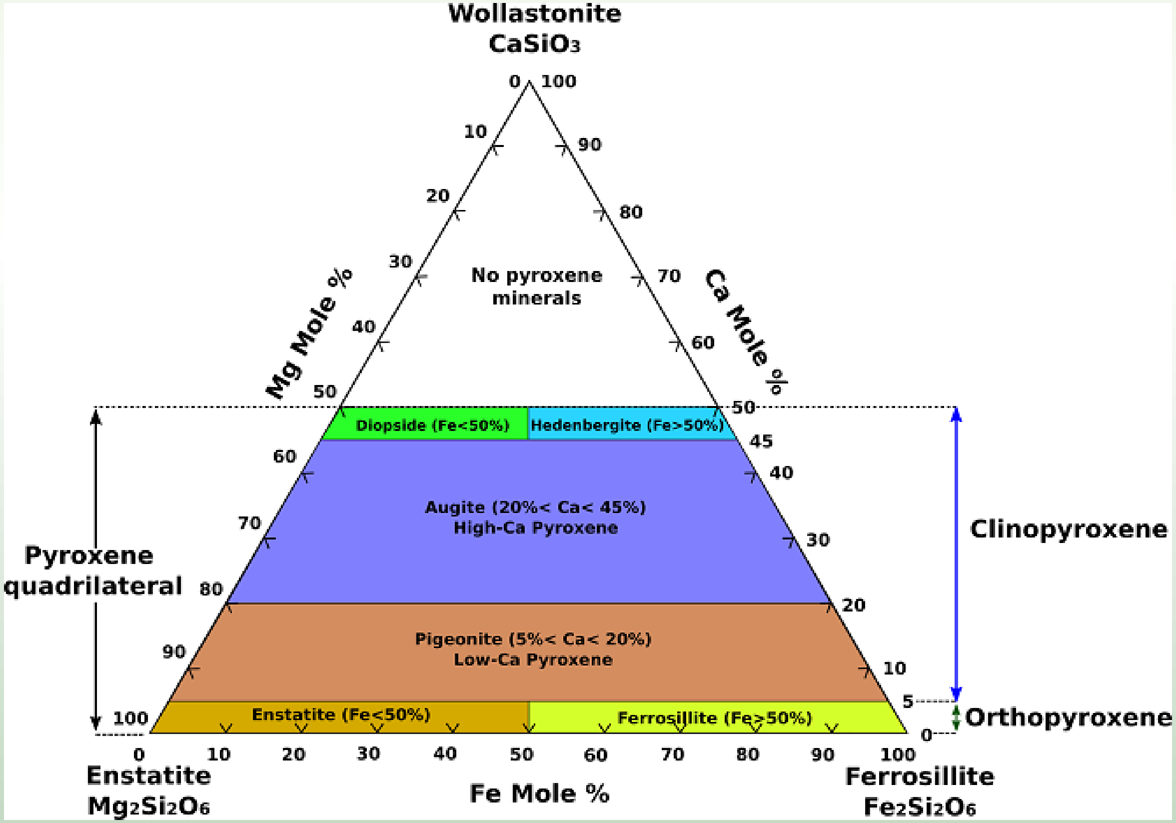
$\square Ca_2(Mg_{4.5-2.5}Fe^{2+}_{0.5-2.5})Si_8O_{22}(OH)_2$

Mg = 5 **4.5** **Actinolite** **2.5** **0 (Fe^{2+} = 5)**

Similar argumentations applied, for example, to

Augite, $[Ca_{0.9-x}(Mg,Fe)_{0.1+x}](Mg,Fe)Si_2O_6$ ($x \leq 0.4$)

Pigeonite, $[(Mg,Fe)_{0.9-x}Ca_{0.1+x}](Mg,Fe)Si_2O_6$ ($x \leq 0.3$)



HOW CAN WE REPRESENT A MINERAL SPECIES?

