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Structure of 16-Hydroxyisosteviol-Derived Dicarboxylic Acid Esters

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Abstract — Dielcometry, method of dipole moments, IR spectroscopy, and computer simulation were used to show that dicarboxylic acid esters derived from 16-hydroxyisosteviol (*ent*-16-hydroxybeyeran-19-oic acid) exist in CCl_4 solutions as tweezer-like or open-chain structures, or dimers with various steric structures, depending on the degree of dilution. Concentrations at which both the esters and parent dicarboxylic acids undergo structural rearrangement were established. The structure of three esters was confirmed by X-ray diffraction.

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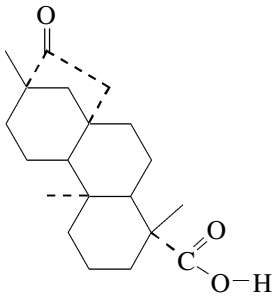
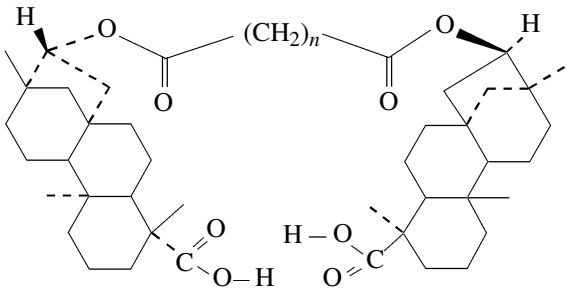
Bis-derivatives of the diterpenoid isosteviol (*ent*-16-oxobeyeran-19-oic acid) (**I**), in which the two *ent*-beyeran carcasses are linked via the C^{19} carboxy groups, are present in crystal as so-called tweezer-like structures [1–3]. The beyeran carcasses in these structures locate one over the other, forming an intramolecular cavity whose size and shape are defined by the length and chemical composition of the spacer [1]. Tweezer-like structures were also revealed in CCl_4 solutions of these compounds by means of dipole moment measurements and computer simulation [4]. We recently synthesized 16-hydroxyisosteviol bis-derivatives **II**–**V** in which the two *ent*-beyeran carcasses are linked with various-length polymethylene spacers already via hydroxyl functions [5]. We considered it important to study the structure of these isosteviol derivatives, too.



I



II–**IV**

n = 1 (**II**), 4 (**III**), 6 (**IV**), 8 (**V**).

Compouds **II**–**V** are dibasic carboxylic acids. Therefore, in solutions, depending on the degree of dilution, they can exist both as acid dimers and as monomers. The fractions of the dimeric and monomeric forms in solution are obviously dependent of the concentration of the acid: With dilution, the fraction of the former decreases and the fraction of the latter increases.

The so-called "critical concentration" at which a solute changes its aggregative state can be determined with high precision by dielcometric titration [6]. The

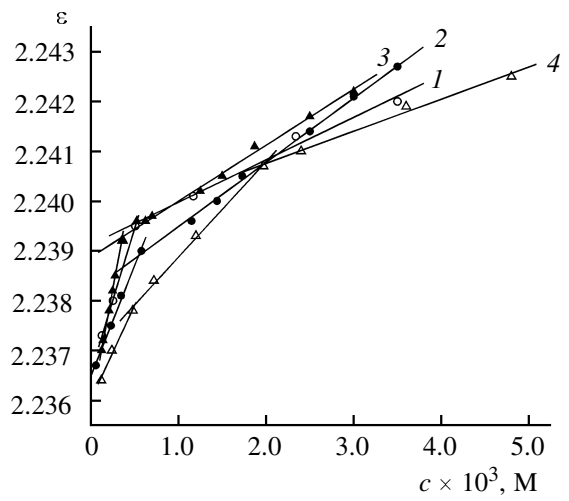


Fig. 1. Plot of dielectric constant (ε) vs. solute concentration (*c*, M). Solute: (*1*) compound **II**; (*2*) compound **III**; (*3*) compound **IV**; and (*4*) compound **V**.

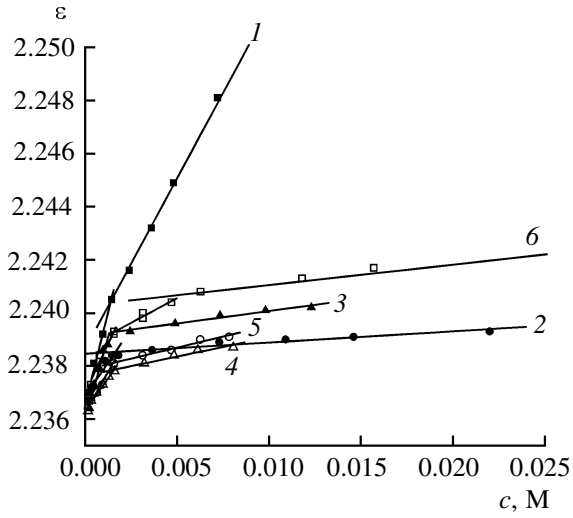


Fig. 2. Plot of dielectric constant (ε) vs. solute concentration (*c*, M). Solute: (*1*) isosteviol (**I**); (*2*) malonic acid (**VII**); (*3*) adipic acid (**VIII**); (*4*) suberic acid (**IX**); (*5*) sebacic acid (**X**); and (*6*) acetic acid (**VI**).

dielectric constant of a medium (ε) containing polar substances is highly sensitive to the structurization degree (i.e. to formation by polar substances of various-polarity aggregates), and dielcometry is used to success in micelle formation research [7–9].

