Densities and Excess Molar Volumes for Acetone + Propionic Acid + Water from (283.15 to 323.15) K at Atmospheric Pressure

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This paper presents experimental densities for the system acetone + propionic acid + water at atmospheric pressure from (283.15 to 323.15) K. A vibrating-tube densimeter provides density measurements over the entire composition range. We have calculated the excess volumes of the mixture and represent them with a Redlich−Kister-type polynomial.

Introduction

In the chemical industry, knowledge of the thermophysical properties of mixtures is of great importance. These properties result from experimental measurements or correlations. Developing accurate correlations requires accurate experimental measurements to ensure that the equation represents the correct physical behavior of the measured property. Two properties of considerable interest are the density and the excess volume of the mixture. Recently, Estrada-Baltazar et al.[1] reported the atmospheric pressure densities from (283.15 to 323.15) K for the pure components and the binary mixtures for acetone, water, and propionic acid. Lebed and Eddin[2] have measured the density of the ternary system acetone + propionic acid + water at 298 K over a reduced range of compositions. They show that the excess volume for the ternary systems along different propionic acid isopleths has a constant value independent of the propionic acid mole fraction. They use a vibrating device and a pycnometer to measure the densities. However, we have found[1] a discrepancy within their measurements for acetone + propionic acid.

This paper is a continuation of our previous work in which we report the atmospheric pressure densities of the ternary system acetone (1) + propionic acid (2) + water (3) from (283.15 to 323.15) K over the entire range of composition using a vibrating-tube densimeter. Another purpose of this work is to check the acetone mole fraction at which the excess volume has a constant value as mentioned by Lebed and Eden.[2] We have calculated excess volumes from the experimental densities and represent them with a Redlich−Kister-type equation.

Experimental Section

We have used an Anton Paar (DMA 5000) vibrating-tube densimeter[1] to measure the densities of the mixture. The densimeter has an uncertainty reported by the manufacturer of ±0.005 kg·m^{-3}, but we believe the accuracy is on the order of ±0.03 kg·m^{-3}. A platinum resistance thermometer with an uncertainty of ±0.01 K on ITS-90 provides temperature measurements. The repeatability of the density and temperature measurements is ±0.001 kg·m^{-3} and ±0.001 K, respectively. The manufacturer has calibrated the apparatus with ultrapure water and air. We have reported the principle of measurement in our previous work[1] together with measured water densities to test the calibration.

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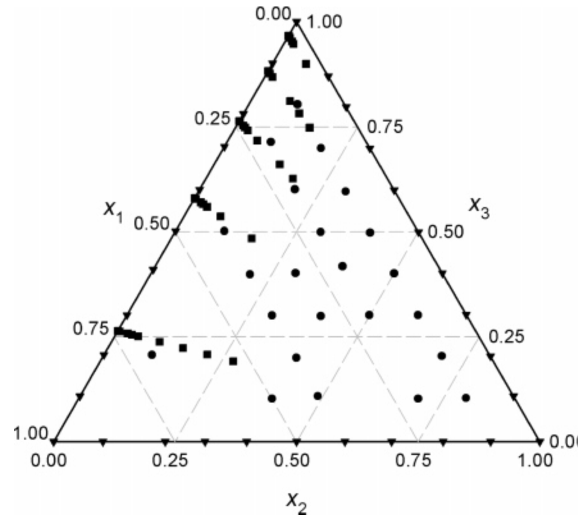

Figure 1. Mole fraction distribution of the density measurements at 298.15 K: ●, this work; ▼, Estrada-Baltazar, et al.;[1] ■, Lebed and Eddin.[2]

Samples

Fermont International supplied the acetone (stated purity 99.7%), and the water and propionic acid came from J. T. Baker. The stated purity for propionic acid was 99%. The water grade was HPLC. Reagents were used as received, and mixtures have been prepared gravimetrically using an analytical balance (Ohaus model AS120S) with a precision of ±0.1 mg. The overall uncertainty in the mole fractions was ±0.2%.

