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SPECTRAL STUDY OF (4'-PHENYL)-1,2,4-TRIAZOL-1-IUM-PHENACYLID (PTPhY) IN TERNARY SOLUTIONS

The molecule of (4'-phenyl)-1,2,4-triazol-1-ium-phenacylid (PTPhY) is studied in two types of ternary solutions. In the first category, the binary solvent contains two hydroxyl miscible liquids, and the second one contains one protic and one non-protic solvents. The potential energy in pairs of the type hydroxyl solvent-ylid is estimated in the frame of the statistical cell model of ternary solutions. From the viewpoint of interactions in the first ylid solvation shell, the statistical average weight of the active solvent differs from its molar fraction in the binary solvent.

Keywords: (4'-phenyl)-1,2,4-triazol-1-ium-phenacylid (PTPhY), electronic absorption spectrum, potential energy in molecular pairs.

1. Introduction

As a spectrally active molecule, we take (4'-phenyl)-1,2,4-triazol-1-ium-phenacylid (PTPhY) belonging to the N-ylid class. N-ylids are substances with zwitterionic character having multiple applications in organic chemistry such as acid-basic indicators, precursors for new heterocyclic substances or as substances modifying the liquid conductivity.

Large pioneering studies regarding N-ylids, especially cycloimmonium-ylids, were made by the team, whose leaders are I. Zugravescu and M. Petrovanu,

Professors at Organic Chemistry Department of Alexandru Ioan Cuza University of Iasi.

Cycloimmonium ylids are N-Ylids with a heterocycle (pyridinium, benzo-[f]-quinolinium, pyridazinium, iso-quinolinium, triazolium, and so on) as a cation and various substituted carbanions. The ylid carbanion can be mono- or bi-substituted. Being little stable, the carbanion monosubstituted cycloimmonium ylids are used in obtaining new compounds, especially by dimerization reactions or by the salt method [1].

Cycloimmonium ylids are spectrally active substances with UV and Vis electronic absorption bands attributed to $\pi \rightarrow \pi^*$ and $n \rightarrow \pi^*$ transitions, respectively [1, 2].

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The visible band of the $n \rightarrow \pi^*$ type appears by the intramolecular charge transfer (ICT) from the ylid carbanion toward the heterocycle. This band is very sensitive to the solvent nature and to the chemical structure of the ylid carbanion. The spectral shifts of the visible ICT band offer information about the strength of intermolecular interactions in cycloimmium ylid solutions [2–4].

In ternary solutions, the position of this band is an indicator both of the solution non-homogeneity and the intermolecular interaction strength, when the binary solvent composition is varied [5, 6].

Our purpose is to evaluate the strength of the specific interactions between the studied ylid and hydroxyl solvents used to achieve the ternary solutions and to characterize the composition of the ylid first solvation shell. As a spectrally active molecule, we consider (4'-Phenyl)-1,2,4-Triazol-1-ium-phenacylid (PTPhY) in two ternary solutions achieved in binary solvents: water (1) + methanol (2) and methanol (1) + benzene (2). For the first set of ternary solutions, the competition between the two hydroxyl solvents will be indicated by the statistical weights of the two solvents in the first solvation shell of ylid. The estimation of the potential energy in the molecular pair ylid-methanol can be made, by basing on the statistic cell model of ternary solutions and using the spectral data obtained for the second set of ternary solutions.

2. Experimental Part

The first binary solvent was made by the hydroxyl liquids: water (1) as active and methanol (2) as little active in the specific interactions with ylid. The second binary solvent was achieved from two miscible spectrally grade liquids (a hydroxyl liquid as an active solvent from the viewpoint of interactions) and a non-hydroxyl one (as an inactive solvent).

In order to realize the ternary solutions, two binary solutions at the same concentration in the studied PTPhY ylid were prepared and were combined in various volumetric ratios. The studied ylid has the chemical structure shown in Fig. 1.

