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Exegesis of Potential of Ionic Liquid for Absorption of Carbon dioxide

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The atmospheric concentration of industrial gases, especially CO_2, has been persistently rising, reaching 424 ppm by November 2024, which correlates with an increase in global temperatures. In view of this, CO_2 mitigation technologies must be developed. As of now, absorption of CO_2 using amines is the most prevalent technology for CO_2 capture from post-combustion flue gas. However, this process requires high energy for solvent regeneration. Therefore, researchers have suggested ways to get around the drawbacks of amine process. Ionic liquids, characterized as salts with melting points below 100°C, have garnered interest in recent years as potential solvents for CO_2 absorption, owing to their low vapor pressures, high thermal stability, and significant CO_2 uptake capacity. This review articulates the molecular mechanisms underlying CO_2 capture with ionic liquids. It explores the properties of ionic liquids, the characterization of CO_2-ionic liquid systems, and the effects of operating conditions on the CO_2 uptake capacity of ionic liquids. It underscores the role of cations, anions, and functional groups in determining the solubility of CO_2 in ionic liquids, as well as their biodegradability and toxicity.

Keywords: Absorption, CO_2 capture, ionic liquids, global warming, solvent regeneration.

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Exegesis of Potential of Ionic Liquid for Absorption of Carbon Dioxide

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Abstract

The atmospheric concentration of industrial gases, especially CO2, has been persistently rising, reaching 424 ppm by November 2024, which correlates with an increase in global temperatures. In view of this, CO2 mitigation technologies must be developed. As of now, absorption of CO2 using amines is the most prevalent technology for CO2 capture from post-combustion flue gas. However, this process requires high energy for solvent regeneration. Therefore, researchers have suggested ways to get around the drawbacks of amine process. Ionic liquids, characterized as salts with melting points below 100°C, have garnered interest in recent years as potential solvents for CO2 absorption, owing to their low vapor pressures, high thermal stability, and significant CO2 uptake capacity. This review articulates the molecular mechanisms underlying CO2 capture with ionic liquids. It explores the properties of ionic liquids, the characterization of CO2-ionic liquid systems, and the effects of operating conditions on the CO2 uptake capacity of ionic liquids. It underscores the role of cations, anions, and functional groups in determining the solubility of CO2 in ionic liquids, as well as their biodegradability and toxicity.

Keywords: Absorption, CO2 capture, ionic liquids, global warming, solvent regeneration.

1. Rationale

The level of CO2 has escalated from around 280 ppm at the onset of the industrial revolution to 427 ppm in February 2025, which leads to the rising in the mean temperature as shown in Figure 1 (Pang 2023). The total energy related to CO2 emissions is comprised of 20% from the industries, 23% transportation, 41% energy sector, and 10% building construction (Shi et al. 2022). High levels of CO2 emissions in the energy sector are predominantly attributed to the use of fossil fuels for heat and power generation (Yang et al. 2022, Tawalbeh et al. 2022). Coal fuel contributes to 43% of CO2 emissions, compared to 37% from oil and 20% from gas (Han et al. 2020). With the surge in energy consumption, it is expected that CO2 emissions will two-fold every year, culminating in a total of 28.8 gigatons by 2050 (Soonsawad et al. 2022). In 2023, carbon dioxide emissions worldwide, attributed to fossil fuels and industrial sectors, were recorded at 37.01 billion metric tons ($GtCO_2$). It is anticipated that emissions will increase by 1.08 % in 2024, reaching an unprecedented level of 37.41 $GtCO_2$. Global emission of CO2 is revealed in Figure 2. Various technologies being developed to harnessing renewable energy sources and hydrogen to achieve sustainable and clean power generation. Meanwhile, technologies for carbon capture, utilization, sequestration, and storage (CCUS) are being recommended for the management of CO2 concentrations or converting them into useful chemical compounds (Yusuf et al. 2023, Alami et al. 2020). Although the CCUS processes may be seen as a viable solution (Suicmez 2019), nevertheless it requires high energy consumptions and quite expensive too (Chen et al. 2022).

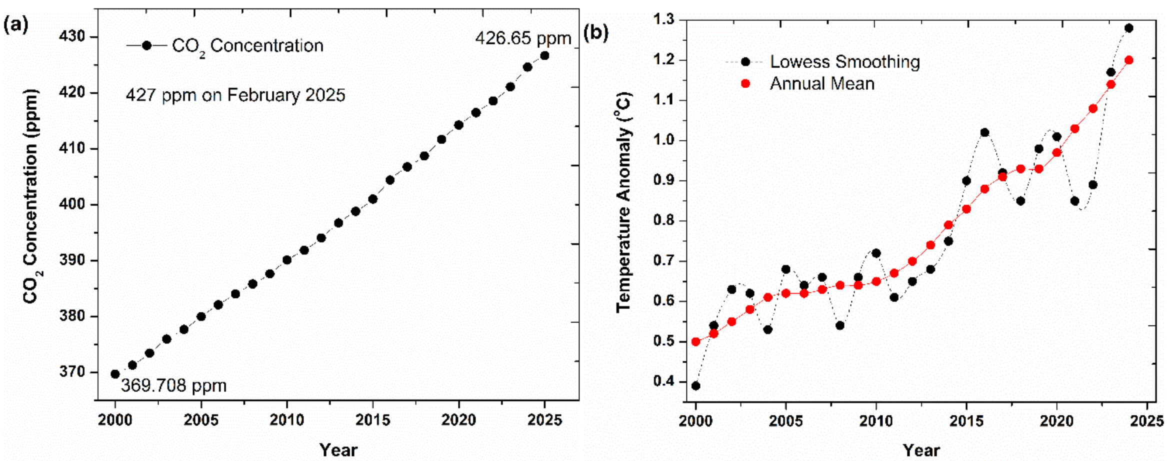

Figure 1 (a) Atmospheric CO2 levels measured by NOAA at Mauna Loa Observatory, Hawaii, (b) Change in global surface temperature and earth's average surface temperature.

At present, the most accepted technique for CO2 capture is reliant on amine-based technologies, notably monoethanolamine (MEA) (Rozanska et al. 2021, Janati et al. 2021, Perumal et al. 2022). The CO2 capture process that incorporates amine-based technology is dictated by energy-intensive chemical reactions, which require substantial heat for the removal of CO2 in the regeneration phase (Janati et al. 2021, Ye et al. 2019, Liu et al. 2020). It is expected that approximately 2.5 - 3.6 GJ of energy will be required to capture 1 ton of CO2 using 30% aqueous solution of MEA, assuming a separation efficiency of 90% (Silva-Beard et al. 2022). By increasing the operating pressure to 150 bar, the energy requirement for this process can be minimized to 0.42 GJ per ton of CO2. Nevertheless, the CO2 capture rate under these conditions is regarded as quite low. Approximately 50% of the energy in amine-based technology is spent on regenerating amine, and the rest energy is allocated for pressurizing the CO2 stream (Panja et al. 2022, Rochelle 2009). Ionic liquids exhibit a significant capacity for absorption, are less corrosive, and are biodegradable. As a result, they have been proposed as alternatives to the current processes involving corrosive, volatile, and deteriorated delicate amine solvents (Dubey et al. 2022). In addition, their non-flammable characteristics and high solubility for CO2 render them an outstanding option for carbon dioxide capture (Elmobarak et al. 2021). Ionic liquids are emphasized in research for their potential to replace conventional solvents, typically volatile organic compounds, aiding in the mitigation of environmental contamination. The adjustable features of ionic liquids facilitate the design of solvents possessing specific properties (Bahadur et al. 2019). In a pioneering study, Blanchard and his co-author (Blanchard et al. 1999) demonstrated for the first time that IL (1-butyl-3-methylimidazolium hexafluorophosphate, [BMIM][PF_6]) can be effectively used in the capture of CO2. Since then, the literature has provided insights into the mechanisms of CO2 capture in both conventional and functionalized ionic liquids. A wide array of conditions and stream compositions, allows for the effective use of ionic liquids in CO2 capture. The evolution of molecular structures in both protic and aprotic ionic liquids has revealed exceptional efficiency in capturing CO2, utilizing a broad spectrum of ionic liquids. The interplay between the anionic portion of ionic liquids and CO2 is vital for the capture of carbon dioxide and could potentially enhance the efficiency compared to standard organic solvents (Carvalho et al. 2009, Wu et al. 2020). Carbon dioxide can be capture by ionic liquids through physical absorption, which do not involve chemical reactions. This methodology revels that the cations embedded in the cyclic configuration of ionic liquids, paired with anions that possess extended distances between oxygen and nitrogen, show intensified electrostatic interactions and hydrogen bonding. Consequently, this leads to an increased absorption of carbon dioxide.

The characteristics of ionic liquids, encompassing solubility, selectivity, viscosity, and volatility, play an important role in CO2 capture processes. The innovations of new ILs, particularly through the synthesis of functionalized ionic liquids with tailored functional groups (Wang et al. 2022) and the implementation of supported ionic liquid membranes, (Wang et al. 2016) has opened avenues for the large-scale utilization of these materials in capturing CO2 from industrial sources, even when CO2 partial pressures are low. Ionic liquids that are cationic and anionic in nature have been effectively employed for the absorption of carbon dioxide from various streams with differing compositions. An important characteristic of these ILs is their reversibility, which supports their potential for large-scale applications and recyclability (Phan et al. 2008). Various studies have aimed at the development of reversible ionic liquids that can be utilized in processes for capturing carbon dioxide. The ionic liquids produced, characterized by their low volatility and thermal stability, have shown efficiency that rivals that of commercial solvents in CO2 capture. However, the biodegradability and toxicity of the most commonly utilized ionic liquids require additional investigation to promote green chemistry and ensure the sustainability of this technological innovation (Singh et al. 2020, Brzęczek-Szafran et al. 2020).

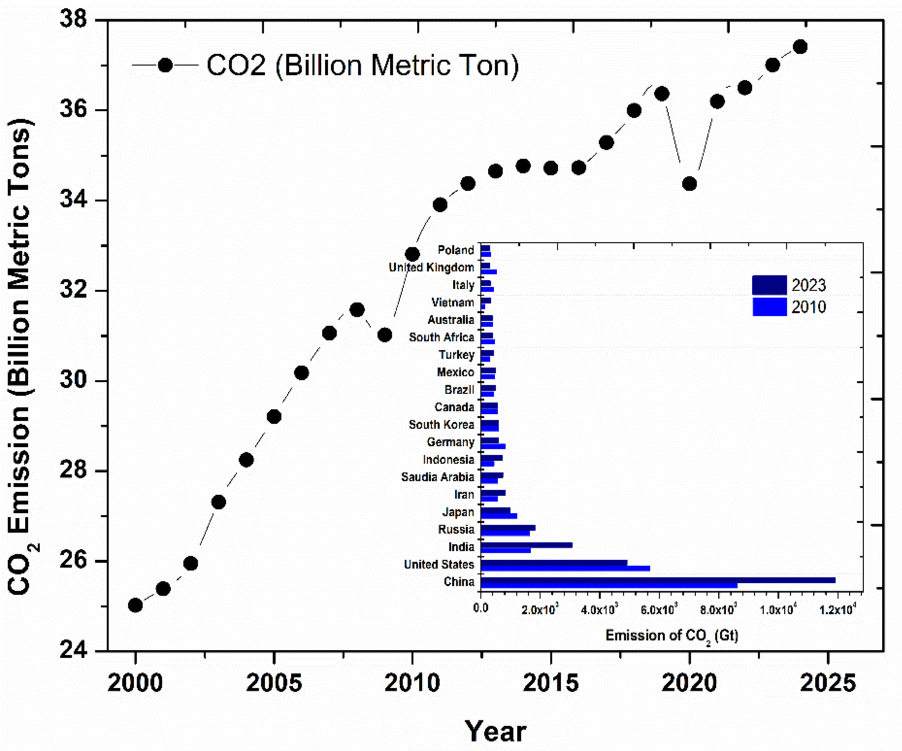

Figure 2 Global emission of CO2 (giga ton) by various countries.

The current study provides a detailed overview of the latest findings and progress in the application of ionic liquids for carbon dioxide capture from industrial flue gases. In addition, the review examines a range of perspectives regarding the use of ILs in CO2 capture, focusing on their application in post-combustion, pre-combustion, and oxy-fuel combustion techniques. The relationship between the effectiveness and efficiency of ionic liquids in CO2 capture and their key properties is noteworthy. The characteristics of ILs, including CO2 solubility, selectivity, viscosity, and cost, were systematically evaluated and comparing these attributes with those of solvents that are commercially available. In addition, the research addressed the role of specific functional groups, including cations and anions, in the optimization of CO2 solubility and selectivity in various ionic liquids. The evaluation also encompassed the potential toxicity and biodegradability of the ILs under consideration. The study reviewed advancements in functionalized ionic liquids and the related evolution of supported Ionic liquid membrane technology was conducted, including an evaluation of their toxicity and biodegradability. The persistent challenges and future research opportunities are encapsulated, along with a guide intended for producers and decision-makers to select the most suitable ionic liquid-based CO2 capture approach.