The plots of the dielectric constants ε of solutions of compounds **II**–**V** in CCl_4 vs. the concentrations of the solutions are presented in Fig. 1, and Fig. 2 shows similar plots for the corresponding dicarboxylic acids, acetic acid, and isosteviol. The results of analysis of the plots are given in Table 1 which lists concentrations at which the solutions radically change their polarity (as evidenced by well-defined inflections in the plots). By analogy with the term "critical micellization concentration" (CMC) widely used in micelle formation research [7–9], we gave these concentrations the name "critical aggregation concentrations" (CAC). Since 16-hydroxyisosteviol (**XI**) and compounds **II**–**V** contain carboxy groups, and all carboxylic acids are known to form H-bonded dimers at certain concentrations in soluions [10], we suggested that in our case the CAC value obtained by dielcometry relates to the concentration range where, at a definite dilution, the fraction of monomers becomes to be larger than that of dimers.

Table 1. Critical aggregation concentrations (CAC) for CCl_4 solutions of dicarboxylic acids and their derived 16-hydroxyisosteviol esters

Acid	CAC (M) × 10^3, acid	Ester	CAC (M) × 10^4, ester
Acetic (**VI**)	1.6	–	–
Isosteviol (**I**)	1.8	–	–
Malonic (**VII**)	1.0	**II**	5.0
Adipic (**VIII**)	1.5	**III**	6.0
Suberic (**IX**)	1.7	**IV**	4.0
Sebacic (**X**)	1.6	**V**	7.0, 25

As seen from Table 1, compounds **II**–**IV** form acid dimers at a concentration that is an order of magnitude lower than the concentration of the dimer formation from the corresponding acids (malonic, adipic, and suberic). This finding means that the former acids are more prone to dimerization than dibasic carboxylic acids. Since the slope of the plot of the ε of a solution vs. the concentration of the solute is proportional to the dipole moment [11], the plots in Figs. 1 and 2 allow us to estimate not only the polarity of the solution, but also the concentration of one or another component. The concentration ranges in the plots for acetic (**VI**), malonic (**VII**), adipic (**VIII**), suberic (**IX**), and sebacic acids (**X**) and isosteviol (**I**) (Fig. 2), from 2×10^{-4} M (measurement start) to CAC ($1.0–1.8 \times 10^{-3}$ M), correspond to the monomeric form. Dimers of monocarboxylic acids are nonpolar, since the dipole moments of their carboxy groups are directed toward each other and mutually compensated. Therefore, the nonzero polarity of the solutions of our considered monocarboxylic acids (acetic acid and isosteviol) at the CAC and above gives evidence

showing that the solutions contain, along with dimers, the polar monomeric form. In accordance with the additivity principle [Eq. (1)] [11], the concentration of the latter is estimated by Eq. (2) which simplifies to Eq. (3), when the dimeric form is nonpolar.

$$\mu^2_{exp} = \mu^2_{mono} n_{mono} + \mu^2_{dimer}(1 - n_{mono}), \quad (1)$$

$$n_{mono} = (\mu^2_{exp} - \mu^2_{dimer})/(\mu^2_{mono} - \mu^2_{dimer}), \quad (2)$$

$$n_{mono} = \mu^2_{exp}/\mu^2_{mono}. \quad (3)$$

Here μ_{mono}, μ_{dimer}, μ_{exp} are the dipole moments of the monomer and dimer, and the experimental dipole moment, respectively, and n_{mono} is the concentration of the monomeric form in the solution. Our measured experimental dipole moment of acetic acid (**VI**) at concentrations below the CAC is 1.57 ± 0.28 D. The theoretical dipole moment μ_{mono} of 1.62 D, necessary for determining n_{mono} of acetic acid (**VI**), was estimated using the C(O)O group dipole moment equal to 1.7 D and directed along the C=O bond [12], as well as the N–O dipole moment of 1.0 D. The theoretical μ_{mono} of 1.62 D is nicely consistent with our experimental value (1.57 D). The experimental dipole moment of a solution of acetic acid (**VI**) at a concentration of above the CAC is 0.5 D, which, according to Eq. (3), corresponds to a 10% content of the monomeric form.

