785. *Molecular Polarisability: The Conformations of Diethyl Oxalate, Malonate, Succinate, Adipate, and Sebacate as Solutes in Carbon Tetrachloride.*

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Dipole moments, molar Kerr constants, etc., are recorded for the esters named in the title. From known bond polarities and polarisabilities, the resultant moments and anisotropies of various conformations of these "flexible" esters are computed *a priori*, and are compared with values from experiment. In ethyl acetate the C_2H_5 group appears to lie in a plane normal to that containing the $Me{\cdot}CO_2$ unit. Diethyl oxalate is probably a mixture of *cis*- and *trans*-isomers, neither of which is planar. Observations on the remaining esters can be interpreted only if with such solutes several (specified) forms are simultaneously present.

Measurements here recorded concern αω-diethyl esters of the type $[CH_2]_n(CO{\cdot}OEt)_2$ having $n = 0$, 1, 2, 4, and 8. They each contain six polar bonds for which a variety of mutual dispositions are possible even if internal rotations are hindered. The literature gives little information on the conformations adopted by such "flexible" molecules as solutes—a state to which our methods, dependent on the analysis of polarisability and polarity into bond values having directional qualities, are conveniently applicable.

Experimental

The esters were purified commercial samples; they were dried with anhydrous magnesium sulphate, then redistilled immediately before solutions were prepared: diethyl malonate, b. p. 198°; diethyl succinate, b. p. 217—218°; diethyl adipate, b. p. 102—106°/4 mm.; diethyl sebacate, b. p. 142—144°/3—5 mm.

Details of procedures, apparatus, computational methods, symbols used, etc., are given in refs. 1—3. For pure carbon tetrachloride (*i.e.*, when $w_2 = 0$ in Table 1) at 25°, the properties indicated have values as follow: ε (dielectric constant) = 2·2270; *d* (density) = 1·58454; *n* (refractive index) = 1·4575; *B* (Kerr constant) = $0{\cdot}070 \times 10^{-7}$.

Previous Measurements.—There are no dipole-moment determinations, made before 1948, listed by Wesson [4] in the M.I.T. Tables, for these esters as solutes in carbon tetrachloride. Since 1948 the annexed have been recorded.

Solute †	Solvent	μ (D)	Ref.	Solute †	Solvent	μ (D)	Ref.
Et_2 malonate	C_6H_6	2·1	5	Et_2 adipate	C_6H_6	2·25	5
,,	,,	2·47—2·51 *	6	,,	,,	2·42	7
,,	Dioxan	2·49—2·52 *	6	,,	,,	2·35—2·39 *	6
Et_2 succinate	C_6H_6	2·13—2·14 *	6	,,	Dioxan	2·38—2·41 *	6
,,	Dioxan	2·15—2·20 *	6	Et_2 sebacate	C_6H_6	2·42—2·45 *	6
				,,	Dioxan	2·43—2·48 *	6

* Only determinations at 20° have been included; ref. 6 contains also measurements at 45° and 70°.
† No earlier estimates exist of the molar Kerr constants of these four esters.

Discussion

Anisotropic Polarisabilities of the Ethoxycarbonyl Group.—Le Fèvre and Sundaram [8] have shown that for methyl acetate the carbon atom, corresponding to *C in Fig. 1, is

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[1] Le Fèvre, "Dipole Moments," Methuen, London, 3rd edn., 1953.

[2] Buckingham, Chau, Freeman, Le Fèvre, Rao, and Tardif, *J.*, 1956, 1405.

[3] Le Fèvre and Le Fèvre, (*a*) *J.*, 1953, 4041; (*b*) *Rev. Pure Appl. Chem.*, 1955, **5**, 261; (*c*) Chap. XXXVI in "Physical Methods of Organic Chemistry," ed. Weissberger, Interscience Pub., New York, London, 3rd edn., Vol. I, p. 2459.

[4] Wesson, "Tables of Electric Dipole Moments," Technology Press, M.I.T., 1948.

[5] Jatkar and Phansalkar, *J. Univ. Poona Sci. and Technol.*, 1953, 45.

[6] Ketelaar and van Meurs, *Rec. Trav. chim.*, 1957, **76**, 437.

[7] Shott-L'vova and Syrkin, *Izvest. Akad. Nauk S.S.S.R., Otdel. Khim. Nauk*, 1954, 381.

[8] Le Fèvre and Sundaram, *J.*, 1962, 3904.