The PTPhY concentration in ternary solutions was very small (10^{-4} – 10^{-5}) mol/L. A Specord UV-Vis Carl Zeiss Jena Spectrophotometer with a data acquisition system was used for the recording of spec-

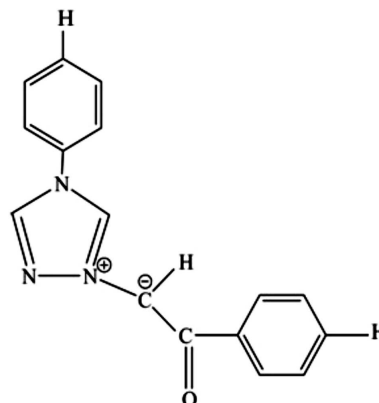


Fig. 1. Chemical structure of the studied 4'-phenyl-1,2,4-triazol-1-ium-phenacylid (PTPhY)

tra. The substance was prepared as indicated in [7, 8]. The ylid purity was checked by the elemental and spectral (IR and NMR) methods.

3. Theoretical Notions Regarding the Intermolecular Interactions in Ternary Solutions

Intermolecular interactions in liquids [9–12] can be classified into universal (long-range) and specific (quasichemical or short-range) interactions.

The universal interactions are given by the radial action of all solvent molecules from the solution on a spectrally active molecule. The universal interactions are non-saturated and non-oriented. Theoretically, they are approximated by the sum of all interactions in pairs of the type “spectrally active molecule-solvent molecule” (at different relative distances).

The specific interactions [11, 12] are oriented and act locally only between some atomic groups (substituents) of molecules.

Usually, the liquid theories are developed only for the universal interactions, and the specific interactions are neglected [10, 11]. The universal interaction can be evaluated by theoretically established formulae, in which microscopic and macroscopic parameters are considered for each type of molecules.

In order to evaluate the contribution of the specific interactions, some empirical scales [13] were proposed or some empirical terms were added to those describing the universal interactions [2, 14]. These terms depend on the local properties of the atomic groups under specific interactions.

Ternary solutions are used in order to obtain liquids with various physical-chemical parameters. When the binary solvent is realized from two liquids with appropriate macroscopic parameters and having different compartments from the viewpoint of specific interactions [15–21], the active solvent action in realizing specific interactions can be emphasized.

Ternary solutions were studied for various types of spectrally active molecules in various binary solvents. Some theories based on experimental data were developed in [15, 5].

To some cycloimmonium ylids, the statistical cell model of ternary solutions was successfully applied [17–21]. In this model, the solvent shells surrounding the spectrally active molecules are considered as being composed of the two solvents in different statistical ratios (active and inactive from the viewpoint of specific interactions) named statistical average weights of each type of a solvent in the shell. They are statistically evaluated because the Brownian motion changes the shell composition. The statistical average weights p_1 and p_2 of the active (1) and inactive (2) solvents in the first solvation shell of a spectrally active molecule can be determined by spectral measurements, and they differ from the molar ratios x_1 and x_2 of the two solvents in the ternary solution. We have

$$p_1 = \frac{\nu_t - \nu_2}{\nu_1 - \nu_2} \text{ and } p_2 = \frac{\nu_1 - \nu_t}{\nu_1 - \nu_2}. \quad (1)$$

The molar fractions of the two liquids in a binary solvent can be expressed as

$$x_1 = \frac{C_1 \frac{\rho_1}{M_1}}{C_1 \frac{\rho_1}{M_1} + C_2 \frac{\rho_2}{M_2}} \text{ and } x_2 = \frac{C_2 \frac{\rho_2}{M_2}}{C_1 \frac{\rho_1}{M_1} + C_2 \frac{\rho_2}{M_2}}. \quad (2)$$

The parameters p_1 and p_2 and x_1 and x_2 are bonded by the relations

$$p_1 = \frac{x_1 \exp\left(-\frac{w_1}{kT}\right)}{x_1 \exp\left(-\frac{w_1}{kT}\right) + x_2 \exp\left(-\frac{w_2}{kT}\right)}, \quad (3)$$

$$p_2 = \frac{x_2 \exp\left(-\frac{w_2}{kT}\right)}{x_1 \exp\left(-\frac{w_1}{kT}\right) + x_2 \exp\left(-\frac{w_2}{kT}\right)}.$$

The parameters from relations (1)–(3) are the following: p_1 and p_2 are the statistical average weights of the two solvents in the first solvation shell of one spectrally active molecule; x_1 and x_2 are the molar ratios in the bulk binary solvent; C_1 and C_2 are the volumetric concentrations of the two solvents in the binary

solvent; ρ_1 and ρ_2 are the densities of the two solvents; M_1 and M_2 are the molar masses of the two solvents; w_1 and w_2 are the potential energies in the molecular pairs of the types “solute–active solvent molecules” and “solute–inactive solvent molecules”, respectively; T – absolute temperature, k is Boltzmann constant, $\nu \text{ cm}^{-1}$ is the wave number in the maximum of the electronic absorption band of the solute (spectrally active) molecule and the indices 1, 2 and t refer to the binary solutions realized in the corresponding active (1) and inactive (2) solvents and in the ternary solution, respectively.

