Electronic Supplementary Material (ESI) for CrystEngComm.
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Supplementary materials

Migration paths of the Na^+-ion diffusion for minerals of the lovozerite group: crystallochemical and DFT modeling

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Table S1. Topological characteristics of the atomic nets for lovozerite group of minerals.

Mineral	Space group	Topological classification	Type of atoms coordination	Point symbol		Transitivity	Tiling	ICSD
Combeite **Litvinskite** **Lovozerite** **Townendite** **Zolotarevite**	$R\bar{3}m$ Cm $C2_1$ $R\bar{3}m$ $R\bar{3}m$	sqc962	3,6-c	$\{6^3\}6\{6^6.8^6.12^3\}$	2-nodal net	[4 2 3 1]	$[6^4.8^3]$	62827 57042 30389 168092 137779
Kapustinite **Kazakovite** **Zirsinalite**	$R\bar{3}m$ $C2/m$ $R\bar{3}cr$	New topology	3,4,6^2-c net	$\{4.8^2\}2\{4^3.8^3\}2\{4^6.8^6.10^3\}$	4-nodal net	[10 10 9 8]	2t-kzd + 6t-jnt-1+ 3t-kds+t-cub+3t-ste	250170 200602 200800
Imandrite	$Pmnn$	New topology	3^2,4^2,6^2-c net	$\{4.5.7\}2\{4.5^2.6^2.8\}2\{4.5^2.7^2.8\}$ $4\{4.7.8\}4\{4^4.5^2.6^2.7^4.8^2.9\}$ $2\{4^6.7^2.8^4.9^2.10\}$	6-nodal net	[9 10 9 7]	2t-kzd + 2t-ukc+ 4t-jnt-1+ t-lov + 4$[4.5.7.8^2]$ + t-bru + t-ste	200805
Tisinalite	$P\bar{3}$	New topology	3,4,6-c net	$\{4.5.7\}2\{4.5^2.6^2.8\}2\{4.5^2.7^2.8\}$ $4\{4.7.8\}4\{4^4.5^2.6^2.7^4.8^2.9\}$ $2\{4^6.7^2.8^4.9^2.10\}$	6-nodal net	[10 9 8 7]	3t-kds+ t-cub+2$[6^3.8^3]$	250068
Koashvite	$Pmnb$	New topology	3^4,4^4,6^3-c net	$\{4.5.7\}\{4.5^2.7\text{^}2.8\}\{4.7.8\}$ $5\{4^2.5.7.8^2\}4\{4^3.7^2.8\}$ $\{4^4.5^2.7^6.8^2.10\}\{4^6.7^2.8^4.9^2.10\}$ $\{4^6.7^2.8^4.9^3\}$	11-nodal net	[16 19 16 10]	2t-kzd+ 4t-jnt-1 +$[4^2.7^2]$+t-kds+ 2$[4.5.7.8^2]$+ t-csv-1 + t-ste+$[4^2.7^4.8^2]$	86517

Table S2. Tiles for atomic net of the combeite, litvinskite, lovozerite, townendite, zolotarevite minerals with **sqc962** topology.

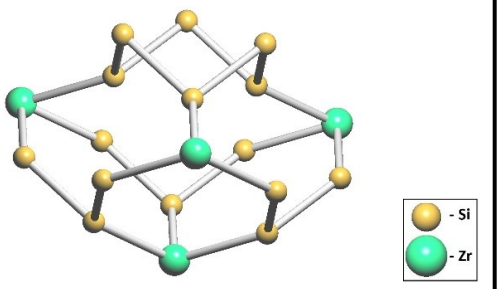
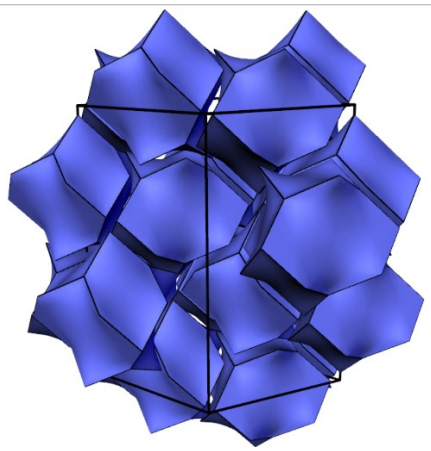
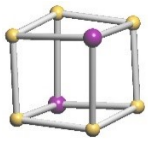
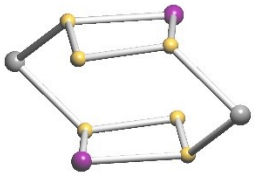
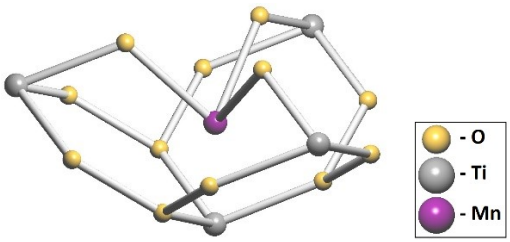
sqc962 (*Combeite, Lovozerite, Litvinskite, Townendite, Zolotarevite*)		
Face symbol:	**[$6^4.8^3$]**	**TILING**
		
V, E, F: **Label:**	**(19, 24, 7)** **t-unknown**	

Table S3. Tiles for atomic net of the tisinalite mineral with new topology obtained by means the geometrically-topological analysis.

