ISSN 1070-3632, Russian Journal of General Chemistry, 2011, Vol. 81, No. 7, pp. 1511–1522. © Pleiades Publishing, Ltd., 2011.
Original Russian Text © S.B. Bulgarevich, M.V. Boiko, M.N. Lyashenko, E.E. Akimova, 2011, published in Zhurnal Obshchei Khimii, 2011, Vol. 81, No. 7, pp. 1163–1174.

Molecular Polarizability of Organic Compounds and Their Complexes: LVI.[1] Molar Volume and Structure in a Solution of the Compounds with Several Axes of Intramolecular Rotation

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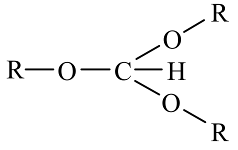
Received June 3, 2010

Abstract—Molar volumes in solutions of compounds like orthoformic esters, trialkyl phosphates, trialkylphosphites, substituted aziridines, cyclopropanes, cyclohexanes, boroxines, *N*-aryl-4-pyridones, decalines, and cyclooctane were determined and discussed. Conformations of alkyl substituents in the esters were found to be similar to the conformations of the corresponding alkanes. Molar volumes of aziridines and cyclopropanes were found to be additive with respect to the molar volumes of bond and group increments. The nature of solvation of the molecules of these compounds was found to be similar to that in the model systems which served for the calculations of the increments. Molar volumes of cyclohexane, decaline, and cyclooctane also were found to be additive with respect to the contributions of the molar volumes of increments of the corresponding bonds and groups. The solvation and the steric structure of substituted boroxines were found to be similar to those of the structurally analogous substituted benzenes. Conformations of *N*-aryl-4-pyridone and its substituted derivatives in solutions were found to be similar to the conformations of biphenyl and its derivatives. A possibility of simplification of the methods for determining the dipole moments and Kerr constants of compounds from their additive molar volumes was demonstrated.

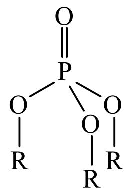
DOI: 10.1134/S1070363211070176

Orthoformic Esters, Trialkyl Phosphates, and Trialkyl Phosphites

We have studied such conformationally mobile systems as orthoformic esters **I**–**IV** and their structural organoelement analogs, trialkyl phosphates **V**–**X** and phosphites **XI**–**XV** and determined molar volumes at infinite dilution of these compounds in benzene and carbon tetrachloride solutions. The experimental data obtained are listed in Table 1.

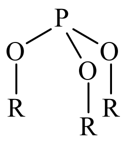


I–**IV**



V–**X**

R = CH_3 (**I, V, XI**); C_2H_5 (**II, VI, XII**); *n*-C_3H_7 (**III, VII**); *iso*-C_3H_7 (**VIII, XIII**); C_4H_9 (**IV**); C_5H_{11} (**IX**); C_6H_5 (**X**).



XI–**XV**

Additive analysis of the molar volumes of compounds **I**–**XV** was started with determining the increment of the molar volume of the homological difference $\Delta V(CH_2)$ per a methylene group. The calculation was performed by comparing the molar volumes of the molecules with the substituents differing by one or more methylene groups. The

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[1] For communication LV, see [1].

Table 1. Molar volumes of the studied compounds in solutions at infinite dilution at 25°C. Determination of dipole moments and Kerr constants of the molecules in solutions is carried out using additivity of molar volumes[a]

Comp. no.	Solvent	β	$_\infty V_2$, cm^3 mol^{-1}	V_{add}, cm^3 mol^{-1}	ε, %	V_{add} by simplified calculation, cm^3 mol^{-1}	Data obtained in this work by simplified procedure		Experimental data		Reference
							μ, D	$_\infty(_mK_2)\times10^{12}$, esu	μ, D	$_\infty(_mK_2)\times10^{12}$, esu	
Orthoformic esters											
I	CCl_4	–0.593	106.7±1.5	–	–	–	–	–	–	–	[2]
II	CCl_4	–0.753	164.0±1.4	–	–	154.7	1.62	–10.9	1.67	–9.1	[2]
III	CCl_4	-0.762	211.7±2.6	–	–	202.7	1.57	–7.3	1.64	–6.1	[2]
IV	CCl_4	–0.782	261.3±2.6	–	–	250.7	1.58	1.9	1.66	1.6	[2]
Trialkyl phosphates											
V	C_6H_6	0.283	115.0±0.6	–	–	–	–	–	–	–	[3]
VI	C_6H_6	0.178	171.3±0.8	–	–	163.0	3.11	–134.8	3.12	–135	[3]
VII	C_6H_6	0.138	221.2±0.5	–	–	211.0	3.16	–184.3	3.18	–184	[3]
VIII	C_6H_6	0.112	228.0±2.3	–	–	211.0	2.80	–127.8	2.84	–128	[3]
IX	C_6H_6	0.080	324.6±0.5	–	–	307.0	3.11	–206.9	3.14	–207	[3]
X	C_6H_6	0.301	261.0±3.8	–	–	–	–	–	–	–	[3]
Trialkyl phosphites											
XI	C_6H_6	0.169	118.0±0.2	–	–	–	–	–	–	–	[3]
XII	C_6H_6	0.086	173.7±1.5	–	–	166.0	1.78	–4.5	1.80	–4.4	[3]
XIII	C_6H_6	0.038	229.2 ±0.7	–	–	214.0	1.84	–47.2	1.82	–47	[3]
XIV	C_6H_6	0.008	570.8±0.3	–	–	550.0	1.68	–153.4	1.75	–153	[3]
XV	C_6H_6	0.271	258.9±3.0	–	–	–	–	–	–	–	[3]
Aziridines											
XVI	C_6H_{12}	–0.024	57.0±0.2	–	–	–	–	–	–	–	[4]
XVII	C_6H_{12}	–0.078	79.5±0.2	75.5	5.1	–	1.30	–10.2	1.31	–10.2	[4]
XVIII	C_6H_{12}	0.199	123.3±0.3	115.6	6.3	–	1.35	–67.6	1.38	–68	[4]
XIX	C_6H_{12}	0.269	129.6±0.9	129.8	0.2	–	2.29	–	2.28	–	[4]
Cyclopropanes											
XX	CCl_4	–0.314	92.0±0.7	94.0 97.7	2.1 6.2	97.7	1.98	–	1.95	–	[5]
XXI	CCl_4	–0.115	175.1±0.2	137.1	21.7	142.8	0	4.38	0	4.4	[5]
XXII	C_6H_{12}	0.786	142.5	138.9 142.6	2.6 0.07	142.6	0	18.8	0	17.2	[6]
XXIII	C_6H_{12}	0.279	155.7	152.0	2.3	157.8	1.99	47.48	2.43	43.6	[6]
XXIV	CCl_4	–0.285	151.7±0.3	149.4	1.5	149.5	1.88	–50.3	1.91	–49.5	[5]
	C_6H_6	0.289	152.3±1.2		1.9		1.86	–61.9	1.90	–61.9	
XXV	C_6H_{12}	0.340	171.5	168.1	2.0	165.9	2.12	17.33	2.13	15.9	[6]
XXVI	CCl_4	–0.172	163.8±0.2	166.0	1.3	163.8	1.95	–103.94	1.95	–104	[5]
	C_6H_6	0.352	164.2±0.6	164.4	0.1	161.6	1.99	–100.5	2.00	–101	
XXVII	C_6H_{12}	0.320	201.4	204.3	1.5	198.7	2.03	27.63	2.04	25.4	[6]
XXVIII	CCl_4	–0.326	168.3±0.4	166.7	0.9	164.5	2.05	44.28	2.05	–44.3	[5]
	C_6H_6	0.269	168.2±0.9	167.3	0.6		2.03	–54.87	2.03	–54.8	
XXIX	C_6H_{12}	0.394	184.4	182.6	1.0	178.8	2.18	–77.00	2.19	–70.7	[6]

