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Isomorphous substitution of strontium by sodium and rare-earth elements in molybdates with the scheelite-type structure $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$, where Ln = La–Lu

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Using the crystal energy theory of isomorphous miscibility, the mixing energies, critical decomposition temperatures, and substitution limits were calculated, and the thermodynamic stability ranges of solid solutions $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ (where Ln represents rare-earth elements, REEs) were determined. It was shown that both the mixing energies and the critical decomposition temperatures increase systematically with the REE atomic number. A thermodynamic stability diagram and dependencies of solubility limits of the solid solutions were built for concentrations ranging from $x = 0$ to $x = 1.0$ with a step of $\Delta x = 0.05$. These diagrams allow one to determine the limits of equilibrium substitution at a given decomposition temperature, decomposition temperatures for a specified substitution limit, or the thermodynamically stable composition regions. The results may be helpful for immobilizing radioactive isotopes of REEs, actinides, and strontium-90 in nuclear waste disposal and developing new inorganic materials for phosphors and lasers.

Keywords: molybdates, rare-earth elements, strontium, solid solution, scheelite-type structure, isomorphous substitution, thermodynamic stability

Ізоморфні заміщення стронцію на натрій та рідкісноземельні елементи в молібдатах зі структурою шеєліту складу $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$, де Ln = La–Lu.
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Із використанням кристалоенергетичної теорії ізоморфної змішуваності розраховано енергії змішування, критичні температури розпаду, границі ізоморфних заміщень, а також визначено області термодинамічної стабільності твердих розчинів $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$, де Ln – рідкісноземельні елементи (РЗЕ). Показано, що енергії змішування та критичні температури розпаду закономірно зростають зі збільшенням атомного номера РЗЕ. Представлено діаграму термодинамічної стабільності, а також куполи розпаду твердих розчинів у діапазоні концентрацій від $x = 0$ до $x = 1{,}0$ з кроком $x = 0{,}05$. Вони дозволяють визначати рівноважні границі заміщення за температурою розпаду, температуру розпаду за заданою границею заміщення або області термодинамічної стабільності. Результати дослідження можуть бути корисними для іммобілізації радіоактивних ізотопів РЗЕ, актиноїдів та стронцію-90 під час захоронення відходів ядерних реакторів, а також у пошуку нових неорганічних матеріалів для люмінофорів і лазерів.

1. Introduction

Currently, aluminophosphate or borosilicate glasses are used as matrices for the disposal of long-lived radioactive waste, particularly compounds of radioactive isotopes of rare-earth elements (REEs), actinides, and strontium-90. However, the service life of such glasses does not exceed 30-40 years [1]. According to [2-3], under conditions typical for deep geological repositories, borosilicate glass can be subject to dissolution upon contact with groundwater

over geological time scales. Meanwhile, existing regulations require the matrix material to ensure environmental safety for more than 10^5 years [4]. Such long-term durability can be achieved by ceramic matrices based on minerals that have demonstrated natural stability for the required period, specifically, solid solutions of molybdates and tungstates of alkaline-earth metals with a scheelite-type structure [3]. Therefore, the guidelines and recommendations issued for International Atomic Energy Agency (IAEA) member states propose using ceramics based on mineral-like phases for radionuclide immobilization. According to IAEA experts, this approach enhances the environmental safety of radioactive waste storage and disposal and thus contributes to the overall safety of nuclear energy.

The use of solid solutions rather than individual chemical compounds allows for the targeted modification of thermal, physicochemical, electrophysical, and other properties through composition- and temperature-dependent property trends. Phase diagrams and even composition-dependent substitution limits have been most comprehensively studied for systems based on intermediate molybdates and tungstates of alkaline-earth elements, lead, and cadmium with the scheelite structure – for example, see [5-12]. In contrast, heterovalent charge-compensating substitutions, where divalent cations are replaced by singly charged alkali metal cations and trivalent rare earth cations, have been studied to a much lesser extent in pseudo-binary systems of the $M^{II}_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ type (where M^{II} is an alkaline earth element and Ln is a lanthanide).

To our knowledge, information on the substitution limits and stability regions of these numerous systems is limited – see, for example, [2, 3, 11, 13–19]. Among the $M^{II}_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems, those based on strontium molybdates are the most promising for immobilizing highly radioactive waste. This is due to the fact that such solid solutions can be used not only for the immobilization of actinides but also for radioactive REE isotopes, which are similar in ionic size. According to [20], REE isotopes may constitute up to 35 wt.% of nuclear reactor waste. The ionic radii of Pr, Nd, Sm, Eu, and Gd for coordination number 6 fall within the range of 1.078–1.130 Å, while those of Cm, Am, Pu, and U range from 1.110 to 1.165 Å [21]. At the same time, it is possible to co-immobilize radioactive strontium-90 [22]. Moreover, solid solutions based on molybdates and tungstates, in which alkaline earth elements are partially substituted by alkali and rare-earth elements, may also find application as laser, luminescent, and other practically important materials [11, 12, 14, 19].

