

The seidozerite supergroup of TS-block minerals: nomenclature and classification, with change of the following names: rinkite to rinkite-(Ce), mosandrite to mosandrite-(Ce), hainite to hainite-(Y) and innelite-1T to innelite-1A

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ABSTRACT

Here we report a nomenclature and classification for the seidozerite-supergroup minerals. The TS (Titanium-Silicate) block is the main structural unit in all seidozerite-supergroup structures; it consists of a central O (O = Octahedral) sheet and two adjacent H (H = Heteropolyhedral) sheets where Si₂O₇ groups occur in the H sheets. The TS block is characterized by a planar minimal cell based on translation vectors, **t**₁ and **t**₂, the lengths of these vectors are $t_1 \approx 5.5$ and $t_2 \approx 7 \text{ \AA}$, and **t**₁ ^ **t**₂ is close to 90°. The forty-five minerals of the seidozerite supergroup are divided into four groups based on the content of Ti and topology and stereochemistry of the TS block: in rinkite, bafertisite, lamprophyllite and murmanite groups, Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn) = 1, 2, 3 and 4 apfu (atoms per formula unit), respectively. All TS-block structures consist either solely of TS blocks or of two types of block: the TS block and an **I** (Intermediate) block that comprises atoms between two TS blocks. Usually, the **I** block consists of alkali and alkaline-earth cations, H₂O groups and oxyanions (PO₄)³⁻, (SO₄)²⁻ and (CO₃)²⁻. The general formula of the TS block is as follows A₂^PB₂^PM₂^HM₄^O(Si₂O₇)₂X_{4+n}, where M₂^H and M₄^O = cations of the H and O sheets; M^H = Ti, Nb, Zr, Y, Mn, Ca + REE, Ca; M^O = Ti, Zr, Nb, Fe³⁺, Fe²⁺, Mg, Mn, Zn, Ca, Na; A^P and B^P = cations at the peripheral (P) sites = Na, Ca + REE, Ca, Zn, Ba, Sr, K; X = anions = O, OH, F, H₂O; X_{4+n} = X₄^O + X_n^P, n = 0, 1, 1.5, 2, 4; X^P = X_M^P and X_A^P = apical anions of M^H and A^P cations at the periphery of the TS block.

KEYWORDS: seidozerite supergroup, TS block, nomenclature, classification, ideal formula, rinkite, bafertisite, lamprophyllite and murmanite groups.

Introduction

BASED on work of Sokolova (2006) and Sokolova and Cámara (2013) and following recommendations of Mills *et al.* (2009), we report here a nomenclature and classification of the seidozerite supergroup which includes 45 well-characterized titanium-disilicate minerals with the TS block (TS = Titanium-Silicate) (Table 1). The seidozerite

supergroup has been approved by CNMNC-IMA (Memorandum 56-SM/16).

The TS-block minerals have very interesting structures with complicated chemical compositions. The TS block consists of a central O (O = Octahedral) sheet and two adjacent H (H = Heteropolyhedral) sheets. Ti is a topology-defining cation of the TS block. Ti occurs in the O sheet and two H sheets. In the O sheet, Nb, Zr, Fe³⁺, Mg and Mn substitute for Ti (in seven TS-block minerals); in the H sheet, only Nb substitutes for Ti (in eight TS-block minerals). Hence when we say Ti-dominant sites, we also include Nb-,

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TABLE 1. Formulae of seidozerite-supergroup minerals*

Mineral Mineral description	Ideal structural formula	Short form of the ideal formula**	Z	Ref.†
Rinkite group , TS block: Ti (+ Nb + Zr) = 1 apfu, Ti occurs in the O sheet				
General formula	$A_2^P M_2^H M_4^O (Si_2O_7)_2 (X_M^O)_2 (X_A^O)_2$			
Rinkite-(Ce) Lorenzen (1884)	$(Ca_3 REE) Na (NaCa) Ti (Si_2O_7)_2 (OF) F_2$	$Na_2 Ca_4 REE Ti (Si_2O_7)_2 OF_3$	2	(1)
Nacareniobsite-(Ce) Petersen <i>et al.</i> (1989)	$(Ca_3 REE) Na_3 Nb (Si_2O_7)_2 (OF) F_2$	$Na_3 Ca_3 REE Nb (Si_2O_7)_2 OF_3$	2	(2)
Mosandrite-(Ce) Brögger (1890)	$(Ca_3 REE) [(H_2O)_2 Ca_{0.5} \square_{0.5}] Ti (Si_2O_7)_2 (OH)_2 (H_2O)_2$		2	(3)
Seidozerite Semenov <i>et al.</i> (1958)	$Na_2 Zr_2 Na_2 Mn Ti (Si_2O_7)_2 O_2 F_2$	$Na_4 Mn Zr_2 Ti (Si_2O_7)_2 O_2 F_2$	2	(4)
Grenmarite Bellezza <i>et al.</i> (2004)	$Na_2 Zr_2 Na_2 Mn Zr (Si_2O_7)_2 O_2 F_2$	$Na_4 Mn Zr_3 (Si_2O_7)_2 O_2 F_2$	2	(5)
Götzenite Sahama and Hytönen (1957)	$Ca_4 Na Ca_2 Ti (Si_2O_7)_2 (OF) F_2$	$Na Ca_6 Ti (Si_2O_7)_2 OF_3$	1	(4)
Hainite-(Y) Blumrich (1893)	$(Ca_3 Y) Na (NaCa) Ti (Si_2O_7)_2 (OF) F_2$	$Na_2 Ca_4 Y Ti (Si_2O_7)_2 OF_3$	1	(6)
Fogoite-(Y) Cámara <i>et al.</i> (2017)	$Ca_2 Y_2 Na_3 Ti (Si_2O_7)_2 (OF) F_2$	$Na_3 Ca_2 Y_2 Ti (Si_2O_7)_2 OF_3$	1	(7)
Batievaite-(Y) Lyalina <i>et al.</i> (2016)	$Ca_2 Y_2 [(H_2O)_2 \square] Ti (Si_2O_7)_2 (OH)_2 (H_2O)_2$	$Ca_2 Y_2 Ti (Si_2O_7)_2 (OH)_2 (H_2O)_4$	1	(8)
Kochite Christiansen <i>et al.</i> (2003b)	$Ca_2 Mn Zr Na_3 Ti (Si_2O_7)_2 (OF) F_2$	$Na_3 Ca_2 Mn Zr Ti (Si_2O_7)_2 OF_3$	2	(9)
Rosenbuschite*** Brögger (1887)	$Ca_6 Zr_2 Na_6 Zr Ti (Si_2O_7)_4 (OF)_2 F_4$	$Na_6 Ca_6 Zr_3 Ti (Si_2O_7)_4 O_2 F_6$	1	(4)
Bafertisite group , TS block: Ti (+ Nb) = 2 apfu, Ti occurs in the H sheets				
General formula	$A^P B^P M_4^O M_2^H (Si_2O_7)_2 (X_M^O)_2 (X_A^O)_2 X_M^P$			
Jinshajiangite Hong and Fu (1982)	$Ba Na Fe_4^{2+} Ti_2 (Si_2O_7)_2 O_2 (OH)_2 F$	$Na Ba Fe_4^{2+} Ti_2 (Si_2O_7)_2 O_2 (OH)_2 F$	8	(10)
Perraultite Chao (1991)	$Ba Na Mn_4 Ti_2 (Si_2O_7)_2 O_2 (OH)_2 F$	$Na Ba Mn_4 Ti_2 (Si_2O_7)_2 O_2 (OH)_2 F$	8	(11)
Surkhobite**** Rastsvetaeva <i>et al.</i> (2008)	$KBa_3 Ca_2 Na_2 Mn_{16} Ti_8 (Si_2O_7)_8 O_8 (OH)_4 (F, O, OH)_8$		2	(12)

Bobshannonite*** Sokolova <i>et al.</i> (2015a)	$\text{KBaNa}_2(\text{Mn,Na})_8(\text{Nb,Ti})_4(\text{Si}_2\text{O}_7)_4\text{O}_4(\text{OH})_4(\text{O,F})_2$	$\text{Na}_2\text{KBa}(\text{Mn,Na})_8(\text{Nb,Ti})_4(\text{Si}_2\text{O}_7)_4\text{O}_4(\text{OH})_4(\text{O,F})_2$	4	(13)
General formula	$\text{A}_2^p\text{M}_4^o\text{M}_2^h(\text{Si}_2\text{O}_7)_2(\text{X}_M^o)_2(\text{X}_A^o)_2(\text{X}_M^p)_2$			
Bafertisite Semenov and Zhang Peishan (1959)	$\text{Ba}_2\text{Fe}_4^{2+}\text{Ti}_2(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2\text{F}_2$	$\text{Ba}_2\text{Fe}_4^{2+}\text{Ti}_2(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2\text{F}_2$	4	(14)
Hejtmanite Vrána <i>et al.</i> (1992)	$\text{Ba}_2\text{Mn}_4\text{Ti}_2(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2\text{F}_2$	$\text{Ba}_2\text{Mn}_4\text{Ti}_2(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2\text{F}_2$	4	(15)
General formula	$\text{A}_2^p\text{B}_2^p\text{M}_4^o\text{M}_2^h(\text{Si}_2\text{O}_7)_2(\text{TO}_4)_2(\text{X}_M^o)_2(\text{X}_A^o)_2$			
Yoshimuraite Watanabe <i>et al.</i> (1961)	$\text{Ba}_4\text{Mn}_4\text{Ti}_2(\text{Si}_2\text{O}_7)_2(\text{PO}_4)_2\text{O}_2(\text{OH})_2$	$\text{Ba}_4\text{Mn}_4\text{Ti}_2(\text{Si}_2\text{O}_7)_2(\text{PO}_4)_2\text{O}_2(\text{OH})_2$	2	(16)
General formula	$\text{A}_2^p\text{B}_2^p\text{A}_{2m}^i\text{M}_4^o\text{M}_2^h(\text{Si}_2\text{O}_7)_2(\text{CO}_3)_m(\text{X}_M^o)_2(\text{X}_A^o)_2(\text{X}_M^p)_2\text{F}_m, m = 2$			
Bussenite Khomyakov <i>et al.</i> (2001)	$\text{Ba}_4(\text{Na}\square)_2(\text{Fe}^{2+}\text{Na})_2\text{Ti}_2(\text{Si}_2\text{O}_7)_2(\text{CO}_3)_2\text{O}_2(\text{OH})_2(\text{H}_2\text{O})_2\text{F}_2$	$\text{Na}_4\text{Ba}_4\text{Fe}_2^{2+}\text{Ti}_2(\text{Si}_2\text{O}_7)_2(\text{CO}_3)_2\text{O}_2(\text{OH})_2(\text{H}_2\text{O})_2\text{F}_2$	2	(17)
General formula	$\text{A}_3^p\text{B}^p\text{M}_8^o\text{M}_4^h(\text{Si}_2\text{O}_7)_4(\text{X}_M^o)_4(\text{X}_A^o)_4(\text{X}_M^p)_3$			
Cámaraite Sokolova <i>et al.</i> (2009)	$\text{Ba}_3\text{NaFe}_8^{2+}\text{Ti}_4(\text{Si}_2\text{O}_7)_4\text{O}_4(\text{OH})_4\text{F}_3$	$\text{NaBa}_3\text{Fe}_8^{2+}\text{Ti}_4(\text{Si}_2\text{O}_7)_4\text{O}_4(\text{OH})_4\text{F}_3$	4	(18)
Lamprophyllite group , TS block: Ti (+ Nb + Fe ³⁺ + Mg) = 3 apfu, Ti occurs in the H sheets (2 apfu) and in the O sheet (1 apfu)				
General formula	$\text{A}_2^p\text{M}_2^h\text{M}_4^o(\text{Si}_2\text{O}_7)_2(\text{X}_M^o)_2(\text{X}_A^o)_2$			
Lamprophyllite-2M Hackman (1894)	$(\text{SrNa})\text{Ti}_2\text{Na}_3\text{Ti}(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	$\text{Na}_3(\text{SrNa})\text{Ti}_3(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	2	(19)
Lamprophyllite-2O Krivovichev <i>et al.</i> (2003)	$(\text{SrNa})\text{Ti}_2\text{Na}_3\text{Ti}(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	$\text{Na}_3(\text{SrNa})\text{Ti}_3(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	2	(19)
Fluorlamprophyllite Andrade <i>et al.</i> (2017)	$(\text{SrNa})\text{Ti}_2\text{Na}_3\text{Ti}(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$	$\text{Na}_3(\text{SrNa})\text{Ti}_3(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$	2	(20)
Nabalamprophyllite-2M Chukanov <i>et al.</i> (2004)	$\text{BaNaTi}_2\text{Na}_3\text{Ti}(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	$\text{Na}_4\text{BaTi}_3(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	2	(21)
Nabalamprophyllite-2O Sokolova and Hawthorne (2008a)	$(\text{BaNa})\text{Ti}_2\text{Na}_3\text{Ti}(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	$\text{Na}_3(\text{BaNa})\text{Ti}_3(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	2	(22)
Barytolamprophyllite Dudkin (1959)	$(\text{BaK})\text{Ti}_2\text{Na}_3\text{Ti}(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	$\text{Na}_3(\text{BaK})\text{Ti}_3(\text{Si}_2\text{O}_7)_2\text{O}_2(\text{OH})_2$	2	(23)
Lileyite Chukanov <i>et al.</i> (2012)	$\text{Ba}_2\text{Ti}_2\text{Na}_2\text{M}^{2+}\text{Mg}(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$	$\text{Na}_2\text{M}^{2+}\text{Ba}_2\text{MgTi}_2(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$	2	(24)
Emmerichite Chukanov <i>et al.</i> (2014)	$\text{Ba}_2\text{Ti}_2\text{Na}_3\text{Fe}^{3+}(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$	$\text{Na}_3\text{Ba}_2\text{Fe}^{3+}\text{Ti}_2(\text{Si}_2\text{O}_7)_2\text{O}_2\text{F}_2$	2	(25)
General formula	$\text{A}_2^p\text{B}_2^p\text{M}_2^h\text{M}_4^o(\text{Si}_2\text{O}_7)_2(\text{TO}_4)_2(\text{X}_M^o)_2(\text{X}_A^o)_2$			
Innelite-1A Kravchenko <i>et al.</i> (1961)	$\text{Ba}_4\text{Ti}_2\text{Na}(\text{NaM}^{2+})\text{Ti}(\text{Si}_2\text{O}_7)_2[(\text{SO}_4)(\text{PO}_4)]\text{O}_2[\text{O}(\text{OH})]$	$\text{Na}_2\text{M}^{2+}\text{Ba}_4\text{Ti}_3(\text{Si}_2\text{O}_7)_2[(\text{SO}_4)(\text{PO}_4)]\text{O}_3(\text{OH})$	1	(26)

(continued)

TABLE 1. (contd.)