2. Standard CO2 Capture Technologies

Amine-based Technologies continue to be the most prevalent technique for the large-scale capture of carbon dioxide from fossil-fuel power plants (Tan et al. 2022). These technologies incorporate a selection of alkanol amines, such as mono-ethanolamine, diethanolamine, triethanolamine, methyl diethanolamine, and di-isopropanol-amine, which possess excellent reactivity with CO2 and are acknowledged for their effectiveness in carbon dioxide capture (Vaidya et al. 2007). Amine-based technologies involve the interaction of flue gas at temperatures ranging from 40 to 60 °C with an absorbent, typically a 30 wt% solution of mono-ethanolamine (MEA), within an absorption tower to CO2 capture. The resulting CO2-laden amine solution is subsequently directed to a regeneration tower, where CO2 is extracted and the MEA is regenerated for reuse. The extracted CO2 can either be sequestered underground or transformed into value-added products (Gautam et al. 2023, Fernández-González et al. 2022). Amine-based technologies are recognized as mature technologies, achieving a Technology Readiness Level exceeding 7. However, their significant drawbacks, including high energy consumption, corrosive properties, solvent degradation in the presence of oxygen, and solvent volatility, hinder their effectiveness for large-scale applications. The corrosive nature necessitates the use of dilution solutions, while solvent degradation and volatility pose environmental contamination risks (Ellaf et al. 2023). Research findings have shown that amine-based technologies, despite their shortcomings in energy efficiency and environmental impact, are limited by a removal-to-uptake ratio that cannot surpass 0.5 mol CO2 per mol MEA (Fan et al. 2023, Liu et al. 2022). In light of this, there is an urgent call for research endeavors that focus on the development of new solvents with enhanced properties, such as low corrosivity, high capacity for CO2 loading, lower volatility, and improved resistance to chemical degradation, all while requiring low energy input for their application in CO2 capture processes. The processes of post-combustion, pre-combustion, and oxy-fuel combustion are widely recognized as the predominant methods employed for the capture of CO2 (Liu et al. 2020). Each of these processes possesses distinct characteristics and specific requirements for effective CO2 capture. The post-combustion approach is considered the most cost-efficient technology for carbon capture, applicable to both old and new systems. In contrast, the pre-combustion and oxy-fuel combustion techniques are exclusively applicable to newly established power plants (Madejski et al. 2022).

In conventional fossil fuel power stations, the post-combustion process is widely utilized for the capture of carbon dioxide. This technique entails the thorough combustion of fuel in one stage, allowing the released heat to be converted into high-pressure steam, which subsequently utilized for the electrical energy. Thus, the removal technique is adept at addressing a diverse range of conditions. The flue gas from the boiler is characterized by substantial quantities of material that are sorted in the coal extraction stage. The presence of sulfur in the flue gas necessitates its passage through a limestone slurry, which serves to remove the sulfur and generate gypsum. The post-combustion process is distinguished by a clean flue gas that contains a carbon dioxide mass fraction of 10% to 16%. While this process exhibits a high selectivity for carbon dioxide, it also results in low-pressure carbon dioxide, which incurs significant costs for pressurization (Raganati et al. 2021).

The pre-combustion methodology consists of vaporizing of fuel, mixed with oxygen followed by stripped with steam to generate syngas. The mixture is conveyed to a water-gas-shift reactor, leading to the formation of hydrogen and carbon dioxide. The gas mixture, which is rich in CO2, undergoes a process of separation, transportation, and sequestration. Meanwhile, the hydrogen-enriched stream serves as a fuel for electricity production. The pre-combustion technique generates a high partial pressure of CO2, which not only improves CO2 extraction but also diminishes the costs associated with gas pressurization. Nevertheless, it is important to note that maintaining high pressure within the water-gas shift reactor incurs additional costs (Rosner et al. 2020).

In the oxy-fuel combustion process, pure oxygen is utilized in high concentrations and combined with fuel to facilitate combustion, thereby generating the requisite heat to produce high-pressure steam and electricity. The flue gas, which primarily contains water vapor and carbon dioxide, undergoes a stripping process, allowing for partial reuse it and maintaining optimal boiler temperatures. The concentrated carbon dioxide stream that is expelled can be injected underground or transformed into alternative products. The implementation of pure oxygen negates the necessity for a nitrogen separation phase. The oxy-fuel combustion technique is proficient in capturing carbon dioxide from flue gases at a minimal cost. However, it is imperative to utilize specialized boilers that can handle the increased temperatures associated with the use of pure oxygen (Abdelaal et al. 2021).

3. The Approach to CO2 Capture Involving the Utilization of Ionic Liquids

The classification of ionic liquids includes two distinct categories based on their molecular structures. The first one is protic ionic liquids, which can donate protons, and another is aprotic ionic liquids, which do not possess this ability. Figure 3 illustrates few examples of protic and aprotic ionic liquid that are applied in carbon capture and storage, with the R groups representing common alkyl substituents.

The main emphasis of initial research on CO2 capture using ionic liquids has been on the efficiency of CO2 uptake across a range of non-grafted ionic liquids. It has been reported that the interactions between the anionic portion of the ionic liquid and CO2 are significant to CO2 uptake, particularly in contrast to conventional organic solvents. The ionic liquid [EMIM][TF_2N] was found to have a high CO2 uptake capability across different operational conditions, while traditional molecular solvents only exhibited significant CO2 absorption at elevated to moderate pressure ranges (Zakrzewska et al. 2020). Increasing the operating pressure and CO2 mole fraction leads to a rise in bubble-point pressure, which can considerably impact the uptake of CO2. This distinctive behavior is characteristic of CO2-IL systems and is classified as type III fluid-phase performance (Kroon et al. 2005). A more nuanced evaluation of CO2-IL systems focuses on high molecular weight liquid polymers. Various protic ionic liquids featuring distinct anions, including [TMGH][2-OP], [TMGH][3-OP], [TMGH][4-OP], [DBUH][2-OP], [DBUH][3-OP], and [DBUH][4-OP] were investigated for their CO2 absorption standard temperature and pressure. Findings indicated that these ionic liquids showed increased CO2 uptake, which can be attributed to strong electrostatic interactions and hydrogen bonding. The most prevalent method for CO2 capture with ionic liquids relies on physical absorption, which does not entail a chemical reaction. Key physical properties of ionic liquids, such as their solubility, selectivity for CO_2, viscosity, and volatility, are crucial to this process. Therefore, section explicates the characteristics of ionic liquids. Table 1 summarizes the common properties of ionic liquids used in CO_2 capture (Hayes et al. 2015).

Table 1 Properties of Ionic Liquids

Name	Ethylammonium nitrate	1-Butyl-3-methylimidazolium hexafluoro phosphate
Chemical structure	$[CH_3CH_2NH_3^+]$ $[NO_3^-]$	$[C_4mim^+]$ $[PF_6^-]$
Appearance	clear, colorless	clear, colorless
Melting point (^oC)	12	10
Boiling point (^oC)	255	409
Density, ρ (g/cm^3)	1.21	1.366
Viscosity, η (Pa s)	35.9×10^{-4}	36.9×10^{-4}
Vapor pressure, P (Pa)	0.49	$<10^{-2}$
Refractive index, n_D	1.4535	1.411
Diffusion coefficient, $D\times10^{-6}$ (cm^2/s)	$[CH_3CH_2NH_3]^+$ 0.158, $[NO_3^-]^-$ 0.151	$[C_4mim]^+$ 1.5, $[PF_6]^-$ 1.8
Liquid-vapor surface tension, γ_{LV} (mN/m)	47.3	43.8
Ionic Conductivity, κ (S/cm)	2.69×10^{-2}	1.4×10^{-3}
Dielectric constant, ε	26.3±0.5	14.0±0.7
molar heat capacity, C (J/mol. K)	206	406
Thermal conductivity, λ (W/m K)	0.245	0.145

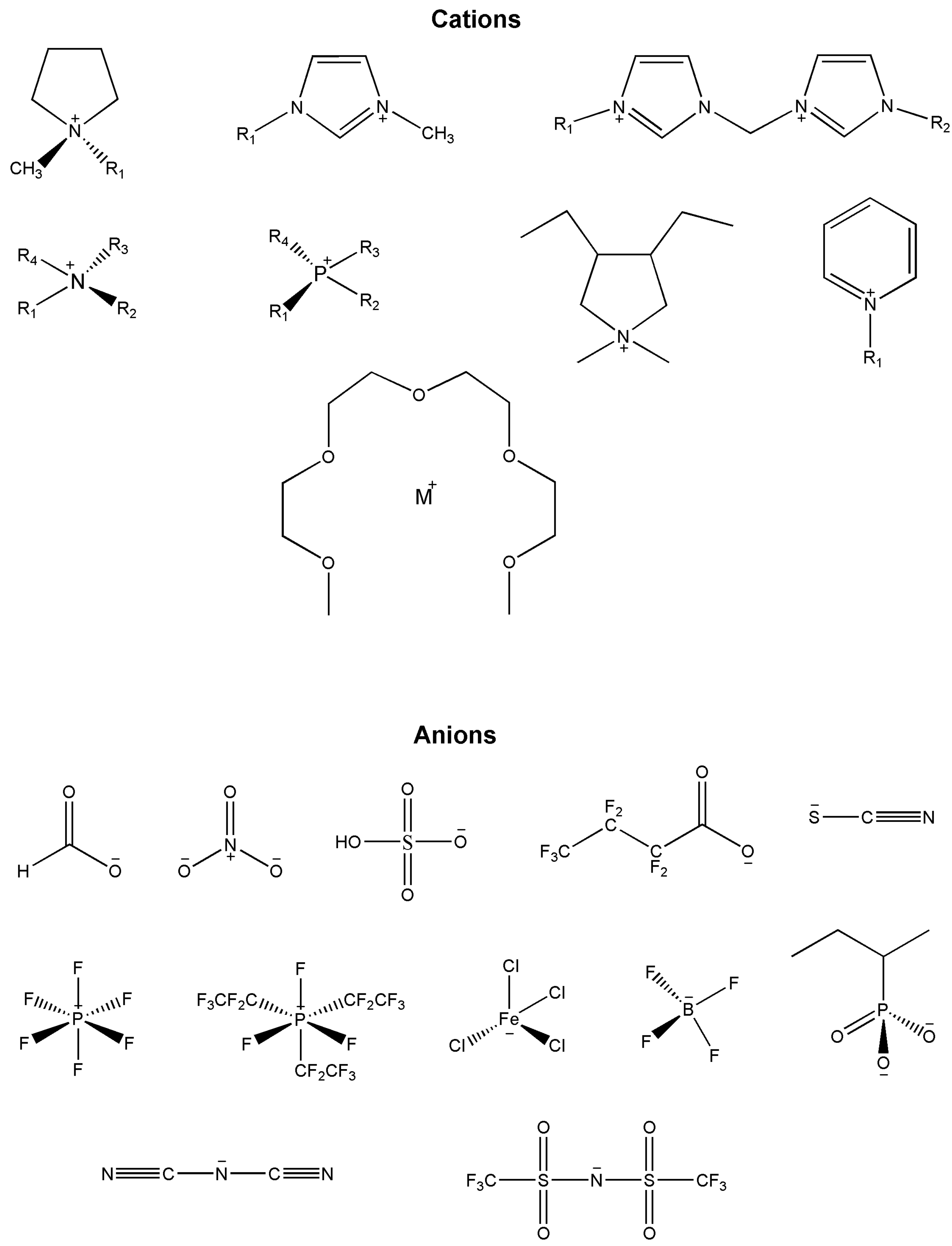

Figure 3 Typical examples of protic and aprotic ionic liquid used in carbon capture technology.

4. Properties of Ionic Liquids

4.1 Density of Ionic liquids

Generally, ionic liquids have a higher density than water; however, guanidinium and pyrrolidinium dicyano-diamide are exceptions, exhibiting densities that range from 0.97 - 0.90 g/cm³. An increase in the carbon count of the alkyl chain corresponds with a reduction in the density of ionic liquids. Moreover, there is a linear decadence in the density of ionic liquids with rising temperatures as depicts in Figure 4 (a-e).

The viscosity of ionic liquids increases with the addition of more carbon atoms in the alkyl group, showcasing a trend that is unlike the viscosity profile seen in conventional organic solvents. Ionic liquids exhibit high viscosity, which is largely a result of hydrogen bonding and Van der Waals interactions. Typically, as the alkyl chain lengthens or fluorination occurs, the molecular interactions tend to increase. Luciana and her co-authors (Tomé et al. 2008) found that the experimental density results for ionic liquids are consistent with the Tait equation (Dymond et al. 1988) for liquid density, as detailed below.

$$\rho = \frac{\rho(T,P=0.1\ MPa)}{\left[1-C\ln\frac{(B+P)}{(B+0.1)}\right]} \tag{1}$$

$$\rho(T,P=0.1\ MPa) = a_1 + a_2T + a_3T^2$$

$$B = b_1 + \frac{b_2}{T}$$

The coefficients a_1, a_2, and a_3 can be adjusted to correspond with the experimental density data for various ionic liquids as a function of temperature. Additionally, the constants C, b_1, and b_2 can be obtained by plotting density against both temperature and pressure, in accordance with the equations provided. Furthermore, Fu et al. (2024) investigated the application of three machine learning algorithms (ANN, XGBoost, LightBGM) to analyze the density and heat capacity of binary systems composed of ionic liquids and water. Their results demonstrate that the ANN-GC model yields superior predictive performance for these properties in the ionic liquid-water system.

