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Article

High-temperature polymorphic transition and crystal structures of feldspar-related $SrZn_2P_2O_8$

Liudmila Gorelova[1], Maria G. Krzhizhanovskaya[1], Valentina A. Yukhno[1], Olga Yu. Shorets[2], Irina A. Volkova[1] and Oleg S. Vereshchagin[3]

[1]Crystallography, Saint Petersburg State University: Sankt-peterburgskij gosudarstvennyj universit, Saint Petersburg, Russian Federation; [2]Institute of Silicate Chemistry RAS: Institut himii silikatov imeni I V Grebensi, Saint Petersburg, Russian Federation; and [3]Mineralogy, Saint Petersburg State University: Sankt-peterburgskij gosudarstvennyj universit, Saint Petersburg, Russian Federation

Abstract

Feldspars are among the most common phases in the Earth's crust and are characterized by wide variations in chemical composition and crystal structure motifs. In this paper, we synthesized $SrZn_2P_2O_8$ and studied it by means of scanning electron microscopy, electron microprobe analysis and powder X-ray diffraction at ambient and high-temperature (up to 900°C) conditions. We have structurally characterized for the first time layered triclinic β-modification of $SrZn_2P_2O_8$ (space group $P\bar{1}$, a = 5.0109(8), b = 8.6202(13), c = 9.7527(15) Å, α = 118.088(3), β = 74.622(6), γ = 87.525(6)° and V = 351.29(10) Å^3), which is structurally related to hexacelsian. The high-temperature study demonstrated that β-$SrZn_2P_2O_8$ transformed irreversibly into the framework monoclinic paracelsian-like α-$SrZn_2P_2O_8$ (space group $P2_1/c$, a = 8.3163(2), b = 9.5023(2), c = 9.0248(2) Å, β = 92.285(1)°, V = 712.60(1) Å^3) above 600°C, which, in turn, is stable up to 900°C, when it melts. Though the crystal structures of α- and β-modification of $SrZn_2P_2O_8$ are different (framework and layered, respectively), their thermal expansion is similar: $\alpha_V \approx 26 \pm 1 \times 10^{-6}$ °C^{-1}, $\alpha_{max}/\alpha_{min} \approx 5$. The possible occurrence of the corresponding minerals in nature is discussed.

Keywords: feldspar; paracelsian; thermal expansion; phase transition; $SrZn_2P_2O_8$; metastable

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Introduction

Feldspars are one of the most important groups of minerals, as they are widespread in the Earth's crust and have been found in a number of celestial bodies (e.g. Wood *et al.*, 1970; Zolensky *et al.*, 2006; Jambon *et al.*, 2008; Chandra *et al.*, 2016; Arai and Maruyama, 2017; Knibbe, 2018). Traditionally (e.g. Ribbe, 1983; Back, 2022) feldspar group minerals include natural compounds having three-dimensional (3D) framework of tetrahedra. This 3D framework is formed by corner-sharing tetrahedra and could have two topologies: feldspar and paracelsian (Smith and Brown, 1988). Krivovichev (2020) drew attention to the fact that minerals with MT_4O_8 general formula, where n is the average charge of the M cation (n = 1–2; M = Na, K, Rb, (NH_4), Ca, Sr, Ba) and k is the average charge of the T cation ($k = 4 - n/4$; T = Be, Zn, Al, B, Fe, Si, As, P), can have other topologies and suggested including them in the feldspar family. According to this approach, feldspar family minerals crystallize in five different topologies. Four of them are TO_4-based [feldspar (3D), paracelsian (3D), svyatoslavite (3D) and dmisteinbergite (layered or 2D)] and one is TO_6-based [hollandite (3D)]. According to this conception, the feldspar family with general formula MT_4O_8, includes 31 mineral species. However, this classification was not approved by International Mineralogical Association (IMA) and contradicts Mills *et al.* (2009), who stated that "…mineral families apply to groups and/or supergroups having similar structural and/or chemical features that make them unique". Most probably, minerals belonging to the feldspar family, suggested by Krivovichev (2020) should be divided into three separate groups, depending on their structural motif, i.e. framework (including feldspar, paracelsian and svyatoslavite topologies), layered (with dmisteinbergite topology) and TO_6-based (i.e. hollandite topology). For further discussion the minerals with dmisteinbergite topology, which include dmisteinbergite, hexacelsian, kokchetavite, cymrite, minjiangite and recently discovered pfaffenbergite and wodegongjieite will be named hexacelsian-type minerals.

There are also a number of synthetic compounds with general formula MT_4O_8. Most of them have feldspar or paracelsian topology, whereas the number of compounds with dmisteinbergite and svyatoslavite topology is relatively small (Czaya, 1972; Dollase and Ross, 1993; David *et al.*, 2013; Dal Bo *et al.*, 2014; Pan *et al.*, 2017; Hwang *et al.*, 2023; Wang *et al.*, 2024). Interestingly, a synthetic

Corresponding author: Liudmila Gorelova; Email: l.gorelova@spbu.ru
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compound with general formula MT_4O_8, in which the T site is occupied by P, Zn or Co could have a topology not known in nature. Notably, two synthetic compounds [α-$CaZn_2P_2O_8$ (Jakeman and Cheetham, 1988) and $SrCo_2P_2O_8$ (El Bali *et al.*, 1993)] have triclinic (space group $P\bar{1}$) layered crystal structures similar to dmisteinbergite/hexacelsian, but not identical to them.

Only two synthetic strontium zinc phosphate are known: $SrZn_2P_2O_8$ (Hemon and Courbion, 1990) and $SrZnP_2O_7$ (Yuan *et al.*, 2007). The well characterized $SrZn_2P_2O_8$ with feldspar-related stoichiometry crystallizes in monoclinic (space group $P2_1/c$) symmetry with paracelsian topology. There are also data on the existence of its metastable high-temperature modification, named β-$SrZn_2P_2O_8$ (Sarver *et al.*, 1961). However, this modification was not structurally characterized and was obtained in conditions that are unattainable today (by rapid cooling in mercury). Though zinc phosphates are not very widespread in nature, to date ~50 minerals with essential P, Zn and O are known.

Here, the thermal behaviour of $SrZn_2P_2O_8$ is described in detail with the focus on formation of different polymorphic modification and their thermal expansion. In addition, assumptions have been made about the possibility of finding related minerals in nature.