Mineral Mineral description	Ideal structural formula	Short form of the ideal formula**	Z	Ref.†
Innelite-2M Sokolova <i>et al.</i> (2011)	$Ba_4Ti_2Na(NaM^{2+})Ti(Si_2O_7)_2[(SO_4)(PO_4)]O_2[O(OH)]$	$Na_2M^{2+}Ba_4Ti_3(Si_2O_7)_2[(SO_4)(PO_4)]O_3(OH)$	2	(26)
General formula	$A_2^P M_2^H M_4^O(Si_2O_7)_2(X_M^O)_2(X_A^O)_2(X_{M,A}^P)_4$			
Epistolite Boeggild (1901)	$(Na\Box)Nb_2Na_3Ti(Si_2O_7)_2O_2(OH)_2(H_2O)_4$	$Na_4TiNb_2(Si_2O_7)_2O_2(OH)_2(H_2O)_4$	1	(27)
Zvyaginite Pekov <i>et al.</i> (2014)	$Na\Box Nb_2NaZn\Box Ti(Si_2O_7)_2O_2(OH)_2(H_2O)_4$	$Na_2ZnTiNb_2(Si_2O_7)_2O_2(OH)_2(H_2O)_4$	4	(28)
General formula	$A_{3m}^I A_2^P M_2^H M_4^O(Si_2O_7)_2(PO_4)_m(X_M^O)_2(X_A^O)_2, m = 2$			
Vuonnemite Bussen <i>et al.</i> (1973)	$Na_6Na_2Nb_2Na_3Ti(Si_2O_7)_2(PO_4)_2O_2(OF)$	$Na_{11}TiNb_2(Si_2O_7)_2(PO_4)_2O_3F$	1	(29)
General formula	$A_{3m}^I A_4^{P[5]} M_2^H [6] M_2^H M_8^O(Si_2O_7)_4(PO_4)_m(X_M^O)_4(X_A^O)_4, m = 2$			
Bornemanite Men'shikov <i>et al.</i> (1975)	$Na_6(Na\Box)Ba_2Ti_2Nb_2(Na_5\Box)Ti_2(Si_2O_7)_4(PO_4)_2O_4(OH)_2F_2$	$Na_6BaTi_2Nb(Si_2O_7)_2(PO_4)_2O_2(OH)F$	1,2	(30)
General formula	$A_2^{P[5]} M_2^{H[6]} M_2^H M_4^O(Si_2O_7)_2X_4^O(X_{M,A}^P)_2$			
Saamite Cámara <i>et al.</i> (2014)	$Ba\Box TiNbNa_3Ti(Si_2O_7)_2O_2(OH)_2(H_2O)_2$	$Na_3BaTi_2Nb(Si_2O_7)_2O_2(OH)_2(H_2O)_2$	2	(31)
General formula	$A_2^{P[5]} M^{H[6]} M^H M_4^O(Si_2O_7)_2X_4^O(X_M^P)(H_2O)_3$			
Kazanskyite Cámara <i>et al.</i> (2012)	$Ba\Box TiNbNa_3Ti(Si_2O_7)_2O_2(OH)_2(H_2O)_4$	$Na_3BaTi_2Nb(Si_2O_7)_2O_2(OH)_2(H_2O)_4$	2	(32)
General formula	$A_8^{P[5]} M_4^{H[6]} M_4^H M_{16}^O(Si_2O_7)_8 X_{16}^O(X_M^P)_4(X_A^P)_3(H_2O)_5$			
Nechelyustovite Németh <i>et al.</i> (2009)	$(Na\Box)\Box_2Ba_4Ti_4Nb_4(Na_{11}\Box)Ti_4(Si_2O_7)_8O_8(OH)_8(H_2O)_{12}$	$Na_6Ba_2Ti_4Nb_2(Si_2O_7)_4O_4(OH)_4(H_2O)_6$	1,2	(33)
General formula	$A_2^P M_2^H M_4^O(Si_2O_7)_2(X_M^O)_2(X_A^O)_2(X_{M,A}^P)_2$			
Delindeite Appleman <i>et al.</i> (1987)	$Ba_2Ti_2(Na_2\Box)Ti(Si_2O_7)_2(OH)_2(H_2O)_2O_2$	$Na_2Ba_2Ti_3(Si_2O_7)_2O_2(OH)_2(H_2O)_2$	8	(34)
Murmanite group. TS block: Ti (+ Mg + Mn) = 4 apfu, Ti occurs in the H sheets (2 apfu) and in the O sheet (2 apfu)				
General formula	$A_2^P M_2^H M_4^O(Si_2O_7)_2(X_M^O)_2(X_A^O)_2(X_{M,A}^P)_4$			
Murmanite Gutkova (1930)	$Na_2Ti_2Na_2Ti_2(Si_2O_7)_2O_4(H_2O)_4$	$Na_4Ti_4(Si_2O_7)_2O_4(H_2O)_4$	1	(35)
General formula	$A_2^P M_2^H M_4^O(Si_2O_7)_2(X_M^O)_2(X_A^O)_2(X_{M,A}^P)_4$			
Calciomurmanite***** Lykova <i>et al.</i> (2016)	$(Ca\Box)Ti_2(Na\Box)Ti_2(Si_2O_7)_2O_2[O(OH)](H_2O)_4$	$NaCaTi_4(Si_2O_7)_2O_3(OH)(H_2O)_4$	1	(36)
Vigrishinite***** Pekov <i>et al.</i> (2013)	$Zn\Box Ti_2Na\Box Ti_2(Si_2O_7)_2O_2O(OH)(H_2O)_4$	$NaZnTi_4(Si_2O_7)_2O_3(OH)(H_2O)_4$	2	(37)

General formula	$A_2^P M_2^H M_4^O (Si_2O_7)_2 (X_{M,A}^O)_4 (X_M^P)_2 (H_2O)_5$		
Kolskyite Cámara <i>et al.</i> (2013)	$(Ca\Box)Ti_2Na_2Ti_2(Si_2O_7)_2O_4(H_2O)_2(H_2O)_5$	$Na_2CaTi_4(Si_2O_7)_2O_4(H_2O)_7$	1 (38)
General formula	$A_2^P M_2^H M_4^O (Si_2O_7)_2 (X_M^O)_2 (X_A^O)_2$		
Schüllerite Chukanov <i>et al.</i> (2011)	$Ba_2Ti_2Na_2Mg_2(Si_2O_7)_2O_2F_2$	$Na_2Ba_2Mg_2Ti_2(Si_2O_7)_2O_2F_2$	1 (39)
General formula	$A_{3m}^I A_2^P M_2^H M_4^O (Si_2O_7)_2 (PO_4)_m (X_{M,A}^O)_4, m = 2$		
Lomonosovite Gerasimovskiy (1950)	$Na_6Na_2Ti_2Na_2Ti_2(Si_2O_7)_2(PO_4)_2O_4$	$Na_{10}Ti_4(Si_2O_7)_2(PO_4)_2O_4$	1 (35)
General formula	$A_{3m}^I A_2^P M_2^H M_4^O (Si_2O_7)_2 [PO_3(OH)][PO_2(OH)_2] (X_M^O)_2 (X_A^O)_2, m = 2$		
Betalomonosovite Gerasimovskiy and Kazakova (1962)	$Na_2\Box_4Na_2Ti_2Na_2Ti_2(Si_2O_7)_2[PO_3(OH)][PO_2(OH)_2]O_2(OF)$	$Na_6Ti_4(Si_2O_7)_2[PO_3(OH)][PO_2(OH)_2]O_3F$	2 (40)
General formula	$A_{3m}^I A_{3t}^I A_2^P M_2^H M_4^O (Si_2O_7)_2 (PO_4)_{m+t} (X_M^O)_2 (X_A^O)_2 F_t,$	$m = 2$ (quadruphite, sobolevite, polyphite); $t = 2$ (quadruphite, sobolevite); $t = 4$ (polyphite)	
Quadruphite Khomyakov <i>et al.</i> (1992)	$Na_6Na_2(CaNa)_2Na_2Ti_2Na_2Ti_2(Si_2O_7)_2(PO_4)_4O_4F_2$	$Na_{14}Ca_2Ti_4(Si_2O_7)_2(PO_4)_4O_4F_2$	1 (41)
Sobolevite Khomyakov <i>et al.</i> (1983)	$Na_6(Na_2Ca)(NaCaMn)Na_2Ti_2Na_2(TiMn)(Si_2O_7)_2(PO_4)_4O_2(OF)F_2$	$Na_{13}Ca_2Mn_2Ti_3(Si_2O_7)_2(PO_4)_4O_3F_3$	2 (42)
Polyphite Khomyakov <i>et al.</i> (1992)	$Na_6(Na_4Ca_2)_2Na_2Ti_2Na_2Ti_2(Si_2O_7)_2(PO_4)_6O_4F_4$	$Na_{18}Ca_4Ti_4(Si_2O_7)_2(PO_4)_6O_4F_4$	1 (42)

*For each group, the content of Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn) apfu is given per (Si₂O₇)₂; for each mineral, the content of Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn) is shown in red; M²⁺ = Fe²⁺, Ca, Mn (lileyite); M²⁺ = Mn, Fe²⁺, Mg, Ca (innelite). **Short formula is given where it is possible; *** formula is given per (Si₂O₇)₄; **** formula is given per (Si₂O₇)₈; *****the ideal formulae are not given due to some problems with structure-refinement results. The general formula of the TS block is A₂^PB₂^PM₂^HM₄^O(Si₂O₇)₂X_{4+n}, where M₂^H and M₄^O = cations of the H and O sheets; A^P and B^P = cations at the peripheral (P) sites; X = anions = O, OH, F, H₂O; X_{4+n} = X₄^O + X_n^O, n = 0, 1, 1.5, 2, 4; X₄^O = anions of the O sheet not bonded to Si: X_M^O = anions at the common vertices of 3M^O and M^H polyhedra; X_A^O = anions at the common vertices of 3M^O and A^P polyhedra (where A^P-X_A^O < 3 Å); X_M^P and X_A^P = apical anions of M^H and A^P cations at the periphery of the TS block; formula A_{3t}^I(PO₄)_tF_t describes the trimeric structure of the I block; m – number of cation I layers, t – number of I layers within the trimeric structure, A_{3m}^I and A_{3t}^I – cations of the I layers except for P⁵⁺. † The most recent reference on the structure: (1) Sample 1991C, Cámara *et al.* (2011); (2) Sokolova and Hawthorne (2008b); (3) Sokolova and Hawthorne (2013); (4) Christiansen *et al.* (2003a); (5) Bellezza *et al.* (2004); (6) Lyalina *et al.* (2015); (7) Cámara *et al.* (2017); (8) Lyalina *et al.* (2016); (9) Christiansen *et al.* (2003b); (10) Cámara *et al.* (2016b); (11) Yamnova *et al.* (1998); (12) Rastsvetaeva *et al.* (2008); (13) Sokolova *et al.* (2015a); (14) bafertisite from Kola, Cámara *et al.* (2016a); (15) Sokolova *et al.* (2016); (16) McDonald *et al.* (2000); (17) Zhou *et al.* (2002); (18) Cámara *et al.* (2009); (19) Krivovichev *et al.* (2003); (20) Andrade *et al.* (2017); (21) Rastsvetaeva and Chukanov (1999); (22) Sokolova and Hawthorne (2008a); (23) Sokolova and Cámara (2008); (24) Chukanov *et al.* (2012); (25) Aksenov *et al.* (2014); (26) Sokolova *et al.* (2011); (27) Sokolova and Hawthorne (2004); (28) Sokolova *et al.* (2017); (29) Ercit *et al.* (1998); (30) Cámara and Sokolova (2007); (31) Cámara *et al.* (2014); (32) Cámara *et al.* (2012); (33) Cámara and Sokolova (2009); (34) Sokolova and Cámara (2007); (35) Cámara *et al.* (2008); (36) Lykova *et al.* (2016); (37) Sokolova and Hawthorne (2017); (38) Cámara *et al.* (2013); (39) Sokolova *et al.* (2013); (40) Sokolova *et al.* (2015b); (41) Sokolova and Hawthorne (2001); (42) Sokolova *et al.* (2005).