TABLE 1.

Incremental Kerr effects, refractive indexes, dielectric constants, and densities of solutions in carbon tetrachloride at 25°.

Diethyl malonate

10^5w_2	2631	3124	3967	4081	4214	4373
$10^7\Delta B$	0·054	0·064	0·079	0·081	0·082	0·084
$-10^4\Delta n$	—	—	—	28	29	30

whence $\Sigma 10^7\Delta B/\Sigma w_2 = 1{\cdot}99$; $\Sigma\Delta n/\Sigma w_2 = -0{\cdot}069$

10^5w_2	390	756	1024	1052	1535	1583	2588	2910	3344
ε^{25}	2·2575	2·2860	2·3046	2·3066	2·3414	2·3450	2·4174	—	2·4708
d_4^{25}	1·58124	1·57826	1·57620	1·57596	—	—	1·56358	1·56070	—

whence $\Delta\varepsilon = 7{\cdot}70w_2 - 12{\cdot}4w_2^2$; $\Sigma\Delta d/\Sigma w_2 = -0{\cdot}818$

Diethyl sucinnate

10^5w_2	2393	2886	3574	4381	4499	6317
$10^7\Delta B$	0·019	0·023	0·029	0·036	0·037	0·051
$-10^4\Delta n$	—	—	—	26	27	37

whence $\Sigma 10^7\Delta B/\Sigma w_2 = 0{\cdot}809$; $\Sigma\Delta n/\Sigma w_2 = -0{\cdot}059$

10^5w_2	642	834	1372	1685	2145	2610	2805	4244
ε^{25}	2·2570	2·2657	2·2905	—	2·3264	2·3469	—	2·4212
d_4^{25}	1·57908	1·57753	1·57297	1·57029	1·56657	1·56278	1·56113	—

whence $\Sigma\Delta\varepsilon/\Sigma w_2 = 4{\cdot}66$; $\Sigma\Delta d/\Sigma w_2 = -0{\cdot}839$

Diethyl adipate

10^5w_2	1317	1475	2017	2089	3059	3270
$10^7\Delta B$	0·017	0·020	0·026	0·028	0·042	0·044
$-10^4\Delta n$	—	—	—	8	14	15

whence $\Sigma 10^7\Delta B/\Sigma w_2 = 1{\cdot}33$; $\Sigma\Delta n/\Sigma w_2 = -0{\cdot}044$

10^5w_2	541	702	1317	1475	2017	2089
ε^{25}	2·2546	2·2629	2·2930	2·3024	2·3285	2·3321
d_4^{25}	1·57976	1·57827	1·57274	1·57128	1·56672	1·56577

whence $\Sigma\Delta\varepsilon/\Sigma w_2 = 5{\cdot}01$; $\Sigma\Delta d/\Sigma w_2 = -0{\cdot}893$

Diethyl sebacate

10^5w_2	1665	2537	3223	3511	3800	5029	5036	5312
$10^7\Delta B$	0·014	—	0·028	—	0·034	0·043	0·044	0·046
$-10^4\Delta n$	—	8	—	11	—	—	—	—

whence $\Sigma 10^7\Delta B/\Sigma \mathrm{w}_2 = 0{\cdot}867$; $\Sigma\Delta n/\Sigma w_2 = -0{\cdot}031$

10^5w_2	253	881	1354	1665	3223	3800	5003	5036
ε^{25}	—	2·2691	2·2920	2·3065	2·3805	2·4068	2·4619	2·4645
d_4^{25}	1·58208	1·57574	1·57095	1·56770	1·55283	—	—	1·53499

whence $\Sigma\Delta\varepsilon/\Sigma w_2 = 4{\cdot}72$; $\Sigma\Delta d/\Sigma w_2 = -0{\cdot}991$

TABLE 2.

Polarisations, dipole moments, and molar Kerr constants (from observations on solutions in carbon tetrachloride at 25°).

Solute	$\alpha\varepsilon_1$	β	γ	δ	$_\infty P_2$ (c.c.)	R_D (c.c.)	μ (D) *	$10^{12}{}_\infty({}_mK_2)$
$CH_2(CO_2Et)_2$	7·70	$-0{\cdot}51_6$	−0·047	28·4	175·2	38·3	2·57	31·6
$[CH_2]_2(CO_2Et)_2$	4·66	$-0{\cdot}52_9$	−0·040	11·6	134·8	42·5	2·10	14·3
$[CH_2]_4(CO_2Et)_2$	5·01	$-0{\cdot}56_3$	−0·030	19·0	166·3	51·5	2·34	27·6
$[CH_2]_8(CO_2Et)_2$	4·72	$-0{\cdot}62_5$	−0·022	12·4	206·1	69·6	2·55	22·8

* Calc. by assuming $_DP = 1{\cdot}05R_D$.

