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Molecular Polarizability of Organic Compounds and Their Complexes: XLIX.[1] Molar Volumes of Polyaryl Systems in Solutions, Extrapolated to Infinite Dilution, Their Additivity, and Steric Structure of the Molecules

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Abstract—Molar volumes of a number of polyaryls and of several model systems at infinite dilution in carbon tetrachloride and benzene were determined. The molar volumes of the compounds under study are additive by bonds, groups, and molecular fragments. The dipole moments and Kerr molar constants of the compounds under study can be found by a simplified additive method. As follows from the additive analysis of the molar volumes of diphenyl, *para*-substituted diphenyls, heteroaromatic analogs, and a number of polyaryls, the molecules of these compounds are acoplanar in the solutions, and the degree of their acoplanarity is the same as in diphenyl.

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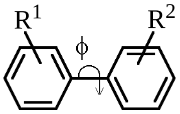
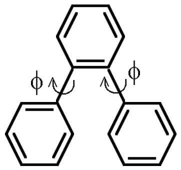
In the previous work [1] we determined the molar volumes ${}_{\infty}V_2$ of a wide series of mono- and polysubstituted benzene compounds with all kinds of substituents at infinite dilution in solutions and demonstrated additivity of these values with respect to molecular fragments and groups. We considered the greatest majority of these conformationally rigid systems mainly with the purpose of creating an additive scheme of group increments of the molar volumes of substituents. We also proposed to substantially modify the procedure for determining dipole moments and Kerr constants of the compounds, by excluding solution densities. We proposed to perform additive calculation of the molar volumes and to use modified formulas for the molar polarizations and Kerr constants.

With the aim to elucidate whether additive analysis of molar volumes give insight into the conformational structure of molecules, we studied in the present work compounds **I**–**XVIII** in which rotation of the aromatic rings around formally single bonds between them is possible.

The resulting molar volumes ${}_{\infty}V_2$ of compounds **I**–**XVIII** and model systems are given in Table 1. The

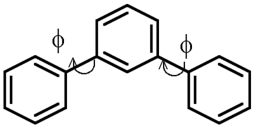


I–VIII

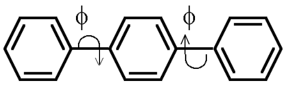


IX,
o-triphenyl

I–VIII, R^1 = H, R^2 = H (**I**), 4-F (**II**), 4-Cl (**III**), 4-Br (**IV**), 4-I (**V**), 4-NO_2 (**VI**); R^1 = 2-NO_2, R^2 = 2'-NO_2 (**VII**); R^1 = 3-NO_2, R^2 = 3'-NO_2 (**VIII**).



X,
m-triphenyl



XI,
p-triphenyl

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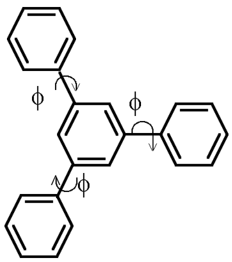
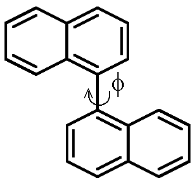
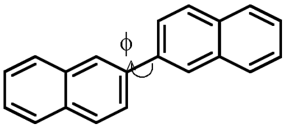
[1] For communication XLVIII, see [1].



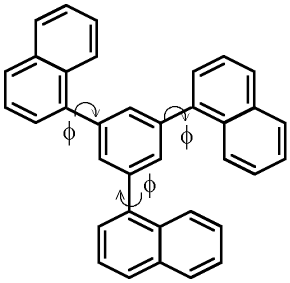
XII,
1,2,5-triphenylbenzene



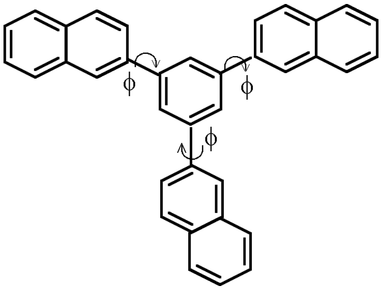
XIII,
1,1'-dinaphthyl



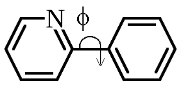
XIV,
1,1'-dinaphthyl



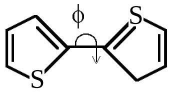
XV,
1,3,5-tri-α-naphthylbenzene



XVI,
1,3,5-tri-β-naphthylbenzene



XVII,
2,2'-dipyridyl



XVIII,
2,2'-dithienyl

experimental values of ${}_{\infty}V_2$ were calculated by extrapolation equation (1) which we derived earlier [1].