Zr-, Fe³⁺- and Mg-dominant sites and (TiMn) sites. Besides Si₂O₇ groups, three other complex anions, (PO₄)³⁻, (SO₄)²⁻ and (CO₃)²⁻, occur outside the TS block in the crystal structures of these minerals. It is very difficult to characterize titanium-disilicate minerals with the TS block as they form intimate intergrowths and twinning is a common feature of many TS-block minerals. Hence crystal-structure solution (and refinement) is not a trivial job. For each mineral, we give references to: (a) the original mineral description; and (b) the most recent work on the crystal structure (Table 1). All other references pertinent to individual mineral species can be found in Sokolova (2006) and Sokolova and Cámara (2013). General structural principles for the seidozerite-supergroup minerals are given in Appendix 1.

We divide the seidozerite-supergroup minerals into four groups based on the content of Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn) (see Table 1 and Appendix 1 for specification of cation sites) and topology and stereochemistry of the TS block.

This is a quantitative classification as minerals of each group have a fixed content of Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn):

Rinkite group	Ti = 1 apfu (atoms per formula unit)
Bafertisite group	Ti = 2 apfu
Lamprophyllite group	Ti = 3 apfu
Murmanite group	Ti = 4 apfu

The four groups correspond to Groups I, II, III and IV of Sokolova (2006). Appendix 2 lists potential seidozerite-supergroup minerals which are not included in the current seidozerite-supergroup nomenclature.

Previous work

The first generalizations on the crystal chemistry of minerals with the TS block were done by Belov (1962–1976, summarized in 1976; e.g. Belov and Organova, 1962) and Pyatenko *et al.* (1976): they considered the TS block as a stable ‘three-layer packet’ characteristic of several Ti-silicate structures. Belov (1976) joined rinkite, mosandrite, seidozerite and rosenbuschite into the ‘rinkite group’ and said that ‘seidozerite-like three-layer packets’ occur in the structures of bafertisite, murmanite, lamprophyllite and innelite; he called TS-block and astrophyllite-group minerals ‘titano-silicate’ analogues of micas.

The alternation of chemically different blocks in a significant number of these structures was

originally described by Egorov-Tismenko and Sokolova (1987, 1990); they considered the sixteen TS-block minerals plus nacaphite, Na₂Ca(PO₄)F (Sokolova *et al.*, 1989), as a unique ‘seidozerite-nacaphite’ series of structures based on the ‘seidozerite block’, and they emphasized the importance of the ‘seidozerite block’ as a basic structural unit. They pointed out that the interlayer composition, i.e. composition of the space between two TS blocks, differs and the topology of the interlayer is related to the structure of nacaphite.

Ferraris *et al.* (1996) introduced a new notation, the HOH layer, for Belov’s ‘seidozerite-like three-layer packet’, where O denotes the sheet of octahedra and H denotes the ‘heterogenous’ silicate sheets. Ferraris *et al.* (1997) called minerals of the ‘seidozerite-nacaphite’ series of Egorov-Tismenko and Sokolova (1987, 1990) ‘heterophyllosilicates’ and ‘seidozerite derivatives’ and considered them as polysomatic and merotype series. Christiansen *et al.* (1999) considered the crystal structures of minerals with HOH sheets as various polytypes and described three types of shift of two H sheets relative to each other, e.g. in seidozerite, lamprophyllite and murmanite.

Sokolova (2006) reviewed structural information for the 24 titanium-disilicate minerals, developed new principles involving the relation between structure topology and chemical composition and divided them into four groups based on the content of Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn) and topology and stereochemistry of the TS block. In Groups I, II, III and IV of Sokolova (2006), Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn) equals 1, 2, 3 and 4 apfu. Therefore Sokolova (2006) has quantitatively classified TS-block minerals. Minerals of each group have structures with a different type of linkage of H and O sheets in the TS block and a different arrangement (stereochemistry) of Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn) polyhedra. For the description of the TS block, Sokolova (2006) used the HOH notation of Ferraris *et al.* (1996), but described the H sheet as a ‘heteropolyhedral sheet’, emphasizing that the H sheet consists of different cation polyhedra [*cf.* ‘heterogenous’ sheet of Ferraris *et al.* (1996)].

The work of Sokolova (2006) resulted in a series of 29 papers on TS-block minerals which we published mainly under the title *From structure topology to chemical composition*. We did not use the latter title for our descriptions of new minerals cámaraite, kazanskiite, saamite, kolskyite, bobshannonite and fogoite-(Y) (Table 1). Following Sokolova (2006) we published a second general

paper on TS-block minerals under the title *From structure topology to chemical composition. XVI. New developments in the crystal chemistry and prediction of new structure topologies for titanium disilicate minerals with the TS block* (Sokolova and Cámara, 2013). In this paper, we introduced a new concept of ‘basic’ and ‘derivative’ structures and, using the relation between basic and derivative structures, predicted 14 new structure types. We published a further paper on explanation of different topologies of Fe^{3+} - and Ti^{4+} -disilicates with HOH layers (Sokolova and Cámara, 2014); and in another paper, we considered the crystal

chemistry of Ba and how Ba affects the topology of TS-block structures (Sokolova and Cámara, 2016). CNMNC-IMA recently reapproved betalomonosovite, a TS-block mineral of the murmanite group (Sokolova *et al.*, 2015b)

The general topology of the TS block

The TS block consists of a central O (O = Octahedral) sheet and two adjacent H (H = Heteropolyhedral) sheets. The O sheet is an array of close-packed octahedra (Fig. 1a) with the formula $M^O X_2^O$, where M^O and X^O are cations and anions of the O sheet. The

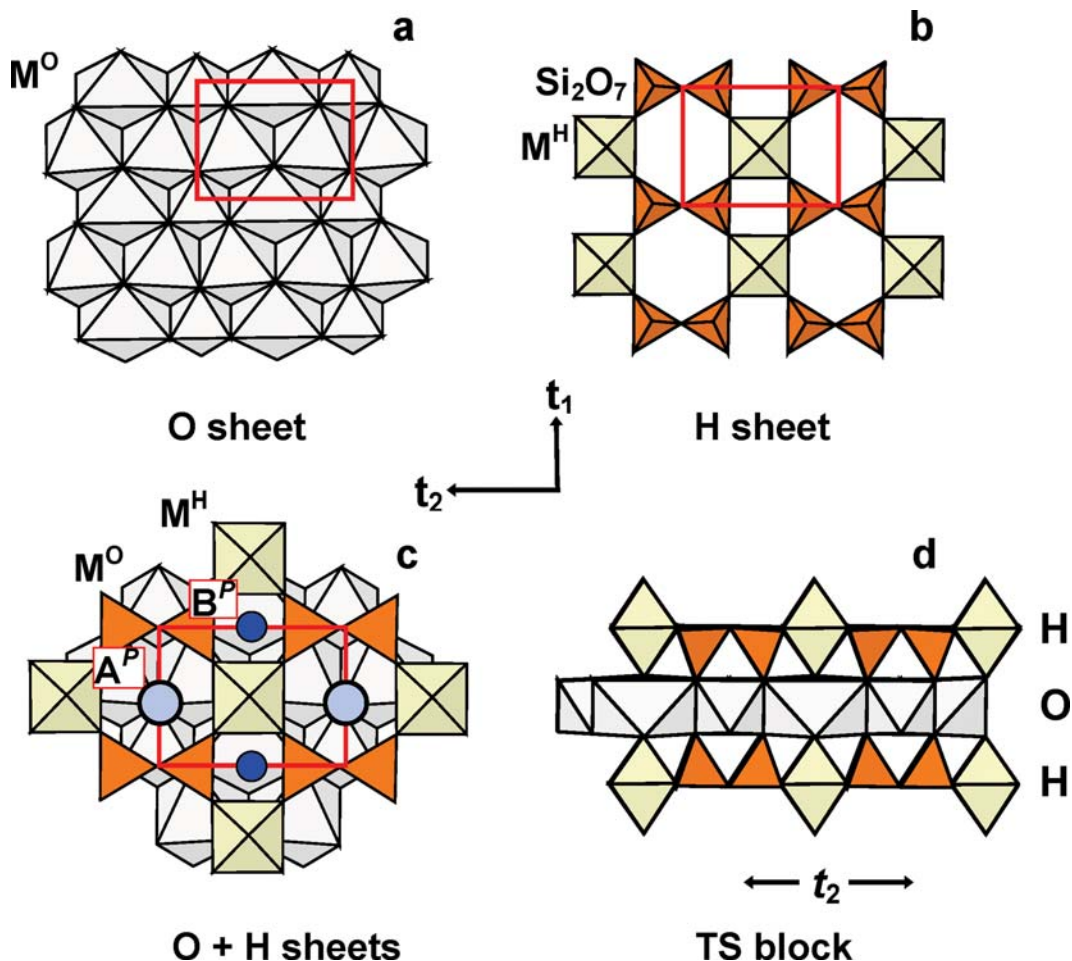


FIG. 1. General topology of the TS (Titanium-Silicate) block: (a) the O (Octahedral) sheet, (b) the H (Heteropolyhedral) sheet of Si_2O_7 groups and M^H polyhedra, (c) O + H sheets and (d) TS block composed of HOH sheets; M^O and M^H octahedra are white and pale yellow, SiO_4 tetrahedra are orange, cations at the peripheral A^P and B^P sites are shown as large pale blue and smaller dark blue spheres, red lines show the minimal cell with $t_1 \approx 5.5 \text{ \AA}$ and $t_2 \approx 7 \text{ \AA}$.

H sheet consists of Si_2O_7 groups and [5–7]-coordinated M^{H} polyhedra in the ratio 1:1 (Fig. 1b). The O and H sheets link together through common vertices of constituent polyhedra (Fig. 1c) to form a TS block (Fig. 1d). The TS block is characterized by a planar minimal cell based on translation vectors, \mathbf{t}_1 and \mathbf{t}_2 , the lengths of these vectors are $t_1 \approx 5.5$ and $t_2 \approx 7 \text{ \AA}$, and $\mathbf{t}_1 \wedge \mathbf{t}_2$ is close to 90° .

There are two peripheral (P) cation sites, A^P and B^P , which occur on the periphery of the TS block (Fig. 1c). The [5–8]-coordinated A^P site can occur in the plane of the H sheet where its constituent cation is bonded to an anion of the O sheet (X_{A}^{O}). The cations occupying the P sites can occur in the intermediate space (out of the H sheet), and, in this case, we consider them as part of the **I** (**I**=Intermediate) block. The B^P cavity is too small to accommodate any cation in the plane of the H sheet, and the B^P cation always occurs in the **I** block.

There are three topologically distinct TS blocks based on three types of linkage of two H sheets and the central O sheet. Linkage 1 occurs where two H sheets connect to the O sheet so that two Si_2O_7 groups on opposite sides of the O sheet link to *trans* edges of the same octahedron of the O sheet (Fig. 2a). Linkage 2 occurs where two Si_2O_7 groups link to two octahedra of the O sheet adjacent along \mathbf{t}_2 (Fig. 2b). Linkage 3 occurs where two Si_2O_7 groups link to two octahedra adjacent approximately along \mathbf{t}_1 (Fig. 2c). Three types of linkage of H and O sheets result in three different topologies of the TS block.

The structural hierarchy of the TS-block structures

All TS-block structures consist either solely of TS blocks or of two types of block: the TS block and an **I** block that comprises atoms between two TS blocks.

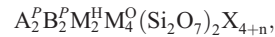
There are four types of self-linkage between adjacent TS blocks. [1] TS blocks link directly through common edges of M^{H} and A^P polyhedra, and common vertices of M^{H} , A^P and Si polyhedra of the H sheets belonging to two TS blocks. [2] TS blocks link through common vertices of Ti (+ Nb) octahedra and the **I** block has one layer of cations ($m=1$). [3] TS blocks do not link directly, additional cations do not occur in the **I** space ($m=0$) and TS blocks are connected through hydrogen bonds of H_2O groups at the X^P sites. [4] TS blocks do not link directly and there are

additional layers of cations (and anions), the **I** block, between adjacent TS blocks ($m=1-6$).

For the concept of ‘basic’ and ‘derivative structures’ (Sokolova and Cámara, 2013), see Appendix 1, (13). There are 40 basic TS-block structures and five derivative TS-block structures: cámaraité, bornemanite, saamite, kazanskyite and nechelyustovite.

The general formula of the TS block

The general formula of the TS block is as follows:



where M_2^{H} and M_4^{O} = cations of the H and O sheets; M^{H} = Ti, Nb, Zr, Y, Mn, Ca + REE [rare-earth elements], Ca; M^{O} = Ti, Zr, Nb, Fe^{3+} , Fe^{2+} , Mg, Mn, Zn, Ca, Na; A^P and B^P = cations at the peripheral (P) sites = Na, Ca + REE, Ca, Zn, Ba, Sr, K; X = anions = O, OH, F, H_2O ; $\text{X}_{4+n} = \text{X}_4^{\text{O}} + \text{X}_n^{\text{P}}$, $n = 0, 1, 1.5, 2, 4$; $\text{X}^{\text{P}} = \text{X}_M^{\text{P}}$ and X_A^{P} = apical anions of M^{H} and A^P cations at the periphery of the TS block. The stoichiometry of the core part of the TS block, $\text{M}_2^{\text{H}} \text{M}_4^{\text{O}} (\text{Si}_2\text{O}_7)_2 \text{X}_4^{\text{O}}$, is invariant in all structures.

