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Refractive Indices and Relative Permittivities of Liquid Mixtures of γ-Butyrolactone, γ-Valerolactone, δ-Valerolactone, or ϵ-Caprolactone + Benzene, + Toluene, or + Ethylbenzene at 293.15 K and 313.15 K and Atmospheric Pressure

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The refractive indices, n_D, and relative permittivities, ϵ, have been measured for the binary liquid mixtures of γ-butyrolactone, γ-valerolactone, δ-valerolactone, or ϵ-caprolactone + benzene, + toluene, or + ethylbenzene over the whole composition range at 293.15 K and 313.15 K and atmospheric pressure. For the pure lactones the dipole moments, μ, the molar polarizability, P_M, and the molar refractivity, R_M, were determined. From the values of ϵ and n_D of the lactone + benzene mixtures, the Kirkwood correlation factor, g, was calculated indicative of the structures of the mixtures.

Introduction

Lactones, especially γ-butyrolactone, which are used as solvents in chemical engineering, have been suggested for liquid−liquid extraction and may be used for the production of biodegradable polymers in the future (e.g., Hutton and Jones, 1963; Awwad et al., 1988). Also, because of their electrochemical behavior, lactones are of considerable interest as solvents in modern lithium batteries (Abraham and Alamgir, 1993; Pistoia, 1994, Avraam et al., 1998). However, despite their potential importance for future technologies, thermodynamic data of lactones and their mixtures are comparatively scarce.

For scientific reasons it is interesting to carry out thermodynamic studies of lactones and their mixtures. A comparison of their properties with those of the well-studied linear esters often reveals characteristic differences. Ring closure in the lactones generally results in an exposure of the ester group because of less steric screening, in an increased polarizability (electron delocalization), and in the case of small cycles in a high ring strain. Consequently, the cyclic, strongly polar lactones exhibit usually higher dipole moments, higher boiling points, enthalpies of vaporization, and gas−liquid critical temperatures than the linear analogues (Kehiaian et al., 1989, 1991).

This work is a continuation of the systematic measurements of the properties of lactones (Klein and Svejda, 1995; Fornefeld-Schwarz and Svejda, 1997; Fornefeld-Schwarz et al., 1997), which will provide the necessary data for improving predictive group theories. In the present work, refractive indices, n_D, and relative permittivities, ϵ, of four pure liquid lactones, γ-butyrolactone, γ-valerolactone, δ-valerolactone, and ϵ-caprolactone, and of their binary mixtures + benzene, + toluene, or + ethylbenzene at 293.15 K and 313.15 K and atmospheric pressure are presented. For the pure lactones the dipole moment, μ, the molar polarizability, P_M, and the molar refractivity, R_M, were calculated. From the values of ϵ and n_D of the lactone + benzene mixtures, the Kirkwood correlation factors, g, of the mixtures were derived.

Experimental Section

γ-Butyrolactone (oxolan-2-one, $C_4H_6O_2$; Fluka AG, Buchs, Switzerland), γ-valerolactone (5-methyloxolan-2-one, $C_5H_8O_2$; Aldrich Chem. Co. Inc., Milwaukee, WI), δ-valerolactone (oxan-2-one, $C_5H_8O_2$; ACROS, Geel, Belgium), ϵ-caprolactone (oxepan-2-one, $C_6H_{10}O_2$; ACROS, Geel, Belgium), benzene (J. T. Baker Chem. B.V., Deventer, The Netherlands), toluene (Riedel-de-Haen, Seelze, Germany), and ethylbenzene (Fluka AG, Buchs, Switzerland) with stated purities of better than 99, 99, 99, 99, 99, 99.7, and 99 mol %, respectively, were stored over molecular sieves (0.4 nm, J. T. Baker Chem. B.V., Deventer, The Netherlands), which were activated at 573 K for 12 h under vacuum prior to use. Carbon tetrachloride (J. T. Baker Chem. B.V., Deventer, The Netherlands), chlorobenzene (J. T. Baker Chem. B.V., Deventer, The Netherlands), 1,2-dichloroethane (Riedel-de-Haen, Seelze, Germany), methanol (Riedel-de-Haen, Seelze, Germany), and acetonitrile (J. T. Baker Chem. B.V., Deventer, The Netherlands) with stated purities of better than 99, 99, 99, 99.8, and 99 mol %, respectively, were needed for the calibration of both the automatic refractometer and the cell for measuring the electric capacity during the determination of ϵ. The lactones and benzene were dried over the molecular sieves in the liquid phase and toluene and ethylbenzene as well as the calibration fluids were dried over the molecular sieves in the gas phase. For γ-butyrolactone, ϵ-caprolactone, benzene, toluene, and ethylbenzene, purities of 99.94, 99.91, 99.99, 99.98, and 99.87 mol %, respectively, were found all determined by gas chromatography (GC; 30 m glass capillary (OV 17), flame ionization detector, and oven temperatures 393, 393, 343, 323, and 373 K, respectively). The purities of γ-valerolactone and δ-valerolactone could not be checked by GC because these materials decompose at elevated temperatures. Traces of water left in the lactones after drying must have been less than 0.001 mol % as checked by Karl Fischer titrations (Fluka AG, Buchs, Switzerland).

The refractive indices, n_D, were measured at 293.15 K and 313.15 K with an automatic refractometer (GPR 11-37 X, Index Instruments, Ramsey, Huntingdon, England)

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Table 1. Refractive Index n_D and Relative Permittivity ϵ of the Calibration Fluids at 293.15 K and 313.15 K and Atmospheric Pressure

	n_D		ϵ	
compound	293.15 K	313.15 K	293.15 K	313.15 K
water	1.333 00[a]	1.330 51[a]		
	1.332 99[b]	1.330 50[c]		
toluene	1.496 77[a]	1.485 17[a]		2.28[d]
	1.496 7[e]	1.485 7[e]		
carbon tetrachloride	1.460 29[a]			
	1.4603[c]			
benzene			2.28[f]	
chlorobenzene			5.71[f]	5.27[d]
1,2-dichloroethane			10.65[f]	9.53[g]
methanol			33.62[f]	29.92[h]
acetonitrile			36.60[i]	33.64[i]