TABLE 3.

Calculations for ethyl acetate.

Fig.	$10^{23}b_1$	$10^{23}b_2$	$10^{23}b_3$	$10^{12}{}_mK$, calc.	$10^{12}{}_\infty({}_mK_2)$
1	0·928	0·949	0·699	+24·1	+20·1
2*a*	0·967	0·880	0·729	+27·7	,,
2*b*	0·929	0·878	0·770	+19·4	,,

elevated 30° from the trigonal carbon plane (cf. ref. 9, p. 4223; ref. 10, M 132). If then the methyl acetate skeleton is retained in ethyl acetate, *C–C can be rotated about O–C* as axis through a range of approximately ±110° from the position supposed in Fig. 1, *i.e.*, in which *C–C is roughly parallel with C–O but elevated above the sp^2-carbon plane. Molecular models show that rotations greater than this result in steric interaction with the carbonyl group. Positions *a* and *b* in Fig. 2 represent the two possible dispositions of the ethyl group when the plane O–*C–C is normal to that of the trigonal carbon valencies. Molecular polarisability semi-axes for the configurations, 1, 2*a*, and 2*b*, have been calculated by addition of bond components and these, together with the resolutes of the permanent dipole moment along the principal axes, lead to estimates of the molar Kerr constant (${}_{\mathrm{m}}K$,calc.) for each structure. Calculations are summarised in Table 3. The following bond polarisability specifications were used: $b_{\mathrm{L}}^{\mathrm{C-C}} = 0{\cdot}099$, $b_{\mathrm{T}}^{\mathrm{C-C}} = b_{\mathrm{V}}^{\mathrm{C-C}} = 0{\cdot}027$, $b_{\mathrm{L}}^{\mathrm{C-H}} = b_{\mathrm{T}}^{\mathrm{C-H}} = b_{\mathrm{V}}^{\mathrm{C-H}} = 0{\cdot}064$, $b_{\mathrm{L}}^{\mathrm{C-O}} = 0{\cdot}081$, $b_{\mathrm{T}}^{\mathrm{C-O}} = b_{\mathrm{V}}^{\mathrm{C-O}} = 0{\cdot}039$, $b_{\mathrm{L}}^{\mathrm{C=O}} = 0{\cdot}230$, $b_{\mathrm{T}}^{\mathrm{C=O}} = 0{\cdot}140$, $b_{\mathrm{V}}^{\mathrm{C=O}} = 0{\cdot}046$ (all $\times 10^{-23}$ c.c.).

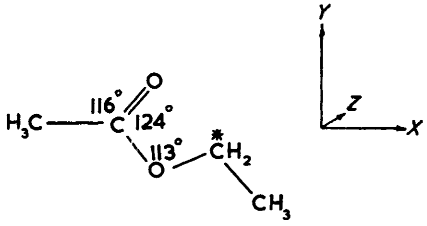

FIG. 1.

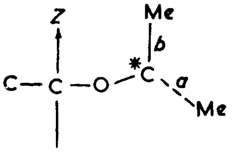

FIG. 2.

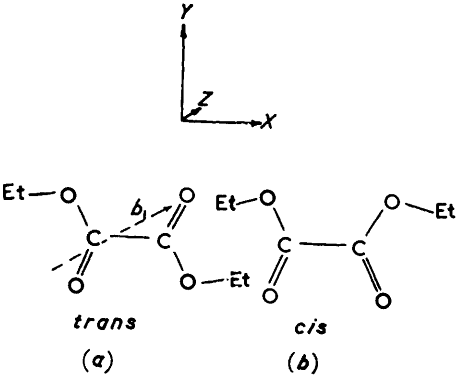

FIG. 3.

