

THERMO-ACOUSTICAL PROPERTIES OF 1,1'-BIS(2,6-DICHLORO-4-HYDROXYPHENYL)CYCLOHEXANE SOLUTIONS AT ATMOSPHERIC PRESSURE

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Abstract— In present work we have reported thermo-acoustical and thermodynamic properties of 1,1'-bis(2,6-dichloro-4-hydroxyphenyl)cyclohexane (CIBC). The density (ρ), viscosity (η) and ultrasonic speed (U) of pure solvents [1, 4-dioxane (DO), chloroform (CF), ethyl acetate (EA), tetrahydrofuran (THF)] and CIBC solutions were investigated at four different temperatures: 298, 303, 308 and 313K to understand the effect of solvents and temperature on molecular interactions. Various acoustical and thermodynamic parameters such as specific acoustical impedance (Z), adiabatic compressibility (K_a), intermolecular free path length (L_f), Rao's molar sound function (R_m), Van der Waals constant (b), internal pressure (π), free volume (V_f), viscous relaxation time (τ) and classical absorption coefficient (α/f^2) were calculated and fairly good corelationship between calculated parameters were obtained. A fairly good to excellent correlation between a given parameter and concentration is observed at all temperatures and solvent systems studied. Gibb's free energy of activation (ΔG^*) is found both concentration and temperature dependent. Both enthalpy of activation (ΔH^*) and entropy of activation (ΔS^*) are found concentration dependent. Thus, acoustical and thermodynamic parameters confirmed presence of strong molecular interactions and structure making nature of the compound.

Index Terms— Density, viscosity, ultrasonic speed, acoustical parameters, thermodynamic parameters, molecular interactions

I. INTRODUCTION

Bisphenols are the important constituents of epoxy resins, plastics, lacquers, etc [1]. They are useful in manufacturing thermally stable polymers and polyester resins [2]. Thermodynamic data are very important tool for understanding the molecular interactions namely solute-solvent and solute-solute, occurring in the solutions. A considerable work on solutions of organic compounds has also been reported in the literature [3,4]. The sound velocity is a purely thermodynamic property. Ultrasonic sound is a viable technology because it is readily available and can be used for wide range of applications in different fields to include consumer industries, pharmaceutical industries, medical field, process industries, chemical industries, among others [5,6]. Ultrasonic sound radiations are used in synthetic organic chemistry, which cause increase of yield, decrease of reaction time, lower reaction temperature, and avoidance of phase transfer catalysis [7-12].

To the best of our knowledge no work has been reported on 1,1'-bis(2,6-dichloro-4-hydroxyphenyl)cyclohexane(CIBC), which prompted us to taken up present work. In present work we have reported measurements of density, ultrasonic speed and viscosity of pure solvents and solutions at different temperatures and evaluated various acoustical and thermodynamic parameters. Fig. 1 shows the structure of 1,1'-bis(2,6-dichloro-4-hydroxyphenyl)cyclohexane (CIBC).

II. EXPERIMENTAL

Materials

The solvents and chemicals used in the present investigation were of AR grade and were further purified according to literature methods [13]. 1,1'-Bis(2,6-dichloro-4-hydroxyphenyl)cyclohexane (CIBC) used in this study was synthesized in our laboratory. 1,4-Dioxane (DO), chloroform (CF), ethyl acetate (EA) and tetrahydrofuran (THF) were supplied by Spectrochem Pvt. Ltd. Mumbai.

Measurements

Apparatus and procedure

All the samples were prepared freshly and retained at the desired temperature for 24 h to ensure their solubility at the temperature. Samples were kept in bottles with PTFE septum under vacuum until further use.

Density, viscosity and ultrasonic speed

Solutions of different concentrations (in molarity, M) were prepared for binary system. The ρ and U measurements were carried out on a Density and Sound Velocity Meter (DSA-5000 M) supplied by Anton Paar GmbH, Graz, Austria. The calibration of DSA was done over a temperature range from 25-40 °C. DSA was thermostated within ± 0.002 °C with Peltier heating device. Viscometric measurements were carried out by using Ubbelohde suspended type viscometer. The repeatability in the viscosity measurements was ± 0.1 %. The viscosity measurements were repeated at least three times for each sample. A constant temperature bath (Nova Instruments, Ahmedabad, Model NV8550E) with an accuracy of ± 0.01 K was used for maintaining constant temperature during viscosity measurements. The flow times of pure solvents and solutions were measured with a digital RACER HS 10W stop watch with an accuracy of ± 0.01 s. The solutions were prepared by mass using an analytical balance (AB204-S; Mettler Toledo, Switzerland) with an uncertainty of $\pm 1 \cdot 10^{-4}$ kg.

