Université de Liège
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The IMA-CNMNC dominant-constituent rule revisited and extended

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The « 50 % rule »

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• Nickel (1992): « … a complete solid-solution series without structural order of the ions defining the end members is **arbitrarily divided at 50 mole %,** and the two portions are given different names… for the sake of brevity, this will be called **the « 50 % rule ».** »

• Nickel & Grice (1998): « In multiple solid-solution series, the 50 % rule is interpreted to mean **predominant occupancy** of a particular structural site…For the purpose of species definition, site **vacancies are to be regarded as atoms**. »

• Wenk & Bulakh (2004): Introduced the name **« 100%/*n* rule »,** with *n* being the number of components (not IMA-CNMNC approved).

The « Dominant Constituent » rule

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• Hawthorne (2002 and pers. commun.): Problems in the **nomenclature of certain end-members** in complex mineral groups (*e.g.*, tourmaline and milarite).

• Cámara *et al*. (2006), Chopin *et al*. (2006), Armbruster *et al*. (2006): IMA-CNMNC-approved reports on the nomenclature of the arrojadite and epidote groups of minerals. In these systems, the dominant-constituent rule has been extended by considering **« a group of atoms with the same valency state »** as a single constituent.

• Hatert & Burke (2008) (Can. Mineral. 46, 717-728): Revision and extension of the **« Dominant constituent rule ».**

Complete solid solutions
Homovalent substitutions at a single site

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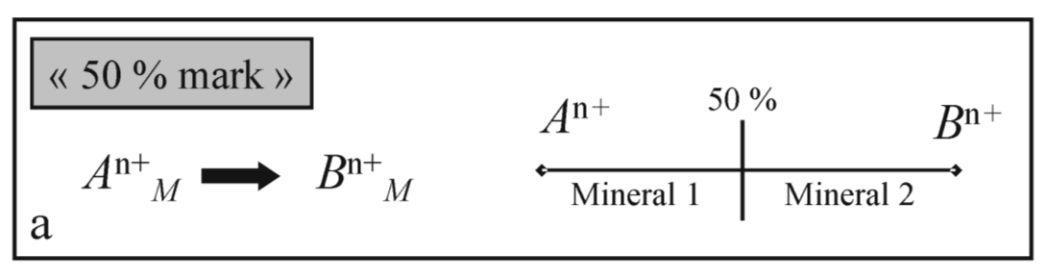

Diopside **Hedenbergite**

$CaMgSi_2O_6 \rightarrow CaFeSi_2O_6$

$Mg^{2+} \rightarrow Fe^{2+}$

Homovalent substitutions at a single site
Multiple solid-solution series

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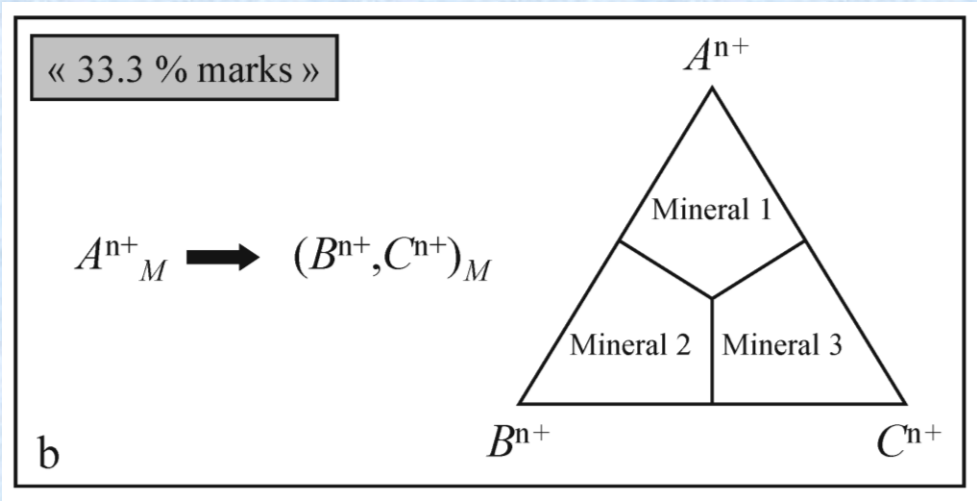


Preisingerite group

Preisingerite, $Bi_3(AsO_4)_2OOH$
Schumacherite, $Bi_3(VO_4)_2OOH$
Petitjeanite, $Bi_3(PO_4)_2OOH$

