Molar Excess Volumes and Molar Excess Enthalpies of Binary Liquid Mixtures of Norbornadiene + Benzene, + Cyclohexane, + Decane, and + Carbon Tetrachloride

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For the binary liquid mixtures of norbornadiene (bicyclo[2.2.1]hepta-2,5-diene) + benzene, + cyclohexane, + decane, or + carbon tetrachloride, the molar excess volumes were determined from density measurements by means of a vibrating glass tube densimeter at 293.15 K and 313.15 K, and the molar excess enthalpies were measured by means of a flow microcalorimeter of Picker type at 293.15 K. All measurements were performed at atmospheric pressure.

Introduction

Norbornadiene (bicyclo[2.2.1]hepta-2,5-diene) is well-known as an important intermediate for organic and polymer synthesis,[1] which exhibits a high chemical reactivity because of the presence of the double bonds and the large ring strain.[2] Very promising technological applications of norbornadiene were found in the last years for solar energy storage[3] or plant growth regulators.[4] However, despite its potential, thermodynamic data for norbornadiene and its mixtures are scarce. As far as we are aware, no measurements of excess enthalpies or excess volumes for systems containing norbornadiene have been reported in the past.

This work continues systematic investigations concerning the excess properties of different types of nonelectrolyte mixtures,[5,6] which will provide the necessary data for improving predictive group theories. For that purpose, norbornadiene offers some special reasons for a study of the excess properties of its binary mixtures: the nonplanar bicyclic structure[7] (Figure 1), the small dipole moment[8] accompanied by a significant quadrupole moment,[9] and the electron delocalization due to the strain-induced overlap of the π orbitals.[9] It is expected that both intermolecular interactions and steric factors will have a notable influence on the measured excess properties of its mixtures.

Experimental Section

Norbornadiene [Sigma-Aldrich Chemie, Steinheim, Germany, inhibited with ≃0.02−0.10% butylhydroxytoluene (BHT)], carbon tetrachloride (J. T. Baker Chemicals B.V., Deventer, The Netherlands), benzene (Sigma-Aldrich Chemie Steinheim, Germany), cyclohexane (J. T. Baker Chemicals B.V., Deventer, The Netherlands), and decane (Acros, Geel, Belgium) with stated purities of better than (98, 99, 99.9, 99, and 99) mol % were stored over a molecular sieve (0.4 nm, J. T. Baker Chemicals B.V., Deventer, The Netherlands, activated at 573 K for more than 12 h under vacuum prior to use). The drying of the chemicals was performed with a molecular sieve in the vapor phase, except for benzene and carbon tetrachloride, where it was carried out in the liquid phase. The purity of the chemicals was checked by gas chromatography, as described in a previous work,[10] and was found to be 99.9 mol % for norbornadiene, 99.99 mol % for benzene, 99.89 mol % for cyclohexane, 99.9 mol % for decane, and 99.99 mol % for carbon tetrachloride. All liquids were thoroughly degassed in a vacuum prior to use.

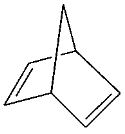

Figure 1. Chemical structure of norbornadiene.

In Table 1, the measured densities ρ of the pure compounds are compared with literature data. Relative atomic masses,[23] $A_r(H) = 1.007\ 95$, $A_r(C) = 12.011$, and $A_r(Cl) = 35.4528$, were used for the calculation of the molar volumes from densities.

Table 1. Density ρ of Pure Components at Atmospheric Pressure Compared with Literature Values

		ρ/g·cm^{-3}	
component	T/K	this work	literature
norbornadiene	293.15	0.906 74	0.906 4[11]
	313.15	0.886 00	
benzene	293.15	0.879 07	0.879 00,[12] 0.879 01[13]
	313.15	0.857 50	0.857 41,[14] 0.857 57[13]
cyclohexane	293.15	0.778 49	0.778 49,[15] 0.778 55[12]
	313.15	0.759 46	0.759 39,[16] 0.759 56[17]
decane	293.15	0.729 91	0.729 91,[15] 0.729 95[18]
	313.15	0.714 70	0.714 69,[19] 0.714 76[18]
carbon tetrachloride	293.15	1.594 20	1.594 17,[20] 1.594 10[21]
	313.15	1.555 22	1.555 22,[15] 1.555 15[22]

The molar excess volumes V^E were calculated from the precise densities of the liquids which were measured by means of a vibrating glass tube densimeter (DMA 02 D, Chempro Paar, Germany) at 293.15 K or 313.15 K and atmospheric pressure. The preparation of the samples

