

DIELECTRIC DISPERSION OF GLYCINE WATER SOLUTION ABSORPTION

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The dielectric coefficients of one-molar water solution of water and glycine at temperature from 20°C up to 50°C in five frequencies in centimetric range are measured. The dielectric spectra taking under consideration other frequencies given in reference are studied.

It is shown that Kirkwood model in which the continuous structures of water-soluble amino-acids are accepted in the capacity of medium consisting of water and bipolar molecules (zwitter-ion) of monomer acid should be revised again.

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INTRODUCTION

The dielectric properties of glycine water solutions are investigated many times [1-14]. The accepted description of equilibrium and dynamic characteristics is based on empiric ratios:

$$\varepsilon_{os} = \varepsilon_{ow} + \delta C \equiv \varepsilon_{ow} + [(\varepsilon_{os} - \varepsilon_{ow})C^{-1}]C, \quad (1)$$

$$\varepsilon'_s - j\varepsilon''_s = \varepsilon_{os} + \delta C(1 + j\omega\tau_1)^{-1} + (\varepsilon_o - \varepsilon_{ow})(1 + j\omega\tau_2)^{-1} \quad (2)$$

where C and τ_1 are molar concentration and time, “s” and “w” indexes are related to solution and water, $\tau_1 > \tau_2$ the rest designations have the usual meaning.

Expression (1) is reliably approved by experiments. The distance $r = 3,2 \text{ \AA}$ between dipole charges in well coincidence with $r = 3,3 \text{ \AA}$ which is the distance between zwitter charges of glycine ion found for $^+\text{NH}_2\text{CH}_2\text{COO}^-$ crystal by X-ray method [15]. This result is considered as the confirmation [10] introduced by Kirkwood [5] on the base of solution model (1) in the form of single zwitter-ions homogeneously distributed in medium with undisturbed water structure.

The aim of investigations described in present article, is in establishment of quality of conformance of equation (2) to dielectric spectrum of glycine one-molar water solution on the base of eigen and reference data overlapping the wavelength range $\lambda = 66,7 - 0,85 \text{ cm}$. The water is chosen in the capacity of control object.

RESULTS AND THEIR DISCUSSION

Experimental test of ratio (2) presenting the dynamic analogue (1) is mainly carried out in long-wave edge of relaxation spectrum with prior equalization of τ_2 to τ_6 and some variations of short-wave region amplitude. The interval of τ_1 obtained designations exceeds the evaluation probable error. Such spread can be considered either as the sequence of initial material limitedness making difficult the spectrum unique decoding or as indication on model principal inadequacy [5].

The dielectric constants ε' and absorption indexes ε'' of water and solution are measured at $\lambda = 5,83; 4,02; 3,23; 2,10; 1,40 \text{ cm}$ and temperatures from 20°C up to 50°C. The measured water ε' and ε'' well coincide with ones calculated by equation (table 1):

$$\varepsilon' - j\varepsilon'' = \varepsilon_{\infty} + \sum_i^3 (\varepsilon_{oi} - \varepsilon_{\infty i}) (1 + j\omega\tau_i)^{-1} \quad (3)$$

where $\varepsilon_{o1} = 80,4; \varepsilon_{o2} = \varepsilon_{\infty 1} = 76,4; \varepsilon_{o3} = \varepsilon_{\infty 2} = 4,58; \varepsilon_{\infty 3} = \varepsilon_{\infty} = 1,78; \tau_1 = 28,6; \tau_2 = 8,92; \tau_3 = 0,046 \text{ c}$ (20°C) [16].

Table 1

The measured ε^* and calculated ε^*_{cal} by (3) the dielectric coefficients of water bidistillate at different wave lengths λ (cm) and 20°C

λ	ε'	ε'_{cal}	ε''	ε''_{cal}
5,83	74,0	72,9	21,2	20,9
4,02	67,8	67,4	26,9	27,3
3,23	61,6	62,2	29,8	31,2
2,10	49,7	48,9	35,6	36,4
1,40	33,2	32,5	36,4	36,3

The dispersion - absorption diagrams of studied solution constructed by our and reference data are given in the figure. In spite of big amount of publications by this system, the initial material either is absent or is given in such form that excludes the possibility of its quantitative consideration. We use ε' and ε'' tabulated in [8, 9] and presented graphically in [11].