Results and Discussion

Atmospheric pressure densities (ρ) from (283.15 to 323.15) K have been measured using a vibrating-tube densimeter. Figure 1 is a plot of the new measurements

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Table 1. Experimental Densities (ρ) and Excess Molar Volumes (V^E) for Acetone (1) + Propionic Acid (2) + Water (3)

x_1	x_2	T/K	ρ/kg·m^{-3}	V^E/cm^3·mol^{-1}	x_1	x_2	T/K	ρ/kg·m^{-3}	V^E/cm^3·mol^{-1}
0.7990	0.1006	283.15	838.300	−0.71187	0.3010	0.4951	283.15	951.092	−1.20111
0.6941	0.0993	283.15	851.832	−1.00337	0.2997	0.5979	283.15	952.539	−0.95859
0.6997	0.1995	283.15	862.898	−0.89911	0.1964	0.0899	283.15	954.236	−1.31407
0.5953	0.2979	283.15	887.333	−1.02676	0.2034	0.1959	283.15	962.779	−1.42915
0.4970	0.1009	283.15	884.180	−1.40052	0.2010	0.2996	283.15	969.037	−1.42947
0.5026	0.2991	283.15	901.998	−1.16366	0.1970	0.3853	283.15	972.980	−1.39578
0.4996	0.3981	283.15	909.420	−1.04679	0.1998	0.4986	283.15	973.993	−1.27951
0.3979	0.1007	283.15	904.234	−1.49148	0.1989	0.5953	283.15	972.714	−1.01305
0.3968	0.2046	283.15	915.335	−1.44093	0.1990	0.6986	283.15	972.672	−0.81723
0.4004	0.2991	283.15	922.398	−1.38669	0.0965	0.1000	283.15	986.781	−0.99224
0.4007	0.3993	283.15	928.632	−1.29812	0.1004	0.2004	283.15	994.357	−1.19604
0.4025	0.4888	283.15	930.254	−1.02074	0.1014	0.3026	283.15	998.125	−1.29528
0.3009	0.0994	283.15	926.944	−1.48504	0.0999	0.4022	283.15	999.916	−1.31201
0.3029	0.2019	283.15	936.594	−1.48468	0.0994	0.5001	283.15	1000.686	−1.31309
0.3015	0.2970	283.15	943.603	−1.44950	0.1000	0.5986	283.15	997.709	−1.12936
0.3009	0.4001	283.15	948.748	−1.36630	0.0996	0.6963	283.15	995.326	−0.93439
					0.1000	0.7962	283.16	991.791	−0.64365
0.7990	0.1006	288.15	832.839	−0.72737	0.3010	0.4951	288.15	945.920	−1.22347
0.6941	0.0993	288.15	846.462	−1.01838	0.2997	0.5979	288.15	947.302	−0.98406
0.6997	0.1995	288.15	857.511	−0.92208	0.1964	0.0899	288.15	949.799	−1.30702
0.5953	0.2979	288.15	882.009	−1.05398	0.2034	0.1959	288.14	958.085	−1.42929
0.4970	0.1009	288.15	879.014	−1.41027	0.2010	0.2996	288.15	964.154	−1.43384
0.5026	0.2991	288.15	896.753	−1.18711	0.1970	0.3853	288.15	968.008	−1.40480
0.4996	0.3981	288.15	904.134	−1.07549	0.1998	0.4986	288.15	968.915	−1.29449
0.3979	0.1007	288.15	899.230	−1.49738	0.1989	0.5953	288.15	967.555	−1.03034
0.3968	0.2046	288.15	910.252	−1.45365	0.1990	0.6986	288.15	967.436	−0.83771
0.4004	0.2991	288.15	917.258	−1.40620	0.0965	0.1000	288.15	982.926	−0.98117
0.4007	0.3993	288.15	923.431	−1.32322	0.1004	0.2004	288.15	989.984	−1.18748
0.4025	0.4888	288.15	924.997	−1.04806	0.1014	0.3026	288.15	993.454	−1.29097
0.3009	0.0994	288.15	922.150	−1.48560	0.0999	0.4022	288.15	995.071	−1.31268
0.3029	0.2019	288.15	931.654	−1.49134	0.0994	0.5001	288.15	995.715	−1.31908
0.3015	0.2970	288.15	938.575	−1.46195	0.1000	0.5986	288.15	992.651	−1.13982
0.3009	0.4001	288.15	943.651	−1.38513	0.0996	0.6963	288.15	990.177	−0.94770
					0.1000	0.7962	288.14	986.542	−0.65742
0.7990	0.1006	293.15	827.330	−0.74376	0.3010	0.4951	293.15	940.720	−1.24730