Materials and methods

Synthesis and primary characterization

The α-$SrZn_2P_2O_8$ phase has been synthesized using a solid-state reactions method from chemically pure $SrCO_3$ (99.99%, Sigma-Aldrich), ZnO (99.99%, Sigma-Aldrich) and $NH_4H_2PO_4$ (99.99%, Sigma-Aldrich) taken in stoichiometric ratios. The reagent mixtures were thoroughly ground in an agate mortar, pressed into pellets, and transferred to platinum crucibles. Crucibles were placed into a muffle furnace and sequentially heated in air at 400°C for 6 hours and at 900°C for 36 hours. The polymorphic transformations of $SrZn_2P_2O_8$ have been studied by solid-state reactions and a melt crystallization method in the temperature range from 800 to 1200°C for 0.5–24 hours.

The phase composition of the samples obtained was monitored by powder X-ray diffraction (PXRD) using a MiniFlex II (Rigaku Oxford Diffraction, Japan) diffractometer ($CuK\alpha_{12}$ radiation, 30 kV/15 mA, Bragg-Brentano geometry, PSD D-Tex Ultra detector). The chemical composition of the obtained compounds was monitored using a S-3400N (Hitachi, Japan) scanning electron microscope (SEM) equipped with AzTec Energy 350 energy dispersive (EDX) spectrometer (Oxford Diffraction, UK).

High-temperature powder X-ray diffraction study

High-temperature (HT) behaviour of $SrZn_2P_2O_8$ has been studied under heating in air by HT powder X-ray diffraction (PXRD) using an Ultima IV (Rigaku, Japan) diffractometer ($CuK\alpha_{12}$ radiation, 40 kV/30 mA, Bragg-Brentano geometry, PSD D-Tex Ultra detector, goniometer radius = 185 mm) with a thermo-attachment in the range of 30–900°C, with temperature steps of 30°C. The fine-powdered sample was deposited on a platinum sample holder (20 × 12 × 1.5 mm) from an ethanol suspension (Filatov, 1971). An external Si standard was used before the measurements to control the 2θ correctness. The calculations of the unit-cell parameters were performed using the program package *Topas 5.0* (Bruker, 2014; Dinnebier *et al.*, 2019). The temperature dependence of the unit-cell parameters was described by linear and/or quadratic polynomial functions, depending on the amount of the experimental points. The calculation and visualization of the thermal expansion parameters tensor was performed using the TTT program package (Bubnova *et al.*, 2013).

Table 1. Crystal data and structure refinement details of triclinic β-$SrZn_2P_2O_7$

Crystal system	Triclinic
Space group, Z	$P\bar{1}$, 2
a (Å)	5.0109(8)
b (Å)	8.6202(13)
c (Å)	9.7527(15)
α (°)	118.088(3)
β (°)	74.622(6)
γ (°)	87.525(6)
V (Å^3)	351.29(10)
Diffractometer	Rigaku Ultima IV
Radiation	$CuK\alpha_{1+2}$
2θ range (°)	5–100
Number of reflections	722
R_p (%)*	4.79
R_{wp} (%)*	6.47
R_{exp} (%)*	1.75
R_B (%)*	3.38
GOF	3.69
Program	*Topas 5.0* (Bruker, 2014)
Starting model	$SrCo_2P_2O_8$ (El Bali *et al.*, 1993)
Impurity phase	3.19 wt.% of Trigonal (?) $SrZn_2P_2O_7$ (Czaya, 1972)

*$R_p = \frac{\sum|Y_{o,m}-Y_{c,m}|}{\sum Y_{o,m}}$; $R_{wp} = \sqrt{\frac{\sum w_m(Y_{o,m}-Y_{c,m})^2}{\sum w_m Y_{o,m}^2}}$; $R_{exp} = \sqrt{\frac{M-P}{\sum w_m Y_{o,m}^2}}$; $R_B = \frac{\sum|I_{o',k}-I_{c,k}|}{\sum I_{o',k}}$

Crystal structure refinement

The crystal structure of β-$SrZn_2P_2O_8$ was refined using a Rietveld refinement method with the use of the Bruker *TOPAS 5.0* software package (Bruker, 2014; Dinnebier *et al.*, 2019). A PXRD pattern was obtained with an Ultima IV (Rigaku, Japan) diffractometer ($CuK\alpha_{12}$ radiation, 40 kV/30 mA, Bragg-Brentano geometry, PSD D-Tex Ultra detector, goniometer radius = 285 mm). The powder XRD plot was collected in the range 5–100° 2θ at ambient temperature. The collecting time was ~14 hours. The structure model of triclinic $SrCo_2P_2O_8$ (El Bali *et al.*, 1993) was used as starting models for the structure refinement. The peak profile was modelled using the Thompson-Cox-Hastings pseudo-Voigt function (TCHZ). Atomic coordinates were refined for all atomic positions (see Supplementary materials – Table S1 and CIF). Isotropic atomic displacement parameters B_{iso} were used for all the atoms; B_{iso} were constrained for groups of atoms (Sr, Zn1–2, P1–2, O1–8) and then refined free of limits. Soft restraints for all P–O bonds in tetrahedra as well as selected distances and angles in zinc polyhedra were realized using the *Topas 5.0* Launch mode with K = 3 weighting factor for penalties. The correctness of the refined structure was confirmed by low values of final agreement factors (Table 1). The observed and calculated powder X-ray diffraction patterns (final Rietveld refinement plot) are shown in Fig. 1. Atomic coordinates and displacement parameters are given in CIF (Supplementary material) and selected interatomic distances are shown in Table 2. The calculated quantity of the impurity phase modelled by the crystal structure of a trigonal $CaZn_2P_2O_7$ (Czaya, 1972) was ~3 wt.%