Naming of the seidozerite supergroup

We chose the name seidozerite for both historical and topological reasons:

- (1) Belov (1962–1976) pioneered the crystal chemistry of the TS-block minerals as we call them now. After solving the crystal structure of seidozerite, a framework of TS-blocks with no intermediate space left between them, Belov used the words ‘seidozerite-like three-layer packet’ to describe the three-sheet nature of the TS-block in several minerals known at that time.
- (2) The alternation of chemically different blocks in a significant number of TS-block structures was originally considered by Egorov-Tismenko and Sokolova (1987, 1990). They considered 17 minerals: seidozerite, rinkite-(Ce), götzenite, rosenbuschite, lamprophyllite, murmanite, epistolite, bafertsite, hejtmánite, innelite, lomonosovite, betalomonosovite, vuonnemite, quadruphite, polyphite, sobolevite and nacaphite as a unique ‘seidozerite-nacaphite’ series of structures based on the ‘seidozerite’ block, and they emphasized importance of the ‘seidozerite’ block as a basic structural unit. The sixteen TS-block minerals considered by Egorov-Tismenko and Sokolova (1987, 1990) (see above) represent the four groups of the

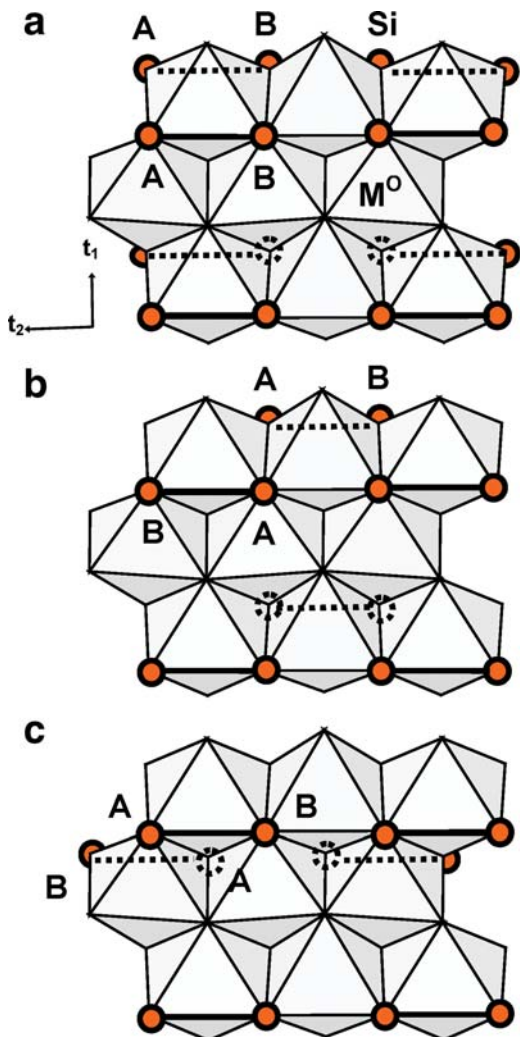


FIG. 2. Schematic representation of different linkages between O and H sheets, i.e. between M^O octahedra and Si_2O_7 groups within one TS block, M^H cations are omitted for clarity: (a) linkage 1; (b) linkage 2; (c) linkage 3. Legend as in Fig. 1, Si_2O_7 groups of two different H sheets are shown schematically as two orange circles connected by a solid (upper surface) or a dashed (lower surface) black line.

seidozerite supergroup: rinkite group (seidozerite, rinkite-(Ce), götzenite, rosenbuschite), bafertisite group (bafertisite, hejmanite), lamprophyllite group (lamprophyllite, vuonnemite, epistolite, innelite) and murmanite group (murmanite, lomonosovite, betalomonosovite, quadruphite, polyphite and sobolevite).

In accord with the original work on TS-block minerals (Belov, 1962–1976; Egorov-Tismenko and Sokolova, 1987, 1990) we chose the following name: seidozerite supergroup of TS-block minerals.

Four groups of the seidozerite-supergroup minerals

We divide the seidozerite-supergroup minerals into four groups based on the content of Ti (+ Nb + Zr + Fe^{3+} + Mg + Mn) and topology and stereochemistry of the TS block. Each group of minerals has the TS block with different: (1) content of Ti (+ Nb + Zr + Fe^{3+} + Mg + Mn); (2) topology of the TS block defined by the type of linkage of H and O sheets; and (3) stereochemistry of Ti (+ Nb + Zr + Fe^{3+} + Mg + Mn) in the TS block. Ideal structural formulae for the 45 seidozerite-supergroup minerals are given in Table 1. Detailed ideal structural formulae for each group are given in Tables 2–5. Crystallographic information for the 45 TS-block minerals is given in Table 6.

Rinkite group

TS block

Ti (+ Nb + Zr) = 1 apfu; Ti occurs in the O sheet; linkage 1 occurs: Si_2O_7 groups of the two H sheets link to trans edges of the large Na polyhedron of the O sheet (Fig. 3a); 1 M^O = Ti, rarely Nb or Zr; 3 M^O are mainly Na, Ca and rarely Mn^{2+} ; $^{[6,7]}M^H$ = Zr, Y, Ca + REE, Ca, Mn; A^P = Na, Ca, Ca + REE (Table 2).

Self-linkage of TS blocks

Self-linkage [1] occurs and TS blocks link directly through common edges of M^H and A^P polyhedra, and common vertices of M^H , A^P and Si polyhedra of the H sheets belonging to two TS blocks.

The crystal structures of the rinkite-group minerals are frameworks of TS blocks (Figs 3b–d).

Bafertisite group

TS block

Ti (+ Nb) = 2 apfu; Ti occurs in the H sheets; linkage 2 occurs: Si_2O_7 groups of the two H sheets link to two M^{2+} octahedra of the O sheet adjacent along t_2 (Fig. 4a); 4 M^O = 4 M^{2+} = Fe^{2+} , Mn^{2+} and (Fe^{2+} Na); $^{[5,6]}M^H$ = Ti, Nb; A^P , B^P = Ba, Na, Sr, K (Table 3).

TABLE 2. Ideal structural formulae of the rinkite-group minerals*, Ti (+ Nb + Zr) = 1 apfu per (Si₂O₇)₂

Mineral	Ideal structural formula							Z	
	A ₂ ^P	M ₂ ^H	M ₄ ^O			(Si ₂ O ₇) ₂	(X _M ^O) ₂	(X _A ^O) ₂	
Rinkite-(Ce)	Ca ₂	(CaREE)	Na(NaCa)	Ti		(Si ₂ O ₇) ₂	(OF)	F ₂	2
Nacareniobsite-(Ce)	(Ca,REE) ₂	(Ca,REE) ₂	Na ₃	Nb		(Si ₂ O ₇) ₂	(OF)	F ₂	2
Mosandrite-(Ce)	Ca ₂	(CaREE)	[(H ₂ O) ₂ Ca _{0.5} □ _{0.5}]	Ti		(Si ₂ O ₇) ₂	(OH) ₂	(H ₂ O) ₂	2
Seidozerite	Na ₂	Zr ₂	Na ₂ Mn	Ti		(Si ₂ O ₇) ₂	O ₂	F ₂	2
Grenmarite	Na ₂	Zr ₂	Na ₂ Mn	Zr		(Si ₂ O ₇) ₂	O ₂	F ₂	2
Götzenite	Ca ₂	Ca ₂	NaCa ₂	Ti		(Si ₂ O ₇) ₂	(OF)	F ₂	1
Hainite-(Y)	Ca ₂	(CaY)	Na(NaCa)	Ti		(Si ₂ O ₇) ₂	(OF)	F ₂	1
Fogoite-(Y)	Ca ₂	Y ₂	Na ₃	Ti		(Si ₂ O ₇) ₂	(OF)	F ₂	1
Batievaite-(Y)	Ca ₂	Y ₂	(H ₂ O) ₂ □	Ti		(Si ₂ O ₇) ₂	(OH) ₂	(H ₂ O) ₂	1
Kochite	Ca ₂	Mn Zr	Na ₃	Ti		(Si ₂ O ₇) ₂	(OF)	F ₂	2
Rosenbuschite	Ca ₄	Ca ₂ Zr ₂	Na ₆	Ti Zr		(Si ₂ O ₇) ₄	(OF) ₂	F ₄	1

* Ideal structural formulae are from Sokolova and Cámara (2013) and Cámara *et al.* (2017) for fogoite-(Y) and Lyalina *et al.* (2016) for batievaite-(Y); the formulae are per (Si₂O₇)₂, except per (Si₂O₇)₄ for rosenbuschite. The invariant core of the TS block, **M₂^HM₄^O(Si₂O₇)₂X₄^O**, is shown in bold: M^O and M^H = cations of the O and H sheets, A^P = cations at the peripheral (P) sites; X^O = anions of the O sheet not bonded to Si; X_M^O = anions at the common vertices of 3M^O and M^H polyhedra; X_A^O = anions at the common vertices of 3M^O and A^P polyhedra.

TABLE 3. Ideal structural formulae of the bafertisite-group minerals*, Ti (+ Nb) = 2 apfu per (Si₂O₇)₂

Mineral	Ideal structural formula									Z
	I block		TS block		I block	TS block				
Jinshajiangite	A ₁₋₂ ^P	B ₀₋₂ ^P	M₄^O	M₂^H	(Si ₂ O ₇) ₂	(X _M ^O) ₂	(X _A ^O) ₂	(X _M ^P) ₀₋₂		8
Perraultite	Ba	Na	Fe₄²⁺	Ti₂	(Si ₂ O ₇) ₂	O ₂	(OH) ₂	F		8
Bobshannonite	Ba K	Na ₂	(Mn,Na)₈	(Nb,Ti)₄	(Si ₂ O ₇) ₄	O ₄	(OH) ₄	(O,F) ₂		4
Bafertisite	Ba ₂		Fe₄²⁺	Ti₂	(Si ₂ O ₇) ₂	O ₂	(OH) ₂	F ₂		4
Hejtmanite	Ba ₂		Mn₄	Ti₂	(Si ₂ O ₇) ₂	O ₂	(OH) ₂	F ₂		4
Yoshimuraite	Ba ₂	Ba ₂	Mn₄	¹⁵¹Ti₂	(Si ₂ O ₇) ₂	O ₂	(OH) ₂		(PO ₄) ₂	2
Bussenite	Ba ₂	Ba ₂	(Fe²⁺Na)₂	Ti₂	(Si ₂ O ₇) ₂	O ₂	(OH) ₂	(H ₂ O) ₂	(CO ₃) ₂ F ₂	2
Cámaraite	A ₃ ^P	B ^P	M₈^O	M₄^H	(Si ₂ O ₇) ₄	(X _M ^O) ₄	(X _A ^O) ₄	(X _M ^P) ₃		4
	Ba ₃	Na	Fe₈²⁺	Ti₄	(Si ₂ O ₇) ₄	O ₄	(OH) ₄	F ₃		4

*Ideal structural formulae are from Sokolova and Cámara (2013), with the anion part modified for bafertisite, hejtmanite and cámaraite in accord with Sokolova and Cámara (2016); formulae are per (Si₂O₇)₂, except per (Si₂O₇)₄ for bobshannonite and cámaraite.

The invariant core of the TS block, **M₄^O(Si₂O₇)₂X₄^O**, is shown in bold; M^O and M^H = cations of the O and H sheets, A^P and B^P = cations at the peripheral (P) sites; X₄^O = anions of the O sheet not bonded to Si; X_M^O = anions at the common vertices of 3 M^O and M^H polyhedra; X_A^O = anions at the common vertices of 3 M^O and A^P polyhedra (where A^P-X_A^O < 3 Å); X_M^P = apical anions of M^H cations at the periphery of the TS block. Constituents of the I block are shown in turquoise colour. Surkhobite (Rastsvetaeva *et al.*, 2008) is not listed here as there are problems with its chemical formula.