The excess function δ_1 is used to describe the homogeneity of the first solvation shell of a solute molecule in the ternary solution [21–23]:

$$\delta_1 = p_1 - x_1. \quad (4)$$

The spectral measurements and knowledge concerning the ternary solution composition offer information regarding the strength of the specific solute – solvent interactions in solutions containing spectrally active molecules and a protic solvent.

A linear dependence of the type (5) [19, 21] was established in the statistical cell model of ternary solutions:

$$\ln \frac{p_1}{1 - p_1} = \ln \frac{x_1}{1 - x_1} + \frac{w_2 - w_1}{kT}. \quad (5)$$

When relation (4) is accomplished by the experimental data, the statistical cell model can be applied to the ternary solutions. The free term in (5) gives the difference between the potential energies in molecular pairs of the type “solute–active solvent (1) molecules” and “solute–inactive solvent (2) molecules”, which cannot be evaluated by other methods. If the non-protic solvent is chosen with appropriate values of the refractive index and dielectric constant comparative to the protic solvent, the difference $w_2 - w_1$ approximates the strength of the hydrogen bond between the –OH groups of solvent molecules and the ylid carbanion with enough precision.

4. Computational Results

The cycloimmonium ylid under study was supposed to a quantum mechanical analysis, by using HyperChem Programs [24–27], and the results are given below (see Table 1).

The optimized structure of the studied ylid is given in Fig. 2. One can observe the co-planarity of the cycles in 4'-phenyl-triazol-1-ium-phenacylid (PTPhY).

The aspect of the spatial distribution of HOMO and LUMO orbitals [25–26] in PTPhY is illustrated in Fig. 3, *a* and *b*.

In Fig. 3, one can observe the redistribution of the electronic cloud by excitation; the negative charge is moved from the carbanion toward the heterocycle after the visible photon absorption. This process determines a decrease of the molecular dipole moment in the excited state of the molecule [2]. In a given solvent, the solvation energy of the studied triazolium ylid is higher in the ground electronic state, as compared with the excited one [28, 29].

Some electro-optical parameters [25–27] of the studied ylid, as computed by HyperChem, are listed in Table 1.

5. Spectral Results and Discussions

The wavenumbers in the maximum of the visible electron absorption band of the studied PTPhY in different binary solvents are listed in Tables 2 and 3. Two sets of ternary solutions are used in this study:

- (I) water (1) + methanol (2) + PTPhY,
- (II) methanol (1) + benzene (2) + PTPhY.

In the first set of ternary solutions, water is considered as an active solvent, because the wavenumber in the maximum of the visible band of PTPhY is the highest in it. The characteristics of the two solutions are given in Tables 2 and 3, which contain the measured refractive index n and electric permittivity ε for each solution, the wavenumber $\bar{\nu}$ cm^{-1} in the maximum of the PTPhY visible absorption band, statistical average weight p_1 of the active molecules

Table 1. Energetic and electro-optical parameters of an isolated PTPhY molecule

Nr.	Property (unit)	T1
1	Total energy (kcal/mol)	66923.321
2	Heat of formation (kcal/mol)	106.923
3	Binding energy (kcal/mol)	-3703.201
4	$\Delta E = E_{\text{LUMO}} - E_{\text{HOMO}} $ (eV)	6.848
6	Log P	1.97
7	Dipole moment (D)	8.594

