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Analysis of enhancement of CO_2 capture through dielectric investigation on amine – Acetate solvent systems

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Abstract

In this study, the dielectric properties such as the static permittivity, the Kirkwood correlation factor, excess permittivity, Bruggeman factor and dipolar excess free energy of binary mixtures (1) n - butylamine with n-butyl acetate, (2) Cyclohexylamine with n-butyl acetate and (3) Diethylamine with n-butyl acetate were investigated at different temperatures of 303K, 313K and 323K using dielectric spectroscopy method. The increase of static permittivity with the increasing concentration of acetate and negative excess permittivity values, are suggestive of dominant specific intermolecular forces, including hydrogen bonding and dipole-dipole interaction between the constituents. This supports the optimization of CO_2 absorption efficiency and is quite informative in the rational design of high-performance solvent systems.

Keywords: Dielectric spectroscopy, static permittivity, binary mixtures, intermolecular interactions, CO_2 absorption efficiency

Introduction

The cumulative increase in carbon dioxide concentrations of the atmosphere, primarily due to the fast industrialization process and burning fossil fuels, is an acute environmental issue that leads to the development of effective carbon capture methods. The process of chemical absorption using liquid solvents is known to be one of the most effective and the most industrial practicable methods out of the existing number of methodologies used. Amine-based solvents have been widely investigated owing to their high reactivity with CO_2 and efficient absorption characteristics; however, traditional systems are limited by challenges such as high energy demand during regeneration, solvent degradation, and corrosion problems [1,2].

To overcome these limitations, recent research has increasingly focused on the development of advanced and hybrid solvent systems, including binary mixtures and blended formulations. The incorporation of organic components and functional additives into amine-based solvents has been shown to significantly enhance CO_2 absorption capacity, reduce viscosity, and improve mass transfer characteristics [1, 2]. In particular, blended amine systems and additive-assisted solvents exhibit improved thermodynamic and kinetic performance due to strengthened intermolecular interactions and optimized solvent structure [3, 4]. To maximize the efficiency of such solvent systems, require a thorough study of the molecular interactions involved on the level of those liquid mixtures. In this context, dielectric spectroscopy has become a highly competitive tool of analysis to investigate intermolecular interactions, dipolar orientation and structural organization of complex liquid systems [1, 2]. The method is useful in characterizing molecular dynamics and provides the information on the mechanisms of interaction, based on which system behavior is determined. Dielectric parameters such as static permittivity, excess permittivity and the Kirkwood correlation factor are necessary data in regard to the presence of hydrogen bonding, polar interaction and nonideal mixing behavior [3, 4]. These parameters are very sensitive to molecular music and structural reordination, thus making them useful tools of understanding non-ideal systems and such processes of interaction at the microscopic level.

Theory

Different mixture formulae can be used to correlate the dielectric parameters with the molecular activities of liquid.

The Kirkwood Model

The Kirkwood correlation factor is a measure of the short-range interaction between the components in the liquid mixtures. For pure liquids and liquid mixtures, it can be described by the following expression [5-7].

$$\frac{4\pi N}{9kT}\left(\frac{\mu_A{}^2\rho_A}{M_A}X_A+\frac{\mu_B{}^2\rho_B}{M_B}X_B\right)g^{eff}=\frac{(\varepsilon_{0m}-\varepsilon_{\infty m})(2\varepsilon_{0m}+\varepsilon_{\infty m})}{\varepsilon_{0m}(\varepsilon_{\infty m}+2)^2} \tag{1}$$

$$\frac{4\pi N}{9kT}\left(\frac{\mu_A{}^2\rho_A g_A}{M_A}X_A+\frac{\mu_B{}^2\rho_B g_B}{M_B}X_B\right)g_f=\frac{(\varepsilon_{0m}-\varepsilon_{\infty m})(2\varepsilon_{0m}+\varepsilon_{\infty m})}{\varepsilon_{0m}(\varepsilon_{\infty m}+2)^2} \tag{2}$$