III. RESULTS AND DISCUSSION

Density, viscosity and ultrasonic speed

Experimentally derived quantities namely ρ , η and U of pure DO, CF, EA, THF and CIBC solutions at four different temperatures: 298, 303, 308 and 313 K are presented in Table 1. The densities of CIBC solutions in all the four solvents increased linearly with concentration (C) and decreased linearly with temperature because of rule of additivity. The densities of the solvents are smaller than that of CIBC, so ρ increased with C in these systems. Both η and U of CIBC solutions increased linearly with C and decreased with T . The variation of η and U with C and T are considerably more than that of ρ due to specific molecular interactions such as association,

dissociation, H-bonding, etc. occurring in the solutions. The ρ , η and U data were correlated with C and T , and excellent correlation of these parameters with C and T is found. Intermolecular motion in solution is affected by molecular interactions [23]. Molecular association leads to changes in both the apparent molecular volume as well as molecular mass and hence the density of the solution. Attractive forces result into molecular association (solvation), i.e. modification of the structure of the solute. The decrease of ρ , η and U with T indicated decrease of cohesive forces [20-22]. The nature of solvent and the solute play an important role in determining all transport and other properties of the solutions. Van der Waals, H-bonding, dipolar and London type interactions result into the aggregation of the solvent molecules around solute molecules and as a consequence structural modification results [19-21, 24].

Various acoustical and thermodynamic parameters of pure solvents and CIBC solutions were derived according to Eqns. 1-12 by using ρ , η and U data at different temperatures and were correlated with C and T . The least-squares equations along with regression coefficients (R^2) are reported in Table 2. Excellent correlation between above mentioned parameters with concentration and temperature is observed. Strong molecular interactions are supported by nonlinear increase of S_n with C and nonlinear decrease with T . Nonlinear variation of S_n with competing solute-solute and solvent-solute interactions with increasing solution concentrations.

Both U and Z were increased with C and decreased with T due to strong molecular interactions. κ_a of solutions was decreased with C and increased with T in all solvents. This can be attributed to the fact that the solvated molecules were fully compressed by the electrical forces of the solute. The strong solvent-solute interactions lead to compressibility. The compressibility of the solution is mainly due to the free solvent molecules. Due to molecular association (solvent-solute interactions) compressibility of the solution was decreased with the increasing solute concentration. Inter molecular free path length is inversely proportional to ultrasonic speed. It was observed from the results that L_f was decreased with C and increased with temperature further supported the presence of strong molecular interactions. $(\alpha/f^2)_{cl}$ decreased with C and temperature. The presence of solvent - solute interactions can also be confirmed from dispersion of ultrasonic speed, which is characterized by relaxation process. According to Eyring rate theory τ is inversely proportional to temperature and hence, increased in the temperature of system caused to decrease in relaxation process. τ is decreased with C and T . Rao's molar sound function (R_m) and Van der Waals constant (b) increased with C and T indicated that there is no complex or aggregate formation taken place in all the systems. The internal pressure (π) decreased with concentration and temperature. The results of π also confirmed our observations for κ_a and L_f . The internal pressure depends on temperature, density, ultrasonic speed and specific heat at a constant pressure, while L_f is temperature dependent.

A variation in the values of π is due to different orientations of CIBC in DO, CF, EA and THF. The free volume (V_f) is inversely proportional to the internal pressure (π) and vice-versa. The ordered structural arrangement is due to decreasing entropy of the system. The lone pairs of electrons of DO, THF, EA and chlorine of CF are electronegative in nature, while hydrogen of CF, methyl and methylene groups are electropositive in nature. The dipole-dipole interactions of the same type leads to structure formation, while of the opposite

type leads to structure breaking tendency. Solvation phenomenon is found minimum in CF as compared to other systems because of above facts. The variation in S_n with C and T also suggested the presence of strong dipole-dipole interactions.

When a solute is added to a solvent, its molecules attract certain solvent molecules toward them. The phenomenon is known as compression and also as limiting compressibility. The aggregation of solvent molecules around solute molecules supported strong solvent-solute interactions and considerable change in structural arrangement. Molecular interactions such as solvent-solute interactions, quantum mechanical dispersive forces and dielectric force may cause high degree of contraction or expansion. The time lag between the excitation and de-excitation processes is observed as an acoustical relaxation. This relaxation process is observed as either an increase in speed with frequency or a decrease in the $(\alpha/f^2)_{cl}$ with frequency. Thermodynamic parameters such as ΔG^* , ΔH^* and ΔS^* were determined according to Eqns. 11 and 12 using viscous relaxation time data as a function of concentration and temperature and are shown in Table 3. The variation of ΔG^* of CIBC solutions with C at different temperatures confirmed concentration dependence of ΔG^* . In DO system ΔG^* was decreased with increasing C and decreased with increasing T , while both ΔH^* and ΔS^* increased with increasing C . In CF and THF systems ΔG^* decreased with increasing C and increased with increasing T , while both ΔH^* and ΔS^* were decreased with increasing C and T . In EA system ΔG^* increased with increasing C and increased with increasing T , while both ΔH^* and ΔS^* are found approximately independent of C . Derived thermodynamic parameters indicated that the condensation and evaporation processes are found concentration and temperature dependent. The negative values of ΔH^* and ΔS^* indicated that activated complexes are in ordered state, i.e. condensation process is predominant over evaporation process, which is further supported by positive values of S_n with C . Thus, thermodynamic parameters supported presence of strong molecular interactions in the solutions of different polarity.