TABLE 4. Ideal structural formulae of the lamprophyllite-group minerals*, Ti (+ Nb + Fe³⁺ + Mg) = 3 apfu per (Si₂O₇)₂

Mineral	Ideal structural formula									Z	
	I block			TS block			I block				
Basic structures											
Lamprophyllite-2M, -2O	A ₂ ^P (SrNa)	B ₂ ^P	M ₂ ^H ¹⁵ lTi ₂	M ₄ ^O Na ₃	Ti	(Si ₂ O ₇) ₂	(X _M ^O) ₂	(X _A ^O) ₂	(X _{M,A} ^P) ₄	2	
Fluorlamprophyllite	(SrNa)		¹⁵ lTi ₂	Na ₃	Ti	(Si ₂ O ₇) ₂	O ₂	(OH) ₂	F ₂	2	
Nabalamprophyllite-2M	BaNa		¹⁵ lTi ₂	Na ₃	Ti	(Si ₂ O ₇) ₂	O ₂	(OH) ₂		2	
Nabalamprophyllite-2O	(BaNa)		¹⁵ lTi ₂	Na ₃	Ti	(Si ₂ O ₇) ₂	O ₂	(OH) ₂		2	
Barytolamprophyllite	(BaK)		¹⁵ lTi ₂	Na ₃	Ti	(Si ₂ O ₇) ₂	O ₂	(OH) ₂		2	
Lileyite**	Ba ₂		¹⁵ lTi ₂	Na(NaM ²⁺)	Mg _{5⁺}	(Si ₂ O ₇) ₂	O ₂	F ₂		2	
Emmerichite	Ba ₂		¹⁵ lTi ₂	Na ₃	Fe _{5⁺}	(Si ₂ O ₇) ₂	O ₂	F ₂		2	
Innelite-1A, -2M **	Ba ₂	Ba ₂	¹⁵ lTi ₂	Na(NaM ²⁺)	Ti	(Si ₂ O ₇) ₂	O ₂	[O(OH)]	[(SO ₄)(PO ₄)]	1,2	
Epistolite	(Na□)		¹⁶ lNb ₂	Na ₃	Ti	(Si ₂ O ₇) ₂	O ₂	(OH) ₂	(H ₂ O) ₄	1	
Zvyaginite	Na□		¹⁶ lNb ₂	NaZn□	Ti	(Si ₂ O ₇) ₂	O ₂	(OH) ₂	(H ₂ O) ₄	4	
Vuonnemite	Na ₂		¹⁶ lNb ₂	Na ₃	Ti	(Si ₂ O ₇) ₂	O ₂	(OH) ₂		1	
Delindeite***	Ba ₂		¹⁶ lTi ₂	Na ₂ □	Ti	(Si ₂ O ₇) ₂	(OH) ₂	(H ₂ O) ₂	O ₂	8	
Derivative structures											
Bornemanite	A ₄ ^P Ba ₂ (Na□)		M ₂ ^H ¹⁵ lTi ₂ ¹⁶ lNb ₂	M ₄ ^O (Na ₅ □)	Ti ₂	(Si ₂ O ₇) ₄	(X _M ^O) ₄	(X _A ^O) ₄	(OH) ₂ F ₂	Na ₆ (PO ₄) ₂	2
Saamite	A ₂ ^P Ba□		M ₂ ^H ¹⁵ lTi ¹⁶ lNb	M ₄ ^O Na ₃	Ti	(Si ₂ O ₇) ₂	(X _M ^O) ₂	(X _A ^O) ₂	(X _{M,A} ^P) ₂ (H ₂ O) ₂		2
Kazanskyite	A ₂ ^P Ba□		M ₂ ^H ¹⁵ lTi ¹⁶ lNb	M ₄ ^O Na ₃	Ti	(Si ₂ O ₇) ₂	(X _M ^O) ₂	(X _A ^O) ₂	(X _M ^P) (H ₂ O)	(H ₂ O) ₃	2
Nechelyustovite	A ₈ ^P Ba ₄ (Na□)□ ₂		M ₂ ^H ¹⁵ lTi ₄ ¹⁶ lNb ₂ ¹⁶ lNb ₂	M ₁₆ ^O (Na ₁₁ □)	Ti ₄	(Si ₂ O ₇) ₈	(X _M ^O) ₈	(X _A ^O) ₈	(X _{M,A} ^P) ₇ (H ₂ O) ₇	(H ₂ O) ₅	1

*Ideal structural formulae are from Sokolova and Cámara (2013), with the anion part modified for bornemanite in accord with Sokolova and Cámara (2016); formulae are per (Si₂O₇)₂, except per (Si₂O₇)₄ for bornemanite and (Si₂O₇)₈ for nechelyustovite.

The invariant core of the TS block, M₂^HM₄^O(Si₂O₇)₂X₄^O, is shown in bold; M^O and M^H = cations of the O and H sheets, A^P and B^P = cations at the peripheral (P) sites; X₄^O = anions of the O sheet not bonded to Si: X_M^O = anions at the common vertices of 3M^O and M^H polyhedra; X_A^O = anions at the common vertices of 3M^O and A^P polyhedra (where A^P - X_A^O < 3 Å); X_M^P and X_A^P = apical anions of M^H and A^P cations at the periphery of the TS block. Constituents of the I block are shown in turquoise color.

** M²⁺ = Fe²⁺, Ca, Mn (lileyite); M²⁺ = Mn, Fe²⁺, Mg, Ca (innelite);

*** due to the Na-H₂O disorder in the O sheet, the stereochemistry of the TS block in delindeite is similar to that of the rinkite group.

TABLE 5. Ideal structural formulae of the murmanite-group minerals*, Ti (+ Mg + Mn) = 4 apfu per (Si₂O₇)₂

Mineral	Ideal structural formula								Z
	I block		TS block				I block		
Murmanite	A ^P ₂	M ^H ₂	M^O(1)₂	M^O(2)₂	(Si₂O₇)₂	(X _M ^O) ₂	(X _A ^O) ₂	(X _{M,A} ^P) ₂₋₄	1
Calciomurmanite	Na ₂	Ti₂	Ti₂	Na₂	(Si₂O₇)₂	O₂	O₂	(H ₂ O) ₄	1
Vigrishinite	(Ca□)	Ti₂	Ti₂	(Na□)	(Si ₂ O ₇) ₂	O₂	[O(OH)]	(H ₂ O) ₄	1
Kolskyite	Zn□	Ti₂	Ti₂	Na□	(Si ₂ O ₇) ₂	O₂	O(OH)	(H ₂ O) ₄	1
Schüllerite	(Ca□)	Ti₂	Ti₂	Na₂	(Si₂O₇)₂	O₂	O₂	(H ₂ O) ₂	1
Schüllerite	Ba ₂	⁵ Ti₂	Mg₂	Na₂	(Si₂O₇)₂	O₂	F₂	(H ₂ O) ₅	1
Lomonosovite	Na ₂	Ti₂	Ti₂	Na₂	(Si₂O₇)₂	O₂	O₂	Na ₆ (PO ₄) ₂	1
Betalomonosovite	Na ₂	Ti₂	Ti₂	Na₂	(Si₂O₇)₂	O₂	(OF)	Na ₂ □ ₄ [PO ₃ (OH)][PO ₂ (OH) ₂]	2
Quadruphite	Na ₂	Ti₂	Ti₂	Na₂	(Si₂O₇)₂	O₂	O₂	Na ₈ Ca ₂ (PO ₄) ₄ F ₂	1
Sobolevite	Na ₂	Ti₂	(TiMn)	Na₂	(Si₂O₇)₂	O₂	(OF)	Na ₉ Ca ₂ Mn(PO ₄) ₄ F ₂	2
Polyphite	Na ₂	Ti₂	Ti₂	Na₂	(Si₂O₇)₂	O₂	O₂	Na ₁₄ Ca ₄ Mn(PO ₄) ₆ F ₄	1

*Ideal structural formulae are from Sokolova and Cámara (2013), except for betalomonosovite (Sokolova *et al.*, 2015b), calciomurmanite (this work) and vigrishinite (Sokolova and Hawthorne, 2017). The invariant core of the TS block, **M^H₂M^O₄(Si₂O₇)₂X₄^O**, is shown in bold; M^O and M^H = cations of the O and H sheets, A^P = cations at the peripheral (P) sites; X₄^O = anions of the O sheet not bonded to Si: X_M^O = anions at the common vertices of 3M^O and M^H polyhedra; X_A^O = anions at the common vertices of 3M^O and A^P polyhedra (where A^P-X_A^O < 3 Å); X_M^P and X_A^P = apical anions of M^H and A^P cations at the periphery of the TS block; (where X^P anions are ligands of P⁵⁺ cations they are considered as part of the I block, shown in turquoise colour); coordination numbers are given for non-octahedral sites in the TS block. Constituents of the I block are shown in turquoise colour.

TABLE 6. Crystallographic information for seidozerite-supergruop TS-block minerals*.

Mineral	Str.**	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	α (°)	β (°)	γ (°)	Sp. gr.	<i>Z</i>	Ref.†
Rinkite group										
Rinkite-(Ce)	B1(RG)	7.441	5.663	18.832	90	101.383	90	$P2_1/c$	2	(1)
Nacareniobsite-(Ce)	B1(RG)	7.468	5.689	18.891	90	101.370	90	$P2_1/c$	2	(2)
Mosandrite-(Ce)	B1(RG)	7.422	5.618	18.723	90	101.423	90	$P2_1/c$	2	(3)
Seidozerite	B2(RG)	5.556	7.075	18.406	90	102.713	90	$P2/c$	2	(4)
Grenmarite	B2(RG)	5.608	7.139	18.575	90	102.600	90	$P2/c$	2	(5)
Götzenite	B3(RG)	9.619	5.723	7.331	89.981	101.132	100.639	$P\bar{1}$	1	(4)
Hainite-(Y)	B3(RG)	9.605	5.693	7.334	89.903	101.082	100.830	$P\bar{1}$	1	(6)
Fogoite-(Y)	B3(RG)	9.575	5.685	7.279	89.985	100.933	101.300	$P\bar{1}$	1	(7)
Batievaite-(Y)	B3(RG)	9.402	5.562	7.378	89.919	101.408	96.621	$P\bar{1}$	1	(8)
Kochite	B3(RG)	10.032	11.333	7.202	90.192	100.334	111.551	$P\bar{1}$	2	(9)
Rosenbuschite	B3(RG)	10.137	11.398	7.2717	90.216	100.308	111.868	$P\bar{1}$	1	(4)
Bafertisite group										
Jinshajiangite	B1(BG)	10.706	13.799	20.760	90.008	94.972	89.984	$C\bar{1}$	8	(10)
Perraultite	B1(BG)	10.731	13.841	20.845	90	95.06	90	$C2$	8	(11)
Surkhobite	B1(BG)	10.723	13.826	20.791	90	95.00	90	$C2$	2	(12)
Bobshannonite	B1(BG)	10.839	13.912	20.980	89.99	95.02	89.998	$C\bar{1}$	4	(13)
Bafertisite	B2(BG)	10.677	13.767	11.737	90.12	112.28	90.02	$C\bar{1}$	4	(14)
Hejtmanite	B2(BG)	10.716	13.795	11.778	90.07	112.24	90.03	$C\bar{1}$	4	(15)
Yoshimuraite	B3(BG)	5.386	6.999	14.748	95.50	93.620	89.980	$P\bar{1}$	2	(16)
Bussenite	B4(BG)	5.399	7.016	16.254	102.44	93.180	90.100	$P\bar{1}$	2	(17)
Cámaraite	D1(BG)	10.697	13.786	21.478	99.345	92.315	89.993	$C\bar{1}$	4	(18)
Lamprophyllite group										
Lamprophyllite-2 <i>M</i>	B1(LG)	19.215	7.061	5.372	90	96.797	90	$C2/m$	2	(19)
Lamprophyllite-2 <i>O</i>	B1(LG)	19.128	7.080	5.382	90	90	90	$Pnmm$	2	(19)
Fluorlamprophyllite	B1(LG)	19.255	7.072	5.381	90	96.794	90	$C2/m$	2	(20)
Nabalamprophyllite-2 <i>M</i>	B1(LG)	19.741	7.105	5.408	90	96.67	90	$P2/m$	2	(21)
Nabalamprophyllite-2 <i>O</i>	B1(LG)	19.564	7.117	5.414	90	90	90	$Pnmm$	2	(22)
Barytolamprophyllite	B1(LG)	19.897	7.117	5.411	90	96.676	90	$C2/m$	2	(23)
Lileyite	B1(LG)	19.905	7.098	5.405	90	96.349	90	$C2/m$	2	(24)
Emmerichite	B1(LG)	19.960	7.099	5.407	90	93.367	90	$C2/m$	2	(25)
Innelite-1 <i>A</i>	B2(LG)	5.423	7.131	14.785	98.442	94.579	90.009	$P\bar{1}$	1	(26)
Innelite-2 <i>M</i>	B2(LG)	5.421	7.125	29.314	90	94.698	90	$P2/c$	2	(26)
Epistolite	B3(LG)	5.460	7.170	12.041	103.63	96.01	89.98	$P\bar{1}$	1	(27)
Zvyaginite	B3(LG)	10.769	14.276	12.101	105.45	95.17	90.04	$C\bar{1}$	4	(28)

Vuonnemite	B4(LG)	5.498	7.161	14.450	92.60	95.30	90.60	$P\bar{1}$	1	(29)
Bornemanite	D1(LG)	5.459	7.142	24.528	96.970	96.927	90.326	$P\bar{1}$	1	(30)
Saamite	D4(LG)	5.437	7.141	21.69	92.97	96.07	90.01	$P\bar{1}$	2	(31)
Kazanskyite	D2(LG)	5.426	7.135	25.514	98.172	90.916	89.964	$P\bar{1}$	2	(32)
Nechelyustovite	D3(LG)	5.447	7.157	47.259	95.759	92.136	89.978	$P\bar{1}$	1	(33)
Delindeite	Related	10.645	13.713	21.600	90	93.804	90	$C2/c$	8	(34)
Murmanite group										
Murmanite	B1(MG)	5.388	7.058	12.176	93.511	107.943	90.093	$P\bar{1}$	1	(35)
Calciomurmanite	B1(MG)	5.347	7.078	12.146	91.827	107.527	90.155	$P\bar{1}$	1	(36)
Vigrishinite	B1(MG)	10.530	13.833	11.659	94.34	98.30	89.90	$C\bar{1}$	4	(37)
Kolskyite	B7(MG)	5.387	7.091	15.473	96.58	93.948	89.818	$P\bar{1}$	1	(38)
Schüllerite	B2(MG)	5.396	7.071	10.226	99.73	99.55	90.09	$P\bar{1}$	1	(39)
Lomonosovite	B3(MG)	5.417	7.119	14.487	99.957	96.711	90.360	$P\bar{1}$	1	(35)
Betalomonosovite	B3(MG)	5.333	14.172	14.509	103.174	96.320	90.278	$P\bar{1}$	2	(40)
Quadruphite	B4(MG)	5.421	7.085	20.364	86.89	94.42	89.94	$P1$	1	(41)
Sobolevite	B5(MG)	7.076	5.411	40.623	90	93.156	90	Pc	2	(42)
Polyphite	B6(MG)	5.393	7.055	26.451	95.216	93.490	90.101	$P\bar{1}$	1	(42)

*The unit-cell parameters are given to the third decimal.