Where μ is the dipole moment in the gas phase, ρ is the density at temperature T, M is the molecular weight, k is the Boltzmann constant, N is the Avogadro's number,ε_0 is the static permittivity and ε_∞ is the static permittivity at high frequency, often represented by the square of refractive index corresponding to sodium D-line. X is the volume fraction and suffices m, A and B represents mixture, liquid A and liquid B respectively. The departure of Kirkwood correlation factor from unity is an indication for the molecular association. It means that if $g > 1$ indicates the parallel orientation among the dipoles, $g < 1$ indicates the anti - parallel orientation among the dipoles and $g = 1$ represents an equilibrium between the multimers or non – association among the dipoles.

Excess permittivity (ε^E)

The excess static permittivity is used to explain the formation of mutimers in the mixture [8-9]. It is defined as,

$$\varepsilon^E = (\varepsilon_{0m} - \varepsilon_{\infty m}) - \left[(\varepsilon_{0A} - \varepsilon_{\infty A})\ X_A + (\varepsilon_{0B} - \varepsilon_{\infty B})\ X_B \right] \qquad (3)$$

The excess permittivity provides qualitative information about multimer formation in the mixture as given below. If $\varepsilon^E = 0$ indicates that there is no interaction between the unlike molecules.

$\varepsilon^E < 0$ indicates the interaction between the molecules in such a way that the effective dipoles get reduced. The two liquids mix in such way that the mixture may form multimers leading to the less effective dipoles.

$\varepsilon^E > 0$ indicates that the two liquids interact in such a way that the effective dipoles increase. This may be due to the formation of monomers and dimers.

Bruggeman factor (f_B)

The Bruggeman factor is another parameter which may be used as an indicator of hetero interaction. The Bruggeman factor f_B is given by [10],

$$f_B = \left[\frac{\varepsilon_{0m} - \varepsilon_{0B}}{\varepsilon_{0A} - \varepsilon_{0B}} \right] \left[\frac{\varepsilon_{0A}}{\varepsilon_{0m}} \right]^{1/3} = (1 - X_B) \qquad (4)$$

From equation (5), a linear relationship is expected when plotted f_B against X_B. Any deviation from this linear relation indicates molecular interactions. It is practically observed that in our experimental data for binary mixtures do not fit well with equation (5).

Dipolar excess free energy (ΔF^E)

The excess Helmholtz free energy of mixing ΔF^E is given by [11],

$$\Delta F^E = \frac{-N}{2} \left[\sum_{r=A,B} \mu_r^2 X_r (R_{fr} - R_{fr0}) + \sum_{r=A,B} \mu_r^2 X^2_r (g_{rr} - 1)(R_{fr} - R_{fr0}) + X_A X_B \mu_A \mu_B (g_{AB} - 1)(R_{fA} + R_{fB} - R_{fA0} - R_{fB0}) \right]$$

$$= \Delta F_0^E + \Delta F_{rr}^E + \Delta F_{AB}^E \qquad (5)$$

This first term ΔF_0^E in equation (7) represents the excess dipolar energy due to long-range electrostatic interaction. The second term ΔF_{rr}^E gives the excess dipolar energy due to short-range interaction between identical molecules and the third term ΔF_{AB}^E gives the excess dipolar energy due to short-range interaction between dissimilar molecules. It gives excess thermodynamic functions in binary mixtures that take into account the contribution due to both short-range and long-range dipolar interactions between both like and unlike molecules is adopted for polar-nonpolar mixtures.