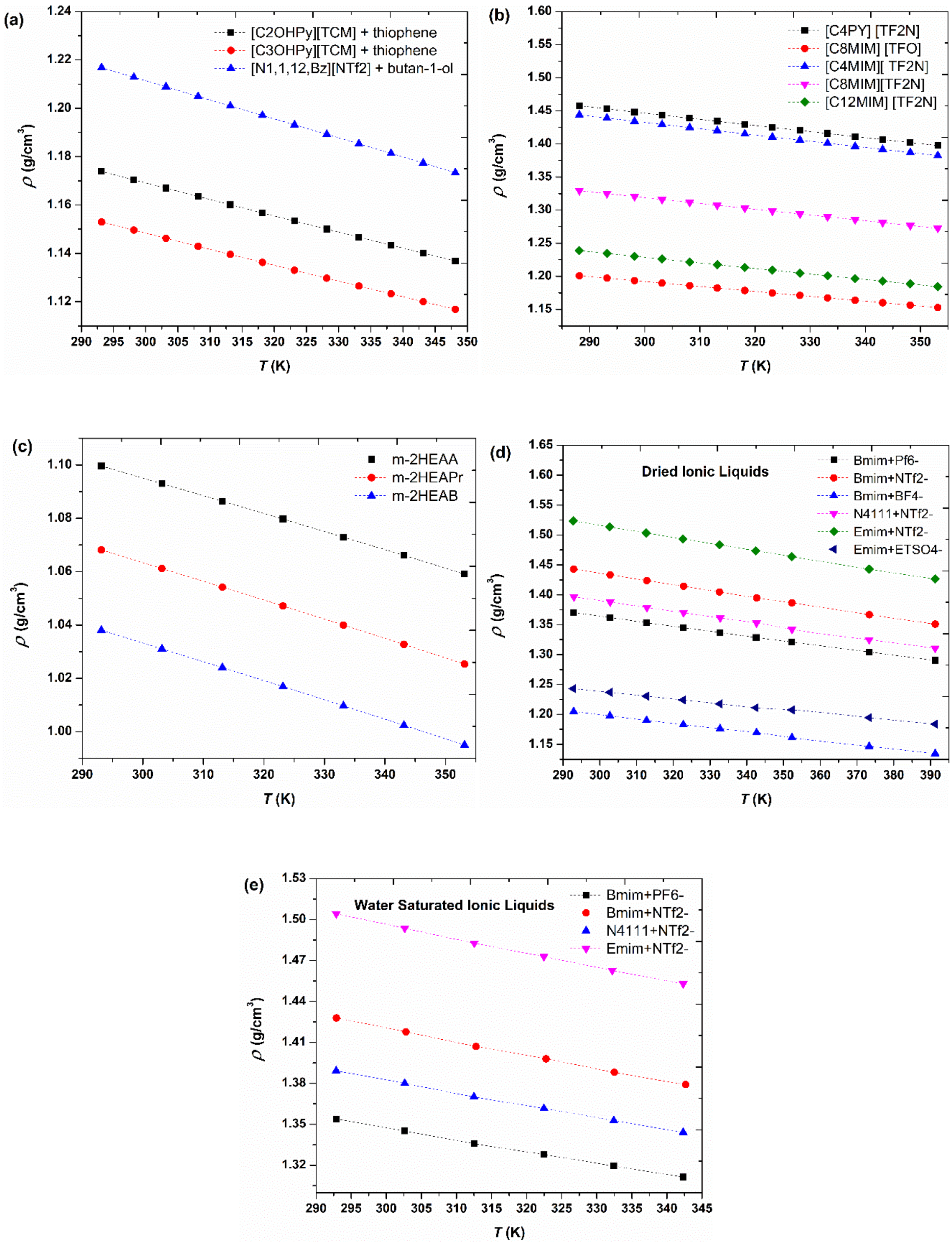

Figure 4 Temperature vs Density (a) Domanska et al. 2019, Fluid Phase Equilib 502:112304; (b) Santos et al. 2016, J Chem Eng Data 61:348-353; (c) Santos et al. 2016, J Chem Eng Data 61:348-353; (d) Jacquemin et al. 2006a, Green Chem 8:172-180; (e) Jacquemin et al. 2006a, Green Chem. 8:172-180.

4.2 Viscosity of Ionic liquids

In the context of CO2 capture, the viscosity of ionic liquids is a vital consideration since increased viscosity may lead to reduced mass transfer and could impede CO2 uptake (Weingartner 2008). Additionally, the viscosity and density of ionic liquids are influenced by the presence of water and other contaminants within them (Jacquemin et al. 2006a). Several ionic liquids form highly viscous gel-like substances, which leads to a diminished capacity in CO2 absorption. However, it is possible to modify the properties of ionic liquids to create a diverse range of viscosities. Different research studies have delved into the relationship between the viscosity of ionic liquids and their temperature, especially for those frequently utilized (Moganty et al. 2010, Crosthwaite et al. 2005, Tsunashima et al. 2007). Findings indicate that most ionic liquids conform to the Arrhenius law, which describes a linear relationship between viscosity and the inverse of temperature. Any deviations from this law are generally elucidated through the Vogel-Fulcher-Tammann equation (Yoshida et al. 2019). The Vogel-Fulcher-Tammann expression of the viscosity is given by-

$$\eta = \eta_0 \exp\left(\frac{B_{VFT}}{T-T_0}\right) \tag{2}$$

Where, T is the absolute temperature, η_0 is the value of the viscosity at the high temperature limit, and B_{VFT} is the quantity related with activation barrier. T_0 is the Vogel temperature. Zhao and his co-authors have synthesized innovative functionalized ionic liquids, namely [N8881][NIA] and [N8881][For], which are distinguished by their low viscosity, high capacity for uptake of CO2, and remarkable recyclability (Zhao et al. 2022). Domanska et al. (2019) and Jacquemin et al. (2006a) also studied the variation of viscosities of ionic liquid such as [C2OHPy][TCM] + thiophene, [C3OHPy][TCM] + thiophene, [$N_{1,1,12,Bz}$][NTf_2] + butan-1-ol, $Bmim^+PF_6^-$, $Bmim^+NTf_2^-$, $Bmim^+BF_4^-$, $N_{4111}{}^+NTf_2^-$, $Emim^+NTf_2^-$, and $Emim^+EtSO_4^-$ with temperature as shown in the Figure 5 (a-c).

Ionic liquids exhibit higher viscosities compared to traditional solvents like water, acetonitrile, and alcohols. Moganty et al. (2010), Tsunashima et al. (2007), Crosthwaite et al. (2005) have sought to engineer ionic liquids with lower viscosities by adjusting the types of cations and anions used. The viscosity enhancement of ionic liquids pertinent to the aforementioned action is arranged in the following order: ammonium [N2228]> phosphonium [P2228]> pyrrolidinium [hmpyrr]> pyridinium [hmpy]> imidazolium [hmim] (Moganty et al. 2010, Tsunashima et al. 2007, Crosthwaite et al. 2005).

The research conducted by Gardas and his co-authors evaluated the transport and thermophysical attributes of ionic liquids, which includes conductivity, thermal conductivity, isobaric electrical expansivity, viscosity, refractive index, and isothermal compressibility (Gardas et al. 2008, 2009). Zailani and his co-author synthesized a series of ammonium-based Protic Ionic Liquids, specifically [EHA][C5], [EHA][C6], [EHA][C7], [BEHA][C5], [BEHA][C6], and [BEHA][C7]. These protic ionic liquids showed remarkable CO2 absorption performance, maintaining efficacy even at a high pressure of 29 bar. Notably, [BEHA][C7] exhibited the highest CO2 uptake capacity, reaching 0.78 mol at this pressure (Zailani et al. 2022).

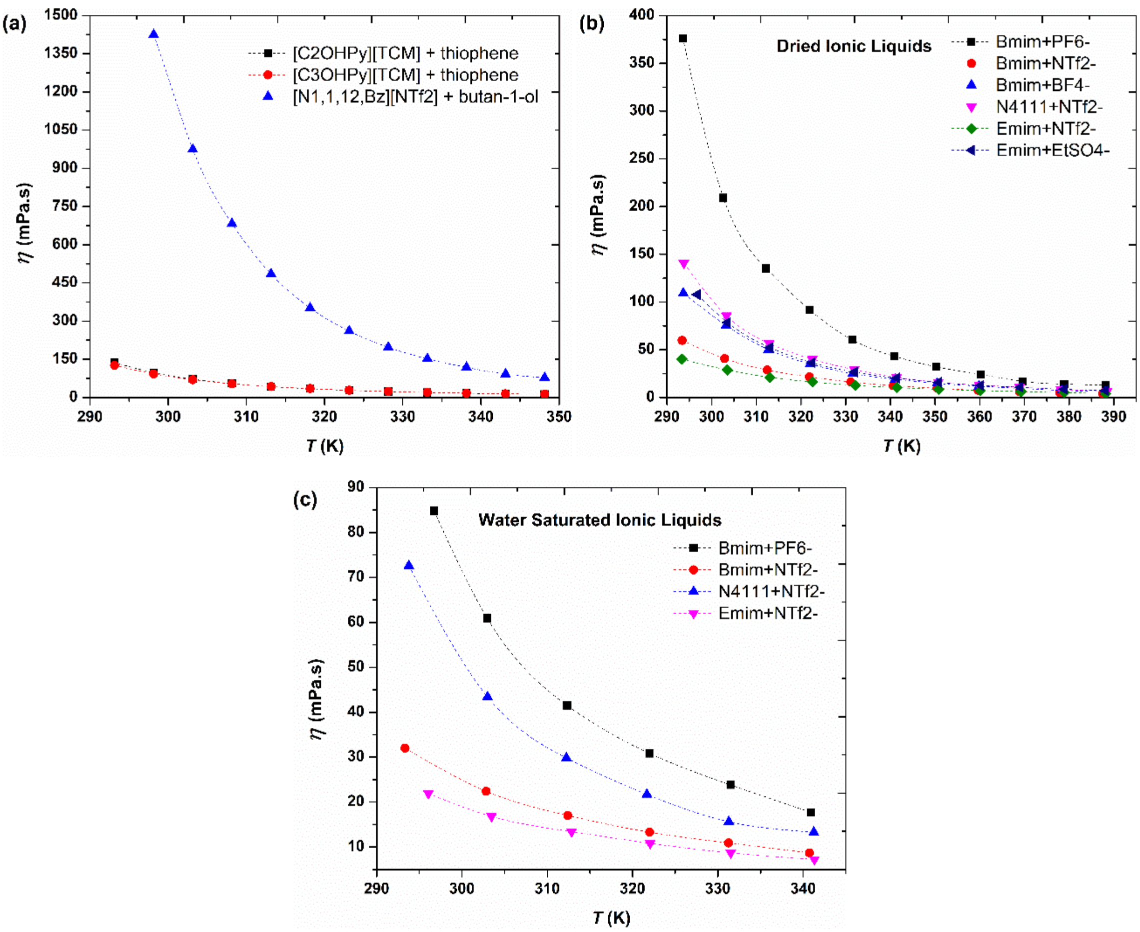

Figure 5 Variation of viscosities with temperature (a) Domanska et al. 2019, Fluid Phase Equilib 502:112304; (b) Jacquemin et al. 2006a, Green Chem. 8:172-180; (c) Jacquemin et al. 2006a, Green Chem. 8:172-180.

CO_2 absorption capacity can be classified in ascending order as [C5], [C6], and [C7]. In-depth analysis of the dynamics of ionic liquids and their molecular simulations were done by Maginn et al. (2009). These simulations primarily focus on the slower dynamics of IL systems, yet they are also capable of measuring viscosities at very short time intervals (Maginn et al. 2009). Viscosity is a critical factor in chemical reactions, especially in dispersion-controlled reactions, where the reaction rate may inversely correlate with the viscosity of the solvent (Weingartner et al. 2008). Consequently, many reactions proceed at a slower rate in ionic liquids compared to conventional solvents, primarily due to the elevated viscosity of ionic liquids. At 298 K, the self-diffusion coefficients for cations and anions are approximately 10–11 m^2/s, compared to the range of 10–10 to 10–9 m^2/s found in simple molecular liquids (Maginn et al. 2009, Weingartner et al. 2008).

The research conducted by Hou and Baltus (2007) developed a distinct correlation for the diffusivity of CO_2 in imidazolium ionic liquids, incorporating factors such as molar mass, viscosity, density, and temperature. Likewise, Ferguson and Scovazzo analyzed gas diffusion in phosphonium ionic liquids (Ferguson et al. 2007). Their research revealed an inverse relationship between the viscosity of phosphonium ionic liquids and their diffusivity. Furthermore, the gas diffusivity observed in phosphonium ionic liquids is related to the viscosity of the solvent, the molar volume of the solvent, and the solute present. On the other hand, (Condemarin et al. 2009) examined gas diffusivities in ammonium ILs and concluded that the diffusivity of gases was contingent upon the solvent's viscosity. These findings illustrate the differences in diffusivity that can be attributed to the type of ionic liquids used. Moreover, the Stokes-Einstein equation illustrated that the diffusivity of gases in ionic liquids is less influenced by viscosity than one would typically assume. Gao et al. (2024) and Melfi et al. (2024) investigated multiple theoretical approaches, including both theoretical and semi-empirical models that combine various theories with equations of state or activity coefficient models, alongside empirical and phenomenological models focused on the viscosity of pure ionic liquids and their mixtures. Nonetheless, this conclusion is debatable, as the Stokes-Einstein equation is primarily applicable to the diffusion of larger solute particles in a medium of smaller molecules (Morgan et al. 2005).

4.3 Solubility of CO_2 in Ionic Liquids

Aki and co-workers inveterate that anionic ionic liquids are the key players in CO_2 capture, whereas protic ionic liquids contribute in a secondary role (Aki et al. 2004). It is also noted that anionic ionic liquids possess a higher uptake of CO_2 than their protic ionic liquid counterparts.

The relationship pertains to the ability of anionic ionic liquids to establish strong Coulombic interactions that contribute to a network facilitating CO2 dissolution and enhancing uptake of CO2. Such interactions facilitate the localization of CO2 within the interstitial spaces of the ILs, resulting in an increase in solubility of CO2 and the observed uptake of CO2 (Shaikh et al. 2022). Through in-situ Attenuated Total Reflectance-Infrared Spectroscopy, Kazarian and co-authors revealed that the anionic nature of [BF4] and [PF6] contributed to an increase in the solubility of CO2 thereby uptake of CO2 (Kazarian et al. 2000). The interaction between CO2 and ionic liquids was emphasized as being consistent with Lewis acid-base interactions. Consequently, the enhanced basicity of [BF4] elucidates the greater solubility of CO2 in [BF4] compared to [PF6]. Likewise, the stronger basic characteristics account for the increased solubility of CO2 in [bmim][PF6] relative to [bmim][BF4]. Through their research, Qin et al. (2024) proposed a range of strategies utilizing the COSMO-RS model to effectively predict the solubility of CO2 and N2, thereby aiding in the identification of optimal ionic liquids for the electrocatalytic conversion of these gases. A database has been established, comprising 3,036 solubility data entries for CO2 and 457 for N2 in ionic liquids, recorded at different temperatures and pressures. The forecasted solubility of CO2 was significantly high, recorded at 43.4%, with R2 values of 0.599 for CO2 and 0.242 for N2 datasets, respectively. Moreover, Glycol ether-functionalized phosphonium and ammonium ILs carrying acetate and Tf2N– anions could dissolve up to 0.55 mol CO2 per mole of ionic liquid (or 5.9 wt% CO 2) at room temperature and atmospheric pressure (Zhao et al. 2022).