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Table 2. Densities ρ and Molar Excess Volumes V^E of Binary Liquid Mixtures with Norbornadiene as One Component at Temperatures of 293.15 K or 313.15 K and Atmospheric Pressure

293.15 K						313.15 K					
x_1	ρ/ g·cm^{-3}	V^E/ cm^3·mol^{-1}	x_1	ρ/ g·cm^{-3}	V^E/ cm^3·mol^{-1}	x_1	ρ/ g·cm^{-3}	V^E/ cm^3·mol^{-1}	x_1	ρ/ g·cm^{-3}	V^E/ cm^3·mol^{-1}
Norbornadiene (1) + Benzene (2)											
0.035 59	0.879 94	0.026	0.426 68	0.890 51	0.136	0.035 59	0.858 46	0.021	0.548 88	0.872 91	0.130
0.105 24	0.881 78	0.059	0.487 98	0.892 20	0.139	0.165 24	0.862 04	0.077	0.618 98	0.874 94	0.122
0.137 54	0.882 61	0.075	0.509 47	0.892 80	0.139	0.243 05	0.864 17	0.106	0.659 06	0.876 09	0.116
0.142 23	0.882 73	0.077	0.551 58	0.893 98	0.136	0.375 43	0.867 95	0.127	0.759 94	0.879 03	0.091
0.148 18	0.882 89	0.080	0.618 98	0.895 92	0.122	0.426 68	0.869 41	0.132	0.856 87	0.881 88	0.056
0.159 24	0.883 20	0.082	0.694 11	0.898 04	0.109	0.466 91	0.870 53	0.136	0.911 07	0.883 40	0.042
0.243 03	0.885 46	0.108	0.759 94	0.899 91	0.092	0.508 99	0.871 77	0.132			
0.281 94	0.886 50	0.119	0.832 60	0.901 99	0.067						
0.363 85	0.888 75	0.133	0.844 73	0.902 32	0.065						
Norbornadiene (1) + Cyclohexane (2)											
0.089 58	0.788 60	0.102	0.438 74	0.830 62	0.278	0.089 58	0.769 44	0.102	0.492 69	0.817 59	0.290
0.102 51	0.790 09	0.114	0.492 69	0.837 44	0.283	0.102 51	0.770 92	0.114	0.507 81	0.819 54	0.284
0.178 48	0.798 92	0.176	0.539 32	0.843 51	0.269	0.178 48	0.779 62	0.178	0.539 32	0.823 50	0.287
0.207 53	0.802 33	0.199	0.620 06	0.854 00	0.260	0.207 53	0.783 00	0.199	0.620 06	0.833 96	0.262
0.247 16	0.807 03	0.224	0.744 49	0.870 63	0.214	0.247 16	0.787 59	0.231	0.744 49	0.850 42	0.211
0.357 20	0.820 50	0.257	0.819 46	0.880 91	0.172	0.357 20	0.800 79	0.276	0.783 51	0.855 70	0.187
0.375 08	0.822 70	0.263	0.853 47	0.885 68	0.146	0.375 08	0.803 03	0.273	0.856 50	0.865 78	0.128
0.394 58	0.825 11	0.269	0.961 88	0.901 18	0.042	0.394 58	0.805 43	0.275	0.961 88	0.880 52	0.042
0.416 97	0.827 91	0.272				0.438 74	0.810 83	0.289			
Norbornadiene (1) + Decane (2)											
0.039 73	0.733 46	0.047	0.497 02	0.788 13	0.358	0.039 73	0.718 06	0.073	0.490 25	0.769 95	0.403
0.044 50	0.733 90	0.052	0.533 83	0.794 09	0.351	0.101 35	0.723 57	0.173	0.589 32	0.786 11	0.360
0.101 35	0.739 24	0.123	0.589 32	0.803 66	0.335	0.188 31	0.732 08	0.280	0.650 89	0.797 36	0.320
0.172 98	0.746 46	0.199	0.596 83	0.805 01	0.333	0.232 31	0.736 72	0.327	0.662 55	0.799 61	0.311
0.188 31	0.748 10	0.211	0.650 89	0.815 26	0.297	0.279 09	0.741 97	0.359	0.784 24	0.825 49	0.213
0.232 31	0.752 90	0.253	0.662 55	0.817 56	0.291	0.391 00	0.755 85	0.402	0.828 95	0.836 37	0.161
0.279 09	0.758 30	0.290	0.773 87	0.841 84	0.202	0.420 80	0.759 86	0.412	0.903 40	0.856 22	0.089
0.366 39	0.769 25	0.337	0.828 95	0.855 48	0.153						
0.420 80	0.776 72	0.354	0.903 40	0.876 00	0.081						
0.490 25	0.787 05	0.361									
Norbornadiene (1) + Carbon Tetrachloride (2)											
0.037 51	1.567 63	−0.034	0.471 56	1.263 67	−0.198	0.040 60	1.527 12	−0.027	0.471 56	1.233 32	−0.169
0.040 61	1.565 33	−0.030	0.474 07	1.261 88	−0.194	0.077 24	1.501 82	−0.049	0.508 48	1.208 49	−0.163
0.077 24	1.539 41	−0.058	0.496 46	1.246 52	−0.200	0.077 42	1.501 78	−0.055	0.520 95	1.200 15	−0.163
0.077 42	1.539 27	−0.057	0.508 48	1.238 21	−0.197	0.103 86	1.483 51	−0.066	0.596 63	1.149 65	−0.155
0.129 45	1.502 61	−0.097	0.520 95	1.229 64	−0.198	0.183 81	1.428 66	−0.110	0.686 73	1.089 91	−0.134
0.183 81	1.464 30	−0.126	0.596 63	1.177 74	−0.188	0.224 21	1.401 03	−0.127	0.716 68	1.070 19	−0.128
0.230 58	1.431 39	−0.145	0.631 18	1.154 16	−0.182	0.299 46	1.349 64	−0.145	0.740 55	1.054 49	−0.120
0.264 52	1.407 57	−0.155	0.634 48	1.151 84	−0.175	0.321 79	1.334 45	−0.149	0.784 24	1.025 87	−0.108
0.269 31	1.404 31	−0.164	0.686 73	1.116 38	−0.168	0.356 36	1.311 00	−0.156	0.839 48	0.989 81	−0.087
0.299 46	1.383 16	−0.169	0.701 06	1.106 66	−0.162	0.356 54	1.310 95	−0.161	0.869 67	0.970 17	−0.073
0.321 79	1.367 56	−0.174	0.716 68	1.096 08	−0.157	0.442 30	1.252 98	−0.167			
0.356 36	1.343 52	−0.186	0.740 55	1.079 90	−0.144						
0.356 55	1.343 35	−0.183	0.784 24	1.050 41	−0.123						
0.399 41	1.313 58	−0.191	0.839 48	1.013 40	−0.101						
0.404 49	1.310 05	−0.192	0.869 67	0.993 22	−0.086						
0.442 30	1.283 85	−0.194	0.923 83	0.957 15	−0.053						
0.464 22	1.268 68	−0.194	0.948 11	0.941 02	−0.034						