3,4,6-c net New topology (*Tisinalite*)			
Face symbol:	**[4^6]**	**[$4^2.8^2$]**	**[$6^3.8^3$]**
			
V, E, F: **Label:**	**(8, 12, 6)** **t-cub**	**(10, 12, 4)** **t-kds**	**(17, 21, 6)** **t-unknown1**

TILING

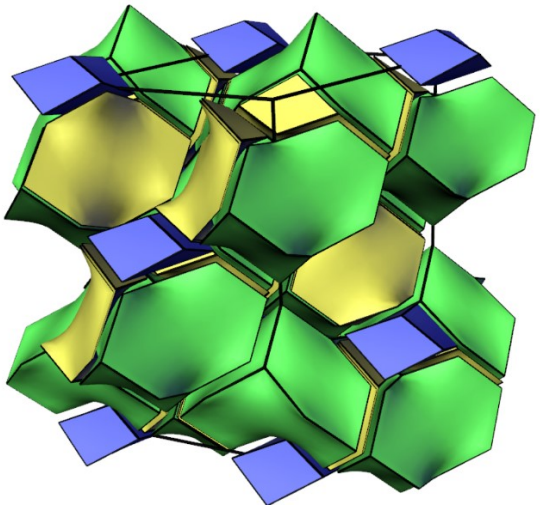
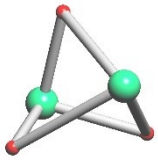
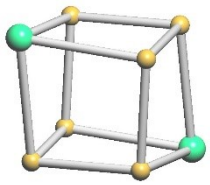
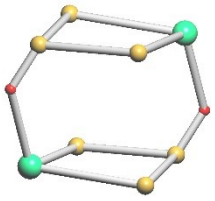
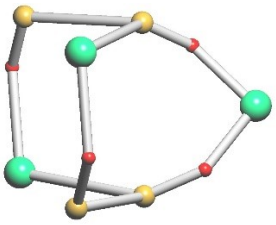
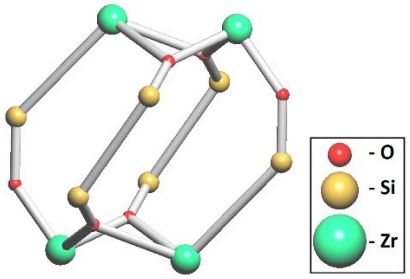


Table S4. Tiles for atomic net of the kapustinite, kazakovite, zirsinalite minerals with new topology obtained by means the geometrically-topological analysis.

3,4,6²-c net New topology (*Kapustinite, Kazakovite, Zirsinalite*)			
Face symbol:	**[4³]**	**[4⁶]**	**[4².8²]**
			
V, E, F: **Label:**	**(5, 6, 3)** **t-kzd**	**(8, 12, 6)** **t-cub**	**(10, 12, 4)** **t-kds**
Face symbol:	**[8³]**	**[4².8⁴]**	
			