$${}_{\infty}V_2 = \frac{M_2(1-\beta)}{\rho_1}. \qquad (1)$$

Here M_2 is the molecular weight of the compound; β, coefficient of the concentration dependence of solution densities; ρ_{12}, $\rho_{12} = \rho_1(1 + \beta\omega)$, and ρ_1, solvent density; and ω, weight fraction of the solute. We also calculated the statistical error of the molar volume ${}_{\infty}V_2$ – $\Delta({}_{\infty}V_2)$ by Eq. (2).

$$\Delta({}_{\infty}V_2) = \frac{M_2\Delta\beta}{\rho_1}. \qquad (2)$$

Here $\Delta\beta$ is the statistical error of β. For other details of determining the molar volumes, see Experimental.

The molar volume of a substance in a liquid, calculated per one molecule, implies the volume of the cavity occupied by this particle in the dynamic structure of the solvent. This volume comprises the intrinsic volume of the particle and the so-called free volume [9]. The intrinsic molar volume of a solute can be considered as its van der Waals volume. It can be calculated if the molecule is considered as a three-dimensional figure constructed from overlapping rigid van der Waals spheres centered on atoms according to the proposed molecular structure [10]. The shape of this figure seems to be completely determined by the molecular structure. The free volume of the cavity is equal to the cavity volume occupied by a particle minus the van der Waals volume of this particle. We suggest that the free volume in the solvent dynamic cavity accommodating the solute molecule is similar in shape to the van der Waals form of the molecule. This is determined by heat motion of solvent molecules about solute molecules, and, finally, by the isotropy of the liquid. Hence, we suggest that the whole cavity occupied by the solute molecule in the dynamic structure of the solvent, too, repeats the shape of the van der Waals figure of the molecule. Naturally, such a cavity shape must be considered as nothing more that the result of averaging over all possible sites of the nearest neighboring solvent molecules with respect to the solute molecule. If the solute molecule undergoes conformational transformations, the shape of its van der Waals figure will change and so will do its volume and also the volume and shape of the molecular cavity. Therefore, we can expect that the molar volumes of solutes extrapolated to infinite dilution can give information about the structure of their molecules in solution.

Previously the concept of the van der Waals molecular volume played a great role in research on crystal structures [10]. Reasoning from the principle of tight packing and from symmetry considerations it was possible to predict the structure of a great number of molecular crystals. The crystal lattices of molecular crystals of organic substances, predicted in such a

Table 1. Molar volumes of polyaryl systems at infinite dilution in solutions, additive molar volumes, and dipole moments and Kerr constants determined from the additive molar volumes at 25°C[a]