[a] This work. [b] Riddick et al. (1986). [c] Index Instruments (1995). [d] Singh and Sinha (1985). [e] Moumouzias and Ritzoulis (1997). [f] Maryott and Smith (1951). [g] Hahn et al. (1993). [h] Gold and Perrine (1967). [i] Jannelli et al. (1983).

at the wavelength of sodium light line D. The refractometer has a resolution of 1×10^{-5} and an accuracy of ±0.00005 for $n_D \leq 1.45$ and of ±0.0001 for $n_D > 1.45$. At the measurements the liquids were conducted to the refractive prism without contact to the atmosphere by means of a flow cell (SGP4, Index Instruments, Ramsey, Huntingdon, England), which was thermostated to ±0.02 K by an external thermostat (F2, Haake, Karlsruhe, Germany). The temperature (according to ITS90) was controlled by a PT-100 thermoresistor calibrated against a calibrated PT-25 thermoresistor (WS 104 HO, Rosemount, Sussex, England) connected to an ASL bridge (A(H)6, Automatic System Labratories, Milton Keynes, England) and measured with an accuracy of ±0.01 K. The refractometer was calibrated with tridistilled, degassed water at $T = 293.15$ K. Afterward the calibration was checked with toluene and carbon tetrachloride, prepared as described above, for which the refractive indices are well-known. The measured values and the reference data are given in Table 1.

Relative permittivities, ϵ, were determined in a self-developed cell for measuring electric capacities (after Wuerflinger (1980), but only for atmospheric pressures as in the present work) connected by shielded, flexible coaxial, electronically compensated cables to a high-precision LCR bridge (Hewlett-Packard, HP 4284 A) with stated accuracy for capacity measurements of 0.05%. A four-terminal pair measurement configuration and a frequency of 1 MHz were employed. The measuring cell, with a content of about 1 cm^3 and entirely closed to the atmosphere, was calibrated with benzene, chlorobenzene, 1,2-dichloroethane, methanol, and acetonitrile at 293.15 K and with toluene, chlorobenzene, 1,2-dichloroethane, methanol, and acetonitrile at 313.15 K. The relative permittivities used for calibration are also summarized in Table 1. Figure 1 shows the calibration curve at $T = 293.15$ K. The cell was thermostated and the temperature measured and controlled in the same way and with the same absolute and relative errors as described above for the measurements of n_D. Depending on the fact that the literature values used for calibration already exhibited a scatter around the straight line calibration curve (Figure 1), the accuracy in ϵ cannot be better than ±1%. However, the reproducibility was found to be better than 0.06%. Also, if the relative permittivities of two liquids, ethylbenzene and acetone, were measured at 293.15 K, which was not used for calibration, values of ϵ of 2.393 and 21.08 were determined as compared to literature values of 2.4042 and 20.90 (Riddick et al., 1986), respectively, which gives $(\epsilon_{exp} - \epsilon_{lit})/\epsilon_{exp}$ of −0.0047 and 0.0085 and indicates the high quality of the present ϵ measurement.

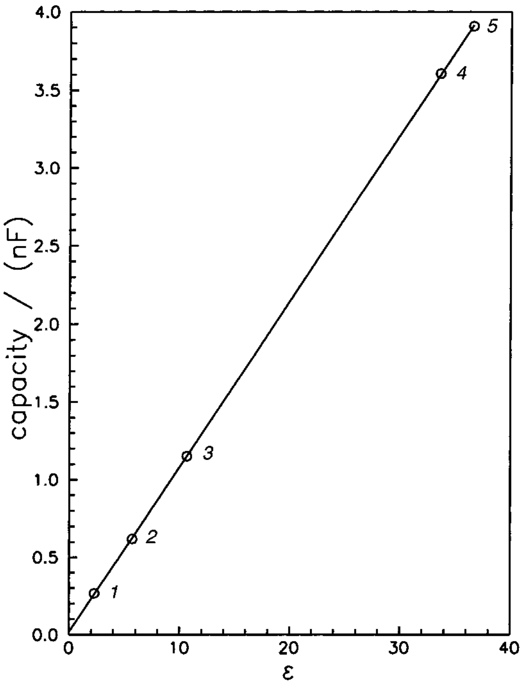

Figure 1. Calibration curve of the cell for measuring the electric capacity of liquids at 293.15 K and atmospheric pressure: (1) benzene; (2) chlorobenzene; (3) 1,2-dichloroethane; (4) methanol; (5) acetonitrile.

Table 2. Refractive Index n_D and Relative Permittivity ϵ of the Pure Compounds at 293.15 K and 313.15 K and Atmospheric Pressure

	n_D		ϵ	
compound	293.15 K	313.15 K	293.15 K	313.15 K
benzene	1.501 13[a]	1.487 77[a]	2.28[a]	2.16[a]
	1.501 12[b]		2.28[c]	
toluene	1.496 77[a]	1.485 17[a]	2.39[a]	2.28[a]
	1.496 7[d]	1.485 7[d]	2.38[d]	2.28[e]
ethylbenzene	1.495 69[a]	1.484 81[a]	2.42[a]	2.28[a]
	1.495 88[b]		2.40[b]	
γ-butyrolactone	1.437 14[a]	1.429 03[a]	42.82[a]	39.91[a]
	1.437 4[f]		39[b]	
			42.35[f]	
γ-valerolactone	1.433 59[a]	1.425 41[a]	36.91[a]	34.47[a]
	1.433 0[g]			
δ-valerolactone	1.459 03[a]	1.451 17[a]	35.78[a]	33.78[a]
ϵ-caprolactone	1.463 61[a]	1.455 83[a]	39.43[a]	36.51[a]

[a] This work. [b] Riddick et al. (1986). [c] Maryott and Smith (1951). [d] Moumouzias and Ritzoulis (1997). [e] Singh and Sinha (1985). [f] Avraam et al. (1998). [g] Landolt−Börnstein (1962).

Mixtures were prepared by mass. The degassed liquids were mixed under vacuum and pressed into the measuring cells without contact to the atmosphere. The final mole fractions were accurate to 0.000 03 (cf. Hahn and Svejda, 1996).