The general number of points allows us to carry out the enough confident comparison of observable and predictable spectra by model 5 in terms of S sum of standard deviations measured of ε' and ε'' on calculated ones.

The analysis validation criterion is the condition $S \leq S_m$ [17] at which the deviation between test and calculation are caused by only measurement errors.

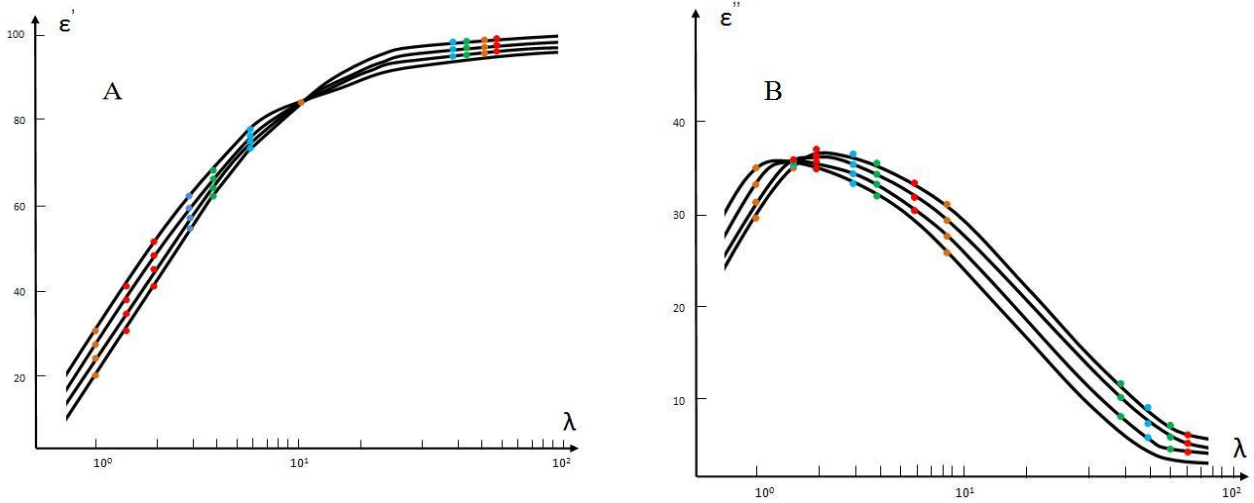


Fig. The dielectric constants ϵ' (A) and absorption indexes ϵ'' (B) 1M of glycine water solution in dependence on wave length λ (cm) at 20 (a); 30 (b); 40 (c); 50° (d): 1 (red) is our data; 2 (green) is [8]; 3 (blue) is [9]; 4 (brown) is [10].

Table 2

The comparison of observable and calculative spectra of one-molar glycine water solution at 20°C.

Ref.	ϵ_{os}	ϵ_{ow}	$\epsilon_{\infty w}$	$\tau_1 \cdot 10^{12} \text{sec}$	$\tau_2 \cdot 10^{12} \text{sec}$	$S(S_m=24,0)$	$S_{dm}(\lambda \gg 33\text{cm})$	$S_{cm}(\lambda < 8,3 \text{ cm})$
[9]	102,6	80,3	5,0	72,0	9,2	114,2	4,4	109,9
[10]	102,6	76,8	5,0	72,0	9,2	60,5	9,4	68,7
[11]	102,6	68,2	3,8	43,6	8,8	48,2	22,7	25,5
[8]	103,6	27,5	—	20,0	—	894,4	281,9	612,5