0.6941	0.0993	293.15	841.037	−1.03436	0.2997	0.5979	293.15	942.039	−1.01045
0.6997	0.1995	293.15	852.079	−0.94605	0.1964	0.0899	293.16	945.314	−1.30345
0.5953	0.2979	293.15	876.644	−1.08228	0.2034	0.1959	293.15	953.339	−1.43198
0.4970	0.1009	293.15	873.799	−1.42234	0.2010	0.2996	293.16	959.242	−1.44104
0.5026	0.2991	293.15	891.468	−1.21205	0.1970	0.3853	293.15	963.000	−1.41574
0.4996	0.3981	293.15	898.810	−1.10513	0.1998	0.4986	293.15	963.804	−1.31079
0.3979	0.1007	293.15	894.172	−1.50577	0.1989	0.5953	293.15	962.360	−1.04805
0.3968	0.2046	293.15	905.122	−1.46848	0.1990	0.6986	293.15	962.179	−0.85890
0.4004	0.2991	293.15	912.073	−1.42724	0.0965	0.1000	293.15	979.002	−0.97317
0.4007	0.3993	293.15	918.196	−1.34986	0.1004	0.2004	293.15	985.559	−1.18168
0.4025	0.4888	293.15	919.712	−1.07668	0.1014	0.3026	293.15	988.740	−1.28898
0.3009	0.0994	293.15	917.314	−1.48954	0.0999	0.4022	293.15	990.188	−1.31519
0.3029	0.2019	293.16	926.678	−1.50096	0.0994	0.5001	293.15	990.721	−1.32702
0.3015	0.2970	293.15	933.507	−1.47650	0.1000	0.5986	293.15	987.566	−1.15139
0.3009	0.4001	293.15	938.509	−1.40506	0.0996	0.6963	293.15	985.011	−0.96209
					0.1000	0.7962	293.15	981.285	−0.67223
0.7990	0.1006	298.15	821.782	−0.76051	0.3010	0.4951	298.15	935.496	−1.27176
0.6941	0.0993	298.15	835.576	−1.05149	0.2997	0.5979	298.15	936.768	−1.03788
0.6997	0.1995	298.14	846.619	−0.97112	0.1964	0.0899	298.16	940.780	−1.30255
0.5953	0.2979	298.15	871.251	−1.11145	0.2034	0.1959	298.15	948.556	−1.43696
0.4970	0.1009	298.15	868.544	−1.43622	0.2010	0.2996	298.16	954.302	−1.45017
0.5026	0.2991	298.15	886.158	−1.23837	0.1970	0.3853	298.14	957.971	−1.42839
0.4996	0.3981	298.15	893.467	−1.13594	0.1998	0.4986	298.15	958.682	−1.32863
0.3979	0.1007	298.15	889.070	−1.51619	0.1989	0.5953	298.15	957.182	−1.06847
0.3968	0.2046	298.15	899.961	−1.48527	0.1990	0.6986	298.15	956.917	−0.88077
0.4004	0.2991	298.15	906.860	−1.44978	0.0965	0.1000	298.15	975.015	−0.96766
0.4007	0.3993	298.15	912.942	−1.37792	0.1004	0.2004	298.15	981.092	−1.17817
0.4025	0.4888	298.15	914.412	−1.10638	0.1014	0.3026	298.15	984.000	−1.28914
0.3009	0.0994	298.16	912.432	−1.49583	0.0999	0.4022	298.15	985.286	−1.31950
0.3029	0.2019	298.16	921.667	−1.51264	0.0994	0.5001	298.15	985.713	−1.33640
0.3015	0.2970	298.15	928.412	−1.49285	0.1000	0.5986	298.15	982.469	−1.16390
0.3009	0.4001	298.15	933.348	−1.42657	0.0996	0.6963	298.15	979.836	−0.97697
					0.1000	0.7962	298.15	976.023	−0.68714
0.7990	0.1006	303.15	816.197	−0.77856	0.3010	0.4951	303.15	930.255	−1.29775
0.6941	0.0993	303.15	830.069	−1.06970	0.2997	0.5979	303.15	931.481	−1.06631
0.6997	0.1995	303.15	841.124	−0.99749	0.1964	0.0899	303.16	936.190	−1.30404
0.5953	0.2979	303.15	865.830	−1.14218	0.2034	0.1959	303.15	943.733	−1.44419
0.4970	0.1009	303.15	863.247	−1.45220	0.2010	0.2996	303.16	949.332	−1.46131
0.5026	0.2991	303.15	880.816	−1.26614	0.1970	0.3853	303.14	952.917	−1.44277
0.4996	0.3981	303.15	888.100	−1.16819	0.1998	0.4986	303.15	953.539	−1.34776
0.3979	0.1007	303.15	883.921	−1.52875	0.1989	0.5953	303.15	951.971	−1.08880