Research has suggested that Lewis acid-base interactions alone do not adequately describe the solubility of CO2 or the CO2 uptake potential of anionic ionic liquids. Thus, mechanism concerning free volume of ionic liquids, which elucidates the differences in CO2 dispersion within these liquids, has been associated with CO2 solubility (Chen et al. 2022, Shaikh et al. 2020). The mechanism governing free volume in ionic liquids is founded on the fact that the addition of CO2 does not lead to a significant change in the volume of free cavities until the CO2 saturation limit is achieved. Studies have revealed that CO2 fills the unoccupied sites within [bmim][PF6] and organizes itself over the anionic component of [PF6] (Kanakubo et al. 2005, Zunita et al. 2022). By adding various anions to the Protonic Ionic Liquid, the solubility of CO2 was significantly improved (Zailani et al. 2022, Farsi et al. 2020). Experiments at 30˚C demonstrated that the gas selectivity in Ionic Liquids is ordered as T7F15CO2 > Methide > TF2N > PF6 > DCA > BF4 > MeSO4 > SCN > NO3 (Wang et al. 2018). The solubility of carbon dioxide (CO2) in various ionic liquids was examined using the COSMO-RS model. The findings indicated that ionic liquids containing fluoride possess enhanced ionic characteristics and demonstrate greater CO2 solubility compared to those lacking a fluoride group (Maiti et al. 2009, Sistla et al. 2011). The trend of anion fluorination was assessed with the widely recognized cationic ionic liquid [bmim]. It was observed that the solubility of CO2 enhances as the number of fluoride groups in the structure increases. CO2 solubility was organized in this manner: bFAP > eFAP > T7F15CO2 > Methide > TF2N > PF6 > TfA > TfO > BF4. Additionally, it was noted that incorporating a longer fluoroalkyl chain into anion ionic liquids, like [FAP], improves the solubility of CO2 (Farsi et al. 2020, Zhang et al. 2008). COSMO-RS testing facilitated a better understanding of the dissolution of CO2 in ionic liquids (Palomar et al. 2011). A wide array of ionic liquids was examined, effectively correlating Henry's law with CO2 solubility and the relevant enthalpy of dissolution in ionic liquids. The results confirmed a linear relationship between CO2 solubility and the exothermic characteristics of the mixture. Palomar et al. (2011) explicates the intermolecular interactions among fluid phases, specifically focusing on hydrogen bonds, electrostatic forces, and van der Waals forces, and their correlation with CO2 solubility in ionic liquids. The findings revealed that van der Waals forces are the primary drivers of CO2 uptake, facilitating its dissolution in ionic liquids. Conversely, the role of hydrogen bonds was negligible, and electrostatic interactions had a limited effect on the enthalpy of dissolution. Palomar et al. (2011) also carried out a COSMO-RS study aimed at discovering new ionic liquids with improved van der Waals interactions to enhance CO2 uptake. Their findings revealed that the presence of bromine in ionic liquids, such as [emim][PBr6], led to both CO2 solubility and uptake. The development of various N-Heterocyclic Anion-based ionic liquids was achieved through Density Functional Theory and COSMO-RS quantum chemical calculations, resulting in CO2 uptake capacities between 0.39 and 1.73 mol/kg, with enthalpy values falling within the range of -43 to -54 kJ/mol (Hospital-Benito et al. 2022).

The solubility of CO2 in ionic liquids was evaluated by incorporating various cations, including ammonium, cholinium, pyridinium, pyrrolidinium, phosphonium, and imidazolium, along with the anion [Tf2N] (Jacquemin et al. 2006a). Cation fluorination, represented by [C6H4F9mim], has the potential to greatly increase CO2 solubility relative to anion fluorination (Almantariotis et al. 2010). The incorporation of long alkyl chains in the phosphonium cation [P666,14] facilitates greater solubility of CO2 (Ramdin et al. 2012). Additionally, the pairing of ionic liquids with traditional bis(trifluoromethyl sulfonyl)amide [Tf2N] anions also contributes to increased CO2 solubility. Several studies have shown that the solubility of CO2 increases with the elongation of the alkyl chain. Studies have revealed that increasing the length of the alkyl chain leads to a greater solubility of CO2. The COSMO method accounts for the acidity of ionic liquids by analyzing their structural features. In the case of ionic liquids, a hydrogen bond can form at the C2 position of the imidazolium ring, which carries a relatively high positive charge. The COSMO method explicates the acidity of ionic liquids based on their structural characteristics. In ionic liquids, a hydrogen bond can form at the C2 position of the imidazolium ring, which exhibits a relatively high positive charge. Consequently, an increased absorption of CO2 can take place at this location through its exchange with hydrogen (Sistla et al. 2011, Shimoyama et al. 2010, Zhang et al. 2020). Experimental results and molecular simulations have confirmed that the introduction of a methyl group in place of the hydrogen proton at the C2 site leads to a slight decrease in CO2 solubility (Aki et al. 2004, Cadena et al. 2004, Shamair et al. 2020). At 25°C, the Henry's constant for CO2 solubility in [bmim][PF6] was recorded at 53.4 bar, while it increased to 61.8 bar in [bmmim][PF6] with the methyl group substitution (Cadena et al. 2004). Despite the extensive use of molecular simulations to investigate the solubility of CO2 in ionic liquids, there has been limited research focused on the development of CO2 solubility isotherms. COSMO facilitates the selection of an appropriate ionic liquid for the absorption of CO2 from flue gas emissions. Various alternative methods that leverage the properties of viscosity or surface tension have been employed to assess the solubility of gases in ionic liquids (Zhai et al. 2022, Abourehab et al. 2022, Shojaeian2020). Further, regular solution theory can be applied to evaluate gas solubility in ionic liquids under low-pressure conditions (Dębski et al. 2019). In regular solution theory, solute activity coefficient, γ_1 is dependent on the liquid molar volume ($\bar{V}_1$) and variations in the solubility parameters of the solute, δ_1 and solvent, δ_2, as expressed-

$$RT \ln \gamma_1 = \bar{V}_1 \Phi_2^2 (\delta_1 - \delta_2)^2 \qquad (3)$$

The identification of the factors within real solution theory allows for the determination of the total solubility isotherm (Nikolenko et al. 2020). The parameter δ_2 can be either undefined or modified to fit the experimental isotherms. Vaporization enthalpies were used, following the correlation $\delta_2 = (\Delta H_{vap} U_2/V_2)$ were used to deduce the δ_2. Nonetheless, it was found that the experimental δ_2 values produced inaccurate predictions for the solubility of CO2 in [hmim]-[Tf2N] when utilizing real solution theory. The underwhelming performance of real solution theory when applying real solubility, as opposed to associated solubility factors, to determine CO2 solubility is not surprising. Typically, the addition of CO2 to ionic liquids at low pressure results in a negative deviation from ideality, as indicated by Raoult's law. This leads to an activity coefficient (γCO2) for ionic liquids that is less than 1. Nonetheless, real solution theory can also account for mixtures that show positive deviations from ideal behavior. In both experimental and simulation contexts, the solubility of CO2, measured by mole fraction, was employed to evaluate CO2 uptake. Various research efforts have indicated that entropy plays a significant role in influencing and regulating the physical absorption of CO2 by ionic liquids (Lin et al. 2019). This facilitates the development of a correlation, as indicated in Eq. (4), which pertains to the solubility of CO2 in ionic liquids over a temperature range of 25 to 93°C.

$$P = m_i^0 e^{\left(\frac{[6.8591-2004.3]}{T}\right)} \tag{4}$$

Blanchard, Aki, and Kumełan were used Eq. (4) for measuring the solubility of CO2 in ionic liquids (Blanchard et al. 2001,Aki et al 2004, Kumełan et al. 2010). A significant number of Ionic liquids demonstrated divergence discrepancies from Eq. (4) (Carvalho et al. 2010, Brennecke et al. 2010). For instance, acetates (m-2-HEAA) and formats (m-2HEAF) enhanced CO2 solubility through the formation of electron donor–acceptor compounds, which do not adhere to Eq. (4). Additionally, other Ionic liquids featuring various anions, such as [doc], [xSO4], [SCN], [mp], and [NO3] along with [bmim][BF4], also did not conform to this standard correlation. Furthermore, few more Ionic liquids, including [PF6], [DCA], and [TfO] did not align with the proposed model, suggesting that the current model requires further improvement.

The findings of Kumełan et al. (2010), Aghaie et al. (2020), and Suzuki et al. (2022) observed that, molecular weight of ionic liquids plays a crucial role in determining the solubility of CO2. Further research has indicated that higher molecular weights of ionic liquids correlate with increased CO2 solubility, even though it was initially considered that solubility was largely dependent on molarity. The solubility data for CO2 aligns with findings documented in the literature (Kumełan et al. 2010, Aghaie et al. 2020, Suzuki et al. 2022). Usually, the solubility of CO2 is expressed in terms of molarity (Jacquemin et al. 2006a,Domanska et al. 2010, Gonçalves et al. 2011). A plot illustrating the relationship between pressure and molarity for multiple ionic liquids results in almost straight lines. The slopes of these lines facilitate the calculation of Henry's constants in terms of molarity. Subsequently, Henry's coefficients are plotted against the molecular weight of the ionic liquid. The trends observed suggest that as the molarity of ionic liquids rises, the Henry's coefficient for CO2 solubility declines.

An alternative method for assessing CO2 solubility in ionic liquids is the free-space technique (Dębski et al. 2019, Domanska et al. 2010, Gonçalves et al. 2011, Song et al. 2020). This method relies on the molar-free volume of the ionic liquids. A robust correlation was found between Henry's Constant and the molar-free volume, indicating that as the molar-free volume increases, Henry's Constant decreases. Van der Waals molar volume correlation was developed by Zhao and co-authors, which is used to deduce to the molar-free volume of ionic liquids (Zhao et al. 2003). An accurate assessment of the van der Waals molar volume was achieved through the free-space method. In addition, many researchers have leveraged the molar-free volume of ionic liquids to assess Henry's Constant across a range of ionic liquids, linking these findings to CO2 solubility (Jacquemin et al. 2006a, Domanska et al. 2010, 119, Gonçalves et al. 2011). Research findings revealed that the molar-free volume of ionic liquids is contingent upon the aromatic imidazolium and pyridine rings, along with the nonaromatic pyrrolidine ring. Additionally, it was confirmed that an increase in the molecular weight of ionic liquids correlates with an increase in their molar-free volume.

The solubility and selectivity of CO2 in the ionic liquids are significantly influenced by the molar-free volume of these substances. Higher molar-free volumes and greater molecular weights of ionic liquids lead to improved CO2 solubility (Shannon et al. 2012). These results corroborate the research concluded by Carvalho et al. (2010), which showed that the solubility of CO2 in ionic liquids is primarily influenced by entropic factors rather than the interactions between solute and solvent. The patterns of solubility as related to molarity or molality exhibit variations when these trends are considered on a mole fraction basis. One persistent observation is that CO2 demonstrates higher solubility in fluorinated ionic liquids compared to non-fluorinated counterparts. Apart from the free-space method, the pattern discussed earlier emphasizes the importance of the interactions between solute and solvent. It is essential to note that the solubility of CO2 is not evaluated based on mole fraction due to the substantial influence of molar volume.

Machine learning (ML) models comprising random forest, artificial neural network, and multiple linear regression were established by using 9864 data points covering 124 ILs and descriptors from the σ-profile for predicting CO2 solubility in ionic liquids. The random forest model yielded the most favorable results, indicated by an R^2 of 0.9754 and a mean absolute error of 0.0257 (Laakso et al. 2025). Furthermore, artificial neural networks, deep learning algorithms, and support vector machines have been employed to forecast solubility in ionic liquids, yielding significant findings that highlight the efficacy of these methodologies (Kazmi et al. 2025).

4.4 Selectivity of Ionic Liquids

Data pertaining to the solubility of CO2 alone is inadequate for determining the CO2 removal efficiency of Ionic Liquid. Furthermore, the selectivity of ionic liquid for CO2 provides additional insights. Although solubility data for CO2 is available in the literature, however, details on its selectivity of CO2 remain limited. In the context of CO2 capture from flue gases, selectivities are primarily influenced by the composition of the flue gas and the ratios of its various components, including CO2/CH4, CO2/H2, and CO2/N2. Additionally, flue gases may contain other contaminants like CO, SOx, and H2S. Thus, the selectivity for CO2 is prioritized over its solubility. Different research studies have assessed the solubility of CO2 in ionic liquids in relation to other constituents of flue gas. The solubility of CO2 in [hmpy][Tf2N] at 298 K was observed to be comparable to that of SO2, with C2H4, C2H6, CH4, O2, and N2 showing progressively lower solubility thereafter (Anderson et al. 2007, Anthony 2005, Lei 2014).