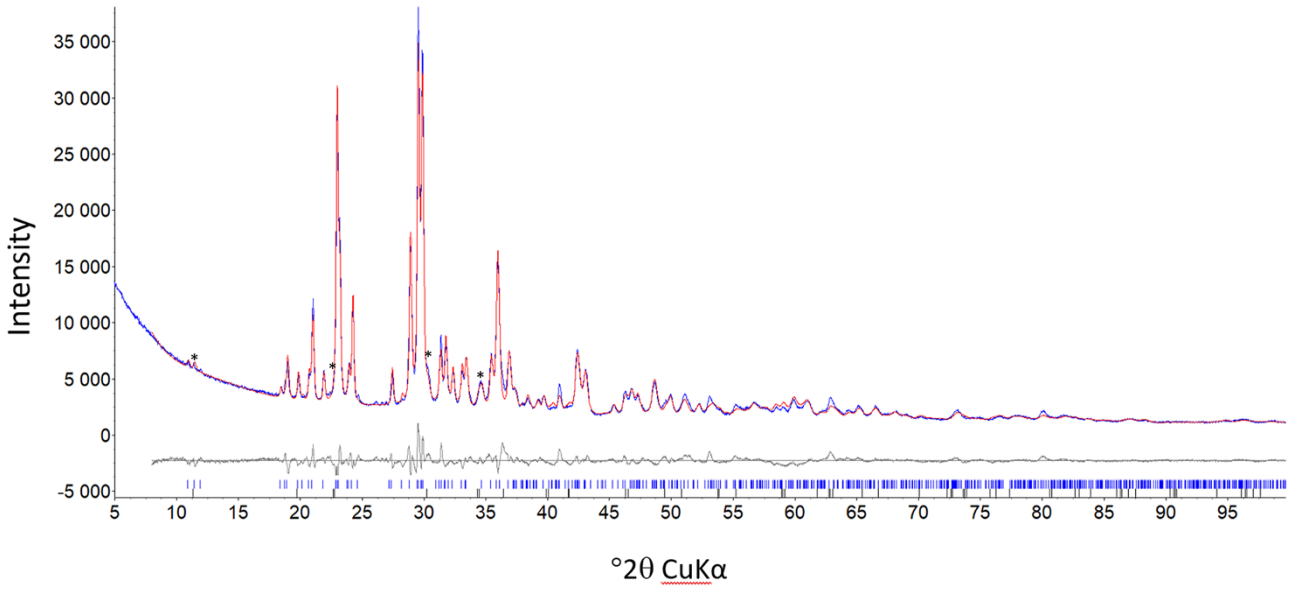


Figure 1. Final Rietveld plot of triclinic β-$SrZn_2P_2O_7$. Blue line shows experimental PXRD data, red line corresponds to the calculated XRD data, grey line is the difference between the measured and calculated XRD patterns. Peak positions of triclinic β-$SrZn_2P_2O_7$ are shown in the lowest part of the figure in blue. Black ticks correspond to the admixture of ~3.1 wt.% of presumably trigonal $SrZnP_2O_7$; its most intensive peaks are marked by asterisks.

Table 2. Selected bond lengths (Å) of triclinic β-$SrZn_2P_2O_7$

Sr1–O7	2.38(5)	Zn1–O6	1.81(5)	P1–O3	1.50(4)
Sr1–O3	2.60(5)	Zn1–O4	2.04(5)	P1–O2	1.54(6)
Sr1–O2	2.63(7)	Zn1–O4	2.13(4)	P1–O4	1.53(5)
Sr1–O3	2.71(5)	Zn1–O5	2.23(5)	P1–O1	1.54(6)
Sr1–O1	2.77(4)	Zn1–O7	2.77(4)	<P1–O>	1.53
Sr1–O7	2.79(4)	<Zn1–O> ^{IV}	2.05		
Sr1–O6	2.80(4)	<Zn1–O> ^{V}	2.19	P2–O7	1.51(5)
Sr1–O8	2.93(4)			P2–O6	1.52(5)
<Sr–O>	2.70	Zn2–O8	1.71(5)	P2–O5	1.55(5)
		Zn2–O1	1.77(5)	P2–O8	1.56(6)
		Zn2–O2	1.94(6)	<P2–O>	1.54
		Zn2–O5	2.02(6)		
		Zn2–O3	2.98(6)		
		<Zn2–O> ^{IV}	1.86		
		<Zn2–O> ^{V}	2.08		

Results and discussion

Formation conditions of different polymorphs of $SrZn_2P_2O_8$

The single-phase sample of α-$SrZn_2P_2O_8$ [space group $P2_1/c$, a = 8.3163(2), b = 9.5023(2), c = 9.0248(2) Å, β = 92.285(1)°, V = 712.60(1) Å^3] has been obtained using solid-state reactions methods at 900°C for 36 hours. We were unable to obtain well-cut crystals, but studies of the melt particles revealed a stepped surface relief and perfect cleavage (Fig. S1a). The compound is chemically homogeneous, free of impurities and is characterized by a predetermined elemental ratio (Sr:Zn:P:O 1:2:2:8; Fig. S1b). All the attempts to synthesize its high-temperature modification using solid-state reactions and melt crystallization methods with different heat or cooling rates and time of heat treatment were unsuccessful. Nevertheless this polymorphic modification has been obtained during the HT PXRD experiment. The α-$SrZn_2P_2O_8$ modification was quickly heated in air up to 900°C with intermediate annealing at 300 and 600°C. Above 900°C the sample melted and further heating was carried out at a rate of 5°C/min up to 1200°C with annealing at each 30°C for ~30 minutes. After that the sample was cooled rapidly to ambient temperature. As a result β-$SrZn_2P_2O_8$ was obtained. The exact reasons for the formation of this phase during the HT PXRD experiment are unclear. As with other metastable phases, we are inclined to consider kinetic causes (long heating, rapid quenching) and crystallization from a superheated (boiling) melt, in which unusual atomic polymerization could exist (e.g. Toda *et al.*, 2021).

Previously, α-$SrZn_2P_2O_8$ doped by different cations has been obtained by different methods (chloride-flux method, solid-state reactions etc.) at the temperature from 550 to 1000°C, depending on the admixtures (Hemon and Courbion, 1990; Yang and Chen, 2006; Yi *et al.*, 2010; Li *et al.*, 2014; Guo *et al.*, 2016; Khidhirbrahmendra *et al.*, 2019; Xu *et al.*, 2020). The existence of high-temperature β-$SrZn_2P_2O_8$ has been mentioned previously only once, by Sarver *et al.* (1961). According to their data the high-temperature polymorph existences between 1035 and 1175°C, when it melts (above 1175°C). They also mentioned that this phase can be quenched at ambient temperature using only extremely

