



Changes to the cerite group nomenclature

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Received: 27 July 2023 – Revised: 6 October 2023 – Accepted: 13 October 2023 – Published: 23 November 2023

Abstract. The cerite and merrillite groups belong to the cerite supergroup. Some nomenclature and classification changes have been made to the cerite group, whereas the merrillite group remains unchanged. Minerals of the cerite group have the general formula $A_9XM[T_7O_{24}\emptyset_4]Z_3$, where T is Si. The cerite group, from now on, is subdivided into two subgroups, cerite and taipingite. The root name will be cerite and taipingite if the Z anions are dominated by (OH) and F, respectively. The prefix ferri- or alumino- will be added if the M cations are dominated by Fe^{3+} or Al, respectively. If the M cation is Mg, there will be no prefix. Taking into account the valency-imposed double site occupancy and the site total charge approach, a double suffix will be used to represent the essential A constituents in the general chemical formula. Cerite-(Ce), aluminocerite-(Ce), ferricerite-(La), and taipingite-(Ce) have been renamed cerite-(CeCa), aluminocerite-(CeCa), ferricerite-(LaCa), and taipingite-(CeCa), respectively. The newly approved mineral aluminotaipingite-(CeCa) also belongs to the taipingite subgroup.

The cerite supergroup (Atencio and Azzi, 2020) consists of two groups of isostructural trigonal $R3c$ (no. 161) minerals, namely, cerite (silicates) and merrillite (phosphates) groups. The merrillite group is subdivided into two subgroups: merrillite (without OH in the \emptyset site) and whitlockite (with OH in the \emptyset site). The nomenclature introduced by Atencio and Azzi (2020) is based on the dominant species of the dominant valence at each site.

The recent discoveries of four new members in the cerite group, following the four valid members already approved, make it necessary to revise the nomenclature of this group. One of these new species, aluminotaipingite-(CeCa) IMA2022-126, has already been approved by the CNMNC-IMA (Commission on New Minerals, Nomenclature and Classification of the International Mineralogical Association) and published (Campostrini et al., 2023); two are under review by the CNMNC-IMA; and one is under study.

The crystal structure of these minerals involves three 8- and 9-fold coordinated A sites, one 6-fold coordinated

X site, one octahedral M site, and three $[TO_3(\emptyset)]$ tetrahedral groups. The crystal structure of cerite supergroup minerals consists of $[M(TO_4)_6]$ clusters linked by $\{A_9X(TO_3\emptyset)\}$ groups.

The general chemical formula of cerite supergroup minerals is $A_9XM[T_7O_{24}\emptyset_4]Z_3$, where the letters, except for O for oxygen, represent groups of atoms (and not structural sites) on which to apply the dominant constituent and valency rule and the endmember concept. A = REE, Ca, Sr, Na, and \square ; X = \square , Ca, Na, and Fe^{2+} ; M = Mg, Fe^{2+} , Fe^{3+} , Al, and Mn; T = Si and P; \emptyset = O and OH; and Z = \square , OH, and F, where REE is rare earth elements of yttrium and lanthanoids (La–Lu) (Atencio and Azzi, 2020). The general structural formula of cerite supergroup minerals is $A_{13}A_2A_3A_3XM_1[T_1T_3T_2T_3T_3O_{24}\emptyset_{13}\emptyset_{10}]Z_1Z_2Z_3$. The letter Z represents the set of anions occurring at three nonequivalent Z1, Z2, and Z3 sites; thus, the composition $Z = F_{1.8}(OH)_{1.2}$ is consistent with the endmember composition $Z = F_3$ (as $F > OH$). Grouping atoms over similar sites,

Table 1. Ideal formula, dominant constituents in the general chemical formula, and unit-cell parameters (*R3c*) for the cerite supergroup minerals.