All assignments suggested up to now are dissatisfied (table 2) in terms of this criterion. The distinctive agreement with experiment only in that range where authors have measured ϵ' and ϵ'' is notable and the appearance of rapidly growing divergences because of overrunning λ takes place. The parameters calculated in [9] by measurements only at four points from $\lambda = 66,7$ up to 33 cm are given in decimetric range $S_{dm} = 4,4$ ($S_m = 8,0$) and $S_{cm} = 109,9$ ($S_m = 16,0$) is given in centimetric one. According to [10] $\epsilon_{\infty 1}$ value should be less than ϵ_{ow} because the amino-acid molecules behave themselves as non-polar ones at corresponding λ can be written by empiric formula:

$$\epsilon_{\infty 1} = \epsilon_{ow} - (\epsilon_{ow} - 1)V \cdot C \cdot 10^{-3}, \quad (4)$$

where V is glycine molar partial volume. In this case S increase is devalued by more than double increase of S_{dm} . The parameter set based on centimetric points leads to

further decrease general S , moreover, the main contribution in S_{cm} is defined by the point at $\lambda = 0,85$ cm where $S=16,3$. At the same time S_{dm} increase shows the choice baselessness of $\tau_1 = 43,6$ psec instead of $\tau_1 = 72,0$ psec [9] giving the well S_{dm} . Finally, $S=0,05$ corresponds to experiment parameters [8] at single $\lambda = 3,20$ cm with general $S=894,4$ (1).

CONCLUSION

The given results allow us to confirm that the dynamic dielectric behavior of glycine one-molar water solution can't be described by ratio (2) at condition of overlapping of enough wide range wave lengths. This conclusion prejudices the use validity of ratio (1) for finding of dipole moment of monomer zwitter-ion of glycine and shows on the necessity of model revision [5] postulating the presence only two dielectrically active types of kinetic units in amino-acid water solutions.

- [1] P.B.Undre, S.N.Helambe, S.B.Jagdale, P.W.Khirade, S.C.Mehrotra. Pramana-J. Phys., 68, 851, 2007.
- [2] B.G. Lone, P. Undre, S.S. Patil, P.W. Khirade, S.C. Mehrotra. J. Mol. Liq., 141, 47, 2008.
- [3] A. Chaudhari, A.G. Shankarwar, B.R. Arbad, S.C. Mehrotra. Journal of Solution Chemistry, vol.33, № 3, 2004, p. 313 – 322.
- [4] Ch.O. Gadjar, S.T. Azizov, Sh.K. Agamuradova. Fizika, т. XIV, №2, s. 56 – 59, 2008. (In Russian).
- [5] J.G. Kirkwood. In: "Proteins, Amino Acids and Peptides", ed. E. J. Cohn, J.T. Edsall, Reinhold. N. Y., 1943, 294.
- [6] W.L. Gent. Trans. Farad. Soc., 50, 1954, 1229.
- [7] K. Dharmalingam, K. Ramachandran, Sivagurunathan, B.P. Undre, P.W. Khirade, S.C. Mehrotra. Mol. Phys., 104, 2835 (2006).
- [8] O. Sandus, B.B. Lubitz. J. Phys. Chem., 65, 1961, 881.
- [9] M.W. Aaron, E.H. Grant. Trans. Farad. Soc., 59, 1963, 85.
- [10] E.H. Grant. In: "Elektronenspinresonanz und andere Spektroskopischen Methoden in Biologie", Akad.-Verlag. Berlin, 1973, s. 273.
- [11] A.M. Bottreau, G. Delbos, C. Marzat, J.M. Salefran,

DIELECTRIC DISPERSION OF GLYCIN WATER SOLUTION ABSORPTION

- J. Moreau*. M. C. R. Acad. Sci., B276, 1973, 373.
- [12] *S.T. Azizov*. Fizika, т. XVII, №2, selection: En, s. 88-90., 2011. (In Russian).
- [13] *A.H. Clark, P.A. Quickenden, A.J. Suggett*. Chem. Soc. Farad. Trans., pt. 2. 70, 1974, 1847.
- [14] *J.L. Salefran, D. Delbos, C. Marzat, A.M. Bottreau*. Annal Sci. Univ. Clermont, Phys., 1977, p. 199.
- [15] *V.P. Pawar, S.C. Mehrotra*. J. Mol. Liq., 95, 63, 2002.
- [16] *A.M. Bottreau, J.M. Moreau, J.M. Laurent, C.J. Marzat*. Chem. Phys., 62, 1975, 300.
- [17] *P. Sivagurunathan, K. Dharmalingam, K. Ramachandran, B.P. Undre, P.W. Khirade, S.C. Mehrotra*, Philos. Mag. Lett., 86, 291, 2006.

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