The exhaust gas emitted from fossil fuel-based power plants comprises 2–3% O2, 8–10% CO2, 18–20% H2O, and 67–72% N2. The substantial selectivity of CO2 suggests that [hmpy][Tf2N] may be an effective option for CO2 capture from these flue gas emissions. The pronounced solubility of hydrocarbons, such as C2H4, C2H6, and CH4 in ionic liquids, specifically [hmpy][Tf2N], could lead to a slight decrease in CO2 selectivity, thereby influencing the overall CO2 uptake. During the CO2 capture process employing [hmpy][Tf2N], SO2 could potentially contend with CO2. The solubility of CO2, C2H4, and C2H6 in ionic liquids rises as the temperature decreases (Kumełan et al. 2005). Conversely, the solubility of CH4 and O2 in [bmim][PF6] remains unaffected by temperature variations. Since cooling the flue gas during CO2 capture is improbable, there is a significant need for ionic liquids that exhibit high CO2 solubility at elevated temperatures. In phosphonium, ammonium, and imidazolium ionic liquids, the solubility of CH4 exhibits minor variations with temperature changes (Carvalho et al. 2011). Carvalho and co-author found that the solubility of CH4 in ionic liquids is influenced by factors other than temperature alone (Carvalho et al. 2010). An increase in temperature leads to a modest rise in the solubility of CH4, although this effect is affected by the polarity of the ionic liquid. The relationship between the selectivities of various ionic liquids for CO2/CH4 and H2S/CH4 can be explained by the Kamlet-Taft β factor, which is based on the solvent's ability for hydrogen bonding and its polarization characteristics. Compared to carbon dioxide, the solubility of carbon monoxide and hydrogen in [bmim][PF6] and [hmim][Tf2N] is significantly reduced, which indicates that these ionic liquids are highly selective for CO2 and show promising potential for CO2 capture (Kumełan et al. 2005a, 2006). Moreover, it has been found that increasing the temperature leads to a rise in the solubility of

H_2 in both [bmpy][Tf2N] and [hmim][Tf2N] (Kumełan et al. 2010, Biswas et al. 2022). Conversely, the solubility of CO_2 in [bmim][PF6] diminishes with increasing temperature, whereas the solubility of CO is unaffected by temperature changes. Likewise, an increase in temperature led to a higher solubility of carbon monoxide in [bmim][CH3SO4] (Kumełan et al. 2007). Jacquemin et al. examined the solubility of several gases in the ionic liquids [bmim][PF6] and [bmim][BF4] at low pressures (Jacquemin et al. 2006b, 2006c). Their analysis showed that hydrogen had the lowest solubility in both ionic liquids, whereas carbon dioxide had the highest. This result aligns with previous findings regarding CO_2 absorption and the increased solubility of H_2 as temperatures decrease. As a result, [bmim][PF6] and [bmim][BF4] are strongly endorsed for CO_2 capture, as the solubility of flue gases is organized in the order of CO_2 > C_2H_6 > CH_4 > Ar > O_2 > N_2 > CO > H_2. How the inclusion of cations in ionic liquids affects hydrogen solubility studies by Jacquemin et al. They found that, the introduction of cations like [N4111], [emim], and [bmim], alongside the anion [Tf2N] resulted in a modest increase in H_2 solubility. Notably, the combination of [Tf2N] and [N4111] yielded the highest solubility for H_2. It was also observed that in this combination, the solubility of H_2 declined as the temperature rose, which is in contrast to the findings related to the combinations of [bmpy]-[Tf2N], [bmim]-[PF6], and [hmim]-[Tf2N].

The research conducted by Yokozeki et al. (2007) indicates that the selectivity of CO_2 in the ionic liquid [bmim][PF6] can reach levels of 30 - 300 under standard operating conditions, which is notably higher than the selectivity of new polymeric membranes, which is between 10 - 30 (Ying et al. 2018). Additionally, the selectivity of CO_2 in [bmim][MeSO4] and [bmim][PF6], determined through the equation of state for a gas mixture of CO_2 and H_2S, was calculated to be in the range of 3.2 - 4 (Shiflett et al. 2010a). The findings indicated significant competition between the two gases, which led to a diminished selectivity for CO_2 in the [bmim][PF6]. Selectivity of CO_2 in the [bmim][MeSO4], relies on the molar ratio of CO_2/H_2S. Selectivity of CO_2 in the range 10 - 13 (Shiflett et al. 2010a, Barzegar et al. 2021). The solubility of hydrogen, oxygen, carbon monoxide, and nitrogen were analyzed in analogous ionic liquids, and the findings revealing significant discrepancies in the reported values (Jacquemin et al. 2006b, Kumełan et al. 2005b, Gomes 2007). For example, the Henry's constant for oxygen in [bmim][PF6] was measured at 650±425 MPa at 283 K, while this value dropped to 51.5±0.6 MPa at the same temperature [Anthony et al. 2002, Kumełan et al. 2005a, 2005b].

The solubility of gases in ionic liquids is associated with their polarity. Simple gases usually interact inadequately with ionic liquids, while gases that feature an electric quadrupole moment, like CO_2 and C_2H_4, show significantly higher solubility (Abbas et al. 2014, Guo et al. 2020). The relationship between gas solubility in ionic liquids and the molar free volume of these solvents indicates that reducing the molar free volume leads to improved standard selectivities for CO_2/CH_4 and CO_2/N_2 (Camper et al. 2004, Finotello et al. 2008). The study conducted by Finotello et al. (2008) examined the selectivity of CO_2, N_2, and CH_3 in pure forms of [bmim][Tf2N] and [bmim][BF4], along with their mixtures. It was noted that the optimal selectivity for these gases was attained when 5 mol % of [bmim][Tf2N] was mixed with an equivalent amount of [bmim][BF4]. Imidazolium-based ionic liquids that have been modified with ethylene glycol exhibited a greater selectivity for CO_2 compared to that for CH_4 and N_2 in gas mixtures comprising CO_2, CH_4, and N_2 (Bara et al. 2007).

The research investigated by Mahurin and co-authors on the Selectivity of CO_2 of a CO_2/N_2 mixture in pyrrolidinium, imidazolium, and pyridinium ionic liquids modified with a benzyl group. The findings indicated that the Selectivity of CO_2 values ranged from 22 -33, implying an increased Uptake of CO_2 (Mahurin et al. 2011). The determination of solubility for mixed gases is often intricate, leading to a limited amount of mixture solubility data available in the literature. The solubility of mixed gases, specifically O_2, CO_2, and CH_4, in the ionic liquid [hmim][Tf2N] has been investigated by Hert et al. (2005). Furthermore, the solubility of O_2 exhibited minimal to no increase when CO_2 was present (Shi et al. 2008). Experiments on CO_2/O_2, after modification, affirmed the results, revealing that the estimated selectivity of CO_2 in the CO_2/O_2 mixture is nearly ideal (Shiflett et al. 2010). In their studies, Shiflett et al. and Jalili et al. explored the solubility of H_2S and CO_2 in Ionic Liquids, including [bmim][PF6], [omim][Tf2N], and [bmim][MeSO4] (Shiflett et al. 2010a, 2010b, Jalili et al. 2010). The results revealed that the solubility of CO_2 and H_2S in [bmim][MeSO4] and [bmim][PF6] is contingent upon the feed composition and the temperature conditions. At a temperature of 298.15 K, the solubility values were observed to range from 1 to 4 and from 1 to 10, respectively. Furthermore, the study also assessed the selectivity of CO_2 in the ionic liquid [omim][Tf2N] at 303.15 K was approximately 3.

In the context of CO_2 removal from natural gas, which is processed at elevated pressures, the selectivity for CO_2 does not correspond with the effectiveness of the CO_2 capture method. As mentioned earlier, in the pre-combustion technique, both H_2 and CO_2 exhibit high selectivity. Thereby, the absorption of CO_2 from natural gas ought to be examined in relation to actual operating conditions. Yokozeki et al., Shi et al., and Kumełan et al. Investigated primarily the selectivity of CO_2 and H_2 (Yokozeki et al. 2007, Shi et al. 2008, Kumełan et al. 2011). The selectivity of CO_2 and H_2 in the ionic liquid [bmim][PF6], showing that increases in temperature and pressure lead to a reduction in both selectivity values (Yokozeki et al. 2007). Furthermore, Kim et al. (2007) revealed that [hmim][Tf2N] exhibits significant selectivity for CO2 in a CO2/N2 mixture. The negligible absorption of N2 by the ionic liquid signifies an exceptional CO2 uptake and high operational efficiency.

In essence, the primary determinant for CO2 absorption via ionic liquids is largely reliant on the gas composition, especially the ratio of CO2 to N2. The selectivity for CO2 in different ionic liquids exceeds that of N2, indicating a highly effective CO2 capture process. Although the standard selectivity of CO2 in a CO2/H2 mixture within ionic liquids is relatively high, it is anticipated that the actual selectivity will decrease at higher temperatures. As the temperature rises, the solubility of H2 in ionic liquids is enhanced, while CO2 experiences a decline in solubility under similar temperature conditions. In the context of natural gas sweetening, it is crucial to eliminate various pollutants, with CO2 and H2S, along with CO2 and CH4, being the most frequently removed. Ionic liquids exhibit a standard selectivity for CO2/CH4 that is similar to that of natural solvents; nevertheless, the actual selectivity for CO2/CH4 in ionic liquids is estimated to fall short of the standard selectivity. In addition, the standard selectivity for the mixture of CO2 and H2S cannot be foreseen, since the solubility of CO2 is greatly diminished by H2S, which exhibits a much higher solubility in ionic liquids. Thus, although both gases can be removed simultaneously, this may not be the most effective strategy, as it could require an additional step to remove CO2 from H2S.

4.5 Volatility of Ionic Liquids

Ionic liquids are often characterized by their low vapor pressure. Nonetheless, Earle and co-workers challenged this assumption by demonstrating that aprotic ionic liquids could be distilled at 300°C under vacuum pressure without any significant signs of decomposition (Earle et al. 2006). At a temperature of 169°C and a pressure of 0.08 bar, the [hmim] [Tf2N] ionic liquids can be distilled while maintaining stability and avoiding substantial decomposition. Esperanca et al. and Carvalho et al. were tried to establish a correlation among the adhered properties of ionic liquids like enthalpy of vaporization (ΔH_{vap}), boiling temperature, vapor phase. Moreover, also determine the dependency of vapor-liquid equilibrium of ionic liquids on vapor phase and enthalpy of vaporization, while ensuring that their decomposition does not occur at high temperatures (Esperança et al. 2010, Carvalho et al. 2011). The vapor phase and enthalpy of vaporization of ionic liquids under extreme vacuum conditions were investigated using line-of-sight mass spectroscopy. The findings revealed that the vapor phase comprises neutral ion pairs, and the enthalpy of vaporization predominantly adheres to the Coulombic relationship between the liquid and vapor states (Armstrong et al. 2007). Additionally, Rai et al. (2011) employed molecular modeling techniques to analyze the vapor phase of ionic liquids. Simulation results suggests that the vapor phase is mainly characterized by single ion pairs, and a substantial amount of ions is observed in larger mass forms, which becomes more pronounced with increasing pressure and temperature. Koddermann et al. and Esperança et al. did experiments to deduce the enthalpy of vaporization of ionic liquids using temperature-programmed desorption, molecular dynamics simulation, the Knudsen method, surface tension, and microcalorimetry (Koddermann et al. 2008, Esperança et al. 2010). Regrettably, these methods do not yield consistent ΔH_{vap} results for ionic liquids. For the ionic liquid [omim][Tf2N], the calculated ΔHvap values were found to be in the range of 150 - 192 kJ/mol (Ludwig et al. 2007). Nevertheless, Rebelo et al. (2005) have reported that the reliable range for ΔH_{vap} is between 120 - 200 kJ/mol. Likewise, [OMIM][BF4] and [BMIM][BF6] have revealed an outstanding CO2 uptake capabilities, ranging from 80.8 - 99.8% and losses confined to 5 - 8% (Swati et al. 2022).

The ΔH_{vap} of imidazolium ionic liquids was determined through far-infrared calculations, which indicated a range of 128 - 165 kJ/mol (Fumino et al. 2010). In contrast, the ΔH_{vap} for a set of twelve ionic liquids was determined using line-of-sight mass spectroscopy (Deyko et al. 2009). The analysis is predicated on the cumulative influence of Coulombic interactions alongside the contributions of van der Waals forces between the two ions, namely the cation and anion. Precise vapor pressure data for nine imidazolium-based ionic liquids has been reported (Rocha et al. 2011). The values were ascertained through the quantitative assessment of structural separation phenomena in ionic liquids, incorporating corrections for the applicable thermodynamic properties. The vapor pressure data for all ionic liquids at 450 K was approximately 0.02 Pa, indicating a very low pressure that falls below typical experimental conditions. Despite this low pressure, the volatility of the ionic liquid is still anticipated. The insignificant volatility of the ionic liquid is not expected to have a detrimental effect on its applications as a green solvent (Kianfar et al. 2020). Noorani and co-authors investigated the CO2 absorption capacity of vinyl imidazolium amino acid-based ionic liquids at around 283 K. Their findings revealed the following order of CO2 absorption capacity: [BIm][L-Pro] < [BIm][L-al] < [BIm][L-Ala] < [BIm][Gly] < [BIm][L-Lys] < [BIm][L-Arg] (Noorani et al. 2022). Among the vinyl imidazolium amino acid-based ionic liquids examined, [BIm][L-Arg] exhibited the highest capacity for CO2 absorption, attributed to the presence of a greater number of amino groups.

