Density, Viscosity, Refractive Index, and Speed of Sound in Binary Mixtures of Acrylonitrile with Methanol, Ethanol, Propan-1-ol, Butan-1-ol, Pentan-1-ol, Hexan-1-ol, Heptan-1-ol, and Butan-2-ol

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Density, viscosity, and refractive index data at 298.15, 303.15, and 308.15 K as well as the speed of sound at 298.15 K in the binary mixtures of acrylonitrile with methanol, ethanol, propan-1-ol, butan-1-ol, pentan-1-ol, hexan-1-ol, heptan-1-ol, and butan-2-ol are presented over the whole range of mixture compositions. From these results, excess molar volume, V^E, deviations in viscosity, $\Delta\eta$, molar refraction, ΔR, speed of sound, Δu, and isentropic compressibility, Δk_S have been calculated. These quantities are fitted to a Redlich−Kister type polynomial equation to derive the binary coefficients and estimate the standard deviations between the experimental and calculated quantities.

Introduction

Acrylonitrile is a versatile liquid which finds use as a monomer in the preparation of polyacrylonitrile. Thus, a study of physical property data on the binary mixtures containing acrylonitrile has attracted considerable interest in the literature (Aminabhavi and Banerjee, 1998; Haijun et al.,1994; Sandhu and Singh, 1992). As a part of our ongoing program of research, we present here the experimental results of density, ρ, viscosity, η, and refractive index, n_D, at 298.15, 303.15, and 308.15 K, as well as the speed of sound, u, at 298.15 K for the binary mixtures of acrylonitrile with methanol, ethanol, propan-1-ol, butan-1-ol, pentan-1-ol, hexan-1-ol, heptan-1-ol, and butan-2-ol. From these data, excess molar volume, V^E, deviations in viscosity, $\Delta\eta$, molar refraction, ΔR, the speed of sound, Δu, and isentropic compressibility, Δk_S, have been calculated. These results are fitted to the Redlich and Kister type polynomial equation (Redlich and Kister, 1948) to derive the binary coefficients and estimate the standard deviations between the experimental and calculated results.

Experimental Section

Materials and Methods. High-purity spectroscopic grade samples of acrylonitrile, pentan-1-ol, hexan-1-ol, and heptan-1-ol were purchased from Fluka. Ethanol from E. Merck and butan-2-ol from BDH were used directly. Methanol, propan-1-ol, and butan-1-ol were purchased from s.d. Fine Chemicals Ltd., Mumbai, India. The GLC analyses of these liquids indicated a mol % purity of >99.0. The analyses were performed on a gas chromatograph, HP Series 6890 using a flame ionization detector with fused silica columns, having a sensitivity better than 10^{-8} g of fatty acid/(μL of the solvent). All of the samples were used without further purification. Experimental values of densities, ρ, and refractive indices, n_D, at the sodium-D line for the pure liquids are compared with the published results at 298.15 K in Table 1.

Experimental details about the preparation of binary mixtures, measurements of mass, density, refractive index, speed of sound, and viscosity of pure liquids and binary mixtures are the same as those described previously (Aralaguppi et al., 1991). The mass measurements (±0.01 mg) were made using an electronic balance (Mettler AE 240). The reproducibility in mole fraction was within ±0.0001 units. Densities of pure liquids and their mixtures were measured using a pycnometer having a bulb volume of 15 cm^3 and a capillary bore with an internal diameter of 1 mm. Density values are accurate to ±0.0002 g·cm^{-3}.

Viscosities were measured using a Cannon Fenske Viscometer (size 75, Industrial Research Glassware Ltd., Roselle, NJ). An electronic digital stopwatch with a readability of ±0.01 s was used for the flow time measurements. The measured viscosity values are accurate to ±0.001 mPa·s. Calibrations of the pycnometer and viscometer are the same as those described earlier (Aminabhavi and Bindu, 1995; Aminabhavi et al., 1994).

The speed of sound values were measured using a variable path single-crystal interferometer (Mittal Enterprises, Model M-84, New Delhi). The interferometer was used at a frequency of 1 kHz and was calibrated using water and benzene. The speed of sound values are accurate to ±2 m·s^{-1}. In all the property measurements, an INSREF

Table 1. Comparison of Experimental Densities (ρ) and Refractive Indices (n_D) of Pure Liquids with Literature Values at 298.15 K