A. Equations

Various acoustical and thermodynamic parameters were determined according to following theoretical equations:

$$\text{Specific acoustical impedance (Z): } Z = U\rho \quad (1)$$

$$\text{Adiabatic compressibility } (\kappa_a): \kappa_a = 1/U^2\rho \quad (2)$$

Internal pressure (π) [14]:

$$\pi = b^*RT (K\eta/U)^{1/2} (\rho^{2/3}/M^{7/6}) \quad (3)$$

Where b^* is the packing factor (2) and K is a constant (4.28×10^9). R is the gas constant $\{8.3143/(J \cdot K^{-1} \cdot mol^{-1})\}$.

$$\text{Free volume } (V_f) [15]: V_f = [MU/K\eta]^{3/2} \quad (4)$$

Inter molecular free path length (L_f) [16]:

$$L_f = K_J \kappa_a^{1/2} \quad (5)$$

where $K_J \{(93.875 + 0.375T) \times 10^{-8}\}$ is a temperature-dependent Jacobson's constant.

Van der Waals constant (b) [17]:

$$b = M/\rho \{1 - [RT/(MU^2)]\} [\sqrt{1 + (MU^2)/3RT} - 1] \quad (6)$$

Where M is the apparent molecular weight of the solution, R is the gas constant and T is the absolute temperature.

Viscous relaxation time (τ):

The resistance offered by viscous force in the flow of sound wave appears as a classical absorption associated with it is the viscous relaxation time: $\tau = 4\eta/3\rho U^2$ (7)

Classical absorption coefficient $(\alpha/f^2)_{cl}$ [18]:

$$(\alpha/f^2)_{cl} = 8\pi^2\eta/3U^3\rho \quad (8)$$

Rao's molar sound function (R_m) [19]:

$$R_m = (M/\rho) U^{1/3} \tag{9}$$

The solvation number (S_n) can be expressed as:

$$S_n = M_2/M_1 [(1-\kappa_a)/\kappa_{a1}] [(100-X)/X] \tag{10}$$

Where M_1 and M_2 are the molecular weights of solvent and solute, respectively.

Thermodynamic parameters [39]:

Free energy of activation (ΔG^*), enthalpy of activation (ΔH^*) and entropy of activation (ΔS^*) can be determined by using viscous relaxation time data at different concentrations and temperatures: $(1/\tau) = (kT/h)e^{\Delta G^*/RT}$ (11)

$$\ln(1/\tau T) = \ln(k/h) + (\Delta S^*/R) - (\Delta H^*/RT) \tag{12}$$

Where k is the Boltzmann constant and h is the Planck's constant.

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Table: 1 The density (ρ), viscosity (η), and ultrasonic speed (U) data for CIBC in DO, CF, EA and THF at 298 K, 303 K, 308 K and 313 K

