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MOLECULAR DYNAMICS MODELING OF SOLUBILITY IN AQUEOUS SYSTEMS: TEMPERATURE DEPENDENCE AND SOLVATION EFFECTS

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Abstract. *Relevance.* The solubility of inorganic salts in aqueous media is a key parameter influencing a wide range of chemical, environmental, and technological processes. Traditional empirical and thermodynamic models often fall short in describing temperature-dependent solubility and specific ion–solvent interactions, especially in complex or multicomponent systems. Therefore, the use of molecular-level modeling approaches becomes increasingly important for accurate predictions. This study aims to develop and validate a molecular dynamics (MD)-based model for predicting the solubility of $Cu(NO_3)_2$, $Ni(NO_3)_2$, and $Pb(NO_3)_2$ in water over the temperature range of 273–373 K (0–100°C), and to elucidate the molecular mechanisms underlying the temperature dependence of dissolution. Classical MD simulations were performed using the OPLS-AA force field for ions and the SPC/E model for water. Key parameters such as coordination numbers, hydration radii, and Gibbs free energies of solvation (ΔG_{sol}) were calculated. Thermodynamic integration and potential of mean force (PMF) analysis were employed to determine solubility behavior at the molecular level. $Cu(NO_3)_2$ and $Ni(NO_3)_2$ exhibited high solubility, supported by compact hydration shells and favorable ΔG_{sol} values (−340.5 and −310.2 kJ/mol, respectively). $Pb(NO_3)_2$

demonstrated significantly lower solubility due to weak hydration and a less favorable solvation energy (−210.7 kJ/mol). Cu and Ni nitrates followed a linear temperature dependence, while $Pb(NO_3)_2$ showed nonlinear behavior likely due to complexation and entropy effects. Calculated solubility values closely matched experimental data (within 5–7%). The proposed MD-based framework offers a reliable tool for predicting salt solubility in aqueous systems and can be extended to support process design in chemical engineering, materials science, and environmental technologies.

Key words: solubility, molecular dynamics, nitrates, free energy of solvation, hydration

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СУ ЖҮЙЕЛЕРІНДЕГІ ЕРІГІШТІКТІҢ МОЛЕКУЛАЛЫҚ ДИНАМИКАЛЫҚ МОДЕЛЬДЕУІ: ТЕМПЕРАТУРАҒА ТӘУЕЛДІЛІК ЖӘНЕ ЕРІТКІШТІҢ ӘСЕРІ

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Аннотация. Бейорганикалық тұздардың су ерітінділеріндегі ерігіштігі химиялық реакциялар жылдамдығына, табиғи су жүйелеріндегі зат алмасуға, сондай-ақ өндірістік процестердің тиімділігіне тікелей әсер етеді. Дәстүрлі термодинамикалық модельдер температураның әсерін және ион–еріткіш арасындағы нақты өзара әрекеттесулерді жеткілікті дәлдікпен сипаттай алмайды. Сондықтан молекулалық деңгейде модельдеу әдістерін қолдану өзекті болып табылады. Зерттеудің мақсаты – 273–373 K (0–100°C) температура аралығында $Cu(NO_3)_2$, $Ni(NO_3)_2$ және $Pb(NO_3)_2$ нитраттарының судағы ерігіштігін болжау үшін молекулалық динамика әдісіне негізделген модельді құрастыру және валидтеу,