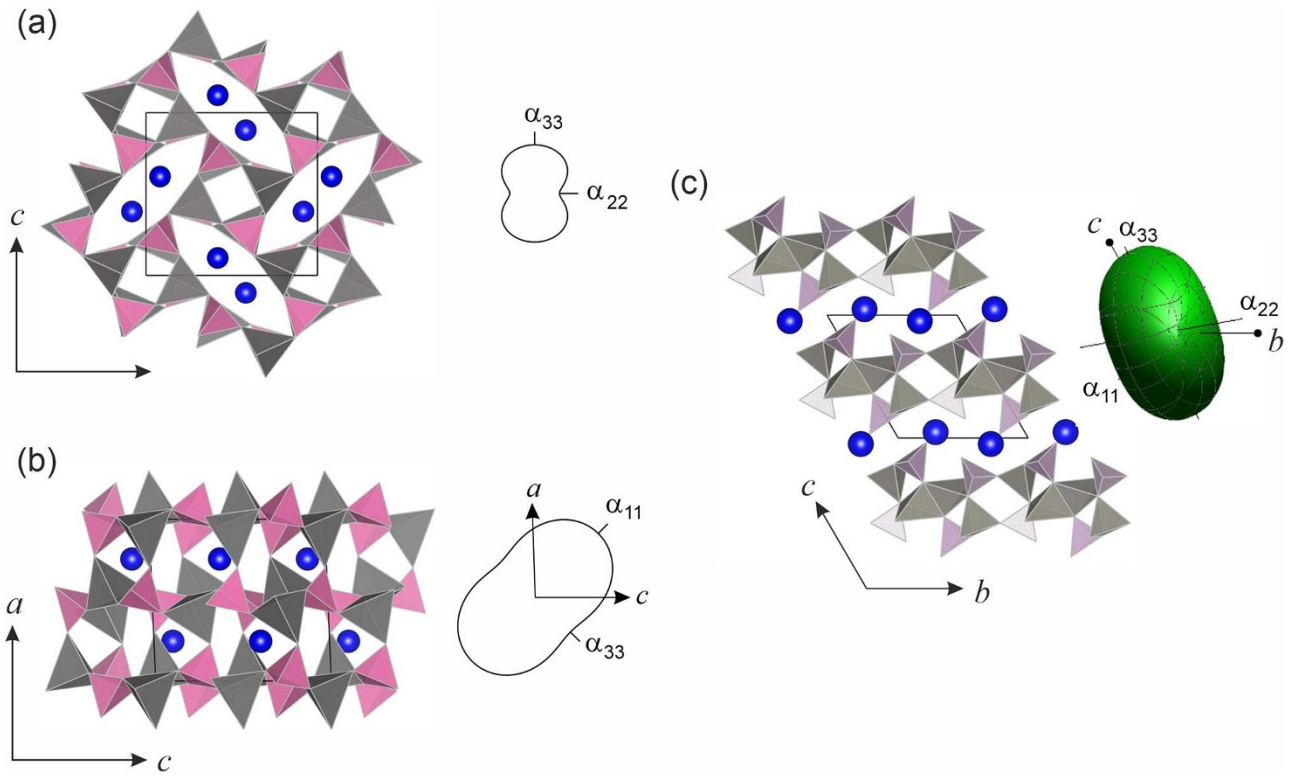


Figure 2. Crystal structures of α- (a, b) and β-$SrZn_2P_2O_8$ (c) with the section indicating thermal deformations. PO_4 and ZnO_4 tetrahedra are given in purple and grey, respectively. Sr atoms are presented as blue spheres.

rapid cooling by pouring a melted batch into liquid Hg, water or over dry ice, whereas the cooling in air always results in the formation of α-$SrZn_2P_2O_8$. However, the authors were unable to obtain any crystallographic data on β-$SrZn_2P_2O_8$.

The stable α-$SrZn_2P_2O_8$ is structurally related to feldspar compounds with paracelsian topology (Fig. 2a,b) and has many structural analogues with different chemical composition (e.g. alumino-, borosilicates, beryllium phosphates, etc.). As far as we know its high-temperature β-modification, has only two direct structural analogues, namely $SrCo_2P_2O_8$ (El Bali *et al.*, 1993) and α-$CaZn_2P_2O_8$ (Jakeman and Cheetham, 1988) (Table 3). However, it could be also considered as a hexacelsian-type compound (see below). $SrCo_2P_2O_8$ has been obtained by slow cooling (10°C/hour) of the melt (obtained at 1200°C) with stoichiometric composition (El Bali *et al.*, 1993). The synthesis of α-$CaZn_2P_2O_8$ is completely different (Jakeman and Cheetham, 1988). The polycrystalline sample was prepared in two steps: (1) dissolving of $CaCO_3$, ZnO and $NH_4H_2PO_4$ in acid solution; (2) the dried powder was ground and fired at 800°C for 24 hours. The single crystals of α-$CaZn_2P_2O_8$ were grown using $ZnCl_2$ as a flux, but Jakeman and Cheetham (1988) did not provide the temperature and speed of their crystallization. It should be noted that similar triclinic crystal structure can also be obtained with a Mg admixture ($CaZn_{2-x}Mg_xP_2O_8$, x = 0–0.75), but a pure Mg analogue cannot be obtained (Jakeman and Cheetham, 1988). It is interesting to note that anhydrous calcium and magnesium phosphates are represented by only two minerals (keplerite and stanfieldite), both of which have been discovered in native Fe-rich meteorites (Britvin *et al.*, 2020, 2021). Thus, it can be assumed that reducing conditions are important for the occurrence of such phosphates in nature.

Crystal structure of β-$SrZn_2P_2O_8$

No crystallographic data were previously available for β-$SrZn_2P_2O_8$ (Sarver *et al.*, 1961). According to our data, the crystal structure of β-$SrZn_2P_2O_8$ (space group $P\bar{1}$, a = 5.0109(8), b = 8.6202(13), c = 9.7527(15) Å, α = 118.088(3), β = 74.622(6), γ = 87.525(6)° and V = 351.29(10) Å^3) can be described as a layered structure (Fig. 2c), consisting of PO_4, ZnO_4 tetrahedra. $Zn2O_4$ tetrahedra are connected to each other *via* corners, whereas $Zn1O_4$ tetrahedra are connected to each other along edges. This type of tetrahedra connection is not common for Zn, but it is known in some crystal structures (e.g. Ghose *et al.*, 1977; Wiebcke, 2002; Harrisson, 2010). Thus the ZnO_4 tetrahedra form Zn_4O_{12} structural units (Fig. 3a). These units form layers connecting *via* PO_4 tetrahedra (Fig. 2c, 4a). The resulting layers are formed by three-, four- and six-membered rings. The interlayer space is occupied by Sr atoms in eight-fold coordination. SrO_8 polyhedra are connected to each other through the vertices and edges and form the chains along the *a* axis (Fig. 3b).