C (mol dm ⁻³) ^a	DO + CIBC			CF + CIBC		
	ρ (kg m ⁻³) ^b	η (mPa s) ^c	U (m s ⁻¹) ^d	ρ (kg m ⁻³) ^b	η (mPa s) ^c	U (m s ⁻¹) ^d
	298 K			298 K		
0.00	1027.60	1.2224	1345.70	1478.33	0.5533	983.86
0.01	1029.08	1.2247	1346.33	1480.60	0.5552	984.96
0.02	1030.36	1.2264	1346.62	1482.58	0.5570	986.05
0.04	1032.96	1.2310	1347.64	1485.69	0.5603	988.18
0.06	1035.52	1.2347	1348.50	1489.20	0.5637	990.51
0.08	1038.21	1.2391	1349.58	1492.56	0.5671	992.61
0.10	1040.55	1.2425	1350.36	1497.72	0.5710	995.00
	303 K			303 K		
0.00	1021.82	1.0939	1323.80	1468.02	0.5270	966.84
0.01	1023.43	1.0960	1324.40	1471.06	0.5291	967.97
0.02	1024.72	1.0976	1324.70	1472.79	0.5306	968.99
0.04	1027.33	1.1015	1325.80	1476.18	0.5338	971.17
0.06	1029.89	1.1052	1326.60	1479.69	0.5374	973.49
0.08	1032.59	1.1091	1327.80	1483.10	0.5406	975.63
0.10	1034.94	1.1123	1328.60	1488.10	0.5445	978.00
	308 K			308 K		
0.00	1016.21	1.0100	1302.02	1458.23	0.5017	949.89
0.01	1017.76	1.0120	1302.62	1461.46	0.5039	951.00
0.02	1019.06	1.0135	1302.93	1463.25	0.5056	952.06
0.04	1021.68	1.0171	1304.10	1466.62	0.5088	954.21
0.06	1024.26	1.0206	1305.08	1470.16	0.5120	956.55
0.08	1026.97	1.0244	1306.22	1473.60	0.5153	958.64
0.10	1029.33	1.0276	1307.07	1478.60	0.5194	961.00
	313 K			313 K		
0.00	1010.46	0.9269	1280.37	1448.46	0.4776	933.02
0.01	1012.09	0.9288	1280.94	1451.80	0.4795	934.05
0.02	1013.39	0.9304	1281.37	1453.59	0.4813	935.27
0.04	1016.02	0.9339	1282.50	1457.00	0.4845	937.30
0.06	1018.61	0.9372	1283.70	1460.56	0.4879	939.77
0.08	1021.34	0.9406	1284.73	1464.05	0.4909	941.75
0.10	1023.70	0.9440	1285.71	1469.09	0.4948	944.22
C (mol dm ⁻³) ^a	EA + CIBC			THF + CIBC		
	ρ (kg m ⁻³) ^b	η (mPa s) ^c	U (m s ⁻¹) ^d	P (kg m ⁻³) ^b	η (mPa s) ^c	U (m s ⁻¹) ^d
	298 K			298 K		
0.00	894.79	0.4274	1140.52	882.33	0.4625	1278.30
0.01	896.50	0.4301	1142.63	884.45	0.4641	1279.68
0.02	897.82	0.4321	1144.36	885.85	0.4653	1280.71
0.04	900.91	0.4367	1148.05	888.84	0.4676	1283.01

0.06	903.54	0.4412	1151.58	891.52	0.4696	1284.99
0.08	906.33	0.4455	1155.09	894.38	0.4715	1287.38
0.10	909.43	0.4504	1159.12	897.55	0.4741	1289.57
		303 K			303 K	
0.00	894.79	0.4050	1118.16	876.83	0.4474	1254.25
0.01	896.50	0.4075	1120.20	878.97	0.4489	1255.69
0.02	897.82	0.4097	1122.04	880.37	0.4500	1256.86
0.04	900.91	0.4141	1125.55	883.39	0.4520	1259.04
0.06	903.54	0.4182	1129.36	886.08	0.4543	1261.30
0.08	906.33	0.4224	1132.78	888.96	0.4568	1263.59
0.10	909.43	0.4273	1136.92	892.15	0.4598	1266.07
		308 K			308 K	
0.00	882.47	0.3846	1095.67	871.30	0.4299	1230.27
0.01	884.20	0.3871	1097.98	873.44	0.4316	1231.88
0.02	885.56	0.3892	1099.69	874.86	0.4331	1233.02
0.04	888.70	0.3938	1103.35	877.89	0.4356	1235.25
0.06	891.38	0.3979	1107.06	880.60	0.4382	1237.62
0.08	894.21	0.4021	1110.58	883.50	0.4410	1239.96
0.10	897.37	0.4070	1114.89	886.71	0.4439	1242.52
		313 K			313 K	
0.00	876.23	0.3644	1073.41	865.73	0.4129	1206.46
0.01	877.99	0.3671	1075.73	867.88	0.4149	1208.22
0.02	879.35	0.3688	1077.35	869.32	0.4164	1209.24
0.04	882.53	0.3736	1081.22	872.37	0.4192	1211.81
0.06	885.24	0.3775	1084.85	875.09	0.4217	1214.08
0.08	888.09	0.3817	1088.47	878.01	0.4245	1216.67
0.10	891.29	0.3866	1092.69	881.23	0.4273	1219.11

^a Molarity of CIBC in DO and CF solutions at different temperatures in mol·dm⁻³.

^b ρ /(kg $\rho \cdot m^{-3}$) = density; ^c η /(mPa · s) = viscosity and ^d U /(m · s⁻¹) = ultrasonic speed.