Results and Discussion

Experimental values of the refractive index and the relative permittivity of the pure components are reported in Table 2 and compared with literature values. The refractive index data for γ-butyrolactone and γ-valerolactone at 293.15 K agree well with the literature values. The difference between the experimental and the literature

Table 3. Experimental Values of the Refractive Index n_D of the Mixtures of the Lactones + Benzene, + Toluene, or + Ethylbenzene at 293.15 K and 313.15 K and Atmospheric Pressure

	n_D	
x_1	293.15 K	313.15 K
γ-Butyrolactone (1) + Benzene (2)		
0.0000	1.501 13	1.487 77
0.0942	1.497 24	1.484 57
0.1920	1.492 47	1.480 60
0.3092	1.486 11	1.474 95
0.4159	1.479 69	1.469 17
0.5252	1.472 62	1.462 73
0.6017	1.467 40	1.457 87
0.7056	1.460 00	1.450 94
0.7847	1.454 06	1.445 38
0.9009		1.436 78
0.9073	1.444 64	
1.0000	1.437 14	1.429 03
γ-Butyrolactone (1) + Toluene (2)		
0.0000	1.496 77	1.485 17
0.1033	1.493 57	1.482 20
0.2059	1.489 61	1.478 69
0.3059	1.485 31	1.474 67
0.4146	1.479 75	1.469 61
0.5058	1.474 57	1.464 82
0.5695	1.470 75	1.461 20
0.6088	1.468 20	1.458 82
0.7129	1.461 07	1.452 07
0.8117	1.453 54	1.444 96
0.9042	1.445 90	1.437 47
1.0000	1.437 14	1.429 03
γ-Butyrolactone (1) + Ethylbenzene (2)		
0.0000	1.495 69	1.484 81
0.0886		1.482 46
0.0888	1.493 13	1.482 43
0.1922	1.489 63	1.479 13
0.2070	1.489 01	1.478 63
0.2106	1.488 89	1.478 52
0.3042	1.485 14	1.474 94
0.3118	1.484 79	1.474 66
0.4103	1.480 23	1.470 43
0.5142	1.474 69	1.465 18
0.6108	1.468 91	1.459 72
0.7236	1.461 28	1.452 48
0.7244	1.461 25	1.452 37
0.8220	1.453 67	1.445 17
0.8987	1.447 00	1.438 68
0.9111	1.445 89	1.437 58
1.0000	1.437 14	1.429 03
γ-Valerolactone (1) + Benzene (2)		
0.0000	1.501 13	1.487 77
0.0943	1.494 98	1.482 47
0.1997	1.487 88	1.476 21
0.3089	1.480 48	1.469 44
0.3951	1.474 54	1.464 00
0.5087	1.466 67	1.456 74
0.6038	1.460 19	1.450 68
0.7013	1.453 50	1.444 42
0.7939	1.447 30	1.438 43
0.8965	1.440 41	1.431 88
1.0000	1.433 59	1.425 41
γ-Valerolactone (1) + Toluene (2)		
0.0000	1.496 77	1.485 17
0.1069	1.491 50	1.480 26
0.1753	1.487 78	1.476 87
0.3007	1.480 75	1.470 26
0.4082	1.474 26	1.464 19
0.4175	1.473 70	
0.5375	1.466 09	1.456 53
0.6261	1.460 29	1.450 99
0.6333	1.459 79	1.450 56
0.7317	1.453 07	1.444 16
0.8216	1.446 76	1.438 04
0.9195	1.439 65	1.431 19
1.0000	1.433 59	1.425 41
γ-Valerolactone (1) + Ethylbenzene (2)		
0.0000	1.495 69	1.484 81
0.1014	1.491 24	1.480 59
0.1807	1.487 30	1.476 95
0.2917	1.481 64	1.471 55
0.4008	1.475 53	1.465 77
0.5082	1.469 10	1.459 65
0.6058	1.462 89	1.453 68
0.6980	1.456 66	1.447 67
0.8082	1.448 74	1.440 04
0.9132	1.440 68	1.432 29
1.0000	1.433 59	1.425 41
δ-Valerolactone (1) + Benzene (2)		
0.0000	1.501 13	1.487 77
0.0953	1.498 59	1.486 13
0.1942	1.495 33	1.483 62
0.3029	1.491 33	1.480 38
0.3994	1.487 31	1.476 98
0.4931	1.483 25	1.473 42
0.6018	1.478 36	1.469 00
0.6909	1.474 13	1.465 16
0.8004	1.468 85	1.460 36
0.8977	1.464 08	1.455 91
1.0000	1.459 03	1.451 16
δ-Valerolactone (1) + Toluene (2)		
0.0000	1.496 77	1.485 17
0.1003	1.494 96	1.483 69
0.1929	1.492 68	1.481 86
0.2954	1.489 81	1.479 39
0.4017	1.486 33	1.476 36
0.4913	1.483 03	1.473 44
0.6010	1.478 63	1.469 43
0.7066	1.473 97	1.465 13
0.7924	1.469 90	1.461 41
0.8951	1.464 70	1.456 55
1.0000	1.459 03	1.451 17
δ-Valerolactone (1) + Ethylbenzene (2)		
0.0000	1.459 69	1.484 81
0.0903	1.494 13	1.483 46
0.2020	1.491 65	1.481 37
0.2994	1.489 09	1.479 11
0.3934	1.486 34	1.476 62
0.4935	1.482 94	1.473 55
0.6049	1.478 69	1.469 65
0.7001	1.474 63	1.465 91
0.8007	1.469 93	1.461 53
0.9043	1.464 52	1.456 43
1.0000	1.459 03	1.451 17
ϵ-Caprolactone (1) + Benzene (2)		
0.0000	1.501 13	1.487 77
0.0996	1.498 21	
0.1042		1.485 77
0.1940	1.494 98	1.483 42
0.2972		1.480 35
0.3040	1.490 92	
0.3734	1.488 12	
0.3966		1.477 06
0.5009		1.473 49
0.5068	1.482 83	
0.5819		1.470 62
0.6255	1.478 05	
0.6913	1.475 40	
0.7000		1.466 41
0.7899		1.463 21
0.7964	1.471 36	
0.8887		1.459 70
0.9199	1.466 65	
1.0000	1.463 61	1.455 83
ϵ-Caprolactone (1) + Toluene (2)		
0.0000	1.496 77	1.485 17
0.0875	1.494 95	1.483 71
0.1085		1.483 34
0.1954	1.492 24	1.481 54
0.3080	1.488 98	1.478 84
0.3118	1.488 87	
0.4016	1.486 04	1.476 29
0.5133		1.472 94
0.5158	1.482 17	
0.6249	1.47822	1.469 30
0.7313	1.474 17	1.465 65
0.8303	1.470 44	1.462 17
0.9344	1.466 27	1.458 27
1.0000	1.463 61	1.455 83
ϵ-Caprolactone (1) + Ethylbenzene (2)		
0.0000	1.495 69	1.484 81
0.0911	1.494 02	1.483 39
0.2040	1.491 48	1.481 32
0.3032	1.488 92	1.479 05
0.3866		1.476 98
0.4127	1.485 75	
0.5190	1.482 35	1.473 19
0.6354	1.478 32	1.469 52
0.7264	1.474 89	1.466 39
0.8240	1.471 08	1.462 84
0.9149	1.467 35	1.459 30
1.0000	1.463 61	1.455 83