5. Task Specific Ionic Liquids

Task-specific ionic liquids, also called functionalized ionic liquids, are designed to improve the performance of conventional ionic liquids for particular applications through alterations in their ionic composition. Over the past ten years, the study of ionic liquids has evolved to encompass three forms of task-specific ionic liquids that specifically address CO2 capture: anionic-functionalized ILs, cationic-functionalized ILs, and dual-functionalized ILs. The objective of optimizing these functional groups is to increase the efficiency of CO2 absorption by strengthening the interaction between carbon dioxide and ionic liquids. A recently developed ionic liquid exhibits a two-dimensional structure composed of 2D-ordered mono-IL configurations (Wang 2022). As noted earlier, the low solubility of CO2 is the key constraint in the capture of CO2 from post-combustion processes that employ ionic liquids. Research has shown that the solubility of CO2 in various ionic liquids, including those with the most favorable physical configurations, is less than 5 mol%. The integration of amine chemistry with ionic liquids has notably boosted the efficiency of CO2 capture. As a result, the adjustment and development of these ionic liquids have proliferated significantly.

5.1 *Cationic functionalized ILs*

The concept of task-specific ionic liquids was initially introduced by Bates et al. (2002) and Davis (2004). The researchers combined an imidazolium cation with a primary amine fraction and a cationic-functionalized IL, achieving a CO2 uptake ratio of 2:1. The results from these studies illustrated that the stoichiometry of CO2 capture was comparable to the maximum theoretical molar limit for CO2 absorption in traditional amine systems. The reversibility of the CO2 uptake implies a potential for an efficient and simple regeneration process. Under vacuum, the produced cationic-functionalized IL was regenerated at temperatures between 80-100ºC. In their study, Ding et al. detail the process of in-situ polymerizing confined imidazolium-based poly ionic liquids (ILpoly) into a metal-organic framework, resulting in the formation of ILpoly-MOF (Ding et al. 2018). The ILpoly-MOF that was created showed excellent CO2 capture abilities, with a notable capacity for CO2 uptake. According to Bernard and co-authors, the interaction of amine with [BEIM]BF4 led to varying CO2 uptake capacities, influenced by the type of amine employed (Bernard et al. 2019). The findings of this study indicate that the mixture of Methyl diethanolamine (MEDA) with [BEIM]BF4 possesses a remarkable ability to uptake CO2 during cycling processes. In addition, it showcases energy efficiency, strong regeneration potential, and a low viscosity profile, which are advantageous for practical use. The compounds [3-AP][TFA] and [MDEA][TFA] were recently subjected to tests to evaluate their CO2 absorption under different mixing ratios, specifically within the range of 2:1 to 1:6. The findings indicated that [3-AP][TFA] attained a CO2 uptake of 0.91 mol CO2 per mol of ionic liquid at a 1:6 ratio, exceeding the performance of [MDEA][TFA]. A ratio of 1:4 was identified as the most effective, yielding a CO2 absorption of 0.93 mol CO2 for every mol of ionic liquid. The outcomes reveal that augmenting the capacity for CO2 absorption does not necessitate a significant quantity of MDEA (Shohrat et al. 2022). Likewise, it was verified that the interaction of mono-ethanolamine (MEA) and di-ethanolamine (DEA) with [Rmim][Tf2N] resulted in different CO2 uptake capacities, as depicted in Figure 6. ILs-amine demonstrates a CO2 uptake that is two orders of magnitude greater than that of IL-DEA (Camper et al. 2008). The potential of ILpoly combined with polyurethane structures is being examined for its effectiveness in CO2 capture. Thus, a range of anionic ionic liquids derived from polyurethane was established, and the study explored the impact of the polyol's chemical structure and various counter-cations (including imidazolium, phosphonium, ammonium, and pyridinium) on the absorption of CO2 at different CO2/CH4 ratios. Dual-functionalized ionic liquids (CAT-ANILs) were created by altering the cationic ionic liquid [bmim] through the introduction of primary and tertiary amines. The resulting cations were then paired with the anionic ionic liquids [DCA] and [BF4] (Sánchez et al. 2007). The developed CAT-ANILs ([bmim][DCA] and [bmim][BF4]) did not exhibit a significant increase in CO2 solubility.

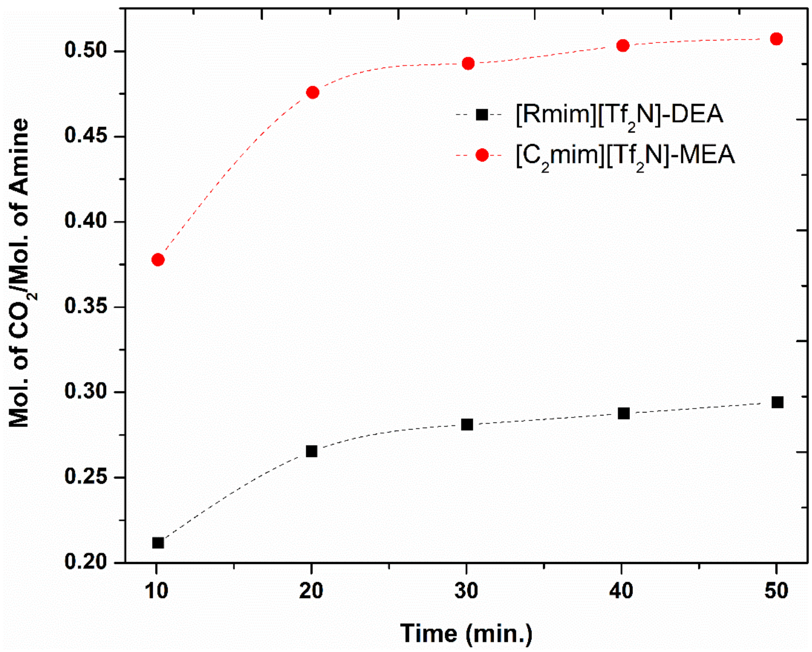

Figure 6 The uptake of carbon dioxide in equimolar concentration of ionic liquids namely, [Rmim][Tf2N]-DEA and [C2mim][Tf2N]-MEA.

The combination of the cationic ionic liquid [bmim] with the anionic ionic liquid containing an amino group, [Ambim], markedly improved CO2 capture at a temperature of 303 K and a pressure of 0.1 MPa, achieving enhancements of 13 and 14 times for [Ambim][BF4] and [Ambim][DCA], respectively (Sánchez et al. 2007). Thus, it was recommended that the presence of amine groups in the cationic ionic liquid contributed to an improvement in CO2 solubility. The isotherms being investigated illustrate that the interaction between CO2 and functionalized ionic liquids is attributed to chemical absorption, indicating that CO2 may be separated from the flue gas stream, even at low pressure levels. The uptake of CO2 was found to be more effective in amine-modified ionic liquids than in the tertiary-amine modified IL [3Amim][BF4]–CO2, due to the notably lower solubility of CO2 in the latter. This observation was intended to minimize the reactivity between tertiary amines and CO2 (Vaidya et al. 2007). The task-specific ionic liquid retained its CO2 uptake capacity when reproduced at 353 K under vacuum condition. Nonetheless, viscosity issues with CO2 were reiterated after the reaction took place. The use of task-specific ionic liquids has yielded favorable results in the realm of CO2 capture. However, their high viscosity presents a challenge that hinders the feasibility of scaling up their application. The application of non-modified amine solutions in room-temperature ionic liquids can efficiently mitigate the viscosity concerns associated with amine-functionalized ionic liquids (Camper 2008). The majority of ionic liquids tend to absorb more CO2 as the operating pressure increases. According to Fatima et al., some non-modified room temperature Ionic liquids (NRTILs) exhibit considerable CO2 uptake even at reduced pressures, owing to their enhanced reactivity with CO2 (Fatima et al. 2021). Thus, a solution consisting of 50 mol% Mono Ethanol Amine (MEA) combined with NRTIL was capable of attaining a CO2 absorption ratio of nearly 2:1, closely aligning with the stoichiometric ratio of the 1 MEA process (Ramdin et al. 2012). This approach facilitates a decrease in the viscosity of ionic liquids from approximately 20 mPa.s to values akin to those found in aqueous MEA solutions, particularly below 3.1 mPa.s. The viscosity of the NRTIL mixed with a 30 wt% MEA solution at 25˚C has been reported to be 2.2 mPa.s. High viscosities observed through molecular simulation was elucidated by Yu et al. (2007). The findings revealed that incorporating an amino group into the imidazolium ring does not impact the anionic configuration, as the anions are uniformly distributed over the –NH2 group, facilitated by strong hydrogen bonding interactions. There was a significant decline in the coefficient of ionic self-diffusion compared to the non-functionalized counterparts, leading to an increase in viscosity. Likewise, Gutowski and co-author employed molecular modeling to provide insights into the significant viscosity increases that occur during the CO2 capture process involving amine-modified ionic liquids

(Gutowski et al. 2008). The conclusion drawn is that the viscosity enhancement is due to the slow translational and rotational movements of amine-modified ionic liquids, in conjunction with the formation of a strong and pervasive network of hydrogen bonds.

5.2 *Anionic functionalization ILs*

Cation-functionalized ionic liquids (CAT-FUNILS), including amine-functionalized cations, are recognized for their effectiveness in CO2 capture during pre-combustion conditions. Nevertheless, to enhance the efficiency and practicality of the process, it is important to optimize the reaction stoichiometry currently set at 1:2. In their study, Gurkan and co-authors found that the 1:2 stoichiometry present in amine-functionalized cation systems correlates with the formation of carbamate during the binding process between an amine and a cationic group (Gurkan et al. 2010). It was proposed that the stoichiometric ratio could be minimized to 1:1 by affixing an amine group to a particular anion group. The stoichiometric ratio of 1:1 was attained using two amino acid-derived ionic liquids, [P666,14][Met] and [P66614][Pro]. Figure 7 illustrates the anticipated isotherms for CO2 capture utilizing anion-functionalized ionic liquids (AN-FUNILS) with this specific stoichiometric ratio. The isotherms can be categorized into two separate elements: a steep increase at low pressure due to chemical absorption and a gradual increase in capacity at elevated pressure resulting from physical absorption. A major aspect of CO2 capture is attributed to chemical absorption, which achieves a stoichiometric ratio of 1:1, as validated by FTIR measurements (Gurkan et al. 2010). Nonetheless, amine-modified ionic liquids are distinguished by their high enthalpy and viscosity. At a temperature of 25˚C, the enthalpies associated with the CO2 capture reactions utilizing [P66614][Met] and [P66614][Pro] were found to be −64 kJ/mol and −80 kJ/mol, respectively. The results suggest that these values correspond to the average physical absorption levels of traditional amines, which lie between -10 and -20 kJ/mol, and the average chemical absorption levels, which are between -85 and -100 kJ/mol. The viscosity of cation-functionalized ionic liquids increases upon reacting with CO2, attributed to the creation of a hydrogen-bonded network. Different studies revealed analogous trends (Chen et al 2022, Goodrich et al. 2011, Shi et al. 2020). The viscosity of the mixture containing CAT-FUNIL ([P66614]) and deprotonated anions from amino acids, including isoleucinate and glycinate, increased by a factor of 240 compared to the pure ionic liquids. As viscosity rises, more energy will be needed to pump the viscous ionic liquid, and concurrently, the effectiveness of CO2 capture will decline because of the decreased diffusion of CO2 within these liquids. In their study, Voskian et al. synthesized an AN-FUNIL from ethylenediamine, which demonstrated a CO2 absorption capacity of around 42 mgCO2/gIL. The high viscosity of the AN-FUNIL probably resulted in kinetic and gas contact challenges for the cell (Voskian et al. 2020). The carbon dioxide capture efficiency of amino acid ionic liquids, like alanine (Ala), arginine (Arg), glycine (Gly), histidine (Hist), lysine (Lys), proline (Pro), serine (Ser), and taurine (Tau) was done by Shahrom and colleagues (Shahrom et al. 2019). Among the various compounds tested, [Lys] showed the most significant CO2 uptake, reaching 15.7 wt%. Regarding molar adsorption, [VBTMA][Arg] demonstrated the greatest CO2 uptake capacity at 0.83 mol/mol, which increased to 1.14 mol/mol after undergoing polymerization. It was noted that the ionic liquid regeneration process improves with increased pressure and decreased temperature, reaching maximum CO2 desorption at 80˚C. Moreover, this material has been shown to possess high recyclability, sustaining 86% of its CO2 uptake capacity after five cycles. A new imidazolium-based TIL (TCMI-IL) has been synthesized recently, employing three amine-based chains (Hafizi et al. 2021). The physical and chemical attributes of this innovative tricationic ionic liquid were evaluated using a simple and efficient production process. The relationship between absorption temperature and ionic liquid content was analyzed at different equilibrium pressures, spanning from 90 to 240 kPa. The tricationic ionic liquid exhibited superior CO2 absorption and remarkable structural flexibility.

Amiri et al. employed cyano-based anion functionalized ionic liquids (AN-FUNILS), namely 1-hexyl-3-methylimidazolium tetracyanoborate ([hmim][TCB]), to facilitate the uptake of CO2 process from a gas mixture comprising CH4 and CO2 (Amiri et al. 2021). The synthesized [hmim] [TCB] revealed a high capacity for CO2 uptake and a viscosity that is lower than that of the organic ionic liquids (DEPG-Selexol). Additionally, the [hmim] [TCB] exhibited an impressive capability to absorb CO2 from a feed gas stream containing 20 to 40 mol % CO2, surpassing the performance of DEPG-Selexol. The remarkable absorption of CO2 persisted even when the concentration was reduced to as low as 5 mol%. The [hmim][TCB] underwent regeneration via swing pressure and temperature methods. The use of AN-FUNILS alongside anions, such as acetate, has been recognized as a promising material for the capture of CO2. Wasewar (2021) investigated the effectiveness of using a combination of AN-FUNILS and acetate ([bmim][acetate]) at a dilution of 14 wt% in solution for capturing CO2. The 14 wt% AN-FUNILS revealed exceptional CO2 uptake, reaching a volumetric capacity of approx. 25 m^3/m^3.