Table: 2 The least-square equations and regression coefficients for CIBC solutions in DO, CF, EA and THF at 298, 303, 308 and 313 K

Parameter	Least square equations (regression coefficients, R ²) [DO+ CIBC]			
	298 K	303 K	308 K	313 K
ρ (kg·m ⁻³) ^a	66.04 C + 1027 (0.999)	67.08 C + 1021 (0.999)	68.08 C + 1016 (0.999)	69.15 C + 1010 (0.999)
η (m·Pa·s) ^b	0.2027 C + 1.2226 (0.9989)	0.1855 C + 1.094 (0.9994)	0.1761 C + 1.0101 (0.9996)	0.1702 C + 0.927 (0.9999)
U (m·s ⁻¹) ^c	95.35 C + 1346 (0.999)	98.51 C + 1324 (0.999)	100.8 C + 1302 (0.999)	102.9 C + 1280 (0.999)
$Z \cdot 10^{-6}$ (kg·m ⁻² ·s ⁻¹) ^d	0.2222 C + 1.3831 (0.9996)	0.2224 C + 1.353 (0.9993)	0.2226 C + 1.3233 (0.9995)	0.224 C + 1.294 (0.9995)
$\kappa_a \cdot 10^{10}$ (Pa ⁻¹) ^e	-1.0306 C + 5.3725 (0.9995)	-1.101 C + 5.5828 (0.9993)	-1.1824 C + 5.8036 (0.999)	-1.2773 C + 6.0353 (0.9994)
$L_f \cdot 10^{11}$ (m) ^f	-0.4677 C + 4.853 (0.9994)	-0.4902 C + 4.9471 (0.9991)	-0.5164 C + 5.044 (0.9993)	-0.5471 C + 5.1437 (0.9994)
$R_m \cdot 10^4$ (m ^{10/3} ·s ^{-1/3} ·mol ⁻¹) ^g	11.936 C + 9.468 (1)	12.001 C + 9.4685 (1)	12.07 C + 9.4686 (1)	12.141 C + 9.4689 (1)
$b \cdot 10^5$ (m ³) ^h	10.397 C + 8.0784 (1)	10.493 C + 8.1137 (1)	10.599 C + 8.1488 (1)	10.701 C + 8.1846 (1)
$\pi \cdot 10^{-8}$ (Pa) ⁱ	-6.8685 C + 5.3383 (0.9985)	-6.6614 C + 5.1576 (0.9984)	-6.5644 C + 5.0608 (0.9983)	-6.4372 C + 4.9497 (0.9984)
$V_f \cdot 10^7$ (m ³) ^j	2.0752 C + 1.0786 (1)	2.4024 C + 1.2432 (1)	2.653 C + 1.3669 (1)	2.9452 C + 1.5161 (1)
$\tau \cdot 10^{13}$ (s) ^k	-0.255 C + 8.758 (0.9842)	-0.2517 C + 8.1439 (0.9956)	-0.257 C + 7.8165 (0.9938)	-0.2373 C + 7.46 (0.9877)

$(\alpha/f^2)_{cl} \cdot 10^{15}$ (s ² m ⁻¹) ^l	-0.8107 C + 12.833 (0.9957)	-0.8101 C + 12.131 (0.9975)	-0.8474 C + 11.838 (0.9973)	-0.8472 C + 11.489 (0.996)
S_n^m	-5E+06 C ⁴ + 1E+06 C ³ - 92294 C ² + 3033.3 C - 13.392 (0.9668)	-5E+06 C ⁴ + 1E+06 C ³ - 88043 C ² + 2792 C - 12.056 (0.9842)	-3E+06 C ⁴ + 807497 C ³ - 68887 C ² + 2457 C - 9.7896 (0.9591)	-3E+06 C ⁴ + 787567 C ³ - 65439 C ² + 2277C - 7.9747 (0.9639)

Least square equations (regression coefficients, R²) [CF+ CIBC]