Table 1. (Contd.)

Comp. no.	Solvent	β	$_\infty V_2$, cm^3 mol^{-1}	V_{add}, cm^3 mol^{-1}	ε, %	V_{add} by simplified calculation, cm^3 mol^{-1}	Data obtained in this work by simplified procedure		Experimental data		Reference
							μ, D	$_\infty(_mK_2)\times10^{12}$, esu	μ, D	$_\infty(_mK_2)\times10^{12}$, esu	
					Cyclopropanes						
XXX	C_6H_{12}	0.326	187.4	192.7	2.9	179.5	2.18	96.55	2.20	88.6	[6]
XXXI	C_6H_{12}	0.371	213.9	214.4	0.2	201.2	1.91	–74.05	1.95	–67.9	[6]
XXXII	C_6H_{12}	0.566	154.8	149.4	3.5	149.4	1.87	–1.2	1.89	–1.1	[6]
XXXIII	C_6H_{12}	0.534	174.6	171.2	2.0	165.8	2.03	86.79	2.06	79.5	[6]
XXXIV	C_6H_{12}	0.629	170.1	173.0	1.7	167.6	1.87	–90.96	1.88	–83.8	[6]
XXXV	C_6H_{12}	0.514	221.1	206.5	6.6	201.1	1.78	–49.30	1.84	–45.3	[6]
					Cycloalkanes						
XXXVI	CCl_4	–1.001	106.3	100.2	5.8	–	0	0.75	0	0.63	[7]
XXXVII	CCl_4	–1.026	125.6±0.9	121.3	3.4	–	0	3.69	0	3.09	[7]
XXXVIII	CCl_4	–0.915	169.6±2.3	166.3	1.9	–	0	2.63	0	2.20	[7]
XXXIX	CCl_4	–0.815	158.4	145.7	8.0	–	–	2.30	0	1.80	[7]
				151.3	4.5						
XL	CCl_4	–0.778	155.1	145.7	6.1	–	–	1.94	0	1.62	[7]
				151.3	2.5						
XLI	CCl_4	–0.854	131.3±1.7	133.6	1.7	–	0	2.00	0	1.68	[7]
					Boroxines						
XLII	C_6H_6	0.058	135.3±0.8	144.7^b	7.0	–	–	3.8	–	3.8	[8]
XLIII	C_6H_6	0.240	271.2±3.4	270.5^b	0.3	–	–	115.9	–	116	[8]
					N-aryl-4-pyridones						
XLIV	C_6H_6	0.289	139.3	152.2	9.3	–	–	–	–	–	[9]
	dioxane	0.139	143.6		6.0						
XLV	C_6H_6	0.233	162.6	155.7	4.2	–	7.01	6103.7	7.0	6101	[9]
	dioxane	0.142	154.8	160.0	3.4		7.19	6857.3	7.1	6471	
XLVI	C_6H_6	0.311	162.2	151.4	6.5	–	7.29	7074.2	7.2	7071	[9]
	dioxane	0.270	146.2	157.9	8.0		7.36	7215.5	7.3	6809	
XLVII	C_6H_6	0.228	163.6	155.7	4.8	–	6.89	7812.7	6.8	7809	[9]
	dioxane	0.120	158.7	160.0	0.7		6.97	8321.3	6.9	7853	
XLVIII	C_6H_6	0.323	159.3	151.4	5.0	–	5.05	4738.2	5.0	4736	[9]
	dioxane	0.248	150.6	157.9	4.8		5.27	5507.8	5.2	5196	
XLIX	C_6H_6	0.406	170.0	157.5	7.4	–	5.26	5143.9	5.2	5142	[9]
	dioxane	0.288	173.4	161.8	6.7		5.69	6502.1	5.7	6137	

[a] β is concentration coefficient, $_\infty V_2$ is molar volume extrapolated to infinite dilution, V_{add} is additive molar volume, μ is dipole moment, $_\infty(_mK_2)$ is Kerr constant. [b] Molar volumes $_\infty V_2$ of model compounds, 1,3,5-trimethylbenzene and 1,3,5-triphennylbenzene are given.

magnitude of the molar volume per one methylene group was calculated from the difference between the molar volumes of the nearest pairs of homologous compounds as the difference between the magnitude for the subsequent and the previous compound in the reaction series.

Orthoformic esters. The magnitudes of $\Delta V(CH_2)$ of the compounds in solutions are as follows: **I** and **II**, 19.0 cm^3 mol^{-1}; **II** and **III**, 15.9 cm^3 mol^{-1}; **III** and **IV**, 16.6 cm^3 mol^{-1}. The average value of $\Delta V(CH_2)$ amounted to 17.2 cm^3 mol^{-1}. For the individual liquid compounds: **I**, 109.6 cm^3 mol^{-1} and **II**, 166.4 cm^3 mol^{-1}

[10], $\Delta V(CH_2) = 18.9$ cm^3 mol^{-1}, which is very close to the value for the same pair in solution.