values is less than 0.05%. The relative permittivity value of γ-butyrolactone at 293.15 K is in agreement with the value given by Avraam et al. (1998) but differs from the value recommended by Riddick et al. (1986).

The measured values for the refractive index, n_D, of the binary mixtures of the lactones + benzene, + toluene, or + ethylbenzene over the whole composition range at 293.15 K and 313.15 K and atmospheric pressure are given in Table 3. As one example, the refractive indices of the mixtures of the lactones + the same solvent, namely, benzene, as a function of the mole fraction at 293.15 K are shown in Figure 2. The overall appearance of the curves does not change with toluene or ethylbenzene as solvents or at the higher temperature.

The experimental values of the relative permittivity, ϵ, of the mixtures at various mole fractions at 293.15 K and

Table 4. Experimental Values of the Relative Permittivity ϵ of the Mixtures of the Lactones + Benzene, + Toluene, or + Ethylbenzene at 293.15 K and 313.15 K and Atmospheric Pressure

293.15 K		313.15 K		293.15 K		313.15 K		293.15 K		313.15 K	
x_1	ϵ	x_1	ϵ	x_1	ϵ	x_1	ϵ	x_1	ϵ	x_1	ϵ
γ-Butyrolactone (1) + Benzene (2)				γ-Butyrolactone (1) + Toluene (2)				γ-Butyrolactone (1) + Ethylbenzene (2)			
0.0000	2.28	0.0000	2.16	0.0000	2.39	0.0000	2.28	0.0000	2.42	0.0000	2.28
0.0982	4.79	0.0894	4.25	0.1189	4.89	0.0872	3.92	0.1243	4.58	0.0887	3.72
0.1977	7.60	0.1913	6.95	0.2339	7.69	0.1051	4.27	0.2484	7.34	0.1828	5.48
0.2945	10.92	0.1973	7.13	0.3459	11.19	0.2196	6.88	0.3581	10.47	0.2050	5.94
0.3837	14.19	0.2984	10.21	0.4419	14.51	0.2946	8.88	0.4570	13.76	0.3057	8.29
0.4959	18.56	0.3964	13.54	0.5433	18.62	0.3989	12.08	0.5448	17.26	0.4200	11.53
0.5904	22.73	0.3986	13.60	0.6396	23.00	0.5038	15.79	0.6763	23.24	0.5007	14.24
0.6888	27.16	0.4878	16.95	0.7273	27.27	0.5215	16.45	0.7799	28.68	0.6091	18.44
0.7893	31.96	0.5952	21.21	0.8250	32.48	0.6006	19.64	0.8724	34.14	0.7042	22.73
0.8939	37.27	0.7057	25.96	0.9180	37.82	0.7011	24.09	0.9484	39.12	0.8084	28.10
1.0000	42.82	0.8071	30.55	1.0000	42.82	0.8184	29.85	1.0000	42.82	0.9047	33.73
		0.9048	35.21			0.9104	34.79			1.0000	39.91
		1.0000	39.91			1.0000	39.91				
γ-Valerolactone (1) + Benzene (2)				γ-Valerolactone (1) + Toluene (2)				γ-Valerolactone (1) + Ethylbenzene (2)			
0.0000	2.28	0.0000	2.16	0.0000	2.39	0.0000	2.28	0.0000	2.42	0.0000	2.28
0.0939	4.77	0.0821	4.17	0.0960	4.46	0.0702	3.66	0.0530	3.41	0.0743	3.55
0.1888	7.43	0.0828	4.20	0.1936	6.71	0.0790	3.83	0.1900	6.28	0.0812	3.67
0.3267	11.90	0.1828	6.86	0.2958	9.67	0.1733	5.92	0.3275	9.71	0.1788	5.54
0.3858	13.97	0.1942	7.18	0.4015	12.93	0.2876	8.82	0.4026	11.93	0.2955	8.21
0.4955	17.78	0.2939	10.11	0.5017	16.32	0.3010	9.19	0.5376	16.29	0.4083	11.24
0.5892	21.23	0.3019	10.35	0.5865	19.54	0.4020	12.11	0.6181	19.21	0.5043	14.13
0.6842	24.73	0.3886	13.06	0.7012	23.95	0.5139	15.68	0.7010	22.60	0.6030	17.48
0.7805	28.39	0.4899	16.34	0.8046	28.13	0.6068	18.86	0.8015	26.84	0.7079	21.38
0.8793	32.23	0.5919	19.79	0.9078	32.54	0.7035	22.40	0.9254	32.72	0.8129	25.71
1.0000	36.91	0.7040	23.69	1.0000	36.91	0.8049	26.32	1.0000	36.91	0.9160	30.36
		0.8117	27.54			0.9062	30.45			1.0000	34.47
		0.8999	30.74			1.0000	34.47				
		0.9137	31.25								
		1.0000	34.47								
δ-Valerolactone (1) + Benzene (2)				δ-Valerolactone (1) + Toluene (2)				δ-Valerolactone (1) + Ethylbenzene (2)			
0.0000	2.28	0.0000	2.16	0.0000	2.39	0.0000	2.28	0.0000	2.42	0.0000	2.28
0.1041	5.05	0.1117	4.85	0.1067	4.97	0.1006	4.23	0.0957	4.04	0.1037	4.03
0.2126	8.27	0.1866	6.86	0.2008	7.14	0.1980	6.35	0.1975	6.08	0.1938	5.77
0.2990	11.01	0.2891	9.77	0.2947	9.99	0.2881	8.64	0.2869	8.27	0.3128	8.44
0.4095	14.74	0.3946	13.00	0.2944	9.92	0.3720	10.92	0.3897	11.02	0.4074	10.95
0.5004	17.92	0.4786	15.65	0.4044	12.89	0.4045	11.84	0.5034	14.55	0.5049	13.81
0.6148	22.26	0.6040	19.83	0.5063	16.02	0.5123	15.20	0.5978	17.77	0.6049	17.13
0.7022	25.35	0.6943	22.88	0.6146	19.74	0.6067	18.33	0.7011	21.79	0.7202	21.39
0.8071	29.24	0.7983	26.55	0.7103	23.55	0.7061	21.86	0.8100	26.39	0.8287	25.87
0.8933	32.50	0.8883	29.72	0.8168	27.83	0.8152	26.10	0.8975	30.52	0.9096	29.46
1.0000	35.78	1.0000	33.78	0.9100	31.78	0.8942	29.15	1.0000	35.78	1.0000	33.78
				1.0000	35.78	1.0000	33.78				
ϵ-Caprolactone (1) + Benzene (2)				ϵ-Caprolactone (1) + Toluene (2)				ϵ-Caprolactone (1) + Ethylbenzene (2)			
0.0000	2.28	0.0000	2.16	0.0000	2.39	0.0000	2.28	0.0000	2.42	0.0000	2.28
0.0999	5.20	0.0962	4.74	0.0893	4.51	0.1061	4.59	0.0879	4.23	0.1034	4.25
0.2040	8.63	0.1907	7.53	0.1870	7.08	0.2161	7.36	0.2325	7.81	0.1827	5.98
0.3160	12.62	0.2906	10.72	0.2868	10.29	0.2431	8.17	0.3186	10.31	0.3091	9.23
0.4058	15.80	0.3954	14.23	0.3939	13.94	0.2965	9.73	0.4349	14.14	0.4025	11.98
0.4600	17.90	0.5097	18.21	0.5040	18.01	0.4177	13.55	0.5003	16.51	0.5042	15.33
0.5228	20.35	0.5853	20.91	0.6030	21.92	0.4898	16.00	0.6218	21.55	0.6002	18.78
0.6471	25.35	0.6322	22.62	0.6877	25.38	0.4967	16.25	0.7009	25.05	0.7007	22.73
0.7482	29.48	0.6477	23.19	0.7930	30.05	0.6113	20.40	0.7807	28.73	0.8022	27.04
0.8581	33.86	0.7095	25.47	0.8975	34.61	0.6818	23.07	0.8800	33.48	0.9024	31.65
1.0000	39.43	0.8043	29.02	1.0000	39.43	0.8127	28.31	1.0000	39.43	1.0000	36.51
		0.8932	32.36			0.9000	32.06				
		1.0000	36.51			1.0000	36.51				