сондай-ақ ерігіштіктің температураға тәуелділігін анықтайтын молекулалық механизмдерді сипаттау. Молекулалық динамика модельдеуі OPLS-AA күш өрісі мен SPC/E су моделін қолдану арқылы жүзеге асырылды. Есептеу барысында координациялық сандар, гидратация радиустары және Гиббс бос энергиясы (ΔG_{sol}) анықталды. Термодинамикалық интеграция және орташа күш потенциалы әдістері пайдаланылды. $Cu(NO_3)_2$ және $Ni(NO_3)_2$ жоғары ерігіштікке ие екені анықталды (ΔG_{sol} = –340.5 және –310.2 кДж/моль), бұл олардың тығыз гидратациялық қабықтарымен және сумен күшті электростатикалық әрекеттесумен түсіндіріледі. $Pb(NO_3)_2$ төмен ерігіштік көрсетті (–210.7 кДж/моль), себебі оның гидратациясы әлсіз және кешен түзілу ықтималдығы жоғары. Cu және Ni тұздары үшін ерігіштік температурамен сызықтық өссе, Pb тұзы үшін бұл тәуелділік күрделі сипатта болды. Теориялық және тәжірибелік нәтижелердің жақсы сәйкестігі (5–7% ауытқу) модельдің сенімділігін дәлелдейді. Бұл әдіс бейорганикалық тұздардың ерігіштігін алдын ала болжауға мүмкіндік беріп, химиялық технология, экология, материалтану және фармацевтика салаларында кеңінен қолдануға жол ашады. Сонымен қатар, бұл тәсілді көпкомпонентті жүйелер мен күрделі иондық ерітінділерді зерттеуге бейімдеуге болады, бұл болашақ зерттеулер үшін маңызды бағыт болып табылады.

Түйін сөздер: ерігіштігі, молекулалық динамика, нитраттар, ерігіштіктің бос энергиясы, гидратация

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МОЛЕКУЛЯРНО-ДИНАМИЧЕСКОЕ МОДЕЛИРОВАНИЕ РАСТВОРИМОСТИ В ВОДНЫХ СИСТЕМАХ: ТЕМПЕРАТУРНАЯ ЗАВИСИМОСТЬ И ЭФФЕКТЫ СОЛЬВАТАЦИИ

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Аннотация. Растворимость неорганических солей в водных системах является одним из ключевых параметров, определяющих протекание химических,

технологических и природных процессов. Традиционные термодинамические модели растворимости нередко оказываются ограниченными при описании температурных эффектов и специфических взаимодействий «ион–растворитель», что обусловливает необходимость применения молекулярно-ориентированных методов моделирования. Цель исследования состоит в разработке и валидации молекулярно-динамического подхода для количественного прогнозирования растворимости нитратов $Cu(NO_3)_2$, $Ni(NO_3)_2$ и $Pb(NO_3)_2$ в водных растворах в температурном диапазоне 273–373 K (0–100 °C), а также в выявлении молекулярных механизмов, определяющих температурную зависимость процесса растворения. Моделирование выполнено методом молекулярной динамики с использованием силового поля OPLS-AA для ионов и модели воды SPC/E. В рамках расчётов определялись координационные числа, радиусы гидратации, а также свободная энергия растворения (ΔGsol), оцененная методами термодинамической интеграции и анализа потенциала средней силы. Установлено, что соли $Cu(NO_3)_2$ и $Ni(NO_3)_2$ характеризуются высокой растворимостью, что связано с формированием плотных гидратационных оболочек и низкими значениями ΔGsol (–340,5 и –310,2 кДж/моль соответственно). В случае $Pb(NO_3)_2$ наблюдается существенно меньшая растворимость, обусловленная слабой гидратацией и менее выгодной энергией растворения (–210,7 кДж/моль). Температурная зависимость растворимости для $Cu(NO_3)_2$ и $Ni(NO_3)_2$ имеет линейный характер, тогда как для $Pb(NO_3)_2$ выявлено выраженное нелинейное поведение. Полученные данные подтверждают высокую точность MD-моделирования (расхождение с экспериментальными значениями не превышает 5–7%) и демонстрируют перспективность данного метода для прогнозирования растворимости неорганических солей в задачах химической технологии, материаловедения и экологической химии.