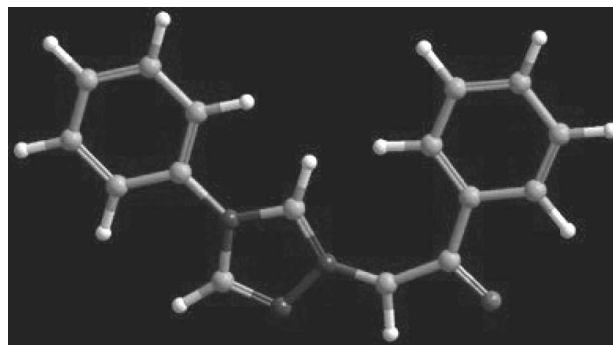
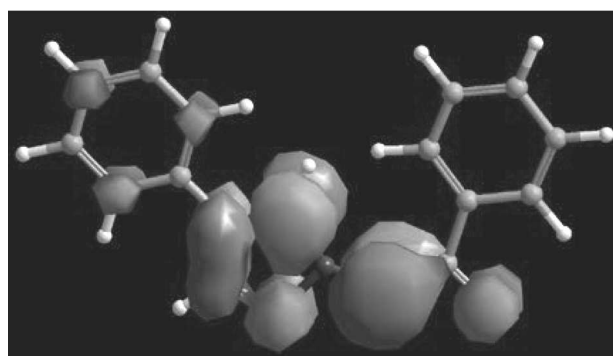
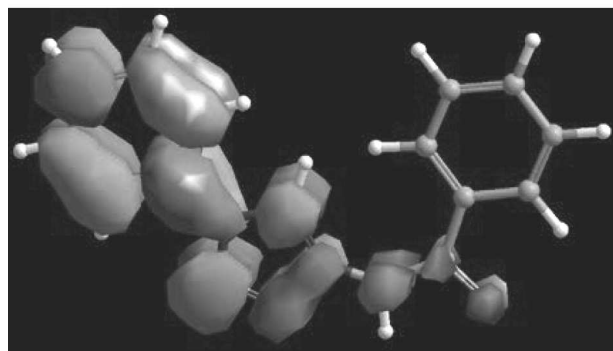


Fig. 2. Optimized structure of the studied PTPhY by HyperChem Programs 8.0.6



a



b

Fig. 3. HOMO (*a*) and LUMO orbitals of PTPhY (*b*)

in the first solvation shell of a PTPhY molecule and the excess function δ_1 .

PTPhY is a polar molecule. Orientation interactions in polar solvents are decisive in its solutions. As it results from Fig. 4, in which a linear dependence between the wavenumber in the maximum of the ICT band and the electric permittivity of the binary sol-

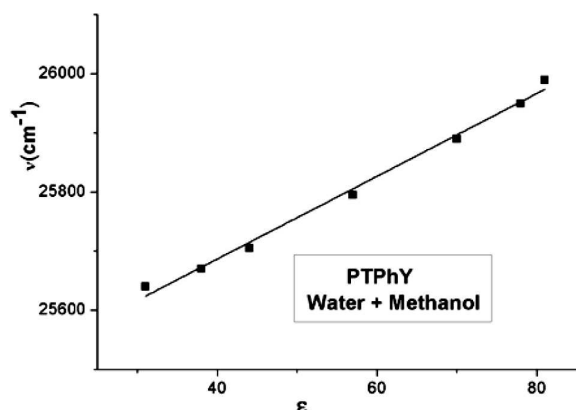


Fig. 4. Wavenumber ν (cm^{-1}) vs. ϵ for ternary solutions water (1) + methanol (2) + PTPhY

