DETERMINATION OF DIPOLE MOMENT OF OXALIC ACID IN DIFFERENT SOLVENTS

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Özet - **Deneysel dielektrik sabitleri kullanılarak okzalik asit çözeltilerinin 20^{0}C de ve farklı çözücülerde hazırlanan çözeltilerinin dipol momentleri belirlenmiştir. Okzalik asitin dipol momenti üzerine çözücülerin etkisi tartışılmıştır. Diğer önemli fiziksel nicelikler olan kırma indisleri, yoğunluklar ve dielektrik sabitleri de belirlenmiştir.**

Anahtar Kelimeler - **Dipol Moment, Debye Teorisi, Kırma İndisi, Dielektrik Sabiti**

Abstract - **The dipole moments of the solutions of oxalic acid in different solvents at 20^{0}C are obtained by using the experimental dielectric constants. The effect of the solvent on the dipole moment of oxalic acid is discussed. Other important physical quantities such as refractive index, density and dielectric constant are also determined.**

Keywords - **Dipole moment; Debye theory; Refractive index, Dielectric Constant.**

I. INTRODUCTION

Because the dipole moment *(μ)* gives information about the molecular shape and the electronic change distribution in the molecule , it is therefore very important in characterizing and in elucidation of the molecular structure of various substances [1,2].

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It was pointed out by Debye that molecules of the so-called polar molecules, though electrically neutral, possess a non vanishing electric dipole moment even in the absence of applied fields and that the magnitude of the molecular dipole moment could be found from the permittivity (dielectric constant) data [2,3]. The dipole moment can be computed from observation of the permittivity determined from electrical methods (static fields) in the low frequency range.

The study of the dielectric constant is so important that it can provide information about the dipole moments and polarizability and about the behaviour of the molecules under the influence of an external or internal electric field. [4]

We use the Clausius-Mosotti equation for calculation of the dipole moments with a high degree of accuracy [1,2,5]. The aim of this paper is to measure some thermodynamic and physical properties relevant with the solutions.

II. EXPERIMENTAL

The density of the solutions, which is required to determine other physical properties, was measured at 20^{0}C by pycnometric method, the pycnometer volume being between 20 and 25mL. The temperature of the thermostatic bath was controlled in the range between 0 ± 0.5^{0}C and 50 ± 0.5^{0}C.

An Abbe refractometer was used to measure the refractive index at 20±0.2^{0}C; the refractometer cell was connected with a temperature-controlled bath. The wavelength is 589.6 nm, Na (D-line).

The dielectric constants measurements were carried out using HP 4192 Ab model Empedans Analyzer for solutions of oxalic acid in the frequency 100kHz at 20^0C with a home-made liquid cell. A parallel plate geometry with a guard ring was used and the liquid volume required is small (about 1ml). The cell was calibrated by measuring, after careful cleaning, the capacity under vacuum.

Solutions were prepared using solvents which have different dielectric constants such as methyl alcohol, ethyl alcohol, n-propyl alcohol, iso-propyl alcohol, cyclohexane and toluene. The concentration range of solutions were 2.00×10^{-3} to 1.00×10^{-3} $molL^{-1}$.

III. RESULTS AND DISCUSSION

In this study the physical quantities such as refractive index, density and dielectric coefficient are measured. The physicochemical properties of oxalic acid solutions in different solvents at 20^0C are shown in Table I.

The dielectric constants were calculated by the following equation,

$$\varepsilon = C / C_0 \tag{1}$$

Where, C_0 is capacitance of condenser in vacuum and C is capacitance of solution in condenser.

