

Densities and Isothermal Compressibilities at Pressures up to 20 MPa of the Systems *N,N*-Dimethylformamide or *N,N*-Dimethylacetamide + α,ω -Dichloroalkane

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Densities of pure *N,N*-dimethylformamide, *N,N*-dimethylacetamide, 1,2-dichloroethane, 1,4-dichlorobutane, and 1,6-dichlorohexane were measured at (288.15, 298.15, 308.15, and 318.15) K at pressures up to 20 MPa, and from them, isothermal compressibilities were obtained. Densities for *N,N*-dimethylformamide or *N,N*-dimethylacetamide + 1,2-dichloroethane, or + 1,4-dichlorobutane, or + 1,6-dichlorohexane at 298.15 K and at pressures up to 20 MPa were measured, and isothermal compressibilities were obtained.

Introduction

To continue with the systematic study of thermodynamic properties of mixtures containing amides and mono- and polychloroalkanes,¹ we present here the densities, ρ , at 298.15 K and at pressures up to 20 MPa of *N,N*-dimethylformamide or *N,N*-dimethylacetamide + 1,2-dichloroethane, or + 1,4-dichlorobutane, or + 1,6-dichlorohexane. This work is part of research to study the intermolecular interactions present in mixtures such as amide + α,ω -dichloroalkane; these interactions could be dipolar like those in the pure amides, and also, acceptor–donor interactions are present in the mixtures of these compounds. Amides are of interest because they are used as simple models in biochemistry.^{2–4} The study of liquid mixtures containing amides could contribute to an understanding of complex molecules of biological interest. Also, *N,N*-dimethylformamide and *N,N*-dimethylacetamide are used as selective solvents for hydrocarbon extraction from petroleum. On the other hand, mono- and polyhaloalkanes represent a class of technically important compounds, used in industry as intermediates or as final products. These compounds are also interesting from a theoretical point of view because of the inter- and intramolecular effects. In the case of α,ω -dichloroalkanes such as those studied in this work, the proximity effect is present.

Densities, ρ , of the pure liquids (*N,N*-dimethylformamide,¹ *N,N*-dimethylacetamide,¹ 1,2-dichloroethane, 1,4-dichlorobutane, and 1,6-dichlorohexane) were measured at (288.15, 298.15, 308.15, and 318.15) K at pressures up to 20 MPa, and from them, thermal expansion coefficients, α , were derived.

Isothermal compressibilities, κ_T , of the pure liquids and their mixtures were calculated, and the excess isothermal compressibilities, κ_T^E , of the mixtures were derived. As far as we know, there are no previous measurements on these mixtures in the literature. We have found values for densities of the *N,N*-dimethylacetamide + 1,2-dichloroethane system not at 298.15 K but at 303.15 K and 0.1 MPa.⁵ From the comparison, it can be said that our data follow the right trend.

Experimental Section

Materials. *N,N*-Dimethylformamide (mole fraction purity > 99 %) and *N,N*-dimethylacetamide (mole fraction purity \geq 99

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%) were obtained from Riedel de Haen. 1,2-Dichloroethane (mole fraction purity > 99.5 %) and 1,4-dichlorobutane (mole fraction purity > 97 %) were obtained from Fluka, and 1,6-dichlorohexane (mole fraction purity of 98 %) was obtained from Aldrich. All the liquids were used without further purification.

In Table 1, the measured densities, ρ , and isothermal compressibilities, κ_T , at 298.15 K, 308.15 K, and 0.1 MPa are compared with literature values.

Apparatus and Procedure. The mixtures were prepared by mass, and the mole fraction uncertainty was estimated to be less than $\pm 10^{-4}$. The densities, ρ , of the pure components were measured at (288.15, 298.15, 308.15, and 318.15) K at pressures up to 20 MPa. For binary mixtures, experimental densities were measured at 298.15 K at pressures up to 20 MPa. The measured densities were determined with a vibrating-tube densimeter with a DMA 512 high-pressure cell. High pressures were generated by a liquid pump (model LC-10 AT of Shimadzu).

The vibrating-tube temperature, T , measured using an Anton-Paar CKT 100 digital thermometer, was stable to better than ± 0.01 K using a Grant LT D6G thermostat. Pressures, p , were measured with a pressure gauge from Druck (model DPI 145) from (0 to 20) MPa, with an uncertainty of 0.005 % full scale.

The Forced Path Mechanical Calibration model¹³ was used to calibrate the densimeter. 1,2-Dichloroethane⁸ was used as a reference liquid for calibration purposes. This liquid was chosen because it is widely studied in the literature and because its density, ρ , is higher than the values of density, ρ , studied in our research. The uncertainty of the reported densities was estimated to be 10^{-4} g·cm⁻³.

Results and Discussion

Some of the measured densities, ρ , for the studied α,ω -dichloroalkanes at (288.15, 298.15, 308.15, and 318.15) K and at pressures, p , up to 20 MPa are reported in Table 2. Some of the isothermal compressibilities, κ_T

$$\kappa_T = \rho^{-1}(\partial\rho/\partial P)_T \quad (1)$$

obtained at (288.15, 298.15, 308.15, and 318.15) K for the pure liquids are given in Table 2. The complete set of densities, ρ , and isothermal compressibilities, κ_T , is given as Supporting