The crystal structures of the most closely related compounds, i.e. triclinic modifications of $SrCo_2P_2O_8$ and $CaZn_2P_2O_8$, are usually described as consisting of PO_4 and $Co2O_4$/$Zn2O_4$ tetrahedra and $Co1O_5$/$Zn1O_5$ distorted trigonal bipyramids with four bonds of ~1.94–2.04 Å and a fifth bond of 2.45 Å and 2.52 Å for Co and Zn, respectively. Although the necessity of the existence of a fifth long bond seems doubtful, the additional bond has to be included in the coordination sphere of Co/Zn atoms according to the bond length analysis (Jakeman and Cheetham, 1988). For the case of β-$SrZn_2P_2O_8$, the fifth Zn–O bond is longer than 2.7 Å, whereas four other bonds are in the range of 1.81–2.23 Å. To understand whether it is necessary to include the fifth oxygen atom in the

Table 3. Crystallographic information of the compounds isostructural to β-$SrZn_2P_2O_8$

Compound	β-$SrZn_2P_2O_8$	$SrCo_2P_2O_8$	α-$CaZn_2P_2O_8$
Space group	*P*−1	*P*−1	*P*−1
a, Å	5.0109(8)	5.014(2)	4.960(2)
b, Å	8.6202(13)	8.639(4)	8.418(4)
c, Å	9.7527(15)	9.691(1)	8.940(4)
α, °	118.088(3)	118.04(3)	113.75(4)
β, °	74.622(6)	75.09(4)	102.45(5)
γ, °	87.525(6)°	86.90(4)	94.20(6)
V, Å^3	351.29(10)	350.41	328.23
Reference	This work	El Bali *et al.* (1993)	Jakeman and Cheetham (1988)

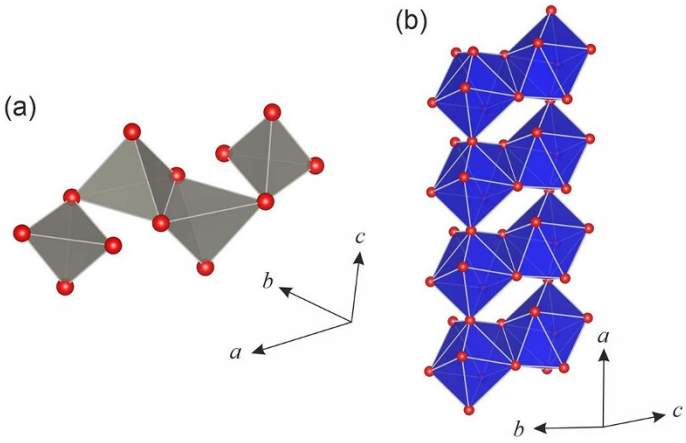


Figure 3. Fragments of β-$SrZn_2P_2O_8$: (a) Zn_4O_{12} structural units; (b) chain of SrO_8 polyhedra. Grey and blue polyhedra show ZnO_n (*n* = 4, 5) and SrO_8 polyhedra, respectively; red spheres indicate oxygen atoms.

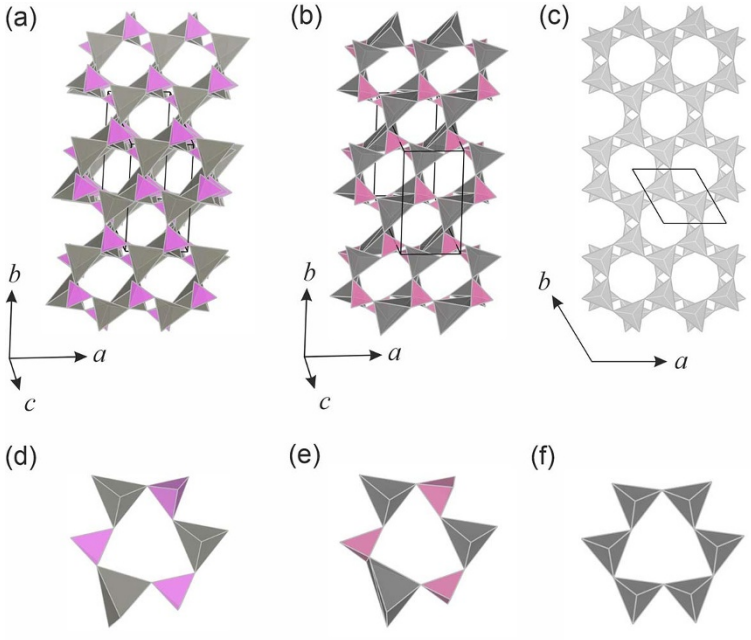


Figure 4. Double layers and six-membered rings in hexacelsian-type compounds: of β-$SrZn_2P_2O_8$ (a, d), α-$CaZn_2P_2O_8$ (b, e) (Jakeman and Cheetham, 1988) and β-dmisteinbergite (c, f) (Gorelova *et al.*, 2023b). PO_4 tetrahedra and ZnO_n (*n* = 4, 5) polyhedra in crystal structures of β-$SrZn_2P_2O_8$ and α-$CaZn_2P_2O_8$ are given in purple and grey, respectively. Grey tetrahedra in β-dmisteinbergite show mixed TO_4 (*T* = Si, Al) tetrahedra.

coordination sphere of Zn, the bond weights (BW) for this cation were calculated (Table S2). The results obtained demonstrate that for the case of $SrCo_2P_2O_8$ and $CaZn_2P_2O_8$ the BW of the fifth Co1–O7 and Zn2–O8 bond are 0.0938 and 0.0361, respectively, i.e. an order of magnitude lower than for other four bonds. The BW for Zn1–O7 in β-$SrZn_2P_2O_8$ is still an order of magnitude lower (0.0011), i.e. including this bond in the coordination sphere of Zn1 is not advisable.