33.3 % boundary

Schoenfliesite group

Schoenfliesite,$MgSn(OH)_6$
Natanite, $FeSn(OH)_6$
Wickmanite, $MnSn(OH)_6$
Mushistonite, $CuSn(OH)_6$
Vismirnovite, $ZnSn(OH)_6$
Burtite, $CaSn(OH)_6$

16.6 % boundary

Independant homovalent substitutions at several sites

Columbite group

$Fe^{2+} \rightarrow Mn^{2+}$
A site

$FeTa_2O_6$ $MnTa_2O_6$

Tantalite-(Fe)	Tantalite-(Mn)
Columbite-(Fe)	Columbite-(Mn)

$Ta^{5+} \rightarrow Nb^{5+}$
B site

$FeNb_2O_6$ $MnNb_2O_6$

Ferrocolumbite, Crystal Park, El Paso So., Colorado, USA
(from Webmineral.com)

Heterovalent substitutions at a single site


Monazite-(Ce), Conselheiro Pena, Minas Gerais, Brazil (from Webmineral.com)

« 50 % mark »

$$A^{n+}{}_M \rightarrow (B^{(n+1)+}{}_{0.5} C^{(n-1)+}{}_{0.5})_M$$

50 %

A^{n+} | $(B^{(n+1)+}{}_{0.5} C^{(n-1)+}{}_{0.5})$

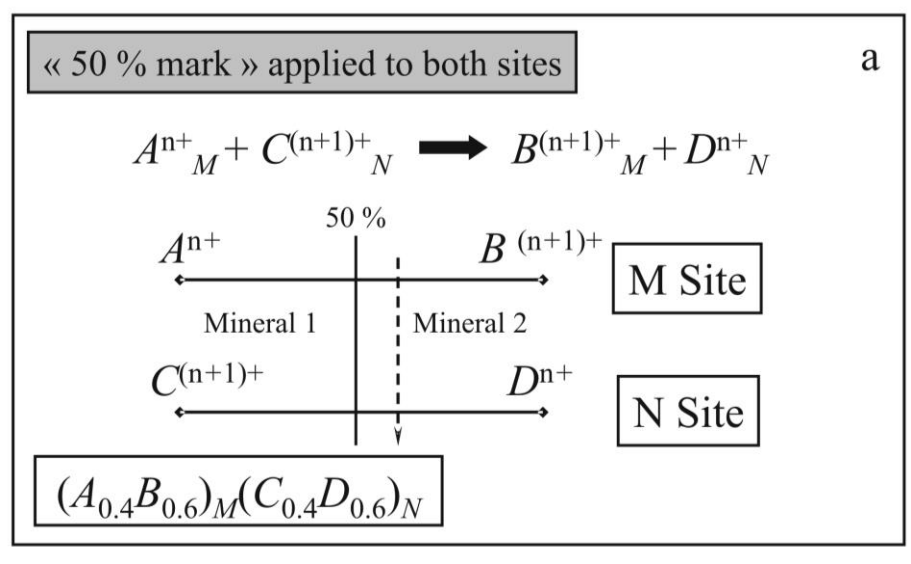
Mineral 1 | Mineral 2

Monazite-(Ce) **Cheralite**

$$Ce(PO_4) \rightarrow (Ca_{0.5}Th_{0.5})(PO_4)$$

$$Ce^{3+} \rightarrow 0.5\ Ca^{2+} + 0.5\ Th^{4+}$$

Coupled heterovalent substitutions at two sites



Albite **Anorthite**

$$Na(AlSi_3O_8) \rightarrow Ca(Al_2Si_2O_8)$$

$$Na^+ + Si^{4+} \rightarrow Ca^{2+} + Al^{3+}$$

Valency-imposed double site-occupancy

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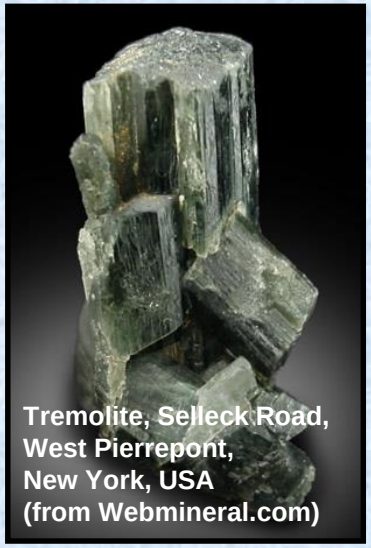
Heterovalent substitutions at one site

