DIPOLE MOMENTS OF TWO DERIVATIVES OF D-GLUCOSE IN LIQUID STATE: APPLICATION OF JATKAR'S EQUATION

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The applicability of Jatkar's equation for the calculation of the dipole moments of polar liquids has been established in the case of two derivatives of D-glucose.

Introduction

Many attempts have been made to express the dielectric constant of a condensed medium possessing permanent dipoles in terms of its dipole moment. Onsager made a new approach to the problem,[1] rejecting Debye's concept[2] of "hindering rotational energy" of molecules in liquid media. Kirkwood[3] generalised Onsager's theory. In recent years, Scholte[4] has suggested the extension of the theory to ellipsoidal molecules. Onsager's approach, however, has met with criticism.[5,6] Some empirical equations[7,8] have also been formulated which connect the dielectric constant of a liquid with its polarisation. Jatkar developed an equation[9] which may be applied to polar liquids. Recently, Phadke[10] has found that Jatkar's equation gives more reliable results than Onsager's in the case of fatty acids. In the present paper, the applicability of Jatkar's equation for the calculation of the dipole moments of two derivatives of D-glucose in liquid state has been examined.

Experimental

The α- and β-isomers of 1, methyl 2, 3, 4, 6 tetramethyl D-glucose were prepared according to the method described by Haworth.[11,12] The α-isomer could be obtained in a pure condition; the β-compound, however, was slightly impure. The physical constants of the compounds prepared by the author are given below:

1, methyl 2, 3, 4, 6 tetramethyl α-D-glucose: $d_D^{27^\circ} = 1{\cdot}1025$; b.p. = 133–35° C. at a pressure of 2·5 mm.; refractive index, $n_D^{27^\circ} = 1{\cdot}4435$; specific rotation, $(\alpha)_D^{27^\circ} = +\,152{\cdot}8°$, in a solution of absolute ethyl alcohol.

1, methyl 2, 3, 4, 6 tetramethyl β-D-glucose: density, $d^{25^\circ} = 1{\cdot}0965$; b.p. = 117° C., at a pressure of 0·75 mm.; refractive index, $n_D^{25^\circ} = 1{\cdot}4439$; specific rotation, $(\alpha)_D^{25^\circ} = +\,9{\cdot}4°$, in absolute ethyl alcohol.

For the measurement of dielectric constants, an apparatus similar to that of Nagamani and Jatkar[13] was employed. The densities of the liquids were determined carefully by means of a pyknometer provided with ground-glass caps; and the refractive indices using an Abbe refractometer.

The dipole moments were calculated by the following expression[9]:

$$_{T}P = (\epsilon - 1) \cdot \frac{M}{d} = (n^2 - 1) \cdot \frac{M}{d} + \frac{4\pi N\mu^2}{3.kT} \cdot \frac{j+1}{j},$$

where

$_{T}P$ = total polarisation; N = Avogadro number;
ϵ = dielectric constant; k = Boltzmann constant;
M = molecular weight; T = temperature in degrees absolute;
d = density;
n = refractive index; μ = dipole moment.

According to Jatkar,[9] j in the above equation must be put as equal to $\frac{1}{2}$ for liquids. The electronic polarisation of the compounds, $_{E}P_{J}$, to be used in Jatkar's equation has been computed from the term $(n^2 - 1)$. M/d. For the α-isomer, $_{E}P_{J}$ works out to be 245·7 and for the other compound 247·3.

The results are recorded in the following tables. For N and k in the above expression, the values given by Birge[14] have been used.

TABLE I

Dipole Moment of 1, *methyl* 2, 3, 4, 6 *tetramethyl* α-*D-glucose*

$t°$ C. ..	30	40	50	60	70	85
d ..	1·0965	1·0876	1·0812	1·0722	1·0636	1·0515
ϵ ..	4·943	4·856	4·756	4·630	4·536	4·407
$_{T}P$ ..	899·0	886·6	868·5	846·4	831·1	810·0
μ ..	1·90	1·91	1·91	1·91	1·91	1·92

TABLE II

Dipole Moment of 1, *methyl* 2, 3, 4, 6 *tetramethyl* β-*D-glucose*

$t°$ C. ..	25	40	50	60	70	82·5
d ..	1·0965	1·0870	1·0795	1·0686	1·0623	1·0563
ϵ ..	5·235	5·049	4·930	4·793	4·680	4·530
$_{T}P$ ..	965·6	931·3	910·2	887·4	866·0	835·4
μ ..	1·97	1·97	1·97	1·97	1·97	1·95

DISCUSSION

The values of the dipole moments recorded in Tables I and II indicate that the moments calculated by the application of Jatkar's equation are remarkably constant over a wide range of temperature for the compounds studied. The dipole moments of these compounds in solutions of benzene and dioxane have also been determined, and are dealt with in a separate paper. The author obtained in solutions of benzene the following values: for the α-isomer, $\mu_{30} = 2{\cdot}08$ D and $\mu_{40} = 2{\cdot}11$ D; and for the β-isomer, $\mu_{30} = 2{\cdot}05$ D and $\mu_{40} = 2{\cdot}06$ D. The corresponding values in dioxane solutions were: $\mu_{30} = 1{\cdot}94$ D and $\mu_{40} = 1{\cdot}99$ D for the former compound and $\mu_{30} = 1{\cdot}99$ D and $\mu_{40} = 2{\cdot}04$ D for the latter. It may be pointed out that the results recorded in Tables I and II agree well with those obtained in solutions of non-polar solvents. In view of this agreement, it is suggested that the dipole moments of carbohydrate derivatives, which are often viscous liquids difficult to crystallise, can be conveniently computed by applying Jatkar's equation to the data obtained for the liquid state.

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