Comp. no.	Solvent	β	${}_{\infty}V_2$, cm^3 mol^{-1}	V_{ad},[b] cm^3 mol^{-1}	ε_V, %	Data obtained in this work by a simplified procedure		Experimental data		Reference
						μ, D	${}_{\infty}({}_mK_2) \times 10^{12}$, CGSE units	μ, D	${}_{\infty}({}_mK_2) \times 10^{12}$, CGSE units	
I	CCl_4	–0.512	147.1 ± 1.3	146.7, 149.7	0.3, 1.8	0	40.4	0	40.5	[3]
II	CCl_4	–0.422	154.5 ± 2.1	153.2, 154.8	0.8, 0.2	1.43	242	1.4	242	[3]
III	CCl_4	–0.374	163.6 ± 6.7	161.0, 162.6	1.6, 0.6	1.57	426	1.6	426	[3]
IV	CCl_4	–0.143	168.2 ± 1.9	164.9, 165.9	2.0, 1.4	1.55	456	1.7	456	[3]
V	CCl_4	0.000	176.8	170.5, 173.3	3.6, 2.0	1.2	650	1.5	671	[3]
VI	CCl_4	–0.477	185.7	161.5, 163.1	13.0, 12.2	4.29	3260	4.4	3265	[3]
VII	C_6H_6	0.367	176.9	176.3, 176.5	0.3, 0.2	5.20	–961.0	5.2	–962	[3]
VIII	C_6H_6	0.406	166.0	176.3, 176.5	6.2, 6.3	4.08	–860.0	4.0	–861	[3]
IX	C_6H_6	0.203	210.1 ± 0.7	206.1, 210.6	1.9, 0.2	0	36.4	0	36.6	[4]
X	C_6H_6	0.201	210.5 ± 2.5	206.1, 210.6	2.1, 0.05	0	95.1	0	95.3	[4]
XI	C_6H_6	0.203	210.0 ± 1.4	206.1, 210.6	1.8, 0.3	0	137.0	0	137.1	[4]
XII	CCl_4	–0.399	270.5 ± 4.5	265.5, 271.5	1.8, 0.4	0	126.0	0	125.5	[4]
XIII	C_6H_6	0.235	222.7 ± 4.3	218.3	2.0	0	147.0	0	145.6	[4]
XIV	C_6H_6	0.247	219.3 ± 7.2	218.3	0.4	0	340.0	0	340.5	[4]
XV	C_6H_6	0.276	378.3 ± 4.1	372.9	1.4	0	369.0	0	369.6	[4]
XVI	C_6H_6	0.289	371.5 ± 6.7	372.9	0.4	0	586.0	0	585.4	[4]
XVII	CCl_4	–0.353	133.4 ± 0.4	129.9	2.6	0.60	13.7	0.61	13.8	[5]
XVIII	CCl_4	–0.240	130.1	–	0.5	0.54	23.2	0.54	33 ± 2	[6]
Benzene	CCl_4	–0.772	87.3 ± 1.3	–	–	–	–	–	–	[1]
	c	–	88.8							[2]
Pyridine	CCl_4	–0.582	79.0	–	–	–	–	2.35	150	[7]
Thiophene	CCl_4	–0.487	79.0	–	–	–	–	0.54	11.1	[6]
Naphthalene	CCl_4	–0.522	123.1 ± 1.5	–	–	–	–	–	–	[8]

[a] (β) Concentration coefficient; (${}_{\infty}V_2$) molar volume at infinite dilution; (ε_V) relative deviation of experimental molar volumes ${}_{\infty}V_2$ from additive molar volumes V_{ad}; (μ) dipole moment; and [${}_{\infty}({}_mK_2)$] Kerr constant. [b] The first value in the column was obtained using increments of molar volumes in solutions and the second value, with the same data for straight liquids [2]. [c] Straight liquid.

way, agree with experimental. Consequently, the shape and volume of molecules play an essential role in the formation of crystal structures. There are reasons to believe that in liquids, too, the molar volumes of solutes and the corresponding van der Waals volumes can provide valuable information about the steric structure of the molecules.

The additive molar volume V_{ad} of a compound in which intramolecular rotation of aromatic rings is possible were calculated by simply summing up the group increments to the molar volume, according to the molecular structure [Eq. (3)].

$$V_{ad} = \sum_i V(\text{ring})_i + nV(\text{C–C}) + \sum_j V(\text{R})_j. \qquad (3)$$

Here $V(\text{ring})_i$ is the molar volume of the ith aromatic ring; V(C–C), increment of the of the molar volume of the bridging C–C bond around which rotation occurs; n, number of such bonds; and $V(\text{R})_j$, increment of the molar volume of the jth substituent in the ring.

For V(ring) we used the molar volumes ${}_{\infty}V_2$ of model compounds: benzene, thiophene, pyridine, and naphthalene. The increment of the molar volume of the bridging bond V(C–C) was found from the ${}_{\infty}V_2$ of 2,2'-dithienyl (**XVIII**) and thiophene (Table 1) by simply subtracting two molar volumes of thiophene from the molar volume of 2,2'-dithienyl: $V(\text{C–C}) = 130.1 - 2 \cdot 79.0$ cm^3 mol^{-1}. We selected these model compounds because of an almost free rotation of the thiophene rings in 2,2'-dithienyl both in the gas phase and, apparently, in solutions [11]. The V(C–C) increment obtained in this way is not complicated by any

Table 2. Group increments of molar volumes $V(R)$, $cm^3\ mol^{-1}$

R	By solutions	By straight liquids	Reference
C–C[a]	–27.9	–	[b]
C–C[c]	–27.5	–	[b]
F	6.5	5.1	[1]
Cl	14.3[d]	12.9	[1]
Br	18.2	16.2	[1]
I	23.8	23.6	[1]
NO_2	14.8[e]	13.4	[1]

[a] Determined by the model compound 2,2'-dithienyl. [b] Present work. [c] Determined by diphenyl. [d] Determined in this work with data in [12]. [e] Determined in this work with data in [13].

conformational features of the model. The negative value of our calculated increment is quite acceptable for the additive approach, and its sign is nothing more than evidence for screening of the bridging bond by rotating aromatic rings. Previously we found the $V(R)_j$ increments from data for monosubstituted benzenes in solutions [1]. These values, together with V(C–C), are given in Table 2.