	ρ/(g·cm^{-3})		n_D	
liquid (mol % purity)	expt	lit.	expt	lit.
acrylonitrile (99.06)	0.8004	0.8003[a]	1.3900	1.3888[b]
methanol (99.7)	0.7869	0.7866[c,d]	1.3278	1.3265[d,e]
		0.7867[e]		
ethanol (99.6)	0.7854	0.7851[d]	1.3605	1.3594[d]
		0.7850[e]		1.3592[e]
propan-1-ol (99.75)	0.7995	0.7997[d]	1.3838	1.3837[d]
butan-1-ol (99.5)	0.8059	0.8060[d]	1.3984	1.3973[d]
pentan-1-ol (99.7)	0.8107	0.8109[f]	1.4090	1.4077[g]
hexan-1-ol (99.75)	0.8147	0.8152[g]	1.4163	1.4160[g]
heptan-1-ol (99.8)	0.8189	0.8197[b]	1.4233	1.4227[b]
butan-2-ol (99.5)	0.8024	0.8024[b]	1.3951	1.3953[b]

[a] Haijun et al., 1994. [b] Riddick et al., 1986. [c] Won et al., 1981. [d] Marsh, 1994. [e] Rodriguez et al., 1996. [f] Garcia et al., 1991. [g] Ortega and Matos, 1986.

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Table 2. Experimental Densities (ρ), Refractive Indices (n_D), Viscosities (η), and the Speed of Sound (u) of the Binary Mixtures at Different Temperatures

x_1	ρ/(g·cm^{-3})	n_D	η/(mPa·s)	u/(m·s^{-1})	x_1	ρ/(g·cm^{-3})	n_D	η/(mPa·s)	u/(m·s^{-1})	x_1	ρ/(g·cm^{-3})	n_D	η/(mPa·s)	u/(m·s^{-1})
Acrylonitrile (1) + Methanol (2)														
298.15 K														
0.0000	0.7869	1.3278	0.545	1108	0.4017	0.7968	1.3621	0.388	1160	0.7966	0.7997	1.3826	0.340	1184
0.1021	0.7906	1.3386	0.483	1124	0.5035	0.7979	1.3687	0.367	1168	0.8985	0.8001	1.3865	0.338	1188
0.2197	0.7938	1.3489	0.435	1140	0.6614	0.7989	1.3766	0.351	1178	1.0000	0.8004	1.3900	0.339	1192
0.3020	0.7953	1.3552	0.410	1150	0.6991	0.7992	1.3787	0.346	1180					
303.15 K														
0.0000	0.7821	1.3265	0.510		0.4017	0.7914	1.3594	0.367		0.7966	0.7943	1.3798	0.325	
0.1021	0.7855	1.3361	0.453		0.5035	0.7924	1.3659	0.354		0.8985	0.7946	1.3835	0.322	
0.2197	0.7887	1.3448	0.410		0.6614	0.7932	1.3718	0.337		1.0000	0.7950	1.3871	0.326	
0.3020	0.7901	1.3530	0.387		0.6991	0.7937	1.3760	0.329						
308.15 K														
0.0000	0.7776	1.3254	0.477		0.4017	0.7861	1.3575	0.348		0.7966	0.7885	1.3774	0.311	
0.1021	0.7807	1.3339	0.428		0.5035	0.7870	1.3630	0.331		0.8985	0.7889	1.3810	0.309	
0.2197	0.7835	1.3441	0.387		0.6614	0.7878	1.3707	0.318		1.0000	0.7891	1.3845	0.312	
0.3020	0.7849	1.3506	0.366		0.6991	0.7881	1.3731	0.315						
Acrylonitrile (1) + Ethanol (2)														
298.15 K														
0.0000	0.7854	1.3605	1.099	1148	0.4030	0.7935	1.3742	0.513	1176	0.8006	0.7981	1.3849	0.363	1189
0.1009	0.7887	1.3646	0.859	1157	0.5025	0.7947	1.3770	0.458	1180	0.8993	0.7993	1.3874	0.348	1191
0.2017	0.7907	1.3679	0.704	1165	0.6044	0.7958	1.3797	0.415	1184	1.0000	0.8004	1.3900	0.339	1192
0.3022	0.7922	1.3711	0.593	1171	0.7032	0.7969	1.3824	0.384	1187					
303.15 K														
0.0000	0.7815	1.3589	0.994		0.4030	0.7886	1.3716	0.480		0.8006	0.7929	1.3824	0.345	