Parameter	298 K	303 K	308 K	313 K
ρ (kg·m ⁻³) ^a	66.04 C + 1027 (0.999)	67.08 C + 1021 (0.999)	68.08 C + 1016 (0.999)	69.15 C + 1010 (0.999)
η (m·Pa·s) ^b	0.1747 C + 0.5534 (0.9995)	0.1716 C + 0.5271 (0.9988)	0.1707 C + 0.502 (0.9984)	0.169 C + 0.4777 (0.9991)
U (m·s ⁻¹) ^c	95.35 C + 1346 (0.999)	98.51 C + 1324 (0.999)	100.8 C + 1302 (0.999)	102.9 C + 1280 (0.999)
$Z \cdot 10^{-6}$ (kg·m ⁻² ·s ⁻¹) ^d	0.3477 C + 1.4546 (0.998)	0.3485 C + 1.4198 (0.9982)	0.3455 C + 1.3858 (0.998)	0.3444 C + 1.3521 (0.9978)
$\kappa_a \cdot 10^{10}$ (Pa ⁻¹) ^e	-2.3925 C + 6.9872 (0.9991)	-2.5542 C + 7.2841 (0.9991)	-2.7029 C + 7.5962 (0.999)	-2.8831 C + 7.9265 (0.9988)
$L_f \cdot 10^{11}$ (m) ^f	-0.9557 C + 5.5346 (0.999)	-0.9994 C + 5.6509 (0.9991)	-1.0358 C + 5.7707 (0.999)	-1.0818 C + 5.8949 (0.9988)
$R_m \cdot 10^4$ (m ^{10/3} ·s ^{-1/3} ·mol ⁻¹) ^g	4.4279 C + 8.0301 (0.9996)	4.4378 C + 8.0373 (0.9996)	4.4597 C + 8.043 (0.9996)	4.4851 C + 8.0487 (0.9996)
$b \cdot 10^5$ (m ³) ^h	4.0404 C + 7.5447 (0.9995)	4.0656 C + 7.585 (0.9995)	4.1042 C + 7.6246 (0.9995)	4.1436 C + 7.6649 (0.9995)
$\pi \cdot 10^{-8}$ (Pa) ⁱ	-2.0005 C + 3.7629 (0.9989)	-1.9872 C + 3.75 (0.9989)	-1.9686 C + 3.7365 (0.9988)	-1.9533 C + 3.7211 (0.999)
$V_f \cdot 10^7$ (m ³) ^j	2.2985 C + 3.4928 (0.9996)	2.3884 C + 3.66 (0.9993)	2.4498 C + 3.8353 (0.9988)	2.529 C + 4.0211 (0.9994)
$\tau \cdot 10^{13}$ (s) ^k	-0.1931 C + 5.1559 (0.9785)	-0.1863 C + 5.1199 (0.9952)	-0.1405 C + 5.0848 (0.9731)	-0.1147 C + 5.0498 (0.9679)
$(\alpha/f^2)_{cl} \cdot 10^{15}$ (s ² m ⁻¹) ^l	-1.5004 C + 10.673 (0.9981)	-1.5048 C + 10.556 (0.9985)	-1.5631 C + 10.443 (0.9997)	-1.5345 C + 10.334 (0.9979)
S_n^m	-7E+06 C ⁴ + 2E+06 C ³ - 106204 C ² + 2909.2 C - 13.116 (0.9498)	-5E+06 C ⁴ + 1E+06 C ³ - 72145 C ² + 2078.5 C - 9.3978 (0.9886)	-5E+06 C ⁴ + 1E+06 C ³ - 70152 C ² + 2004.2 C - 8.5199 (0.9932)	-3E+06 C ⁴ + 678245 C ³ - 53489 C ² + 1802.6 C - 7.8856 (0.9999)

Least square equations (regression coefficients, R²) [EA+ CIBC]

Parameter	298 K	303 K	308 K	313 K
ρ (kg·m ⁻³) ^a	66.04 C + 1027 (0.999)	67.08 C + 1021 (0.999)	68.08 C + 1016 (0.999)	69.15 C + 1010 (0.999)
η (m·Pa·s) ^b	0.2265 C + 0.4276 (0.9996)	0.2187 C + 0.4052 (0.9993)	0.2203 C + 0.3848 (0.9996)	0.2179 C + 0.3646 (0.9999)
U (m·s ⁻¹) ^c	95.35 C + 1346 (0.999)	98.51 C + 1324 (0.999)	100.8 C + 1302 (0.999)	102.9 C + 1280 (0.999)
$Z \cdot 10^{-6}$ (kg·m ⁻² ·s ⁻¹) ^d	0.3302 C + 1.0208 (0.9995)	0.3295 C + 0.9938 (0.9994)	0.329 C + 0.9671 (0.9994)	0.3276 C + 0.9409 (0.9994)
$\kappa_a \cdot 10^{10}$ (Pa ⁻¹) ^e	-4.0027 C + 8.5868 (0.9995)	-4.306 C + 8.9965 (0.9994)	-4.641 C + 9.4339 (0.9994)	-4.9903 C + 9.8977 (0.9993)
$L_f \cdot 10^{11}$ (m) ^f	-1.4467 C + 6.1356 (0.9995)	-1.5209 C + 6.2802 (0.9994)	-1.6013 C + 6.4311 (0.9994)	-1.6815 C + 6.5873 (0.9994)
$R_m \cdot 10^4$ (m ^{10/3} ·s ^{-1/3} ·mol ⁻¹) ^g	25.61 C + 10.292 (1)	25.786 C + 10.295 (1)	25.963 C + 10.297 (1)	26.141 C + 10.3 (1)
$b \cdot 10^5$ (m ³) ^h	23.075 C + 9.2035 (1)	23.35 C + 9.2532 (1)	23.63 C + 9.3038 (1)	23.915 C + 9.3555 (1)
$\pi \cdot 10^{-8}$ (Pa) ⁱ	-6.775 C + 3.1121 (0.995)	-6.7719 C + 3.0965 (0.9949)	-6.7494 C + 3.0839 (0.9948)	-6.727 C + 3.0674 (0.9947)
$V_f \cdot 10^7$ (m ³) ^j	14.217 C + 4.0545 (0.9995)	14.827 C + 4.2821 (1)	15.442 C + 4.4897 (1)	16.192 C + 4.7204 (0.9999)
$\tau \cdot 10^{13}$ (s) ^k	0.1921 C + 4.8972 (0.9764)	0.1735 C + 4.8619 (0.9845)	0.2561 C + 4.8413 (0.9877)	0.3073 C + 4.8134 (0.9885)