Dipole moments of molecular systems are calculated by dielectric constant measurement of solutions which were prepared in non-polar solvents. The total molar polarization can be obtained by applying the Clasius-Mosotti equation [1,6]:

$$P_s = ((\varepsilon_s-1)/(\varepsilon_s+2))\,((M_1X_1 + M_2X_2)/\rho_s)) \tag{2}$$

Where, X_2 is mol fraction of solute, X_1 is mol fraction of solvents, M_1 and M_2 are molecular weight of solvent and solute, respectively.

$$P_s = P_1X_1 + P_2X_2 \tag{3}$$

There are two molar polarization terms. P_s is a functional term which has two parameters. $P_s=f(X_1,X_2)$. In this study, solutions in different proportions were prepared, then ε_s and ρ_s of solutions were determined. The different P_s values were plotted against X_2. While mole fraction of solute led to zero at limiting position, P_s, , limit value of molar polarization can also be extrapolated [7].

$$\lim_{X_2\to 0} P_s = P_2 \tag{4}$$

P_2, molar polarization of solute was obtained by using extrapolation equation.

P_2 of the solutions which were calculated by using Eq. (2) were plotted against X_2, mole fractions of solute in the solutions [7]. While mole fraction of solute leads to zero at limiting position, P_s, , limit value of molar polarization were extrapolated. P_2 of the solutions are shown in Fig. 1.