Table 1. Densities, ρ , and Calculated Isothermal Compressibility Values, κ_T , for the Pure Components at (298.15 and 308.15) K and 0.1 MPa and Those from the Literature

component	$\rho/(\text{g}\cdot\text{cm}^{-3})$ at 298.15 K		$10^4\kappa_T/\text{MPa}^{-1}$ at 298.15 K		$\rho/(\text{g}\cdot\text{cm}^{-3})$ at 308.15 K		$10^4\kappa_T/\text{MPa}^{-1}$ at 308.15 K	
	this work	lit.	this work	lit.	this work	lit.	this work	lit.
<i>N,N</i> -dimethylformamide	0.9438	0.9439 ⁶	6.51	6.50 ⁶	0.9342	0.93396 ¹¹	6.98	
<i>N,N</i> -dimethylacetamide	0.9370	0.9363 ⁶	6.71	6.39 ⁷	0.9269	0.92630 ¹²	6.76	
1,2-dichloroethane	1.2455	1.2456 ⁸	7.97	8.20 ⁹	1.2309	1.2309 ⁸	8.63	
1,4-dichlorobutane	1.1337	1.1333 ¹⁰	6.90		1.1224		7.39	
1,6-dichlorohexane	1.0638	1.0637 ¹⁰	6.44		1.0541		7.03	

Table 2. Experimental Values of Density, ρ , and Calculated Isothermal Compressibility, κ_T , for the Pure α,ω -Dichloroalkanes Studied at Pressure, p , and Temperature, T

p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$
1,2-Dichloroethane											
$T = 288.15 \text{ K}$			$T = 298.15 \text{ K}$			$T = 308.15 \text{ K}$			$T = 318.15 \text{ K}$		
0.1	1.2599	7.32	0.1	1.2455	7.97	0.1	1.2310	8.63	0.1	1.2164	9.49
2.0	1.2616	7.23	2.0	1.2474	7.88	2.0	1.2330	8.51	2.0	1.2185	9.32
4.1	1.2636	7.14	4.1	1.2494	7.79	4.1	1.2352	8.37	4.1	1.2209	9.13
6.1	1.2654	7.06	6.1	1.2514	7.70	6.1	1.2373	8.25	6.1	1.2231	8.94
8.1	1.2672	6.97	8.1	1.2532	7.62	8.1	1.2393	8.13	8.1	1.2252	8.76
10.1	1.2690	6.88	10.0	1.2551	7.53	10.1	1.2413	8.00	10.1	1.2275	8.57
12.1	1.2707	6.80	12.1	1.2573	7.44	12.1	1.2434	7.87	12.1	1.2296	8.40
14.1	1.2724	6.71	14.2	1.2590	7.35	14.2	1.2453	7.75	14.2	1.2316	8.21
16.3	1.2742	6.62	16.2	1.2608	7.26	16.2	1.2472	7.63	16.3	1.2338	8.02
18.2	1.2758	6.54	18.3	1.2628	7.17	18.3	1.2492	7.50	18.2	1.2355	7.86
20.0	1.2773	6.46	20.2	1.2645	7.09	20.2	1.2510	7.38	20.2	1.2375	7.67
1,4-Dichlorobutane											
$T = 288.15 \text{ K}$			$T = 298.15 \text{ K}$			$T = 308.15 \text{ K}$			$T = 318.15 \text{ K}$		
0.1	1.1437	6.43	0.1	1.1337	6.90	0.1	1.1223	7.39	0.1	1.1120	8.01
2.0	1.1452	6.35	2.0	1.1352	6.82	2.0	1.1239	7.28	2.0	1.1137	7.87
4.1	1.1467	6.27	4.1	1.1368	6.73	4.1	1.1256	7.17	4.1	1.1155	7.72
6.1	1.1481	6.19	6.1	1.1384	6.65	6.1	1.1272	7.07	6.1	1.1173	7.57
8.1	1.1495	6.12	8.1	1.1398	6.57	8.1	1.1288	6.96	8.1	1.1189	7.42
10.1	1.1510	6.03	10.1	1.1414	6.48	10.1	1.1304	6.85	10.1	1.1206	7.27
12.1	1.1524	5.96	12.1	1.1428	6.40	12.1	1.1319	6.75	12.1	1.1221	7.13
14.2	1.1538	5.88	14.1	1.1442	6.32	14.1	1.1335	6.65	14.2	1.1239	6.98
16.3	1.1552	5.80	16.2	1.1458	6.23	16.2	1.1350	6.54	16.3	1.1254	6.83
18.3	1.1565	5.72	18.3	1.1472	6.15	18.3	1.1365	6.43	18.3	1.1270	6.68
20.2	1.1578	5.65	20.2	1.1487	6.07	20.2	1.1380	6.33	20.2	1.1284	6.54
1,6-Dichlorohexane											
$T = 288.15 \text{ K}$			$T = 298.15 \text{ K}$			$T = 308.15 \text{ K}$			$T = 318.15 \text{ K}$		
0.1	1.0737	6.24	0.1	1.0638	6.44	0.1	1.0546	7.03	0.1	1.0451	7.61
2.0	1.0750	6.16	2.0	1.0652	6.39	2.0	1.0559	6.93	2.0	1.0466	7.48
4.1	1.0763	6.08	4.1	1.0667	6.35	4.1	1.0574	6.82	4.1	1.0481	7.33
6.1	1.0776	6.00	6.1	1.0680	6.30	6.1	1.0589	6.72	6.1	1.0497	7.19
8.1	1.0789	5.93	8.1	1.0694	6.26	8.1	1.0602	6.61	8.1	1.0512	7.06
10.1	1.0802	5.85	10.1	1.0707	6.21	10.1	1.0617	6.51	10.1	1.0526	6.91
12.1	1.0815	5.77	12.1	1.0719	6.17	12.1	1.0631	6.40	12.1	1.0541	6.78
14.2	1.0828	5.69	14.2	1.0733	6.13	14.1	1.0645	6.30	14.2	1.0556	6.64
16.3	1.0840	5.62	16.4	1.0748	6.08	16.2	1.0658	6.20	16.3	1.0571	6.49
18.3	1.0853	5.54	18.3	1.0761	6.04	18.3	1.0672	6.09	18.3	1.0583	6.36
20.2	1.0865	5.47	20.2	1.0773	6.00	20.3	1.0685	5.99	20.2	1.0596	6.23