With a **pertinent name**, accompanied by an **ideal chemical formula**.

- **Jacobsite**, ideally $\mathbf{MnFe_2O_4}$
- **Jacobsite-*Q***, ideally $\mathbf{MnFe_2O_4}$

Note that the ideal formula should correspond to an *endmember* composition.

But some exceptions exist…..

Mineral Formula: Endmember Formula *vs.* Ideal Formula

Magnesio-hornblende $^{A}\square^{B}Ca_2{}^{C}(Mg_4Al)^{T}(Si_7Al)O_{22}(OH)_2$

can be represented as

50% tremolite $^{A}\square^{B}Ca_2{}^{C}(Mg_5)^{T}Si_8O_{22}(OH)_2$

50% tschermakite $^{A}\square^{B}Ca_2{}^{C}(Mg_3Al_2)^{T}(Si_6Al_2)O_{22}(OH)_2$

…$^{C}(Mg_5)^{T}(Si_8)$…	**…$^{C}(Mg_4Al)^{T}(Si_7Al_1)$…**	**…$^{C}(Mg_3Al_2)^{T}(Si_6Al_2)$…**
Tremolite (endmember)	**Magnesio-hornblende** (intermediate-member)	Tschermakite (endmember)
ideal formula	ideal formula	ideal formula

Amphibole general chemical formula

$A\ B_2\ C_5\ T_8\ O_{22}\ W_2$

Amphibole structural formula

$A\ M(4)_2\ [M(1)\ M(2)_2\ M(3)_2]\ [T(1)_4\ T(2)_4]\ O_{22}\ O(3)_2$

$A = A$

$B_2 = {}^{[6\text{-}8]}M(4)_2$

$C_5 = {}^{[6]}[M(1)\ M(2)_2\ M(3)_2]$

$T_8 = {}^{[4]}[T(1)_4\ T(2)_4]$

$W_2 = O(3)_2$

Grouping of some crystallographic sites for nomenclature purpose (allowed by the guidelines of Hatert & Burke, 2008)

Amphibole chemical formula

$A\ B_2\ C_5\ T_8\ O_{22}\ W_2$

Amphibole structural formula

$A\ M(4)_2\ [M(1)\ M(2)_2\ M(3)_2]\ [T(1)_4\ T(2)_4]\ O_{22}\ O(3)_2$

Magnesio-hornblende

$^{A}\square\,^{B}Ca_2\,^{\mathbf{C}}\mathbf{(Mg_4Al)}^{\mathbf{T}}\mathbf{(Si_7Al)}O_{22}(OH)_2$

$^{A}\square\ ^{M(4)}Ca_2\ [^{M(1)}Mg\ ^{\mathbf{M(2)}}\mathbf{(AlMg)}\ ^{M(3)}Mg_2]\ [^{\mathbf{T(1)}}\mathbf{(Si_3Al)}\ ^{T(2)}Si_4]\ O_{22}\ ^{O(3)}(OH)_2$

Reducible to the end-members

50% tremolite

$^{A}\square\ ^{M(4)}Ca_2\ [^{M(1)}Mg\ ^{\mathbf{M(2)}}\mathbf{(Mg^{2+}_2)}\ ^{M(3)}(Mg_2)]\ [^{\mathbf{T(1)}}\mathbf{(Si^{4+}_4)}\ ^{T(2)}(Si_4)]\ O_{22}\ ^{O(3)}(OH)_2$