Materials and Methods

The materials used in the current experiment were of AR grade, and they were purchased all at SRL, India. After calibration with standard liquids such as carbon tetrachloride, benzene, toluene and chlorobenzene, the Static permittivity ε_{0m} at 1 KHz was measured with a digital VLCR-7 meter supplied by M/S Vasavi electronics, India. The square refractive Index of sodium D-line at an optical frequency was determined to calculate the permittivity of that frequency $\varepsilon_{\infty m}$, and this was calculated using an Abbe refractometer. The uncertainties on the values of statical permittivity, refractive index and density stood at 0.0005, 0.0002 and 0.0001 g/cc respectively. Measurements were carried out at temperatures of 303±1K, 313±1K, and 323±1K with a water circulating thermostat set up.

Results and Discussion

Table 1- 4 showed that the dielectric parameters such as static permittivity, High frequency permittivity, Kirkwood correlation factor, Excess permittivity, Bruggeman factor and dipolar excess free energy for the following binary mixtures (1) n-Butylamine+n-Butyl acetate, (2) Cyclohexylamine+n-Butyl acetate, and (3) Diethylamine+n-Butyl acetate at 303K, 313K, and 323K.

Table 1: Values of ε_{0m}, $\varepsilon_{\infty m}$, g^{eff}, g_f, ε^E, f_B, ΔF_0^E, ΔF_{rr}^E, ΔF_{ab}^E and ΔF^E of binary mixtures of Butyl acetate with n-butylamine as a function of mole fraction at 303K, 313K and 323K

T/K	X_2	ε_{0m}	$\varepsilon_{\infty m}$	g^{eff}	g_f	ε^E	f_B	ΔF_0^E /Jmole^{-1}	ΔF_{rr}^E /Jmole^{-1}	ΔF_{ab}^E /Jmole^{-1}	ΔF^E /Jmole^{-1}
303	0	5.261	1.9243	0.97	1	0	1	0	0	0	0
	0.1	5.18	1.9254	1.01	0.95	-0.0182	0.87	6.69	-0.63	0.52	6.58
	0.2	5.126	1.9268	1.06	0.93	-0.0097	0.79	8.99	-1.59	0.44	7.84
	0.3	5.072	1.9277	1.12	0.92	-0.0007	0.7	10.5	-2.85	-0.19	7.46
	0.4	4.991	1.9288	1.18	0.92	-0.0189	0.58	14.12	-4	1.28	11.4
	0.5	4.91	1.9299	1.26	0.92	-0.0372	0.44	16.54	-4.74	2.99	14.79
	0.6	4.856	1.9307	1.36	0.91	-0.0281	0.36	15.11	-5.34	1.99	11.76
	0.7	4.802	1.9324	1.48	0.93	-0.0199	0.27	12.76	-5.38	1.1	8.48
	0.8	4.748	1.9335	1.63	0.95	-0.0111	0.18	9.48	-4.65	0.24	5.07
	0.9	4.694	1.9363	1.82	0.97	-0.004	0.09	5.24	-2.94	-0.06	2.23
	1	4.64	1.9421	2.06	1	0	0	0	0	0	0
	0	5.207	1.916	0.99	1	0	1	0	0	0	0
	0.1	5.153	1.9188	1.04	0.95	0.0046	0.91	3.49	-0.41	0	3.05
	0.2	5.072	1.9193	1.08	0.92	-0.0156	0.78	9.46	-1.33	0.03	8.16