Table 1 (Continued)

x_1	x_2	T/K	ρ/kg·m^{-3}	V^E/cm^3·mol^{-1}	x_1	x_2	T/K	ρ/kg·m^{-3}	V^E/cm^3·mol^{-1}
0.3968	0.2046	303.15	894.759	−1.50382	0.1990	0.6986	303.15	951.641	−0.90316
0.4004	0.2991	303.15	901.617	−1.47412	0.0965	0.1000	303.15	970.952	−0.96411
0.4007	0.3993	303.15	907.659	−1.40723	0.1004	0.2004	303.15	976.584	−1.17694
0.4025	0.4888	303.15	909.089	−1.13716	0.1014	0.3026	303.15	979.227	−1.29119
0.3009	0.0994	303.16	907.498	−1.50433	0.0999	0.4022	303.15	980.359	−1.32542
0.3029	0.2019	303.16	916.618	−1.52646	0.0994	0.5001	303.15	980.685	−1.34708
0.3015	0.2970	303.15	923.287	−1.51116	0.1000	0.5986	303.15	977.356	−1.17733
0.3009	0.4001	303.15	928.161	−1.44963	0.0998	0.6963	303.15	974.649	−0.99247
					0.1000	0.7962	303.15	970.757	−0.70262
0.7990	0.1006	308.15	810.567	−0.79755	0.3010	0.4951	308.15	924.989	−1.32491
0.6941	0.0993	308.15	824.515	−1.08911	0.2997	0.5979	308.15	926.176	−1.09584
0.6997	0.1995	308.15	835.589	−1.02506	0.1964	0.0899	308.15	931.544	−1.30770
0.5953	0.2979	308.15	860.374	−1.17422	0.2034	0.1959	308.15	938.866	−1.45337
0.4970	0.1009	308.15	857.898	−1.46975	0.2010	0.2996	308.15	944.325	−1.47406
0.5026	0.2991	308.15	875.440	−1.29545	0.1970	0.3853	308.15	947.833	−1.45861
0.4996	0.3981	308.15	882.702	−1.20163	0.1996	0.4986	308.15	948.372	−1.36805
0.3979	0.1007	308.15	878.722	−1.54327	0.1989	0.5953	308.15	946.743	−1.11018
0.3968	0.2046	308.15	889.513	−1.52400	0.1990	0.6986	308.15	946.355	−0.92656
0.4004	0.2991	308.15	896.336	−1.49990	0.0965	0.1000	308.15	966.837	−0.96291
0.4007	0.3993	308.15	902.348	−1.43807	0.1004	0.2004	308.15	972.025	−1.17739
0.4025	0.4888	308.15	903.746	−1.16951	0.1014	0.3026	308.15	974.419	−1.29487
0.3009	0.0994	308.16	902.518	−1.51520	0.0999	0.4022	308.15	975.406	−1.33281
0.3029	0.2019	308.15	911.525	−1.54209	0.0994	0.5001	308.15	975.632	−1.35877
0.3015	0.2970	308.15	918.119	−1.53071	0.1000	0.5986	308.15	972.224	−1.19159
0.3009	0.4001	308.15	922.946	−1.47421	0.0996	0.6963	308.15	969.445	−1.00840
					0.1000	0.7962	308.15	965.480	−0.71837
0.7990	0.1006	313.15	804.884	−0.81686	0.3010	0.4951	313.15	919.699	−1.35344
0.6941	0.0993	313.15	818.907	−1.10923	0.2997	0.5979	313.15	920.848	−1.12626
0.6997	0.1995	313.15	830.011	−1.05367	0.1964	0.0899	313.16	926.842	−1.31347
0.5953	0.2979	313.15	854.884	−1.20776	0.2034	0.1959	313.15	933.959	−1.46462
0.4970	0.1009	313.15	852.499	−1.48897	0.2010	0.2996	313.16	939.285	−1.48861
0.5026	0.2991	313.15	870.023	−1.32588	0.1970	0.3853	313.15	942.710	−1.47547
0.4996	0.3981	313.15	877.278	−1.23679	0.1998	0.4986	313.15	943.179	−1.38948
0.3979	0.1007	313.15	873.474	−1.55977	0.1989	0.5953	313.15	941.490	−1.13222
0.3968	0.2046	313.15	884.229	−1.54617	0.1990	0.6986	313.15	941.056	−0.95095
0.4004	0.2991	313.15	891.017	−1.52715	0.0965	0.1000	313.15	962.647	−0.96328
0.4007	0.3993	313.15	897.004	−1.47018	0.1004	0.2004	313.15	967.418	−1.17956
0.4025	0.4888	313.15	898.376	−1.20304	0.1014	0.3026	313.15	969.574	−1.30009