313.15 K and atmospheric pressure are listed in Table 4. A plot of the relative permittivities of the mixtures of the lactones + the same solvent, comparable to Figure 2, would result in almost a single curve over the whole concentration range, because the influence of the different lactones on ϵ of the mixtures is rather similar. Therefore, in Figure 3 the relative permittivities of the mixtures of the *same* lactone + the three solvents, benzene, toluene, and ethylbenzene, at 293.15 K and atmospheric pressure are shown as an example. Again the shape of the curves for the other lactones and/or the higher temperature does not change either. The experimental refractive indices and relative permittivities of all of the binary mixtures at both temperatures were smoothed by an equation of the form

$$A = \sum_{i=0} b_i {x_1}^i \tag{1}$$

where A is either n_D or ϵ and x_1 the respective lactone mole fraction. The adjustable parameters b_i were obtained by linear regression and are summarized in Tables 5 and 6 along with the standard deviation σ, calculated by the expression

$$\sigma = \sqrt{\frac{1}{n-p}\sum_n (A_{\mathrm{exp}} - A_{\mathrm{cal}})^2} \tag{2}$$

where A_{exp} and A_{cal} are the experimental data and calcu-

Table 5. Coefficients b_i and Standard Deviations σ for the Fit of the Refractive Indices n_D to Equation 1 at Temperatures T and Atmospheric Pressure

system	T/K	b_0	b_1	b_2	b_3	$\sigma \times 10^5$
γ-butyrolactone (1) + benzene (2)	293.15	1.501 18	−0.039 52	−0.032 23	0.007 76	5
	313.15	1.487 82	−0.031 68	−0.034 34	0.007 28	6
γ-butyrolactone (1) + toluene (2)	293.15	1.496 85	−0.029 63	−0.026 25	−0.003 75	7
	313.15	1.485 20	−0.026 83	−0.023 43	−0.005 86	6
γ-butyrolactone (1) + ethylbenzene (2)	293.15	1.495 77	−0.028 65	−0.016 98	−0.012 89	7
	313.15	1.484 92	−0.027 10	−0.013 93	−0.014 74	8
γ-valerolactone (1) + benzene (2)	293.15	1.501 16	−0.065 19	−0.007 54	0.005 19	4
	313.15	1.487 81	−0.055 92	−0.013 54	0.007 07	4
γ-valerolactone (1) + toluene (2)	293.15	1.496 94	−0.050 21	−0.013 19		7
	313.15	1.485 28	−0.045 92	−0.014 01		6
γ-valerolactone (1) + ethylbenzene (2)	293.15	1.495 65	−0.042 09	−0.019 87		8
	313.15	1.484 75	−0.039 21	−0.020 03		6
δ-valerolactone (1) + benzene (2)	293.15	1.501 18	−0.025 41	0.027 06	0.010 36	6
	313.15	1.487 84	−0.015 88	−0.032 86	0.012 11	6
δ-valerolactone (1) + toluene (2)	293.15	1.496 84	−0.016 96	−0.024 19	0.003 36	3
	313.15	1.485 19	−0.012 79	−0.023 97	0.002 77	3
δ-valerolactone (1) + ethylbenzene (2)	293.15	1.495 72	−0.016 60	−0.017 53	−0.002 55	3
	313.15	1.484 84	−0.013 91	−0.016 41	−0.003 31	4
ϵ-caprolactone (1) + benzene (2)	293.15	1.501 21	−0.029 03	−0.019 72	0.011 24	9
	313.15	1.487 87	−0.018 71	−0.026 12	0.012 86	9
ϵ-caprolactone (1) + toluene (2)	293.15	1.496 82	−0.019 96	−0.019 72	0.006 52	4
	313.15	1.485 17	−0.014 69	−0.021 09	0.006 45	2
ϵ-caprolactone (1) + ethylbenzene (2)	293.15	1.495 71	−0.017 26	−0.017 90	0.003 08	3
	313.15	1.484 81	−0.013 74	−0.018 01	0.002 78	2