	0.3	5.045	1.9196	1.16	0.93	0.0184	0.74	8.02	-2.69	-0.05	5.28
313	0.4	4.964	1.9218	1.22	0.92	-0.0034	0.6	12.02	-3.9	0	8.12
	0.5	4.883	1.9224	1.3	0.91	-0.0237	0.46	14.82	-4.72	0.01	10.11
	0.6	4.829	1.9246	1.4	0.89	-0.0185	0.37	13.74	-5.44	0	8.3
	0.7	4.748	1.9254	1.51	0.9	-0.039	0.23	14.16	-4.68	-0.04	9.44
	0.8	4.694	1.9304	1.66	0.93	-0.0367	0.14	11	-3.68	-0.06	7.26
	0.9	4.667	1.9315	1.87	0.96	-0.0034	0.09	4.9	-3.11	0	1.8
	1	4.613	1.9354	2.12	1	0	0	0	0	0	0
	0	5.18	1.9132	1.02	1	0	1	0	0	0	0
	0.1	5.126	1.9166	1.06	0.95	0.0041	0.91	3.49	-0.28	0	3.21
	0.2	5.045	1.9188	1.11	0.91	-0.0177	0.78	9.54	-1.09	0.04	8.49
	0.3	5.018	1.9193	1.18	0.91	0.0162	0.74	8.07	-2.54	-0.04	5.49
	0.4	4.937	1.9199	1.25	0.92	-0.0039	0.6	12.11	-3.79	0	8.33
	0.5	4.829	1.9216	1.32	0.9	-0.0522	0.42	17.78	-4.19	0	13.6
323	0.6	4.802	1.9221	1.43	0.88	-0.0183	0.37	13.85	-5.51	0	8.34
	0.7	4.721	1.9243	1.54	0.88	-0.0401	0.23	14.27	-4.78	-0.05	9.45
	0.8	4.667	1.9271	1.7	0.91	-0.0355	0.14	11.09	-3.81	-0.05	7.23
	0.9	4.613	1.9307	1.89	0.96	-0.0316	0.05	6.93	-1.63	-0.04	5.26
	1	4.586	1.9335	2.17	1	0	0	0	0	0	0

Table 2: Values of ε_{0m}, $\varepsilon_{\infty m}$, g^{eff}, g_f, ε^E, f_B, ΔF_0^E, ΔF_{rr}^E, ΔF_{ab}^E and ΔF^E of binary mixtures of Butyl acetate with Cyclohexylamine as a function of mole fraction at 303K, 313K and 323K