Trialkyl phosphates. The magnitudes of $\Delta V(CH_2)$ of the compounds in solutions are as follows: **V** and **VI**, 18.8 cm^3 mol^{-1}; **VI** and **VII**, 16.6 cm^3 mol^{-1}; **VII** and **IX**, 17.2 cm^3 mol^{-1}. The average value of $\Delta V(CH_2)$ is 17.6 cm^3 mol^{-1}. For the individual liquids: **V**, 115.4 cm^3 mol^{-1}, and **VI**, 170.4 cm^3 mol^{-1} [10], $\Delta V(CH_2) = 18.3$ cm^3 mol^{-1}. For a pair of compounds in solution with a substituent of normal and *iso*-structure, **VI** and **VIII**, $\Delta V(CH_2) = 18.9$ cm^3 mol^{-1}.

Trialkyl phosphites. In solutions, for the compounds **XI** and **XII** $\Delta V(CH_2) = 18.6$ cm^3 mol^{-1}; **XII** and **XIV**, 16.6 cm^3 mol^{-1}. The average value of $\Delta V(CH_2)$ is 17.6 cm^3 mol^{-1}. The individual liquids: **XI**, 118.0 cm^3 mol^{-1}, and **XII**, 172.6 cm^3 mol^{-1} [10], $\Delta V(CH_2) = 18.2$ cm^3 mol^{-1}. For a pair of compounds in solution with a normal substituent, **XII**, and a substituent with *iso*-structure, **XIII**, $\Delta V(CH_2) = 18.5$ cm^3 mol^{-1}.

It is interesting to note that the increment $\Delta V(CH_2)$ for the CH_2 group nearest to those attached to the ether oxygen in all trialkyl esters is significantly higher than the increments $\Delta V(CH_2)$ for the more distant groups. The increment of this nearest CH_2 group is close to a similar increment for the pairs of compounds containing substituents of normal and *iso*-structures. Obviously, this is due to the presence of the branched structure in the molecule near the CH_2 group, hindering the solvation by the solvent molecules and increasing the magnitude of the molar volume increment. Increments of the more remote methylene groups are close in magnitude to the increment $\Delta V(CH_2)$ for the previously studied trialkylamines [$\Delta V(CH_2) = 16.6$ cm^3 mol^{-1}] and saturated hydrocarbons [$\Delta V(CH_2) = 16.7$ cm^3 mol^{-1}], (Table 2), indicating the conformational similarity of these substituents and the peculiarities of their solvation in solutions.

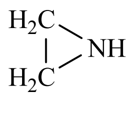
In [2, 3], whose data on the dipole moments and Kerr constants we used to determine the ${}_{\infty}V_2$ values for the orthoformates, trialkyl phosphates, and trialkyl phosphites, it was concluded that none of the possible fixed conformations of alkyl substituents in the molecules was preferable, and these conformations transformed into each other due to rotation around the ordinary C–C, C–O, and P–O bonds. On the average, for their molecular conformations a simple model is valid with approximate symmetry about the axis passing through the carbon or phosphorus atom in the groups O_3CH, O_3PO, and O_3P. Here is a complete analogy with the molecular conformations of trialkylamines that we have considered previously by the method of molar volumes [1].

It is interesting to compare the molar volumes of trimethyl phosphate (**V**) and trimethylphosphite (**XI**): 115.0 and 118.0 cm^3 mol^{-1}, respectively (Table 1). The coordination P=O bond contributes to a decrease rather than increase in the molar volume, due to compression of the molecule **XI** by the coordination bond in the compound **V**. We have observed such a decrease earlier for aromatic derivatives of phosphine oxide and phosphine (${}_{\infty}V_2$, cm^3 mol^{-1}): 226.2, [$(C_6H_5)_3PO$]; 229.6, [$(C_6H_5)_3P$]; 271.1, [$(4\text{-}CH_3C_6H_4)_3PO$]; 291.8, [$(4\text{-}CH_3C_6H_4)_3P$] [13].

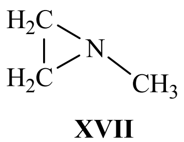
However, for triphenyl phosphate (**X**) and triphenyl phosphite (**XV**) the opposite pattern was observed: ${}_{\infty}V_2$ = 261.0 and 258.9 cm^3 mol^{-1}, respectively. Despite the presence of coordination P=O bond in the molecule **X**, the molar volume of compound is not reduced due to the compression at the coordination of the phosphorus lone pair (LP), but slightly increases as compared to the molar volume of compound **XV**. If this is not an experimental error, the only explanation is the electrostatic attraction of *ortho*-hydrogen atoms of the phenyl rings in the molecule **X** to the phosphoryl oxygen, which leads to the formation of a some kind of six-membered ring, which impedes the access of solvent molecules at the solvation, and thus increases the molar volume of compound **X** compared with compound **XV**. Note that according to the conclusions in [3] based on the data on dipole moments and Kerr constants used by us for determining the molar volumes of compounds **X** and **XV**, the location of the phenyl rings of the molecules toward the P=O bond or LP of phosphorus and in the opposite direction is equally probable. This confirms the possibility of formation of intramolecular six-membered ring, as described above.

Substituted Aziridine and Cyclopropane

We have studied the molar volumes at infinite dilution of substituted aziridines **XVI–XIX** and cyclopropanes **XX–XXXV** in benzene, cyclohexane and carbon tetrachloride. The experimental data are listed in the Table 1.



XVI

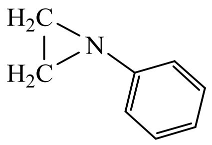


XVII

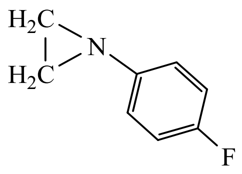
Table 2. Increments of bond (ΔV) and group (**V**) molar volumes of the studied compounds