Schorl → **Elbaite**

$$NaFe^{2+}_3Al_6(Si_6O_{18})(BO_3)_3(OH)_4 \rightarrow Na(Li_{1.5}Al_{1.5})Al_6(Si_6O_{18})(BO_3)_3(OH)_4$$

$$Fe^{2+} \rightarrow 0.5\ Li^{+} + 0.5\ Al^{3+}$$

Coupled heterovalent substitutions at two sites



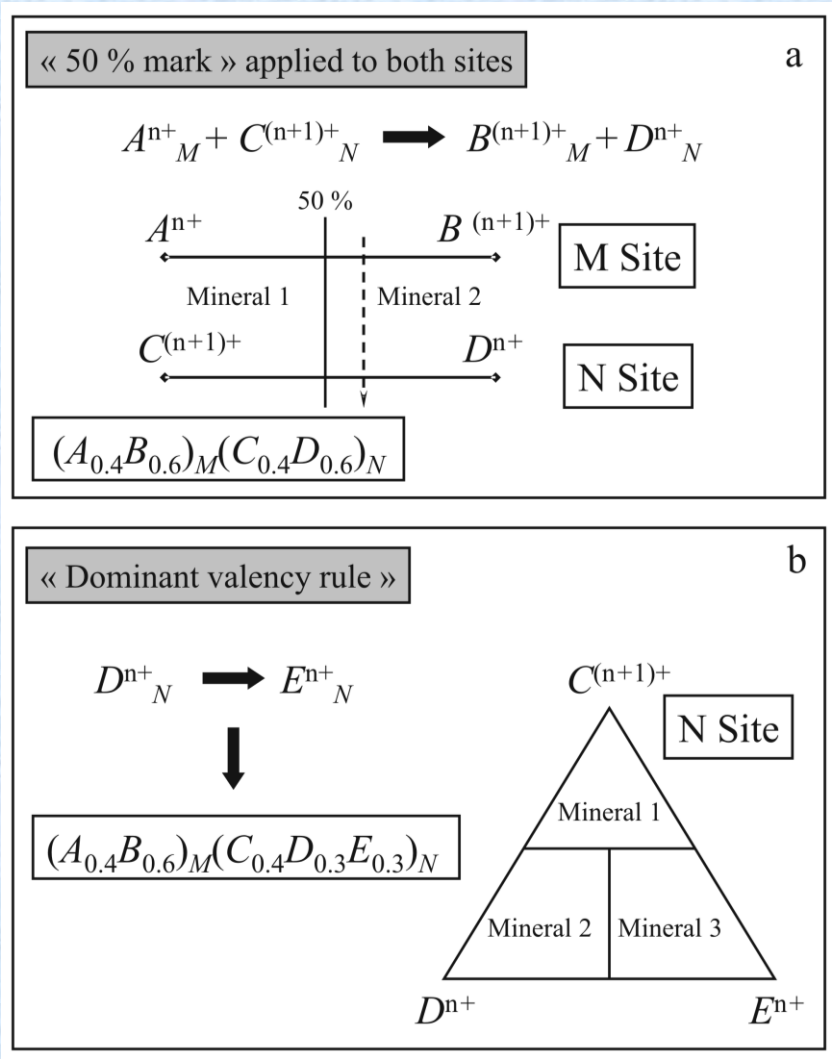
Tremolite, Selleck Road, West Pierrepont, New York, USA (from Webmineral.com)

Tremolite → **Richterite**

$$\square Ca_2Mg_5(Si_8O_{22})(OH)_2 \rightarrow Na(NaCa)Mg_5(Si_8O_{22})(OH)_2$$

$$\square_A + Ca^{2+}{}_B \rightarrow Na^{+}{}_A + Na^{+}{}_B$$

Coupled heterovalent-homovalent substitutions



Albite **Anorthite**

$Na(AlSi_3O_8) \rightarrow Ca(Al_2Si_2O_8)$

Coupled heterovalent substitution

$Na^+ + Si^{4+} \rightarrow Ca^{2+} + Al^{3+}$

$(Na_{0.6}Ca_{0.4})Al_{1.4}Si_{2.6}O_8$
(Albite)

Homovalent substitution

$Na^+ \rightarrow K^+$

$(Ca_{0.4}Na_{0.35}K_{0.25})Al_{1.4}Si_{2.6}O_8$

$CaAlSi_3O_8$ = New mineral species?
NO! Ca- and K-rich albite!