50% tschermakite

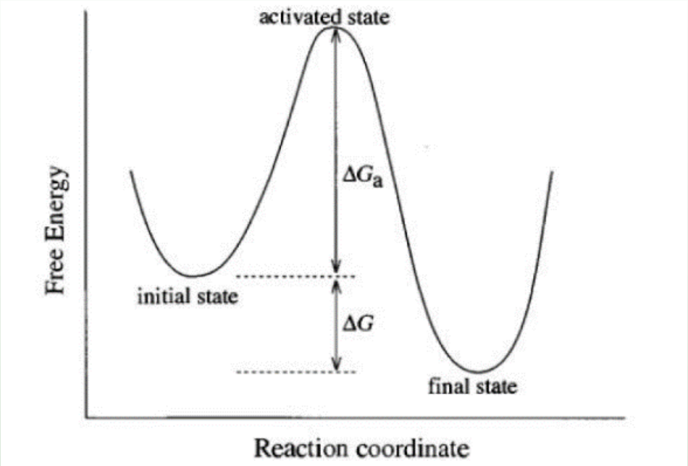
$^{A}\square\ ^{M(4)}Ca_2\ [^{M(1)}Mg\ ^{\mathbf{M(2)}}\mathbf{(Al^{3+}_2)}\ ^{M(3)}(Mg_2)]\ [^{\mathbf{T(1)}}\mathbf{(Si^{4+}_2Al^{3+}_2)}\ ^{T(2)}(Si_4)]\ O_{22}\ ^{O(3)}(OH)_2$

Tremolite and tschermakite formulae are *irreducible*.

MINERAL FORMED UNDER NON-AMBIENT CONDITIONS

Many minerals may be formed under conditions of relative HT and/or HP and may therefore be metastable at ambient conditions.

- For some minerals, the reaction rates from a metastable to a stable status are very low, so that they may persist for billions of years.
- *e.g.,* transformation of diamond to graphite is so very slow that it is possible to **characterize diamond from laboratory experiments *using normal procedures***.



- For other minerals, the reaction rates can be quick enough that they tend to hydrate/dehydrate or melt/evaporate when removed from their place of origin and thus not persist under ambient conditions.
- *e.g.*, mercury is liquid at room temperature, but it crystallizes below –39 °C in *R*-3*m* space-group type.

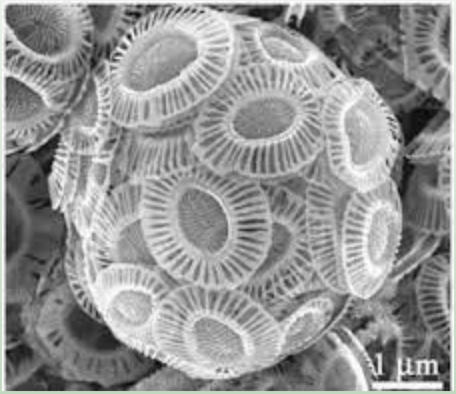
It exists cold geological environments at the Earth's surface where solid mercury may occur; northern regions of Siberia with T < –39 °C (and likely in Antarctica).

According to the IMA-CNMNC guidelines (Nickel and Grice 1998), metastable mineral substances (ephemeral minerals) can be accepted as mineral species if they can be adequately characterized by using *special procedure in the investigation*.

CHAPTER 4: BIOMINERALS
Biologic *vs.* geological processes

Biominerals are all those mineral substances in which organisms played an important role, but at the same time a geological process was involved in their formation.

- *Fossils* are constituted by biominerals, since their skeletons were formed by biological processes, and were then affected by diagenesis.
- *e.g.*, an organism excretes a liquid that may crystallize as a result of evaporation (geological process) on a natural surface. This substance may be approved as a mineral such as urea in guano deposits.



Chapter 5: Exceptions to the CNMNC rules

IMPORTANT message to the scientific community

The IMA-CNMNC does not wish to impose an arbitrary set of rigid rules, but rather to provide consistent guidelines to define new minerals and to rationalize mineral nomenclature

In this regard, consider the mineral redefinition/discreditation process.

According to Nickel and Grice (1998), redefinition/discreditation of a mineral species **requires a re-examination of the type specimen**, a comparison of the new data with the original, and justification for the redefinition/discreditation.