However, most publications focus primarily on studying the synthesis conditions and properties of materials, without predicting their behavior during practical use. It is well known [23] that solid solutions are prone to decomposition upon cooling, which can lead to the degradation of materials based on them, altering their properties and making them unreproducible. In this regard, it is desirable to know the limits of isomorphous substitution and thermodynamic stability under synthesis, operational conditions, and even during the expected storage. Experimental determination of substitution limits and stability regions using X-ray diffraction analysis by the annealing and quenching method is complicated by the difficulty of achieving equilibrium at low temperatures due to the slow diffusion rate in the solid phase, as well as the possibility of partial decomposition of the solid solution upon cooling from high temperatures. Additionally, the isostructurality of alkali-earth metal molybdates and sodium-REE double molybdates makes their identification challenging.

The lack of sufficient information about the substitution limits and thermodynamic stability regions of solid solutions forces researchers to select material compositions and synthesis conditions either by analogy with related systems or by "trial and error." Such an approach may result in unnecessary consumption of expensive reagents and increased research time. Hence, it is reasonable to complement experimental methods with computational ones, which do not have these limitations. As an example of such an approach, one can refer to studies [24-25] in which the synthesis conditions for samples of the $Y_{1-x}Sc_xPO_4$ system were selected based on the calculated results presented in [26].

Considering the above, the present study aimed to predict the limits of isomorphous substitutions and the thermodynamic stability of solid solutions $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$, where Ln = La–Lu.

2. Initial data and calculation methodology

In the crystal-energy theory of isomorphous substitutions developed by Urusov, the main challenge in determining the limits of isomorphous substitutions lies in evaluating the mixing energy (Q_{mix}) [23].

Since the components of the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems are isostructural, this energy can be calculated as the sum of two contributions: one resulting from the difference in the degree of ionicity of the chemical bond in the system components (Q_ε), and the other – from the difference in the sizes of the substituting structural units (Q_R), as expressed by equation (1):

$$Q_{mix} = Q_\varepsilon + Q_R = \\ =1390\times m\times z_m\times z_x\times\alpha\times(\Delta\varepsilon)^2/(2\times R) + \\ + C\times m\times n\times z_m\times z_x\times(\Delta R/R_1)^2,\ \text{kJ/mol} \quad (1)$$

where: $m = 2$ is the the number of distinct structural units in the components within the pseudobinary approximation of the scheelite structure; sodium and lanthanide ions, statistically occupying cationic positions in the scheelite-type structures $Na_{0.5}Ln_{0.5}MoO_4$, are considered as one structural unit, and the molybdate anion as the second;

$z_m = z_x = 2$ are the formal (integer) charges of the substituting (z_m) and common (z_x) structural units of the components;

$\alpha = 1.723$ is the reduced Madelung constant, calculated by Templeton's formula [27];

$C = 20(2\Delta_X + 1)$ is a constant dependent on the properties of the components, where Δ_X is the difference in the electronegativities between the cations (taken from [28]) and the MoO_4^{2-} anion, the electronegativity of which, following the recommendation of [29], is assumed to be equal to the electronegativity of the oxide anion O^{2-} (3.758). The choice of the electronegativity scale from [28], as opposed to those of other authors, was based on the fact that the electronegativity values in this scale vary with regular periodicity: they increase consistently in the $Ce^{3+} - Eu^{3+}$ series from 1.348 to 1.433 and in the $Gd^{3+} - Yb^{3+}$ series from 1.386 to 1.479, with sharp drops at the $Eu^{3+} - Gd^{3+}$ (from 1.433 to 1.386) and $Yb^{3+} - Lu^{3+}$ (from 1.479 to 1.431) transitions. These features are associated with the electronic configuration of the REEs: europium and gadolinium have a half-filled 4f shell (7 electrons), while ytterbium and lutetium have a filled 4f shell (14 electrons). The transitions from europium to gadolinium and from ytterbium to lutetium correspond to the first appearance of an electron in the 5d subshell.