V, E, F: **Label:**	**(11, 12, 3)** **t-jnt-1**	**(16, 20, 6)** **t-ste**	
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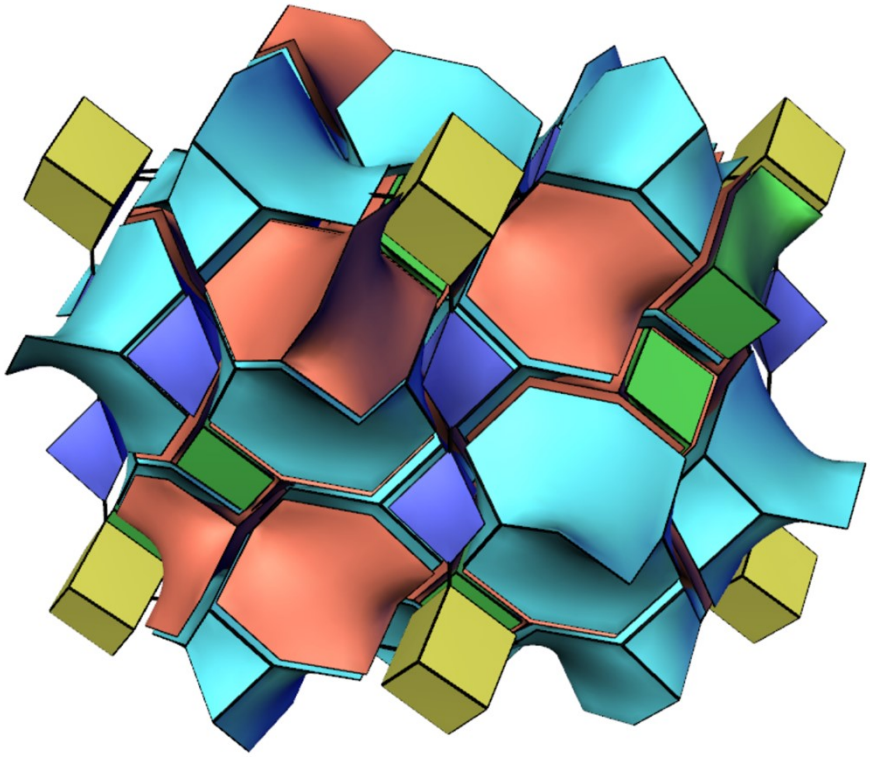
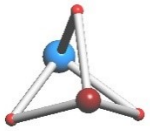
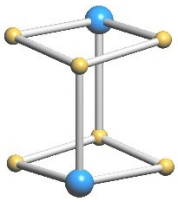
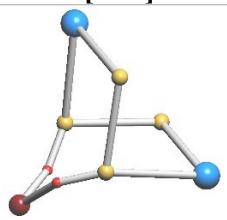
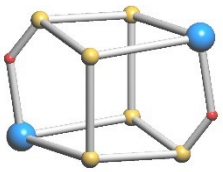
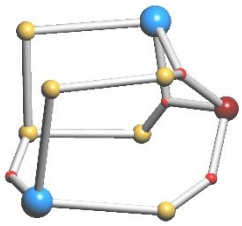
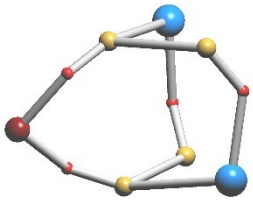
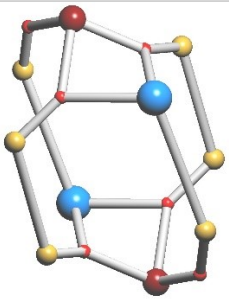
			

Table S5. Tiles for atomic net of the imandrite mineral with $3^2,4^2,6^2$T18 topology obtained by means the geometrically-topological analysis.

$3^2,4^2,6^2$T18 (*Imandrite*)				
Face symbol:	**[4^3]**	**[$4^2.6^2$]**	**[6.7^2]**	**[$4^2.5^4$]**
				
V, E, F: **Label:**	**(5, 6, 3)** **t-kzd**	**(8, 10, 4)** **t-lov**	**(9, 10, 3)** **t-ukc**	**(10, 14, 6)** **t-bru**
Face symbol:	**[4.5.7.8^2]**	**[8^3]**	**[$4^2.8^4$]**	
				
