Densities and Dielectric Permittivities of Four Polyhydric Alcohols

O. V. Grineva,* V. I. Zhuravlev, and N. V. Lifanova

Faculty of Physical Chemistry, Chemistry Department, Moscow State University, 117234 Moscow, Russia

The densities of 2-methyl-2,4-pentanediol, 2,5-hexanediol, 1,7-heptanediol, and 1,2,6-hexanetriol were measured in the range $20 \leq t/°C \leq 70$. The dielectric permittivities of the same polyhydric alcohols were determined at 1 MHz between 10 and 200 °C. The results were compared with literature data.

Introduction

The density and dielectric permittivity are important properties of matter and of liquids in particular. The dielectric permittivity provides useful information on the intermolecular interactions in liquids. In our previous work (Zhuravlev, 1992) we used experimental densities and dielectric constants of pure propanediols and its solutions to calculate some related properties and then to discuss intermolecular association.

In this work we reported densities and dielectric permittivities of three diols and one triol. The substances under investigation are widely used in industry and scientific research, but information about its physical properties, except for the properties of 2-methyl-2,4-pentanediol, are very scant.

Experimental Section

Materials. The samples of 2-methyl-2,4-pentanediol, 2,5-hexanediol, and 1,2,6-hexanetriol were from Merck-Schuchardt. According to the supplier, the purities of the materials were better than 99%, 98%, and 97%, respectively. The 1,7-heptanediol was from Ferak Laborat Berlin (West) with purity "rein".

Immediately prior to use the samples were fractionally distilled under reduced pressure. The middle fractions were used.

Apparatus and Procedures. Densities were measured using glass monocapillary pycnometers which held ca. 20 cm^3 of liquid. The pycnometers were thermostated to within ±0.02 °C. The temperatures were checked by a calibrated platinum resistance thermometer. The pycnometers were calibrated with bidistilled deionized water.

The density measurements were made in 3−4 pycnometers and repeated 3−5 times, so the total number of measurements was 12−15 at each temperature. The reproducibility of results was within $\pm 5 \times 10^{-5}$ g·cm^{-3}. The absolute accuracy was estimated to be within $\pm 1 \times 10^{-4}$ g·cm^{-3}.

Dielectric permittivity measurements were carried out at 1 MHz by using a bridge scheme. The measuring cell was a coaxial capacitor type. It was equipped with E7-12 digital device for measurements of *L*, *C*, and *R* (*L* = inductance, *C* = capacitance, and *R* = resistance). The cell, having a stainless steel jacket, was thermostated to within ±0.02 °C. The temperatures were measured by a calibrated platinum resistance thermometer.

The cell was calibrated with standard pure liquids: chlorobenzene (ϵ = 5.690 at 20 °C and 5.612 at 25 °C), 1-butanol (ϵ = 17.8 at 20 °C and 13.1 at 60 °C), acetone (ϵ = 20.7 at 25 °C), ethanol (ϵ = 24.35 at 25 °C and 22.8 at 35 °C), and bidistilled water (ϵ = 80.37 at 20 °C and 78.54 at 25 °C). The dielectric constants for standards were taken from the literature (Akhadov, 1972; Weast and Lide, 1989−1990).

Experiments were performed 4−5 times at each temperature. The reproducibility of dielectric permittivity measurements was better than ±0.5%, and the accuracy was estimated to be ±1%.

Results and Discussion

Density. Experimental values for density (ρ) for the four polyhydric alcohols are given in Table 1. We also listed some literature values. We have not included results for 2-methyl-2,4-pentanediol and 1,2,6-hexanetriol where the authors present only equations without experimental data.

Our results for 2-methyl-2,4-pentanediol agree with those of Marks (1967) and Mellan (1962) within $\pm 2 \times 10^{-4}$ g·cm^{-3}. Our density values for 1,2,6-hexanetriol are in agreement with those of Tess *et al.* (1957) with the same accuracy, but the density at 20 °C by Marks (1967) is greater than ours by 3.4×10^{-3} g·cm^{-3}. We suspect this difference is due to impurities in the sample of 1,2,6-hexanetriol used by Marks (1967).

The densities of 2,5-hexanediol and 1,7-heptanediol are available in the literature only at room temperature. As $d^{20}{}_{20}$ = 0.9617 corresponds to ρ^{20} = 0.959 97 g·cm^{-3} our density value for 2,5-hexanediol at 20 °C is in agreement with that of Curme and Johnston (1953) within $\pm 2 \times 10^{-5}$ g·cm^{-3}. From Table 1, there are no dependable results for the density of 1,7-heptanediol. There is considerable difference between various literature sources, and besides that, the literature density data are appreciably greater than ours. All the cited works concerning 1,7-heptanediol were devoted to syntheses, but not a study of the ρ properties of diols; we suppose that samples of 1,7-heptanediol contained some impurities (water in particularly), and so its density values were greater.

Dielectric Permittivity. Experimental values for the dielectric permittivity (ϵ) are given in Table 2. We also listed all values in the temperature range studied, which were found in the literature. Again we do not include results where only an equation was given.