This value exceeds that of physical ionic liquids, which is approximately 3 m^3/m^3; nonetheless, it remains below 30 wt % aqueous MEA in the solution, roughly 65 m^3/m^3. The findings of Maginn et al. indicated that the CO2 absorption in the [bmim][acetate] system is a result of the acetate anion facilitating proton removal from the C2 position of the imidazolium ring, culminating in the formation of acetic acid (Maginn et al. 2005). In contrast, Shiflett et al.(2008) argued that the acetic acid production method outlined by Maginn et al. (2005) is not very efficient. Additional experimental investigations revealed the generation of acetic acid within the reactor. The authors described the phase characteristics of the CO2+[bmim][acetate] system as distinctly atypical, marked by significant intermolecular forces and intricate reactions. Lately, advancements have been made in the development of hybrid materials that utilize ionic liquids supported on inexpensive renewable resources, like the microporous structure of carbonized agave bagasse fibers, to enhance the capacity for CO2 uptake.

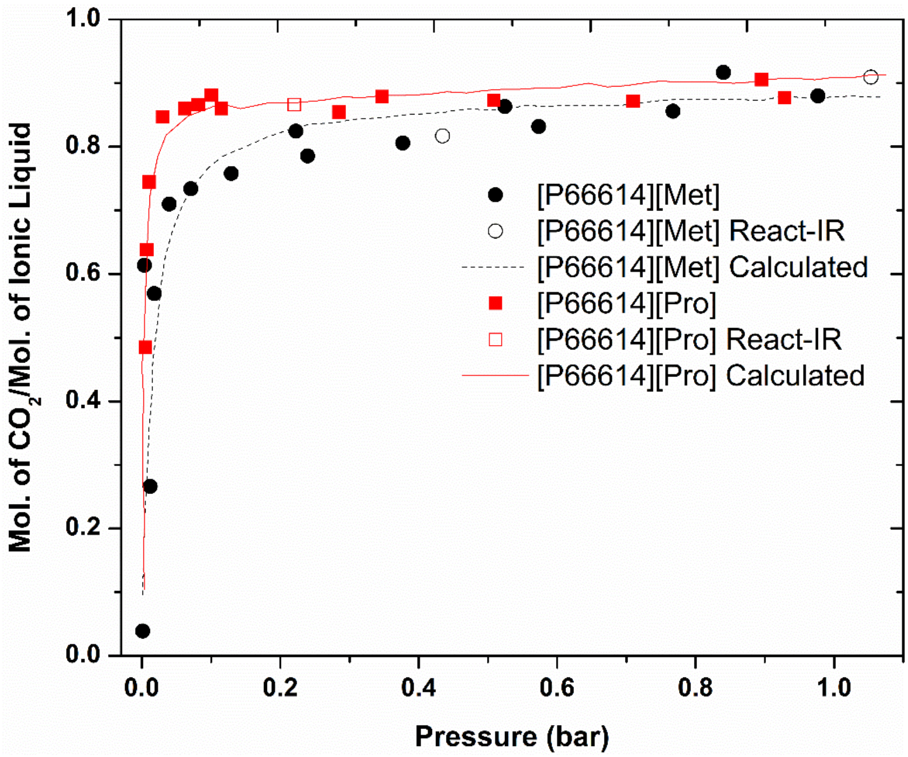

Figure 7 The absorption of carbon dioxide at 22°C by [P66614][Pro] and [P66614][Met]. Reproduced with the consent of Gurkan et al. 2010, J. Am. Chem. Soc. 132, 2116-2117 & Ramdin et al. 2012, Ind. Eng. Chem. Res. 51, 8149-8177.

As mentioned earlier, the ionic liquid 1-butyl-3-methylimidazolium acetate (Isaacs-Páez et al. 2022) possesses an outstanding ability to absorb CO2, exhibiting a high affinity for CO2. The CO2 absorption capacity was analyzed following the addition of this ionic liquid to acid-washed carbonized fibers, carbonized fibers, and impregnated carbonized fibers, using various mass ratios of CO2. At a mass ratio of 1:103, the combination of Carbonized fibers ionic liquid

(CF-IL) led to an increase in CO2 uptake from 0.77 mmol CO2/g IL for the ionic liquid to 1.29 mmol CO2/g IL for the CF-IL. The tests performed over a duration of 50 minutes demonstrated that the new combination improved the CO2 uptake rate from 0.012 to 0.02 mmol.CO2/min.g, suggesting a significant potential for CO2 capture. The work of Wang et al. involved the alteration of superbase-derived protic ionic liquids (S-DPILs), referred to as (MTBD), by the inclusion of weak proton donors, comprising different partially fluorinated alcohols such as HFPD, TFPA, TFE, pyrrolidone, phenol, and imidazole (Wang et al. 2010). Each of the combinations exhibited remarkable properties for capturing CO2. Notably, the [MTBDH+]/[TFE-] pair displayed a rapid CO2 uptake, a low viscosity of 8.63 cP at 23°C, and a substantial CO2 uptake capacity of 1.13 mol CO2 per mol of S-DPILs. Furthermore, reports indicate that the S-DPILs exhibited a negligible loss in capacity after undergoing several CO2 uptake cycles. The regeneration of these S-DPILs was achieved by employing nitrogen aeration at 80°C. A distinct form of hybrid material, which is a polyamine-based protic ionic liquid (PIL), was generated by incorporating tetraethylenepentammonium nitrate [TEPA][NO3] into SBA-15 along with mesoporous silica (Zhang et al. 2019). The newly developed hybrid adsorbent demonstrated a CO2 uptake rate of 147×10^{-3} mmol/g.s, which is three times greater than that of current IL-functionalized and amine-modified support systems. Furthermore, the CO2 uptake capacity can be increased to 2.15 mmol/g by elevating the temperature to 333 K and lowering the pressure to 0.15 bar, indicating its excellent performance in low-pressure CO2 environments. The compound underwent regeneration through nitrogen aeration at a temperature of 373 K, which restored around 90% of its original CO2 uptake capacity. Figure 8 provides an overview of the CO2 solubility for various functionalized ionic liquids like [Guad-(6,6),(1,1),(1,1)][DCA] and [Guad-(6,6),(1,1),(1,1)][TCM] (Krolikowski et al. 2023).

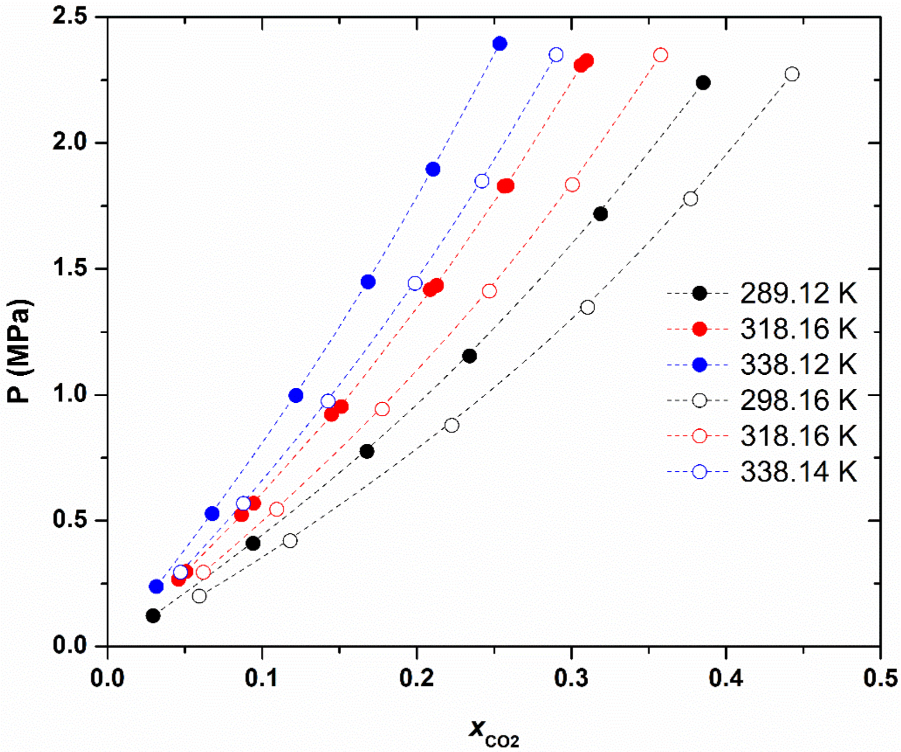

Figure 8 Comparison of experimental data for the solubility of CO2 in: [Guad- [Guad-(6,6),(1,1),(1,1)][DCA] at 298.12 K (●); 318.16 K (●); and 338.12 K (●); and [Guad-(6,6),(1,1),(1,1)][TCM] at 298.17 K (○); 318.16 K (○); and 338.15 K (○).

6. The Biodegradable Nature of Ionic Liquids

The molecular structure of ionic liquids, which encompasses anions, cations, and functional groups, plays a crucial role in determining their biodegradability. Consequently, biodegradability is typically assessed and related to the molecular structure. Additionally, the biodegradability of ionic liquids is also contingent upon the application conditions and the point of effluent discharge (Singh et al. 2020, Brzęczek-Szafran et al. 2020). The evaluation of the biodegradability of different chemical substances was carried out following the standards set forth by the Organization for Economic Co-operation and Development (OECD) (Wu et al. 2019). The Organization for Economic Co-operation and Development is an intergovernmental organization comprising 38 member states, dedicated to fostering economic progress and international trade. Various methodologies are in accordance with OECD regulations, such as die-away test (OECD 301A), modified Sturm test (OECD 301B), closed bottle test (OECD 301D), aerobic mineralisation in surface water-simulation biodegradation test (OECD 309), ASTM D 5988 test, CO2 headspace test (ISO 14593). Different techniques are founded on individual concepts that involve analyzing CO2 production, dissolved organic carbon, and O2 uptake as criteria for assessing biodegradability. The determination of biodegradability suitability is reliant on the physical properties of the ionic liquid. Gathergood et al. (2004) and Garcia et al. (2005) were pioneers in identifying the biodegradability of imidazolium ionic liquids. The results from the closed bottles of [bmim][X] ionic liquids, with X being Br, BF4, PF6, TF2N, DCA, and octyl sulfate, indicated that the biodegradability of [bmim][X] ionic liquids is very minimal, less than 5%. In contrast, octyl sulfate ionic liquid showed a moderate biodegradability of 25%. Consequently, these ionic liquids do not meet the criteria to be labelled as "biodegradable" or environmentally friendly. Furthermore, it has been established that a minimum biodegradability of 60% is necessary for an ionic liquid to be considered green in a standard 28-day testing period (Garcia et al. 2005, Gathergood et al. 2006). To enhance the biodegradability of the ionic liquids discussed earlier, Gathergood et al. (2004) utilized the instructions provided by Boethling et al. (2007). Although these requirements are primarily intended as general guidelines, they can additionally essential prerequisites for the formulation of biodegradable ionic liquids. To improve the biodegradability of ionic liquids, the alkyl side chain of the imidazolium cation was modified by the addition of either an ester or an amide group (Buettner et al. 2022). Findings revealed that extending the length of the ester alkyl chain in the modified cation led to enhanced biodegradability. Incorporating a methyl group at the C2 position of the imidazolium ring led to only a slight increase in biodegradability relative to the C2-unsubstituted ionic liquids (Buettner et al. 2022). In contrast, the ester-functionalized ionic liquids showed enhanced biodegradability relative to the non-modified ionic liquids. The incorporation of the [mim-ester] cation and the [octyl sulfate] anion resulted in a biodegradability exceeding 60%. Therefore, the findings indicate that the combination of ester-modified imidazolium cations and an [octyl sulfate] anion results in biodegradable ionic liquids (Gathergood et al. 2006, Verma et al. 2022).

In their study, Morrissey and co-authors assessed the biodegradability of a wide range of imidazolium-based ionic liquids employing the CO2 headspace test (Morrissey et al. 2009). The ionic liquids tested incorporated ester and ether groups within their alkyl chain structure. The presence of ester groups in ionic liquids contributed to their biodegradability, while those containing ether functionalities exhibited very limited biodegradability. Likewise, the biodegradability of ester-functionalized pyridinium ionic liquids, characterized by a cation associated with multiple anions such as bromide, iodide, bis(trifluoromethyl sulfonyl)imide, PF6, and octyl sulfate, employing the CO2 headspace test. The study revealed that pyridinium ionic liquids with ester side chains exhibited considerable biodegradability, whereas those with alkyl side chains devoid of ester functionalities were not biodegradable. The findings suggest that the anion's contribution to biodegradability is not substantial (Mena et al. 2020, Harjani et al. 2009, Zhang et al. 2010). An investigation into the biodegradability of pyridinium and thiazolium ionic liquids, characterized by various functionalities such as acetal, carbamate, ethyl ether side chains, hydroxyethyl side chains, and methyl was carried out by Ford and coauthors (Ford et al. 2010). The study revealed that pyridinium ionic liquids possessing the hydroxyethyl functionality were highly biodegradable. Conversely, thiazolium ionic liquids with ether, carbamate, acetal, and hydroxyethyl functionalities showed reduced biodegradability. Moreover, both phosphonium and ammonium ionic liquids, in conjunction with the octyl sulfate anion, was found to be low (Kowalska et al. 2021).