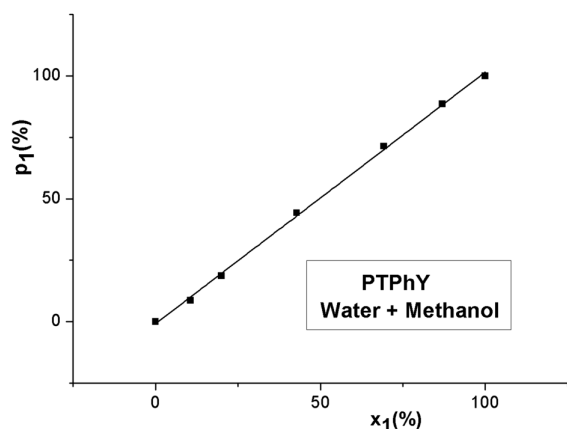


Fig. 5. p_1 vs. x_1 for ternary solutions water (1) + methanol (2) + PTPhY

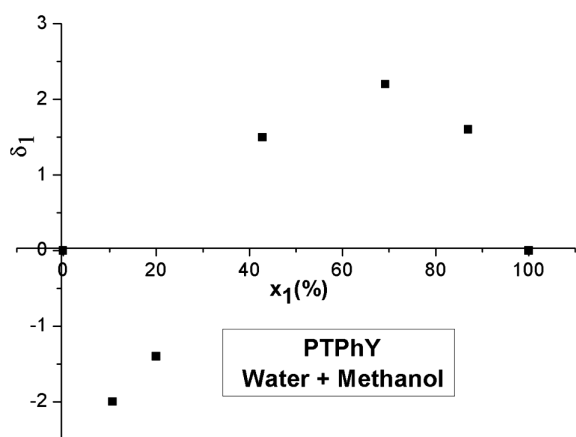


Fig. 6. Excess function δ_1 vs. x_1 for ternary solutions water (1) + methanol (2) + PTPhY

vent for ternary solutions of the type (I) is evidenced, the molecular interactions of the dipolar type are predominant in these solutions.

For the water molar concentration smaller than 40%, the conditions $p_1 < x_1$ and $\delta_1 = p_1 - x_1 < 0$ are accomplished in solutions of the type (I), as it can be seen in Figs. 5 and 6. This results in that the water molar concentration in the rest of a solution is higher than in the first solvation shell of PTPhY. For molar concentrations $x_1 > 40\%$, the first solvation shell of PTPhY becomes enriched in the water molecules, and $\delta_1 > 0$.

There is a linear dependence between $\ln \frac{p_1}{1-p_1}$ and $\ln \frac{x_1}{1-x_1}$ for the two sets of the analyzed ternary solutions of PTPhY (see Figs. 7 and 11), proving the applicability of the statistical cell model of ternary solutions to this kind of mixtures. The slope of the dependences is near the unity, and the intercept is proportional to the difference between the potential energies of the molecular pairs of the types “PTPhY- active solvent (1)” and “PTPhY-inactive solvent (2)”. The values of the slope and intercept of lines of the type (4) are given in Table 4.

Table 2. Characteristics of binary solvent water (1) + methanol (2) and wavenumbers in the maximum of the visible band of PTPhY

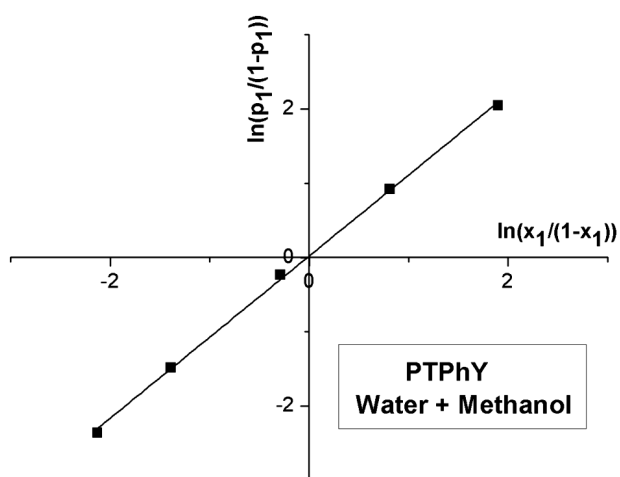
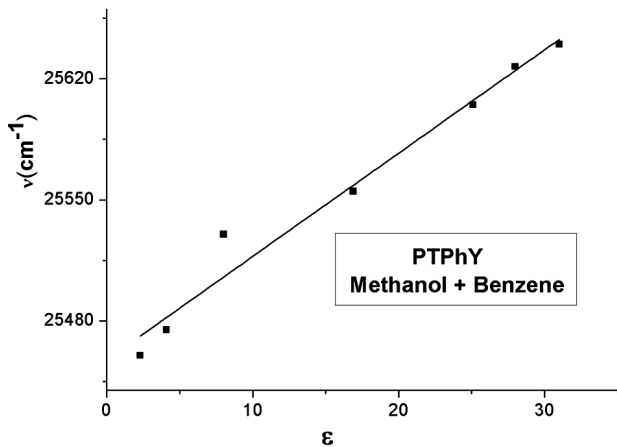
Nr.	$C_1\%$	$x_1\%$	n	ϵ	$\bar{\nu}$ (cm^{-1})	p_1	δ_1
1	0	0	1.331	31	25640	0	0
2	5	10.6	1.337	38	25670	8.6	-2.0
3	10	20.0	1.341	44	25705	18.6	-1.4
4	25	42.8	1.354	57	25795	44.3	1.5
5	50	69.2	1.373	70	25890	71.4	2.2
6	75	87.0	1.387	78	25950	88.6	1.6
7	100	100	1.396	81	25990	100	0