Bond or group	ΔV, $cm^3\ mol^{-1}$	V, $cm^3\ mol^{-1}$	Compound	Reference
CH_2	17.2^a	–	Orthoformic esters in solutions in C_6H_6 and CCl_4	–
	17.6^a	–	Trialkylphosphates in solutions in C_6H_6 and CCl_4	–
	17.6^a	–	Trialkylphosphшtes in solutions in C_6H_6 and CCl_4	–
	16.6^a	–	Trialkylphosphites in solutions in C_6H_6 and CCl_4	[1]
	16.7^a	–	Acyclic saturated hydrocarbons in solutions in CCl_4	[1]
	25.1	–	Cyclopropane from phenylcyclopropane as individual liquid	–
	17.7	–	Cyclohexane in solutions in CCl_4	–
C–H	13.0	–	Saturated hydrocarbons, methane in solutions in CCl_4	[11]
	12.3^b	–	Aromatic compounds in solutions in CCl_4	[12]
C–C	–11.0	–	Saturated hydrocarbons, ethane in solutions in CCl_4	[12]
	–16.6	–	Cyclohexane in solutions in CCl_4	–
N–H	11.6	–	Ammonia in solutions in C_6H_6	[1]
C=O	17.4	–	Acetone in solutions in C_6H_6	–
$N–C_6H_5$	70.2	–	Diphenylamine in solutions in C_6H_6	–
$C–C_6H_5$	64.7	–	Toluene in solutions in C_6H_6	–
$N–CH_3$	30.1	–	Trimethylamine in solutions in C_6H_6	–
C–Cl	24.3	–	Carbon tetrachloride in solutions in C_6H_6	–
C–Br	24.2	–	Carbon tetrachloride in solutions in C_6H_6	–
CH_3	–	16.4	Toluene in solutions in CCl_4	[11]
F	–	6.5	Fluorobenzene in solutions in CCl_4	[11]
Cl	–	12.1	Fluorobenzene in solutions in C_6H_6	[11]
		14.3	in solutions in CCl_4	
Br	–	18.2	Bromobenzene in solutions in CCl_4	[11]

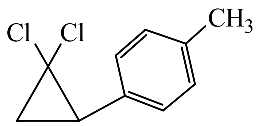
[a] The values averaged over the class. [b] With respect to benzene and naphthalene.



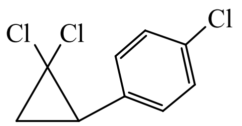
XVIII



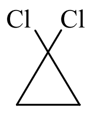
XIX



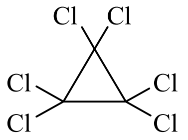
XXV



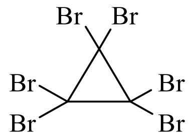
XXVI



XX



XXI



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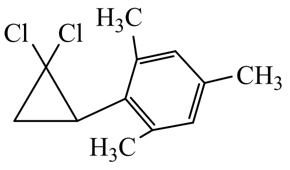
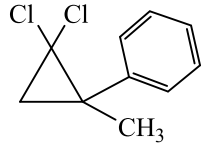
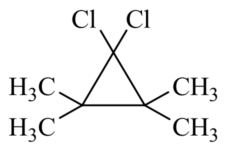


XXVII

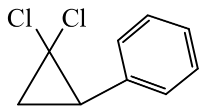


XXVIII

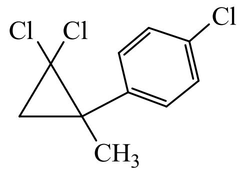
XX **XXI** **XXII**



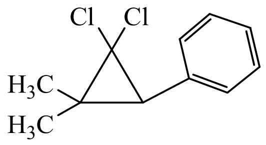
XXIII



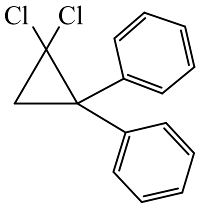
XXIV



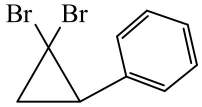
XXIX



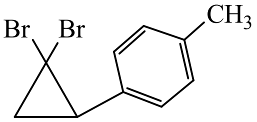
XXX



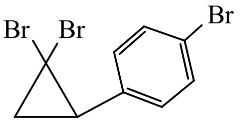
XXXI



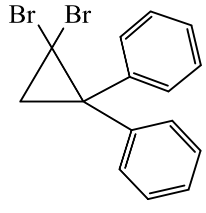
XXXII



XXXIII



XXXIV



XXXV

The comparison of molar volumes of phenylcyclopropane (126.9 $cm^3 mol^{-1}$), styrene oxide (113.5 $cm^3 mol^{-1}$) as individual liquids [10], and *N*-phenylaziridine **XVIII** (123.3 $cm^3 mol^{-1}$) in solution (Table 1) shows that these values are close to each other. The styrene oxide molecule contains by one hydrogen atom less than the molecule of *N*-phenylaziridine. Adding the increment of the molar volume of C–H (13.0 $cm^3 mol^{-1}$, Table 2) to the molar volume of styrene oxide gives a value almost coinciding with the molar volumes of *N*-phenylaziridine and phenylcyclopropane. Hence we can conclude that the molar volumes of cyclopropane, aziridine, and oxirane rings are virtually identical. The increments of molar volumes of lone electron pairs of the heteroatoms nitrogen and oxygen are also approximately equal for these rings, and are close to the molar volume increment of C–H bond.

Calculation of Additive Molar Volumes of Aziridines

***N*-Methylaziridine (XVII)**. The additive molar volume was calculated on the basis of molecular structure by subtracting the molar volume increment of the NH bond, ΔV(NH) from the molar volume of aziridine **XVI** and adding the increment of the N–CH_3 bond, ΔV(N–CH_3). The molar volume increment of the NH bond was calculated from the molar volume of ammonia solution (34.7 $cm^3 mol^{-1}$ [1]) by dividing it by 3, and the molar volume increment of the N–CH_3 bond was calculated from the molar volume of trimethylamine in solution (90.2 $cm^3 mol^{-1}$ [1]) by dividing it by 3 (Table 2).

$$V_{\text{add}}(\mathbf{XVII}) = {}_{\infty}V_2(\mathbf{XVI}) - \Delta V(\text{NH}) + \Delta V(\text{N–CH}_3) = 75.5\ \text{cm}^3\,\text{mol}^{-1}.$$

Here and further, the data required to calculate the increments of bonds and groups are given in Table 2.

***N*-Phenylaziridine (XVIII)**. The additive molar volume was calculated on the basis of its molecular structure by subtracting the molar volume increment of NH bond, ΔV(N–H) from the molar volume of compound **XVI**, and adding the increment of N–C_6H_5 bond, ΔV(N–C_6H_5). The molar volume increment of the NH bond was calculated from the molar volume of ammonia, and the molar volume increment of N–C_6H_5 bond was calculated on the basis of the molar volume of diphenylamine in solution (151.9 $cm^3 mol^{-1}$ [13]): $\Delta V(\text{N–C}_6\text{H}_5) = {}_{\infty}V_2[(\text{diphenylamine}) - \Delta V(\text{N–H})]/2$.

$$V_{\text{add}}(\mathbf{XVIII}) = {}_{\infty}V_2(\mathbf{XVI}) - \Delta V(\text{N–H}) + \Delta V(\text{N–C}_6\text{H}_5) = 115.6\ \text{cm}^3\,\text{mol}^{-1}.$$

***N-p*-fluorophenylaziridine (XIX)**. The additive molar volume of this compound was calculated by adding the group increment of the molar volume of substituent F in the aromatic ring, V(F), to the molar volume of compound **XVIII**.

$$V_{\text{add}}(\mathbf{XIX}) = {}_{\infty}V_2(\mathbf{XVIII}) + V(\text{F}) = 129.8\ \text{cm}^3\,\text{mol}^{-1}.$$

The comparison of the additive values of molar volume with the experimental values (Table 1) shows that the molar volumes of the studied aziridines **XVII**–**XIX** are additive with respect to the bond and group increments of the molar volumes of molecules. Hence, the nature of solvation of the molecules of compounds **XVII**–**XIX** is similar to those which occurs in model compounds, used for the obtaining the necessary increments.

