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Thermophysical and sonochemical behaviour of binary mixtures of decan-1-ol with halohydrocarbons at (T = 293.15 and 313.15) K

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ABSTRACT

Densities and ultrasonic velocities of binary mixtures of decan-1-ol with 1,2-dichloroethane, 1,2-dibromoethane, and 1,1,2,2-tetrachloroethene have been measured over the entire range of composition at T = (293.15 and 313.15) K and at atmospheric pressure. From these results, the excess molar volumes, molar free volumes, excess molar isentropic compressibilities, limiting excess partial molar volumes, and isentropic compressibilities, intermolecular free lengths, and available volumes by three methods, thermal expansion coefficients, parameters related to space-filling ability, intermolecular free lengths, and molecular radii have been calculated. The experimental ultrasonic velocities have been analyzed in terms of the ideal mixture relations of Nomoto and Van Dael, Jacobson's free length, Schaaff's collision factor, Flory's statistical, and Prigogine–Flory–Patterson theories and thermoacoustical parameters.

1. Introduction

The variations in the volumetric and acoustic properties of binary mixtures of alkanols containing haloalkanes, acetonitrile, ethylacetate, and ethenyl ethanoate, with the molecular size, shape, chain-length, and degree of molecular association of normal alkanols and branched alkanols have been reported earlier [1–10]. Alkanols are polar and self-associated liquids, and the dipolar association of alkanols decreases when they are mixed with polar compounds containing halogen atoms, due to some sort of specific intermolecular interactions between the hydroxyl oxygen of alkanols and the haloalkanes [11–23]. In an attempt to explore the nature of interactions occurring between the mixing components, we report here the experimental values of densities and ultrasonic velocities for the binary mixtures of decan-1-ol with 1,2-dichloroethane (DCE), 1,2-dibromoethane (DBE), and 1,1,2,2-tetrachloroethene (TCE) at T = (293.15 and 313.15) K over the entire range of mixture mole fraction and at the atmospheric pressure. From the experimental values of density and ultrasonic velocity, the excess molar volumes, V^{E}, molar free volumes, V_f, thermal expansion coefficients, α, excess molar isentropic compressibilities, $K^{E}_{S,m}$, limiting excess partial molar volumes, $\overline{V}^{E,0}_{i}$, and isentropic compressibilities, $\overline{K}^{E,0}_{m,i}$, intermolecular free lengths, L_f, and available volumes, V_a, by three different methods and parameters V_f/V related to space-filling ability have been calculated. These excess functions have been fitted to the Redlich–Kister polynomial equations to derive the binary coefficients and the standard errors between the experimental and the calculated quantities. The experimental ultrasonic velocities have been analyzed in terms of Nomoto's relation (N), Van Dael's ideal mixture relation (VD), Jacobson's free length theory (FLT), Schaaffs' collision factor theory (CFT), thermoacoustical parameters (TAP), Flory's statistical theory (FT). and Prigogine–Flory–Patterson (PFP) theory.

2. Experimental

2.1. Materials

The mole fraction purity of the liquids from s.d. fine Chemical Ltd. were as follows: 1,2-dichloroethane (0.997), 1,2-dibromoethane (0.995), 1,1,2,2-tetrachloroethene (0.994), and decan-1-ol (0.997). Prior to experimental measurements, all liquids were stored in dark bottles over 0.4 nm molecular sieves to reduce water content and were partially degassed with a vacuum pump under nitrogen atmosphere. The purities of all the samples determined by chromatographic analysis were better than 0.995 on a molar basis. Density and ultrasonic velocity values of the pure liquids and their mixtures at T = (293.15 and 313.15) K were measured with an Anton Paar digital densimeter (model DSA 5000) operated in the static mode and automatically thermostatted within ±0.001 K.

The densities have precision better than $\pm 10^{-3}$ kg · m^{-3} and the velocity of sound values are accurate to ±0.01 m · s^{-1}. Densities and ultrasonic velocities of the pure liquids are in good agreement with the values found in the literature as shown in table 1.

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TABLE 1
Physical properties of pure liquid components.

Pure liquid	T/K	ρ/(g · cm^{-3})		u/(m · s^{-1})		α/kK^{-1}	
		Expt.	Lit.	Expt.	Lit.	Expt.	Lit.
Decan-1-ol	293.15	0.829991	0.8299[a]	1396.37	1397.23[g]	0.8212	0.8400[e]
1,2-DCE	293.15	1.252742	1.25209[b]	1212.75	1194.06 (298.15 K)[h]	1.1643	1.141[b]
1,2 -DBE	293.15	2.179604	2.1791[b]	1006.95	993.73 (298.15 K)[f]	0.9584	0.964 (298.15 K)[c]
1,1,2,2-TCE	293.15	1.622395	1.62283[b]	1053.84	1032.1 (303.15 K)[i]	1.0254	1.030 (298.15 K)[d]

[a] Reference [2].
[b] Reference [23].
[c] Reference [12].
[d] Reference [8].
[e] Reference [20].
[f] Reference [21].
[g] Reference [19].
[h] Reference [4].
[i] Reference [8].