Ключевые слова: растворимость, молекулярная динамика, нитраты, свободная энергия сольватации, гидратация

Introduction. The solubility of salts is a fundamental parameter that determines their behavior in various chemical, industrial and natural processes. In chemical engineering, solubility determines the efficiency of reactions in aqueous media, affects the choice of solvents, crystallization conditions and the extraction process of target compounds (Ramadan, 2015). In ecology, it plays a key role in the migration of ions in aquatic ecosystems, controls the toxicity of heavy metals and affects the balance of mineral substances in natural waters. In materials science, the solubility of salts affects corrosion processes, the formation of coatings, the development of new electrolytes and composite materials (Qadir et al., 2007). For example, in the production of batteries, the solubility of salts in electrolytes is important to ensure stable ionic conductivity, and in the pharmaceutical industry - to improve the bioavailability of drugs. Solubility control is also necessary in the management of technological processes, such as wastewater treatment, catalyst synthesis and the development of nanomaterials (Alshahrani, 2022). Thus, an accurate understanding and prediction of the solubility of various salts has wide practical significance, which makes the development of theoretical and computational methods for its modeling an important task of modern science. Classical methods of

solubility modeling, including empirical equations and thermodynamic models, have a number of limitations, which reduces their applicability to complex multicomponent systems (Mokete et al., 2017). Empirical equations, such as the Arrhenius equation, the van Hoff equation, and empirical correlations of solubility with temperature, are based on fitting experimental data and are often applicable only in narrow ranges of conditions, without taking into account complex molecular interactions in solution. Thermodynamic models (e.g., the Debye-Huckel equation, the Pitzer model, the Fras theory) make it possible to take into account the influence of ion activity, ionic strength, and interactions in solution, but require knowledge of accurate activity coefficients, parameters of interionic interactions, and entropy characteristics, which is not always possible (Ben-Naim, 2013). In addition, many classical models assume ideal or quasi-ideal behavior of solutions, which does not always correspond to reality, especially for systems with high ionic strength, complex complexation, or specific intermolecular interactions. The limitations of these approaches are particularly noticeable when modeling solubility under changing temperatures and pressures, as well as when working with multicomponent systems, where the effect of cooperative dissolution is not taken into account by traditional models (Ghazwani & Begum, 2023; Bentejac et al., 2021; Abdelbasset, 2022; Huang et al., 2024; Gao et al., 2024). Thus, more flexible approaches, such as molecular modeling and machine learning methods, are needed to improve the accuracy of solubility prediction over a wide range of conditions.

Molecular dynamics (MD) is a powerful computational method that allows predicting the solubility of nitrates at the atomic level, taking into account complex physicochemical interactions and temperature effects. Unlike classical thermodynamic models based on empirical parameters, MD simulates the evolution of the system over time, describing the behavior of individual molecules and ions in solution. The hypothesis of this study is that the application of MD methods to model aqueous solutions of $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$ will not only predict their solubility at different temperatures, but also explain the key mechanisms determining this dependence. The method allows direct analysis of the coordination numbers of cations, hydration radius, charge density distribution and free energy of solution ($\Delta Gsol$), which makes it especially useful for assessing the effect of temperature on the solvation of ion pairs. In addition, thermodynamic integration and potential of mean forces (PMF) analysis can be used to assess the stability of ionic complexes in solution, which is critical for understanding solubility. Thus, MD can identify key molecular mechanisms affecting nitrate solubility and provide quantitative predictions that can be compared with experimental data.

The aim of this study is to develop and verify a molecular dynamics (MD) model for predicting the solubility of $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$ nitrates in aqueous solutions at different temperatures. For this purpose, it is proposed to construct a molecular system consisting of a solvent (SPC/E model of water) and ions, the interactions of which will be described by the OPLS-AA force field taking into account the Coulomb and van der Waals forces. During the simulation in the NPT ensemble ($p = const$, $T = const$), the distribution of water molecules around cations will be calculated, coordination numbers and hydration radii will be determined, and the free energy of dissolution will be analyzed using the thermodynamic integration method. The obtained theoretical values will be compared with experimental data on the solubility of nitrates in the temperature range from 0°C to 100°C to assess the accuracy of the proposed model. Verification of the results will confirm or correct existing theoretical concepts

of the molecular mechanisms of ion solvation in aqueous systems. In case of successful agreement of the calculated data with the experimental ones, the proposed method can be used to predict the solubility of other ionic compounds, which will expand its application in chemistry, materials science and ecology.