Configuration 2*b* affords best agreement with experiment. If from the polarisability tensor for this structure, the elements of which are referred to the axes *X*, *Y*, *Z* of Fig. 1, we subtract the contributions of three C–H bonds and of the link C–C, we derive the semi-axes b_i' specifying the group CO_2Et and their locations within the reference co-ordinate axes:

	Direction cosines with *X*	*Y*	*Z*
$b_1' = 0{\cdot}618$	+0·922	−0·379	+0·077
$b_2' = 0{\cdot}679$	+0·378	+0·926	+0·023
$b_3' = 0{\cdot}551$	−0·081	+0·009	+0·997

For geometrical simplification in the succeeding calculations b_3' has been taken as coincident with the *Z* direction. Following Le Fèvre and Sundaram [8] we accept the ethoxycarbonyl group moment components as $\mu_X = +0{\cdot}75$, $\mu_Y = +1{\cdot}55$, and $\mu_Z = -0{\cdot}66$ D.

Diethyl Oxalate.—Dougill and Jeffrey (ref. 10, M 167) have shown by *X*-ray diffraction that the solid-state isomer of dimethyl oxalate is the *trans*-form alone. The spectroscopic studies of Mizushima [11] and Miyazawa [12,13] indicate that in the liquid and the gaseous

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[9] O'Gorman, Shand, and Schomaker, *J. Amer. Chem. Soc.*, 1950, **72**, 4222.

[10] Sutton, " Tables of Interatomic Distances and Configuration in Molecules and Ions," *Chem. Soc. Spec. Publ.* No. 11, 1958.

[11] Mizushima, " Internal Rotation and Molecular Configuration," Academic Press Inc., New York, 1954, p. 75.

[12] Miyazawa and Kurantani, *J. Chem. Soc. Japan*, 1951, **72**, 804.

[13] Miyazawa, *J. Chem. Soc. Japan*, 1954, **75**, 540.

states this substance exists as a mixture of (presumably flat) *cis*- and *trans*-isomers, with no *gauche*-conformation present.

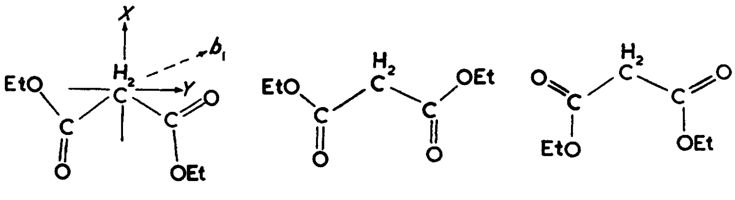
Fig. 3*a* and *b* represent diagrammatically the *trans*- and the *cis*-form, respectively, constructed with non-planar CO_2Et groups as derived from 2*b* above; the *cis* is generated from the non-polar *trans*-configuration by a 180° rotation of one ethoxycarbonyl group about the central C–C bond as axis. This results in a non-vanishing resultant moment (1·32 D) in the *Z* direction, in addition to that along the $-Y$ axis. In form 3*a*, the semi-axes b_1 and b_2 are located in the *X*,*Y* plane with b_1 50° from *X*; in form 3*b* the principal polarisabilities b_1, b_2, and b_3 coincide with *X*, *Y*, and *Z*, respectively. Calculations are summarised in Table 4.

TABLE 4.

Calculations for diethyl oxalate.

Fig.	$10^{23}b$, calc.	μ, calc. (D)	$10^{12}{}_{m}K$, calc.	Fig.	$10^{23}b$, calc.	μ, calc. (D)	$10^{12}{}_{m}K$, calc.
3*a*, *trans*	$b_1 = 1·403$ $b_2 = 1·317$ $b_3 = 1·129$	0	+2·9	3*b*, *cis*	$b_1 = 1·353$ $b_2 = 1·367$ $b_3 = 1·129$	3·4	+91·2

For an equivalent mixture of *cis*- and *trans*-isomers the following are predicted: μ,calc. $= 2·3_8$ D, ${}_{m}K$, calc. $= +47 \times 10^{-12}$, in good agreement with the observed values of $2·4_1$ D and $+45·4 \times 10^{-12}$, respectively (as recorded by Le Fèvre, Le Fèvre, and Oh, ref. 14, p. 223). If, however, the ethoxycarbonyl group polarisabilities are derived from structure 1 (Fig. 1) for ethyl acetate, then the calculated molar Kerr constants for diethyl oxalate conformations are $+10·2 \times 10^{-12}$ (*trans*) and $+232 \times 10^{-12}$ (*cis*), whereupon a 1 : 1 ratio gives the correct $\mu_{\text{resultant}}$, but yields an ${}_{m}K$, calc. of $+121 \times 10^{-12}$, which is too high. For a structure intermediate between 3*a* and *b*, with the two trigonal carbon planes at right angles, μ,calc. $= 2·3_8$ D and ${}_{m}K$, calc. $= -32 \times 10^{-12}$.