0.1009	0.7841	1.3620	0.787		0.5025	0.7898	1.3745	0.431		0.8993	0.7939	1.3847	0.332	
0.2017	0.7859	1.3649	0.648		0.6044	0.7909	1.3772	0.392		1.0000	0.7950	1.3871	0.326	
0.3022	0.7874	1.3687	0.551		0.7032	0.7920	1.3796	0.364						
308.15 K														
0.0000	0.7772	1.3568	0.907		0.4030	0.7835	1.3692	0.451		0.8006	0.7873	1.3795	0.329	
0.1008	0.7796	1.3602	0.724		0.5025	0.7846	1.3719	0.405		0.8993	0.7883	1.3821	0.318	
0.2017	0.7812	1.3633	0.602		0.6044	0.7855	1.3746	0.371		1.0000	0.7891	1.3845	0.312	
0.3022	0.7824	1.3663	0.513		0.7032	0.7864	1.3771	0.347						
Acrylonitrile (1) + Propan-1-ol (2)														
298.15 K														
0.0000	0.7995	1.3838	1.941	1216	0.4079	0.8009	1.3868	0.688	1198	0.8002	0.8004	1.3889	0.393	1190
0.1031	0.8003	1.3846	1.409	1212	0.5104	0.8007	1.3873	0.578	1195	0.9032	0.8004	1.3896	0.360	1191
0.2030	0.8007	1.3853	1.074	1207	0.6066	0.8005	1.3879	0.497	1192	1.0000	0.8004	1.3900	0.339	1192
0.3070	0.8008	1.3860	0.850	1202	0.7057	0.8005	1.3884	0.435	1190					
303.15 K														
0.0000	0.7955	1.3819	1.722		0.4079	0.7959	1.3847	0.635		0.8002	0.7953	1.3863	0.373	
0.1031	0.7961	1.3824	1.264		0.5104	0.7959	1.3851	0.538		0.9032	0.7950	1.3865	0.343	
0.2030	0.7962	1.3830	0.975		0.6066	0.7955	1.3855	0.465		1.0000	0.7950	1.3871	0.326	
0.3070	0.7962	1.3838	0.778		0.7057	0.7953	1.3858	0.412						
308.15 K														
0.0000	0.7916	1.3797	1.543		0.4079	0.7912	1.3821	0.590		0.8002	0.7897	1.3837	0.355	
0.1031	0.7916	1.3803	1.139		0.5104	0.7908	1.3825	0.503		0.9032	0.7894	1.3842	0.328	
0.2030	0.7917	1.3809	0.888		0.6066	0.7904	1.3829	0.438		1.0000	0.7891	1.3845	0.312	
0.3070	0.7916	1.3816	0.710		0.7057	0.7900	1.3833	0.389						
Acrylonitrile (1) + Butan-1-ol (2)														
298.15 K														
0.0000	0.8059	1.3984	2.532	1244	0.4063	0.8045	1.3960	0.849	1215	0.8074	0.8019	1.3924	0.429	1195
0.1054	0.8056	1.3978	1.797	1236	0.5073	0.8039	1.3955	0.690	1209	0.9006	0.8012	1.3910	0.386	1193
0.2059	0.8054	1.3976	1.363	1228	0.6039	0.8033	1.3945	0.581	1204	1.0000	0.8004	1.3900	0.339	1192
0.3050	0.8050	1.3966	1.065	1222	0.6962	0.8027	1.3935	0.499	1200					
303.15 K														
0.0000	0.8018	1.3961	2.209		0.4063	0.8000	1.3937	0.776		0.8074	0.7967	1.3898	0.407	
0.1054	0.8016	1.3957	1.596		0.5073	0.7992	1.3926	0.637		0.9006	0.7959	1.3884	0.369	
0.2059	0.8011	1.3953	1.221		0.6039	0.7984	1.3921	0.539		1.0000	0.7950	1.3871	0.326	
0.3050	0.8004	1.3947	0.965		0.6962	0.7976	1.3906	0.468						
308.15 K														
0.0000	0.7982	1.3924	1.949		0.4063	0.7955	1.3914	0.714		0.8074	0.7914	1.3865	0.385	
0.1054	0.7976	1.3936	1.424		0.5073	0.7945	1.3902	0.594		0.9006	0.7904	1.3854	0.352	
0.2059	0.7970	1.3931	1.102		0.6039	0.7936	1.3891	0.505		1.0000	0.7891	1.3845	0.312	
0.3050	0.7963	1.3921	0.881		0.6962	0.7926	1.3881	0.442						