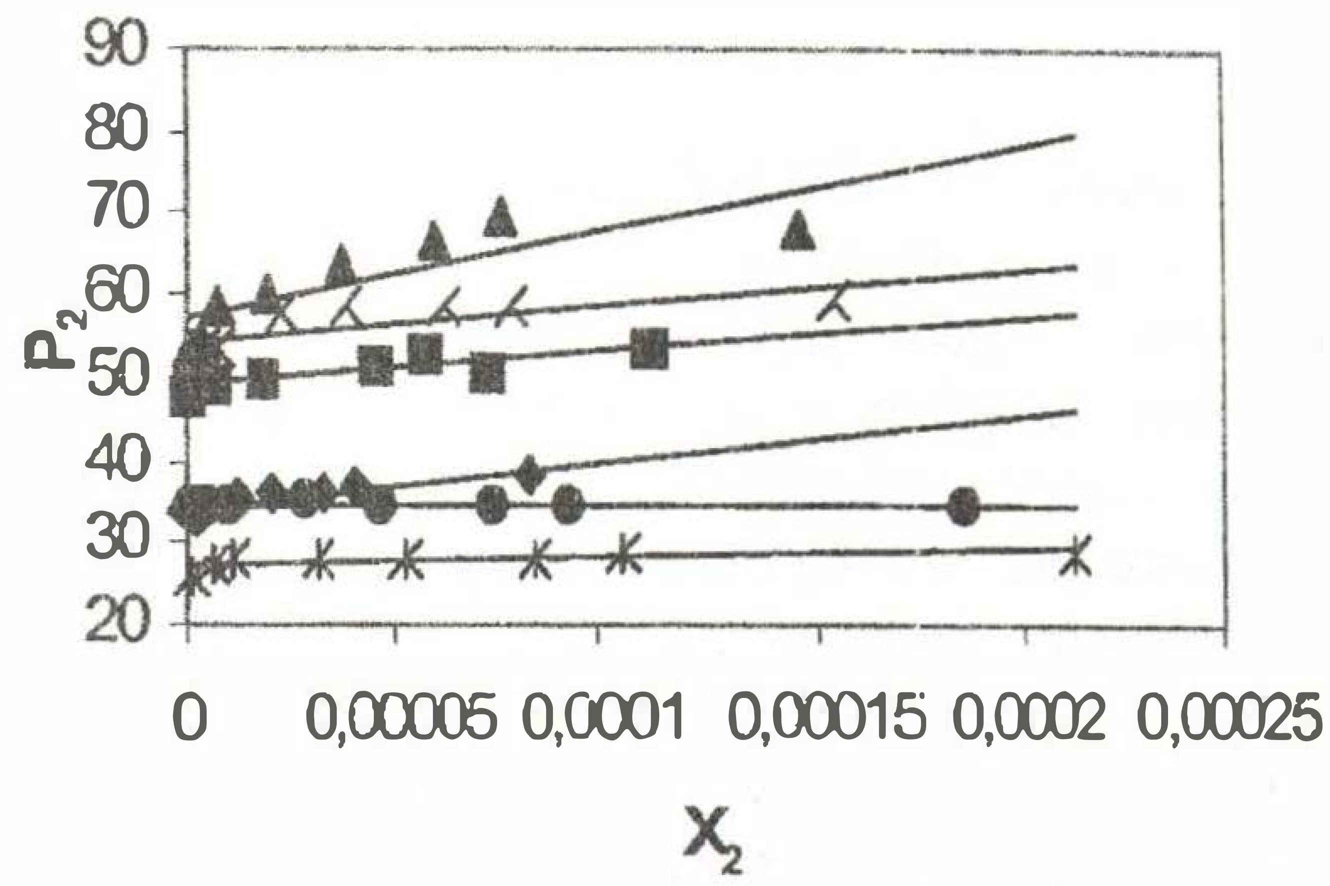

Fig. 1. P_2, molar polarizations of the oxalic acid solutions in different solvents at 20^0C. The compositions are methyl alcohol (♦), ethyl alcohol (■), n-propyl alcohol (▲), iso-propyl alcohol x, cyclohexane (*), toluene (•).

From Lorenz-Lorentz equations, R_2 molar refractivity value of solute was obtained. It is given by;

$$R_{1,2} = \left(\frac{n^2-1}{n^2+2}\right)\left(\frac{X_1M_1 + X_2M_2}{\rho_s}\right) \tag{5}$$

where, n is refractive index of the solutions, M_1 and M_2 are molecular weight of solvent and solute, respectively and ρ_s is density of the solutions [8,9,10]. The different $R_{1,2}$ values were plotted against X_1. While mole fraction of solvent led to one at limiting position, $R_{1,2}$, limit value of molar refractive can also be extrapolated. R_2, molar refractive value of the solute was obtained by using extrapolation equation.

$$\lim_{X_1\to 0} R_{1,2} = R_2 \tag{6}$$

R_2 of the solutions which were calculated by using Eq. (5) were plotted against X_1, mole fractions of solvent in the solutions . While mole fraction of solvent leads to zero at limiting position, R_s, , limit value of molar refractivity were extrapolated. R_2 of the oxalic acid solutions are shown in Fig. 2.

Table I. Physicochemical properties of oxalic acid solutions in different solvents at 20°C.