Generally all three of these compounds (β-$SrZn_2P_2O_8$, $SrCo_2P_2O_8$ and α-$CaZn_2P_2O_8$) with layered triclinic crystal structures have similarities with hexacelsian-type minerals. The main difference being that in hexacelsian-type minerals TO_4 tetrahedra are joined to each other *via* corners, whereas some of the *T* atoms in crystal structures of β-$SrZn_2P_2O_8$, $SrCo_2P_2O_8$ and α-$CaZn_2P_2O_8$ are connected to each other *via* edges. Most probably, this difference leads to a decrease of symmetry in the

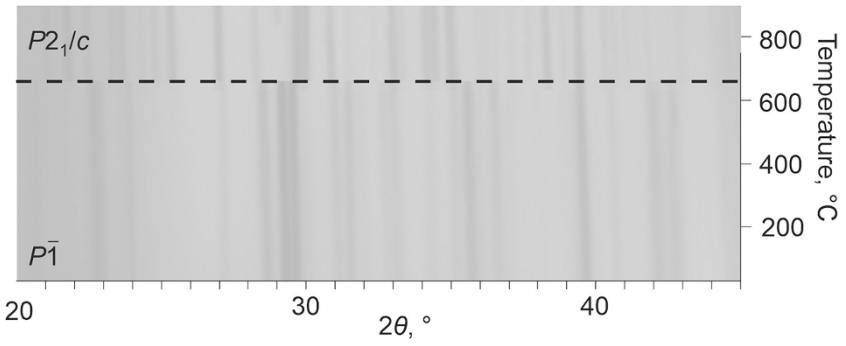


Figure 5. The evolution of the PXRD patterns of β-$SrZn_2P_2O_8$ in the range 30–900°C.

crystal structure of β-$SrZn_2P_2O_8$, $SrCo_2P_2O_8$ and α-$CaZn_2P_2O_8$ to triclinic. Nevertheless layers consist of six-membered rings of TO_n polyhedra (Fig. 4) in all types of crystal structures. In all cases the *M* cations are located in the interlayer space.

It is interesting to note that both $SrCo_2P_2O_8$ and $CaZn_2P_2O_8$ do not form framework crystal structures with paracelsian topology unlike $SrZn_2P_2O_8$. $SrCo_2P_2O_8$ crystallizes only in triclinic (space group $P\bar{1}$) symmetry (El Bali *et al.*, 1993) with layered crystal structure, whereas $CaZn_2P_2O_8$ has triclinic (space group $P1$; α-$CaZn_2P_2O_8$) and hexagonal (space group $P\bar{3}$; β-$CaZn_2P_2O_8$) polymorphs (Czaya, 1972; Jakeman and Cheetham, 1988), but both of them are layered too. A number of closely related compounds also do not exhibit similar polymorphism. Thus, $BaZn_2P_2O_8$ crystallizes only in monoclinic symmetry (space group $P2_1/c$) with framework paracelsian topology (Lucas *et al.*, 1998). $CaCo_2P_2O_8$ and $BaCo_2P_2O_8$ form completely different crystal structures (Faza *et al.*, 1950; Bircsak and Harrison, 1998; David *et al.*, 2013). We can assume that the key to polymorphism is not only the density of oxygen layers (as was suggested earlier), but also the fundamentally different thermal behaviour of large cations [e.g. Ca (R = 1.00 Å), Sr (R = 1.18 Å), Ba (R = 1.42 Å); Shannon, 1976], that lead to the limited isomorphism and changes in their coordination polyhedra.

Temperature behaviour of different polymorphs of $SrZn_2P_2O_8$

According to the HT PXRD data, α-$SrZn_2P_2O_8$ is stable up to 900°C, above which it starts to melt, whereas β-$SrZn_2P_2O_8$ is less stable and transforms into α-modification above 630°C (Fig. 5).

The temperature dependencies for the unit-cell parameters of both $SrZn_2P_2O_8$ modifications are shown in Fig. 6. The volume thermal expansion of framework α-$SrZn_2P_2O_8$ equals 25 × 10^{-6} °C^{-1} that is close to the average volume expansion coefficient (α_V = 23 × 10^{-6} °C^{-1}) for different compounds with paracelsian topology (Gorelova *et al.*, 2023a). The thermal expansion of α-modification has sharply anisotropic character ($\alpha_{max}/\alpha_{min}$ = 4.9) with the maximal expansion close to the *a* axis and minimal along *b* axis (Table 4, Figs 2a, 2b and 6a). It should be noted that though the anisotropic expansion is typical for paracelsian-like phases, the directions of maximal and minimal expansion are usually in the plane of the layer formed by four- and eight-membered rings of TO_4 tetrahedra (T = Si, Al, B). In the case of α-$SrZn_2P_2O_8$ the direction of maximal expansion is perpendicular to these layers and is located along the flexible crankshaft chains of TO_4 tetrahedra (T = Zn, P), that is more typical for compounds with feldspar topology. A similar behaviour has been described previously for $BaAs_2Zn_2O_8{\cdot}H_2O$ (Gorelova *et al.*, 2022).

The layered β-$SrZn_2P_2O_8$ shows very similar thermal behaviour despite a different structural motif. Its volume expansion and degree of anisotropy are slightly large (α_V = 27 × 10^{-6} °C^{-1}; $\alpha_{max}/\alpha_{min}$ = 5.6). The direction of maximal thermal expansion almost coincides with the *c* axis, i.e. it is perpendicular to the layer plane (Table 4, Figs 2c and 6b), which is generally typical for layered crystal structures. Additionally, such a sharp expansion along the *c* axis can be due to the so-called 'preparing' of the crystal structure to a phase transition into α-modification. The thermal expansion within the layer plane is quite anisotropic too (α_{11}/α_{22} = 4.1), that can be explained by the low symmetry of the studied compound, for which the shear character of thermal deformations is typical (Filatov, 1990, 2011).

Possible natural formation conditions

According to the International Mineralogical Association (IMA) List of Minerals, 47 minerals contain essential Zn, P and O, while only two of them are anhydrous, namely kuksite $Pb_3Zn_3TeO_6(PO_4)_2$ (Kim *et al.*, 1990) and tululite $Ca_{14}(Fe^{3+},Al)(Al,Zn,Fe^{3+},Si,P,Mn,Mg)_{15}O_{36}$ (or $Ca_{14}(Fe^{3+}O_6)[(Si,P)O_4][(Al,Zn)_7O_{13}]$; Khoury *et al.*, 2016). Kuksite was found in several Au, Ag-related deposits in Russia (Kim *et al.*, 1990; Kondratieva *et al.*, 2021) and the USA (e.g. Kampf *et al.*, 2009, 2022; Mills *et al.*, 2010; Yang *et al.*, 2021) and is always formed as a secondary mineral at low temperatures (below 250°C), whereas its synthetic analogue has been prepared above 500°C by solid-state methods (Mill', 2009b; 2009a). Tululite is only found in combustion metamorphic rocks in central Jordan (Khoury *et al.*, 2016; Sokol *et al.*, 2020; Galuskina *et al.*, 2021) and is formed at ~800–850°C and ambient pressures.