0.3009	0.0994	313.16	897.485	−1.52808	0.0999	0.4022	313.15	970.418	−1.34126
0.3029	0.2019	313.16	906.387	−1.55945	0.0994	0.5001	313.15	970.550	−1.37131
0.3015	0.2970	313.15	912.918	−1.55210	0.1000	0.5986	313.15	967.073	−1.20675
0.3009	0.4001	313.15	917.695	−1.49989	0.0996	0.6963	313.15	964.230	−1.02525
					0.1000	0.7962	313.15	960.187	−0.73420
0.7990	0.1006	318.15	799.151	−0.83739	0.3010	0.4951	318.15	914.381	−1.38319
0.6941	0.0993	318.15	812.629	−1.08275	0.2997	0.5979	318.15	915.499	−1.15775
0.6997	0.1995	318.15	824.395	−1.08430	0.1964	0.0899	318.15	922.078	−1.32161
0.5953	0.2979	318.15	849.359	−1.24317	0.2034	0.1959	318.15	929.001	−1.47788
0.4970	0.1009	318.15	847.045	−1.51015	0.2010	0.2996	318.15	934.198	−1.50458
0.5026	0.2991	318.15	864.570	−1.35819	0.1970	0.3853	318.15	937.562	−1.49429
0.4996	0.3981	318.15	871.821	−1.27343	0.1998	0.4986	318.15	937.952	−1.41166
0.3979	0.1007	318.15	868.173	−1.57861	0.1989	0.5953	318.15	936.214	−1.15505
0.3968	0.2046	318.15	878.897	−1.57023	0.1990	0.6986	318.15	935.740	−0.97592
0.4004	0.2991	318.15	885.661	−1.55632	0.0965	0.1000	318.15	958.377	−0.96551
0.4007	0.3993	318.15	891.630	−1.50406	0.1004	0.2004	318.15	962.762	−1.18377
0.4025	0.4888	318.15	892.979	−1.23796	0.1014	0.3026	318.15	964.692	−1.30708
0.3009	0.0994	318.15	892.393	−1.54323	0.0999	0.4022	318.15	965.403	−1.35130
0.3029	0.2019	318.15	901.205	−1.57905	0.0994	0.5001	318.15	965.448	−1.38522
0.3015	0.2970	318.15	907.679	−1.57539	0.1000	0.5986	318.15	961.896	−1.22234
0.3009	0.4001	318.15	912.407	−1.52684	0.0996	0.6963	318.15	958.993	−1.04218
					0.1000	0.7962	318.15	954.885	−0.75038
0.7990	0.1006	323.14	793.362	−0.85846	0.3010	0.4951	323.15	909.032	−1.41378
0.6941	0.0993	323.15	807.589	−1.15770	0.2997	0.5979	323.14	910.127	−1.19036
0.6997	0.1995	323.15	818.740	−1.11681	0.1964	0.0899	323.15	917.273	−1.33097
0.5953	0.2979	323.15	843.789	−1.27963	0.2034	0.1959	323.14	923.997	−1.49182
0.4970	0.1009	323.15	841.534	−1.53215	0.2010	0.2996	323.15	929.095	−1.52231
0.5026	0.2991	323.15	859.073	−1.39150	0.1970	0.3853	323.15	932.382	−1.51382
0.4996	0.3981	323.15	866.330	−1.31155	0.1998	0.4986	323.14	932.701	−1.43470
0.3979	0.1007	323.15	862.816	−1.59833	0.1989	0.5953	323.15	930.910	−1.17819
0.3968	0.2046	323.15	873.517	−1.59522	0.1990	0.6986	323.15	930.403	−1.00142
0.4004	0.2991	323.14	880.261	−1.58637	0.0965	0.1000	323.14	954.047	−0.96798
0.4007	0.3993	323.15	886.223	−1.53927	0.1004	0.2004	323.15	958.428	−1.20163
0.4025	0.4888	323.14	887.549	−1.27389	0.1014	0.3026	323.15	959.767	−1.31412
0.3009	0.0994	323.15	887.264	−1.56005	0.0999	0.4022	323.15	960.350	−1.36128
0.3029	0.2019	323.15	895.988	−1.60010	0.0994	0.5001	323.15	960.316	−1.39921
0.3015	0.2970	323.15	902.398	−1.59946	0.1000	0.5986	323.14	956.695	−1.23807
0.3009	0.4001	323.14	907.086	−1.55479	0.0996	0.6963	323.15	953.738	−1.05936
					0.1000	0.7962	323.15	949.575	−0.76725

