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GAS TRANSPORT AND STRUCTURAL EFFECTS IN [EMIM][SCN] AND [EMIM][DCA] IONIC LIQUIDS: A MOLECULAR DYNAMICS STUDY

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Annotatsiya. 1-etil-3-metilimidazoliy sianid ([EMIM][SCN]) va 1-etil-3-metilimidazoliy disianid ([EMIM][DCA]) ion suyuqliklarida karbonat angidrid (CO_2), vodorod sulfidi (H_2S) va metan (CH_4) gazlarining strukturaviy va transport xossalari 298 K va 373 K haroratlarda atomistik molekulyar dinamika modellashtirish yordamida o‘rganildi. Asosiy e’tibor gazlarning o‘z-o‘zidan diffuziya koeffitsientlariga hamda gazlarning erishi natijasida ion suyuqlik mikrostrukturasi qanday o‘zgarishiga qaratildi; bu esa kation–kation radial taqsimot funksiyalari (RTF) orqali tavsiflandi. Natijalar shuni ko‘rsatadiki, gazlarning erishi ion suyuqlik strukturasiga sezilarli ta’sir ko‘rsatmaydi, biroq H_2S CO_2 va CH_4 ga nisbatan biroz kuchliroq lokal tartiblanishni yuzaga keltiradi. Gazlarning harakatchanligi $D(CH_4) > D(CO_2) > D(H_2S)$ tartibida bo‘lib, bu gaz-anion o‘zaro ta’sir kuchi bilan izohlanadi. Barcha sharoitlarda [EMIM][DCA] [EMIM][SCN] ga nisbatan yuqori diffuziya koeffitsientlarini ko‘rsatadi, bu uning pastroq yopishqoqligi bilan bog‘liq. Haroratning oshishi diffuziyani sezilarli darajada kuchaytiradi, bu esa yopishqoqlikning kamayishi hamda o‘zaro ta’sirlarning zaiflashuvi bilan izohlanadi. Olingan natijalar sianofunksional ion suyuqliklarda anion tuzilishi, gaz–anion o‘zaro ta’sirlari va transport xossalari o‘rtasidagi bog‘liqlikni molekulyar darajada tushuntirib beradi hamda tabiiy gazni tozalash jarayonlari uchun samarali absorbentlarni tanlashda muhim ahamiyatga ega.

Kalit so‘zlar: Ion suyuqliklar; molekulyar dinamika; radial taqsimot funksiyasi; o‘z-o‘zidan diffuziya; o‘rtacha kvadrat siljish; gaz transporti; [EMIM][SCN]; [EMIM][DCA]; CO_2; H_2S; CH_4.

Аннотация. Структурные и транспортные свойства диоксида углерода (CO_2), сероводорода (H_2S) и метана (CH_4) в ионных жидкостях 1-этил-3-метилимидазолий тиоцианат ([EMIM][SCN]) и 1-этил-3-метилимидазолий дицианамид ([EMIM][DCA]) были исследованы с использованием атомистического молекулярно-динамического моделирования при

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температурах 298 K и 373 K. Особое внимание уделено коэффициентам самодиффузии газов и влиянию растворения газов на микроструктуру ионных жидкостей, характеризуемую радиальными функциями распределения (RDF) катион–катион. Результаты показывают, что растворение газов приводит лишь к незначительным изменениям структуры ионной жидкости, при этом H_2S вызывает несколько более выраженное локальное упорядочение по сравнению с CO_2 и CH_4. Подвижность газов подчиняется закономерности $D(CH_4) > D(CO_2) > D(H_2S)$, что отражает различия в силе взаимодействия газ–анион. Во всех условиях [EMIM][DCA] демонстрирует более высокие коэффициенты диффузии по сравнению с [EMIM][SCN], что связано с его более низкой вязкостью. Повышение температуры существенно увеличивает диффузию, что обусловлено как снижением вязкости, так и ослаблением специфических межмолекулярных взаимодействий. Полученные результаты дают молекулярно-уровневое представление о взаимосвязи между структурой аниона, взаимодействиями газ–анион и транспортными свойствами в циано-функционализированных ионных жидкостях, что имеет важное значение для разработки эффективных абсорбентов для очистки природного газа.