There is no single mineral with essential Zn, P and O, which contains Sr^{2+} or Ba^{2+}. In addition, only 11 minerals with essential Zn, P and O contain Ca^{2+} and only five of them contain Pb^{2+}. Among the calcium minerals are: batagayite $CaZn_2(Zn,Cu)_6(PO_4)_4[PO_3(OH)]_3{\cdot}12H_2O$ (Yakovenchuk *et al.*, 2018), ehrleite $Ca_2ZnBe(PO_4)_2(PO_3OH){\cdot}4H_2O$ (Robinson *et al.*, 1985), falsterite $Ca_2MgMn^{2+}{}_2Fe^{2+}{}_2Fe^{3+}{}_2Zn_4(PO_4)_8(OH)_4(H_2O)_{14}$ (Kampf *et al.*, 2012), guimarãesite $Ca_2Be_4Zn_5(PO_4)_6(OH)_4{\cdot}6H_2O$ (Chukanov *et al.*, 2008), hillite $Ca_2Zn(PO_4)_2{\cdot}2H_2O$ (Yakubovich *et al.*, 2003), jahnsite-(CaMnZn) $CaMn^{2+}Zn_2Fe^{3+}{}_2(PO_4)_4(OH)_2{\cdot}8H_2O$ (Grey *et al.*, 2020), jungite $Ca_2Zn_4Fe^{3+}{}_8(PO_4)_9(OH)_9{\cdot}16H_2O$ (Moore and Ito, 1980), scholzite and parascholzite $CaZn_2(PO_4)_2{\cdot}2H_2O$ (Strunz, 1948; Strunz and Tennyson, 1956; Sturman *et al.*, 1981), skorpionite $Ca_3Zn_2(PO_4)_2(CO_3)(OH)_2{\cdot}H_2O$ (Krause *et al.*, 2008) and, already mentioned above, tululite. Among lead minerals are: cuprodongchuanite $Pb_4CuZn_2(PO_4)_4(OH)_2$ (Sun *et al.*, 2021), cuprozheshengite $Pb_4CuZn_2(AsO_4)_2(PO_4)_2(OH)_2$ (Sun *et al.*, 2024a), dongchuanite $Pb_4ZnZn_2(PO_4)_4(OH)_2$ (Li *et al.*, 2023),

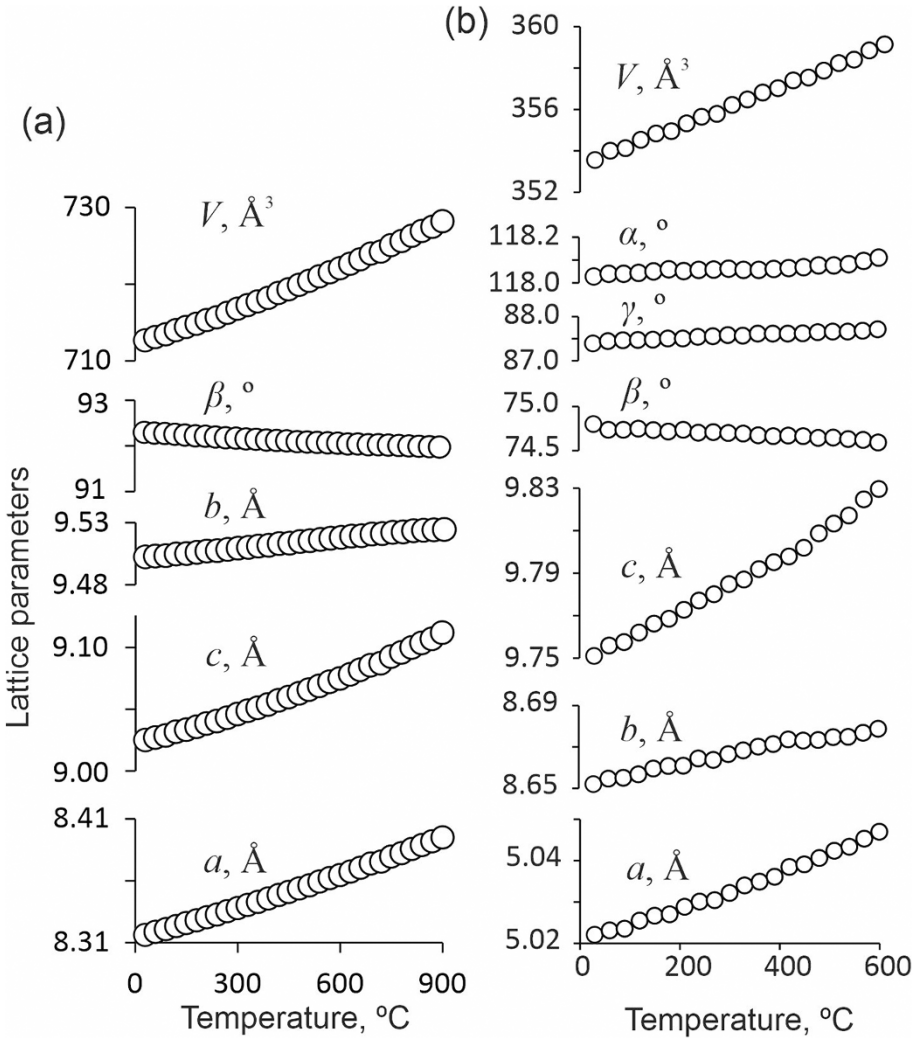


Figure 6. Unit-cell parameters of α-$SrZn_2P_2O_8$ (a) and β-$SrZn_2P_2O_8$ (b) at different temperatures. Errors are smaller than symbols.