$n = 8$ is the coordination number of the substituting structural unit in the pseudobinary representation of the scheelite-type structure;

$R_{Na,Ln-M}$ is the interatomic distance between the cation and the tetrahedral anion in $Na_{0.5}Ln_{0.5}MoO_4$, calculated from the unit cell parameters reported in [30];

ΔR is the difference in the "cation – tetrahedral anion" interatomic distances between $SrMoO_4$ and $Na_{0.5}Ln_{0.5}MoO_4$;

$\Delta R/R_1$ is the relative difference in the "cation – tetrahedral anion" interatomic distances in the system components (dimensional parameter);

R_1 is the "cation – tetrahedral anion" interatomic distance in the component with the smaller cation radius;

$\Delta\varepsilon$ is the difference in the ionicity degree of the chemical bond in the system components in the pseudobinary approximation of the structure. The ionicity degree ε in crystals was determined based on the electronegativity difference between the tetrahedral anion and the cations, according to the data from [31].

The critical decomposition temperatures T_{cr} were calculated within the approximation of regular solid solutions using Eq. 2 [23]:

$$T_{cr} = Q_{mix}/2kN, \quad (2)$$

where k is the Boltzmann constant, and N is Avogadro's number. Since the size mismatch parameter $\Delta R/R_1$ was significantly less than 0.1 (Table 1), the calculation of the equilibrium substitution limits as a function of temperature in accordance with [23] was performed in the approximation of regular solid solutions using the Becker equation (Eq. 3) [32]:

$$-(1-2x)/\ln[x/(1-x)] = R_g\times T_d/Q_{mix} \quad (3)$$

where x is the molar fraction of the dissolved component, R_g is the universal gas constant, and T_d is the decomposition temperature of the solid solution. The values of R_g and Q_{mix} in both latter cases were expressed in calories [23].

The error in calculating the critical (maximum) decomposition temperature of solid solutions was ±100 K, and the mixing energy Q_{mix}, considering the input data's uncertainty, had an error of up to ±13% [23].

Table 1. Some initial data, calculated mixing energies Q_R, and critical decomposition temperatures of solid solutions in the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems

Ln	R(Na,Ln–M), Å	$\chi = ((\chi(Na) + \chi(Ln))/2 + \chi(Sr))/2$	$\Delta\chi = 3.758 - \chi$	C, kJ	$\Delta R/R_1$	Q_R, kJ/mol	T_{cr}, K
La	3.872	1.158	2.600	124.0	0.0139	1.53	91
Ce	3.854	1.163	2.595	123.8	0.0186	2.74	163
Pr	3.837	1.170	2.588	123.5	0.0232	4.25	253
Nd	3.827	1.165	2.585	123.4	0.0258	5.26	314
Sm	3.807	1.179	2.579	123.2	0.0313	7.72	460
Eu	3.798	1.186	2.574	123.0	0.0337	8.94	533
Gd	3.791	1.173	2.585	123.4	0.0356	10.01	597
Tb	3.775	1.179	2.579	123.2	0.0400	12.62	753
Dy	3.768	1.182	2.576	123.0	0.0419	13.82	825
Ho	3.762	1.184	2.574	123.0	0.0436	14.96	893
Er	3.752	1.186	2.572	122.9	0.0464	16.93	1010
Tm	3.742	1.190	2.568	122.7	0.0492	19.01	1135
Yb	3.738	1.196	2.562	122.5	0.0503	19.83	1184
Lu	3.732	1.184	2.574	123.0	0.0520	21.29	1271

Note: The interatomic distance $R(SrMoO_4)$ = 3.926 Å was calculated based on the unit cell parameters of $SrMoO_4$ (a = 5.3944, c = 12.02 Å) [33].

3. Results of calculations and discussion

3.1. Energies of mixing of solid solutions

Some initial data and calculation results are summarized in Table 1 and Figure 1*a*. As seen from the provided data, with the increase of the atomic number of REE, the contributions to the total mixing energy due to differences in the sizes of the substituting structural units, Q_R, change smoothly, increasing significantly from 1.53 to 21.29 kJ/mol. The contributions to the mixing energy due to differences in the degree of bond ionicity of the components, Q_ε (Table 2 and Figure 1*b*), are much smaller (ranging from 0.48 to 2.01 kJ/mol) and increase slightly with increasing atomic number of the REE, with two maxima for $Sr_{1-x}(Na_{0.5}Eu_{0.5})_xMoO_4$ and $Sr_{1-x}(Na_{0.5}Yb_{0.5})_xMoO_4$, which are due to the aforementioned structure of the electronic shells of the REEs.