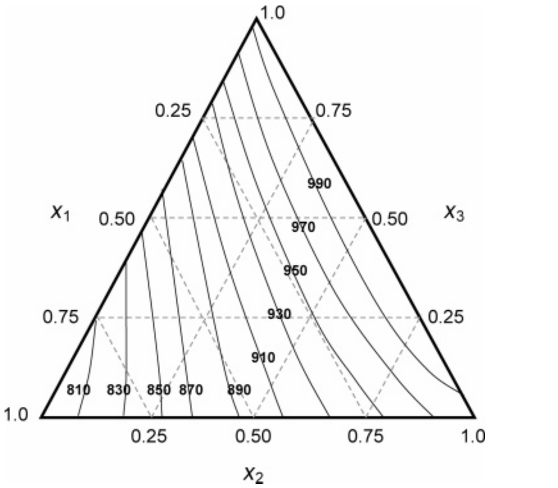

Figure 2. Constant density curves for the system acetone (1) + propionic acid (2) + water (3) at 298.15 K. Density units are kg·m^{-3}.

Table 2. Parameters for the Calculation of the Excess Volume of the Binary Systems Using Equation 3

T/K	$a_0^{(ij)}$	$a_1^{(ij)}$	$a_2^{(ij)}$	$a_3^{(ij)}$	σ/cm^3·mol^{-1}
		Acetone (1) + Water (3)			
283.15	−5.8009	2.4595	−0.4733	−1.0377	0.0130
288.15	−5.8080	2.4001	−0.4001	−1.0604	0.0133
293.15	−5.8246	2.3504	−0.3350	−1.0747	0.0135
298.15	−5.8874	2.3127	0.0000	−1.0976	0.0163
303.15	−5.9121	2.2822	0.0000	−1.1016	0.0152
308.15	−5.9447	2.2599	0.0000	−1.1006	0.0144
313.15	−5.9846	2.2436	0.0000	−1.0854	0.0138
318.15	−6.0349	2.2408	0.0000	−1.0821	0.0132
323.15	−6.0877	2.2479	0.0000	−1.0972	0.0128
		Propionic Acid (2) + Water (3)			
283.15	−4.6576	0.8885	−0.7599	0.0000	0.0142
288.15	−4.6334	0.7705	−0.7411	0.0000	0.0129
293.15	−4.6206	0.6733	−0.7429	0.0000	0.0109
298.15	−4.6120	0.5826	−0.7429	0.0000	0.0097
303.15	−4.6082	0.5047	−0.7523	0.0000	0.0083
308.15	−4.5651	0.4285	−0.8915	0.0000	0.0140
313.15	−4.6112	0.2293	−0.7738	0.3910	0.0045
318.15	−4.6120	0.1426	−0.8021	0.4681	0.0037
323.15	−4.6229	0.0600	−0.7921	0.5255	0.0026
		Acetone (1) + Propionic Acid (2)			
283.15	−3.2615	−0.8322	−0.3720	0.0000	0.0176
288.15	−3.3278	−0.8512	−0.3984	0.0000	0.0103
293.15	−3.4589	−0.8732	−0.4233	0.0000	0.0105
298.15	−3.5943	−0.8966	−0.4491	0.0000	0.0106
303.15	−3.7352	−0.9239	−0.4742	0.0000	0.0108
308.15	−3.8824	−0.9530	−0.5010	0.0000	0.0109
313.15	−4.0354	−0.9844	−0.5286	0.0000	0.0110
318.15	−4.1957	−1.0219	−0.5575	0.0000	0.0112
323.15	−4.3646	−1.0637	−0.5852	0.0000	0.0122

along with those existing in the literature at 298.15 K, and Table 1 contains the experimental results. We have compared our experimental results with values reported by Lebed and Eddin[2] at 298.15 K. Although they did not measure at exactly the same mole fractions, our density values agree with theirs within 0.009 kg·m^{-3}. Figure 2 presents constant density curves for the ternary system at 298.15 K.