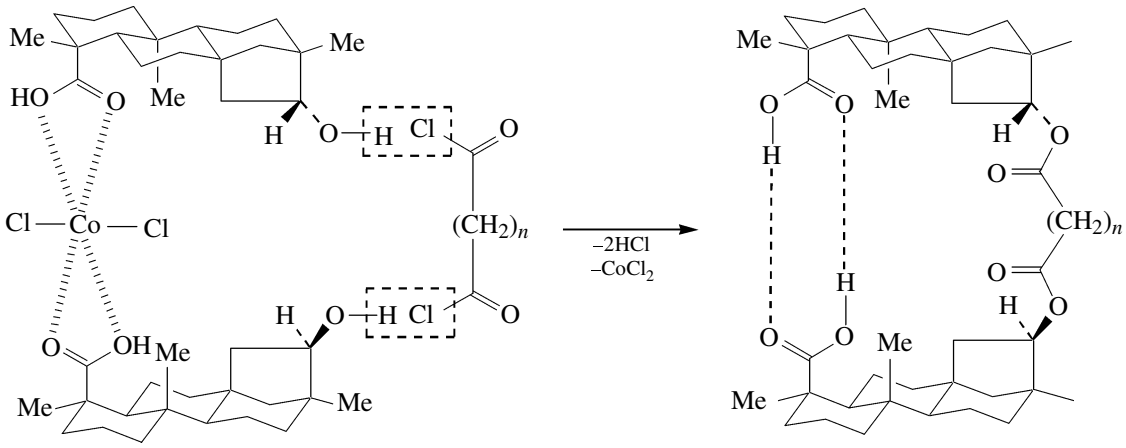
Isosteviol (**I**) contains, along with carboxyl, a keto group, and, therefore, the dipole moment of its dimer should be nonzero. In calculation of the theoretical dipole moment of isosteviol and its dimer by the vector additive scheme [11, 13], we used the same dipole moment of the carboxy group as in acetic acid, and the dipole moments of cyclopentanone C_{sp^3}–C_{sp^2} and C=O bonds were taken to be 0.7 and 1.7 D, respectively [11]. The H–C_{sp^3} dipole moment was always taken to be 0.28 D [11]. The geometries of isosteviol and its dimer was optimized by the PM3 method [14] using the Gaussian98 program [15]. The theoretical dipole moment of the monomerc form of isosteviol (3.77 D) is close to experimental measured at concentrations below the CAC (3.95 ± 0.42 D), whereas the polarity of the dimeric form of isosteviol (0.26 D) is lower than the value (1.09 D) corresponding to the ε of the solution above the CAC point. Consequently, in this concentration range (1.8×10^{-3}–1.44×10^{-2} M) the solution contains, along with dimers of isosteviol, its monomeric form. According to Eq. (2), the content of the latter is 8%.

Calculation of the dipole moments of dimeric dicarboxylic acids **VII**–**X** should involve special conformational analysis aimed at determining mutual orientation of the "terminal" carboxy groups in the dimers. Therefore, we restricted ourselves to the determination of experimental dipole moments of the monomeric forms at concentrations below the CAC. The following experimental values were obtained, D: 3.0 ± 0.44 (**VII**), 3.20 ± 0.51 (**VIII**), 3.0 ± 0.35 (**IX**), and 3.20 ± 0.38 D (**X**). The published dipole moments of dicarboxylic acids **VII**–**X** [16] were measured at concentrations above the CAC (when solutions contain, along with the monomeric form, a minor amount of the less polar dimeric form). The measurements were performed in dioxane which in itself is able to associate with acids, and, therefore, published values are regularly underestimated compared to our results, equaling 2.6 (**VII**), 2.2 (**VIII**), 2.36 (**IX**), and 2.46 D (**X**) [16]. At the same time, the dipole moment of acetic acid, measured in benzene at concentrations below the CAC (1.50 D [16]), is almost coinciding with our value (1.57 D).

Even though compounds **II**–**V** are, too, dibasic acids, we can suggest that they will differ in behavior in solution from ordinary dicarboxylic acids. The results of ab initio calculations [17], vibration spectroscopy [17, 18], and X-ray diffraction study with full electron density analysis [19], dicarboxylic acids (up to sebacic) in crystal, solution, and liquid and gaseous states exist as open-chain structures combined to form hydrogen-bonded dimers of the tape type.

A characteristic feature of isosteviol (**I**) and, correspondingly, 16-hydroxyisosteviol (**XI**) which is the starting materal for the synthesis of esters **II**–**V** is that the carboxy and keto (or hydroxy) groups at the termini of the rigid *ent*-beyeran carcass locate strictly on one side of the carcass. As a result, the molecule looks like a rigid "∏-shaped bracket," with the CO_2H and OH groups at its termini. It can be suggested that during synthesis of compounds **II**–**V**, due to the presence in the reaction mixture of $CoCl_2$, a transition state (TS) arises, in which the mutual arrangement of the reagent molecules predetermines formation of a tweezer-like structure with an intramoleclar hydrogen bond.

Whether such a cyclic TS forms or not depends on the length of the polymethylene chain (spacer) in the acid chloride. Malonic acid chloride has an ideally sized spacer. Computations by the PM3 method [14] using the Gaussian98 program [15] show that the tweezer-like structure of compound **II** is preferred by 25.1 kJ mol^{-1} over open-chain. Actually, by X-ray diffraction data, compound **II** exists in crystal as a tweezer-like structure with an intramolecular hydrogen bond between the carboxy groups. Thus, we can suggest with assurance that the tweezer-like mono-



TS **II**, $n = 1$

molecular form of compound **II**, which exists in CCl_4 solutions at concentrations below the critical dimerization concentration, unlike what is observed with ordinary dicarboxylic acids, is already a kind of a "dimer," since it contains two hydrogen-bonded CO_2H groups belonging to two isosteviol fragments. At the same time, in compounds with a longer polymethylene spacer between two isosteviol fragments such a hydrogen-bonded tweezerlike structure becomes strained and straightens out, so that the carboxy groups become free. According to PM3 computations, the attendant energy gain, for example, for sebacic ester **V**, is 29.3 kJ mol^{-1}.

To establish the structure of compound **II** in solution, we applied the method of dipole moments [7], which was previously used to success in determining the structures of different classes of organic and organoelement compounds in solutions [4, 13, 20]. We used the same bond and group dipole moments as in isosteviol. The theoretical dipole moment (1.72 D) calculated by the vector additive scheme from the X-ray crystal molecular geometry of compound **II** proved to be much underestimated compared with experimental (4.5 D, Table 2). However, PM3 geometry optimization of compound **II** revealed its more polar form in which the spacer conformation differs from that in crystal.