Information. Density data were fitted to linear equations, and analytical differentiation was done to obtain the isothermal compressibilities. The uncertainty of the reported isothermal compressibilities was estimated to be $\pm 10^{-6} \text{ MPa}^{-1}$. For given values of p and T , for example, 20 MPa and 298.15 K, the density, ρ , decreases following the sequence 1,2-dichloroethane > 1,4-dichlorobutane > 1,6-dichlorohexane > *N,N*-dimethylformamide¹ > *N,N*-dimethylacetamide,¹ and the isothermal compressibility, κ_T , decreases following the same sequence. As an example, the isothermal compressibility values, κ_T , obtained for the studied α,ω -dichloroalkanes at 298.15 K are represented against pressure in Figure 1. From this figure and Figure 1 from García-Giménez et al. (2007),¹ it is observed that the behavior of the two amides is alike, while that of the pure α,ω -dichloroalkanes studied in this work is quite different. It can be concluded that the structural and interaction differences between the two amides are less important than those between the α,ω -dichloroalkanes.

Thermal expansion coefficients, α , are obtained by using the following equation

$$\alpha = -\rho^{-1}(\delta\rho/\delta T)_p \quad (2)$$

Density data were fitted to linear equations, and analytical differentiation was done to obtain thermal expansion coefficients. The uncertainty of the reported thermal expansion coefficients was estimated to be $\pm 10^{-5} \text{ K}^{-1}$. We have obtained the following values of α for the pure liquids at 298.15 K and 0.1 MPa: α (*N,N*-dimethylformamide) = $9.8 \cdot 10^{-4} \text{ K}^{-1}$; α (*N,N*-dimethylacetamide) = $9.6 \cdot 10^{-4} \text{ K}^{-1}$; α (1,2-dichloroethane) = $1.2 \cdot 10^{-3} \text{ K}^{-1}$; α (1,4-dichlorobutane) = $9.4 \cdot 10^{-4} \text{ K}^{-1}$; and α (1,6-dichlorohexane) = $8.9 \cdot 10^{-4} \text{ K}^{-1}$. The values found in the literature for the pure liquids are α (*N,N*-dimethylformamide) = $9.75 \cdot 10^{-4} \text{ K}^{-1}$,¹¹ α (*N,N*-dimethylacetamide) = $9.60 \cdot 10^{-4} \text{ K}^{-1}$,¹² and α (1,2-dichloroethane) = $11.41 \cdot 10^{-4} \text{ K}^{-1}$.⁶ We did not find the value of the thermal expansion coefficient, α , for

Table 3. Experimental Values of Density, ρ , and Calculated Isothermal Compressibility, κ_T , for the Studied Mixtures at Pressure, p , and 298.15 K