According to [23], in general, if the differences in the degree of bond ionicity between the components of the system are less than 0.05, the value of Q_ε will be negligible and can be neglected. This is also because the errors in determining the electronegativity, which served as a basis for calculating Q_ε, are about 0.05, which is significantly greater than the inaccuracies in determining the unit cell parameters, on the basis of which the Q_R energy was initially calculated.

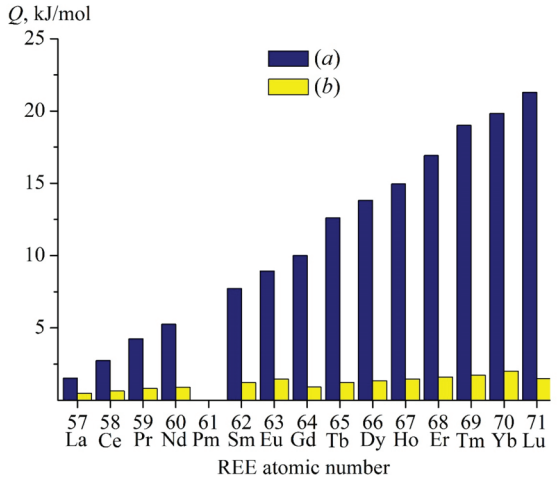

Figure 1. Dependencies of the calculated mixing energies Q_R (*a*) and Q_ε (*b*) of the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems on the REE atomic number.

In this case, $\Delta\varepsilon$ ranges from 0.014 to 0.028 (Table 2), and the values of Q_ε are significantly smaller (Figure 1*b*) than Q_R (Figure 1*a*). Therefore, for all systems, we neglected the Q_ε values.

3.2. Decomposition temperatures of solid solutions

Based on the calculated decomposition temperatures (T_d) of the limited solid solution series, $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$, for substitution limits of x = 0.05, 0.10, 0.15, and 0.20 (Table 3), and on the calculated critical decomposition temperatures (T_{cr}) (Table 1), the dependen-

Table 2. Some initial data and calculated mixing energies Q_ε of the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ solid solutions

Ln	χ(Ln)	$\chi(MoO_4) - \chi(Na_{0.5}Ln_{0.5})$	$\varepsilon(Na_{0.5}Ln_{0.5}MoO_4)$	$\Delta\varepsilon$*	Q_ε, kJ/mol
La	1.327	2.583	0.766	0.014	0.48
Ce	1.348	2.572	0.764	0.016	0.63
Pr	1.374	2.559	0.762	0.018	0.81
Nd	1.382	2.555	0.761	0.019	0.90
Sm	1.410	2.541	0.758	0.022	1.22
Eu	1.433	2.529	0.756	0.024	1.45
Gd	1.386	2.553	0.761	0.019	0.91
Tb	1.410	2.541	0.758	0.022	1.23
Dy	1.426	2.533	0.757	0.023	1.34
Ho	1.433	2.529	0.756	0.024	1.47
Er	1.438	2.527	0.755	0.025	1.60
Tm	1.455	2.518	0.754	0.026	1.73
Yb	1.479	2.506	0.752	0.028	2.01
Lu	1.431	2.530	0.756	0.024	1.48

*Note: $\Delta\varepsilon = \varepsilon(SrMoO_4) - \varepsilon(Na_{0.5}Ln_{0.5}MoO_4)$; the value of $\varepsilon(SrMoO_4) = 0.780$ is defined based on the data from [31], derived from $\chi(MoO_4) = 3.758$, $\chi(Sr) = 1.139$, and $\chi(Na) = 1.024$.

cies of decomposition temperatures on the REE atomic numbers have been plotted for all systems (Figure 2).

These dependencies allow for the graphical determination of the equilibrium substitution limits (x) at a given T_d or the T_d for given substitution limits [34]. The intersection points of the isotherm, drawn from the given decomposition temperature with a vertical line drawn from the REE number, allow us to determine the composition region where the substitution limit is located. Interpolation of the segment of this vertical between the two nearest curves provides the substitution limit. The calculated critical decomposition temperatures for the unlimited solid solution series of the considered systems (Table 1, Fig. 2, curve *e*, at $x = 0.5$)) range from 91 K to 1271 K and increase with the atomic number of REE in the La–Lu series.

3.3. Regions of thermodynamic stability

It is known that as the temperature decreases, the equilibrium limits of isomorphous substitutions decrease [23]. This continues until the diffusion rate becomes so low that the reduction in solubility regions practically stops, i.e., spontaneous "quenching" occurs, and the solid solutions become metastable. When studying related systems, it was previously assumed [34] that spontaneous "quenching" may be close to the minimum temperature at which the diffusion rate becomes sufficient for forming solid solutions when synthesized from the initial substances.