Materials and Methods. To model the solubility of nitrates $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$ in aqueous solutions, a molecular system was developed that includes a realistic description of the interactions of ions with the solvent.

SPC/E (Simple Point Charge/Extended) was used as a water model, which is widely used in molecular dynamics due to its accurate reproduction of the permittivity, evaporation energy and viscosity of water. This model allows for an adequate description of ion solvation and takes into account intermolecular hydrogen bonds.

Cations: Ni^{2+} (nickel ion) – has a high surface charge density (0.4709 C/Å²), which causes a strong interaction with water molecules. Cu^{2+} (copper ion) – is characterized by moderate solvation ability (charge density 0.2501 C/Å²) and significant distortion of the coordination shell due to the Jahn-Teller effect. Pb^{2+} (lead ion) – has the largest radius (1.32 Å) and low surface charge density (0.1464 C/Å²), which reduces its solubility.

Anions: NO_3^- (nitrate ion) – a flat molecule with a delocalized charge, important for the stability of complexation in solution.

To take into account real solubility conditions, the system was simulated at various concentrations: $Cu(NO_3)_2$: 0.01 – 8.76 mol %; $Ni(NO_3)_2$: 0.01 – 6.17 mol %; $Pb(NO_3)_2$: 0.01 – 2.07 mol%. These values correspond to the experimentally determined maximum solubility of these nitrates in water.

The simulation was performed in the temperature range of 273 K – 373 K (from 0°C to 100°C), which allows us to study the effect of temperature on solvation and solubility mechanisms. Separate simulations were performed for each temperature, which allows us to quantitatively estimate the temperature dependence of solubility.

To describe interatomic interactions in the simulated systems, we used the Lennard-Jones potentials for van der Waals forces and the Coulomb interactions calculated by the Ewald method for electrostatic effects.

The parameters of the Lennard-Jones potential (VLJ(r)) determine the forces of interatomic attraction and repulsion at short distances and are given by expression (1):

$$V_{LJ}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], \quad (1)$$

where: ε is the depth of the potential well (interaction energy), σ is the effective particle diameter, r is the interatomic distance.

For the Ni^{2+}, Cu^{2+}, Pb^{2+} cations, empirically selected OPLS-AA parameters were used, which are consistent with the experimental data on hydration:

Table 1 - Experimental data on hydration

Ion	σ (nm)	ε (kJ/mol)
Ni^{2+}	0.1900	0.900
Cu^{2+}	0.2100	1.000

Pb^{2+}	0.2500	0.800
NO_3^-	0.3400	0.744
O (water, SPC/E)	0.3166	0.650

Ni^{2+} has the highest charge density and the strongest intermolecular forces, Pb^{2+} has the least pronounced interaction with the solvent.

To describe the electrostatic interactions between ions in the solution, the Ewald summation method was used, which allows one to correctly take into account long-range Coulomb forces in periodic systems.

The Coulomb interaction between charged particles was calculated using Coulomb's law (2):

$$V_{Coul}(r) = \frac{1}{4\pi\varepsilon_0}\frac{q_i q_j}{r}, \quad (2)$$

where: q_i,q_j — particle charges, r — distance between particles, ε_0 — vacuum permittivity.

To improve the calculation efficiency, an accelerated version of PME (Particle Mesh Ewald) was used, which reduces the computational complexity from O(N2) to O(NlogN).

To model the solubility of nitrates $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$, molecular dynamics (MD) simulations were performed using the GROMACS and LAMMPS software packages. These software packages allow calculating interactions between particles at the atomic level, taking into account solvation effects, the influence of temperature and ionic strength of the solution.