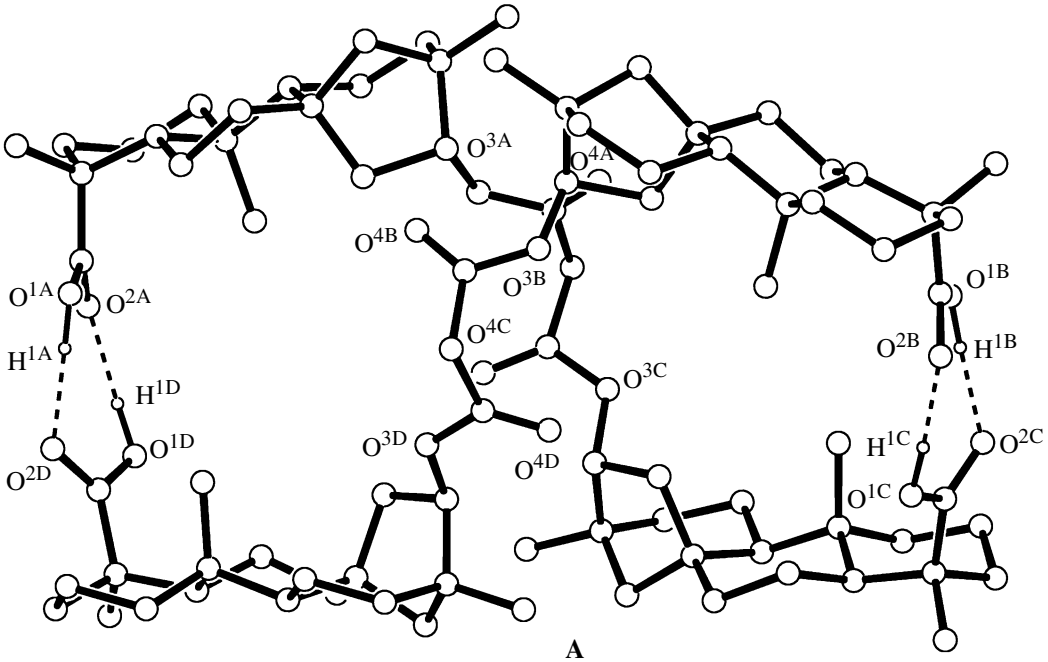
Table 2. Dipole moments of compounds **II**–**V** at concentrations below and above the critical aggregation concentration (CAC)

Comp. no.	μ, D (below CAC)	μ, D (above CAC)
II	4.50 ± 0.55	3.12 ± 0.32
III	4.70 ± 0.40	4.20 ± 0.38
IV	4.97 ± 0.48	4.00 ± 0.35
V	4.94 ± 0.66	4.50 ± 0.44, 3.28 ± 0.51

Dihedral angles, deg (see Fig. 3)	X-ray diffraction	PM3
$C^{13A}C^{16A}O^{16A}C^{21A}$	164	166
$C^{16A}O^{16A}C^{21A}C^{22}$	–178	–11
$O^{16A}C^{21A}C^{22}C^{21B}$	–90	–134
$C^{21A}C^{22}C^{21B}O^{16B}$	–93	–62
$C^{22}C^{21B}O^{16B}C^{16B}$	–180	–43
$C^{21B}O^{16B}C^{16B}C^{13B}$	171	–93

The dipole moment of the latter structure, calculated by the vector additive scheme, was 3.70 D, which is lower than experimental by 0.8 D. This difference can be explained by the presence in the concentration range below the CAC point of an open-chain monomeric form of compound **II**. The dipole moment of this form, calculated by the vector additive scheme, is 8.94 D, and its fraction in the solution, estimated by Eq. (2), is 10%.

Let us consider the possible dimeric forms of compound **II**, which can exist at concentrations above the CAC. According to PM3 computations, dimer **A** is preferred, but it is also the least polar. Its dipole moment calculated by the vector additive scheme is 0.7 D. Dimer **B** is more polar (1.32 D) but less favored by energy (by 12.6 kJ mol^{-1}) compared to dimer **A**. Computer simulation revealed one more, quite an unusual type of dimer. According to PM3 data, as the two tweezer-like forms of compound **II** approach each other (Fig. 3), they grab each other to form a pseudocatenane-type dimer **C**. As this takes place, the intramolecular $RCO_2H\cdots(O)HOCR$ hydrogen bonds in each of the two tweezer-like structures are cleaved, and the structures interpenetrate so that