(*a*) (*b*) (*c*)

FIG. 4.

Diethyl Malonate.—Polarisability semi-axes, resultant dipole moments, and molar Kerr constants computed for conformations 4*a*—*c* of diethyl malonate are listed in Table 5.

TABLE 5.

Calculations for diethyl malonate.

$10^{23}b$, calc.	μ, calc. (D)	$10^{12}{}_{m}K$, calc.	$10^{23}b$, calc.	μ, calc. (D)	$10^{12}{}_{m}K$, calc.	$10^{23}b$, calc.	μ, calc. (D)	$10^{12}{}_{m}K$, calc.
Form 4*a*			Form 4*b*			Form 4*c*		
$b_1 = 1·569$ $b_2 = 1·533$ $b_3 = 1·284$	2·0	+56·6	$b_1 = 1·582$ $b_2 = 1·520$ $b_3 = 1·284$	3·6	+181	$b_1 = 1·502$ $b_2 = 1·600$ $b_3 = 1·284$	2·1	−28·9

Models give little guidance in choosing from the infinitude of possible conformations; we therefore consider the simplest, *i.e.*, those in which the unit $O_2C{\cdot}C{\cdot}CO_2$ is planar. In each case b_3 is coincident with the *Z* axis; b_1 and b_2 lie along the *X* and the *Y* direction, respectively, for structures 4*b* and *c*; b_1 for configuration 4*a* is located 60° from *X* as indicated.

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[14] Le Fèvre, Le Fèvre, and Oh. *Austral, J. Chem.*, 1957, **10**, 218.

The observed values from Table 2 are: $\mu = 2{\cdot}57$ D, and ${}_{\infty}({}_{\mathrm{m}}K_2) = 31{\cdot}6 \times 10^{-12}$. Clearly none of the three structures considered is present alone. A mixture of all three can be made to give a resultant dipole moment and molar Kerr constant compatible with experiment.

Esters of Formula $[\mathrm{CH_2}]_n(\mathrm{CO_2Et})_2$, *where* n = 2, 4, *and* 8.—*X*-Ray crystallographic investigations (ref. 10, M 166, M 203, M 226) show that the solid-state configuration for succinic, adipic, and sebacic acid is one in which the carbon atoms of the methylene groups have a planar, extended, zig-zag arrangement and the carbonyl groups, which are *trans* to each other, are substantially in this plane (the slight deviations reported are generally attributable to effects of hydrogen-bonding with closely neighbouring acid molecules).

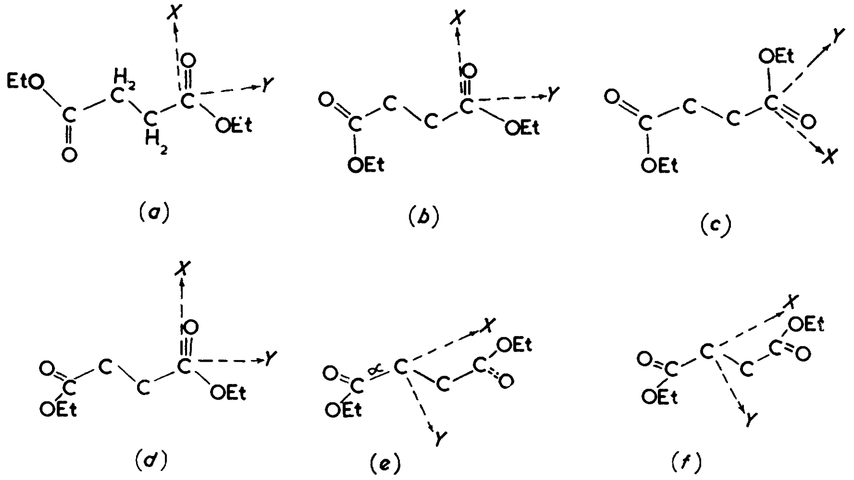

FIG. 5.