The dominant-valency rule

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A group of atoms with the same valency state has to be considered as a single constituent

Arrojadite group

- Arrojadite-(KNa) = $KNaNa_2CaNa_2Fe_{13}Al(PO_4)_{11}(PO_3OH)(OH)_2$
- $(Ba_{0.40}K_{0.35}Na_{0.25})(Na_{0.6}\square_{0.4})Na_2CaNa_2Fe_{13}Al(PO_4)_{11}(PO_3OH)(OH)_2$

  ↳ arraojadite-(KNa), not arrojadite-(BaNa)!

Epidote group

- Clinozoisite = $CaCaAlAlAl(Si_2O_7)(SiO_4)O(OH)$
- *A*2 occupancy $(Ce_{0.35}La_{0.05}Ca_{0.30}Sr_{0.20}Pb_{0.10})$

  ↳ clinozoisite subgroup, not allanite subgroup!

Clinozoisite, Alchuri, Shigar Skardu district, Pakistan (from Webmineral.com)

The dominant-valency rule

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Pumpellyite group

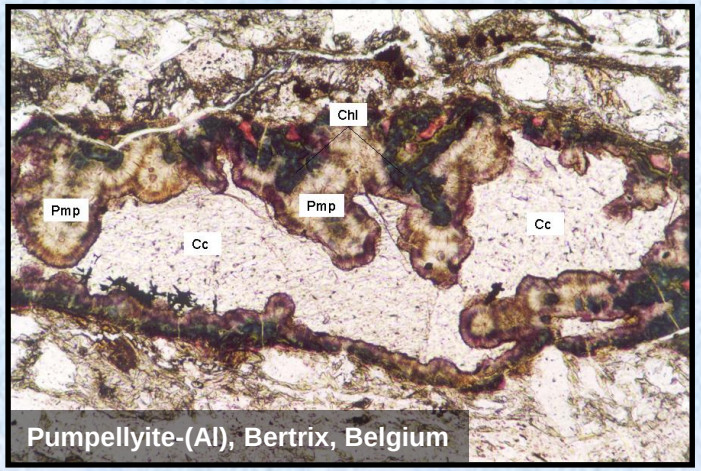
- Pumpellyite-(Al) end member = $Ca_2AlAl_2(SiO_4)(Si_2O_7)(OH)_3$
- $(Ca_{1.99}Na_{0.01})(Al_{0.42}Fe^{2+}_{0.33}Mg_{0.24}Mn_{0.01})Al_2(SiO_4)(Si_2O_7)(OH)_{2.42}\bullet 0.58H_2O$

↳ pumpellyite-(Fe^{2+}), not pumpellyite-(Al)!

Triploidite group

- Staněkite = $Mn^{2+}Fe^{3+}(PO_4)O$
- Triploidite = $Mn^{2+}_2(PO_4)(OH)$
- $(Mn^{2+}_{1.60}Fe^{3+}_{0.40})(PO_4)[O_{0.40}(OH)_{0.35}F_{0.25}]$

↳ triploidite, not « oxytriploidite »!



Pumpellyite-(Al), Bertrix, Belgium

Grouping of crystallographic sites

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Amphibole group

- Nomenclature based on the formula $AB_2C_5T_8O_{22}W_2$

  → *C* represents the group of five *apfu* in the *M*(1), *M*(2), and *M*(3) sites

Olivine group

- Fayalite = Fe_2SiO_4
- Forsterite = Mg_2SiO_4

  → The *M*(1) and *M*(2) sites are considered as a whole for nomenclature purpose

Fayalite,
Coso Hot Springs, Inyo County, USA
(from Webmineral.com)

Necessary to avoid the proliferation of mineral species in complex groups

Conclusions

- Nomenclature of minerals in complete solid-solutions series remains determined by the dominant constituent rule.

- For coupled heterovalent-homovalent substitutions, the "dominant valency rule" has to be applied. This rule is an extension of the dominant constituent rule in which a group of atoms with the same valency state is considered as a single constituent.