Ключевые слова: ионные жидкости; молекулярная динамика; радиальная функция распределения; самодиффузия; среднеквадратичное смещение; транспорт газов; [EMIM][SCN]; [EMIM][DCA]; CO_2; H_2S; CH_4

Abstract. Structural and transport properties of carbon dioxide (CO_2), hydrogen sulfide (H_2S), and methane (CH_4) in the ionic liquids 1-ethyl-3-methylimidazolium thiocyanate ([EMIM][SCN]) and 1-ethyl-3-methylimidazolium dicyanamide ([EMIM][DCA]) were investigated using atomistic molecular dynamics simulations at 298 K and 373 K. Particular attention was given to gas self-diffusion coefficients and the influence of gas dissolution on the ionic liquid microstructure, characterized by cation-cation radial distribution functions (RDFs). The results show that gas dissolution induces only minor perturbations in the ionic liquid structure, with H_2S producing slightly stronger local ordering effects compared to CO_2 and CH_4. Gas mobility follows the consistent trend $D(CH_4) > D(CO_2) > D(H_2S)$ in both systems, reflecting differences in gas–anion interaction strength. Across all conditions, [EMIM][DCA] exhibits higher diffusivities than [EMIM][SCN], in line with its lower viscosity. Increasing temperature significantly enhances diffusion, indicating the combined influence of reduced viscosity and weakened specific interactions. These findings provide molecular-level insight into the relationship between anion structure, gas-anion interactions, and transport properties in cyano-functionalized ionic liquids, with direct

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implications for the design of efficient absorbents in natural gas sweetening processes.

Keywords: Ionic liquids; molecular dynamics; radial distribution function; self-diffusion; mean square displacement; gas transport; [EMIM][SCN]; [EMIM][DCA]; CO_2; H_2S; CH_4

1. INTRODUCTION.

The removal of acid gases, principally CO_2 and H_2S, from natural gas streams is critical industrial process that directly affects pipeline integrity, combustion efficiency, and environmental compliance [1, 2]. Conventional aqueous amine-based technologies, although widely implemented, are associated with significant drawbacks, including high regeneration energy requirements, solvent degradation, and corrosion-related issues [3, 4]. These limitations have driven the search for alternative solvent systems with improved physicochemical performance. Room-temperature ionic liquids (RTILs) have attracted considerable attention as tunable, non-volatile solvents for gas capture and separation, combining negligible vapor pressure, wide liquid-phase stability windows, and the structural flexibility afforded by independent cation and anion selection [5-8]. Among these, imidazolium-based ionic liquids containing cyano-functionalized anions, such as thiocyanate ([EMIM][SCN]) and dicyanamide ([EMIM][DCA]), are of particular interest owing to their relatively low viscosities, which are advantageous for mass transfer and process efficiency. [9, 10].

Recent molecular simulation studies have provided valuable insights into the thermodynamics of gas absorption in these systems, including free energy profiles and solvation structures. [11], However, despite their industrial relevance, quantitative information on gas transport properties remains extremely limited. In particular, no self-diffusion data have been reported for CO_2, H_2S, and CH_4 in [EMIM][SCN], and only scarce experimental data exist for [EMIM][DCA]. This lack of transport data represents a significant barrier to the development of predictive models for gas absorption kinetics and process design.

In this work, fully atomistic molecular dynamics simulations are employed to investigate the structural and transport properties of CO_2, H_2S, and CH_4 in [EMIM][SCN] and [EMIM][DCA] at 298 K and 373 K. Gas self-diffusion coefficients are evaluated from mean square displacement analysis, while cation–cation RDFs are used to probe structural perturbations upon gas dissolution. The aim of this study is to establish clear relationships between anion structure, gas–anion interactions, and transport behavior, thereby providing molecular-level insights relevant to the rational design of ionic liquids for natural gas sweetening applications.