Table 3. Characteristics of binary solvent methanol (1) + benzene (2) and wavenumbers in the maximum of the visible band of PTPhY

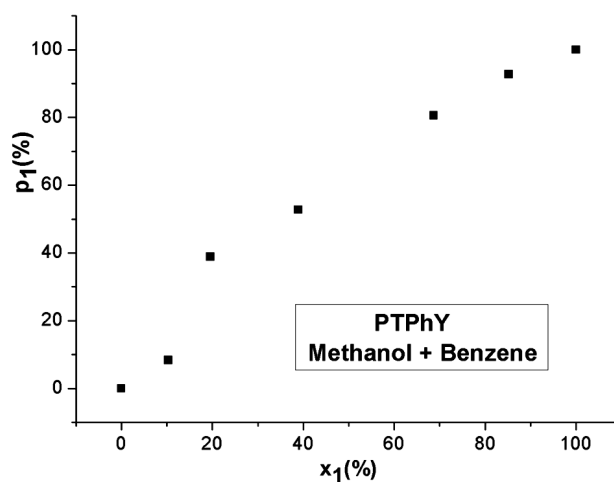
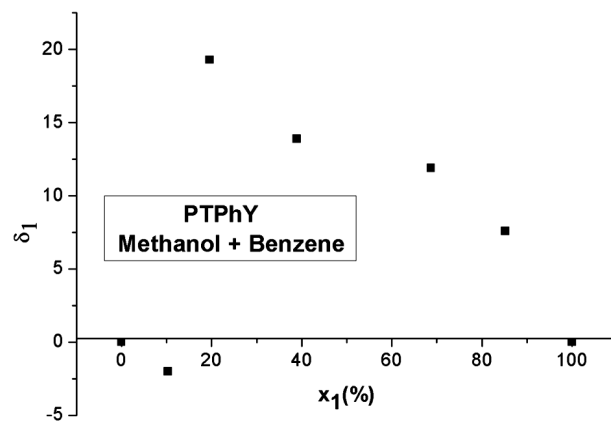
Nr.	$C_1\%$	$x_1\%$	n	ϵ	$\bar{\nu}$ (cm^{-1})	p_1	δ_1
1	0	0.0	1.331	2.3	25460	0.0	0.0
2	5	10.3	1.340	4.1	25475	8.3	-2.0
3	10	19.6	1.361	8.0	25530	38.9	-19.3
4	25	38.9	1.387	16.9	25555	52.8	13.9
5	50	68.7	1.432	25.1	25605	80.6	11.9
6	75	85.2	1.483	28.0	25627	92.8	7.6
7	100	100	1.501	31.0	25640	0.0	0.0

Table 4. Regression coefficients in the equation $\ln \frac{p_1}{1-p_1} = m \ln \frac{x_1}{1-x_1} + n$ for PTPHY

Solvent	$m \pm \Delta m$	$n \pm \Delta n$	R	SD	N	$\omega_2 - \omega_1 (\times 10^{-22}, \text{J})$
Water + methanol	1.092 ± 0.018	0.020 ± 0.004	0.99	0.057	5	0.83 ± 0.17
Methanol + benzene	1.162 ± 0.141	0.592 ± 0.205	0.94	0.448	5	24.53 ± 8.49

Fig. 7. $\ln \frac{p_1}{1-p_1}$ vs. $\ln \frac{x_1}{1-x_1}$ for ternary solutions: water (1) + methanol (2) + PTPHYFig. 8. Wavenumber ν (cm^{-1}) vs. ϵ for ternary solutions methanol (1) + benzene (2) + PTPHY

In solutions of type (II) achieved in the binary solvent methanol (1) + benzene (2), the complex realized by hydrogen bonds between PTPHY and methanol molecules has also an important dipolar moment, so, in its ternary solutions, the orientation interactions are dominant. Figure 8 shows this fact

Fig. 9. p_1 vs. x_1 for ternary solutions water (1) + methanol (2) + PTPHYFig. 10. Excess function δ_1 vs. x_1 for ternary solutions (II): methanol (1) + benzene (2) + PTPHY

by the linear dependence between the wavenumber in the maximum of the PTPHY visible absorption band and the electric permittivity of the binary solvent.