- Coupled heterovalent substitutions at a single or at two sites may produce end-member formulae with valency-imposed double site-occupancy.

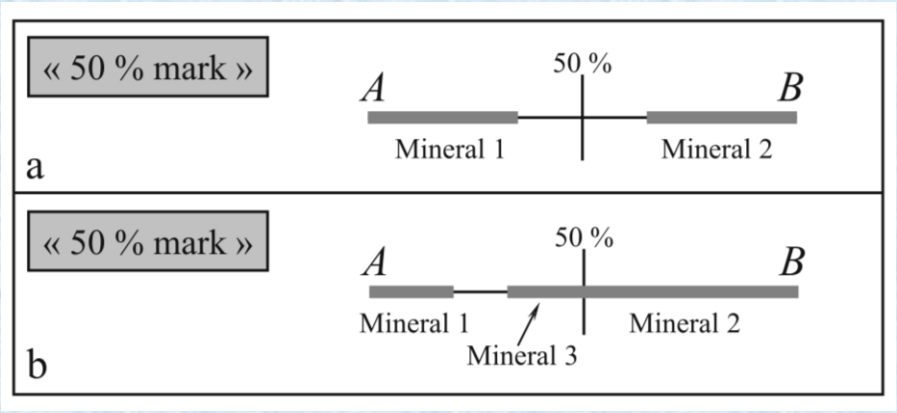
- A grouping of crystallographic sites may be required for complex crystal structures, in order to avoid the proliferation of new mineral species.

Acknowledgements

- Frank Hawthorne, Christian Chopin, and Thomas Armbruster, who initiated the discussion on the application of the dominant-constituent rule.

- Several CNMNC members who helped to improve the text of this revision, especially Gunnar Raade, Paul Keller and André-Mathieu Fransolet.

Binary partial solid-solution series




Hematite + rutile,
Norro Horizonte, Bahia, Brazil
(from Webmineral.com)

Hematite – Ilmenite

Fe_2O_3 – $FeTiO_3$

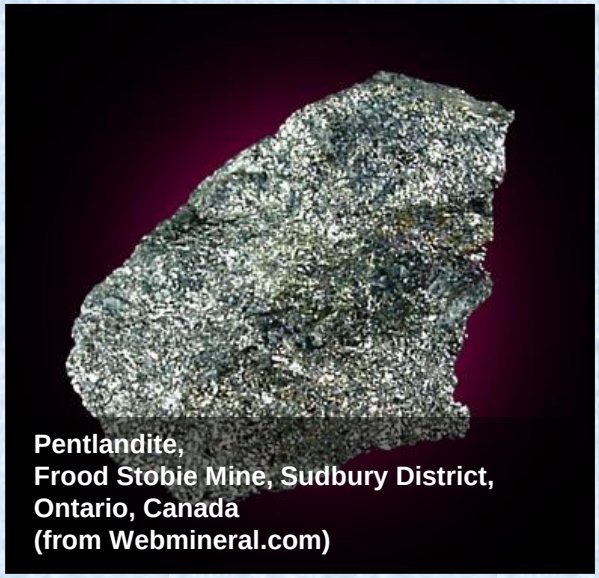
Solid solution limited to small ranges near the end members

Sphalerite – Rudashevskyite

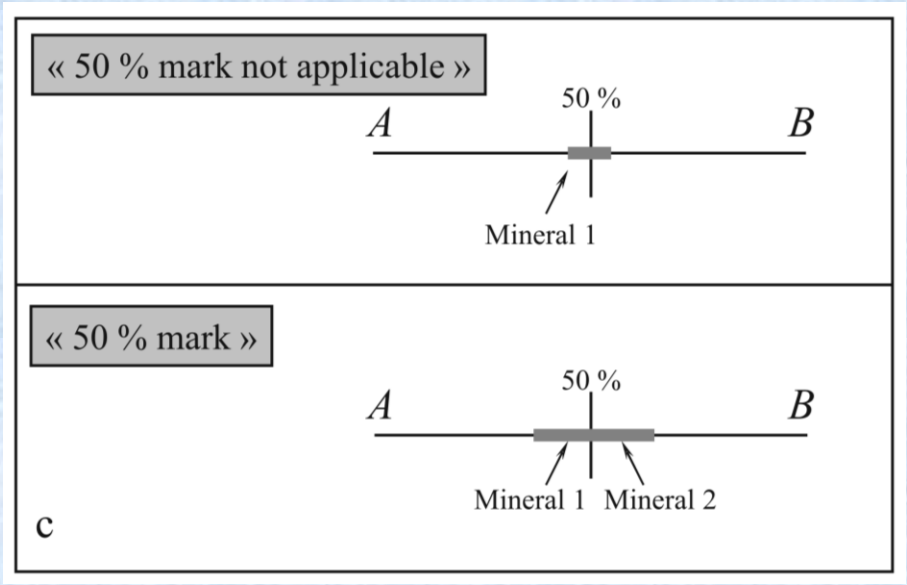
Solution of FeS in ZnS ending at 66 mol. % FeS