Table 4. Thermal expansion coefficients (TECs) (×10^6 °C^{-1}) of $SrZn_2P_2O_8$ along the principle axes of the thermal expansion tensor and along the crystallographic axes

Compound (space group)	ΔT °C	α_{11}	α_{22}	α_{33}	$\mu_{(\alpha 33\wedge c)}$	α_a	α_b	α_c	α_α	α_β	α_γ	α_V	$\alpha_{max}/\alpha_{min}$
$SrZn_2P_2O_8$ ($P2_1/c$)	30–900	14.3(1)	2.9(1)	7.8(2)	44.6(9)	10.84(1)	2.9(1)	11.0(2)	–	−3.98(9)	–	25.0(2)	4.9
$SrZn_2P_2O_8$ ($P-1$)	30–600	10.2(2)	2.5(2)	14.1(3)	14.3(2)	8.7(2)	5.3(2)	13.6(3)	0.86(8)	−3.7(2)	5.6(2)	26.7(4)	5.6

zheshengite $Pb_4ZnZn_2(AsO_4)_2(PO_4)_2(OH)_2$ (Sun *et al.*, 2024b) and, mentioned above, kuksite. It is interesting to note that all the Pb-dominant minerals except kuksite were discovered recently, have supergene origin (low temperatures, low pressures) and are members of the dongchuanite group (Sun *et al.*, 2024a; 2024b). The Ca-dominant minerals are extremely rare and most of them (except scholzite and parascholzite) are found in only 1–2 localities (mindat.org, Ralph *et al.*, 2025). Notably all these minerals are secondary low-temperature minerals.

It should be noted that none of the mentioned minerals contain Sr, even in trace amounts, although Sr is usually dispersed in calcium minerals (e.g. apatite group minerals; Pekov *et al.*, 1996). Furthermore Sr-containing minerals rarely have layered structures (exceptions are lamprophyllite and Sr-rich borates; e.g. Pekov *et al.*, 2004; Pekov, 2005; Ralph *et al.*, 2025). It is the structural motif of these minerals that may explain the absence of calcium (see below).

The crystal structures of the minerals mentioned above, can be formed by different combinations of Zn- and P-based polyhedra: phosphorous is always surrounded by four oxygen atoms, whereas zinc can be coordinated by four and/or six oxygen atoms. The crystal structures of kuksite, tululite, ehrleite, falsterite, skorpionite, scholzite and parascholzite are based on layers of corner-sharing ZnO_4 and PO_4 tetrahedra (Taxer, 1975; Hawthorne and Grice, 1987; Taxer and Bartl, 1997; Krause *et al.*, 2008; Mills *et al.*, 2010; Kampf *et al.*, 2012; Khoury *et al.*, 2016; Tobase *et al.*, 2019). In crystal structures of guimarãesite, hillite and jahnsite-(CaMnZn) phosphorous is coordinated by four oxygen atoms, whereas zinc is coordinated by six oxygens

(Yakubovich *et al.*, 2003; Chukanov *et al.*, 2008; Grey *et al.*, 2020). Pb-dominant minerals, related to the dongchuanite group, have a layered crystal structure. The layers are formed by TO_4 (T = Zn, P, As) tetrahedra and XO_6 octahedra (X = Zn, Cu), i.e. in their crystal structures zinc is surrounded by four and six oxygen atoms (Sun *et al.*, 2024a; 2024b). A similar tendency is in the crystal structure of batagayite, in which layers are formed by PO_4 and ZnO_4 tetrahedra and TO_6 (T = Zn, Cu, Mg) octahedra (Yakovenchuk *et al.*, 2018).

Nevertheless, to date three Sr-dominant minerals are known in the feldspar family, namely slawsonite $SrAl_2Si_2O_8$ (Griffen *et al.*, 1977), pekovite $SrB_2Si_2O_8$ (Pautov *et al.*, 2004) and strontiohurlbutite $SrBe_2P_2O_8$ (Rao *et al.*, 2014). All of them belong to the paracelsian topology, i.e. have framework crystal structures. An interesting fact is that pekovite has both Ca- and Ba-dominant analogues, namely danburite (Phillips *et al.*, 1974) and maleevite (Pautov *et al.*, 2004), whereas slawsonite has only a Ba-dominant analogue, namely paracelsian (Smith, 1953) and strontiohurlbutite has only a Ca-dominant analogue, namely hurlbutite (Lindbloom *et al.*, 1974). Notably, minerals with the composition of $CaAl_2Si_2O_8$ and $BaBe_2P_2O_8$ are known in nature, but crystallize in other topologies. $CaAl_2Si_2O_8$ is known in feldspar (anorthite; Wainwright and Starkey, 1971), dmisteinbergite (dmisteinbergite; Chesnokov *et al.*, 1990; Zolotarev *et al.*, 2019), svyatoslavite (svyatoslavite; Chesnokov *et al.*, 1989; Krivovichev *et al.*, 2012) and hollandite (stöfflerite; Tschauner and Ma, 2017) topologies. $BaBe_2P_2O_8$ is known in dmisteinbergite topology only (minjiangite; Rao *et al.*, 2015). The recent discovery of two new hexacelsian-type metastable minerals of the feldspar family, namely pfaffenbergite $KNa_3(Al_4Si_{12})O_{32}$ (Silvio *et al.*, 2026) and wodegongjieite $KCa_3(Al_7Si_9)O_{32}$ (Mugnaioli *et al.*, 2022), is one more confirmation that layered modification of $SrZn_2P_2O_8$ can be also found in nature.

Based on that we assume that the zinc phosphate minerals with both feldspar- and hexacelsain-type crystal structures (i.e. different polymorphic modifications of $SrZn_2P_2O_8$ or $CaZn_2P_2O_8$), can be found in nature. The α-modification of the $SrZn_2P_2O_8$ phase with the paracelsian structure may be found in nature under high-temperature and low-pressure conditions. However, the existence of a β-modification of $SrZn_2P_2O_8$ is questionable, as this phase is undoubtedly metastable and requires very specific formation conditions (e.g. superheated melt).

Conclusion

During this work, the crystal structure of β-$SrZn_2P_2O_8$ was determined for the first time. It has been shown that β-$SrZn_2P_2O_8$ can be synthesized by the rapid cooling of stoichiometric $SrZn_2P_2O_8$ melt in air. According to the obtained results, the triclinic (space group $P\bar{1}$) crystal structure of β-$SrZn_2P_2O_8$ is layered and close to $SrCo_2P_2O_8$ and α-$CaZn_2P_2O_8$. The β-$SrZn_2P_2O_8$ transforms into stable α-modification with framework crystal structure of paracelsian topology when heated above 630°C. The thermal expansion coefficients of both $SrZn_2P_2O_8$ modifications were determined. The volume expansion ($\alpha_V = 26 \pm 1 \times 10^{-6}$ °C^{-1}) and the anisotropy of thermal expansion are similar for both phases despite the fact that they have significantly different structures. We assume the possibility of discovering a new feldspar- and hexacelsian-type minerals in nature.

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