O3A
O4A
O4B
O3B
O1A
O2A
O1B
H1A
O4C
O2B
H1B
H1D
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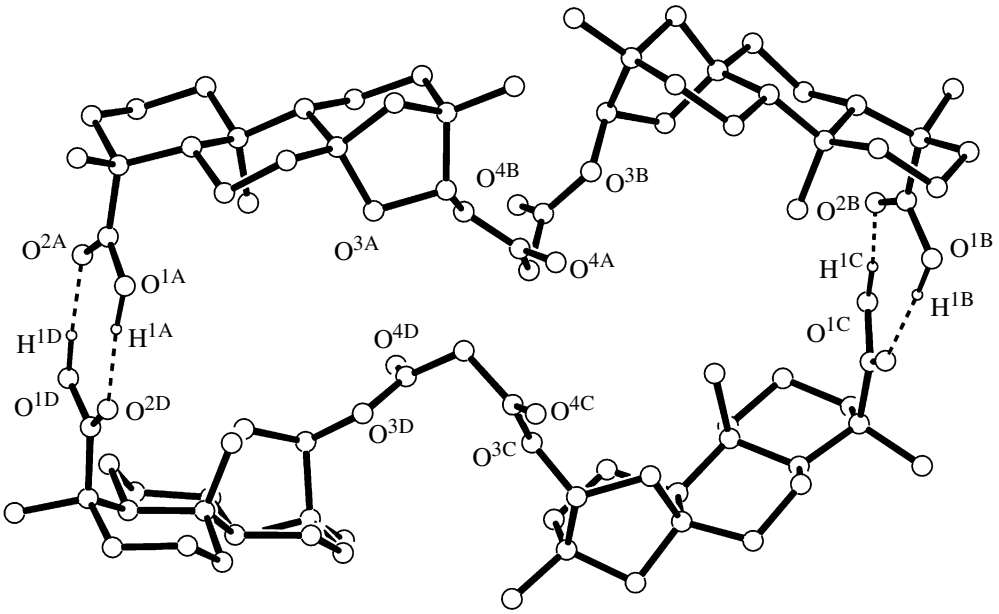
O1D
O3D
H1C
O2C
O2D
O4D
O1C

A


O4B
O3B
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O3A
O4A
O1B
O1A
H1C
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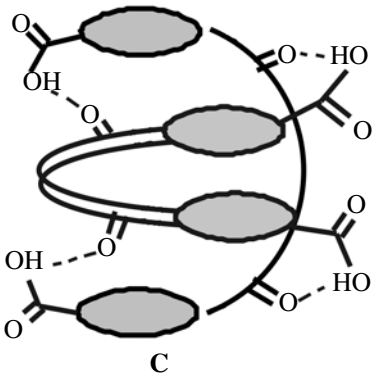
O4C
O3D
O3C

B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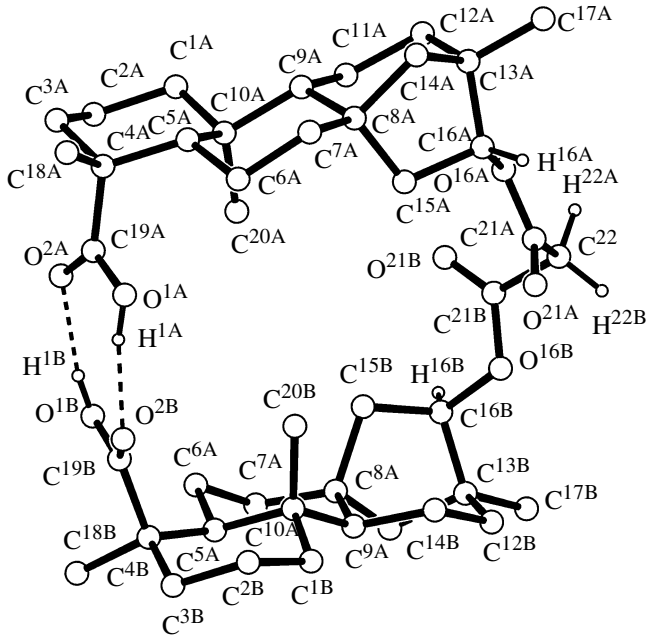

Fig. 3. Molecular geometry of compound **II** in crystal by X-ray diffraction data. Shown are carboxyl and spacer methylene hydrogens and hydrogens at C^{16}. The intramolecular hydrogen bond is shown by the dashed line.

the carboxyl hydroxyls of one of the molecules are hydrogen-bonded with the ester carbonyls of the other. Thus, four intermolecular $RCO_2H\cdots O{=}COR$ hydrogen bonds arise instead of two intramolecular $RCO_2H\cdots(O)HOCR$ hydrogen bonds. The relative energy of dimer **C** is about 12.6 kJ mol^{-1}, but its vector additive dipole moment is higher (1.96 D). To explain the experimental polarity of the solution of compound **II** at concentrations above the CAC (3.1 D, Table 2), we suggested formation in the solution, along with dimer **C**, of a highly polar (8.94 D) open-chain monomeric form. Its fraction estimated by Eq. (2) is 8%.

Probably, the three dimeric forms simulated with compound **II** as an example can also be present in CCl_4 solutions of compounds **II**–**V** at concentrations

Table 3. Optical density ratios D^{3525}/D^{2670} for compounds **I**–**V** in CCl_4 solutions

I	II	III	IV	V	c, M
0.20	–	–	–	–	1×10^{-2}
0.38	–	–	–	0.02	6×10^{-3}
0.55	–	–	–	0.04	4×10^{-3}
0.60	–	0.08	–	0.06	2.0×10^{-3}
1.04	0.002	0.10	–	0.08	2×10^{-4}–6×10^{-4}