We calculate the excess molar volume using

$$V^{\mathrm{E}} = \frac{x_1M_1 + x_2M_2 + x_3M_3}{\rho} - \left(\frac{x_1M_1}{\rho_1} + \frac{x_2M_2}{\rho_2} + \frac{x_3M_3}{\rho_3}\right) \quad (1)$$

where ρ is the mixture density and x_i, ρ_i, M_i are the mole fraction, density, and molecular weight of pure component

Table 3. Parameters for the Redlich−Kister Equation for Acetone (1) + Propionic Acid (2) + Water (3)

T/K	A	B_2	σ/cm^3·mol^{-1}
283.15	3.6487	−5.0784	0.0264
288.15	3.2750	−5.2196	0.0261
293.15	3.1683	−5.0301	0.0265
298.15	3.1244	−4.8616	0.0263
303.15	3.0207	−4.7258	0.0267
308.15	2.7987	−4.5730	0.0274
313.15	2.8481	−4.2152	0.0273
318.15	2.8058	−4.1271	0.0278
323.15	2.7083	−3.8128	0.0279

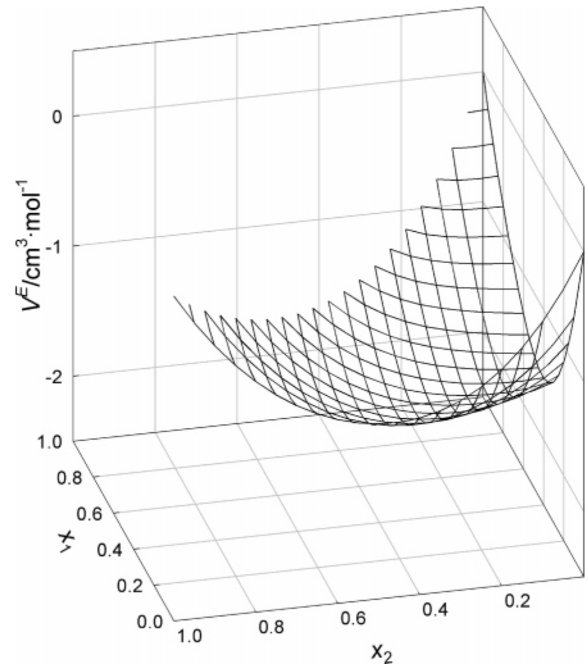

Figure 3. Excess molar volume for the system acetone (1) + propionic acid (2) + water (3) at 298.15 K.

i. Excess volumes appear in Table 1 and can be represented with a modified Redlich−Kister[3]-type equation

$$V^{\mathrm{E}}_{123} = V^{\mathrm{E}}_{12} + V^{\mathrm{E}}_{23} + V^{\mathrm{E}}_{13} + x_1x_2x_3[A + B_1(x_1 - x_2) + B_2(x_2 - x_3) + B_3(x_1 - x_3) + ...] \quad (2)$$

with

$$V^{\mathrm{E}}_{ij} = x_ix_j\sum_{k=0}^{n} a_k^{(ij)}(x_i - x_j)^k \quad (3)$$

where V^{E}_{ijk} is the excess molar volume of the ternary system acetone (1) + propionic acid (2) + water (3) and V^{E}_{ij} are the functions for the excess molar volumes of the binary systems. Estrada-Baltazar et al.[1] present excess molar volumes for the binaries. Unfortunately, that work contains a calculation error, and we have submitted a correction[4] with this paper to correct the error. We have recalculated the values using eq 3. Table 2 contains the parameters $a_k^{(ij)}$ for the binary systems. Two parameters, A and B_2, are sufficient to represent the excess volumes. These values result from fitting eq 2 to the calculated excess volumes using a least-squares method. Table 3 contains values for the parameters along with their standard deviations defined as

$$\sigma = \left[\frac{\sum (V^{\mathrm{E}}_{\mathrm{exptl}} - V^{\mathrm{E}}_{\mathrm{calcd}})^2}{n - m}\right]^{1/2} \quad (4)$$