$(\alpha/f^2)_{cl} \cdot 10^{15}$ (s^2m^{-1}) ^l	-0.9759 C + 8.8409 (0.9981)	-1.0121 C + 8.7121 (0.9938)	-1.0931 C + 8.5737 (0.998)	-1.0053 C + 8.466 (0.9963)
S_n^m	-5E+06 C ⁴ + E+06 C ³ - 82255 C ² + 2431.2 C - 11.191 (0.9839)	-5E+06 C ⁴ + 1E+06 C ³ - 77714 C ² + 2336.1 C - 10.642 (0.9681)	-5E+06 C ⁴ + 1E+06 C ³ - 78473 C ² + 2322.1 C - 10.288 (0.9895)	-5E+06 C ⁴ + 1E+06 C ³ - 74041 C ² + 2242 C - 9.4809 (0.9728)

Parameter	Least square equations (regression coefficients, R ²) [THF+ CIBC]			
	298 K	303 K	308 K	313 K
ρ (kg·m ⁻³) ^a	66.04 C + 1027 (0.999)	67.08 C + 1021 (0.999)	68.08 C + 1016 (0.999)	69.15 C + 1010 (0.999)
η (m·Pa·s) ^b	0.1118 C + 0.4629 (0.9966)	0.1196 C + 0.4474 (0.9959)	0.1366 C + 0.4301 (0.999)	0.1399 C + 0.4134 (0.9975)
U (m·s ⁻¹) ^c	95.35 C + 1346 (0.999)	98.51 C + 1324 (0.999)	100.8 C + 1302 (0.999)	102.9 C + 1280 (0.999)
$Z \cdot 10^{-6}$ (kg·m ⁻² ·s ⁻¹) ^d	0.2887 C + 1.1285 (0.9998)	0.2898 C + 1.1004 (0.9988)	0.29 C + 1.0726 (0.9986)	0.2909 C + 1.0452 (0.9986)
$\kappa_a \cdot 10^{10}$ (Pa ⁻¹) ^e	-2.3132 C + 6.9305 (0.9988)	-2.5061 C + 7.2437 (0.9988)	-2.7061 C + 7.5758 (0.9985)	-2.9339 C + 7.9276 (0.9983)
$L_f \cdot 10^{11}$ (m) ^f	-0.9275 C + 5.5121 (0.9988)	-0.9832 C + 5.6352 (0.9988)	-1.0383 C + 5.763 (0.9986)	-1.1008 C + 5.8953 (0.9984)
$R_m \cdot 10^4$ (m ^{10/3} ·s ^{-1/3} ·mol ⁻¹) ^g	128.822 C + 8.8723 (0.9999)	28.469 C + 8.8737 (0.9999)	28.296 C + 8.8743 (0.9999)	28.643 C + 8.873 (0.9999)
$b \cdot 10^5$ (m ³) ^h	24.873 C + 7.6447 (0.9999)	25.145 C + 7.6816 (0.9999)	25.424 C + 7.719 (0.9999)	25.709 C + 7.7571 (0.9999)
$\pi \cdot 10^{-8}$ (Pa) ⁱ	-10.692 C + 3.8442 (0.9923)	-10.648 C + 3.8381 (0.9922)	-10.643 C + 3.8306 (0.9919)	-10.57 C + 3.8116 (0.9925)
$V_f \cdot 10^7$ (m ³) ^j	16.237 C + 3.1668 (1)	16.559 C + 3.2394 (1)	16.864 C + 3.34 (1)	17.398 C + 3.4431 (1)
$\tau \cdot 10^{13}$ (s) ^k	-0.1911 C + 4.37 (0.975)	-0.2205 C + 4.3454 (0.9828)	-0.3793 C + 4.3221 (0.9728)	-0.4284 C + 4.2777 (0.9935)
$(\alpha/f^2)_{cl} \cdot 10^{15}$ (s^2m^{-1}) ^l	-1.0359 C + 7.141 (0.9976)	-1.0201 C + 6.9635 (0.9964)	-1.2129 C + 6.7941 (0.9928)	-1.2245 C + 6.5979 (0.9977)
S_n^m	-7E+06 C ⁴ + 2E+06 C ³ - 116944 C ² + 3724.9 C - 18.045 (0.9816)	-6E+06 C ⁴ + 1E+06 C ³ - 106299 C ² + 3481.5 C - 16.393 (0.9556)	-6E+06 C ⁴ + 1E+06 C ³ - 105165 C ² + 3400.1 C - 15.28 (0.9818)	-5E+06 C ⁴ + 1E+06 C ³ - 86457 C ² + 2975 C - 11.772 (0.9591)

^a ρ /(kg · m⁻³) = density.