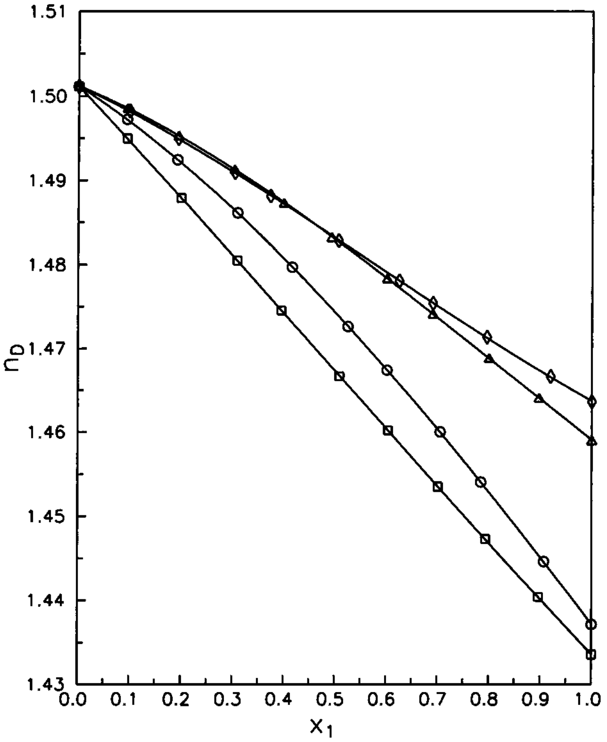

Figure 2. Variation of the refractive index n_D at 293.15 K and atmospheric pressure with the mole fraction x_1 of the mixtures: (○) γ-butyrolactone (1) + benzene (2); (□) γ-valerolactone (1) + benzene (2); (△) δ-valerolactone (1) + benzene (2); (◊) ϵ-caprolactone (1) + benzene (2).

lated values, respectively, n is the number of experimental points, and p is the number of coefficients.

Because of the high boiling points (>473 K) of the pure lactones, it is difficult to measure μ of these substances in the gas phase. Therefore, the method of infinite dilution of the lactones dissolved in the nonpolar liquid benzene, which may suppress interactions between the lactone molecules, has been applied in this work to determine the dipole moments. According to Böttcher and Bordewijk (1978), the following relationship was used:

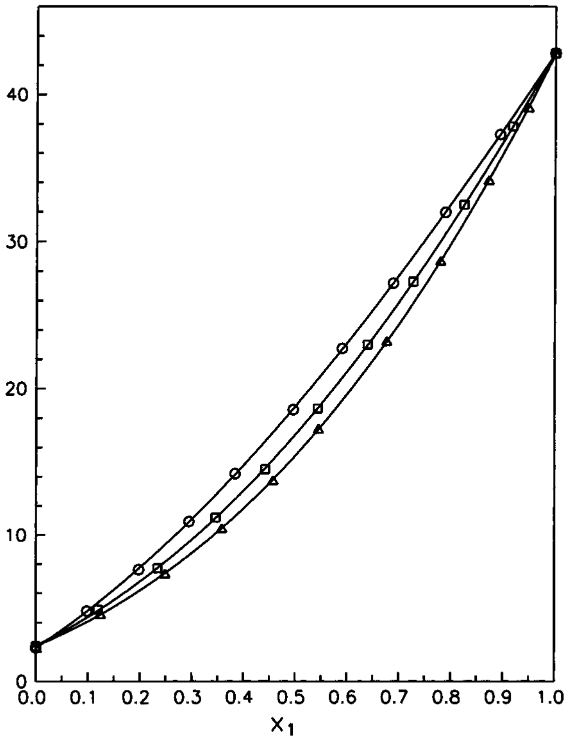

Figure 3. Variation of the relative permittivity ϵ at 293.15 K and atmospheric pressure with the mole fraction of γ-butyrolactone, x_1: (○) + benzene (2); (□) + toluene (2); (△): + ethylbenzene (2).

$$\frac{4\pi N_A \mu^2}{9kTV_2} = \frac{3}{(\epsilon_2 + 2)^2}\left[\left(\frac{\partial \epsilon}{\partial x_1}\right)_{x_1=0} - 2n_{D,2}\left(\frac{\partial n_D}{\partial x_1}\right)_{x_1=0}\right] \quad (3)$$

N_A is Avogadro's number, k Boltzmann's constant, and V_2 the molar volume of benzene (=component 2), which was calculated from the molar mass, $M_2 = 78.113\ 64$ kg kmol^{-1}, and density, $\rho_2 = 879.01$ kg m^{-3}, of benzene taken from Klein and Svejda (1995). To the experimental points of ϵ and n_D of the mixtures in the range of $x_1 = 0-0.30$ of the lactones (=component 1) was fitted a curve, and its slope was determined at $x_1 \simeq 0$, which equals the values of the differential quotients needed in eq 3. The dipole moments

Table 6. Coefficients b_i and Standard Deviations σ for the Fit of the Relative Permittivities ϵ to Equation 1 at Temperatures T and Atmospheric Pressure