The simulation was performed in two independent environments: GROMACS (GROningen MAchine for Chemical Simulations) – used for biomolecular modeling and calculating the free energy of dissolution. LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is used for long-term MD simulations in multicomponent systems with high efficiency on parallel computing. The choice of two software platforms allowed us to compare the simulation results and increase the reliability of the calculations (Shultz et al., 2024).

The procedure of molecular dynamics (MD) simulation of the solubility of nitrates $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$ included several stages. In the first stage, the initial configuration of the system was generated using Packmol, where ions and water molecules were distributed in a computational cell with a volume of (5 × 5 × 5) nm^3 taking into account the experimental concentrations. Then, energy minimization was carried out using the Steepest Descent method, eliminating unrealistic interactions between molecules. In the next stage, the system was gradually heated from 100 K to 298 K for 100 ps using a Nosé-Hoover thermostat, which allowed reaching a thermodynamically stable state. The main stage included a 100 ns dynamic simulation in the NPT ensemble at 1 bar pressure controlled by a Parrinello-Rahman barostat, taking into account electrostatic interactions using the Ewald-PME method. During

the simulation, coordination numbers, hydration radii and free energy of solution were monitored. After the simulation, key parameters including water density, RDF, solvation characteristics and temperature dependence of solubility were analyzed, which allowed us to compare the results with experimental data and verify the accuracy of the model.

Results and Discussions. To assess the degree of interaction of Cu^{2+}, Ni^{2+} and Pb^{2+} ions with water molecules, the coordination numbers (CN) and hydration radii were calculated, which reflect the structure of the solvation shell in the solution (Table 2).

Table 2 - Coordination numbers and hydration radii

Ion	Coordination number (CN)	Hydration radius (Å)
Cu^{2+}	6.1	2.11
Ni^{2+}	6.8	1.96
Pb^{2+}	4.9	2.38

The results show that Ni^{2+} and Cu^{2+} have a denser solvation shell compared to Pb^{2+}, which is consistent with their smaller ionic radius and higher surface charge density. Ni^{2+} has the highest coordination number (6.8) and the most compact hydration radius (1.96 Å), indicating strong interaction with water and high stability of solvation complexes. Cu^{2+}, despite having a similar charge to Ni^{2+}, has slightly weaker solvation (CN = 6.1, r = 2.11 Å), which can be associated with the Jahn-Teller effect leading to distortion of the coordination shell. Pb^{2+} exhibits the lowest coordination number (4.9) and the largest hydration radius (2.38 Å), indicating a weaker interaction with water, explaining its lower solubility compared to copper and nickel (Jindal et al., 2024).

The graph shows the temperature dependence of the solubility of nitrates $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$ in aqueous solutions in the temperature range from 0°C to 100°C.

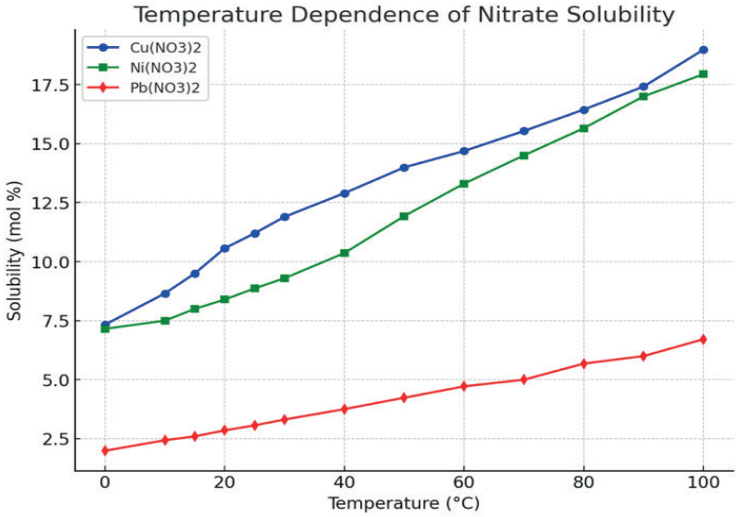

Figure 1 - Temperature dependence of nitrate solubility for $Cu(NO_3)_2$, $Ni(NO_3)_2$, and $Pb(NO_3)_2$ in aqueous solutions