Table 2 (Continued)

x_1	ρ/ (g·cm^{-3})	n_D	η/ (mPa·s)	u/ (m·s^{-1})	x_1	ρ/ (g·cm^{-3})	n_D	η/ (mPa·s)	u/ (m·s^{-1})	x_1	ρ/ (g·cm^{-3})	n_D	η/ (mPa·s)	u/ (m·s^{-1})
Acrylonitrile (1) + Pentan-1-ol (2)														
298.15 K														
0.0000	0.8107	1.4090	3.388	1279	0.4053	0.8080	1.4033	1.064	1240	0.8042	0.8034	1.3951	0.464	1202
0.1032	0.8102	1.4078	2.405	1271	0.5035	0.8070	1.4021	0.847	1229	0.9004	0.8020	1.3927	0.401	1196
0.2077	0.8095	1.4063	1.777	1260	0.6091	0.8059	1.3998	0.668	1219	1.0000	0.8004	1.3900	0.339	1192
0.3006	0.8089	1.4050	1.384	1251	0.7025	0.8047	1.3979	0.558	1210					
303.15 K														
0.0000	0.8071	1.4070	2.925		0.4053	0.8036	1.4010	0.965		0.8042	0.7981	1.3927	0.436	
0.1032	0.8063	1.4055	2.107		0.5035	0.8023	1.3995	0.774		0.9004	0.7965	1.3900	0.382	
0.2077	0.8056	1.4041	1.580		0.6091	0.8009	1.3975	0.619		1.0000	0.7950	1.3870	0.326	
0.3006	0.8047	1.4030	1.240		0.7025	0.7997	1.3952	0.520						
308.15 K														
0.0000	0.8034	1.4048	2.543		0.4053	0.7995	1.3989	0.879		0.8042	0.7932	1.3902	0.416	
0.1032	0.8026	1.4035	1.860		0.5035	0.7981	1.3973	0.715		0.9004	0.7913	1.3874	0.364	
0.2077	0.8017	1.4024	1.413		0.6091	0.7966	1.3949	0.577		1.0000	0.7891	1.3845	0.315	
0.3006	0.8007	1.4005	1.122		0.7025	0.7951	1.3927	0.488						
Acrylonitrile (1) + Hexan-1-ol (2)														
298.15 K														
0.0000	0.8147	1.4163	4.394	1310	0.4105	0.8111	1.4093	1.300	1257	0.8056	0.8048	1.3957	0.495	1218
0.1023	0.8141	1.4149	3.139	1298	0.5081	0.8098	1.4058	1.006	1248	0.9019	0.8029	1.3903	0.410	1204
0.2036	0.8133	1.4132	2.308	1284	0.6117	0.8080	1.4027	0.774	1240	1.0000	0.8004	1.3900	0.339	1192
0.3089	0.8123	1.4113	1.705	1270	0.7084	0.8064	1.4002	0.617	1230					
303.15 K														
0.0000	0.8113	1.4140	3.733		0.4105	0.8069	1.4077	1.175		0.8056	0.7999	1.3957	0.466	
0.1023	0.8102	1.4132	2.727		0.5081	0.8055	1.4052	0.916		0.9019	0.7973	1.3901	0.388	
0.2036	0.8094	1.4115	2.030		0.6117	0.8037	1.4002	0.712		1.0000	0.7950	1.3871	0.326	
0.3089	0.8080	1.4096	1.522		0.7084	0.8017	1.3958	0.571						
308.15 K														
0.0000	0.8078	1.4122	3.213		0.4105	0.8027	1.4051	1.063		0.8056	0.7947	1.3902	0.439	
0.1023	0.8068	1.4112	2.380		0.5081	0.8010	1.4015	0.840		0.9019	0.7922	1.3853	0.370	
0.2036	0.8057	1.4099	1.799		0.6117	0.7989	1.3996	0.661		1.0000	0.7891	1.3845	0.312	