7. The Toxic Nature of Ionic Liquids

The investigation of toxicology is fundamental for elucidating the effects of ionic liquids on both human being and the environment systems. The evaluation of IL toxicity is conducted using established protocols, including those set by ASTM, ISO, or OECD. The reaction of microorganisms, used as a testing model, to ionic liquid exposure is indicative of toxicity, commonly measured in terms of LC50, IC50, or EC50 values. Important insights into the toxicity of ionic liquids have been discussed in various reviews, where the toxicity is particularly noteworthy (Zhao et al. 2007, Petkovic et al. 2011, Flieger et al. 2020, Gonçalves et al. 2021). In the evaluation of ionic liquid toxicity, the cation is deemed essential, while the anion has a negligible effect on this assessment (Yan et al. 2019, Cho et al. 2021, Matzke et al. 2007, Couling et al. 2006). Two aquatic test models were employed to evaluate the ecotoxicity of quaternary phosphonium, quaternary imidazolium, pyridinium, and ammonium ionic liquids. Findings revealed that the EC50-based toxicities of all the ionic liquids were lies between approximately 104 - 106, exceeding the toxicity levels of conventional solvents (Wells et al. 2006). In addition, the toxicity of the ionic liquid containing a chloride anion lessened with an increase in the alkyl chain length of the imidazolium cation (Romero et al. 2008, Hernández-Fernández et al. 2022). This pattern has been identified in ammonium, pyridinium (Fütyu et al. 2022), pyrrolidinium (Ghanem et al. 2023), phosphonium (Sani et al. 2019), and morpholinium (Baruah et al. 2022) ionic liquids. Furthermore, the marine toxicity of ionic liquids with diverse head groups was explored by Stolte et al. (2007). Their findings revealed a correlation between the lipophilicity of ionic liquids and their ecotoxicity, indicating that toxicity levels rose with increasing lipophilicity (Padilla et al. 2021). A larger alkyl chain not only boosts the hydrophobic characteristics of ionic liquids (ILs) but also leads to a rise in toxicity as the chain length increases. Additionally, the toxicity is further augmented by the number of alkyl chains attached to the cation.

Quantitative structure property relationship (QSPR) model to evaluating and calculating the toxicity associated with ionic liquids was developed by Couling et al. (2006). This model indicates a toxicity ranking among cations, arranged from least to most toxic as follows: ammonium, pyridinium, imidazolium, triazolium, and tetrazolium. Nevertheless, this trend is not commonly observed, as pyridinium and ammonium ionic liquids tend to be more toxic than imidazolium ionic liquids (Stolte et al. 2007, Pretti et al. 2009). Although the anion plays a secondary role in the toxicity of ionic liquids, it can significantly enhance or mitigate their toxic effects. Frade et al. compiled toxicity data for marine organisms, revealing the following trend in anion toxicity: [Tf2N] > [PF6] > [BF4] > [Cl] > [DCA] > [Br] (Frade et al. 2010). Anions that are fluorinated, such as BF4, and Tf2N exhibit toxicity and represent a major environmental threat (Vieira et al. 2019).

The toxicity of ionic liquids is not uniform; each type presents its own toxicity profile, with [C8mim]Cl being notably toxic. A key determinant of ionic liquids' toxicity is the length of the alkyl chain present in the cations. The toxicity of ionic liquids escalates with the elongation of the cation's alkyl chain. Figure 9 Illustrates the correlation between the length of the alkyl chain in ionic liquids and the EC50 values observed in IPC-81 cells. The data indicates a nearly exponential decline in the EC50 value corresponding to the elongation of the alkyl chain from 2 to 10 carbons. The EC50 value for the short-chain [C2mim]Cl is 7.2 mmol/L (equivalent to 1100 mg/L or approximately 0.1 wt%), which is significantly greater than that of [C8mim]Cl (Kuroda et al. 2022).

In conclusion, multiple testing models have been employed to measure toxicity, and these models can exhibit varying responses to comparable ionic liquids. Therefore, it is crucial to avoid transferring data from one test model to another. Nonetheless, it is reliably noted that toxicity tends to increase with the elongation of the alkyl chain and the number of alkyl chains in the cation. Lastly, the morpholinium cation and the DCA anion are considered to be an effective options for lessening toxicity (Hernández-Fernández et al. 2022, Cłapa et al. 2021).

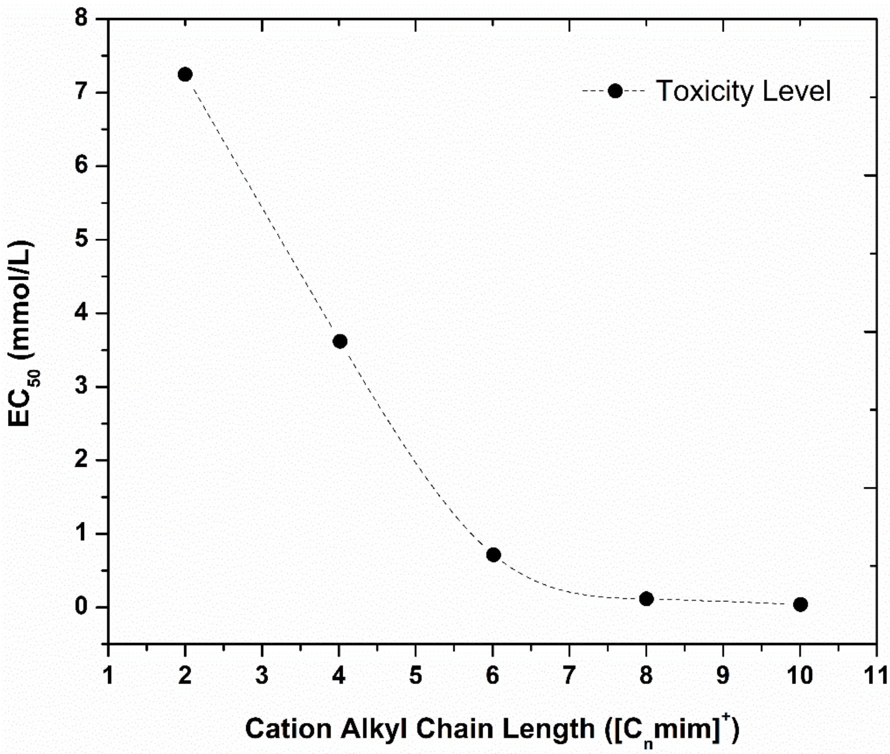

Figure 9 The correlation between alkyl chain length and the EC50 value of [Cnmim]Cl in relation to IPC-81 cells.

8. Ionic Liquids' Efficiency in Comparison to Commercial Solvents for CO2 Capture

The absorption of CO2 through ionic liquids is contingent upon their characteristics and interactions with the solvents involved in the process. Thus, in comparing the performance of ionic liquids to that of commercial solvents for CO2 uptake, one must evaluate characteristics such as absorption capacity, viscosity, selectivity, stability, and cost. The choice of solvent for carbon dioxide capture will depend on various factors, including partial pressure of the gas, operational conditions, and the properties of the products and contaminants involved (Haider et al. 2022). The effectiveness of ionic liquids for CO2 absorption is compared to that of commercially available solvents. The solvents Fluor, Purisol, Rectisol, and Selexol were assessed independently based on their physical CO2 uptake, whereas Sulfolane and Sulfinol were utilized in conjunction with DIPA and MDEA, respectively (Elmobarak et al. 2023). The econamine technique requires the incorporation of Fluor with minimum of 30 wt% MEA to ensure optimal CO2 uptake through chemical absorption (Chao et al. 2021). The financial outlay for implementing various ionic liquids in large-scale CO2 capture processes is significantly elevated, being 10 to 20 times more than that of standard solvents (Ramdin et al. 2012, Hospital-Benito et al. 2021). In this regard, the successful application of ionic liquids is reliant on additional properties of these liquids. As discussed earlier, ILs usually possess a higher viscosity than commercial solvents like DIPA and MEA, which does not constitute an advantage for their application in CO2 uptake. Yet, considering that ionic liquids are consistently applied in a diluted manner, with viscosities that are not considerably greater than that of water, the issue of viscosity challenge is rendered negligible. A key characteristic of ionic liquids that facilitates their application in CO2 uptake is their significantly lower vapor pressure in comparison to conventional solvents currently in use. Most of the Ionic liquids put forward exhibit lower vapor pressures and viscosities in solution, which are comparable to the successful application of the Selexol method.

The low volatility of ionic liquids is another attribute that underpins their effectiveness in CO2 uptake. As the most prevalent method for carbon dioxide absorption, the MEA process is plagued by considerable volatility and thermal degradation. These factors considerably impact both the efficiency and cost-effectiveness of the CO2 uptake process (Ochedi et al. 2021, Gusnawan et al. 2020). The findings of Goff et al. reveal an overall loss of MEA at the stripper, quantified between 80 and 540 g/ton, across a temperature range of 110 to 30°C. This loss incurs solvent replacement costs estimated to be between \$0.19 and \$2.31 per ton (Goff et al. 2004, Davis et al. 2009). The results of the Aspen Plus simulation demonstrate that ionic liquids might be an economically viable solution for CO2 uptake in the context of pre-combustion (Hospital-Benito et al. 2021). The findings of the study indicated that the ionic liquid [P2228][CNPyr] can undergo regeneration at a pressure of 1 bar. The expense associated with the absorption of CO2 was established at \$40 per ton of CO2. Performing the regeneration of the ionic liquid at 1 bar and at higher temperatures would be in line with the operational conditions of flue gas. Thus, preventing the high costs of equipment that are typically required for vacuum regeneration processes. Furthermore, this would reduce the utility expenses and lessen the heat transfer disparity between processes. The analysis of direct costs alone indicated a minimum cost of \$64.1 per ton of CO2, calculated from an ionic liquid price of \$50 per kilogram at scale. It is plausible that future solvent innovations could decrease this cost to under \$40 per ton of CO2.

Taking this into account, the inherent low volatility and thermal stability of ionic liquids under diverse operational conditions imply their economic viability for CO2 capture. Indeed, some studies have aimed to combine ionic liquids with monoethanolamine to tackle the volatility and thermal stability issues that MEA presents. The combination of [bpy][BF4] with MEA can lead to a reduction in reboiler duty costs by approximately 15% and a decrease in CO2 capture expenses by about 7.44% (Akinola et al. 2019). One more advantage of using ionic liquids for CO2 capture is their diminished corrosivity towards carbon steel relative to the MEA process. Furthermore, certain ILs have been identified as effective anti-corrosion agents (Kobzar et al. 2021). The existing body of research concerning the corrosion and degradation properties of ionic liquids is limited, indicating a need for further investigation in this area. Nevertheless, certain commonly utilized ionic liquids can become corrosive when they interact with copper alloys, particularly at higher temperature conditions (Yavuz et al. 2022, Jiang et al. 2022).

The preceding analysis of the costs involved in the ionic liquids process relative to its performance suggests that this technology is indeed attractive. Furthermore, the tunable characteristics of ionic liquids can be harnessed to design and produce cost-effective, thermally stable ionic liquids with a high capacity for CO2 uptake and selectivity. Ionic liquids can function independently or be mixed with traditional solvents. Moreover, they can be designed to perform effectively in conjunction with various conventional solvents. To illustrate, at post-combustion conditions with extremely low CO2 partial pressure, the integration of high-energy efficiency amine-modified ionic liquids, utilizing reaction stoichiometry, can be a more effective approach for CO2 capture compared to the standalone use of Sulfinol or MEA. Conversely, processes characterized by high partial pressures of CO2 in conjunction with ionic liquids may be applied, as detailed in Table 1, owing to the substantial solubility of CO2 present under these conditions. The integration of supported ionic liquid membranes could lead to a better price-performance ratio for ionic liquids.

9. Concluding Remarks and Future Directions

Attaining an effective separation of greenhouse gases, notably CO2, from flue gas is a challenging endeavor. The substantial energy requirements and associated cost for CO2 uptake from flue gas render ionic liquids an impractical choice for large-scale applications. A range of novel ionic liquid separation techniques and materials have been recommended to resolve this concern. This article assessed the literature on the CO2 capture process that incorporates ionic liquids. Researchers examined various trends related to the selectivity and solubility of CO2 in a range of ionic liquids. Furthermore, they investigated the effects of cations, anions, and functional groups on the physical attributes, biodegradability, volatility, and toxicity of these ionic liquids.

In post-combustion method, the solubility of CO2 in standard ionic liquids through physical methods is markedly lower than that of the amine approach. Furthermore, an increase in the molar free volume, molecular weight, and accessible volume of ionic liquids leads to a decrease in Henry's constant. Thus, the solubility of CO_2 in ionic liquids was analyzed in terms of molality (mol/kg), or molarity (mol/m3) rather than through a mole fraction perspective. The capacity for CO_2 absorption has been significantly enhanced by altering conventional Ionic Liquids to include an amine component, facilitating a chemical reaction between CO_2 and the amine.

An essential attribute for industrial separation processes is the selectivity of CO_2. The evaluation of selectivity for CO_2 revealed that it tends to exhibit greater solubility in ionic liquids than other gases, including H_2, N_2, and O_2. On a different note, ionic liquids demonstrate a high solubility for both H_2S and SO_2 gases. This indicates that the selectivity of CO_2 is likely to be excellent in CO_2/simple-gas systems, although it will be lower in CO_2/sour-gas systems. To address this challenge, the selectivity for CO_2 might be increased through the utilization of ionic liquids that possess a low molar-free volume. The high viscosity of modified and unmodified ionic liquids serves as a major impediment to their use in industrial applications. The insights provided in this review can aid in the development of Ionic Liquids with minimal viscosity. Furthermore, the scarce information regarding the biodegradability and toxicity of ionic liquids suggests that many frequently utilized ionic liquids are both nonbiodegradable and significantly toxic. Nevertheless, certain trends have emerged that indicate the possibility of developing relatively safe ionic liquids.

Additionally, in the context of ionic liquids commercialization, various obstacles must be resolved, including additional data is essential concerning chemical and thermal stability, corrosivity, water solubility, diffusion coefficients, viscosity, density, specific heat, the heat of fusion, surface tension, biodegradability, and toxicity. Furthermore, at present, the laboratory-scale cost associated with ionic liquids is nearly $1000 per kilogram, rendering them 100 to 1,000 times more expensive than traditional solvents. Nonetheless, the cost benchmark for conventional solvents is not available, as ionic liquids are intricate particles that necessitate additional innovative stages in their production and purification.

Competing Interests

The authors declare that they have no competing interests.

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