T/K	**X_2**	**ε_{0m}**	**$\varepsilon_{\infty m}$**	**g^{eff}**	**g_f**	**ε^E**	**f_B**	**ΔF_0^E /Jmole^{-1}**	**ΔF_{rr}^E /Jmole^{-1}**	**ΔF_{ab}^E /Jmole^{-1}**	**ΔF^E /Jmole^{-1}**
	0	5.261	1.9243	0.97	1	0	1	0	0	0	0
	0.1	4.991	1.9379	0.93	0.95	-0.1979	0.61	30.25	-1.12	0.13	29.25
	0.2	4.91	1.9569	0.94	0.94	-0.204	0.49	34.12	-1.41	0.08	32.8
	0.3	4.829	1.9659	0.96	0.94	-0.2057	0.37	37.07	-1.61	-0.12	35.34
	0.4	4.775	1.9836	0.99	0.94	-0.1901	0.29	35.69	-1.67	-0.3	33.71
303	0.5	4.748	2.0028	1.03	0.95	-0.1628	0.25	29.86	-1.75	-0.36	27.75
	0.6	4.721	2.0167	1.07	0.97	-0.1057	0.21	24.56	-1.76	-0.27	22.53
	0.7	4.667	2.0432	1.11	0.97	-0.102	0.12	21.42	-1.37	-0.35	19.69
	0.8	4.64	2.0612	1.17	0.98	-0.0639	0.08	14.7	-1.1	-0.19	13.41
	0.9	4.613	2.0857	1.23	0.99	-0.0332	0.04	7.56	-0.65	-0.07	6.84
	1	4.586	2.1066	1.31	1	0	0	0	0	0	0
	0	5.207	1.916	0.99	1	0	1	0	0	0	0
	0.1	4.964	1.9324	0.96	0.95	-0.1767	0.64	27.17	-0.4	0.13	26.9
	0.2	4.856	1.9524	0.96	0.93	-0.2141	0.47	35.14	-0.69	0.05	34.5
	0.3	4.802	1.9631	0.99	0.94	-0.1935	0.39	34.75	-0.96	-0.09	33.7
	0.4	4.748	1.9735	1.02	0.95	-0.1737	0.3	33.72	-1.18	-0.25	32.29
313	0.5	4.721	1.9983	1.06	0.95	-0.1551	0.26	28.24	-1.47	-0.33	26.44
	0.6	4.694	2.0164	1.1	0.96	-0.1054	0.22	23.26	-1.65	-0.28	21.32
	0.7	4.64	2.0372	1.14	0.96	-0.099	0.13	20.45	-1.34	-0.35	18.76
	0.8	4.613	2.0521	1.2	0.98	-0.0608	0.09	14.06	-1.15	-0.18	12.73
	0.9	4.586	2.0788	1.27	0.98	-0.0354	0.04	7.24	-0.72	-0.08	6.44
	1	4.559	2.0944	1.35	1	0	0	0	0	0	0
	0	5.18	1.9132	1.02	1	0	1	0	0	0	0
	0.1	4.937	1.9296	0.98	0.95	-0.1785	0.64	27.41	0.3	0.14	27.85
	0.2	4.802	1.9502	0.98	0.92	-0.2451	0.43	39.22	0.19	-0.02	39.4
	0.3	4.748	1.9606	1	0.93	-0.226	0.34	38.72	-0.19	-0.2	38.33
	0.4	4.721	1.9634	1.05	0.95	-0.1734	0.3	34.03	-0.68	-0.25	33.1
	0.5	4.694	1.9915	1.09	0.95	-0.1598	0.26	28.51	-1.2	-0.36	26.96
323	0.6	4.667	2.0158	1.12	0.95	-0.1181	0.22	23.49	-1.56	-0.36	21.57
	0.7	4.613	2.0318	1.17	0.96	-0.1086	0.13	20.65	-1.33	-0.42	18.9
	0.8	4.586	2.0483	1.23	0.97	-0.0738	0.09	14.19	-1.22	-0.27	12.71
	0.9	4.559	2.0512	1.32	0.99	-0.0263	0.04	7.31	-0.8	-0.04	6.47
	1	4.532	2.0742	1.41	1	0	0	0	0	0	0

Table 3: Values of ε_{0m}, $\varepsilon_{\infty m}$, g^{eff}, g_f, ε^E, f_B, ΔF_0^E, ΔF_{rr}^E, ΔF_{ab}^E and ΔF^E of binary mixtures of Butyl acetate with Diethylamine as a function of mole fraction at 303K, 313K and 323K

T/K	**X_2**	**ε_{0m}**	**$\varepsilon_{\infty m}$**	**g^{eff}**	**g_f**	**ε^E**	**f_B**	**ΔF_0^E /Jmole^{-1}**	**ΔF_{rr}^E /Jmole^{-1}**	**ΔF_{ab}^E /Jmole^{-1}**	**ΔF^E /Jmole^{-1}**
	0	5.261	1.9243	0.97	1	0	1	0	0	0	0
	0.1	4.937	1.9188	0.94	0.95	-0.1807	0.79	31.09	-1.52	0.58	30.15
	0.2	4.721	1.9179	0.93	0.93	-0.2516	0.65	46.68	-2.63	0.99	45.03
	0.3	4.559	1.913	0.94	0.92	-0.2588	0.54	53.65	-3.51	0.78	50.92