Our results for 2-methyl-2,4-pentanediol are in excellent agreement (within ±1%) with those of Ikada (1971) and Haranadh (1963) in the entire temperature range and of Moriamez *et al.* (1961) at 25 °C. The ϵ values of McDuffie and Litovitz (1962) for 2-methyl-2,4-pentanediol and 1,2,6-hexanetriol are greater than ours by 1.5−4%, and values

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Table 1. Experimental Densities of Some Polyhydric Alcohols

	2-methyl-2,4-pentanediol ρ/(g·cm^{-3})		1,2,6-hexanetriol ρ/(g·cm^{-3})	
t/°C	this work	lit.	this work	lit.
20	0.9218	0.92109 (Ikada, 1971) 0.9216 (Mellan, 1962) 0.9220 (Marks, 1967)	1.1030	d^{20}_{4} = 1.1030 (Tess *et al.*, 1957) 1.1064 (Marks, 1967)
30	0.9145	0.91390 (Ikada, 1971) 0.9145 (Mellan, 1962)	1.0970	d^{30}_{4} = 1.0972 (Tess *el al.*, 1957)
40	0.9072		1.0909	
50	0.8999	0.89965 (Ikada, 1971)	1.0849	
60	0.8926		1.0788	
70	0.8853		1.0726	

	2,5-hexanediol ρ/(g·cm^{-3})		1,7-heptanediol ρ/(g·cm^{-3})	
t/°C	this work	lit.	this work	lit.
20	0.95995	d^{20}_{20} = 0.9617 (Curme and Johnston, 1953)	0.9552	d^{20}_{4} = 0.9571 (Bel'skii *et al.*,1963) d^{25}_{4} = 0.9556 (Polyakova and Belov, 1964) d^{25}_{4} = 0.9569 (Huber, 1951) d^{25}_{4} = 0.9570 (Burdick and Adkins, 1934)
30	0.9533		0.9493	
40	0.9466		0.9434	
50	0.9398		0.9375	
60	0.9328		0.9315	
70	0.9256		0.9256	

Table 2. Dielectric Permittivities of Some Polyhydric Alcohols

	2-methyl-2,4-pentanediol					1,2,6-hexanetriol	
		lit.[a]					lit.[a]
t/°C	this work	Ikada (1971)	Moriamez *et al.* (1961)	Haranadh (1963)	McDuffie and Litovitz (1962)	this work	McDuffie and Litovitz (1962)
10	27.5	27.67			$28.4^{11.5}$	31.3	$31.5^{12.1}$
15	26.7					30.6	
20	25.9	25.86				29.8	
25	25.1		25.0			29.0	
30	24.4	24.36		24.4		28.2	
40	22.9	22.91				26.7	
50	21.6	21.50	22.9^{49}	21.0^{55}		25.3	
60	20.3	20.10				24.0	
70	19.1		20.3^{72}			22.7	
80	17.9			18.0		21.6	
90	16.8					20.5	
100	15.8					19.5	
110	14.8					18.5	
120	13.9					17.6	
130	13.0					16.7	
140	12.2					15.9	
150	11.4					15.2	
160	10.7					14.5	
170	10.0					13.8	
180	9.4					13.2	
190	8.8					12.6	
200						12.0	

t/°C	2,5-hexanediol (this work)	1,7-heptanediol (this work)	t/°C	2,5-hexanediol (this work)	1,7-heptanediol (this work)
7.5	23.0		80.0	15.7	15.8
10.0	23.5	2.9 (glass)	90.0	14.7	14.8
12.5	23.6		100.0	13.7	13.9
15.0	23.5	3.0 (glass)	110.0	12.8	13.0
		23.6 (supercooled)	120.0	11.9	12.2
17.5	23.3		130.0	11.2	11.4
20.0	23.0	22.9	140.0	10.5	10.7
25.0	22.4	22.2	150.0	9.8	10.0
30.0	21.8	21.5	160.0	9.2	9.3
40.0	20.4	20.3	170.0	8.7	8.7
50.0	19.2	19.1	180.0	8.2	8.2
60.0	18.0	17.9	190.0	7.7	7.7
70.0	16.8	16.8	200.0	7.3	7.3

[a] Superscript numbers indicate temperatures at which dielectric measurements were carried out.

of Moriamez *et al.* (1961) at 49 and 72 °C for 2-methyl-2,4-pentanediol are greater than ours by 5.5−7.5%.

There are no available dielectric constant data for 2,5-hexanediol and 1,7-heptanediol. 1,7-Heptanediol adheres to a glass at 17−19 °C, so we give the dielectric permittivity at 15 °C in the glass and the supercooled liquid state.

Registry Numbers Supplied by the Author. 1,7-Heptanediol, 629-30-1; 2,5-hexanediol, 2935-44-6; 1,2,6-hexanetriol, 106-69-4; 2-methyl-2,4-pentanediol, 107-41-5.

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