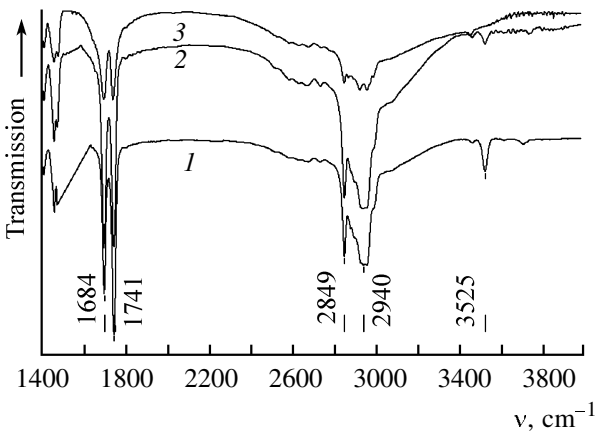

Fig. 4. IR spectra of isosteviol (**I**). (*1*) Solution in CCl_4, c 0.00048 M; (*2*) solution in CCl_4, c 0.0144 M; and (*3*) KBr pellet.

above the CAC. The only difference is that the molecules with longer spacers between the *ent*-beyeran carcasses will be more flexible and less folded, and will prefer dimeric form **B**. However, this will not affect considerably the polarity of solutions with concentrations above the CAC, since, in force of the mentioned features of the steric structure of compounds **II**–**V**, their dimeric forms will be roughly close in polarity (1–2 D). The most important factor here will be the presence in solutions of highly polar open-chain monomolecular forms. Their dipole moments estimated by the vector additive scheme for the PM3-optimized molecular geometries are, too, close for compounds **II**–**V** (8.94 D for malonic ester **II** and 9.30 D for sebacic ester **V**). Therefore, we can conclude that the fractions of these monomolecular forms in CCl_4 solutions at concentrations above the CAC will be close to each other (8–10%).

Evidence for this assumption was provided by the IR spectra of isosteviol (**I**) and compounds **II**–**V**.[1] As follows from the variation in the intensity of the stretching vibration band of the free carboxyl OH group (3525 cm^{-1}), in going from crystal to CCl_4 solution and with the subsequent dilution of the latter, the fraction of the polar monomolecular form tends to increase. This tendency is most pronounced with isosteviol (**I**) (Fig. 4).

Comparing the IR spectra measured in KBr pellets and in dilute CCl_4 solutions, we can see that in the solutions the stretching vibration bands of the free

[1] Detailed IR spectral analysis of compounds **I**–**V** will be reported in our further publication.

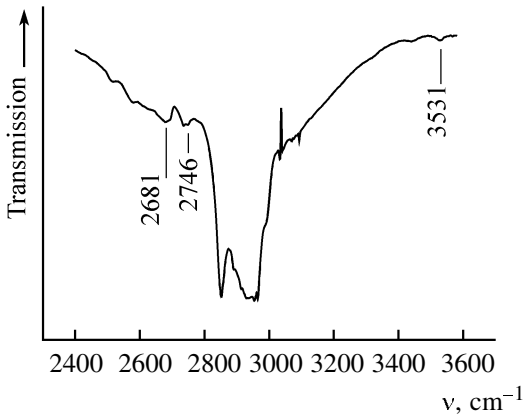

Fig. 5. IR spectrum of sebacic diester **V**. Solution in CCl_4, c 0.00011 M.

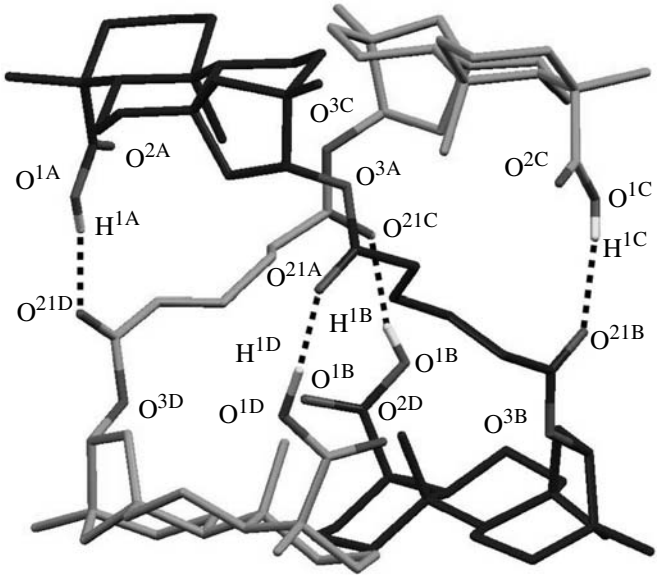

Fig. 6. Molecular geometry and hydrogen bonds (dashed lines) in the crystal of compound **III**. Numbering is shown only for carboxyl and ester oxygens and hydrogens involved in hydrogen bonding.

hydroxy group ν(OH) at 3525 cm^{-1} and free carbonyl group ν(C=O) of the carboxyl function (the latter band appears in the same region as that of the isosteviol keto group, i.e., at 1740 cm^{-1}) are stronger.

The percentages of the monomolecular forms of compounds **I**–**V** in CCl_4 can be directly estimated from the ratios of the optical densities of the free and associated carboxyl OH bands D^{3525}/D^{2670}, listed in Table 3. As seen from Table 3, at 10^{-3} M concentrations the fraction of the polar monomolecular form for isosteviol is 30–40% and no more than 6–8% for adipic and sebacic esters **III** and **V**. At concentrations of 10^{-4} M, the fraction of monomolecular isosteviol increases to 50%, whereas the fractions of monomolecular compounds **III** and **V** remain unchanged (8%). Even though the fraction of the monomers in the latter cases are small, their free OH stretching vibration bands are visible (Fig. 5). With malonic and suberic esters **II** and **IV**, no spectral evidence for the presence in solutions of the monomolecular forms of these compounds was obtained. Thus, by IR spectroscopy we could confirm the dielcometric and dipole-moment data showing that compounds **III** and **V** at concentrations above the CAC point can exist by about 8% in the polar monomolecular form.