p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$
<i>N,N</i> -Dimethylformamide (x) + 1,2-Dichloroethane ($1 - x$)								
$x = 0.0805$			$x = 0.1978$			$x = 0.3020$		
0.1	1.2212	7.79	0.1	1.1862	7.69	0.1	1.1549	7.48
2.0	1.2230	7.69	2.0	1.1880	7.57	2.0	1.1566	7.38
4.0	1.2248	7.58	4.0	1.1897	7.46	4.0	1.1582	7.27
6.0	1.2267	7.47	6.0	1.1915	7.34	6.0	1.1599	7.17
8.0	1.2285	7.37	8.0	1.1932	7.22	8.0	1.1616	7.07
10.0	1.2304	7.26	10.0	1.1950	7.10	10.0	1.1632	6.96
12.0	1.2322	7.15	12.0	1.1967	6.98	12.0	1.1649	6.85
14.0	1.2339	7.05	14.0	1.1983	6.87	14.0	1.1664	6.75
16.0	1.2356	6.94	15.9	1.1999	6.76	16.0	1.1680	6.65
18.0	1.2372	6.84	18.0	1.2015	6.64	18.0	1.1695	6.55
20.0	1.2390	6.73	20.0	1.2031	6.52	20.0	1.1711	6.44
$x = 0.3970$			$x = 0.4988$			$x = 0.6023$		
0.1	1.1265	7.43	0.1	1.0957	7.16	0.1	1.0645	7.08
2.0	1.1280	7.32	2.0	1.0972	7.08	2.0	1.0659	6.98
4.0	1.1296	7.21	4.0	1.0987	7.00	4.0	1.0674	6.88
6.0	1.1314	7.09	6.0	1.1002	6.92	6.0	1.0688	6.78
8.0	1.1328	6.98	8.0	1.1018	6.83	8.0	1.0703	6.69
10.0	1.1345	6.86	10.0	1.1033	6.75	10.0	1.0718	6.58
11.9	1.1360	6.76	12.0	1.1048	6.67	12.0	1.0732	6.49
14.0	1.1376	6.64	14.0	1.1062	6.59	13.9	1.0746	6.40
16.0	1.1390	6.53	16.0	1.1077	6.51	16.0	1.0759	6.30
18.0	1.1405	6.43	18.0	1.1090	6.43	18.0	1.0773	6.20
20.0	1.1421	6.31	20.0	1.1106	6.34	20.0	1.0786	6.10
$x = 0.7054$			$x = 0.8005$			$x = 0.9071$		
0.1	1.0336	6.95	0.1	1.0052	6.81	0.1	0.9728	6.66
2.0	1.0350	6.86	2.0	1.0065	6.73	2.0	0.9740	6.59
4.0	1.0364	6.76	4.0	1.0079	6.65	4.0	0.9752	6.51
6.0	1.0377	6.66	6.0	1.0092	6.56	6.0	0.9765	6.43
8.0	1.0392	6.57	8.0	1.0105	6.48	8.0	0.9778	6.35
10.0	1.0406	6.47	9.9	1.0118	6.40	10.0	0.9791	6.27
11.9	1.0419	6.38	12.0	1.0132	6.32	12.0	0.9803	6.19
14.0	1.0432	6.28	14.0	1.0144	6.24	14.0	0.9815	6.11
16.0	1.0445	6.18	16.0	1.0157	6.16	16.0	0.9826	6.04
18.0	1.0457	6.09	17.9	1.0169	6.08	18.0	0.9838	5.96
20.0	1.0471	5.99	20.0	1.0182	6.00	20.0	0.9851	5.88
<i>N,N</i> -Dimethylformamide (x) + 1,4-Dichlorobutane ($1 - x$)								
$x = 0.1003$			$x = 0.1923$			$x = 0.2994$		
0.1	1.1190	6.82	0.1	1.1051	7.00	0.1	1.0879	6.89
2.0	1.1204	6.74	2.0	1.1065	6.90	2.0	1.0893	6.80
4.0	1.1220	6.66	4.0	1.1081	6.80	4.0	1.0908	6.72
6.0	1.1234	6.57	6.0	1.1095	6.70	6.0	1.0923	6.63
8.0	1.1249	6.49	8.0	1.1110	6.59	8.0	1.0937	6.55
10.0	1.1264	6.40	10.0	1.1126	6.49	10.0	1.0952	6.46
12.0	1.1278	6.32	11.9	1.1139	6.39	12.0	1.0966	6.37
14.0	1.1292	6.24	13.9	1.1153	6.29	14.0	1.0979	6.29
16.0	1.1306	6.16	16.0	1.1168	6.18	16.0	1.0992	6.20
18.0	1.1320	6.08	18.0	1.1181	6.08	18.0	1.1006	6.12
20.0	1.1334	6.00	20.0	1.1195	5.98	20.1	1.1022	6.03
$x = 0.4006$			$x = 0.5022$			$x = 0.6004$		
0.1	1.0712	6.96	0.1	1.0524	6.77	0.1	1.0340	6.86
2.0	1.0726	6.88	2.0	1.0538	6.69	2.0	1.0353	6.76
4.0	1.0740	6.79	4.0	1.0552	6.61	4.0	1.0367	6.67
6.0	1.0754	6.70	6.0	1.0566	6.53	6.0	1.0381	6.57
8.0	1.0769	6.61	8.0	1.0579	6.45	8.0	1.0394	6.48
10.0	1.0784	6.52	10.0	1.0593	6.36	10.0	1.0408	6.38
12.0	1.0798	6.43	11.9	1.0606	6.28	12.0	1.0421	6.29
14.0	1.0811	6.35	13.9	1.0620	6.20	14.0	1.0434	6.19
16.0	1.0825	6.26	16.0	1.0633	6.12	16.0	1.0446	6.10
18.0	1.0838	6.18	17.9	1.0645	6.05	18.0	1.0459	6.00
20.0	1.0853	6.09	20.0	1.0659	5.96	20.0	1.0472	5.91
$x = 0.7029$			$x = 0.7943$			$x = 0.9006$		
0.1	1.0131	6.82	0.1	0.9934	6.69	0.1	0.9689	6.63
2.0	1.0144	6.73	2.0	0.9947	6.62	2.0	0.9702	6.54
4.0	1.0158	6.63	4.0	0.9960	6.54	4.0	0.9714	6.45
6.0	1.0170	6.54	6.0	0.9973	6.47	6.0	0.9726	6.37
8.0	1.0184	6.45	8.0	0.9985	6.40	8.0	0.9739	6.28
10.0	1.0197	6.35	10.0	0.9999	6.32	10.0	0.9752	6.18
12.0	1.0211	6.26	12.0	1.0012	6.25	12.0	0.9764	6.10
14.0	1.0224	6.17	14.0	1.0023	6.18	14.0	0.9775	6.01
16.0	1.0235	6.08	16.0	1.0035	6.11	16.0	0.9787	5.92
18.0	1.0247	5.99	18.0	1.0049	6.04	18.0	0.9798	5.84
20.0	1.0261	5.90	20.0	1.0061	5.97	20.0	0.9810	5.75