**Structure type: B (basic) or D (derivative) (Sokolova and Cámara, 2013); (RG = Rinkite group, BG = Bafertisite group, LG = Lamprophyllite group, MG = Murmanite group).

† The most recent reference on the structure as in Table 1.

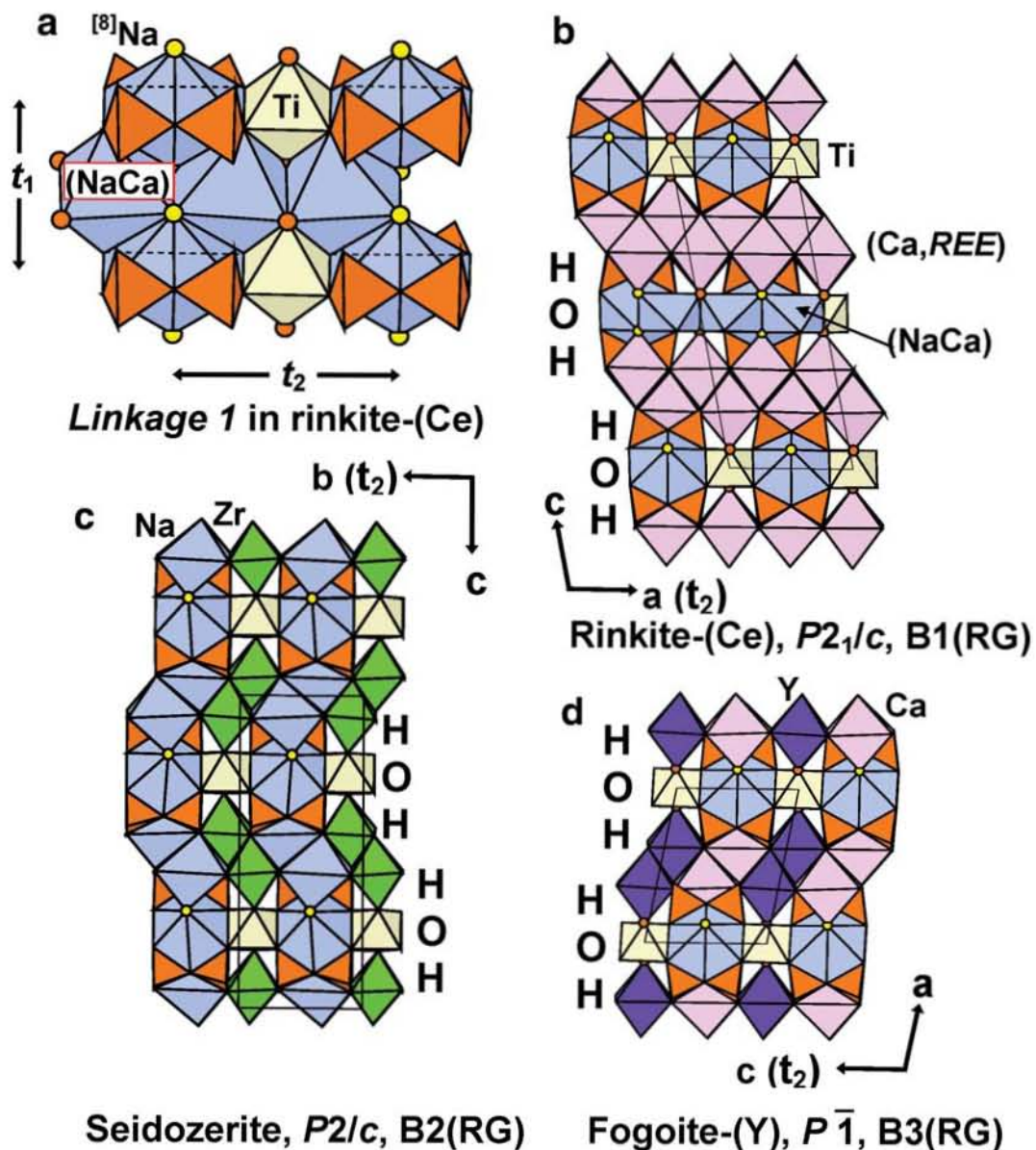


FIG. 3. Rinkite group: linkage 1 of H and O sheets in rinkite-(Ce) (a), only the Si_2O_7 groups of the H sheets are shown, M^{H} and A^{P} polyhedra are omitted for clarity, positions of the Si_2O_7 groups of the lower H sheet are shown by dashed lines; the basic crystal structures of rinkite-(Ce) (b), seidozerite (c) and fogoite-(Y) (d). Si, Na, Ti, Zr, Y and Ca polyhedra are orange, blue, pale yellow, green, purple and pink, respectively. F atoms and (O,F) anions are shown as small yellow and orange spheres. Captions (b–d): mineral name, space group, structure type where B = Basic structure, RG = Rinkite Group.

Self-linkage of TS blocks

Two types of self-linkage of TS blocks occur: [2] TS blocks link through common vertices of Ti

octahedra and the I block has one layer of cations ($m = 1$) in bobshannonite (Fig. 4b), jinshajiangite, perraultite and surkhobite; and [4] TS blocks do not

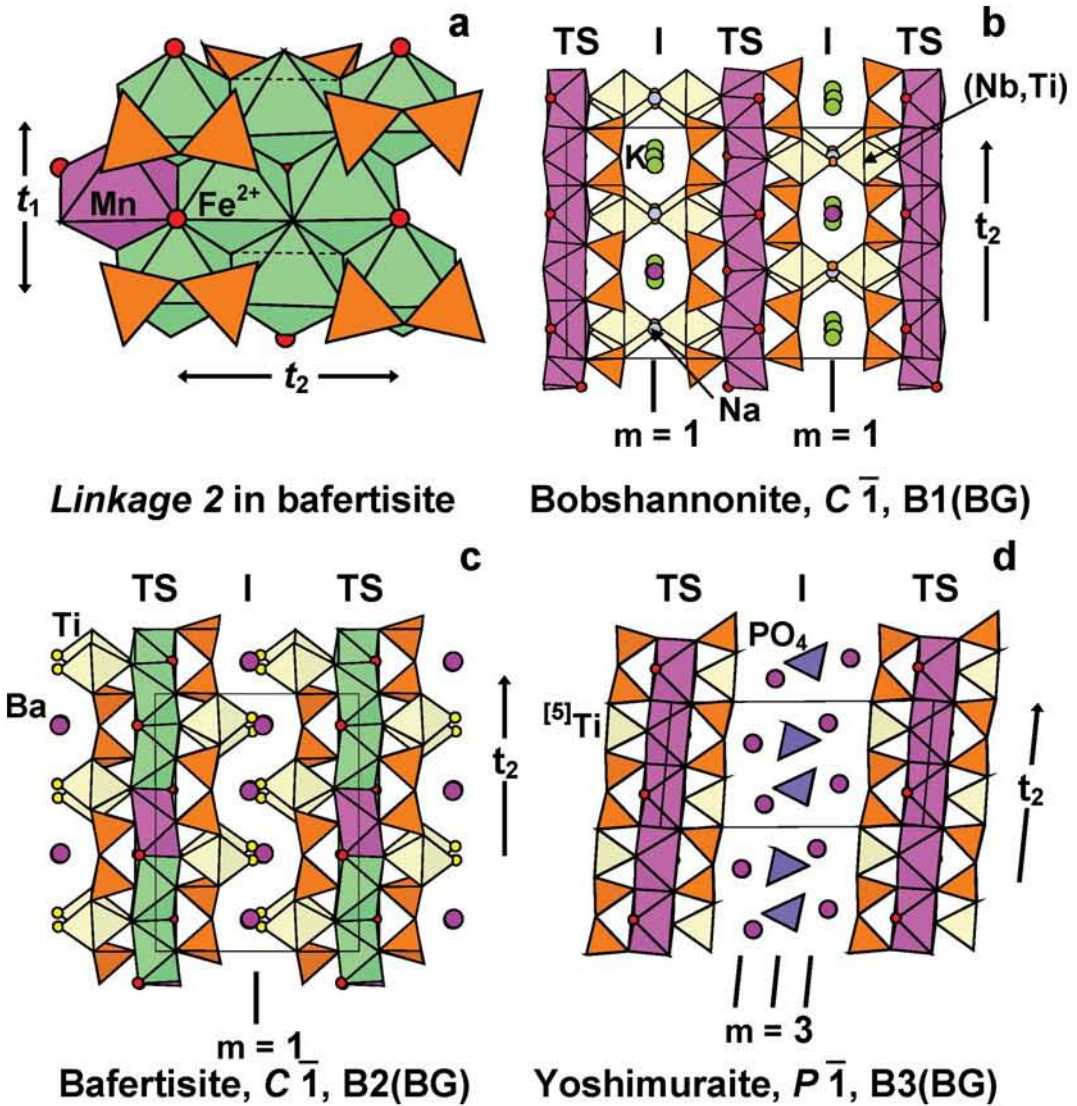


FIG. 4. Bafertisite group: linkage 2 of H and O sheets in bafertisite (a), the basic crystal structures of bobshannonite (b), bafertisite (c) and yoshimuraite (d). Legend as in Fig. 2; Ti (+ Nb), Fe^{2+} and Mn polyhedra are pale yellow, green and magenta, respectively; Ba, K and Na atoms are shown as large raspberry and green spheres and medium blue spheres; F atoms, (OF) anions and OH groups are shown as small yellow, orange and red spheres, respectively. Captions (b–d): mineral name, space group, structure type where B = Basic structure, BG = Bafertisite Group. Labels TS and I show position of TS and I blocks in a structure, and short black lines show position of cation layers (m = number of layers) in the I block.

link directly, and there are additional layers of cations (and anions), the I block, between adjacent TS blocks ($m = 1-4$) (Figs 4c,d).

The crystal structures of the bafertisite-group minerals are alternation of the TS and I blocks.

Lamprophyllite group

TS block

Ti (+ Nb + Fe^{3+} + Mg) = 3 apfu; Ti occurs in the O sheet (1 apfu) and H sheets (2 apfu); linkage 1

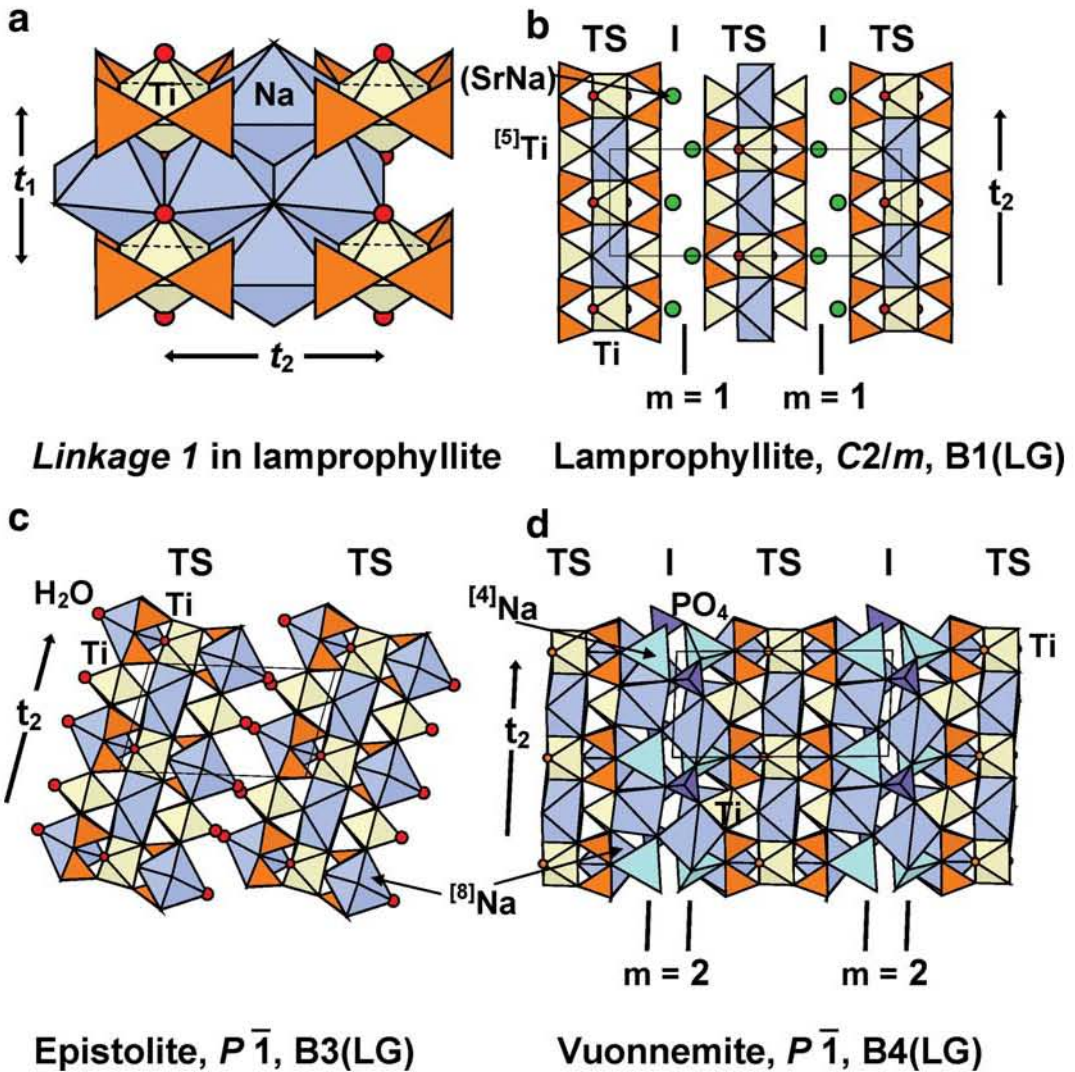


FIG. 5. Lamprophyllite Group: linkage 1 of H and O sheets in lamprophyllite (a), the basic crystal structures of lamprophyllite (b), epistolite (c) and vuonnemite (d). Legend as in Fig. 3; Ti, $^{[6,8]}\text{Na}$ and $^{[4]}\text{Na}$ polyhedra are pale yellow, navy blue and turquoise, respectively; P tetrahedra are purple; (SrNa) atoms are shown as large dark-green spheres; F atoms, (OF) anions and OH groups are shown as small yellow, orange and red spheres; H₂O groups are shown as medium red spheres. Captions (b–d): mineral name, space group, structure type where B=Basic structure, LG=Lamprophyllite Group. Labels TS and I show position of TS and I blocks in a structure, and short black lines show position of cation layers (m =number of layers) in the I block.