Calculation of Additive Molar Volumes of Cyclopropanes

1,1-Dichlorocyclopropane (XX). Additive calculation was carried out by two methods. First, based on previous findings that the molar volumes of cyclopropane and aziridine rings are approximately the same: $V_{\text{add}}(\mathbf{XX}) = {}_{\infty}V_2(\mathbf{XVI}) - \Delta V(\text{N–H}) + 2\Delta V(\text{C–Cl})$. Here ΔV(C–Cl) is the bond increment of the molar volume of the C–Cl bond obtained by dividing of the molar volume of liquid CCl_4 as an individual liquid by four, $V(CCl_4)$ = 97.1 $cm^3 mol^{-1}$, 25ºC [2]. $V_{\text{add}}(\mathbf{XX})$ =

94.0 $cm^3 mol^{-1}$. Second, proceeding from the molar volume of phenylcyclopropane, according to the scheme considering the structure of molecules: V_{add}(**XX**) = V(phenylcyclopropane) – $\Delta V(C–C_6H_5)$ – ΔV(C–H) + 2ΔV(C–Cl) = 97.7 $cm^3 mol^{-1}$. The $\Delta V(C–C_6H_5)$ magnitude was calculated according to the scheme: $\Delta V(C–C_6H_5)$ = $_\infty V_2$(toluene) – 3ΔV(C–H), where ΔV(C–H) is the bond increment for alkanes. As expected, the results are similar.

The schemes of the additive calculation of other substituted cyclopropanes are given below. They are composed according to the structures of these compounds.

$$V_{add}(\mathbf{XXI}) = {}_\infty V_2(\mathbf{XX}) - 4\,\Delta V(C–H) + 4\,\Delta V(C–Cl) = 137.1\ cm^3\,mol^{-1}.$$

A large divergence of the additive and the experimental values may be due to mutual steric approach of the C–Cl bonds around the three-membered ring, but as will be shown later, this probably is a result of the experimental error in determining the density in [5].

Hexabromocyclopropane (XXII). The additive calculation was carried out in two ways. First, based on previous findings that the molar volumes of cyclopropane and aziridine rings are approximately the same: V_{add}(**XXII**) = $_\infty V_2$(**XVI**) – ΔV(N–H) – 4ΔV(C–H) + 6ΔV(C–Br) = 138.9 $cm^3 mol^{-1}$. Here ΔV(C–Br) is the bond increment of the molar volume of the C–Br bond, obtained by dividing the molar volume of CBr_4 as an individual fluid by four {$V(CBr_4)$ = 97.0 $cm^3 mol^{-1}$, 20ºC [14]}). Second, we proceeded from the molar volume of phenylcyclopropane, in accordance with the structure of molecules: V_{add}(**XXII**) = $_\infty V_2$(phenylcyclopropane) – $\Delta V(C–C_6H_5)$ – 5 ΔV(C–H) + 6ΔV(C–Br) = 142.6 $cm^3 mol^{-1}$. Like above, the results obtained are similar.

$$V_{add}(\mathbf{XXIII}) = {}_\infty V_2(\mathbf{XX}) - 4\Delta V(C–H) + 4\Delta V(C–C) + 12\Delta V(C–H) = 152.0\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXIV}) = {}_\infty V_2(\text{phenylcyclopropane}) - 2\Delta V(C–H) + 2\Delta V(C–Cl) = 149.4\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXV}) = {}_\infty V_2(\mathbf{XXIV}) + V(CH_3) = 168.1\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXVI})\text{ in }CCl_4 = {}_\infty V_2(\mathbf{XXIV}) + V(Cl) = 166.0\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXVI})\text{ in }C_6H_6 = {}_\infty V_2(\mathbf{XXIV}) + V(Cl) = 164.4\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXVII}) = {}_\infty V_2(\mathbf{XXV}) + 2V(CH_3) = 204.3\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXVIII})\text{ in }CCl_4 = {}_\infty V_2(\mathbf{XXIV}) - \Delta V(C–N) + \Delta V(C–N) + 3\,\Delta V(C–H) = 166.7\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXVIII})\text{ in }C_6H_6 = {}_\infty V_2(\mathbf{XXIV}) - \Delta V(C–H) + \Delta V(C–C) + 3\,\Delta V(C–H) = 167.3\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXIX}) = {}_\infty V_2(\mathbf{XXVIII}) + V(Cl) = 182.6\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXX}) = {}_\infty V_2(\mathbf{XXIV}) - 2\,\Delta V(C–H) + 2\,\Delta V(C–C) + 6\,\Delta V(C–H) = 192.7\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXXI}) = {}_\infty V_2(\mathbf{XXIV}) - \Delta V(C–H) + \Delta V(C–C_6H_5) = 214.4\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXXII}) = \mathbf{V}(\text{phenylcyclopropane}) - 2\Delta V(C–H) + 2\Delta V(C–Br) = 149.4\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXXIII}) = {}_\infty V_2(\mathbf{XXXII}) + V(CH_3) = 171.2\ cm^3\,mol^{-1};$$

$$V_{add}(\mathbf{XXXIV}) = {}_\infty V_2(\mathbf{XXXII}) + {}_\infty V\,(Br) = 173.0\ cm^3\,mol^{-1};$$

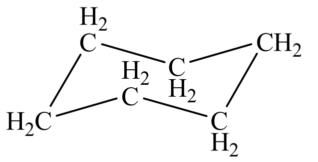
$$V_{add}(\mathbf{XXXV}) = {}_\infty V_2(\mathbf{XXXII}) - \Delta V(C–H) + \Delta V(C–C_6H_5) = 206.5\ cm^3\,mol^{-1}.$$

Additive analysis of the examined cyclopropanes showed that the additivity of molar volumes of bond and group increments of substituents generally is well satisfied for them (Table 1). Hence, the nature of solvation of the molecules of compounds **XX**–**XXXV** is similar to that in the model compounds taken for obtaining the necessary increments (Table 2). It seems somewhat surprising that a large discrepancy was observed between the values for hexachlorocyclopropane **XXI**. If this discrepancy is valid, then similar difference should be observed for compounds **XXII** and **XXIII** where the steric hindrance between substituents is no less than that in the molecule **XXI**, but for these compounds the difference between the experimental and calculated values is quite reasonable. Therefore, we suggest that the discrepancy between the additive and the experimental values of **XXI** is due to errors in determining density of solutions in [5], whose data we used.