(from carefully degassed liquids, under vacuum, with vapor space correction), their transfer to the vibrating tube (without losses by evaporation or contact to air), and the experimental setup (like measurement and control of the temperature) have been described in a previous paper.[24] In summary, the following uncertainties were found: ±0.003 K for the temperature; 3×10^{-5} for the final mole fractions; 2×10^{-5} g·cm^{-3} at 293.15 K and 1×10^{-4} g·cm^{-3} at 313.15 K for the density, with a reproducibility of 3×10^{-6} g·cm^{-3} at both temperatures; 0.003 cm^3·mol^{-1} for the molar excess volumes at about equimolar composition.

The molar excess enthalpies H^E were measured with a dynamic flow calorimeter of Picker type (Setaram, France) at 293.15 K and at atmospheric pressure, as described in detail elsewhere.[25] The composition of each mixture was determined by its density,[6] which was measured in a thermostatically controlled flow densimeter (DMA 602, Chempro Paar, Germany) connected in series immediately behind the calorimeter. From these densities and the measured excess volumes of the systems, the mole fraction of the mixture could be calculated to an estimated uncertainty of ±0.0001. The calorimeter was thermostated to ± 0.03 K or better and controlled by calibrated Pt-100 thermoresistors. It was checked routinely by measurements on the system benzene + cyclohexane, and the agreement with these literature data[6] was found to be within less than 1% over the central range of the concentration. The reproducibility of the H^E data, even at low concentration ranges, appeared to be better by about 1 order of magnitude, as can be noticed on the figures. All points were taken at several different days and still show only little scatter about the fitting curve.