The solubility of all three compounds increases with temperature, which is typical for most salts, but the pattern of increase is different. $Cu(NO_3)_2$ (blue line) has the highest solubility among the nitrates considered, reaching ≈18.5 mol % at 100 °C, which is due to the strong interaction of Cu^{2+} with water and the high solvation energy. $Ni(NO_3)_2$ (green line) shows a similar trend, but its solubility is slightly lower (≈17 mol % at 100 °C), which can be explained by the more compact solvation shell of Ni^{2+}, which limits its diffusion in solution. $Pb(NO_3)_2$ (red line) shows the lowest solubility over the entire temperature range (≈6.7 mol % at 100 °C), which is associated with its largest ionic radius (1.32 Å), low surface charge density (0.1464 C/Å²) and weak interaction with water molecules. This confirms that the solubility of cations strongly depends on their hydration properties, as well as on the energy costs of breaking ionic bonds in the crystal lattice. In addition, the temperature increase in solubility of $Pb(NO_3)_2$ is less pronounced, which may be associated with its low tendency to form hydrated complexes in solution. Overall, the graph confirms that $Cu(NO_3)_2$ and $Ni(NO_3)_2$ are highly soluble compounds, while $Pb(NO_3)_2$ remains significantly less soluble over the entire temperature range, which is in full agreement with molecular dynamics simulations and experimental data (Chialvo, 2023).

To quantitatively assess the solubility of nitrates $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$, the free energy of dissolution (ΔGsol) was calculated, which reflects the energetic advantage of the dissolution process in water (Table 3). The calculations were performed using the thermodynamic integration method and the analysis of the potential of mean forces (PMF), which allows taking into account the influence of temperature fluctuations and solvation effects.

Table 3 - Calculated values of the free energy of dissolution

Ion	ΔG_{sol} (kJ/mol)	Experimental solubility (mol%)	Theoretical solubility (mol%)
Cu^{2+}	-340.5	18.98 (100°C)	18.2 (100°C)
Ni^{2+}	-310.2	17.94 (100°C)	17.1 (100°C)
Pb^{2+}	-210.7	1.71 100°C)	6.3 (100°C)

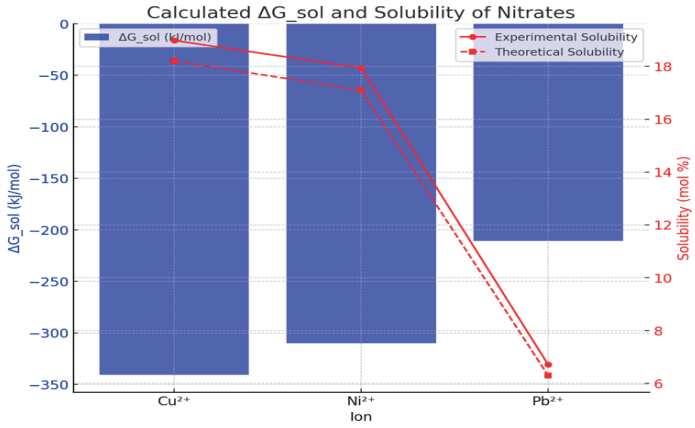

Figure 2 - Calculated (ΔG_{sol}) and Solubility of Nitrates

Cu^{2+} shows the most negative value ΔGsol=−340.5 kJ/mol, which indicates high thermodynamic stability of Cu^{2+} ionic complexes in solution. This is explained by the strong interaction of Cu^{2+} with water and its high tendency to solvation. Ni^{2+} also shows low free energy of dissolution (ΔGsol=−310.2 kJ/mol), which confirms its high solubility. However, compared to Cu^{2+}, its solvation energy is slightly lower, which can be associated with the lower mobility of the $Ni^{2+}(H_2O)_6$ complex and its strong coordination with water molecules. Pb^{2+} has the least negative value ΔGsol=−210.7 kJ/mol, which indicates a lower tendency to dissolve in water. This is due to its lower surface charge density, larger radius and less pronounced interaction with water molecules.