Table 3. Calculated decomposition temperatures (T_d, K) of solid solutions in the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems at substitution limits of $x = 0.05$, 0.10, 0.15, and 0.20

Ln	T_d, K, for x value			
	0.05	0.10	0.15	0.20
La	56	66	74	79
Ce	100	119	132	142
Pr	155	185	205	220
Nd	192	229	253	272
Sm	282	336	372	399
Eu	326	389	431	462
Gd	365	435	482	517
Tb	461	549	608	652
Dy	504	601	666	714
Ho	546	650	721	773
Er	618	736	816	875
Tm	694	826	916	982
Yb	724	862	956	1025
Lu	777	926	1026	1100

It was previously established [3] that the minimum temperature for solid-phase synthesis of a solid solution of molybdate with a composition close to $Ca_{0.5}Li_{0.25}Gd_{0.25}MoO_4$, from $CaMoO_4$, Gd_2O_3, and $Li_2Mo_4O_{13}$ is in the temperature range of 823 to 873 K, i.e., on average around 848 K. This suggests that the temperature for spontaneous "quenching" upon cooling of $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ solid solutions is also

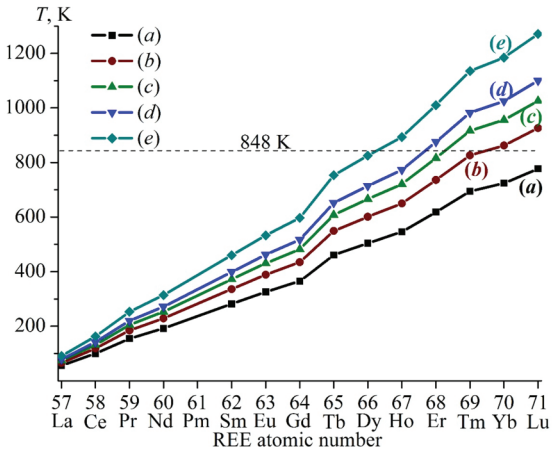

Figure 2. Decomposition temperatures of solid solutions in the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems as a function of the rare-earth element atomic number (thermodynamic stability diagram) for substitution limits of $x = 0.05$ (*a*), 0.10 (*b*), 0.15 (*c*), 0.20 (*d*), and 0.50 (*e*).

close to 848 K. Therefore, at approximately 848 K, the diffusion rate is such that not only does the solid-phase reaction begin to form from the starting materials, but upon cooling below this temperature, spontaneous "quenching" of the solid solutions will occur and become metastable.

Therefore, it can be assumed that unlimited solid solutions of the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems, which are stable at temperatures above the critical points (Figure 2, above curve *e*), may decompose upon cooling below the critical temperatures, forming regions of limited miscibility. This occurs if diffusion rates and time are sufficient for the formation and growth of stable nuclei of a new phase.

Solid solutions containing REEs from La to Tb will be thermodynamically stable above the critical temperatures and metastable below them – i.e., they are unlikely to decompose at any temperature.

Solid solutions containing REEs from Er to Lu will be thermodynamically stable above the critical temperatures, unstable in the temperature range between the critical temperatures and ~848 K (where decomposition into two solid solutions may occur), and metastable at temperatures below ~848 K.

For each $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ system, decomposition temperatures were calculated over the composition region $1.0 > x > 0$ (in increments of $x = 0.05$) and dependences of solubility limits for isomorphous substitution were built (Fig. 3). These dependences allow us to more accurately graphically determine the decomposition temperature at a given substitution limit or the equilibrium substitution limit at a given decomposition temperature for each specific system and to identify thermodynamically stable regions.

Continuous solid solution series are thermodynamically stable above the peaks of the dependences of solubility limits for isomorphous substitution. Two regions of limited miscibility exist below the peaks but above the curves. Below the dependencies, mixtures of two solid solutions based on each component of the systems are expected to form.

3.4. Comparison of the calculated results with literature data

To our knowledge, the literature contains no data on the critical decomposition temperatures, solubility limits in cases of partial miscibility, or the thermodynamic stability of solid solutions in the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems. Previous studies [19, 35] have focused mainly on synthesis conditions and specific properties of solid solutions where Ln = Nd and Eu, with synthesis temperatures falling within the thermodynamically stable regions predicted in our work. In particular, in the $Sr_{1-x}(Na_{0.5}Nd_{0.5})_xMoO_4$ system [35], single-phase scheelite-type samples were synthesized at 1073 K for $x = 0$–1.0, with unit cell parameters decreasing systematically as the neodymium content increased. This trend suggests unlimited miscibility of the components and is consistent with our calculations predicting a continuous solid solution series stable at the synthesis temperature and down to the critical value of 314 K, below which they can persist as a metastable phase. Similarly, in the $Sr_{1-x}(Na_{0.5}Eu_{0.5})_xMoO_4$ system [19], single-phase scheelite-type samples were synthesized at 1023 K for $x = 0$–0.6, with unit cell parameters systematically decreasing with increasing Eu content. This behavior is also consistent with our predictions that the $Sr_{1-x}(Na_{0.5}Eu_{0.5})_xMoO_4$ solid solutions remain thermodynamically stable at the synthesis temperature and down to the critical point of 533 K, below which they may exist as metastable phases.