0.3089	0.8043	1.4076	1.365		0.7084	0.7969	1.3956	0.533						
Acrylonitrile (1) + Heptan-1-ol (2)														
298.15 K														
0.0000	0.8189	1.4233	5.652	1330	0.4142	0.8140	1.4151	1.627	1278	0.8027	0.8065	1.4008	0.540	1221
0.1047	0.8180	1.4215	4.015	1315	0.5106	0.8124	1.4125	1.238	1266	0.9033	0.8038	1.3956	0.425	1206
0.2060	0.8169	1.4202	2.967	1302	0.6206	0.8104	1.4085	0.891	1250	1.0000	0.8004	1.3900	0.339	1192
0.3057	0.8156	1.4174	2.212	1291	0.7044	0.8088	1.4052	0.705	1236					
303.15 K														
0.0000	0.8153	1.4211	4.759		0.4142	0.8100	1.4131	1.441		0.8027	0.8014	1.3986	0.508	
0.1047	0.8145	1.4194	3.469		0.5106	0.8081	1.4106	1.189		0.9033	0.7987	1.3931	0.403	
0.2060	0.8132	1.4179	2.587		0.6206	0.8059	1.4066	0.815		1.0000	0.7950	1.3871	0.326	
0.3057	0.8115	1.4155	1.958		0.7044	0.8040	1.4030	0.652						
308.15 K														
0.0000	0.8119	1.4197	4.045		0.4142	0.8058	1.4111	1.296		0.8027	0.7966	1.3963	0.478	
0.1047	0.8107	1.4175	3.000		0.5106	0.8039	1.4085	1.013		0.9033	0.7932	1.3906	0.383	
0.2060	0.8093	1.4159	2.273		0.6206	0.8014	1.4040	0.750		1.0000	0.7891	1.3845	0.312	
0.3057	0.8078	1.4134	1.730		0.7044	0.7994	1.4009	0.605						
Acrylonitrile (1) + Butan-2-ol (2)														
298.15 K														
0.0000	0.8024	1.3951	2.925	1230	0.4055	0.7996	1.3924	0.775	1224	0.8030	0.7994	1.3900	0.418	1217
0.1033	0.8014	1.3946	1.828	1210	0.5087	0.7992	1.3921	0.630	1213	0.8992	0.7998	1.3895	0.378	1204
0.2014	0.8007	1.3937	1.319	1222	0.6049	0.7990	1.3911	0.536	1220	1.0000	0.8004	1.3900	0.339	1192
0.3010	0.8001	1.3934	0.990	1206	0.7009	0.7991	1.3904	0.456	1210					
303.15 K														
0.0000	0.7983	1.3921	2.417		0.4055	0.7948	1.3898	0.704		0.8030	0.7940	1.3873	0.391	
0.1033	0.7968	1.3920	1.567		0.5087	0.7943	1.3893	0.582		0.8992	0.7944	1.3867	0.358	
0.2014	0.7963	1.3914	1.165		0.6049	0.7938	1.3885	0.499		1.0000	0.7950	1.3871	0.326	
0.3010	0.7954	1.3908	0.887		0.7009	0.7936	1.3876	0.438						
308.15 K														
0.0000	0.7939	1.3910	2.011		0.4055	0.7898	1.3872	0.644		0.8030	0.7885	1.3843	0.373	
0.1033	0.7926	1.3898	1.361		0.5087	0.7892	1.3864	0.539		0.8992	0.7889	1.3839	0.342	
0.2014	0.7916	1.3891	1.024		0.6049	0.7887	1.3857	0.465		1.0000	0.7891	1.3845	0.312	
0.3010	0.7907	1.3882	0.799		0.7009	0.7884	1.3849	0.413						