Table 1 compares the additive molar volumes V_{ad} with the experimental molar volumes ${}_\infty V_2$. As seen from Table 1, in the majority of cases the calculated values well fit experimental. The relative deviation of calculation from experiment (ε_V) does not exceed 4%, except for 4-nitrodiphenyl (**VI**) (13%) and 3,3'-dinitrodiphenyl (**VIII**) (6.3%), which is attributable, first of all, to the low solubility of these compounds and to the resulting inaccuracy in their density estimates. In the majority of cases this deviation does not exceed 2%. Such result is quite acceptable for the additive approximation, since the fit of calculated to experimental values compares with the errors in those latter.

The fact that the additive values fit experiment suggests that the aromatic rings in the molecules under study are well solvated with solvent molecules from all sides. However, the same is not true of the bridging bonds linking these rings, since the V(C–C) increment is below zero. This fact alone allows us to conclude that the aromatic rings in the molecules under study are acoplanar. Further evidence for this conclusion can be obtained by analyzing bond rather than group increments of molecular molar volumes. To construct a bond scheme for calculation of the molar volumes of aromatic compounds, one should first find the C–H and aromatic C–C bond increments of the molar volume ΔV(C–H) and ΔV(C–C), respectively. These values can be calculated from ${}_\infty V_2$ for benzene and naphthalene by equations set (4) constructed with account for the number of the mentioned bonds in the molecules.

$$
\begin{aligned}
{}_\infty V_2(\text{benzene}) &= 6\Delta V(\text{C–H}) + 6\Delta V(\text{C–C}),\\
{}_\infty V_2(\text{naphthalene}) &= 8\Delta V(\text{C–H}) + 11\Delta V(\text{C–C}) \qquad (4)
\end{aligned}
$$

Substitution of the ${}_\infty V_2$ values for benzene and naphthalene, taken from Table 1, into Eqs. (4) gives the following values of the required increments: ΔV(C–H) 12.3 and ΔV(C–C) 2.2 $cm^3\ mol^{-1}$. These values are above zero, which points to the fact that solvent molecules solvate both exocyclic C–H and endocyclic C–C bonds in benzene and naphthalene.

Now we can find the bridging C–C increment of the molar volume [ΔV(C–C)]. To this end, we should subtract ${}_\infty V_2$ for two thiophene molecules from ${}_\infty V_2$ for 2,2'dithienyl. But first we should subtract the ΔV(C–H) increments of two excluded bonds from the ${}_\infty V_2$ of thiophene. This results in Eq. (5).

$$\Delta V(\text{C–C}) = V(\text{C–C}) + 2\Delta V(\text{C–H}). \qquad (5)$$

By substituting the above numeral data into Eq. (5) we obtain ΔV(C–C) = –3.3 $cm^3\ mol^{-1}$.

Similar calculation can be also carried out directly with data for diphenyl, using an evident equality: $\Delta V(\text{C–C}) = {}_\infty V_2(\text{diphenyl}) - 2[{}_\infty V_2(\text{benzene}) - \Delta V(\text{C–H})] = -2.9\ cm^3\ mol^{-1}$. As a result, we obtain a negative ΔV(C–C) increment close to –3.3 $cm^3\ mol^{-1}$. The negative values of this increment, notwithstanding the fact that the bridging bond between rings is longer than the ring aromatic C–C bond [11], can be accounted for by acoplanarity of diphenyl aromatic rings in compounds **I**–**VIII**, 2,2'-dithienyl (**XVIII**), and the other aromatic systems **IX**–**XVIII** (Table 1).