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2. COMPUTATIONAL METHODS

2.1. Molecular Models and System Preparation

All MD simulations were carried out using the GROMACS-2021.4 software package with GPU acceleration. The two ionic liquids investigated in this work were [EMIM][SCN] and [EMIM][DCA]. Force field parameters for both ILs were adopted from the literature [12], and the intermolecular parameters for CO_2 [13], H_2S [14] and CH_4 [15] were taken from dedicated parameterization studies. Initial simulation boxes were constructed using the PACKMOL software , with each system containing 500 $[EMIM]^+$ cations paired with 500 $[SCN]^-$ or 500 $[DCA]^-$ anions for the respective ILs. Prior to equilibration, each assembly was subjected to energy minimization via the steepest descent algorithm to remove steric clashes. Subsequently, the systems were equilibrated for 100 ns in the isothermal–isobaric (NPT) ensemble at 298 K and 1 bar. A semi-isotropic Parrinello-Rahman barostat was employed with a compressibility of 4.5×10^{-5} bar^{-1} and a pressure coupling time constant of 1.0 ps, while temperature control was achieved using a Nosé–Hoover thermostat with a coupling constant of 1.0 ps. Van der Waals and short-range electrostatic interactions were truncated at a cutoff distance of 1.3 nm, and long-range electrostatics were treated by the particle mesh Ewald (PME) method using a real-space cutoff of 1.3 nm and a reciprocal-space grid spacing of 0.15 nm.

2.2. MSD and RDF Simulations

For gas-IL production simulations, 24 gas molecules were introduced into each equilibrated IL box, corresponding to a low-concentration regime that avoids artificial clustering while ensuring adequate statistical sampling, followed by energy minimization and a 5 ns NVT equilibration at the target temperature.

Production NVT runs of 100 ns were then performed at each temperature (298 K and 373 K). Self-diffusion coefficients D were extracted from the linear regime of the ensemble-averaged MSD using the Einstein relation, with fitting performed over the final 10 ns where diffusive behavior is well established.

To improve statistical reliability, three independent replicas were simulated for each gas-IL temperature combination, and reported values are arithmetic means with standard deviations.

$EMIM^+$-$EMIM^+$ center-of-mass RDFs were computed over the full 100 ns production trajectory using the GROMACS gmx rdf utility (bin width 0.002 nm) for both pure IL and gas-loaded systems to quantitatively assess gas-induced structural perturbations.

3. RESULTS AND DISCUSSION

3.1. Structural Analysis: Radial Distribution Functions

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The $EMIM^+$–$EMIM^+$ center-of-mass radial distribution functions (RDFs) for pure and gas-loaded [EMIM][SCN] and [EMIM][DCA] at 298 K are shown in Figure 1. In both ionic liquids, the first coordination shell peak appears at r ≈ 0.42 nm with g(r) ≈ 1.47–1.49, followed by a broader second maximum at r ≈ 0.88 nm, consistent with established structural features of imidazolium-based systems. Notably, [EMIM][SCN] exhibits a slightly higher and sharper first peak compared to [EMIM][DCA], indicating more pronounced short-range ordering of the cationic network. This difference arises from the linear geometry of the SCN^- anion, which promotes more directional interactions and tighter packing, whereas the more delocalized and bifurcated structure of DCA^- allows greater orientational flexibility and reduced structural ordering.

Upon gas dissolution, distinct trends emerge depending on the nature of the gas molecule. For CO_2, the RDFs of both ionic liquids remain largely unchanged relative to their pure counterparts, with only minor variations in peak intensity. This indicates that CO_2 primarily occupies interstitial free volume and interacts moderately through quadrupole–charge interactions, stronger than **CH_4** but weaker than H_2S**,** without significantly disrupting the underlying cationic structure.