Table 3. Estimated Parameters of Excess and Deviation Funtions for Mixtures

function	temp/K	A_0	A_1	A_2	σ
		Acrylonitrile (1) + Methanol (2)			
$V^E \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−0.671	−0.323	−0.069	0.004
	303.15	−0.619	−0.367	−0.119	0.009
	308.15	−0.597	−0.284	−0.033	0.006
$\Delta R \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−3.475	−0.775	−0.149	0.006
	303.15	−3.550	−0.697	−0.343	0.028
	308.15	−3.574	−0.705	−0.346	0.010
$\Delta\eta/(mPa \cdot s)$	298.15	−0.291	−0.111	−0.083	0.001
	303.15	−0.258	−0.103	−0.113	0.002
	308.15	−0.249	−0.087	−0.054	0.001
$\Delta u/(m \cdot s^{-1})$	298.15	71.95	19.80	−10.44	0.158
$\Delta k_s/(TPa^{-1})$	298.15	−83.50	−3.20	22.46	0.315
		Acrylonitrile (1) + Ethanol (2)			
$V^E \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−0.378	−0.613	−0.512	0.007
	303.15	−0.362	−0.401	−0.216	0.007
	308.15	−0.310	−0.379	−0.306	0.005
$\Delta R \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−0.318	0.008	−0.053	0.002
	303.15	−0.347	0.114	−0.160	0.008
	308.15	−0.362	0.010	−0.059	0.002
$\Delta\eta/(mPa \cdot s)$	298.15	−1.039	−0.590	−0.342	0.004
	303.15	−0.912	−0.500	−0.293	0.003
	308.15	−0.810	−0.434	−0.243	0.002
$\Delta u/(m \cdot s^{-1})$	298.15	40.60	9.91	7.26	0.208
$\Delta k_s/(TPa^{-1})$	298.15	−67.17	21.97	−17.31	0.262
		Acrylonitrile (1) + Propan-1-ol (2)			
$V^E \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−0.268	−0.398	−0.154	0.004
	303.15	−0.186	−0.335	−0.166	0.010
	308.15	−0.158	−0.239	−0.034	0.007
$\Delta R \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−0.202	0.076	−0.063	0.001
	303.15	−0.154	0.084	−0.216	0.006
	308.15	−0.171	0.043	−0.035	0.001
$\Delta\eta/(mPa \cdot s)$	298.15	−2.210	−1.388	−0.849	0.009
	303.15	−1.909	−1.173	−0.709	0.007
	308.15	−1.669	−1.033	−0.644	0.006
$\Delta u/(m \cdot s^{-1})$	298.15	−37.31	15.07	9.90	0.305
$\Delta k_s/(TPa^{-1})$	298.15	55.62	20.51	−20.42	0.441
		Acrylonitrile (1) + Butan-1-ol (2)			
$V^E \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−0.153	−0.149	0.018	0.004
	303.15	−0.116	−0.203	−0.088	0.008
	308.15	−0.095	−0.094	0.023	0.004
$\Delta R \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−2.065	0.332	−0.171	0.007
	303.15	−2.042	0.297	0.040	0.009
	308.15	−1.913	−0.110	0.405	0.017
$\Delta\eta/(mPa \cdot s)$	298.15	−2.929	−1.900	−1.057	0.015
	303.15	−2.479	−1.559	−0.812	0.011
	308.15	−2.115	−1.311	−0.683	0.010
$\Delta u/(m \cdot s^{-1})$	298.15	−32.61	9.34	−7.04	0.242
$\Delta k_s/(TPa^{-1})$	298.15	63.62	1.50	6.98	0.284
		Acrylonitrile (1) + Pentan-1-ol (2)			
$V^E.10^6/(m^3.mol^{-1})$	298.15	−0.097	−0.142	−0.056	0.001
	303.15	−0.052	−0.226	0.041	0.007
	308.15	−0.089	−0.119	−0.016	0.001
$\Delta R \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−5.397	1.324	−0.561	0.008
	303.15	−5.340	1.362	−0.513	0.007
	308.15	−5.345	1.276	−0.347	0.010
$\Delta\eta/(mPa \cdot s)$	298.15	−4.035	−2.502	−1.388	0.019
	303.15	−3.375	−2.025	−1.085	0.015
	308.15	−2.831	−1.656	−0.841	0.012
$\Delta u/(m \cdot s^{-1})$	298.15	−24.23	33.43	4.19	0.264
$\Delta k_s/(TPa^{-1})$	298.15	83.20	20.26	−25.79	0.536
		Acrylonitrile (1) + Hexan-1-ol (2)			
$V^E \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−0.003	−0.305	−0.147	0.009
	303.15	0.052	−0.066	0.142	0.018
	308.15	0.087	−0.264	−0.202	0.005
$\Delta R \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−9.968	2.448	−1.601	0.025
	303.15	−9.883	2.573	−0.258	0.047
	308.15	−9.746	2.132	−1.471	0.030
$\Delta\eta/(mPa \cdot s)$	298.15	−5.349	−3.128	−1.660	0.016
	303.15	−4.375	−2.391	−1.182	0.011
	308.15	−3.624	−1.906	−0.921	0.009
$\Delta u/(m \cdot s^{-1})$	298.15	−7.12	−31.80	22.89	1.618
$\Delta k_s/(TPa^{-1})$	298.15	61.86	−53.32	40.20	1.967
		Acrylonitrile (1) + Heptan-1-ol			
$V^E \times 10^6/(m^3 \cdot mol^{-1})$	298.15	0.225	−0.158	−0.415	0.003
	303.15	0.251	−0.326	−0.514	0.016
	308.15	0.258	−0.114	−0.238	0.003
$\Delta R \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−14.84	5.420	−2.292	0.023
	303.15	−14.65	5.360	−2.358	0.022
	308.15	−14.66	5.408	−2.446	0.028
$\Delta\eta/(mPa \cdot s)$	298.15	−6.890	−3.709	−2.050	0.026
	303.15	−5.503	−2.788	−1.609	0.030
	308.15	−4.577	−2.141	−0.926	0.009
$\Delta u/(m \cdot s^{-1})$	298.15	21.98	−6.15	−41.61	0.328
$\Delta k_s/(TPa^{-1})$	298.15	73.35	−6.39	43.50	1.179
		Acrylonitrile (1) + Butan-2-ol (2)			
$V^E \times 10^6/(m^3 \cdot mol^{-1})$	298.15	0.937	0.028	−0.078	0.006
	303.15	1.058	−0.016	0.116	0.019
	308.15	1.101	0.030	−0.071	0.010
$\Delta R \times 10^6/(m^3 \cdot mol^{-1})$	298.15	−2.102	0.134	−0.181	0.008
	303.15	−2.010	0.034	0.062	0.010
	308.15	−2.162	0.198	−0.253	0.004
$\Delta\eta/(mPa \cdot s)$	298.15	−3.935	−3.362	−2.530	0.042
	303.15	−3.100	−2.533	−1.845	0.030
	308.15	−2.451	−1.907	−1.287	0.019
$\Delta u/(m \cdot s^{-1})$	298.15	24.50	−112.52	−43.10	7.695
$\Delta k_s/(TPa^{-1})$	298.15	−29.86	−139.8	104.8	11.004

model 016 AP thermostat was used at a constant digital temperature display accurate to ±0.01 K. The results of ρ, n_D, η, and u compiled in Table 2 represent the averages of three independent measurements for each composition of the mixture.