occurs: Si₂O₇ groups of the two H sheets link to *trans* edges of the small Ti octahedron of the O sheet (Fig. 5a); 1 M^O=Ti, rarely Fe³⁺, Mg; 3 M^O=mainly Na, rarely Zn; subordinate Ca, Mn, Fe²⁺, Mg; $^{[5,6]}\text{M}^{\text{H}}$ =Ti, Nb; A^P=Ba, Na, (SrNa), (BaK), (BaNa); B^P=Ba (Table 4).

Self-linkage of TS blocks

Two types of self-linkage of TS blocks occur: [3] TS blocks do not link directly, additional cations do not occur in the I space ($m=0$) and TS blocks are connected through hydrogen bonds of H₂O groups at the X^P sites as in

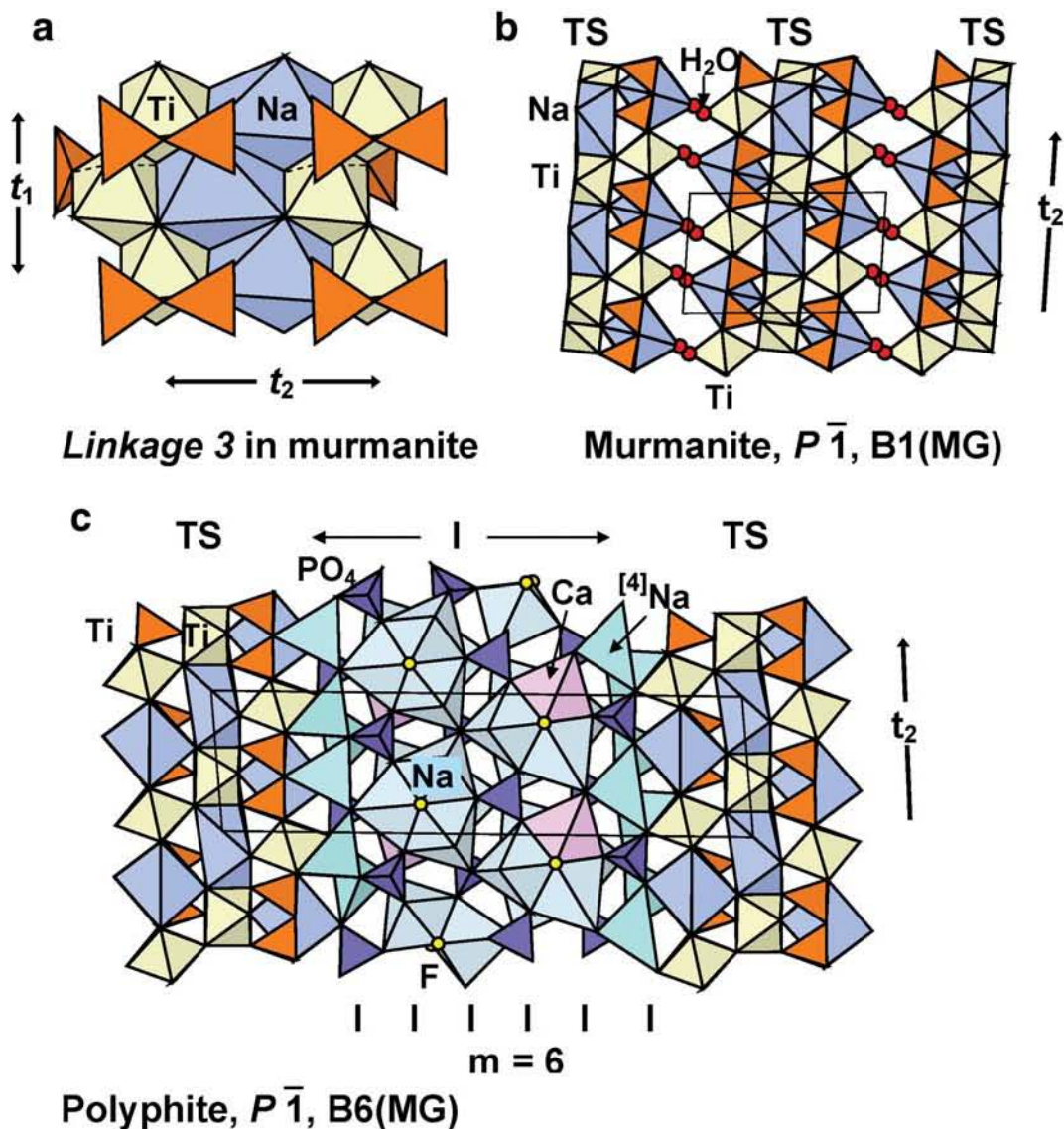


FIG. 6. Murmanite group: linkage 3 of H and O sheets in murmanite (a), the basic crystal structures of murmanite (b) and polyphite (c). Legend as in Fig. 3; Ti, [^{6,8}]Na, [⁴]Na polyhedra and Ca-dominant polyhedra are pale yellow, navy blue, turquoise and pale pink, respectively; P tetrahedra are purple; F atoms and H₂O groups are shown as small yellow and medium red spheres. Captions (b,c): mineral name, space group, structure type where B = Basic structure, MG = Murmanite Group. Labels TS and I show the position of TS and I blocks in a structure, and short black lines show the position of cation layers (m = number of layers) in the I block.

epistolite (Fig. 5c); and [4] TS blocks do not link directly and there are additional layers of cations in the I block between adjacent TS blocks as in lamprophyllite and vuonnemite (Figs 5b,d).

Polytypism is common for lamprophyllite, nabalamprophyllite and inelite (Table 1).

Murmanite group

TS block

Ti (+ Mg + Mn) = 4 apfu; Ti occurs in the O sheet (2 apfu) and H sheets (2 apfu); linkage 3 occurs: Si₂O₇ groups of the two H sheets link to two Ti octahedra

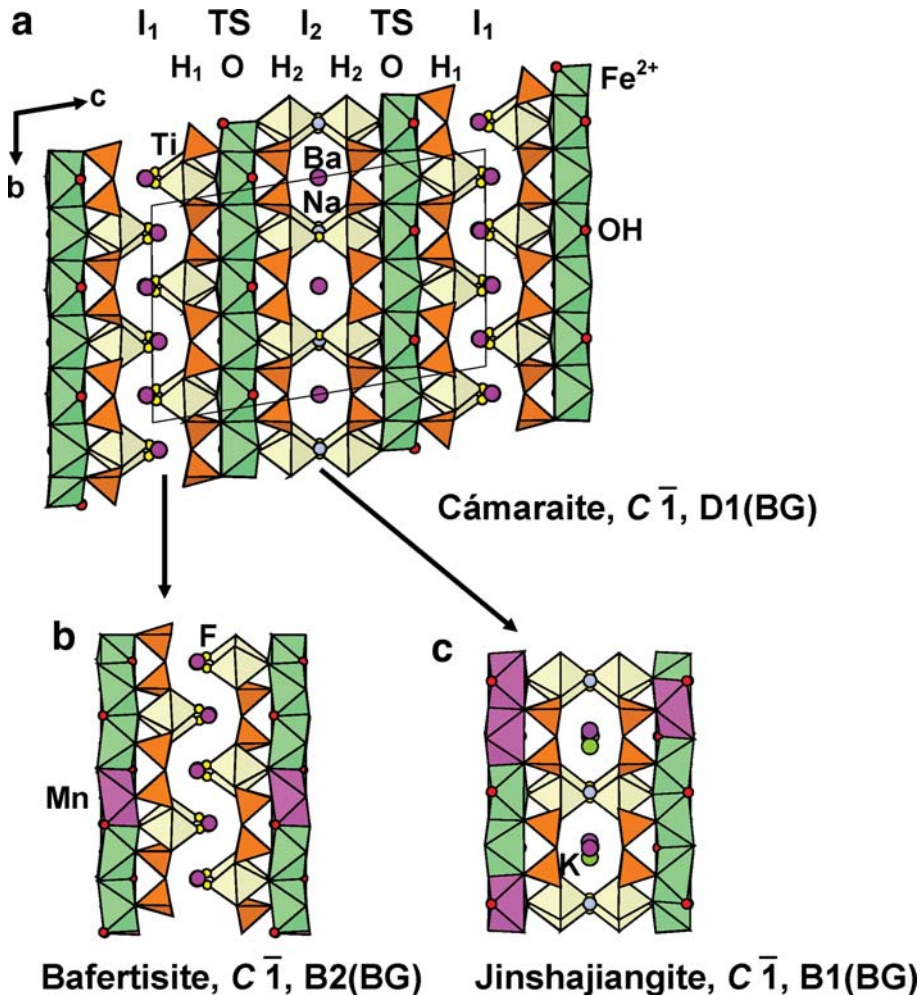


FIG. 7. The derivative (D) structure of cámaraites (bafertisite group) (a) can be built of the fragments of the basic (B) structures of the minerals of the same group: bafertisite (b) and jinshajiangite (c). Legend as in Fig. 4.

of the O sheet adjacent along t_1 (Fig. 6a); $2M^O = \text{Ti}$, (TiMn), rarely Mg; $2M^O = \text{Na}$; $^{[6,5]}M^H = \text{Ti}$; $A^P = \text{Na}$, rarely Ca, Ba and Zn (Table 5).

Self-linkage of TS blocks

Two types of self-linkage of TS blocks occur: [3] TS blocks do not link directly, additional cations do not occur in the I space ($m = 0$) and TS blocks are connected through hydrogen bonds of H_2O groups at the X^P sites as in murmanite (Fig. 6b); and [4] TS blocks do not link directly and there are additional layers of cations in the I block between adjacent TS blocks as in polyphite ($m = 6$) (Fig. 6c).

In rinkite and lamprophyllite groups, topology of the TS block is identical (defined by linkage 1) but stereochemistry is different: in the rinkite group, Si_2O_7 groups link to the large Na polyhedron of the O sheet; in the lamprophyllite group, Si_2O_7 groups link to the small Ti octahedron of the O sheet.

For each group, only basic structures are shown in Figs 3–6. Figure 7a shows the derivative structure of cámaraites (bafertisite group) which can be built of the structural fragments of two minerals of the same group: bafertisite (Fig. 7b) and jinshajiangite (Fig. 7c).

Naming of the groups

Since 1965, several 'group' names were used for TS-block minerals: lomonosovite group, murmanite-lomonosovite group, rosenbuschite group, götzenite-seidozerite-rosenbuschite group, rinkite group, epistolite group, lamprophyllite group, etc, not mentioning numerous series. However, none of those groups was defined quantitatively on the content of Ti and topology of the main structural unit, the TS-block, and none of those groups was approved by the CNMNC-IMA.

We name each group after the oldest mineral, i.e. the mineral described prior to all other minerals of the group (Table 1):

Rinkite group ¹	rinkite-(Ce) (Lorenzen, 1884)
Bafertsite group	bafertsite (Semenov and Zhang Peishan, 1959)
Lamprophyllite group	lamprophyllite (Hackman, 1894)
Murmanite group	murmanite (Gutkova, 1930).

Changing names

Rinkite group: rinkite-(Ce), mosandrite-(Ce) and hainite-(Y)

Rare-earth elements are chemically essential constituents and need to have their own position in the mineral formula to keep neutral-charge stoichiometry. Hence the Levinson suffix should be applied to a mineral with Y and/or lanthanoids (Ln: La–Lu) regardless of whether Y and/or lanthanoids are dominant at particular crystallographic sites. The three minerals of the rinkite group have been renamed as follows: rinkite → rinkite-(Ce), mosandrite → mosandrite-(Ce) and hainite → hainite-(Y).