In contrast, H_2S produces a subtle but reproducible sharpening of the first RDF peak in [EMIM][SCN], while only minor changes are observed in [EMIM][DCA]. This behavior reflects the ability of H_2S to form directional interactions with the SCN^- anion, including hydrogen-bonding interactions, which locally enhance structural ordering and slightly perturb the ionic network. The effect is less pronounced in [EMIM][DCA], where the interaction sites are more symmetrically distributed.

For CH_4, no measurable changes in the RDFs are observed in either ionic liquid, and the profiles remain indistinguishable from those of the pure systems within statistical uncertainty. This is consistent with the nonpolar and spherically symmetric nature of CH_4, which prevents the formation of specific interactions with the ionic liquid components and results in behavior characteristic of an inert species occupying transient free volume cavities.

Overall, the magnitude of structural perturbation follows the order H_2S> CO_2> CH_4, reflecting the hierarchy of gas-anion interaction strengths. This structural trend provides a direct molecular-level basis for understanding the differences in gas mobility discussed in the following section.

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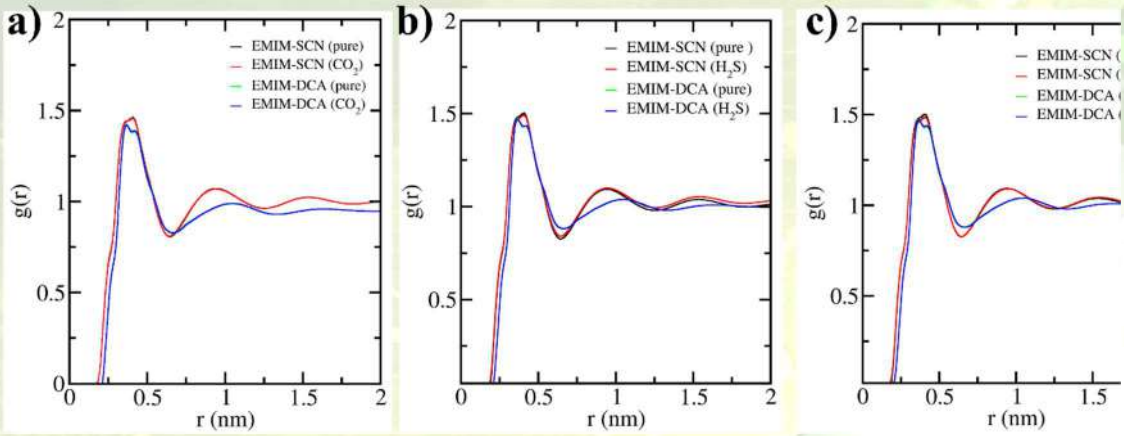


Figure 1. $EMIM^+$–$EMIM^+$ center-of-mass radial distribution functions g(r) for pure and gas-loaded [EMIM][SCN] and [EMIM][DCA] at 298 K: (a) CO_2, (b) H_2S, and (c) CH_4. The IL microstructure remains largely unchanged upon gas dissolution in all cases.

3.2. Self-Diffusion Coefficients

The self-diffusion coefficients of CO_2, H_2S, and CH_4 in [EMIM][SCN] and [EMIM][DCA] at 298 K and 373 K are summarized in Table 1. At 298 K, both ionic liquids exhibit a consistent diffusivity trend of $D(CH_4) > D(CO_2) > D(H_2S)$. This ordering reflects differences in gas–anion interaction strength, where more strongly interacting species experience greater frictional resistance and therefore diffuse more slowly.

Across all systems and temperatures, [EMIM][DCA] exhibits higher diffusivities than [EMIM][SCN]. At 298 K, diffusivity ratios range from approximately 1.2 for H_2S to over 2.4 for CH_4. This behavior is consistent with the lower viscosity of [EMIM][DCA], which facilitates molecular mobility. In addition to viscosity effects, the larger enhancement observed for CH_4 is likely related to differences in free volume characteristics, as CH_4 does not form specific interactions with either anion and is therefore more sensitive to the underlying liquid structure.