	0.4	4.424	1.9102	0.97	0.92	-0.2522	0.45	54.21	-4.24	0.33	50.29
303	0.5	4.262	1.9099	0.98	0.92	-0.2608	0.34	58.16	-4.49	-0.46	53.21
	0.6	4.127	1.9094	1	0.91	-0.2554	0.24	55.15	-4.31	-1.21	49.63
	0.7	4.046	1.9085	1.06	0.93	-0.1909	0.18	43.76	-4.05	-1.15	38.57
	0.8	3.965	1.9074	1.13	0.95	-0.1318	0.12	30.21	-3.35	-0.81	26.04
	0.9	3.884	1.9066	1.2	0.97	-0.0638	0.06	16.19	-2.04	-0.29	13.86
	1	3.803	1.9058	1.3	1	0	0	0	0	0	0
	0	5.207	1.916	0.99	1	0	1	0	0	0	0
	0.1	4.91	1.9149	0.96	0.95	-0.161	0.81	28.02	-0.68	0.56	27.9
	0.2	4.667	1.9138	0.95	0.92	-0.2616	0.65	47.94	-1.59	1.03	47.38
	0.3	4.532	1.9105	0.97	0.93	-0.2466	0.55	51.44	-2.54	0.82	49.72
	0.4	4.397	1.9077	0.99	0.92	-0.2429	0.46	52.39	-3.54	0.37	49.22
313	0.5	4.208	1.9061	0.99	0.91	-0.2801	0.32	60.46	-3.82	-0.64	56.01
	0.6	4.046	1.905	1.01	0.89	-0.3041	0.21	61.38	-3.5	-1.84	56.03
	0.7	3.938	1.9041	1.05	0.9	-0.2696	0.12	53.43	-2.86	-2.18	48.38
	0.8	3.884	1.9011	1.13	0.93	-0.1845	0.08	36.2	-2.45	-1.38	32.37
	0.9	3.83	1.8975	1.22	0.96	-0.0897	0.04	18.96	-1.53	-0.46	16.98
	1	3.776	1.8948	1.34	1	0	0	0	0	0	0
	0	5.18	1.9132	1.02	1	0	1	0	0	0	0
	0.1	4.883	1.9121	0.99	0.95	-0.1614	0.84	30.25	0.17	0.57	29.99
	0.2	4.613	1.9108	0.96	0.91	-0.2893	0.66	34.12	-0.3	1.08	53.05
	0.3	4.478	1.9096	0.98	0.91	-0.277	0.56	37.07	-1.35	0.84	55.25
	0.4	4.37	1.9072	1.01	0.92	-0.247	0.46	35.69	-2.71	0.39	50.52
	0.5	4.181	1.905	1.01	0.9	-0.2843	0.32	29.86	-3.14	-0.67	57.19
323	0.6	3.992	1.9038	1.02	0.88	-0.3357	0.19	24.56	-2.7	-2.33	60.64
	0.7	3.884	1.9005	1.06	0.88	-0.2993	0.1	21.42	-2.16	-2.69	52.66
	0.8	3.83	1.8972	1.14	0.91	-0.2143	0.06	14.7	-1.83	-1.77	36.26
	0.9	3.803	1.8964	1.25	0.96	-0.0958	0.04	7.56	-1.63	-0.53	16.98
	1	3.749	1.8871	1.37	1	0	0	0	0	0	0

The static permittivity (ε_{0m}) of the binary mixtures of n-butyl acetate and the amines n-Butylamine, Cyclohexylamine and Diethylamine show a systematic decrease with an increase in the mole fraction of butyl acetate (X_2) which extends in the available range of temperatures studied at 303-323 K. This reduction can be attributed to the relative lower polarity of butyl acetate when compared to the constituent amines which in turn reduces the overall dipole moment of the mixtures. Moreover, increased temperature raises thermal agitation, which disturbs the alignment of dipoles, and thus, causes one more decrease in ε_{0m}. On the other hand, the high-frequency permittivity ($\varepsilon_{\infty m}$) shows a minor gain with increasing acetate concentration, which is the sign of an increase in the number of the electronic polarization processes. Similar trends have been reported in other polar binary systems which show non- ideological dielectric behaviour [12,13].