system	T/K	b_0	b_1	b_2	b_3	σ
γ-butyrolactone (1) + benzene (2)	293.15	2.28	23.13	22.12	−4.73	0.05
	313.15	2.18	21.16	20.56	−3.98	0.02
γ-butyrolactone (1) + toluene (2)	293.15	2.44	17.00	23.95	−0.55	0.05
	313.15	2.35	15.67	21.90		0.03
γ-butyrolactone (1) + ethylbenzene (2)	293.15	2.40	14.73	19.59	6.04	0.04
	313.15	2.31	14.11	15.41	8.11	0.03
γ-valerolactone (1) + benzene (2)	293.15	2.26	25.20	15.10	−5.68	0.05
	313.15	2.14	23.78	12.50	−3.99	0.02
γ-valerolactone (1) + toluene (2)	293.15	2.39	19.28	18.97	−3.86	0.08
	313.15	2.29	18.12	16.81	−2.76	0.01
γ-valerolactone (1) + ethylbenzene (2)	293.15	2.42	17.67	13.26	3.43	0.07
	313.15	2.30	15.47	15.08	1.62	0.02
δ-valerolactone (1) + benzene (2)	293.15	2.34	23.76	20.30	−10.49	0.06
	313.15	2.15	22.94	13.20	−4.59	0.04
δ-valerolactone (1) + toluene (2)	293.15	2.44	22.36	7.89	3.19	0.05
	313.15	2.28	17.70	15.57	−1.87	0.04
δ-valerolactone (1) + ethylbenzene (2)	293.15	2.40	15.86	15.11	2.40	0.04
	313.15	2.31	14.64	15.67	1.12	0.04
ϵ-caprolactone (1) + benzene (2)	293.15	2.29	27.72	17.31	−7.87	0.05
	313.15	2.13	26.34	12.33	−4.32	0.03
ϵ-caprolactone (1) + toluene (2)	293.15	2.37	22.07	20.46	−5.51	0.06
	313.15	2.25	20.43	17.11	−3.32	0.04
ϵ-caprolactone (1) + ethylbenzene (2)	293.15	2.49	16.76	25.83	−5.60	0.09
	313.15	2.27	17.36	16.88		0.02

Table 7. Calculated Values of the Dipole Moment μ/D, Molar Refractvity R_M/(cm^3 mol^{-1}), Molar Polarizability P_M/(cm^3 mol^{-1}) of the Pure Lactones at 293.15 K and 313.15 K and Atmospheric Pressure Using Molar Mass M/(kg kmol^{-1}) and Density ρ/(kg cm^{-3}) from the Literature[a]

		R_M		P_M			ρ	
compound	μ	293.15 K	313.15 K	293.15 K	313.15 K	M	293.15 K	313.15 K
γ-butyrolactone	4.19	19.97	20.00	706.70	669.50	86.090 44	1129.62	1109.82
γ-valerolactone	4.24	24.69	24.73	755.47	716.95	100.117 32	1055.07	1036.22
δ-valerolactone	4.22	24.70	24.74	714.01	666.74	100.117 32	1108.15	1089.88
ϵ-caprolactone	4.35	29.25	29.29	902.95	847.69	114.144 20	1076.05	1058.94

[a] Fornefeld-Schwarz and Svejda (1997).

of the pure lactones (in D, where 1 D = 3.335 64 × 10^{-30} C m) thus determined at 293.15 K and atmospheric pressure are listed in Table 7. The dipole moment of γ-butyrolactone corresponds well to the literature value of 4.19 D (Wallmark et al., 1970). Slight deviations of μ were found for similar measurements at 313.15 K (not shown here) and attributed to known higher experimental errors at this higher temperature.

In addition to the dipole moment, the molar refractivity, R_M, defined by the Lorentz−Lorenz equation

$$R_M = \frac{n_D^2 - 1}{n_D^2 + 2}\frac{M}{\rho} \tag{4}$$

and the molar polarization, P_M, of the pure lactones at 293.15 K and 313.15 K and atmospheric pressure

$$P_M = \frac{(\epsilon - \epsilon_\infty)(2\epsilon + \epsilon_\infty)}{9\epsilon}V \tag{5}$$

were calculated and are also given in Table 7. ϵ_∞ is the high-frequency permittivity of the lactone for which the usual approximation $\epsilon_\infty = 1.1n_D^2$ was adopted in this work. The molar masses and densities of the lactones needed for the calculation of the molar volume, V, were taken from Fornefeld-Schwarz and Svejda (1997) and are also summarized in Table 7 for the convenience of the reader. The molar refractivity R_M is almost independent of temperature as demanded by theory whereas the molar polarization P_M decreases strongly with increasing temperature. The value of the molar polarization of γ-butyrolactone at 293.15 K, 706.70 cm^3 mol^{-1}, again agrees with the value given by Avraam et al. (1998), 699.39 cm^3 mol^{-1}, by 1%.

Finally, the data of the refractive index and of the relative permittivity of the mixtures of the lactones + benzene were used to calculate the Kirkwood correlation factor, g, from the Kirkwood−Fröhlich equation for mixtures (Prestbo and McHale, 1984), which provides a measure of the average relative orientation of neighboring dipoles of the lactones in the solution

$$g = \frac{9kTV}{4\pi x_1 N_A \mu_1^2}\frac{(2\epsilon + \epsilon_{\infty,1})^2}{\epsilon(\epsilon_{\infty,1} + 2)^2}\left[\frac{\Phi_1(\epsilon - \epsilon_{\infty,1})}{(2\epsilon + \epsilon_{\infty,1})} + \frac{\Phi_2(\epsilon - \epsilon_{\infty,2})}{(2\epsilon + \epsilon_{\infty,2})}\right] \tag{6}$$

ϵ is again the experimentally observed dielectric constant of the mixture, $\epsilon_{\infty,i}$ (=$1.1n_{D,i}^2$) is the high-frequency permittivity of component i numbered as before, μ_1 is the dipole moment of the lactone (from Table 7), and Φ_i is the volume fraction of each component. (Ideal volume fractions were used as discussed previously (Hahn et al., 1993).) The molar volumes V of the mixtures needed for the evaluation of eq 6 were calculated from a Redlich−Kister fit of the excess molar volumes, V^E, of the mixtures:

$$V_E = x_1 x_2 \sum_{i=0}^{2} A_i(x_1 - x_2)^i \tag{7}$$

In Table 8 the Redlich−Kister coefficients of the lactone (1) + benzene (2) mixtures are summarized (Klein and Svejda, 1995; Klein, 1997).