It still remains unclear why compound **V** has two CAC points. Probably, the flexibility of this molecule allows existence of a greater number of dimers of various polarity than in the other compounds in question.

Evidence for the existence of dimers simulated with compound **II** as an example was obtained by X-ray diffraction analysis of esters **III**–**V**. Compound **III** exists in crystal as the dimer shown in Fig. 6. This dimer has the same pseudocatenane structure as dimer **C** predicted by PM3 computations. According to X-ray diffraction data, suberic ester **IV** exists in crystal as an unfolded structure like **B** (Fig. 7).

Thus, the dielcometric experiments, method of dipole moments, IR spectroscopy, and computer simulation show that esters **II**–**V** in CCl_4 solutions of $4–7 \times 10^{-4}$ M concentrations, which we named critical aggregation concentrations (CAC) undergo structural rearrangement. Below the CAC range, the solutions contain both tweezer-like (with an intramolecular hydrogen bond between the carboxy groups) and open-chain monomolecular forms. Above the CAC range, the solutions contain, along with lowpolarity ester **II**–**V** dimers of various structure, highly polar monomolecular forms (6–8%).

EXPERIMENTAL

Compounds **II**–**V** were synthesized as described above [5]. The dipole moments were all determined in CCl_4 soutions by the second Debye method [11], using the dielectric constants measured on a device described in [21] and the refractive indices at 20°C. Table 2 lists the dipole moments of compounds **II**–**V**, determined at concentrations below and above the CAC.

The IR spectra were measured on Bruker Vector 22 Fourier IR spectrometer (resolution 4 cm^{-1}) in KBr

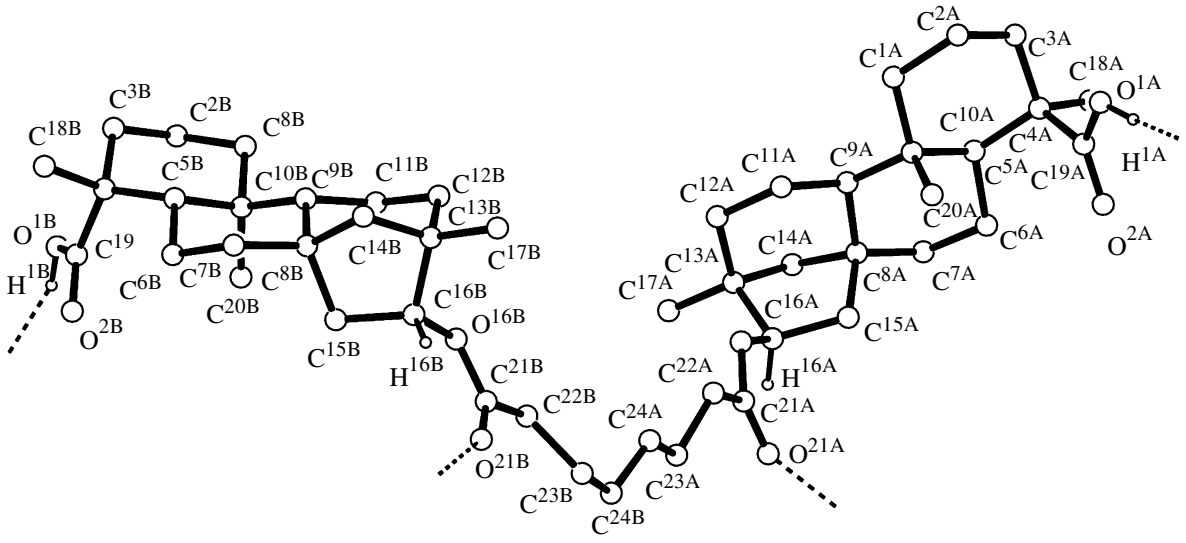

Fig. 7. Molecular geometry of compound **IV** in crystal. Shown are carboxyl hydrogens and hydrogens at C^{16}. Intermolecular hydrogen bonds are shown by dashed lines.

pellets for solids and in cells of various thickness for CCl_4 solutions.

Crystal data (except for structural factors) for compounds **I**, **III**, and **IV** are deposited in the Cambridge Structural Database, entry nos. CCDC 609479 (**II**), 609480 (**III**), and 609478 (**IV**). Details of the experiment and features of the crystal and molecular structure of the compounds will be reported elsewhere.