The deviation of the effective Kirkwood correlation factor (g_{eff}) from unity clearly confirms the presence of significant intermolecular interactions in all the studied systems. At higher mole fractions, values of g_{eff} greater than unity indicate cooperative interactions between unlike molecules, characterized by a tendency for parallel alignment of dipoles. In contrast, the corrective factor ($g_f < 1$) reflects the presence of antiparallel dipolar orientations, highlighting the non-ideal nature of the mixtures. These findings suggest that both parallel (cooperative) and antiparallel interactions coexist within the systems, which is a characteristic feature of hydrogen-bonded liquid mixtures [14].

The values of excess permittivity (ε^E) remain negative throughout the composition range of all systems studied, i.e. there are strong intermolecular interactions. Such interactions mainly occur through hydrogen bonding between amine (–NH2) and ester (–COO2) moieties and dipole-dipole interaction, which then play roles in forming of molecular complexes. The Diethylamine + n-Butyl acetate mixture is characterized by the most negative values of ε^E, which suggests a greater extent of molecular association. These types of negative deviations are typical of those systems where intermolecular association causes the effective dipole moment to be lower than in the solution in the absence of the intermolecular association. [15,16]

The Bruggeman factor (f_B) value has a significant deviation of one and thus denotes strong non-ideal behaviour in the mixtures. It is notable that the concentration of n-butyl acetate was found to decrease f_B, which is indicative of structural rearrangement in the system. This effect can be attributed to distortion of the self-association structures of the pure amine molecules as well as simultaneous resulting formation of new heteromolecular interactions of the constituent species. The occurrence of such changes is an indication of the existence of micro- heterogeneity and formation of molecular complexes in the mixtures.

The fact that the excess Helmholtz free energy, in all the systems considered is positive and rather large suggests that there are particular intermolecular interactions between molecules that are stronger than any dispersion forces. The size of ΔF^E is in the following sequence: Diethylamine > Cyclohexylamine > n-Butylamine. This arrangement implies that Diethylamine has a more intense binding with butyl acetate thus enhancing a higher degree of association of the molecules within the system. Intermolecular interactions are good to allow structuring of the molecules. Organized solvents are used to increase the solubility of CO_2 and greatly increase transfer of mass. The strength of interaction should be moderate enough to ensure the maximum absorption and regeneration energy consumption is achieved. The observations, hence, enhance the rational design of the high-performance amine based solvent systems to use in the carbon capture applications [17, 18].

Conclusion

The current paper underlines the importance of dielectric and thermodynamic characteristics of amine-acetate binary mixtures to the CO_2 capture performance. The fact that the values of static permittivity (ε_{0m}) and excess permittivity value (ε^E) remains negative and persistent, is evidence that there are strong specific intermolecular forces, i.e. the hydrogen bonding force, or the intermolecular dipole force. These reactions cause the formation of structured molecular environment conducive to CO_2 absorption through the promotion of gas-solvent interactions and solubility. Abnormalities in the Kirkwood correlation factor and Bruggeman factor additionally show non-ideal mixing behavior and micro-heterogeneity in the systems. The purpose of such structural organization is reported to enhance the higher mass transfer and diffusion of CO_2, the efficiency of absorption, and solvent performance. The increased level of molecular association found in the case of the Diethylamine + n-butyl acetate mixture in the elucidated systems gives the latter a better chance of occurrence in the CO_2 uptake process. A positive free energy ΔF^E value of the excess shows that particular intermolecular interactions are effective and preferential over the dispersive forces, which is desirable in the solubility of CO_2. However, very powerful interactions can act to slow the regeneration of solvents and increase the amount of energy needed. Therefore, a good ratio between intensity of interaction and mobility of molecules are also necessary to enhance high absorption efficiency and low regeneration energy. On the whole, the findings indicate the applicability of dielectric parameters to correlate the molecular interactions with the CO_2 capture performance. These observations can be effective basis of an intelligent design of more sophisticated amine - acetate solvents that has better CO_2 absorption capacity, volume transfer properties and consumes less energy thus qualifying to be a potential solution to carbon capture methods that are sustainable.

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