It follows from Figs. 9 and 10 that the methanol molecules are dominant in the first solvation shell of ylid. For $x_1 < 20\%$, the benzene molecules are pre-

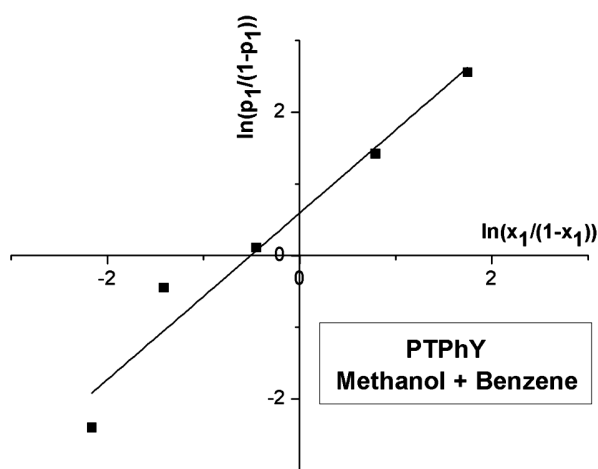


Fig. 11. $\ln \frac{p_1}{1-p_1}$ vs. $\ln \frac{x_1}{1-x_1}$ for ternary solutions (II): methanol (1) + benzene (2) + PTPHY

dominant in the first solvation shell of PTPHY, as this indicated by Fig. 10. For $x_1 > 20\%$, the active solvent from the viewpoint of specific interactions is dominant both in the solution and in the first solvation shell of the studied molecule.

Figure 11 implies that the intercept of line (5) is non-null and positive for type-II solutions, proving $\omega_2 - \omega_1 > 0$. In the other words: $|\omega_1| > |\omega_2|$. The difference approximates the strength of the hydrogen bond of the type “PTPHY–methanol molecules”.

The data obtained in this research prove the applicability of the statistical cell model to ternary solutions of the studied triazolium ylid and offer information about the hydrogen bond strength, when the two solvents (one protic and other non-protic) from the binary solvent are characterized by the appropriate values of refractive indices and electric permittivities.

6. Conclusions

The presented spectral results prove that (4'-phenyl)-1,2,4-triazol-1-ium-phenacylid (PTPHY) is a polar molecule, which can form hydrogen-bonded complexes with hydroxyl solvents.

The strengths of the PTPHY hydrogen bond with water and methanol have comparable values, because the intercept of line (4) is null for the solutions of type (I).

The first solvation shell of PTPHY is non-homogeneous; it has different composition, as compared with the rest of the solution.

The differences between the molar fractions of the two solvents and their average statistical weights in the first solvation shell of the spectrally active molecule are indicators of the anisotropy of the PTPHY ternary solutions.

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ДОСЛІДЖЕННЯ СПЕКТРІВ
(4'-ФЕНІЛ)-1,2,4-ТРИАЗОЛ-1-ІУМ-ФЕНАЦІЛІДА
(РТPhY) У ТЕРНАРНИХ РОЗЧИНАХ

Резюме

Вивчається молекула (4'-феніл)-1,2,4-триазол-1-ІУМ-фенацілід (РТPhY) у тернарних розчинах двох типів. У першому випадку, бінарний розчинник складається з двох гідроксильних змішаних рідин, і у другому випадку з протієвого і непротієвого розчинників. Потенціальна енергія в парах гідроксильний розчинник-ліди оцінена в рамках статистичної осередкової моделі тернарних розчинів. З точки зору взаємодій в першій сольватній оболонці ліди, статистична середня вага активного розчинника відрізняється від його молярної фракції в бінарному розчиннику.