The effect of screening of the C–C bond shows itself in the molar volumes of alkyl molecules. According to [9], the molar volumes of CH_4 and C_2H_6 in CCl_4 are 52 and 67 $cm^3\ mol^{-1}$, respectively. Consequently, the ΔV(C–H) increment per one C–H bond is 13 $cm^3\ mol^{-1}$, which comprises 1/4 of the molar volume of CH_4. Then, the ΔV(C–C) increment per one C–C bond in ethane is 67 – 6.13 = –11 $cm^3\ mol^{-1}$. The negative increment, rather large in its absolute value, points to the fact that the single C–C bond in ethane is completely screened by bulky C–H bonds. This fact provides further evidence for the conclusion that diphenyl and its substituted and structural analogs are acoplanar in solutions. Rotating rings in these molecules screen the bridging C–C bond, which explains the negative bridging bond increments of the molar volume. Note that this result was obtained for organic molecules in solutions by the gravimetric method by studying the concentration dependence of solution densities.

In this work we used the experimental data obtained by using the Kerr effect and dipole moment methods (Table 1 and references therein). Note that the conformations of such compounds as diphenyl and its *para*-substituted derivatives in solutions are difficult to study be these methods, because the dipole moments of the molecules are equal to zero or its direction coincides with the axis of intramolecular rotation [14]. A characteristic feature of such systems is that the dipole component of the Kerr constant is independent of the dihedral angle between the aryl ring planes. Therefore, changes in their Kerr constant are contributed exclusively by the anisotropic component that is generally smaller than the dipole component. For these reasons, the molar Kerr constant depends only slightly the angle between the aryl ring planes [14]. As a result, we consider incorrect the conclusion of Chau et al. [3], based on the Kerr constants, that diphenyl and its *para*-substituted derivatives are planar in solutions. The conclusion in the cited work that the arrangement of the rings in 2,2'-dinitrodiphenyl (**VII**) and 3,3'-dinitrodiphenyl (**VIII**) is close to orthogonal seems to be correct.

The Kerr effects of the polyaryls under study give the following estimates for the rotation angles of aromatic rings: *o*-triphenyl (**IX**) +55°C, +55°C; *m*-triphenyl (**X**) +20°C, ±20°C; *p*-triphenyl (**XI**) +20°C, ±20°C; 1,3,5-triphenylbenzene (**XII**) +38°C, +38°C, +38°C; 1,1'-dinaphthyl (**XIII**) +48°C; 2,2'-dinaphthyl (**XIV**) 0°C; 1,3,5-tri-α-naphthylbenzene (**XV**) +26°C, +26°C, +26°C; and 1,3,5-tri-β-naphthylbenzene (**XVI**) +20°C, +20°C, +20°C [4]. Similar data for 2,2'-dipyridyl [5] and 2,2'-dithienyl (**XVIII**) [6] point to the fact that the heteroatoms in these compounds are *trans* relative to each other, and the rotation angles are 10–17°C for 2,2'-dipyridyl and 20–25°C for 2,2'-dithienyl. According to the method of dipole moments only [15], the acoplanarity of 2,2'-dipyridyl is 17–20°C. This conformation is confirmed by the Kerr effect and the molecular polarizability tensors calculated by the field scheme; the angle between the rings is 19°C [14].

The available published data for other physical methods show that the angle between the aromatic planes in diphenyl is sensitive to the aggregative state of the compound. In crystal, diphenyl (**I**) is planar [16]. By the gas-phase electron diffraction data in [17], this angle is 44°C. The monograph [11] gives angles of 42°C and 44°C for diphenyl (**I**) and 4,4'-difluorodiphenyl, respectively. The conformation of 1,3,5-triphenylbenzene (**XII**) in the gas phase is also similar [11]. In solutions, the angle between the rings spans the range 24–47°C, by IR spectroscopy [18], electronic spectroscopy [19], Faraday effect [20], and Rayleigh scattering [19]. Quantum-chemical calculations, too, lead to similar conclusions [19, 21]. Diphenyl derivatives **I**–**VIII**, too, are nonplanar (40–80°C), as evidenced by photoelectron spectroscopy [22], refractometry [23], and dipole moment measurements [24].

In crystal, 2,2'-dipyridyl (**XVII**) has a planar *trans* conformation [25], and the same is true in solutions, according to NMR data [26]. However, Gupta [27], based on IR spectral data, concluded that the pyridine rings in solutions do not lie in one plane. A slightly different angle (65±7°C) was estimated from the Cotton–Mutton effect [28]. Quantum-chemical calculations [29] result in a planar trans structure, except for the CNDO method and its modifications (ϕ 90–125°C) [29, 30].