Results and Discussion

Experimental values of ρ, n_D, η, and u are used to calculate the mixing functions using the general type equation (Aminabhavi and Bindu, 1995; Aminabhavi et al., 1994):

$$V^E \text{ (or } \Delta Y) = V_m \text{ (or } Y_m) - [V_1 \text{ (or } Y_1)]c_1 - [V_2 \text{ (or } Y_2)]c_2 \quad (1)$$

where V_m refers to the molar volume of the mixture which is calculated as

$$V_m = (M_1x_1 + M_2x_2)/\rho_m \quad (2)$$

Here, M_1 and M_2 are molecular weights of components 1 and 2; V_i ($=M_i/\rho_i$) represents the molar volume of the pure components; Y_m refers to the mixture properties, viz., n_D, η, u, and k_S, while Y_i refers to the properties of pure components ($i = 1, 2$). The quantity ΔY refers to ΔR, $\Delta\eta$, Δu, and Δk_S. For the calculation of ΔR and Δk_S, the volume fraction, ϕ_i was used in place of c_i, while for the remaining quantities and V^E, the mole fraction, x_i, was used (Aminabhavi and Bindu, 1995; Aminabhavi et al., 1994). ϕ_i was calculated as

$$\phi_i = \left(\frac{x_iV_i}{\sum_i x_iV_i}\right) \quad (3)$$

The mixing functions, viz., V^E, ΔR, $\Delta\eta$, Δu, and Δk_S, are fitted to the Redlich−Kister equation (Redlich and Kister, 1948):

$$V^E \text{ (or } \Delta Y) = c_1c_2\sum_{i=1}^{2} A_i(c_2 - c_1)^{i-1} \quad (4)$$

where the coefficients A_i ($i = 0-2$) were obtained by the method of least-squares using the Marquardt algorithm (Marquardt, 1963). In solving eq 4 for ΔR and Δk_S, the volume fraction, ϕ_i, is used in place of c_i, and for the remaining quantities, the mole fraction, x_i, is used. The values of standard deviation, σ, are computed for each of the functions (V^E, ΔR, $\Delta\eta$, Δu, and Δk_S). The calculated values of A_0, A_1, and A_2 along with the σ values are given in Table 3. While minimizing the function, we found that the best fits were obtained by solving eq 4 up to the third degree; i.e., $A_i = 0-2$.

Figure 1 displays the plots of V^E vs x_1 (referring to acrylonitrile) at 298.15 K for all of the binary mixtures. Variations in the V^E vs x_1 curves are quite different depending upon the nature of the second component in the mixture. For instance, the negative V^E observed for the acrylonitrile + methanol, + ethanol, or + propan-1-ol mixture is attributed to the self-associating effect of alcohols, in addition to the large differences in the molar volumes of the component liquids, indicating varying specific interactions between the hydroxy group of the alkanols and the cyanide group of acrylonitrile. These values increase systematically with an increase in the size of the alkanols. For mixtures containing higher alkanols, viz., acrylonitrile + butan-1-ol or + pentan-1-ol, no sharp minima are observed in the V^E plots and such curves for

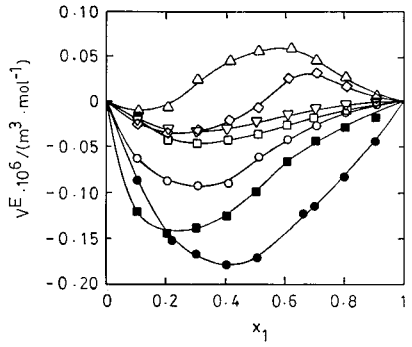

Figure 1. Excess molar volume vs mole fraction of acrylonitrile with (●) methanol, (■) ethanol, (○) propan-1-ol, (□) butan-1-ol, (▽) pentan-1-ol, (◇) hexan-1-ol, and (△) heptan-1-ol at 298.15 K.

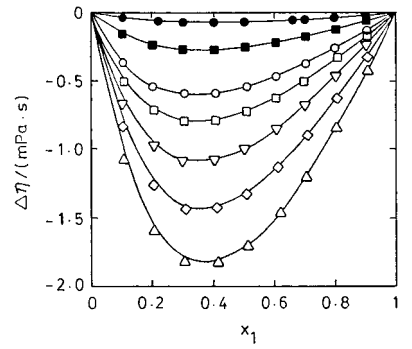

Figure 2. Deviation in viscosity vs mole fraction of acrylonitrile at 298.15 K. Symbols are the same as those given in Figure 1.

these mixtures vary identically. In the case of mixtures of acrylonitrile + hexan-1-ol or + heptan-1-ol, the sigmoidal shapes from negative to positive values are observed, indicating the varying interactions depending upon the composition of acrylonitrile in the binary mixtures. The values of V^E for mixtures of acrylonitrile + butan-2-ol are quite large, indicating the dispersion type interactions, and this curve is not presented because it is out of the scale set for other mixtures.

The effect of temperature on V^E is not the same in all the cases; i.e., with acrylonitrile + methanol, + ethanol, + propan-1-ol, or + butan-1-ol mixtures, the negative values of V^E decrease with increasing temperature, whereas with acrylonitrile + pentan-1-ol, + hexan-1-ol, + heptan-1-ol, and + butan-2-ol, the V^E values do not show any systematic variation with increasing temperature. In view of the limited temperature range studied, the temperature dependencies of V^E vs x_1 curves are not displayed.