- This recommendation should always be followed, but….. in case of the mineral redefinition/discreditation based on the original chemical and/or structural data, **does it make sense to reanalyze the type specimen?**

→ *Exceptions are always possible!*

First examples of exceptions

Approved proposal with the type specimen not reanalyzed

- The name "hibschite" (IMA-approved mineral) was discredited in favor of grossular as Si is the dominant cation at the *Z* site (Grew et al. 2013): $^{X}(Ca_3)^{Y}(Al_2)^{Z}(Si_{3-x}\square_x)O_{12-4x}(OH)_{4x}$ where $x < 1.5$

- "Ferri-ottoliniite" (IMA-approved in 2001) was discarded in the amphibole nomenclature because it does not obey the new rules for classification (Hawthorne et al. 2012).

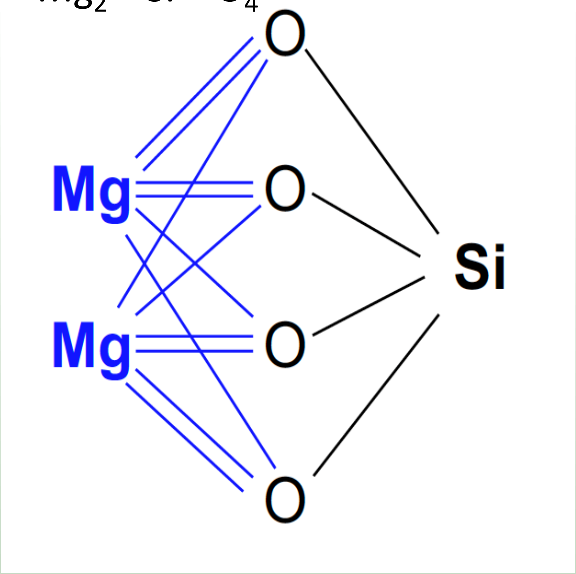
- Executive decision taken by the CNMNC officers:

➢ Potassium is known to be essential in nepheline; thus, the nepheline formula in the CNMNC list was changed from $NaAlSiO_4$ to $Na_3K(Al_4Si_4O_{16})$. Chemical analyses of nepheline from the type locality (Monte Somma-Vesuvius area, Italy) match the latter formula (CNMNC Newsletter No. 42, April 2018).

<u>Second example of exceptions</u>
<u>Approved proposal divergent from the IMA-polymorph recommendation</u>

In the spinel nomenclature (Bosi et al. 2019), we encountered a problem with ringwoodite (spinel structure) and forsterite (olivine structure), ideally Mg_2SiO_4, as **they have the same local bond topology!**

$^{[6]}Mg_2\ ^{[4]}Si\ ^{[4]}O_4$



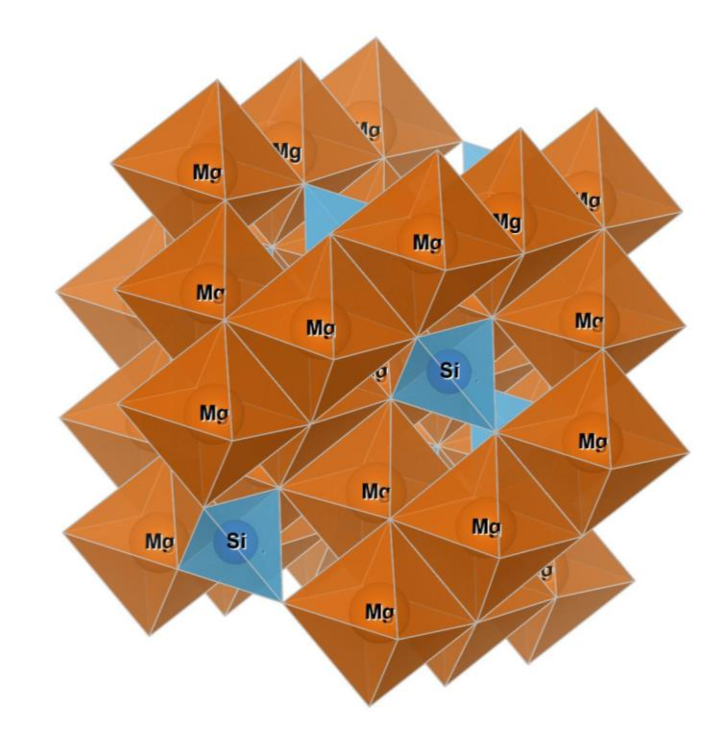
***IMA**: polymorphic forms of a mineral are regarded as different species if their structures are topologically different!*