Table 3 (Continued)

p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$
<i>N,N</i> -Dimethylformamide (x) + 1,6-Dichlorohexane ($1 - x$)								
	$x = 0.0986$			$x = 0.2013$			$x = 0.3197$	
0.1	1.0564	6.60	0.1	1.0486	6.81	0.1	1.0382	6.65
2.0	1.0577	6.55	2.0	1.0499	6.72	2.0	1.0395	6.58
4.0	1.0591	6.49	4.0	1.0513	6.63	4.0	1.0408	6.52
6.0	1.0604	6.44	6.0	1.0526	6.54	6.0	1.0422	6.45
7.9	1.0618	6.39	8.0	1.0540	6.45	8.0	1.0435	6.38
10.0	1.0631	6.33	10.0	1.0555	6.36	10.0	1.0449	6.31
12.0	1.0645	6.27	12.0	1.0568	6.27	12.0	1.0462	6.25
14.0	1.0658	6.22	14.0	1.0581	6.18	14.0	1.0475	6.18
16.0	1.0671	6.16	15.9	1.0593	6.09	16.0	1.0488	6.12
18.0	1.0685	6.11	18.0	1.0606	6.00	17.9	1.0499	6.06
20.0	1.0698	6.05	20.0	1.0620	5.91	20.0	1.0515	5.99
	$x = 0.4014$			$x = 0.5033$			$x = 0.6037$	
0.1	1.0301	6.88	0.1	1.0190	6.68	0.1	1.0073	6.67
2.0	1.0314	6.78	2.0	1.0203	6.63	2.0	1.0086	6.64
4.0	1.0328	6.68	4.0	1.0217	6.58	4.0	1.0099	6.61
6.0	1.0342	6.58	6.0	1.0230	6.53	5.9	1.0112	6.59
8.0	1.0355	6.48	8.0	1.0244	6.48	8.0	1.0126	6.56
10.0	1.0369	6.37	10.0	1.0257	6.43	10.0	1.0139	6.53
12.0	1.0382	6.27	12.0	1.0270	6.38	11.9	1.0151	6.51
13.9	1.0395	6.17	14.0	1.0283	6.33	14.0	1.0166	6.48
15.9	1.0407	6.07	16.0	1.0296	6.28	16.0	1.0180	6.45
18.0	1.0420	5.97	18.0	1.0309	6.23	18.0	1.0191	6.43
20.0	1.0432	5.87	20.0	1.0322	6.18	20.0	1.0205	6.40
	$x = 0.7034$			$x = 0.8019$			$x = 0.9008$	
0.1	0.9943	6.63	0.1	0.9800	6.75	0.1	0.9636	6.30
2.0	0.9956	6.57	2.0	0.9813	6.67	2.0	0.9648	6.27
4.0	0.9969	6.50	4.0	0.9826	6.59	4.0	0.9661	6.24
6.0	0.9982	6.43	6.0	0.9839	6.50	6.0	0.9673	6.20
8.0	0.9995	6.36	8.0	0.9851	6.42	8.0	0.9685	6.17
10.0	1.0008	6.29	10.0	0.9864	6.33	10.0	0.9698	6.14
12.0	1.0020	6.23	12.0	0.9876	6.25	12.0	0.9708	6.11
14.0	1.0033	6.16	14.0	0.9890	6.17	14.0	0.9719	6.08
16.0	1.0045	6.09	15.9	0.9901	6.09	16.0	0.9731	6.04
18.0	1.0056	6.03	17.9	0.9912	6.01	18.0	0.9743	6.01
20.0	1.0070	5.96	20.0	0.9925	5.92	20.0	0.9758	5.98
<i>N,N</i> -Dimethylacetamide (x) + 1,2-Dichloroethane ($1 - x$)								
	$x = 0.0977$			$x = 0.2003$			$x = 0.2988$	
0.1	1.2100	7.73	0.1	1.1744	7.47	0.1	1.1413	7.38
2.0	1.2118	7.62	2.0	1.1760	7.40	2.0	1.1429	7.29
4.0	1.2136	7.51	4.0	1.1777	7.32	4.0	1.1446	7.21
6.0	1.2154	7.40	6.0	1.1795	7.24	6.0	1.1461	7.12
8.0	1.2172	7.29	8.0	1.1812	7.16	8.0	1.1478	7.04
10.0	1.2190	7.17	10.0	1.1829	7.08	10.0	1.1495	6.95
12.0	1.2208	7.06	12.0	1.1846	7.00	12.0	1.1511	6.87
14.0	1.2224	6.95	14.0	1.1863	6.92	14.0	1.1526	6.78
16.0	1.2241	6.84	16.0	1.1878	6.85	16.0	1.1542	6.70
18.0	1.2258	6.73	18.0	1.1895	6.77	18.0	1.1557	6.62
20.0	1.2275	6.62	20.1	1.1911	6.69	20.0	1.1572	6.53
	$x = 0.4022$			$x = 0.4999$			$x = 0.6007$	
0.1	1.1079	7.25	0.1	1.0774	7.14	0.1	1.0471	6.96
2.0	1.1095	7.17	2.0	1.0788	7.05	2.0	1.0484	6.89
4.0	1.1110	7.08	4.0	1.0804	6.96	4.0	1.0498	6.80
6.0	1.1126	6.99	6.0	1.0818	6.87	6.0	1.0512	6.72
8.0	1.1141	6.90	8.0	1.0833	6.78	8.0	1.0527	6.64
10.0	1.1157	6.81	10.0	1.0848	6.68	10.0	1.0542	6.55
12.0	1.1172	6.72	11.9	1.0862	6.60	12.0	1.0555	6.47
14.0	1.1187	6.63	14.0	1.0877	6.50	14.0	1.0568	6.39
15.9	1.1201	6.55	16.0	1.0891	6.41	16.0	1.0581	6.31
17.9	1.1215	6.47	18.0	1.0904	6.32	18.0	1.0595	6.23
20.0	1.1231	6.37	20.0	1.0919	6.23	20.0	1.0608	6.15
	$x = 0.7008$			$x = 0.7988$			$x = 0.8997$	
0.1	1.0181	6.79	0.1	0.9905	6.73	0.1	0.9632	6.58
2.0	1.0194	6.72	2.0	0.9918	6.65	2.0	0.9644	6.51
4.0	1.0209	6.64	4.0	0.9931	6.56	4.0	0.9656	6.44
6.0	1.0221	6.56	6.0	0.9943	6.48	6.0	0.9669	6.37
8.0	1.0235	6.48	8.0	0.9956	6.40	8.0	0.9680	6.31
10.0	1.0248	6.40	10.0	0.9969	6.31	10.0	0.9694	6.24
12.0	1.0261	6.32	12.0	0.9982	6.23	12.0	0.9706	6.17
14.0	1.0274	6.25	14.0	0.9994	6.15	14.0	0.9717	6.10
16.0	1.0287	6.17	16.0	1.0006	6.07	16.0	0.9729	6.04
18.0	1.0299	6.10	18.0	1.0018	5.99	18.0	0.9734	5.97
20.0	1.0312	6.02	20.0	1.0030	5.91	20.1	0.9754	5.90