Table 8. Redlich–Kister Fit (Equation 7) of the Excess Volume V^E, Coefficients A_i, and Standard Deviations σ (All in cm^3 mol$^-$1) at Temperatures T and Atmospheric Pressure as Taken from the Literature[a,b]

system	T/K	A_0	A_1	A_2	σ
γ-butyrolactone (1) +	293.15	−2.544	0.799	−0.289	0.001
benzene (2)	313.15	−2.929	0.872	−0.260	0.002
γ-valerolactone (1) +	293.15	−1.490	0.633	−0.220	0.003
benzene (2)	313.15	−1.800	0.681	−0.154	0.004
δ-valerolactone (1) +	293.15	−2.699	0.988	−0.287	0.002
benzene (2)	313.15	−3.120	0.998	−0.305	0.002
ϵ-caprolactone (1) +	293.15	−2.343	1.082	−0.273	0.002
benzene (2)	313.15	−2.776	1.112	−0.406	0.003

[a] Molar mass of benzene, M = 78.113 64 kg kmol^{-1}, and its density, ρ = 879.01 kg m^{-3} and 857.57 kg m^{-3}, at 293.15 K and 313.15 K, respectively. Klein and Svejda (1995). [b] Klein (1997).

Table 9. Calculated Values of the Kirkwood Correlation Factor g (Equation 6) of the Mixtures of the Lactones + Benzene at 293.15 K and 313.15 K and Atmospheric Pressure

293.15 K		313.15 K		293.15 K		313.15 K	
x_1	g	x_1	g	x_1	g	x_1	g
γ-Butyrolactone (1) + Benzene (2)				γ-Valerolactone (1)+ Benzene (2)			
0.0982	0.76	0.0894	0.74	0.0939	0.79	0.0821	0.78
0.1977	0.77	0.1913	0.78	0.1888	0.80	0.0828	0.78
0.2945	0.81	0.1973	0.79	0.3267	0.84	0.1828	0.82
0.3837	0.83	0.2984	0.81	0.3858	0.87	0.1942	0.83
0.4959	0.85	0.3964	0.84	0.4955	0.89	0.2939	0.86
0.5904	0.88	0.3986	0.84	0.5892	0.92	0.3019	0.86
0.6888	0.90	0.4878	0.87	0.6842	0.94	0.3886	0.88
0.7893	0.92	0.5952	0.90	0.7805	0.96	0.4899	0.91
0.8939	0.94	0.7057	0.92	0.8793	0.98	0.5919	0.93
1.0000	0.96	0.8071	0.94	1.0000	1.00	0.7040	0.96
		0.9048	0.96			0.8117	0.98
		1.0000	0.98			0.8999	1.00
						0.9137	1.01
						1.0000	1.03
δ-Valerolactone (1) + Benzene (2)				ϵ-Caprolactone (1) + Benzene (2)			
0.1041	0.77	0.1117	0.75	0.0999	0.81	0.0962	0.80
0.2126	0.79	0.1866	0.78	0.2040	0.84	0.1907	0.84
0.2990	0.80	0.2891	0.80	0.3160	0.88	0.2906	0.87
0.4095	0.82	0.3946	0.82	0.4058	0.90	0.3954	0.91
0.5004	0.84	0.4786	0.84	0.4600	0.92	0.5097	0.95
0.6184	0.86	0.6040	0.86	0.5228	0.95	0.5853	0.97
0.7022	0.88	0.6943	0.88	0.6471	0.99	0.6322	0.99
0.8071	0.89	0.7983	0.90	0.7482	1.02	0.6477	0.99
0.8933	0.90	0.8883	0.91	0.8581	1.05	0.7095	1.01
1.0000	0.92	1.0000	0.93	1.0000	1.09	0.8043	1.04
						0.8932	1.07
						1.0000	1.10

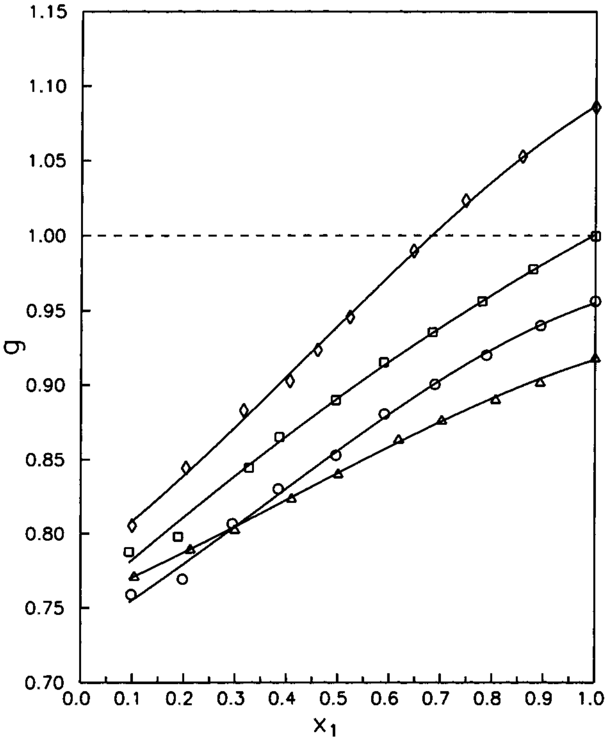

Figure 4. Variation of the Kirkwood correlation factor, g, at 293.15 K and atmospheric pressure with the mole fraction x_1 of the mixtures: (○) γ-butyrolactone (1) + benzene (2); (□) γ-valerolactone (1) + benzene (2); (△) δ-valerolactone (1) + benzene (2); (◇): ϵ-caprolactone (1) + benzene (2).

The Kirkwood correlation factors, calculated for the mixtures of the lactones + benzene at 293.15 K and 313.15 K and atmospheric pressure, are given in Table 9 and plotted for the temperature of 293.15 K in Figure 4. Kirkwood correlation factors for mixtures with toluene and ethylbenzene are not shown because eq 6 does not account for the dipole moment of these slightly polar solvents. The overall appearance of the curves does not change at the higher temperature. Kirkwood g factors greater than 1 are indicative of a tendency toward parallel alignment of dipoles, values less than 1 are obtained when antiparallel alignment is favored, and a value of unity is expected when orientational ordering is absent. As can be seen in Figure 4, the deviations from $g = 1$ are small, indicating the absence of strong short-range orientational correlations despite the relatively strong dipole moments of the lactones as compared to those of the linear esters (e.g., ethylethanoate, μ = 1.88 D (Riddick et al., 1986)). Nevertheless, g is less than unity almost throughout the whole mole fraction range, showing that an antiparallel orientation is favored, as has also been found by Avraam et al. (1998). However, compared, e.g., to strongly associating alcohols ($g \sim 3-5$, Sastry and Valand (1998)), the orientational effects in the lactone mixtures with benzene (g ~0.82) are still surprisingly low.

Acknowledgment

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