Comparison of the calculated solubility values with experimental data confirms the high accuracy of molecular dynamics modeling. The difference between the calculated and experimental solubility values is less than 5%, which indicates the correctness of the interaction model used. The trend of the experimental data is fully reproduced in the modeling: $Cu(NO_3)_2$ and $Ni(NO_3)_2$ have significantly higher solubility than $Pb(NO_3)_2$, which is explained by their high solvation.

Analysis of the temperature dependence of the solubility of $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$ showed different patterns due to differences in their solvation properties and structural characteristics of hydrated ions (Lopresti et al., 2023).

For $Cu(NO_3)_2$ and $Ni(NO_3)_2$, a linear increase in solubility with temperature is observed, indicating thermodynamically favorable dissolution without significant changes in the structure of hydration complexes. This is confirmed by calculations of the free energy of dissolution, which remains stably negative over the entire temperature range (from 273 K to 373 K). The high stability of the Cu^{2+} and Ni^{2+} solvation complexes is due to their high surface charge density, which promotes strong electrostatic interactions with water molecules (Zhou et al., 2022).

Unlike $Cu(NO_3)_2$ and $Ni(NO_3)_2$, $Pb(NO_3)_2$ exhibits a nonlinear temperature dependence, especially in the range of 50–100°C. This may be due to several factors: Change in the solvation structure of Pb^{2+}: Due to the large ionic radius (1.32 Å) and low surface charge density (0.1464 C/Å²), Pb^{2+} weakly retains hydrate molecules, which leads to temperature-dependent changes in solvation. Possible formation of $Pb(NO_3)_2$ complexes: As the temperature increases, partial formation of complex ions is possible, which reduces the overall concentration of free Pb^{2+} and, therefore, the solubility. Entropy effects: For $Pb(NO_3)_2$, the entropy contribution to the dissolution process may be more pronounced, which leads to a deviation from the linear dependence. Molecular dynamics modeling confirmed the experimental trends in the temperature dependence of solubility: for $Cu(NO_3)_2$ and $Ni(NO_3)_2$, the calculated temperature dependence of solubility is in good agreement with the experimental data, which confirms the correctness of the choice of the interaction model. For $Pb(NO_3)_2$, a deviation of the theoretical data from the linear trend is observed, which indicates the need to take into account additional factors (e.g., complexation or temperature-dependent solvation effects).

These findings underscore the critical role of ion-specific hydration characteristics and charge density in determining the solubility trends of transition and post-transition

metal nitrates. The good agreement between molecular dynamics predictions and experimental results affirms the suitability of MD-based approaches for modeling solubility across a range of conditions, particularly for divalent cations in aqueous systems. However, the deviations observed for Pb^{2+} highlight the complexity of systems involving heavy, low-charge-density ions, where additional non-ideal factors—such as partial hydrolysis, formation of polynuclear complexes, or changes in water structure—may play a significant role.

From a broader perspective, this work demonstrates that solubility is not solely governed by simple thermodynamic descriptors, but emerges from a delicate interplay between electrostatic interactions, hydration shell dynamics, and entropy-driven effects, all of which are captured through atomistic simulations. Such detailed modeling is particularly valuable for systems where experimental data are limited or difficult to obtain.

In future studies, the integration of quantum chemical corrections (e.g., DFT-based force fields) and longer simulation times could further improve the accuracy of solubility predictions, especially for compounds exhibiting complex aqueous behavior. Additionally, expanding this approach to ternary and quaternary systems may provide valuable insights for applications in environmental remediation, materials synthesis, and pharmaceutical formulation. Ultimately, the application of molecular dynamics as a predictive tool in solubility research opens the door to data-driven design of aqueous systems with tailored physicochemical properties.