Concentration (mole/l)	Physicochemical Properties of Oxalic acid		
	ρ (g/ml)[a]	ε[a]	n[a]
Methyl Alcohol			
$2.00x10^{-3}$	0.7944	53.08	1.3297
$1.00x10^{-3}$	0.7940	34.83	1.3295
$8.00x10^{-4}$	0.7935	27.46	1.3295
$5.00x10^{-4}$	0.7926	25.36	1.3295
$3.00x10^{-4}$	0.7917	23.15	1.3294
$1.00x10^{-4}$	0.7913	17.89	1.3294
$5.00x10^{-5}$	0.7907	17.21	1.3292
$1.00x10^{-5}$	0.7902	15.73	1.3292
Ethyl Alcohol			
$2.00x10^{-3}$	0.8116	50.61	1.3631
$1.00x10^{-3}$	0.8107	44.18	1.3630
$8.00x10^{-4}$	0.8105	28.89	1.3630
$5.00x10^{-4}$	0.8104	24.74	1.3629
$3.00x10^{-4}$	0.8101	21.50	1.3629
$1.00x10^{-4}$	0.8095	21.06	1.3629
$5.00x10^{-5}$	0.8090	21.03	1.3628
$1.00x10^{-5}$	0.8089	16.39	1.3628
n-Propyl Alcohol			
$2.00x10^{-3}$	0.8180	42.00	1.3844
$1.00x10^{-3}$	0.8072	41.58	1.3843
$8.00x10^{-4}$	0.8065	26.06	1.3843
$5.00x10^{-4}$	0.8063	19.23	1.3842
$3.00x10^{-4}$	0.8062	13.25	1.3842
$1.00x10^{-4}$	0.8060	12.21	1.3842
$5.00x10^{-5}$	0.8053	8.900	1.3840
$1.00x10^{-5}$	0.8044	8.460	1.3840
Iso-Propyl Alcohol			
$2.00x10^{-3}$	0.7892	11.84	1.3766
$1.00x10^{-3}$	0.7883	11.06	1.3765
$8.00x10^{-4}$	0.7874	10.90	1.3765
$5.00x10^{-4}$	0.7874	10.81	1.3764
$3.00x10^{-4}$	0.7873	10.26	1.3764
$1.00x10^{-4}$	0.7865	8.000	1.3763
$5.00x10^{-5}$	0.7865	7.890	1.3763
$1.00x10^{-5}$	0.7856	7.670	1.3763
Cyclohexane			
$2.00x10^{-3}$	0.7782	2.100	1.4520
$1.00x10^{-3}$	0.7780	2.070	1.4519
$8.00x10^{-4}$	0.7780	2.060	1.4519
$5.00x10^{-4}$	0.7776	2.050	1.4518
$3.00x10^{-4}$	0.7768	2.050	1.4518
$1.00x10^{-4}$	0.7699	2.040	1.4517
$5.00x10^{-5}$	0.7619	1.980	1.4517
$1.00x10^{-5}$	0.7605	1.930	1.4516
Toluene			
$2.00x10^{-3}$	0.9621	2.720	1.5185
$1.00x10^{-3}$	0.9620	2.700	1.5184
$8.00x10^{-4}$	0.9602	2.700	1.5183
$5.00x10^{-4}$	0.9546	2.700	1.5183
$3.00x10^{-4}$	0.9500	2.690	1.5182
$1.00x10^{-4}$	0.9493	2.680	1.5181
$5.00x10^{-5}$	0.9407	2.640	1.5181
$1.00x10^{-5}$	0.9368	2.630	1.5180

a: Ref. [11]