Results

The experimental values of the molar excess volume V^E and molar excess enthalpies H^E are presented in Tables 2

Table 3. Molar Excess Enthalpies H^E of Binary Liquid Mixtures with Norbornadiene as One Component at 293.15 K and Atmospheric Pressure

x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}	x_1	H^E/J·mol^{-1}
		Norbornadiene (1) + Benzene (2)			
0.0222	23.1	0.3112	211.3	0.6859	198.1
0.0506	49.9	0.3262	217.7	0.6958	193.9
0.0634	61.1	0.3852	230.9	0.7213	184.6
0.0853	78.3	0.4164	236.5	0.7627	162.2
0.1302	115.3	0.4469	238.8	0.7963	146.1
0.1361	117.3	0.4857	238.5	0.8425	116.4
0.1553	132.1	0.5141	239.0	0.8671	101.8
0.1874	151.3	0.5633	232.3	0.9142	67.5
0.2392	179.9	0.5976	226.6	0.9401	48.2
0.2586	190.1	0.6321	217.9	0.9627	30.4
		Norbornadiene (1) + Cyclohexane (2)			
0.0437	49.7	0.3913	268.8	0.7726	194.2
0.0694	76.0	0.4276	277.4	0.8060	172.1
0.0967	101.9	0.4394	278.3	0.8506	137.9
0.1330	133.3	0.4895	278.9	0.8713	124.1
0.1484	146.5	0.5600	273.9	0.8722	121.0
0.1841	173.7	0.5705	272.8	0.8831	111.5
0.2273	203.3	0.6046	265.7	0.9055	91.1
0.2548	218.9	0.6609	247.6	0.9334	67.6
0.2805	231.8	0.6981	234.1	0.9706	28.8
0.3269	249.3	0.7473	209.2		
0.3340	253.0	0.7632	200.2		
		Norbornadiene (1) + Decane (2)			
0.0462	103.2	0.2890	434.6	0.6619	399.6
0.0703	151.2	0.3399	462.0	0.7239	352.8
0.0946	197.0	0.4020	478.7	0.7695	307.8
0.1375	270.1	0.4485	487.1	0.8163	252.8
0.1605	299.7	0.4500	486.2	0.8837	171.7
0.1970	349.0	0.5002	474.9	0.9414	91.4
0.2115	368.4	0.5559	457.9		
0.2488	399.2	0.6385	416.3		
		Norbornadiene (1) + Carbon Tetrachloride (2)			
0.0402	−33.0	0.2429	−159.1	0.6378	−191.5
0.0409	−34.2	0.2776	−173.0	0.6747	−180.4
0.0691	−56.8	0.3163	−187.0	0.7266	−163.3
0.0991	−77.6	0.3622	−198.8	0.7671	−146.5
0.1344	−100.4	0.3927	−204.6	0.8069	−125.4
0.1570	−115.6	0.4476	−210.8	0.8447	−105.3
0.1844	−131.0	0.4953	−212.6	0.8912	−75.6
0.1844	−130.2	0.5065	−211.4	0.9214	−56.1
0.2067	−142.8	0.5680	−204.3	0.9591	−29.6

and 3, respectively, at various mole fractions x_i of the mixtures. All of the measured excess properties have been fitted to Redlich−Kister-type polynomials

$$Z^E_{\text{calc}} = x_1 x_2 \sum_{i=0}^{k} A_i (x_1 - x_2)^i \tag{1}$$

where $Z^E = V^E$ or H^E.

The coefficients A_i are summarized in Table 4 together with the standard deviation σ, defined as

$$\sigma^2 = \sum_N [Z^E - Z^E_{\text{calc}}]^2/(N - m) \tag{2}$$

where Z^E is the experimental excess property, N is the number of data points, and m is the number of coefficients A_i, and the maximum deviation δ is

$$\delta = \max |Z^E - Z^E_{\text{calc}}| \tag{3}$$

The coefficients A_i and the deviations σ and δ are given in the same units as the corresponding excess properties.

Discussion

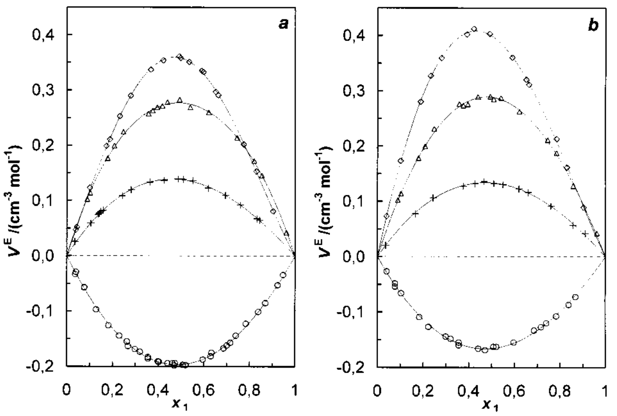

Figure 2. Molar excess volume V^E versus mole fraction x_1 of the binary liquid mixtures of norbornadiene (1): (+) + benzene (2), (△) + cyclohexane (2), (◇) + decane (2), or (○) + carbon tetrachloride (2) at (a) 293.15 K or (b) 313.15 K and atmospheric pressure.