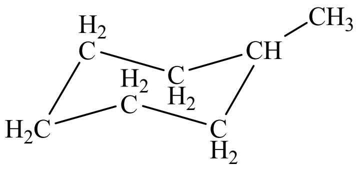
Note that, according to the Kerr effect and dipole moments [4–6], the molecular conformations of phenylaziridine and arylcyclopropane molecules differ by the orientation of the aromatic ring with respect to the three-membered ring, but this does not affect the magnitude of their molar volumes. In *N*-phenylaziridine (**XVIII**) and *N*-*p*-fluorophenylaziridine (**XIX**) the aromatic ring is roughly perpendicular to the aziridine ring bisector plane passing through the nitrogen atom and the midpoint of the C–C three-membered ring. This creates the best conditions for conjugation of the nitrogen LP with the π-system of the aromatic ring. In the case of arylcyclopropanes, the plane of aromatic ring is turned relative to the plane of the C_{ar}–C–CH_3 or C_{ar}–C–H bond at the angle about 60º to the direction of eclipsing one C–C bond of the cyclopropane ring. The turn is caused by the bulky substituent CH_3 when it is adjacent to the aryl ring. In the compounds **XXXI** and **XXXV** both the phenyl rings of the molecules are turned conrotatory from the C_{ar}–C–C_{ar} plane at the angle 70º, which agrees with the data of X-ray analysis, whereby this angle is 80º [6].

Cyclohexanes, Decalines, and Cyclooctane

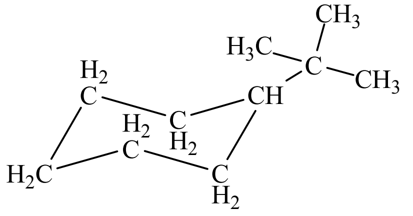
We studied the molar volumes of cyclohexane, cyclooctane,and decalin series **XXXVI–XLI** at infinite dilution in carbon tetrachloroide. The experimental data are listed in Table 1.



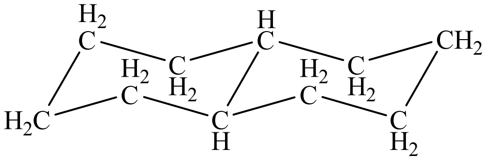
XXXVI



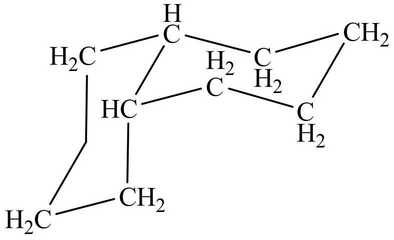
XXXVII



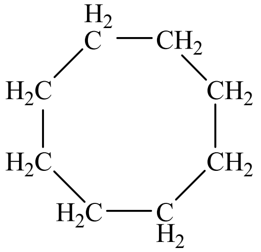
XXXVIII



XXXIX



XL



XLI

Let us estimate the molar volume of cyclohexane **XXXVI** from the increment of the molar volume of methylene difference for saturated hydrocarbons with an open chain, $\Delta V(CH_2)$ = 16.7 cm^3 mol^{-1}, Table 2): V_{add}(**XXXVI**) = $6\Delta V(CH_2)$ = 100.2 cm^3 mol^{-1} . There is a good match of the additively calculated and the experimental values (Table 1). However, as expected, the experimental value is higher, although slightly, than the additive one, because at the solvation of the cyclic molecule the access of solvent molecules inside the ring is hindered compared with open-chain hydrocarbons.

Methylcyclohexane (XXXVII): V_{add}(**XXXVII**) = ${}_\infty V_2(C_6H_{12})$ – ΔV(C–H) + ΔV(C–C) + $3\Delta V$(C–H) = 121.3 cm^3 mol^{-1}.

tert**-Butylcyclohexane (XXXVIII)**: V_{add}(**XXXVIII**) = ${}_\infty V_2(C_6H_{12})$ – ΔV(C–H) + 4 ΔV(C–C) + $9\Delta V$(C–H) = 166.3 cm^3 mol^{-1}.

As seen from Table 1, the consistence of the experimental and calculated additive molar volumes of compounds **XXXVII** and **XXXVIII** is quite acceptable.

Decalin isomers XXXIX and XL. The decalin structure can formally be represented as two cyclohexane structures, which implies additive scheme of calculation: V_{add}(**XXXIX**, **XL**) = 2 ${}_\infty V_2$(**XXXVI**) – $6\Delta V$(C–H) – ΔV(C–C) = 145.7 cm^3 mol^{-1}, that matches well enough the experimental value (Table 1). Additive calculations of these compounds can be further refined, if we define the increment of the molar volume of C–C bond ΔV(C–C) directly from cyclohexane proceeding from the obvious equality: ΔV(C–C) = [${}_\infty V_2(C_6H_{12})$ – $12\Delta V$(C–H)]/6 = –16.6 cm^3 mol^{-1}. Hence, we have V_{add}(**XXXIX**, **XL**) = 151.3 cm^3 mol^{-1}. This result is somewhat better than the preceding (Table 1). As expected, such an approximate calculation still is markedly deviated from the experiment, therewith the experimental values of molar volumes are larger than additive ones, since the presence of a C–C bond common for two rings hinders access of solvent molecules at the solvation and creates an additional molar volume compared to monocyclic molecule. It is not clear why the experimental value of molar volume of the *cis*-decalin is smaller than that of the *trans*-decalin, both in solution and as individual liquids (154.0 and 159.0 $cm^3\,mol^{-1}$ for *cis*- and *trans*-decalin, respectively [10]), although it seems that solvation and self-solvation of the *cis*-structure should be somewhat difficult as compared with the *trans*-structure.

Cyclooctane (XLI). Let us calculate the molar volume of **XLI** like in the case of cyclohexane (**XXXVI**): V_{add}(**XLI**) = 8 $\Delta V(CH_2)$ = 133.6 $cm^3\,mol^{-1}$. A good coincidence of the additive value of the molar volume from the methylene difference increment for the open-chain hydrocarbons (Table 1) indicates that the cyclooctane ring is solvated with solvent molecules like the open chain of a saturated hydrocarbon.