$^{[6]}Mg_2\,^{[4]}Si\,^{[4]}O_4$: ringwoodite *vs*. forsterite

Geometric elements shared by the polyhedra

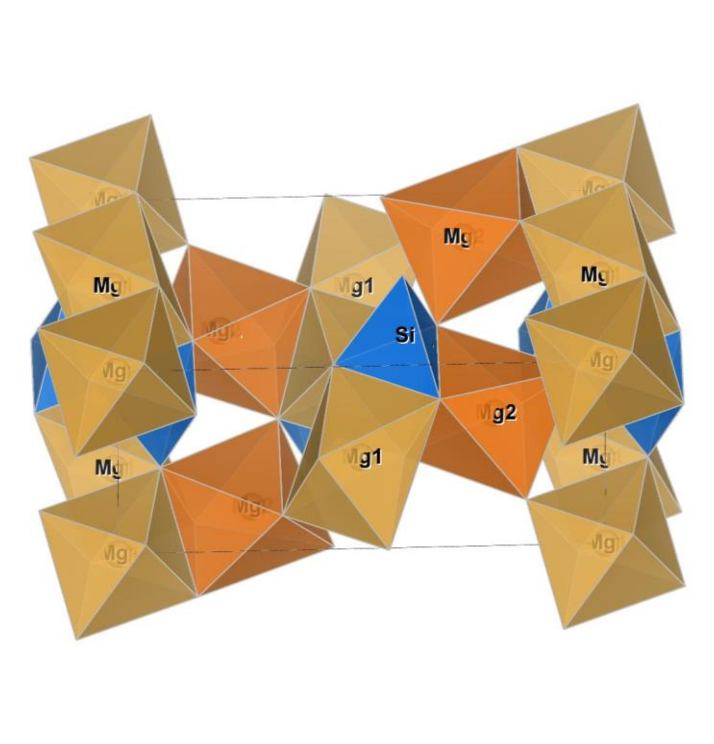
Ringwoodite

(*Fd*-3*m*) - **CCP**



Forsterite

(*Pbnm*) - **HCP**



Thus, we proposed that ringwoodite-forsterite polymorphic forms can be regarded as different species because their **structures are significantly different** in terms of **arrangement of polyhedra**.

*It means that the **type of connection of polyhedra** (corner-, edge- and face-sharing) as well as their relative orientation lead to very different ordering schemes, resulting in pronounced differences among structures even with the same bond topology.*

→ *CNMNC guidelines have to be modified, replacing "Topologically similar polymorphs" by "Structurally similar polymorphs"*

In summary

- ✓ Mineral is a solid chemical substance that formed by a geological process.

- ✓ Mineral species differ from each other depending on their composition, structure and in some cases from their history in the scientific literature.

- ✓ Mineral species can be represented by a pertinent name and an ideal formula.

- ✓ Substances formed under non-ambient conditions can be accepted as mineral species if they can be adequately characterized by using special procedure in the investigation.

- ✓ Biominerals are minerals in which organisms played an important role, but a geological process was also involved in their formation.

- ✓ The IMA-CNMNC does not wish to impose rigid rules, but rather to provide a set of guidelines. Exceptions are always taken into consideration by the CNMNC.

electronic structure
chemical bonding
atomic arrangement
(basic building block for solid)

MANY THANKS FOR YOUR ATTENTION !!!