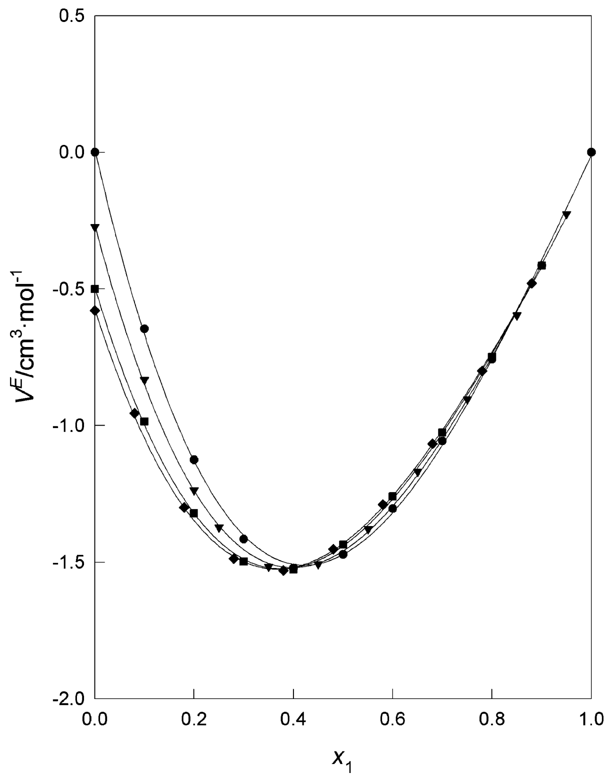

Figure 4. Excess molar volume for the system acetone (1) + propionic acid (2) + water (3) at 298.15 K as a function of the mole fraction of acetone at different constant mole fraction compositions of propionic acid: ●, $x_2 = 0$; ▼, $x_2 = 0.05$; ■, $x_2 = 0.1$; ◆, $x_2 = 0.12$. The solid line is a polynomial regression to emphasize the crossing point.

In eq 4, n is the number of experimental points, and m is the number of parameters. Visak et al.[5] used eq 2 to correlate the excess volumes of water + butyl acetate + methanol, and they show the equivalence between eq 2 and an equation proposed by Cibulka.[6] When correlating the excess molar volumes for ternary systems, it is common[6] to consider the V_{ij}^{E}'s as the excess molar volume functions for the binary systems, but they do not correspond to the excess molar volumes of the binaries because $x_i + x_j$ does not equal unity.[6] However, eq 2 satisfies the binary limit. Figure 3 shows a surface of the excess molar volume at 298.15 K. The calculated excess volume is negative for the mole fractions considered in this work. Figure 4 shows the variation of the excess molar volume with respect to the acetone mole fraction for different propionic acid isopleths. Our measurements show that the excess volume has a constant value of approximately -1.5 cm^3 mol^{-1} at $x_1 = 0.42$, whereas Lebed and Eddin[2] calculated a constant value of the excess volume of -1.35 cm^3 mol^{-1} but at $x_1 = 0.46$. The difference could be caused by the experimental error in the measurements and the purity of the samples used by Lebed and Eddin.[2] We should mention that Lebed and Eddin do not provide a clear explanation of what type of error they have in their measurements. However, recently the same research group[7] has measured the density of acetic acid + water + 1,4-dioxane using the same equipment. They describe it as a VIP-2 vibration densitometer. In this work, they mention that they also measured the density picnometrically. They give a relative error in the determination of the density of 0.01%, which corresponds to a maximum of 0.1 kg·m^{-3} for the densities. The crossing mole fraction agrees with the value of Lebed and Eddin[2] within the uncertainty of the measurements.

Conclusions

We have measured the liquid densities of the ternary system propionic acid (1) + acetone (2) + water (3) using a vibrating-tube densimeter. Excess molar volumes have been calculated and correlated to a Redlich−Kister-type equation. This equation uses two characteristic parameters and the expressions for the binary excess molar volumes to produce an average standard deviation of 0.0265 cm^3·mol^{-1} and an average percentage error of 4.7 from the calculated excess volumes. Our calculated excess volumes have the same behavior as those calculated by Lebed and Eddin.[2] When the excess volumes are plotted for different isopleths, the curves for this mixture cross at a single value for a given mole fraction composition of one of the other components as suggested by Lebed and Eddin.[2]

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