For CO_2 in [EMIM][DCA] at 298 K, the computed diffusion coefficient (4.743×10^{-6} cm² s⁻¹) is lower than the available experimental value (~1.156×10^{-5} cm² s⁻¹). This discrepancy is consistent with the known tendency of standard fixed-charge models to overestimate ionic liquid viscosity, which is partially mitigated in the present work through the use of virtual-site corrections. Nevertheless, the agreement remains within the expected range for classical molecular dynamics simulations, supporting the reliability of the observed trends.

Temperature has a pronounced effect on gas mobility in both ionic liquids. Increasing the temperature from 298 K to 373 K leads to a significant enhancement in diffusion coefficients, with increases ranging from approximately 2.7 to 7.1

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times depending on the gas and ionic liquid. These increases exceed the proportional change expected from temperature alone, suggesting that, in addition to viscosity reduction, weakening of specific gas–anion interactions contributes to enhanced mobility.

Notably, H_2S shows a strong temperature dependence, particularly in [EMIM][DCA], where its diffusivity approaches that of CO_2 at 373 K. This behavior suggests that hydrogen-bonding interactions, which restrict H_2S mobility at lower temperature, are progressively disrupted upon heating. In contrast, CH_4 exhibits consistently high diffusivity across both temperatures, consistent with its weak interaction with the ionic liquid.

Overall, the diffusion behavior follows the inverse order of gas–anion interaction strength, providing a coherent connection between microscopic interaction mechanisms and macroscopic transport properties. These findings, when considered together with the RDF analysis, demonstrate that gas mobility in ionic liquids is governed by a combination of interaction strength, viscosity, and available free volume.

Table 1.

Self-diffusion coefficients ($D \times 10^{-6}$ cm^2 s^{-1}) of CO_2, H_2S, and CH_4 in [EMIM][SCN] and [EMIM][DCA] at 298 K and 373 K. ΔT denotes the multiplicative increase upon heating from 298 K to 373 K.

Ionic liquid	CO_2		H_2S		CH_4	
	298K	373K	298K	373K	298K	373K
[EMIM][SCN]	2.519	9.430	2.249	11.904	4.000	12.460
[EMIM][DCA]	4.743	19.327	2.768	19.625	9.700	27.800

4. CONCLUSIONS

This study employed fully atomistic molecular dynamics simulations to investigate the structural and transport properties of CO_2, H_2S, and CH_4 in the ionic liquids [EMIM][SCN] and [EMIM][DCA] at 298 K and 373 K. The results provide a consistent molecular-level picture linking gas–anion interactions, ionic liquid structure, and gas mobility.

The analysis of radial distribution functions demonstrates that gas dissolution does not significantly disrupt the ionic liquid microstructure, although subtle differences arise depending on gas–anion interaction strength. In particular, H_2S induces a measurable increase in local structural ordering in [EMIM][SCN], while CO_2 and CH_4 exhibit minimal structural impact. These findings confirm that

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specific interactions, rather than simple steric effects, govern structural perturbations in these systems.

Self-diffusion coefficients reveal a consistent hierarchy of $D(CH_4) > D(CO_2) > D(H_2S)$, reflecting the inverse relationship between gas mobility and interaction strength. [EMIM][DCA] exhibits systematically higher diffusivities than [EMIM][SCN], primarily due to its lower viscosity and more favorable free volume characteristics. Temperature is found to strongly enhance gas mobility, with increases exceeding those expected from viscosity reduction alone, indicating the important role of thermally weakened gas–anion interactions.

Taken together, these results establish clear structure–transport relationships in cyano-functionalized ionic liquids and demonstrate that gas mobility is governed by a combination of interaction strength, liquid structure, and temperature. From a practical perspective, [EMIM][DCA] appears more suitable for applications requiring rapid gas transport, whereas [EMIM][SCN] may offer advantages in systems where stronger gas–anion interactions are desirable.

Overall, this work provides a quantitative molecular basis for understanding and predicting gas transport in ionic liquids, contributing to the rational design of advanced absorbents for natural gas sweetening and related separation processes.

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