In the present work we examine the various possible isomers generated by rotations of the terminal ethoxycarbonyl groups relative to each other and to the methylene carbon chain. Fig. 5*a* represents a non-polar *trans*-type structure closely analogous to the solid-state configuration of succinic acid; 5*b* is formed from 5*a* by rotation of one ethoxycarbonyl group through 180°, and 5*c* by rotation of both ethoxycarbonyl groups 180° from their respective positions in 5*a*. Calculated values of the molecular polarisabilities, dipole moments, and molar Kerr constants are listed in Table 6. C–C–C bond angles for the methylene carbon atoms have been taken as 110° throughout. The reference co-ordinate axes have been chosen so that *X*, *Y*, and *Z* coincide with the principal axes b_1', b_2', and b_3' respectively, of the ethoxycarbonyl group upon which they have been superimposed in the diagrams 5*a*—*c*.

The observed values are: $\mu = 2{\cdot}10$ D, and ${}_{\infty}({}_{\mathrm{m}}K_2) = +14{\cdot}3 \times 10^{-12}$. None of the

TABLE 6.

Calculations for diethyl succinate

$10^{23}b$, calc.	Direction cosines with *X*	*Y*	*Z*	μ, calc.	$10^{12}{}_{\mathrm{m}}K$, calc.	$10^{23}b$, calc.	Direction cosines with *X*	*Y*	*Z*	μ, calc.	$10^{12}{}_{\mathrm{m}}K$ calc.
		Form 5*a*						Form 5*b*			
$b_1 = 1{\cdot}763$	+0·916	+0·401	0			$b_1 = 1{\cdot}720$	+0·928	+0·372	0		
$b_2 = 1{\cdot}721$	−0·401	+0·916	0	0	+4·7	$b_2 = 1{\cdot}764$	−0·372	+0·928	0	3·4	+106
$b_3 = 1{\cdot}439$	0	0	+1			$b_3 = 1{\cdot}439$	0	0	+1		
		Form 5*c*									
$b_1 = 1{\cdot}808$	+0·920	+0·392	0								
$b_2 = 1{\cdot}676$	−0·392	+0·920	0	0	+5·3						
$b_3 = 1{\cdot}439$	0	0	+1								

conformations 5*a*—*c* can be present alone nor will any mixture of these give both the right dipole moment and molar Kerr constant; *e.g.*, a mixture of polar form 5*b* (39%) with non-polar form 5*a* or 5*c* (61%) yields the observed dipole moment, but the resultant ${}_{\rm m}K$, calc. becomes (44·6—44·7) × 10^{-12}. The low value of ${}_\infty({}_{\rm m}K_2)$ suggests the participation in the equilibrium mixture of structures in which the group $O_2C{\cdot}C{\cdot}C{\cdot}CO_2$ is non-planar. Accordingly *gauche*-type dispositions of the ethoxycarbonyl groups must also be considered. Fig. 5*d* represents one such group *trans* and the other *gauche* (achieved by rotation of the CO_2Et group through ±120° from the *trans*-position as in 5*a*); 5*e* is a *gauche,-gauche*-type structure in which the group moments are anti-parallel, to give a non-polar isomer; 5*f* is a polar *gauche,gauche*-arrangement in which the carbonyl groups both project above the plane of the methylene carbon atoms. Calculated values for conformations 5*d*—*f* are summarised in Table 7. The axes *X*, *Y*, and *Z* for the *trans,gauche*-form coincide with b_1', b_2', and b_3', respectively, of the CO_2Et group (indicated in Fig. 5*d*); for the configurations 5*e* and *f*, *X* is collinear with the longitudinal axis of the α-C–C bond, and *Y* is perpendicular to *X* and in the plane of the C_4 chain; *Z* is normal to this plane.

TABLE 7.

Calculations for diethyl succinate.

$10^{23}b$, calc.	Direction cosines with *X*	Direction cosines with *Y*	Direction cosines with *Z*	μ, calc.	$10^{12}{}_{\rm m}K$, calc.
Form 5*d*					
$b_1 = 1·665$	+0·944	−0·131	+0·303	2·9	−26·4
$b_2 = 1·752$	+0·180	+0·974	−0·140		
$b_3 = 1·507$	−0·276	+0·186	+0·943		
Form 5*e*					
$b_1 = 1·779$	+0·829	+0·347	−0·438	0	+3·4
$b_2 = 1·482$	+0·007	+0·778	+0·629		
$b_3 = 1·661$	+0·559	−0·524	+0·643		
Form 5*f*					
$b_1 = 1·749$	+0·984	+0·181	0	2·9	−47·8
$b_2 = 1·560$	−0·181	+0·984	0		
$b_3 = 1·613$	0	0	+1		

Accord with experiment can be attained only if we regard the dissolved species as a mixture of several rotational isomers.