¹Based on private communication of A.J. Erdmann, Berzelius (1842) reported that in 1840, Erdmann described a mineral which contained La and Ce and named that new mineral mosandrite after Carl Gustaf Mosander who had discovered La in 1839. However neither chemical analysis nor mineral formula or any numerical data were reported by Berzelius (1842) for mosandrite. A sound description of mosandrite, including chemical analysis and optics, was given by Brögger (1890). Hence we consider rinkite-(Ce) the oldest mineral with a proper mineral description. For rinkite-(Ce), the complete mineral description was reported by Lorenzen (1884), hence it takes precedence over the description of mosandrite-(Ce) by Brögger (1890).

Lamprophyllite group: innelite-1A

Sokolova *et al.* (2011) reported an occurrence of the two polytypes of innelite and named them innelite-1T (triclinic symmetry) and innelite-2M (monoclinic symmetry). In the current polytype nomenclature (Guinier *et al.*, 1984) adopted by IUCr and IMA [the recommendations and guidelines of the CNMNC-IMA are summarized in Nickel, 1993], A stands for the Anorthic (=Triclinic) symmetry. Hence in accord with (Guinier *et al.*, 1984), the name of the triclinic polytype of innelite has been changed: innelite-1T → innelite-1A.

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APPENDIX 1. GENERAL STRUCTURAL PRINCIPLES FOR SEIDOZERITE-SUPERGROUP MINERALS

(modified after Sokolova and Cámara, 2013)

- (1) The TS (Titanium-Silicate) block consists of a central O (Octahedral) sheet and two H (Heteropolyhedral) sheets of M^H cation polyhedra and Si_2O_7 groups. The O sheet is commonly an array of close-packed octahedra with the formula $M^OX_2^O$, where M^O and X^O are cations and anions of the O sheet. The two H sheets of one TS block are attached to the O sheet in the same way. The A^P and B^P cations and X^P anions constitute the peripheral (*P*) part of the TS block. The TS block is characterized by a planar cell based on minimal lengths of translational vectors, $t_1 \approx 5.5$ and $t_2 \approx 7 \text{ \AA}$, and $t_1 \wedge t_2 \approx 90^\circ$.
- (2) All TS-block structures consist either solely of TS blocks or of two types of block: the TS block itself and an **I** (Intermediate) block that comprises all atoms between two TS blocks. TS-block structures have the minimal translations, $t_1 \approx 5.5$ and $t_2 \approx 7 \text{ \AA}$ of the TS block, whereas the third translation varies depending on size of the **I** block.
- (3) There are three topologically distinct TS blocks based on three types of linkage of two H sheets and the central O sheet. *Linkage 1* occurs where two H sheets connect to the O sheet so that two Si_2O_7 groups on opposite sides of the O sheet link to *trans* edges of the same octahedron of the O sheet. *Linkage 2* occurs where two Si_2O_7 groups link to two octahedra of the O sheet adjacent along t_2 . *Linkage 3* occurs where two Si_2O_7 groups link to two octahedra adjacent approximately along t_1 .
- (4) Cations in each sheet of the TS block are arranged in a close-packed layer, where each cation is surrounded by six other cations. The three layers of the TS block constitute a three-layered or cubic close-packing of cations with an ABC repeat.
- (5) The three possible linkages of H sheets and O sheets result from the close-packing of cations with the HOH = ABC repeat: they correspond to three possible translations between A and C, $(2/3 \ 1/3 \ 1)t$, $(2/3 \ 2/3 \ 1)t$ and $(1/3 \ 1/3 \ 1)t$, where t = minimal cation-cation distance in the ABC close-packing.
- (6) The different types of linkages of O and H sheets in the TS block are a result of the bond-

valence requirements of anions shared by the O and H sheets, excluding the anions of the Si_2O_7 group. The type of linkage is not related to the topology or chemical composition of the **I** block.

- (7) Ti occurs in the O sheet and two H sheets. In the O sheet, Nb, Zr, Fe^{3+} , Mg and Mn substitute for Ti (in seven TS-block minerals); in the H sheet, only Nb substitutes for Ti (in eight TS-block minerals). Hence when we say Ti-dominant sites, we also include Nb-, Zr-, Fe^{3+} -, and Mg-dominant sites and (TiMn) sites.
- (8) There are four groups of structures, each characterized by different content of Ti (+ Nb + Zr + Fe^{3+} + Mg + Mn) and topology and stereochemistry of the TS block:

Rinkite group: Ti (+Nb + Zr) = 1 apfu; Ti occurs in the O sheet; linkage 1 occurs: Si_2O_7 groups link to the large Na polyhedron of the O sheet; 1 $M^O = Ti$, rarely Nb or Zr; 3 M^O are mainly Na, Ca and rarely Mn^{2+} ; $^{[6,7]}M^H = Zr, Y, Ca + REE, Ca, Mn$; $A^P = Na, Ca, Ca + REE$.

Bafertisitite group: Ti (+Nb) = 2 apfu; Ti occurs in the H sheets; linkage 2 occurs: Si_2O_7 groups link to two M^{2+} octahedra of the O sheet adjacent along t_2 ; 4 $M^O = 4 M^{2+} = Fe^{2+}, Mn$ and $(Fe^{2+}Na)$; $^{[5,6]}M^H = Ti, Nb$; $A^P, B^P = Ba, Na, Sr, K$.

Lamprophyllite group: Ti (+ Nb + Fe^{3+} + Mg) = 3 apfu; Ti occurs in the O and H sheets; linkage 1 occurs: Si_2O_7 groups link to the small Ti octahedron of the O sheet; 1 $M^O = Ti$, rarely Fe^{3+} , Mg; 3 $M^O =$ mainly Na, rarely Zn, subordinate Mn, Fe^{2+} , Mg and Ca; $^{[5,6]}M^H = Ti, Nb$; $A^P = Ba, Na, (SrNa), (BaK), (BaNa)$; $B^P = Ba$.

Murmanite group, Ti (+ Mg + Mn) = 4 apfu; Ti occurs in the O and H sheets; linkage 3 occurs: Si_2O_7 groups link to two Ti octahedra of the O sheet adjacent along t_1 ; 2 $M^O = Ti, (TiMn)$, rarely Mg; 2 $M^O = Na$; $^{[6,5]}M^H = Ti$; $A^P =$ mainly Na, rarely Ca, Ba and Zn.

In rinkite and lamprophyllite groups, topology of the TS block is identical (defined by linkage 1) but stereochemistry is different: in the rinkite group, Si_2O_7 groups link to the large Na polyhedron of the O sheet; in the lamprophyllite group, Si_2O_7 groups link to the small Ti octahedron of the O sheet.

- (9) The maximal possible content of Ti (+ Nb + Zr + Fe³⁺ + Mg + Mn) in the TS block is 4 apfu.
- (10) The topology and stereochemistry of the TS block are strongly related to the stereochemistry of Ti. The stability of the TS block is due to an extremely wide range in mainly Ti(+ Nb)–O bond-lengths, 1.66–2.38 Å, which allows the chemistry of the TS block to vary drastically while retaining close-packing of the cations.
- (11) The TS block propagates close-packing of cations into the **I** block. All cations of the **I** block are arranged as close-packed layers where m is the number of such layers.
- (12) There are four types of self-linkage between adjacent TS blocks:

[1] TS blocks link directly through common edges of M^H and A^P polyhedra, and common vertices of M^H, A^P and Si polyhedra of the H sheets belonging to two TS blocks. This type of self-linkage of TS blocks occurs in the crystal structures of the rinkite group.

[2] TS blocks link through common vertices of Ti(+ Nb) octahedra and the **I** block has one layer of cations (m = 1).

[3] TS blocks do not link directly, additional cations do not occur in the **I** space (m = 0), and TS blocks are connected through hydrogen bonds of H₂O groups at the X^P sites.

[4] TS blocks do not link directly, and there are additional layers of cations in the **I** block (m = 1–6).

- (13) There are two types of TS-block structures: A ‘basic structure’ has the following four characteristics: (1) there is only one type of TS block; (2) two H sheets of the TS block are identical; (3) there is only one type of **I** block or it is absent; (4) there is only one type of self-linkage of TS blocks.

‘Basic structures’ obey the general structural principles of Sokolova (2006).

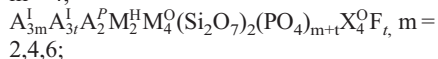
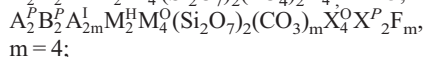
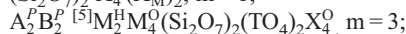
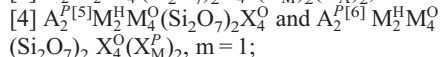
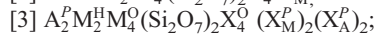
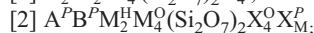
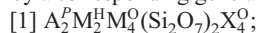
A ‘derivative structure’ has one or more of the three following characteristics: (1) there is more than one type of TS block; (2) there is more than one type of **I** block; (3) there is more than one type of self-linkage of TS blocks.

A ‘derivative structure’ is related to two or more ‘basic structures’ of the same group: it can be derived by adding these structures via sharing the central O sheet of the TS blocks of adjacent structural fragments which represent ‘basic structures’. The five known derivative structures (bafertsite group: cámaraité;

lamprophyllite group: bornemanite, saamite, kazanskyite and nechelyustovite) contain Ba as an essential **I**-block cation.

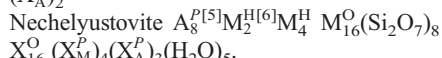
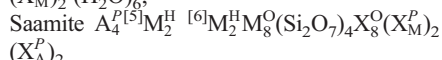
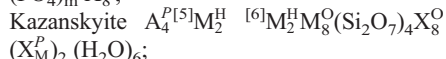
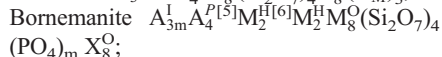
- (14) The general structural formula of the TS block is A₂^PB₂^PM₂^HM₄^O(Si₂O₇)₂X_{4+n}, where M₂^H and M₄^O = cations of the H and O sheets; M^H = Ti, Nb, Zr, Y, Mn, Ca + REE, Ca; M^O = Ti, Zr, Nb, Fe³⁺, Fe²⁺, Mg, Mn, Zn, Ca, Na; A^P and B^P = cations at the peripheral (P) sites = Na, Ca + REE, Ca, Zn, Ba, Sr, K; X = anions = O, OH, F, H₂O; X_{4+n} = X₄^O + X_n^P, n = 0, 1, 1.5, 2, 4; X^P = X_M^P and X_A^P = apical anions of M^H and A^P cations at the periphery of the TS block. The stoichiometry of the core part of the TS block, M₂^HM₄^O(Si₂O₇)₂X₄^O, is invariant in all structures.}

- (15) Each type of a basic structure with a type-[1–4] self-linkage of TS blocks can be characterized by a corresponding general structural formula:



where m = number of cation layers in the **I** block adjacent to the TS block, t = number of cation layers in the trimeric structure of the **I** block, A_{3m}^I and A_{3t}^I are the cations of the m and t layers of the **I** block different from P⁵⁺; T = P⁵⁺, S⁶⁺ for the formula [4] with m = 3.

- (16) The general structural formulae of the derivative structures can be derived by summation of the general structural formulae of related basic structures:



To emphasize the number of structural components in derivative structures, their formulae are given here per (Si₂O₇)₄ and (Si₂O₇)₈, although, some of these formulae can be written per (Si₂O₇)₂.

APPENDIX 2. POTENTIAL SEIDOZERITE-SUPERGROUP MINERALS

Here we list three insufficiently characterized minerals (there is no structure information for all three of them) which potentially can be included in the seidozerite supergroup: shkatulkalite, $\text{Na}_{10}\text{MnTi}_3\text{Nb}_3(\text{Si}_2\text{O}_7)_6(\text{OH})_2\text{F}\cdot 12\text{H}_2\text{O}$ (Men'shikov *et al.*, 1996); bykovaite, $\text{BaNa}\{(\text{Na}, \text{Ti})_4[(\text{Ti}, \text{Nb})_2(\text{OH}, \text{O})_3\text{Si}_4\text{O}_{14}](\text{OH}, \text{F})_2\}$ (Khomyakov *et al.*, 2005) and phosphoinnelite, $\text{Ba}_4\text{Na}_3\text{Ti}_3\text{Si}_4\text{O}_{14}(\text{PO}_4, \text{SO}_4)_2(\text{O}, \text{F})_3$ (Pekov *et al.*, 2006). These three minerals need determination of their crystal structures.

For example, consider phosphoinnelite. Pekov *et al.* (2006) described phosphoinnelite as a P-dominant structural analogue of innelite. The ideal formula of phosphoinnelite contains 25 anions (see above). The structure topology of innelite, ideally $\text{Ba}_4\text{Na}(\text{NaM}^{2+})\text{Ti}_3(\text{Si}_2\text{O}_7)_2 [(\text{SO}_4(\text{PO}_4)]\text{O}_2[\text{O}(\text{OH})]$, requires 26 anions pfu (Tables 1,4; Sokolova *et al.*, 2011). Therefore the formula of phosphoinnelite is not correct as it does not correspond to the structure topology of the innelite structure type.