Table 3 (Continued)

p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$	p/MPa	$\rho/(\text{g}\cdot\text{cm}^{-3})$	$10^4\kappa_T/\text{MPa}^{-1}$
<i>N,N</i> -Dimethylacetamide (x) + 1,4-Dichlorobutane ($1 - x$)								
	$x = 0.0975$			$x = 0.2001$			$x = 0.2996$	
0.1	1.1163	6.80	0.1	1.0978	6.81	0.1	1.0793	6.86
2.0	1.1177	6.72	2.0	1.0993	6.73	2.0	1.0807	6.77
4.0	1.1193	6.64	4.0	1.1008	6.65	4.0	1.0821	6.69
6.0	1.1207	6.57	6.0	1.1022	6.57	6.0	1.0836	6.60
8.0	1.1222	6.49	8.0	1.1036	6.49	8.0	1.0845	6.51
10.0	1.1237	6.41	10.0	1.1052	6.41	10.0	1.0864	6.42
12.0	1.1251	6.33	12.0	1.1066	6.33	12.0	1.0878	6.33
14.0	1.1265	6.25	14.0	1.1079	6.26	14.0	1.0891	6.24
16.0	1.1279	6.17	16.0	1.1093	6.18	16.0	1.0905	6.16
18.0	1.1293	6.10	18.0	1.1106	6.10	18.0	1.0918	6.07
20.0	1.1308	6.02	20.0	1.1120	6.02	20.0	1.0933	5.98
	$x = 0.4017$			$x = 0.5009$			$x = 0.5981$	
0.1	1.0600	6.76	0.1	1.0407	6.86	0.1	1.0217	6.84
2.0	1.0613	6.69	2.0	1.0420	6.77	2.0	1.0230	6.75
4.0	1.0628	6.63	4.0	1.0434	6.68	4.0	1.0244	6.66
6.0	1.0642	6.56	6.0	1.0449	6.59	6.0	1.0256	6.57
8.0	1.0655	6.50	8.0	1.0462	6.50	8.0	1.0270	6.48
10.0	1.0670	6.43	10.0	1.0476	6.41	10.0	1.0285	6.39
12.0	1.0683	6.37	12.0	1.0489	6.32	12.0	1.0298	6.30
14.0	1.0697	6.30	14.0	1.0503	6.23	14.0	1.0310	6.21
16.0	1.0710	6.24	16.0	1.0515	6.14	16.0	1.0323	6.13
18.0	1.0723	6.18	17.9	1.0527	6.06	18.0	1.0335	6.04
20.0	1.0738	6.11	20.0	1.0541	5.97	20.0	1.0348	5.95
	$x = 0.6987$			$x = 0.8010$			$x = 0.9012$	
0.1	1.0011	6.71	0.1	0.9800	6.68	0.1	0.9586	6.56
2.0	1.0023	6.64	2.0	0.9812	6.60	2.0	0.9598	6.49
4.0	1.0037	6.58	4.0	0.9826	6.52	4.0	0.9610	6.41
6.0	1.0050	6.51	6.0	0.9838	6.44	6.0	0.9622	6.34
8.0	1.0063	6.45	8.0	0.9850	6.36	8.0	0.9635	6.26
10.0	1.0076	6.38	10.0	0.9863	6.27	10.0	0.9647	6.18
12.0	1.0089	6.31	11.9	0.9876	6.20	12.0	0.9659	6.11
14.0	1.0102	6.25	14.0	0.9888	6.11	14.0	0.9671	6.03
16.0	1.0114	6.18	16.0	0.9900	6.03	16.0	0.9682	5.96
18.0	1.0127	6.12	18.0	0.9911	5.95	18.0	0.9693	5.89
20.0	1.0140	6.05	20.0	0.9924	5.87	20.0	0.9705	5.81
<i>N,N</i> -Dimethylacetamide (x) + 1,6-Dichlorohexane ($1 - x$)								
	$x = 0.1002$			$x = 0.1985$			$x = 0.3002$	
0.1	1.0545	6.75	0.1	1.0452	6.60	0.1	1.0345	6.64
2.0	1.0558	6.66	2.0	1.0466	6.54	2.0	1.0359	6.57
4.0	1.0572	6.57	4.0	1.0479	6.48	4.0	1.0372	6.50
6.0	1.0586	6.49	6.0	1.0493	6.42	6.0	1.0385	6.44
8.0	1.0600	6.40	8.0	1.0506	6.36	8.0	1.0399	6.37
10.0	1.0614	6.31	10.0	1.0520	6.29	10.0	1.0413	6.30
12.0	1.0627	6.22	12.0	1.0533	6.23	12.0	1.0425	6.23
14.0	1.0639	6.14	14.0	1.0547	6.17	14.0	1.0438	6.16
16.0	1.0653	6.05	16.0	1.0559	6.11	16.0	1.0451	6.10
18.0	1.0665	5.97	18.0	1.0571	6.05	18.0	1.0463	6.03
20.0	1.0679	5.88	20.0	1.0584	5.99	20.0	1.0477	5.96
	$x = 0.4040$			$x = 0.4943$			$x = 0.6007$	
0.1	1.0231	6.63	0.1	1.0123	6.77	0.1	0.9988	6.53
2.0	1.0244	6.57	2.0	1.0136	6.67	2.0	1.0000	6.49
4.0	1.0257	6.51	4.0	1.0149	6.56	4.0	1.0014	6.45
6.0	1.0271	6.45	6.0	1.0163	6.46	6.0	1.0026	6.40
8.0	1.0284	6.39	8.0	1.0174	6.35	8.0	1.0039	6.36
10.0	1.0298	6.33	10.0	1.0189	6.24	10.0	1.0052	6.32
12.0	1.0310	6.27	12.0	1.0202	6.13	12.0	1.0065	6.28
14.0	1.0324	6.21	14.0	1.0214	6.03	14.0	1.0076	6.24
16.0	1.0336	6.15	16.0	1.0226	5.93	16.0	1.0090	6.20
18.0	1.0349	6.10	18.0	1.0238	5.83	18.0	1.0102	6.16
20.0	1.0362	6.04	20.0	1.0250	5.72	20.0	1.0115	6.12
	$x = 0.7006$			$x = 0.8012$			$x = 0.8994$	
0.1	0.9853	6.54	0.1	0.9704	6.69	0.1	0.9546	6.55
2.0	0.9865	6.48	2.0	0.9716	6.60	2.0	0.9557	6.47
4.0	0.9879	6.42	4.0	0.9729	6.52	4.0	0.9570	6.39
6.0	0.9891	6.37	6.0	0.9742	6.43	6.0	0.9582	6.31
8.0	0.9904	6.31	8.0	0.9754	6.34	8.0	0.9594	6.23
10.0	0.9916	6.25	10.0	0.9767	6.25	10.0	0.9606	6.14
12.0	0.9929	6.19	12.0	0.9779	6.16	12.0	0.9618	6.06
14.0	0.9941	6.14	14.0	0.9790	6.07	14.0	0.9630	5.98
16.0	0.9953	6.08	16.0	0.9802	5.99	16.0	0.9640	5.90
18.0	0.9965	6.02	18.0	0.9814	5.90	18.0	0.9652	5.82
19.9	0.9976	5.97	20.0	0.9826	5.81	20.0	0.9664	5.73