Conformations of diethyl adipate (6*a*—*f*) and diethyl sebacate (7*a*—*f*) analogous to structures 5*a*—*f* have been similarly examined. The physical constants thus calculable are listed in Tables 8 and 9, respectively.

The observed quantities are for diethyl adipate, μ = 2·34 D and ${}_\infty({}_{\rm m}K_2) = +27·6 \times 10^{-12}$; and for diethyl sebacate, μ = 2·55 D and ${}_\infty({}_{\rm m}K_2) = +22·8 \times 10^{-12}$. As for diethyl succinate, conformations 6 (or 7) *a*—*c*, *i.e.*, with the group $O_2C{\cdot}[C]_{4\text{ or }8}{\cdot}CO_2$ planar, cannot alone account for the observed quantities. Agreement with experiment can be achieved only if we regard each of the esters in this solvent environment as a mixture of all possible isomers.

TABLE 8.

Calculations for diethyl adipate.

$10^{23}b$, calc.	Direction cosines with *X*	Direction cosines with *Y*	Direction cosines with *Z*	μ, calc.	$10^{12}{}_{\rm m}K$, calc.
Form 6*a*					
$b_1 = 2·115$	+0·962	−0·271	0	0	+7·0
$b_2 = 2·133$	+0·271	+0·962	0		
$b_3 = 1·749$	0	0	+1		
Form 6*b*					
$b_1 = 2·078$	+0·956	+0·292	0	3·4	+119
$b_2 = 2·170$	−0·292	+0·956	0		
$b_3 = 1·749$	0	0	+1		
Form 6*c*					
$b_1 = 2·215$	+0·902	+0·432	0	0	+8·3
$b_2 = 2·034$	−0·432	+0·902	0		
$b_3 = 1·749$	0	0	+1		
Form 6*d*					
$b_1 = 2·025$	+0·977	−0·035	+0·211	2·9	−59·5
$b_2 = 2·151$	+0·061	+0·991	−0·117		
$b_3 = 1·822$	−0·205	+0·127	+0·970		
Form 6*e*					
$b_1 = 2·172$	+0·882	+0·356	−0·307	0	+4·5
$b_2 = 2·000$	−0·470	+0·639	−0·608		
$b_3 = 1·826$	−0·020	+0·681	+0·732		
Form 6*f*					
$b_1 = 2·149$	+0·965	+0·262	0	2·9	−101
$b_2 = 1·926$	−0·262	+0·965	0		
$b_3 = 1·923$	0	0	+1		

TABLE 9.

Calculations for diethyl sebacate.

$10^{23}b$, calc.	Direction cosines with			μ, calc.	$10^{12}{}_{\mathrm{m}}K$, calc.	$10^{23}b$, calc.	Direction cosines with			μ, calc.	$10^{12}{}_{\mathrm{m}}K$, calc.
	X	Y	Z				X	Y	Z		
		Form 7*a*						Form 7*d*			
b_1 = 2·836	+0·988	+0·152	0			b_1 = 2·742	+0·988	+0·097	+0·123		
b_2 = 2·940	−0·152	+0·988	0	0	+13·9	b_2 = 2·957	−0·087	+0·993	−0·086	2·9	−121
b_3 = 2·369	0	0	+1			b_3 = 2·448	−0·130	+0·074	+0·989		
		Form 7*b*						Form 7*e*			
b_1 = 2·976	+0·966	+0·259	0			b_1 = 2·970	+0·897	+0·399	−0·191		
b_2 = 2·980	−0·259	+0·966	0	3·4	+151	b_2 = 2·689	−0·441	+0·785	−0·435	0	+8·8
b_3 = 2·369	0	0	+1			b_3 = 2·487	−0·023	+0·475	+0·880		
		Form 7*c*						Form 7*f*			
b_1 = 3·026	+0·882	+0·471	0			b_1 = 2·955	+0·933	+0·360	0		
b_2 = 2·750	−0·471	+0·882	0	0	+16·4	b_2 = 2·648	−0·360	+0·933	0	2·9	−204
b_3 = 2·369	0	0	+1			b_3 = 2·543	0	0	+1		

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