V, E, F: **Label:**	**(13, 16, 5)** **t-unknown1**	**(11, 12, 3)** **t-jnt-1**	**(16, 20, 6)** **t-ste**	
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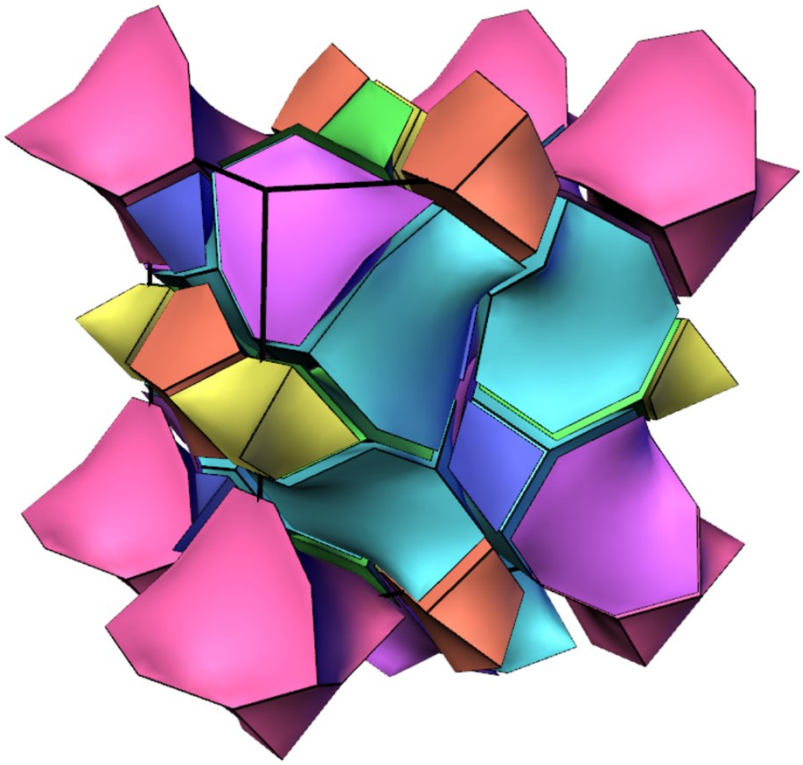
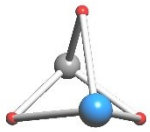
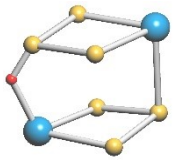
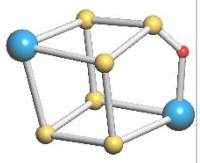
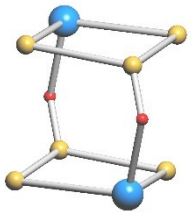
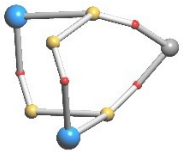
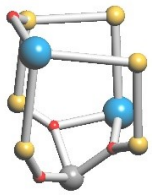
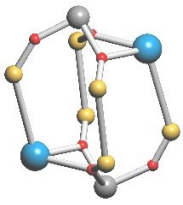
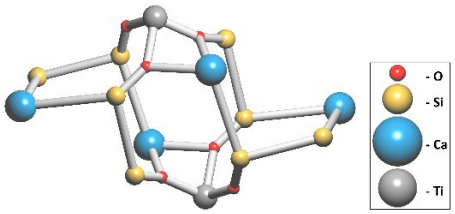
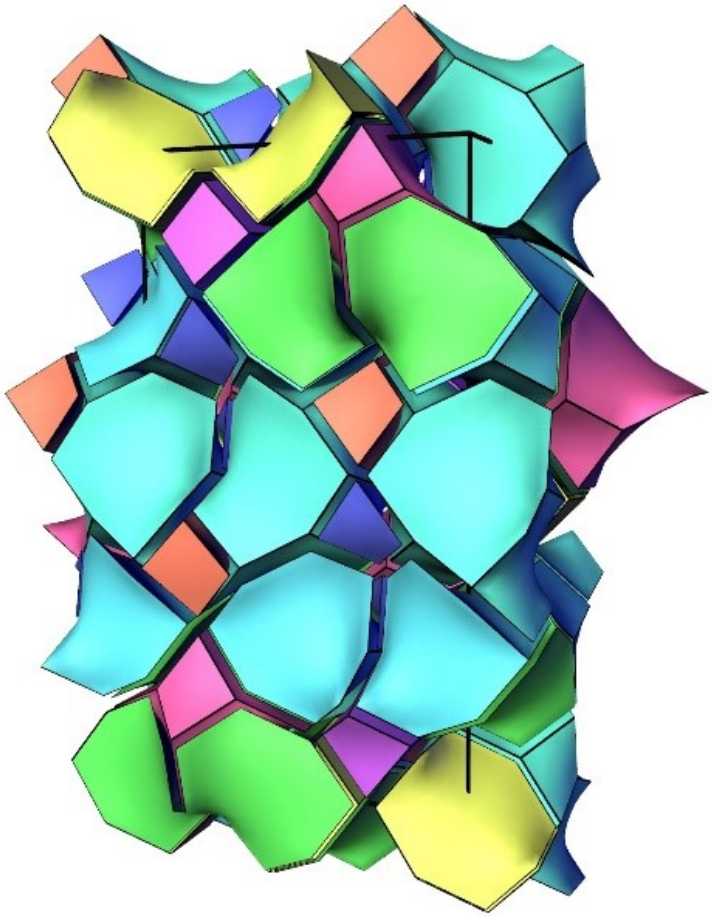
				

Table S6. Tiles for atomic net of the koashvite mineral with new topology obtained by means the geometrically-topological analysis.

$3^4,4^4,6^3$-c net New topology (*Koashvite*)				
Face symbol:	**[4^3]**	**[$4^2.7^2$]**	**[$4^4.5^2$]**	**[$4^2.8^2$]**
				
V, E, F: **Label:**	**(5, 6, 3)** **t-kzd**	**(9, 11, 4)** **t-unknown1**	**(9, 13, 6)** **t-csv-1**	**(10, 12, 4)** **t-kds**
Face symbol:	**[8^3]**	**[$4.5.7.8^2$]**	**[$4^2.8^4$]**	**[$4^2.7^4.8^2$]**
				
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TILING