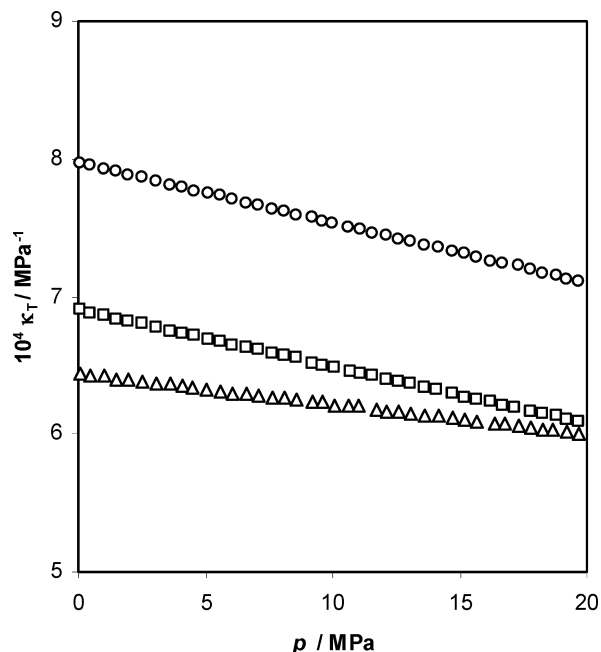


Figure 1. Isothermal compressibility, κ_T , of the studied α,ω -dichloroalkanes plotted against pressure at $T = 298.15$ K: \circ , 1,2-dichloroethane; \square , 1,4-dichlorobutane; \triangle , 1,6-dichlorohexane.

1,4-dichlorobutane and for 1,6-dichlorohexane in the literature. As can be seen, there is a good agreement between the values of thermal expansion coefficients, α , obtained by us and literature values.

For N,N -dimethylformamide or N,N -dimethylacetamide + 1,2-dichloroethane, or + 1,4-dichlorobutane, or + 1,6-dichlorohexane mixtures, some of the experimental densities, ρ , and isothermal compressibilities, κ_T , calculated with eq 1 are presented in Table 3. The complete set of the obtained values is given as Supporting Information. From the experimental values, it can be observed that the isothermal compressibility, κ_T , decreases as the length of the aliphatic chain of the α,ω -dichloroalkane of the mixture increases. The same behavior is found in our previous work.¹ The values of isothermal compressibilities, κ_T , decrease as the length of the aliphatic chain of the 1-chloroalkane of the mixtures studied increases. The same behavior is found in the literature for series of nonsaturated hydrocarbons,¹⁴ alcohols,^{15,16} etc. However, a different behavior is found for series such as n -alkane,¹⁷ for example. Thereby, we can conclude that even $(\delta V^E/\delta P)_T$ and the isothermal compressibility, κ_T , are related properties. Their behavior in function of the molecular structure related parameters such as, for example, the length of the aliphatic chain can be different. The reason can be that the isothermal compressibility, κ_T , depends on the molar volume of the studied system which involves the structural effects in the systems, besides the molecular interactions.