According to the data on the Kerr effect and dipole moment [7], cyclohexane **XXXVI**, methylcyclohexane **XXXVII**, and *tert*-butylcyclohexane **XXXVIII** exist in solution as *chair* conformers, with methyl and *tert*-butyl groups in the compounds **XXXVII** and **XXXVIII** located in the equatorial positions of the cyclohexane ring. The preferred conformations for molecules of decalins **XXXIX**, **XL** and cyclooctane **XLI** in the solutions were not established in [7].

Finally, we compare the values of methylene differences for different hydrocarbons.

We estimate the increment of the molar volume of methylene group $\Delta V(CH_2)$ in cyclopropanes. Based on the calculation of the molar volume of cyclopropane: $\Delta V(CH_2)$ = [V(phenylcyclopropane) – $\Delta V(C–C_6H_5)$ + ΔV(C–H)]/3 = 25.1 $cm^3\,mol^{-1}$.

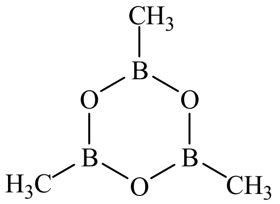
The volume of methylene group in cyclohexane $\Delta V(CH_2) = {}_{\infty}V_2$(cyclohexane)/6 = 17.7 $cm^3\,mol^{-1}$.

For the open chain saturated hydrocarbons $\Delta V(CH_2)$ = 16.7 $cm^3\,mol^{-1}$ (Table 2).

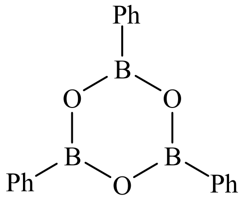
As seen, with increase in the length of hydrocarbon chain the difficulties of its solvation decrease, and the increment of the methylene difference $\Delta V(CH_2)$ falls.

Trimethyl- and Triphenylboroxines

We studied the molar volumes ${}_{\infty}V_2$ at infinite dilution in benzene of trimethyl- and triphenylboroxines **XLII**, **XLIII**. The experimental data are listed in Table 1.



XLII



XLIII

The geometry of boroxine and benzene rings are similar [15], so the most suitable model compound for **XLII** is mesitylene, and for **XLIII,** 1,3,5-triphenylbenzene. We determined the molar amount of mesitylene at infinite dilution in cyclohexane from the data of [16]: β = 0.0681, ${}_{\infty}V_2$ = 144.7 $cm^3\,mol^{-1}$. The molar volume of 1,3,5-triphenylbenzene at infinite dilution in carbon tetrachloroide is 270.5 ± 4.5 $cm^3\,mol^{-1}$ [12].

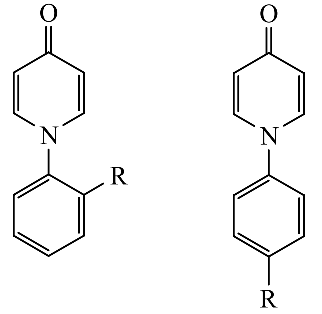
By comparing the molar volumes of 1,3,5-trimethylbenzene with that of trimethylboroxine **XLII**, and triphenylbenzene with triphenylboroxine **XLIII**, Table 1, we can see their similarity. We suggest that at the comparison with the model compounds of a completely different class matching of the molar volumes is quite satisfactorily. From this comparison follows that the solvation and the spatial structure of substituted boroxines **XLII** and **XLIII**, and of the respective substituted benzene derivatives in solutions are also close. The phenyl rings in triphenylboroxine apparently are also turned conrotatory, like in 1,3,5-triphenylbenzene [12]. According to [8], the location of the phenyl rings in triphenylboroxine is close to coplanar with the boroxine ring, the rotation angle of the phenyls to the boroxine ring plane is approximately equal to 17°.

A discrepancy between the values of molar volumes of boroxines **XLII** and **XLIII** and related model can be commented as follows. The boroxine ring is somewhat less than the benzene ring [15], moreover, instead of C–H bonds in the benzene ring, in boroxine there are LP on the oxygen atoms. It is obvious that the latter have a smaller molar volume than the molar volume increment of C–H bond. Therefore, the molar volume of the molecule **XLII** is somewhat less than the molar volume of the mesitylene molecule. In the case of **XLIII** the decrease in the molar volume of this molecule in comparison with symmetric triphenylbenzene is not so large. Most likely, this is due to the planarization of the phenyl rings with respect to boroxine ring compared with model compounds, due to electrostatic attraction of *ortho*-hydrogen atoms of the phenyl rings in **XLIII** to oxygen atoms of the boroxine ring. Hence, an additional molar volume appears which is inaccessible for the solvent molecules

N-Aryl-4-pyridones

We studied the molar volumes of *N*-aryl-4-pyridones **XLIV**–**XLIX** at infinite dilution in dioxane and benzene. The experimental data are listed in Table 1.

First, we performed estimative conformational analysis of unsubstituted compound **XLIV**, based on the molar volume of biphenyl in carbon tetrachloride solutions (147.1 cm^3 mol^{-1}) [12] and the increment of the C=O molar volume, which was calculated from the molar volume of acetone in benzene solution (73.4 cm^3 mol^{-1}) [17] by the scheme: $\Delta V(C{=}O) = V(CH_3COCH_3) - 6\Delta V(C{-}H) - 2\Delta V(C{-}C) = 17.4$ cm^3 mol^{-1}. Hence, $V_{add}(\mathbf{XLIV}) = {}_\infty V_2(\text{biphenyl}) - \Delta V(C{-}H) + \Delta V(C{=}O) = 152.2$ cm^3 mol^{-1}. In this case, the increment ΔV(C–H) refers to benzene derivatives, Table 2. In this calculation we assumed that the molar volume of the quinoid ring is approximately equal to the molar volume of benzene, and the increment of the molar volume of the N–C bridge bond is approximately equal to the increment of molar volume of the C–C bridge bond in biphenyl [12]. An acceptable agreement between the experimental and calculated values for this molecule (Table 1) leads to the conclusion that the conformation of the *N*-phenyl-4-pyridone (**XLIV**) and biphenyl in solutions are similar. The biphenyl rings are acoplanar, and turned relative to each other at the angle of 44° [12]. Acoplanarity of the rings contributes to their solvation. For this reason the additively calculated volume of **XLIV** is relatively close to the value found experimentally. Additive calculation of molar volumes of the other compounds, **XLV**–**XLIX**, was carried out by adding to the molar volume of the unsubstituted molecule **XLIV** the group increments of molar volumes of the substituents (Table 2). The results are shown in Table 1. There is acceptable, for the additive scheme, agreement between calculated and experimental values, especially for dioxane as solvent in which the solubility of these compounds is higher and the density of solutions of compounds, as a function of their concentrations, can be determined more accurately (Table 1). A general conclusion is that the conformations of compounds **XLIV**–**XLIX** in solutions are approximately the same and are similar to the conformation of biphenyl and its derivatives in solutions [12]. Note that in [9], whose data were taken for the determining the molar volumes of compounds **XLIV**–**XLIX**, the mutual orientation of the rings in the molecules has not been established, since the calculated Kerr constants are not very sensitive to the angle of the rings relative to each other. At the same time, the data obtained by the method of molar volumes testify in favor of the acoplanar arrangement of rings in the molecules **XLIV**–**XLIX**.