4. Conclusions

1. Within the framework of the crystal energy theory of isomorphous substitution, the mixing energies (interaction parameters), critical decomposition (stability) temperatures, and substitution limits were calculated, and the

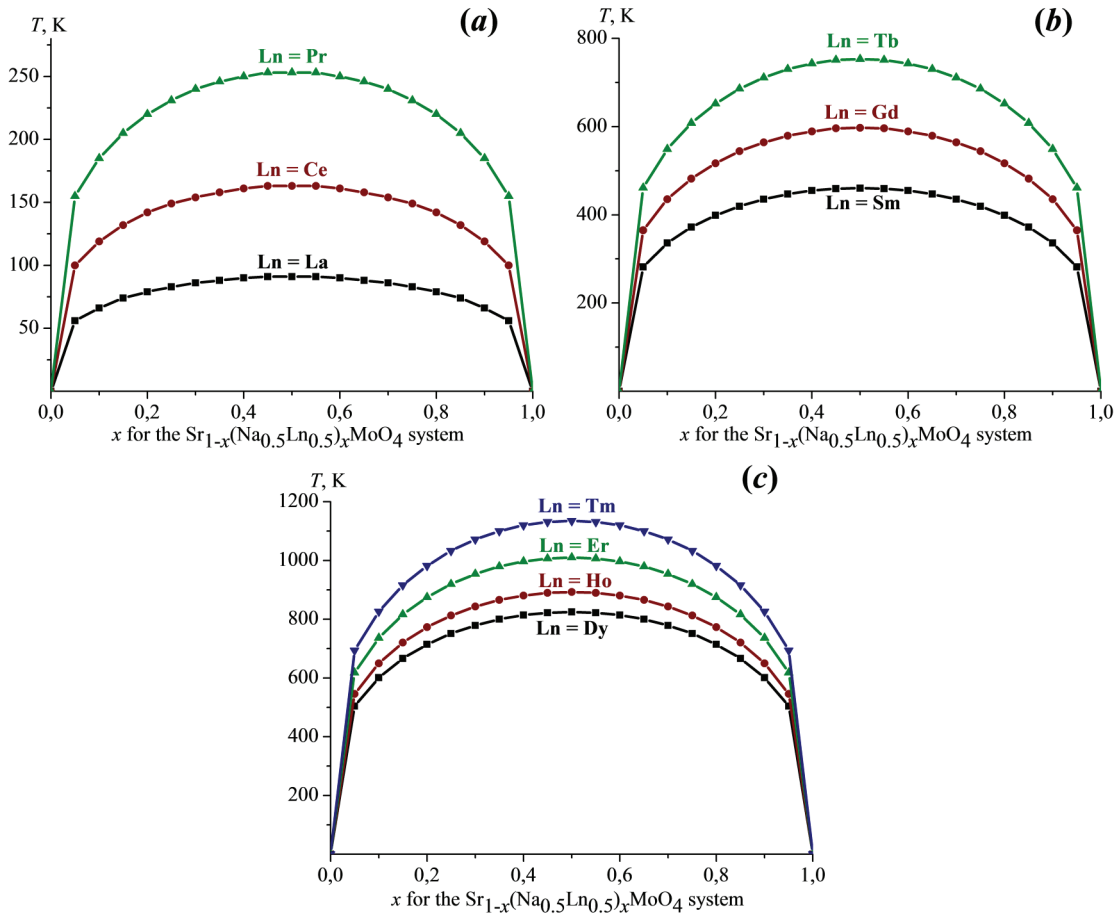

Figure 3. Dependences of solubility limits for isomorphous substitution in $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ solid solutions ($1.0 > x > 0$): (*a*) Ln = La, Ce, and Pr; (*b*) Ln = Sm, Gd, and Tb; (*c*) Ln = Dy, Ho, Er, and Tm.

thermodynamic stability of solid solutions in the systems $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ (where Ln = rare-earth elements) was assessed.