The "excess" compressibility, κ_T^E , defined as

$$\kappa_T^E = -V^{-1}(\delta V^E/\delta P)_T = \kappa_T - \phi_1\kappa_1 - \phi_2\kappa_2 \quad (3)$$

where ϕ_1 and ϕ_2 are the volume fractions, is widely used. Values for κ_T^E were obtained with eq 3 using the volume fractions, ϕ_1 and ϕ_2 , and isothermal compressibility, κ_T , obtained at 298.15 K and 0.1 MPa by fitting the experimental data against the molar fraction of the amide. The values for κ_T^E are represented against the mole fraction of the amide, x_1 , in Figures 2 and 3.

The excess isothermal compressibility values, κ_T^E , increase in the following sequences: N,N -dimethylformamide + 1,2-

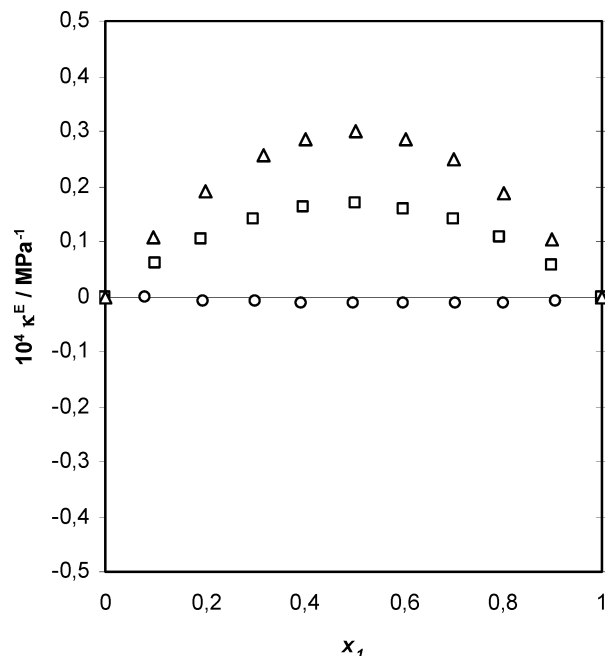


Figure 2. Excess isothermal compressibility, κ_T^E , represented against mole fraction of N,N -dimethylformamide for the mixtures with \circ , 1,2-dichloroethane; or \square , 1,4-dichlorobutane; or \triangle , 1,6-dichlorohexane at $T = 298.15$ K and 0.1 MPa.

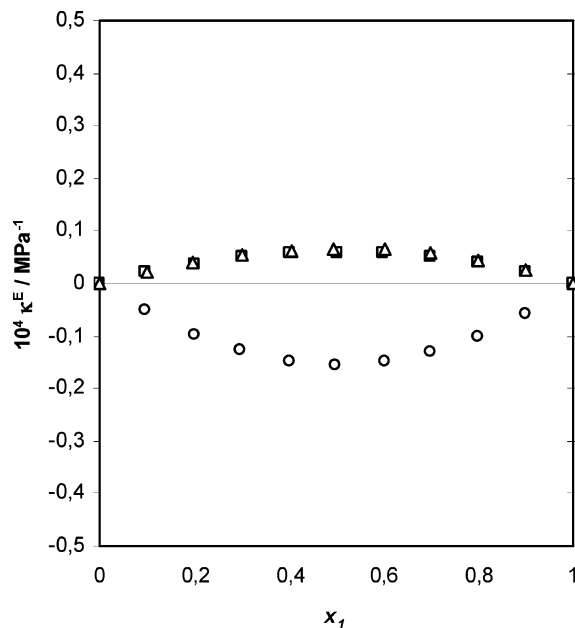


Figure 3. Excess isothermal compressibility, κ_T^E , represented against mole fraction of N,N -dimethylacetamide for the mixtures with \circ , 1,2-dichloroethane; or \square , 1,4-dichlorobutane; or \triangle , 1,6-dichlorohexane at $T = 298.15$ K and 0.1 MPa.

dichloroethane < N,N -dimethylformamide + 1,4-dichlorobutane < N,N -dimethylformamide + 1,6-dichlorohexane and N,N -dimethylacetamide + 1,2-dichloroethane < N,N -dimethylacetamide + 1,4-dichlorobutane \approx N,N -dimethylacetamide + 1,6-dichlorohexane. On the other hand, the excess isothermal compressibility values, κ_T^E , for the mixture N,N -dimethylformamide + 1,2-dichloroethane show practically zero deviation from ideality.

In any case, the explanation of the volumetric behavior of the studied mixtures is difficult from only this kind of measurements, given the variety and complexity of the interactional and geometric effects present in the pure α,ω -

dichloroalkanes and amides, for example, the dipole–dipole interactions and the specific acceptor–donor interactions present in the mixtures.

Supporting Information Available:

Experimental densities, ρ , and isothermal compressibilities, κ_T , calculated with eq 1, for the studied α,ω -dichloroalkane and for *N,N*-dimethylformamide or *N,N*-dimethylacetamide + 1,2-dichloroethane, or + 1,4-dichlorobutane, or + 1,6-dichlorohexane mixtures. This material is available free of charge via the Internet at <http://pubs.acs.org>.

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Received for review June 13, 2007. Accepted September 13, 2007. P. García-Giménez acknowledges the financial support received from DGA, Departamento de Educación y Ciencia, and the European Social Fund (B020/2003).

JE700339F