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REFERENCES

1. Al'fonsov, V.A., Andreeva, O.V., Bakaleinik, G.A., Beskrovnyi, D.V., Gubaidullin, A.T., Kataev, V.E., Kovylyaeva, G.I., Konovalov, A.I., Korochkina, M.G., Latypov, Sh.K., Litvinov, I.A., Musin, R.Z., and Strobykina, I.Yu., *Zh. Obshch. Khim.,* 2003, vol. 73, no. 7, p. 1186.
2. Alfonsov, V.A., Bakaleynik, G.A., Gubaidullin, A.T., Kataev, V.E., Kovyljaeva, G.I., Konovalov, A.I., Litvinov, I.A., Strobykina, I.Yu., Andreeva, O.V., and Korochkina, M.G., *Mendeleev Commun.,* 2000, no. 5, p. 177.
3. Alfonsov, V.A., Andreeva, O.V., Bakaleynik, G.A., Beskrovny, D.V., Kataev, V.E., Kovyljaeva, G.I., Litvinov, I.A., Militsina, O.I., and Strobykina, I.Yu., *Mendeleev Commun.,* 2003, vol. 13, no. 5, p. 234.
4. Kataev, V.E., Strobykin, S.I., Timosheva, A.P., Al'fonsov, V.A., Korochkina, M.G., and Strobykina, I.Yu., *Zh. Obshch. Khim.,* 2005, vol. 75, no. 2, p. 272.
5. Kataev, V.E., Militsina, O.I., Strobykina, I.Yu., Kovylyaeva, G.I., Musin, R.Z., Fedorova, O.V., Rusinov, G.L., Zueva, M.N., Mordovskoi, G.G., and Tolstikov, A.G., *Khim.-Farm. Zh.,* 2006, vol. 40, no. 9, p. 12.
6. Gur'yanova, E.N., Gol'dshtein, I.P., and Romm, I.P., *Donorno-aktseptornaya svyaz'* (Donor–Acceptor Bond), Moscow: Khimiya, 1973.
7. Zhil'tsova, E.P., Timosheva, A.P., Shagidullina, R.A., Mustafina, A.R., Kudryavtseva, L.A., Kataev, V.E., Kazakova, E.Kh., Nikolaev, V.F., and Konovalov, A.I., *Zh. Obshch. Khim.,* 2001, vol. 71, no. 3, p. 419.
8. Zhil'tsova, E.P., Timosheva, A.P., Kudryavtseva, L.A., Kataev, V.E., Sal'nikov, Yu.I., Ryzhkina, I.S., and Shagidullina, R.A., *Zh. Obshch. Khim.,* 2002, vol. 72, no. 7, p. 1088.
9. Zakharova, L.Ya., Valeeva, F.G., Kudryavtsev, D.B., Ibragimova, A.R., Kudryavtseva, L.A., Timosheva, A.P., and Kataev, V.E., *Kinet. Katal.,* 2003, vol. 44, no. 4, p. 599.
10. Iogansen, A.V., *Spectrochim. Acta, Part A,* 1999, vol. 55, no. 8, p. 1585.
11. Minkin, V.I., Osipov, O.A., and Zhdanov, Yu.A., *Dipole Moments in Organic Chemisty,* Leningrad: Khimiya, 1968.

12. Gordon, A.J. and Ford, R.A., *The Chemist's Companion, A Handbook of Practical Data, Techniques, and References,* New York: Wiley, 1972.

13. Semenov, V., Gubaidullin, A., Kataeva, O., Lodochnikova, O., Timosheva, A., Kataev, V., Giniyatullin, R., Nikolaev, A., Chernova, A., Shagidullin, R., Nafikova, A., and Reznik, R., *Struct. Chem.,* 2006, vol. 17, no. 4, p. 409.

14. Stewart, J.J.P., *J. Comput. Chem.,* 1989, vol. 10, p. 209.

15. Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman, J.R., Zakrzewski, V.G., Montgomery, J.A., Stratmann, R.E., Jr., Burant, J.C., Dapprich, S., Millam, J.M., Daniels, A.D., Kudin, K.N., Strain, M.C., Farkas, O., Tomasi, J., Barone, V., Cossi, M., Cammi, R., Mennucci, B., Pomelli, C., Adamo, C., Clifford, S., Ochterski, J., Petersson, G.A., Ayala, P.Y., Cui, Q., Morokuma, K., Malick, D.K., Rabuck, A.D., Raghavachari, K., Foresman, J.B., Cioslowski, J., Ortiz, J.V., Baboul, A.G., Stefanov, B.B., Liu, G., Liashenko, A., Piskorz, P., Komaromi, I., Gomperts, R., Martin, R.L., Fox, D.J., Keith, T., Al-Laham, M.A., Peng, C.Y., Nanayakkara, A., Challacombe, M., Gill, P.M.W., Johnson, B., Chen, W., Wong, M.W., Andres, J.L., Gonzalez, C., Head-Gordon, M., Replogle, E.S., and Pople, J.A., *Gaussian 98, Rev. A.9,* Pittsburgh PA: Gaussian, 1998.

16. McClellan, A.L., *Tables of Experimental Dipole Moments,* San Francisco: Freeman, 1963, vol. 1.

17. Tarakeshwar, P. and Manogaran, S., *Theochem,* 1996, vol. 362, p. 77.

18. Wolfs, I. and Desseyn, H., *Appl. Spectrosc.,* 1996, vol. 50, no. 8, p. 1000.

19. Gopalan, R.S., Kumaradhas, P., Kulkarni, G.U., and Rao, C.N.R., *J. Mol. Struct.,* 2000, vol. 521, p. 97.

20. Kataev, V.E., Ishmaeva, E.A., Patsanovskii, I.I., Kataev, A.V., Vechorek, V., Yarkova, E.G., Zygo, K., and Petrusevich, K.M., *Zh. Obshch. Khim.,* 1998, vol. 68, no. 11, p. 1798.

21. Nigmatullin, R.Sh., Vyaselev, M.R., and Shatunov, V.S., *Zavod. Lab.,* 1964, no. 30, p. 500.