2. It was shown that in these systems, as the atomic number of the REE increases, the mixing energy values systematically rise from 1.53 to 21.29 kJ/mol due to an increase in the size mismatch parameter $\Delta R/R_1$ from 0.0139 to 0.0520, which is due to the growing differences in the sizes of the substituting structural units (Sr and REEs).

3. It was established that the contributions to the total mixing energy Q_{mix} caused by differences in ionic radii (Q_R) exceed those caused by differences in ionicity of components (Q_ε), making the latter negligible.

4. The critical decomposition temperatures of the solid solutions increase proportionally with the mixing energy, from 91 K to 1271 K.

5. A thermodynamic stability diagram was built for all $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems, as well as the dependence of the solubility limits on isomorphic substitution in the concentration range from $x = 0$ to 1.0 with a step of $\Delta x = 0.05$. These diagrams allow one to graphically determine the decomposition temperature for a given composition, the limit of equilibrium substitution at a given decomposition temperature, and also to estimate thermodynamically stable regions over a wide range of compositions and temperatures.

6. The predicted results regarding isomorphous substitution are consistent with previously reported experimental data in the literature for the $Sr_{1-x}(Na_{0.5}Ln_{0.5})_xMoO_4$ systems with Ln = Nd and Eu.

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References

1. Grechanovsky A.E., Eremin N.N., Urusov V.S. *Phys. Solid State,* **55**, 1929 (2013). https://doi.org/10.1134/S1063783413090138
2. Bosbach D., Rabung T., Brandt F., Fanghänel T. *Radiochim. Acta,* **92**, 639 (2004). https://doi.org/10.1524/ract.92.9.639.54976
3. Meng C., Li W., Ren C., Zhao J. *J. Mater. Sci.,* **55**, 2741 (2020). https://doi.org/10.1007/s10853-019-04223-y
4. Skiter E., Vtornikova E. *Nuclear and Radiation Safety*, No. 2 (78), 36 (2018). https://doi.org/10.32918/nrs.2018.2(78).06
5. Li D., Huang Zh., Nie Zh., Zhang L., Bai Y., Zhang X., Song Y., Wang Y. *J. Alloy. Compd.,* 650, 799 (2015). https://doi.org/10.1016/j.jallcom.2015.07.005
6. Mokhosoev M.V., Alekseev F.P., Lutsyk V.I. *Diagrammy sostoyaniya molibdatnykh i vol'framtnykh system* [State diagrams of molybdate and tungsten systems]. Novosibirsk, Nauka, 1978, 320 p. (In Russian)
7. Hallaoui A., Taoufyq A., Arab M., Bakiz B., Benlhachemi A., Bazzi L., Villain S., Valmalette J.-C., Guinneton F., Gavarri J.-R. *J. Solid State Chem.,* 227, 186 (2015). http://dx.doi.org/10.1016/j.jssc.2015.04.004
8. Hallaoui A., Taoufyq A., Arab M., Bakiz B., Benlhachemi A., Bazzi L., Valmalette J.-C., Villain S., Guinneton F., Gavarri J.-R. *Mater. Res. Bull.,* 79, 121 (2016). https://doi.org/10.1016/j.materresbull.2016.03.015
9. Singh N.K., Sharma S., Choudhary R.N.P. *Indian J. Pure Ap. Phy.,* 37, 595 (1999).
10. Zhuravlev V.D., Reznitskikh O.G., Velikodnyi Yu.A., Patrusheva T.A., Sivtsova O.V. *J. Solid State Chem.,* 184, 2785 (2011). https://doi.org/10.1016/j.jssc.2011.08.003
11. Zhuravlev V.D., Reznitskikh O.G. *J. Struct. Chem.*, 53, 100 (2012). https://doi.org/10.1134/S002247661201012X
12. Gupta S.K., Sudarshan K., Yadav A.K., Gupta R., Bhattacharyya D., Jha S.N., Kadam R.M. *Inorg. Chem.,* 57, 821 (2018). https://doi.org/10.1021/acs.inorgchem.7b02780
13. Ansari A.A., Alam M., Parchur A.K. *Appl. Phys. A*, 116, 1719 (2014). https://doi.org/10.1007/s00339-014-8308-4