^b η /(mPa · s) = viscosity.

^c U /(m · s⁻¹) = ultrasonic speed.

^d $Z \cdot 10^{-6}$ /(kg·m⁻²·s⁻¹) = specific acoustical impedance.

^e $\kappa_a \cdot 10^{10}$ /(Pa⁻¹) = adiabatic compressibility.

^f $L_f \cdot 10^{11}$ /(m) = intermolecular free path length.

^g $R_m \cdot 10^4$ /(m^{10/3}·s^{-1/3}·mol⁻¹) = Rao's molar sound function

^h $b \cdot 10^5$ /(m³) = Van der Waals constant.

ⁱ $\pi \cdot 10^{-8}$ /(Pa) = internal pressure.

^j $V_f \cdot 10^7$ /(m³) = free volume.

^k $\tau \cdot 10^{13}$ /(s) = viscous relaxation time

^l $(\alpha/f^2)_{cl} \cdot 10^{15}$ /(s²m⁻¹) = Classical absorption coefficient.

^m S_n = Solvation number

Table: 3 Thermodynamic parameters (ΔG^* , ΔH^* and ΔS^*) derived using τ data for CIBC in 1, 4-dioxane, chloroform, ethylacetate and tetrahydrofuran solutions

System	C (mol dm ⁻³) ^a	ΔG^* / (J mol ⁻¹) ^a				ΔH^* / (kJ mol ⁻¹) ^b	ΔS^* / (J K ⁻¹ mol ⁻¹) ^c
		298 K	303 K	308 K	313 K		
DO+ CIBC	0.01	4195.24	4192.45	4129.82	4115.06	5.57	4.68
	0.02	4194.71	4191.79	4129.00	4114.48	5.57	4.69
	0.04	4194.07	4190.16	4126.97	4112.80	5.60	4.76
	0.06	4191.96	4188.95	4125.41	4110.56	5.60	4.78
	0.08	4190.79	4186.98	4123.63	4109.00	5.60	4.79
	0.10	4188.90	4185.58	4122.58	4108.23	5.58	4.73
System	C (mol dm ⁻³) ^a	ΔG^* / (J mol ⁻¹) ^a				ΔH^* / (kJ mol ⁻¹) ^b	ΔS^* / (J K ⁻¹ mol ⁻¹) ^c
		298 K	303 K	308 K	313 K		
CF+ CIBC	0.01	2881.95	3003.56	3028.22	3099.54	-1.47	-14.59
	0.02	2881.18	3002.43	3027.83	3099.18	-1.48	-14.63
	0.04	2879.87	3000.29	3026.88	3098.89	-1.51	-14.71

	0.06	2877.55	2999.10	3024.02	3097.06	-1.51	-14.71
	0.08	2876.37	2997.15	3023.36	3096.10	-1.52	-14.75
	0.10	2872.96	2994.82	3022.11	3094.24	-1.56	-14.86
System	C (mol dm ⁻³) ^a	ΔG^* / (J mol ⁻¹) ^a				ΔH^* / (kJ mol ⁻¹) ^b	ΔS^* / (J K ⁻¹ mol ⁻¹) ^c
		298 K	303 K	308 K	313 K		
EA+ CIBC	0.01	2756.70	2872.72	2904.13	2978.23	-1.69	-14.91
	0.02	2757.51	2874.21	2905.97	2978.56	-1.68	-14.89
	0.04	2759.19	2876.20	2909.79	2983.54	-1.75	-15.13
	0.06	2762.17	2877.17	2911.15	2985.52	-1.73	-15.07
	0.08	2763.36	2879.19	2914.55	2988.79	-1.78	-15.23
	0.10	2764.47	2880.83	2916.35	2992.38	-1.82	-15.38
System	C (mol dm ⁻³) ^a	ΔG^* / (J mol ⁻¹) ^a				ΔH^* / (kJ mol ⁻¹) ^b	ΔS^* / (J K ⁻¹ mol ⁻¹) ^c
		298 K	303 K	308 K	313 K		
THF+ CIBC	0.01	2416.93	2568.51	2624.18	2722.50	-3.65	-20.35
	0.02	2415.74	2565.54	2624.39	2723.19	-3.70	-21.35
	0.04	2410.77	2559.67	2620.69	2720.38	-3.76	-20.69
	0.06	2405.92	2555.28	2618.26	2717.60	-3.81	-20.86
	0.08	2398.95	2551.98	2616.56	2715.33	-3.91	-21.17
	0.10	2395.54	2549.70	2613.34	2712.44	-3.92	-21.19

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