Table 4. Coefficients A_i and Standard (σ) and Maximum (δ) Deviations of the Redlich−Kister Equation (Eq 1) for the Experimental Excess Data at Temperature T

excess property	T/K	A_0	A_1	A_2	σ	δ
			Norbornadiene (1) + Benzene (2)			
V^E/cm^3·mol^{-1}	293.15	0.551	−0.095		0.002	0.004
V^E/cm^3·mol^{-1}	313.15	0.532	−0.064		0.002	0.003
H^E/J·mol^{-1}	293.15	957.4	−87.6	−28.9	0.9	1.4
			Norbornadiene (1) + Cyclohexane (2)			
V^E/cm^3·mol^{-1}	293.15	1.108	−0.05	0.179	0.003	0.006
V^E/cm^3·mol^{-1}	313.15	1.152	−0.113		0.003	0.006
H^E/J·mol^{-1}	293.15	1123.3	−48.2		1.1	2.1
			Norbornadiene (1) + Decane (2)			
V^E/cm^3·mol^{-1}	293.15	1.432	−0.233	−0.477	0.002	0.004
V^E/cm^3·mol^{-1}	313.15	1.595	−0.534	−0.208	0.003	0.006
H^E/J·mol^{-1}	293.15	1912.5	−409.7	113.1	2.3	3.8
			Norbornadiene (1) + Carbon Tetrachloride (2)			
V^E/cm^3·mol^{-1}	293.15	−0.787	0.055		0.002	0.005
V^E/cm^3·mol^{-1}	313.15	−0.665	0.073		0.003	0.003
H^E/J·mol^{-1}	293.15	−847.0	52.2	27.5	0.7	1.7

The molar excess volumes of the investigated systems are shown in Figure 2. The corresponding Redlich−Kister plots are almost symmetrical. The mixture of norbornadiene + carbon tetrachloride exhibits only negative V^E values with minima of $\simeq -0.2$ cm^3·mol^{-1} at 293.15 K and -0.16 cm^3·mol^{-1} at 313.15 K. The other three systems show positive molar excess volumes in the entire concentration range. The maximum values rise in the sequence benzene < cyclohexane < decane. Except for the mixture with benzene, in the other systems the values at the extrema rise with temperature.

The measured molar excess enthalpies are plotted in Figure 3 and exhibit shapes similar to those of the V^E vs x_1 curves. Also the molar excess enthalpies of the system norbornadiene + carbon tetrachloride are negative, with a minimum of about -200 J·mol^{-1}. The H^E curves of the other three systems show positive values throughout the concentration range, and the maximum value increases from about 230 J·mol^{-1} up to almost 500 J·mol^{-1}, in the same sequence as the V^E: benzene < cyclohexane < decane.

Positive values of V^E and of H^E for the system norbornadiene + benzene indicate that a structural order in the pure liquids is broken by the mixing process without being compensated by strong interactions between norbornadiene and benzene molecules. Apparently, both molecules, although being fairly polar, are hindered sterically to reach an optimal fit for a strong attraction. This is further supported by the results for cyclohexane as a mixing partner. Both systems behave very similarly, obviously only the ring structures of benzene and of cyclohexane have an influence on the excess properties. Larger excess values of

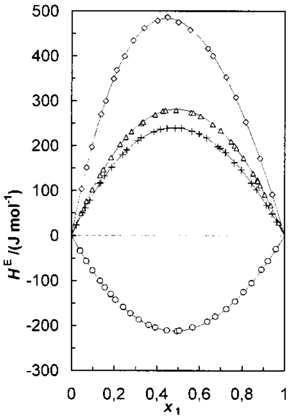

Figure 3. Molar excess enthalpy H^E versus mole fraction x_1 of the binary liquid mixtures of norbornadiene (1): (+) + benzene (2), (△) + cyclohexane (2), (◇) + decane (2), or (○) + carbon tetrachloride (2) at 293.15 K and atmospheric pressure.

mixtures with decane are well-known from many systems, they stem from the large surfaces of linear alkanes by which they interact with other molecules.

However, the negative values of V^E and of H^E for the system norbornadiene + carbon tetrachloride show that strong attractive interactions are possible, if a small molecule like CCl_4 is not sterically hindered to approach the polar norbornadiene molecule in an optimal way. This would explain the negative excess volumes and the exothermal excess enthalpies observed in this system.

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