Figure 2 shows the plots of $\Delta\eta$ vs x_1 for acrylonitrile + *n*-alkanol mixtures at 298.15 K. For all these mixtures, the $\Delta\eta$ values are negative throughout the mixture composition and exhibit quite opposite trends to those of V^E curves. For the binary mixtures containing lower alkanols, sharp minima are not observed, but with an increase in the size of the alkanols, the $\Delta\eta$ curves exhibit sharper minima, indicating varying molecular interactions between the mixing molecules depending upon their sizes. The same dependencies are also observed at 303.15 and 308.15 K, but these curves are not displayed so as to avoid any redundancy. With increasing temperature, the values of $\Delta\eta$ also increase for all of the mixtures.

Figure 3 depicts the plots of ΔR vs ϕ_1 at 298.15 K. It is found that the values of ΔR decrease with an increase in the molecular size of the alkanols. For the acrylonitrile + methanol, + ethanol, or + propan-1-ol mixtures, the negative ΔR values are quite identical over the whole range

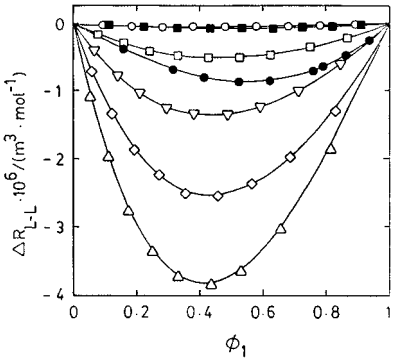

Figure 3. Deviation in molar refraction vs volume fraction of acrylonitrile at 298.15 K. Symbols are the same as those given in Figure 1.

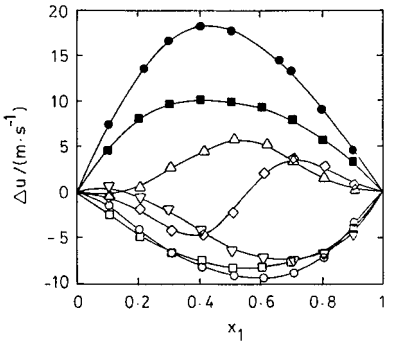

Figure 4. Deviation in speed of sound vs mole fraction of acrylonitrile at 298.15 K. Symbols are the same as those given in Figure 1.

of mixture compositions. For the remaining mixtures, the ΔR values are more negative and show a decrease according to the following sequence: butan-1-ol > methanol > pentan-1-ol > hexan-1-ol > heptan-1-ol. For the binary mixtures containing pentan-1-ol, hexan-1-ol, or heptan-1-ol, the ΔR vs ϕ_1 curves exhibit sharper minima.

From the plots of Δu vs x_1 presented in Figure 4, we find that the values of Δu are positive for mixtures of acrylonitrile + methanol or + ethanol. On the other hand, for mixtures of acrylonitrile with propan-1-ol, butan-1-ol, and pentan-1-ol, the Δu values are negative. In the case of mixtures of acrylonitrile with hexan-1-ol or heptan-1-ol, the curves are sigmoidal. In general, the Δu values for mixtures with *n*-alkanols do not show any systematic trend.

The results of Δk_S vs ϕ_1 displayed in Figure 5 also do not exhibit any systematic trend with the size of the alkanols. In the case of mixtures of acrylonitrile + methanol or + ethanol, the Δk_S values are negative, whereas for all the remaining mixtures, the values of Δk_S are positive.

In the case of acrylonitrile + butan-2-ol mixtures, we have just presented the estimated parameter values for ΔR, $\Delta \eta$, Δu, and Δk_S, but the results are not displayed graphically to minimize the number of curves. The results of ΔR lie much lower than that observed for the acrylonitrile + heptan-1-ol mixture, but the results of $\Delta \eta$ lie between acrylonitrile + butan-1-ol and acrylonitrile + pentan-1-ol mixtures. The Δu results are between mixtures of acrylonitrile containing heptan-1-ol and ethanol mixtures. The values of Δk_S lie between the binary mixtures of acrylonitrile containing ethanol and propan-1-ol.

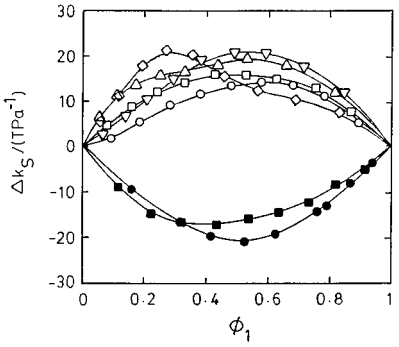

Figure 5. Deviation in isentropic compressibility vs volume fraction of acrylonitrile at 298.15 K. Symbols are the same as those given in Figure 1.

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