R = H (**XLIV**); CH_3 (**XLV, XLVII**); Cl (**XLVI, XLVIII**); Br (**XLIX**).

Next, we have demonstrated a possibility of significant simplification of methods for determining the dipole moments and Kerr constants of the compounds, for which can be used the additive scheme of calculation of molar volumes. We calculated the dipole moments μ and Kerr constants ${}_\infty({}_mK_2)$ of the studied compounds by the simplified procedure proposed in [11] using the additive calculated values and the transformed Fujita (1) and LeFevre (2) formulas for polarization and molar Kerr constant, respectively:

$$ {}_\infty P_2 = \frac{\varepsilon_1 - 1}{\varepsilon_1 + 2}\,{}_\infty V_2 + \frac{3\alpha\varepsilon_1 M_2}{(\varepsilon_1 + 2)^2 M_1}\,V_1, \tag{1}$$

$$ {}_\infty({}_mK_2) = {}_sK_1\rho_1{}_\infty V_2 + (\gamma + \delta - H\gamma - J\alpha\varepsilon_1){}_sK_1\rho_1(M_2/M_1)V_1. \tag{2}$$

These formulas are equivalent to those well-known in the literature used to determine the dipole moments and Kerr constants [11]. Here V_1 is the molar volume of solvent. In [11] a detailed interpretation of these formulas is given. In the formula (1) and (2) instead of ${}_\infty V_2$ the value of V_{add} from Table 1 is used. The results of determining the values of μ and ${}_\infty({}_mK_2)$ of the studied compounds in comparison with previously published experimental data is given in Table 1. The calculation of the V_{add} values in some cases was specifically simplified compared with the described above at the additive analysis of molar volumes $_\infty V_2$ of the studied compounds. The approximate calculation of V_{add} for the compounds **II**–**IV** was carried out along the scheme: $V_{add} = {}_\infty V_2(\mathbf{I}) + n\Delta V(CH_2)$, where $\Delta V(CH_2)$ is the average increment of the CH_2 groups for individual alkanes as liquids, equal to 16.0 cm^3 mol^{-1} [1], n is the total number of such groups in the molecule. An approximate calculation for the compounds **VI**–**IX** was carried out along the scheme: $V_{add} = {}_\infty V_2(\mathbf{V}) + n\Delta V(CH_2)$, designations are the same. An approximate calculation for the compounds **XII**–**XIV** was carried out along the scheme: $V_{add} = {}_\infty V_2(\mathbf{XI}) + n\Delta V(CH_2)$, designations are the same. The calculation for compounds **XVII**–**XIX** coincides with the above formulas given in the text. The calculation for substituted cyclopropanes was carried out proceeding from the data for phenylcyclopropane as an individual fluid by adding and subtracting the respective increments of the bond and group molar volumes (Table 2). The calculation of V_{add} for a number of cyclohexanes, decalins, and cyclooctanes **XXXVI**–**XLI**, and for substituted boroxines **XLII**–**XLII** and *N*-aryl-4-pyridones **XLV**–**XLIX** corresponds to the calculations given above in the text.

In some cases the "simplified" and other calculations of the V_{add} values show that the calculated values of dipole moments and Kerr constants are close to the published [2–9] that have been obtained by the full and throughout determination of these quantities in solution. In the calculations we used the values of concentration coefficients α, γ, and δ from the cited publications, and used them for determining the values of $_\infty V_2$ of the compounds considered in this work. As seen from Table 1, the dipole moments and Kerr constants found in such a simplified manner in most cases coincide with those known from the literature.

We conclude therefore that in most cases the methods of determination of μ and $_\infty(_mK_2)$ can be significantly simplified, by rejecting the determination of the solution density; instead may be calculated the additive molar volumes of molecules of compounds under study and may be used the modified Le Febvre and Fujita formulas. Such a simplification is the more accurate the closer the V_{add} and $_\infty V_2$ values.

EXPERIMENTAL

Experimental dependences of a solution densitiy on its concentration for the determination of molar volume at infinite dilution $_\infty V_2$ were taken from [2–9]. We selected the systems containing at least five concentrations and the corresponding densities and other properties of solutions. The linear dependences $\rho_{12} = \rho_1(1+\beta\omega)$ were treated by the method of least squares for finding values of β, correlation coefficients were no less than 0.99. When the dependence of solution density on the concentration for a given compound was not published, we used published value of β. The calculation of the experimental values of molar volumes of solutes $_\infty V_2$ we carried out by extrapolation formula (3) derived by us earlier [11].

$$_\infty V_2 = [M_2(1 - \beta)]/\rho_1. \tag{3}$$

At the calculating the dipole moments and Kerr constants from the additive molar volumes V_{add}, the necessary data on the quantities of α, β, and δ were taken from the same cited papers.

At finding experimental values of molar volumes of compounds we used the following values of the properties of solvents. Carbon tetrachloroide: ρ_1 = 1.5845 g cm^{-3}, ε_1 = 2.2270 at 25ºC [18]. Dioxane: ρ_1 = 1.02687 g cm^{-3}, ε_1 = 2.209 at 25ºC [18]. Benzene: ρ_1 = 0.87378 g cm^{-3}, ε_1 = 2.2725 at 25ºC [19]. Cyclohexane: ρ_1 = 0.77389 g cm^{-3}, ε_1 = 2.0199 at 25ºC [6]. The other properties of solvents needed to calculate the Kerr constants are given in [18].

Dipole moments of compounds are expressed in Debye (D), the Kerr constant in CGSE units (esu). Conversion factors from units CGSE to SI units are as follows: 1 C m = 0.2998×10^{30} D, 1 m^5 B^{-2} mol^{-1} = 0.8988×10^{15} esu mol^{-1}.

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