14. Meshkova S.B., Topilova Z.M., Dotsenko V.P., Kovalevskaya I.P., Kiriyak A.V. *Functional Materials*, 11, 290 (2004). http://functmaterials.org.ua/contents/11-2/FM112-33.pdf
15. Schmidt M., Heck S., Bosbach D., Ganschow S., Waltherd C., Stumpf T. *Dalton Trans.,* 42, 8387 (2013). https://doi.org/10.1039/C3DT50146A
16. Chang L.L.Y. *J. Inorg. Nucl. Chem.,* 31, 2003 (1969). https://doi.org/10.1016/0022-1902(69)90014-1
17. Cho Y.-S., Huh Y.-D. *Bull. Korean Chem. Soc.,* 32, 1353 (2011). https://doi.org/10.5012/bkcs.2011.32.4.1353
18. Dudnikova V.B., Antonov D.I., Zharikov E.V., Eremin N.N. *Phys. Solid State*+, 64, 1713 (2022). https://doi.org/10.21883/PSS.2022.11.54195.413
19. Li X., Hu Y.-H., Wang Y.-H., Fu Ch.-J., Wu H.-Y., Kang F.-W., Ju G.-F., Mou Zh.-F. *Journal of Guangdong University of Technology,* 27, 32 (2010). https://caod.oriprobe.com//articles/26031729/On_the_Synthesis_of_NaxSr1_2xMoO4_Eu3_x_and_Their_Luminescent_Properti.htm
20. Boatner L.A. *Rev. Mineral. Geochem.,* 48, 87 (2002). https://doi.org/10.2138/rmg.2002.48.4
21. Shannon R.D. *Acta Cryst.* A32, 751 (1976). https://doi.org/10.1107/S0567739476001551
22. Belov A.A., Shichalin O.O., Papynov E.K., Buravlev I.Y., Portnyagin A.S., Azon S.A., Fedorets A.N., Vornovskikh A.A., Kolodeznikov E.S., Gridasova E.A., Pogodaev A., Kondrikov N.B., Shi Y., Tananaev I.G. *Materials,* 16, 5838 (2023). https://doi.org/10.3390/ma16175838
23. Urusov V.S. *Teoriia izomorfnoi smesimosti* [Theory of isomorphous miscibility], Nauka, Moskva. 1977. 251 p. (In Russian)
24. Spassky D., Vasil'ev A., Nagirnyi V., Kudryavtseva I., Deyneko D., Nikiforov I., Kondratyev I., Zadneprovski B. *Materials*, 15, 6844 (2022). https://doi.org/10.3390/ma15196844
25. Voznyak-Levushkina V.S., Arapova A.A., Spassky D.A., Nikiforov I.V., Zadneprovski B.I. *Phys. Solid State,* 64, 567 (2022). https://doi.org/10.1134/S1063783422110130
26. Get'man E.I., Radio S.V., Ardanova L.I. *Inorg. Mater.,* 54, 596 (2018). https://doi.org/10.1134/S0020168518060031
27. Templeton D.H. *J. Chem. Phys.,* 21, 2097 (1953). https://doi.org/10.1063/1.1698788
28. Li K., Xue D. *J. Phys. Chem. A,* 110, 11332 (2006). https://doi.org/10.1021/jp062886k
29. Batsanov S.S. *Russ. Chem. Rev.,* 37, 332 (1968). https://doi.org/10.1070/RC1968v037n05ABEH001639
30. Yevdokimov A.A., Yefremov V.A., Trunov V.K., Kleynman I.A., Dzhurinskiy B.F. *Soyedineniya redkozemel'nykh elementov. Molibdaty, vol'framaty* [Compounds of rare earth elements. Molybdates, tungstates]. Moskva: Nauka, 1991, 267 p. (in Russian)
31. Batsanov S.S. *Strukturnaya khimiya. Fakty i zavisimosti* [Structural chemistry. Facts and

dependencies]. Moskva: Dialog-MGU, 2000. (in Russian)
32. Becker R. *Z. Metallkunde,* 29, 245 (1937). (in German)
33. Gürmen E., Daniels E., King J.S. *J. Chem. Phys.,* 55, 1093 (1971). https://doi.org/10.1063/1.1676191
34. Get'man E.I., Mariichak O.Y., Ardanova L.I., Radio S.V. *In:* Fesenko O., Yatsenko L. (eds) Nanomaterials and Nanocomposites, Nanostructures, and Their Applications. NANO 2023. *Springer Proceedings in Physics,* 253, 453 (2024). Vol. 253. P. 453–468. https://doi.org/10.1007/978-3-031-67519-5_31
35. Tokarev M.G., Potanina E.A., Orlova A.I., Khainakov S.A., Boldin M.S., Lantsev E.A., Sakharov N.V., Murashov A.A., Garcia-Granda S., Nokhrin A.V., Chuvil'deev V.N. *Inorg Mater.,* 55, 730 (2019). https://doi.org/10.1134/S0020168519070203