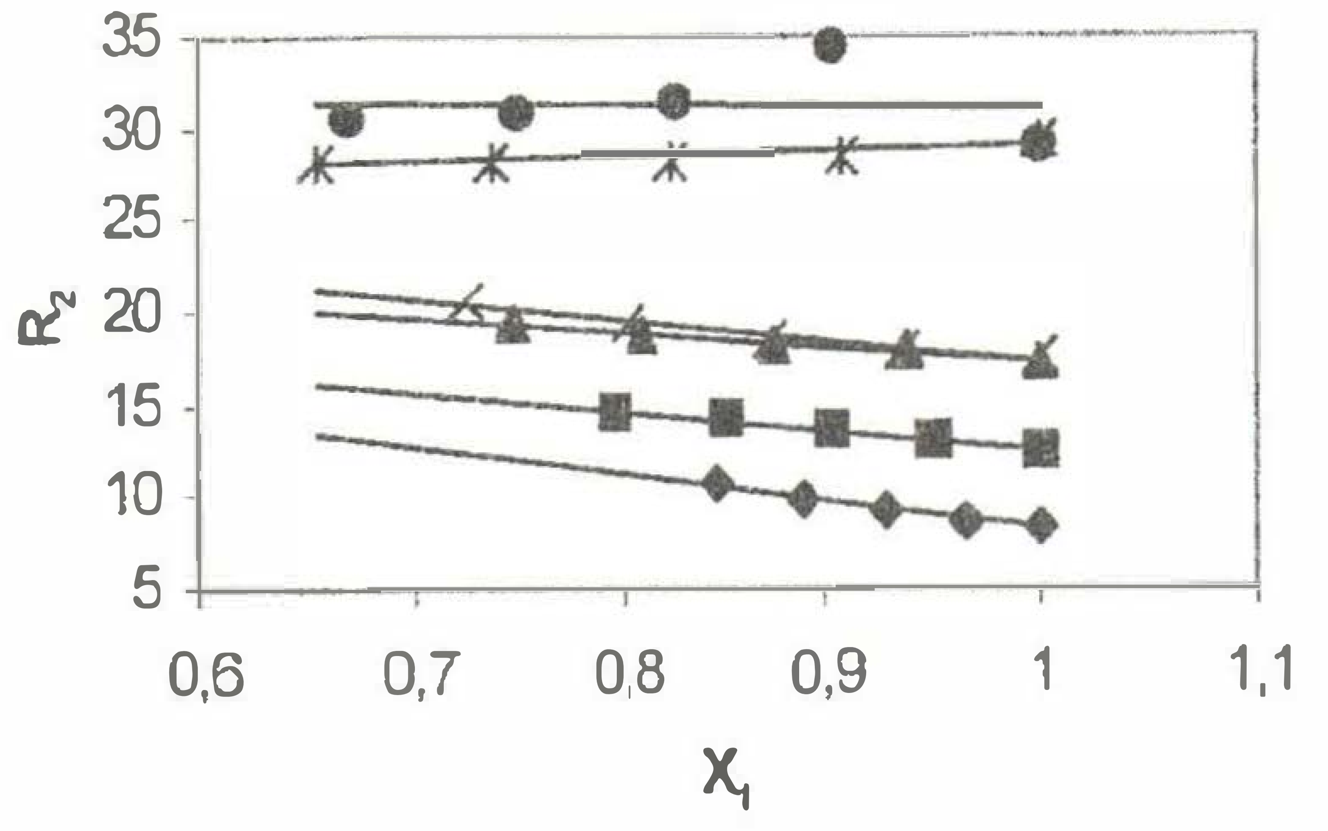

Fig. 2. R_2, molar refractivity of the oxalic acid solutions in different solvents at 20°C. The compositions are methyl alcohol (♦), ethyl alcohol (■), n-propyl alcohol (▲), iso-propyl alcohol x, cyclohexane (*), toluene (●).

P_2 and R_2 values are reported here. Dipole moment of solute in Debye was calculated by using P_2 molar polarization and R_2 molar refractivity term [7].

$$\mu = 0,0128\ [(P_2\text{-}R_2).T]^{1/2} \qquad (7)$$

Physical means of 1Debye is 10^{-18}esybxcm. In this study, obtained dipole moment is known as continuous dipole moment. If a molecular system has polar atomic groups and asymmetric geometry, dipole moment of the molecular system can be calculated by above equations.

P_2 and R_2 of the oxalic acid solutions which were calculated by using [12] Eq. (2-5) are shown in Table II. The concentrations of the oxalic acid solutions are $2x10^{-3}$M. Table II. shows the calculated dipole moments of oxalic acid solutions by Eq. (7).

Table 2. Molar polarizability,P_2 ; molar refractivity, R_2 and dipole moment,μ values of oxalic acid solutions in different solvents at 20°C.

Solvent	Oxalic acid		
	P_2 (cm^3mol^{-1})	R_2 (cm^3mol^{-1})	μ (D)
Methyl Alcohol	33.751	32.394	0.2553
Ethyl Alcohol	46.805	28.542	0.9366
n-propyl Alcohol	58.737	29.663	1.1817
İso-propyl alcohol	53.458	32.740	0.9975
Cyclohexane	30.414	29.328	0.2283
Toluene	29.911	28.622	0.2489

IV. CONCLUSIONS

When the solvents are compared with each other, it can be seen that dipole moments of prepared solutions with n-propyl alcohol are much greater than the other solvents. The result is shown in Table. II. H-bonding can be reveal at this solution. Weak energy interactions caused by the geometric structure of molecular systems are changed and system has asymmetric structure. It is determined that dipole moments of oxalic acid-cyclohexane and oxalic acid-toluene systems are lower than the other systems (Table). According to the results, interactions are weak in this systems and the solvents have non-polar property.

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