- **Sphalerite: ZnS to $(Zn_{0.50}Fe_{0.50})S$**
- **Rudashevskyite: $(Zn_{0.50}Fe_{0.50})S$ to $(Zn_{0.34}Fe_{0.66})S$**

Binary partial solid-solution series



Pentlandite,
Frood Stobie Mine, Sudbury District,
Ontario, Canada
(from Webmineral.com)

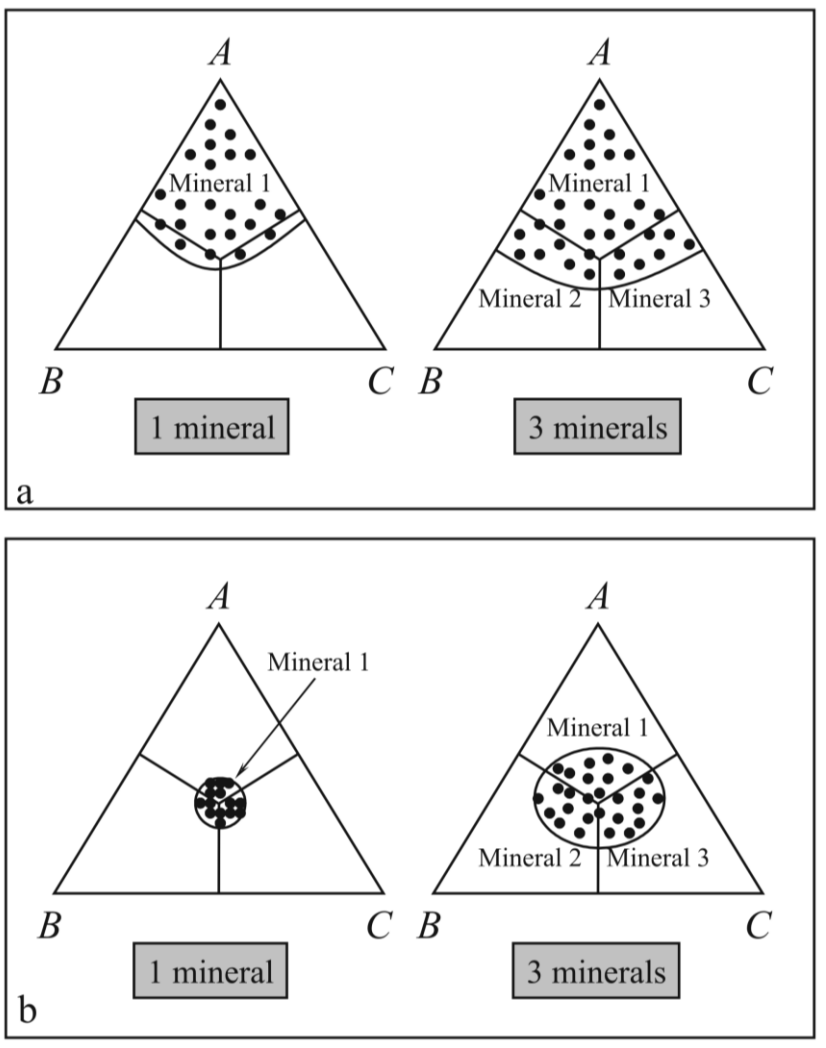


Pentlandite

$Fe(Fe,Ni)_8S_8$

Compositions centered around Fe:Ni = 1:1

Ternary partial solid-solution series



Composition extending substantially beyond the boundary

➡ **Necessary to define new mineral species**

Cluster around the 33.3 % mark

➡ **Only one mineral species**

Extended compositional field

➡ **Several mineral species**