TABLE 2
Densities, ρ, ultrasonic velocities, u, isentropic compressibilities, κ_S, excess molar volumes, V^E, free volume, V_f, excess molar isentropic compressibilities, $K^E_{S,m}$, and thermal expansion coefficients, α, for {halohydrocarbons (1) + decan-1-ol (2)}.

x_1	ϕ_1	$\rho \cdot 10^{-3}$/(kg · m^{-3})	u/(m · s^{-1})	κ_S/(TPa^{-1})	$10^6 \cdot V^E$/(m^3 · mol^{-1})	$10^6 \cdot V_f$/(m^3 · mol^{-1})	$10^{14} \cdot K^E_{S,m}$/(m^5 · N^{-1} · mol^{-1})	α/kK^{-1}
1,2-Dichloroethane (1) + decan-1-ol (2) (T = 293.15 K)								
0.0000	0.0000	0.829991	1396.37	617.91	0.0000	1.6855	0.000	0.8212
0.0692	0.0299	0.841579	1382.81	621.41	0.2266	1.7565	0.083	0.8451
0.1136	0.0504	0.849567	1373.90	623.58	0.3615	1.8006	0.132	0.8564
0.2034	0.0957	0.867401	1355.32	627.62	0.5867	1.8854	0.222	0.8702
0.2938	0.1470	0.887762	1335.62	631.45	0.7761	1.9623	0.303	0.8694
0.3645	0.1920	0.905827	1319.66	633.91	0.8835	2.0220	0.356	0.8653
0.5070	0.2987	0.949509	1287.54	635.30	0.9567	2.1790	0.411	0.8864
0.6043	0.3875	0.986214	1265.40	633.25	0.9490	2.3237	0.418	0.9245
0.6990	0.4903	1.029228	1244.63	627.20	0.8785	2.5245	0.392	0.9969
0.7455	0.5482	1.053665	1235.13	622.12	0.8227	2.6426	0.366	1.0406
0.7816	0.5972	1.074539	1228.31	616.82	0.7604	2.7749	0.338	1.0946
0.8142	0.6448	1.094992	1222.53	611.04	0.6903	2.8721	0.308	1.1286
0.8429	0.6897	1.114401	1218.09	604.78	0.6217	2.9572	0.276	1.1576
0.9034	0.7948	1.160555	1211.63	586.94	0.4209	3.1071	0.187	1.2063
0.9579	0.9041	1.209391	1210.43	564.36	0.1957	3.1386	0.084	1.2132
1.0000	1.0000	1.252742	1212.75	542.74	0.0000	3.0128	0.000	1.1643
1,2-Dichloroethane (1) + decan-1-ol (2) (313.15 K)								
0.0000	0.0000	0.816264	1328.65	693.98	0.0000	2.1836	0.000	0.8428
0.0692	0.0301	0.827391	1314.94	699.00	0.2517	2.2673	0.099	0.8567
0.1136	0.0507	0.835077	1305.73	702.37	0.3986	2.3253	0.162	0.8663
0.2034	0.0963	0.852221	1287.38	708.00	0.6490	2.4538	0.262	0.8923
0.2938	0.1479	0.871824	1267.75	713.68	0.8548	2.6037	0.354	0.9237
0.3645	0.1931	0.889228	1251.27	718.27	0.9706	2.7368	0.424	0.9506
0.5070	0.3002	0.931327	1217.81	724.00	1.0505	3.0199	0.505	1.0003
0.6043	0.3892	0.966695	1195.06	724.32	1.0411	3.2249	0.514	1.0317
0.6990	0.4920	1.008071	1174.28	719.39	0.9700	3.4235	0.474	1.0599
0.7455	0.5499	1.031546	1164.76	714.56	0.9143	3.5238	0.438	1.0752
0.7816	0.5989	1.051572	1157.84	709.36	0.8530	3.5914	0.400	1.0832
0.8142	0.6464	1.071237	1151.93	703.50	0.7782	3.6586	0.361	1.0938
0.8429	0.6912	1.089861	1147.37	696.98	0.7077	3.7228	0.320	1.1066
0.9034	0.7959	1.134212	1140.50	677.82	0.4935	3.8514	0.205	1.1369
0.9579	0.9048	1.181341	1136.85	654.97	0.2366	3.9698	0.090	1.1690
1.0000	1.0000	1.223382	1136.03	633.37	0.0000	4.0825	0.000	1.2025
1,2-Dibromoethane (1) + decan-1-ol (2) (293.15 K)								
0.0000	0.0000	0.829991	1396.37	617.91	0.0000	1.6885	0.000	0.8212
0.0713	0.0335	0.873696	1363.08	616.02	0.3262	1.7885	0.057	0.8953
0.1171	0.0566	0.903742	1341.81	614.57	0.5087	1.8698	0.092	0.9527
0.1704	0.0849	0.940915	1317.21	612.55	0.6841	1.9833	0.128	1.0275
0.2858	0.1532	1.030687	1265.99	605.36	0.9382	2.0635	0.171	1.0482
0.3911	0.2250	1.125696	1218.27	598.54	1.0568	2.0875	0.223	1.0246
0.5100	0.3199	1.252151	1167.73	585.68	1.0542	2.0490	0.233	0.9593
0.5430	0.3494	1.291442	1153.37	582.09	1.0466	2.0197	0.242	0.9258
0.5903	0.3944	1.351801	1134.09	575.16	0.9972	2.0172	0.236	0.9127
0.6875	0.4986	1.492469	1095.33	558.48	0.8289	2.0213	0.220	0.8972
0.7289	0.5486	1.560167	1079.96	549.56	0.7475	2.0243	0.205	0.8955
0.7873	0.6259	1.665231	1059.70	534.76	0.6156	2.0482	0.174	0.9118
0.8411	0.7052	1.773358	1042.20	519.16	0.4875	2.0566	0.143	0.9202
0.9006	0.8037	1.908196	1025.52	498.30	0.3299	2.0319	0.099	0.9150
0.9495	0.8947	2.033543	1015.59	476.77	0.1783	2.0233	0.045	0.9285
1.0000	1.0000	2.179604	1006.95	452.49	0.0000	2.0390	0.000	0.9584

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