Cerite group	Ideal formula	A ₉	X	M	T ₇	O ₂₄	Ø ₄	Z ₃	Unit-cell parameters (<i>a</i> , <i>c</i> , <i>V</i>)	Ref.
Cerite subgroup										
Cerite-(CeCa)	(Ce ₇ Ca ₂)Mg(SiO ₄) ₃ (SiO ₃ OH) ₄ (OH) ₃	Ce ₇ Ca ₂	□	Mg	Si	O	OH	OH	10.779 38.0610 3829.73	1
Ferricerite-(LaCa)	(La ₆ Ca ₃)Fe ³⁺ (SiO ₄) ₃ (SiO ₃ OH) ₄ (OH) ₃	La ₆ Ca ₃	□	Fe ³⁺	Si	O	OH	OH	10.7493 38.318 3834.37	2
Aluminoerite-(CeCa)	(Ce ₆ Ca ₃)Al(SiO ₄) ₃ (SiO ₃ OH) ₄ (OH) ₃	Ce ₆ Ca ₃	□	Al	Si	O	OH	OH	10.6450 38.019 3730.98	3
Taipingite subgroup										
Taipingite-(CeCa)	(Ce ₇ Ca ₂)Mg(SiO ₄) ₃ (SiO ₃ OH) ₄ F ₃	Ce ₇ Ca ₂	□	Mg	Si	O	OH	F	10.7246 37.9528 3780.4	4
Alumino Taipingite-(CeCa)	(Ce ₆ Ca ₃)Al(SiO ₄) ₃ (SiO ₃ OH) ₄ F ₃	Ce ₆ Ca ₃	□	Al	Si	O	OH	F	10.658 37.865 3725	5
Merrillite group										
Merrillite subgroup										
Merrillite	Ca ₉ NaMg(PO ₄) ₇	Ca ₉	Na	Mg	P	O	O	□	10.3444 37.0182 3430.5	6
Ferrimerrillite	Ca ₉ NaFe ²⁺ (PO ₄) ₇	Ca ₉	Na	Fe ²⁺	P	O	O	□	10.372 37.217 3467	7
Keplerite	Ca ₉ (Ca _{0.5} □ _{0.5})Mg(PO ₄) ₇	Ca ₉	Ca _{0.5} □ _{0.5}	Mg	P	O	O	□	10.3330 37.0668 3427.4	8
Mayhite	Ca ₉ (Ca _{0.5} □ _{0.5})Fe ²⁺ (PO ₄) ₇	Ca ₉	Ca _{0.5} □ _{0.5}	Fe ²⁺	P	O	O	□	10.456 37.408 3541.6	9
Deynekoite	Ca ₉ Fe ³⁺ (PO ₄) ₇	Ca ₉	□	Fe ³⁺	P	O	O	□	10.372 37.217 3467	10
Changesite-(Y)	(Ca ₈ Y)Fe ²⁺ (PO ₄) ₇	Ca ₈ Y	□	Fe ²⁺	P	O	O	□	10.3957 37.207 3482.27	11
Whitlockite subgroup										
Whitlockite	Ca ₉ Mg(PO ₄) ₆ (PO ₃ OH)	Ca ₉	□	Mg	P	O	O ₃ OH	□	10.330 37.103 3428.79	12
Strontio whitlockite	Si ₉ Mg(PO ₄) ₆ (PO ₃ OH)	Si ₉	□	Mg	P	O	O ₃ OH	□	10.644 39.54 3880	13
Hedegaardite	(Ca ₈ Na)(Ca _{0.5} □ _{0.5})Mg(PO ₄) ₆ (PO ₃ OH)	Ca ₈ Na	Ca _{0.5} □ _{0.5}	Mg	P	O	O ₃ OH	□	10.3519 37.064 3439.7	14
Wopmayite	(Ca ₆ Na ₃)Mn(PO ₄) ₃ (PO ₃ OH) ₄	Ca ₆ Na ₃	□	Mn	P	O	OH	□	10.3926 37.1694 37.1694	15

¹ Moore and Shen (1983), ² Pakhomovskiy et al. (2002), ³ Nestola et al. (2009), ⁴ Qu et al. (2020), ⁵ Campostrini et al. (2023), ⁶ Xie et al. (2015), ⁷ Britvin et al. (2016), ⁸ Britvin et al. (2021), ⁹ Hwang et al. (2019), ¹⁰ Galuskin et al. (2023), ¹¹ Li et al. (2022), ¹² Calvo and Gopal (1975), ¹³ Britvin et al. (1991), ¹⁴ Witzke et al. (2015), ¹⁵ Cooper et al. (2013).

such as $A(1,2,3)$, $T(1,2,3)$, and $Z(1,2,3)$, helps prevent the proliferation of mineral species with endmember formulae based on the structural formula, where each structural sites can be used (Nickel and Grice, 1998) to define an endmember formula (Hawthorne, 2002). For example, the three independent anion Z sites may result in an endmember composition like $F_2(OH)$. In this way, cerite nomenclature is based on the chemical formula, and, in principle, only the chemical information is needed for the mineral identification.

The cerite group, from now on, is subdivided into two subgroups, cerite and taipingite.

The root name will be cerite and taipingite if the Z anions are dominated by (OH) and F , respectively. The prefix ferri- or alumin- will be added if the M cations are dominated by Fe^{3+} or Al , respectively. If the M cation is Mg , there will be no prefix. Taking into account the valency-imposed double site occupancy (Hatert and Burke, 2008; Hatert et al., 2013) and the site total charge approach of Bosi et al. (2019), a double suffix will be used to represent the essential A constituents in the general chemical formula. Cerite-(Ce), aluminocerite-(Ce), ferricerite-(La), and taipingite-(Ce) have been renamed cerite-(CeCa), aluminocerite-(CeCa), ferricerite-(LaCa), and taipingite-(CeCa), respectively. The newly approved mineral aluminotaipingite-(CeCa) also belongs to the taipingite subgroup.

The charge balance of cerite group minerals is according to the following substitution mechanism: $A[REE_8\Box]^{+24} + M(Fe,Al)^{3+} = A[REE_6(Ca,Sr)_3]^{+24} + M(Fe,Al)^{3+} = A[REE_7(Ca,Sr)_2]^{+25} + M(Mg,Fe)^{2+}$.

The nomenclature of merrillite group remains as it current is. Table 1 summarizes all the currently valid species in the cerite supergroup.

Data availability. No data sets were used in this article.

Author contributions. All authors contributed to the conception of the project and the writing of the paper.

Competing interests. At least one of the (co-)authors is a guest member of the editorial board of *European Journal of Mineralogy* for the special issue “New minerals, nomenclature, and classification: EJM support”. The peer-review process was guided by an independent editor, and the authors also have no other competing interests to declare.

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Special issue statement. This article is part of the special issue “New minerals: EJM support”. It is not associated with a conference.

Acknowledgements. We acknowledge Sergey Krivovichev, Anthony Kampf, the anonymous referee, and all members of the IMA Commission on New Minerals, Nomenclature and Classification for their helpful suggestions and comments.

Financial support. This research has been supported by FAPESP (Fundação de Amparo à Pesquisa do Estado de São Paulo; project 2019/23498-0) and CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico; project 303431/2019-9).

Review statement. This paper was edited by Sergey Krivovichev and reviewed by Anthony Kampf and one anonymous referee.

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