Our present and published data allows us to conclude that the conformations of the systems under study should be similar to the conformations of diphenyl, and the aryl rotation angle ϕ is no less than 24–47°C. Therefore, our studied molecules with possible intramolecular rotation of aromatic rings are all acoplanar in solutions.

We also calculated Kerr constants $_\infty({}_mK_2)$ for diphenyl, its substituted derivatives, and a series of polyaryls, as well as dipole moments μ for substituted diphenyl and 2,2'-dipyridyl, using the additive V_ad values calculated by the new simplified procedure. Obviously, the dipole moments of centrosymmetrical polyaryl molecules are equal to zero. The Kerr constants and dipole moments were calculated by our modified formulas of Le Fevre (6) and Fouillite (7) for Kerr constant $_\infty({}_mK_2)$ and molar polarization $_\infty P_2$.

$$_\infty({}_mK_2) = {}_sK_1\rho_1{}_\infty V_2 + (\gamma + \delta - \mathrm{H}\gamma - J\alpha\varepsilon_1){}_sK_1\rho_1\frac{M_2}{M_1}V_1, \tag{6}$$

$$_\infty P_2 = \frac{\varepsilon_1 - 1}{\varepsilon_1 + 2}{}_\infty V_2 + \frac{3\alpha\varepsilon_1 M_2}{(\varepsilon_1 + 2)^2 M_1}V_1. \tag{7}$$

Here V_1 is the molar volume of the solvent. Detailed decoding of these formulas is given in [1]. We substituted V_ad for $_\infty V_2$ in these formulas. We used our refined data for the concentration coefficients β of solution densities from the works cited in Table 1. The α, γ, and δ concentration coefficients of other solution properties and for the molar refractions of the compounds were taken from these works. When calculating the dipole moment, we accepted, as did the authors of these works, the deformation polarization to be by a factor of 1.05 greater than the molar refraction. The calculation results are given in Table 1, where they are compared with the cited experimental data.

As seen from Table 1, our calculated Kerr constants and dipole moments very well fit the published values. In essence, this is complete coincidence, taking into consideration the usual statistical errors in dipole moments and Kerr constants (1–3%), which were not published at that time. Therefore, dipole moments and Kerr constants in solutions can now be determined by substantially simplified procedure, at least for those classes of compounds, for which an additive scheme for calculation of molar volumes is available.

EXPERIMENTAL

The experimental concentration dependences of solution densities for the compounds under study, necessary for calculation of molar volumes at infinite dilution $_\infty V_2$, were taken from [3–8, 12, 13]. Systems containing no less than five concentrations and their corresponding densities and other solution properties were chosen. The β values were found by least-squares treatment of the linear dependences of solution densities $\rho_{12} = \rho_1(1 + \beta\omega)$ (ρ_1 is the solvent density and ω, weight fraction of the solute). The resulting correlation coefficients were no less than 0.99.

Analysis the concentration dependences of solution densities for 4-iododiphenyl [3] led us to conclude that the solution densities almost coincide with the density of the straight solvent at sufficiently low concentrations. This allowed us to accept β as zero. Unfortunately, in the cited works experimental concentration dependences of solution densities are given not for all compounds. For 4-nitrodiphenyl (**VI**) [3], 2,2'-dinitrodiphenyl (**VII**), 2,2'-dithienyl (**XVIII**) [6], pyridine [7], and thiophene [6] we used published β values. For 3,3'-dinitrodiphenyl (**VIII**) we also give the published β value of 0.406 [3]. The concentration dependences of solution densities for this compound, published in [3], were difficult to refine by statistical treatment.

The experimental molar volumes we determined with the following parameters of solvents as individual liquids: carbon tetrachloride: ρ_1 1.5845 g cm^{-3}, ε_1 2.2270, and n_1 1.4575 at 25°C [3]; and benzene: ρ_1 0.8738 g cm^{-3}, ε_1 2.2725, and n_1 1.4976 at 25°C [3].

The dipole moments were measured in Debyes (D) and Kerr constants, in CGSE units. The coefficients of transforming CGSE units into SI units are the following: 1 Cm = 0.2998×10^{30} D, 1 m^5 V^{-2} mol^{-1} = 0.8988×10^{15} CGSE units mol^{-1}.

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