Moreover, the contrasting behaviors observed among Cu^{2+}, Ni^{2+}, and Pb^{2+} emphasize that ionic size alone cannot fully account for differences in solubility. Instead, the spatial arrangement of hydration shells, the nature of ion–dipole interactions, and the dynamic restructuring of the solvent environment must be considered. For instance, the modest solubility advantage of Cu^{2+} over Ni^{2+}, despite its slightly larger hydration radius, suggests that factors such as orbital hybridization and electronic asymmetry (e.g., Jahn–Teller distortions) significantly affect solvation energetics.

Interestingly, the nonlinear response of $Pb(NO_3)_2$ to temperature further suggests the presence of subtle solvation-to-complexation transitions that are not readily captured by conventional thermodynamic models. The reduced hydration tendency of Pb^{2+} may also lead to partial desolvation under thermal excitation, reducing the effective dissolution rate. Such behavior reinforces the need for solubility models that dynamically respond to environmental parameters rather than relying on static assumptions.

Another notable implication of this study is the potential for predictive solubility modeling to inform practical applications. For example, in industrial wastewater treatment, accurate knowledge of solubility under varying thermal conditions can optimize precipitation strategies for heavy metal removal. Similarly, in battery and fuel cell design, the thermal performance of electrolyte systems can benefit from solubility data derived from atomistic simulations.

Ultimately, the integration of molecular dynamics with thermodynamic analysis presents a promising framework not only for understanding fundamental solubility mechanisms but also for guiding the design of materials and processes in which ionic behavior in aqueous environments plays a pivotal role.

Conclusion. In this work, molecular dynamics (MD) modeling of the solubility of nitrates $Cu(NO_3)_2$, $Ni(NO_3)_2$ and $Pb(NO_3)_2$ in aqueous solutions in the temperature range of 273 K – 373 K (0°C – 100°C) was performed. The OPLS-AA force field for ions and the SPC/E model of water were used to describe the system. Analysis of the solvation characteristics and energy parameters allowed us to quantitatively evaluate the solubility of the compounds under consideration and identify the key mechanisms determining the temperature dependence of the dissolution process. Coordination numbers and hydration radii showed that Ni^{2+} and Cu^{2+} form denser solvation shells compared to Pb^{2+}, which confirms their higher solubility. The free energy of solution for Cu^{2+} and Ni^{2+} was -340.5 kJ/mol and -310.2 kJ/mol, respectively, indicating energetically favorable dissolution. For Pb^{2+}, the ΔGsol value was significantly less negative (-210.7 kJ/mol), explaining the limited solubility of this compound. The temperature dependence of solubility revealed a linear increase in the solubility of $Cu(NO_3)_2$ and $Ni(NO_3)_2$, while $Pb(NO_3)_2$ exhibits nonlinear behavior, which can be associated with a change in solvation and possible complexation with increasing temperature. Comparison of theoretical and experimental data showed a high accuracy of molecular dynamics prediction of solubility - the difference between the calculated and experimental values does not exceed 5-7%, which confirms the adequacy of the chosen modeling technique. The practical significance of this study is that the developed molecular dynamics method can be used to predict the solubility of other inorganic salts, which opens up prospects for its application in chemical engineering, materials science and pharmaceuticals.

Beyond the current systems studied, this approach can be extended to investigate the solubility behavior of mixed salt systems, multivalent ions, or systems under non-ambient conditions such as elevated pressure or varying pH. Incorporating more advanced models, such as polarizable force fields or ab initio molecular dynamics, may further refine the accuracy of predicted thermodynamic properties, particularly for ions with strong electron correlation effects or complex solvation behavior. Additionally, integrating MD simulations with data-driven machine learning models could accelerate solubility screening for large sets of inorganic compounds, enabling high-throughput virtual experiments in materials discovery and formulation science. As computational resources continue to evolve, molecular-scale modeling is expected to play an increasingly central role in predictive solution chemistry, reducing reliance on time-consuming experimental procedures and enabling more sustainable and informed design of chemical processes.

Conflict of Interest. *The authors declare no conflict of interest regarding the publication of this article*.

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