CONFORMATION AROUND SEVERAL EQUIVALENT BONDS. POLYMETHOXY DERIVATIVES OF BENZENE

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Dedicated to Academician J. Mostecký on the occasion of his 60th birthday.

Dipole moments of benzene methoxy derivatives *I—IX* were measured in benzene solution and discussed in terms of the conformation around the C_{ar}—O bonds, exploiting the method of graphical comparison and systematic introduction of substituents. In the case of 1,2-dimethoxybenzene several explanations are in accord with the dipole moment data. However, considering all available evidence, most probable seems to be the presence of two conformers, one of which is non-planar with two non-equivalent methoxy groups (*IC*). The conformation of 1',2,3-trimethoxybenzene is similar to that found for many derivatives in the crystalline phase (*VC*), only the outer methoxy groups are probably slightly deviating from the coplanar position.

On model compounds of different kind we have examined a general problem: conformation around two equivalent single bonds attached to a common central atom. Early work summarized in ref.[1] lead us to conclude that conformations of simple monofunctional compounds are largely retained in gem-derivatives unless the steric hindrance is too strong. This was confirmed by later results[2–6]. A logical extension of these investigations points to aromatic *ortho* derivatives with equal substituents. In these compounds the two axes of rotation are separated by two atoms but the steric hindrance is more significant. In addition to the latter factor, the conformation is controlled by conjugation with the benzene nucleus, favouring more or less the planar forms, and by electrostatic forces. In general, three planar conformers are possible of which the unsymmetrical one (*e.g. IB*) is always stabilized by electrostatic attraction but the steric repulsion in it is intermediate between the two symmetrical forms; compare the situation with gem-derivatives[1] where steric and electrostatic effects are operating in the same direction. In one or more conformers the steric hindrance can evercome the resonance energy so that planarity is no more retained. For these reasons even a reference to monofunctional compounds[1] cannot help in predicting conformation; rather another *ortho* derivative would be needed as model compound, bearing a non-rotating *ortho*-substituent of the same steric size and of similar charge distribution.

In this communication we are dealing with 1,2-dimethoxy and 1,2,3-trimethoxy derivatives of benzene. The conformation of methoxybenzene is planar in the gas phase[7-10] and with all probability also in solution[11-14]; some divergent claims based on measurement[15] of the Kerr constant or on approximate calculations[16,17] cannot be given credit. In the molecule of 1,2-dimethoxybenzene (*I*) the conjugation is weakened[11,18,19] and the torsional barrier lowered[14], hence the occurrence of various non-planar conformers is made possible[13,14,17,18,20,21]. However, a more detailed description was only seldom attempted. Most often, still an equilibrium of the two planar forms was assumed[12,13,22]: *IA* denoted* as *anti-anti* or (180°, 0°), and the less populated *IB* denoted as *syn-anti* or (0°, 0°), the latter being possibly slightly non-planar[13]. Recently, convincing arguments in favour of non-planar conformations have been collected[14]; most probable appeared the form *IC* (possibly with some admixture of *IB*) according to the PE spectra combined with STO-3G calculations, but *ID* was the most stable form according to the calculations themselves[14]. Further authors[18,23] believed a C_2 symmetrical conformer (near to *ID*) to be the most abundant. Finally, a quite improbable distorted conformation was claimed with the oxygen atoms out of the ring plane[24]. The last result throws doubts on the applicability of the Kerr constant; further arguments come from PES[14], quantum chemical calculations[14,17], and little telling X-ray results[14], but most attention has been given to dipole moments[12,13,19-25]. In particular their temperature dependence was considered as significant, although it could not be unambiguously explained[13,14] and even the experimental results[20,21] are not quite consistent. However, the main weakness of the reasoning based on dipole moments is that it has referred only to a single compound, 1,2-dimethoxybenzene; therefore it is too sensitive to the adopted value of the OCH_3 group moment. In this work we have exploited the method of introducing substituents with known bond moments[26] and evaluated the results using graphical representation[27]. In Table I we report the dipole moments of the derivatives *II−IV*.


(180, 0)   (0, 0)   (90, 0)   (90, 270)

IA   *IB*   *IC*   *ID*

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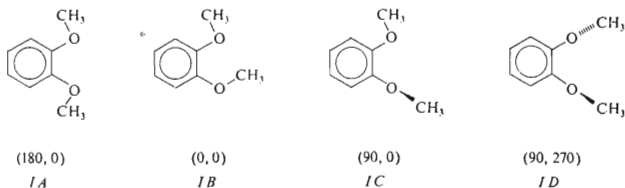
* The simplest possibility how to denote generally the conformation of polymethoxybenzenes is giving successively the angles of each $O-CH_3$ bond with the ring plane, see formulae *IA−ID* and *VA−VD*. This notation differs from ref.[14] in that all the angles are measured in the same direction.

As regards 1,2,3-trimethoxybenzene (V), we are faced with a more complex problem which has been less studied. A compilation[14] of X-ray data obtained on various derivatives revealed almost exclusively the conformation VC (180°, 90°, 0°) for the pertinent fragment, but no supporting evidence was obtained from solution properties or from calculations[14]. The same conformation was tentatively assumed when interpreting the dipole moment of V, although it would require a specially modified value of the OCH_3 group moment[12]. Alternatively, the dipole moment was discussed in terms of planar conformations VA (0°, 0°, 0°) and VB (180°, 0°, 0°), the latter being considered more probable[13]. Therefore, measurement on further derivatives with proper substituents appears mandatory. In this communication we report the dipole moments of compounds $VI - IX$ (Table I). Use of unsymmetrical substituents CHO and COOR is possible in this case since the methoxy groups themselves are positioned symmetrically. In our previous work[1-5,27] only symmetrical substituents were used for such purposes, as a rule Cl, Br, or NO_2. Recently, we have measured the dipole moment of 3,4,5-trimethoxybenzamidoxime[28] but the conformation of the methoxy groups could not be deduced quite safely from this single value.

(0, 0, 0)   (180, 0, 0)   (180, 90, 0)
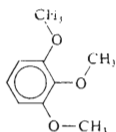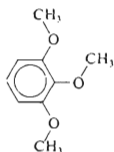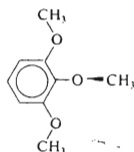
VA VB VC

EXPERIMENTAL

Compounds $II-IV$, VI, $VIII$. IX (Table I) were prepared according to the literature[29-33], their identity was checked by melting point determination and in some cases also by mass spectroscopy. The technique of dipole moment measurement was described[34]. The molar refractions were calculated from experimental values for 1,2-dimethoxybenzene[22] and 1,2,3-trimethoxybenzene[13], and from increments for further functional groups[35]. Conjugation of the latter with the benzene nucleus was expressed by the following exaltations: CN $0·9$ cm³, CHO $1·2$ cm³, COOR $0·7$ cm³; the extra-conjugation of two groups in the position *para* was neglected. The dipole moment data are assembled in Table I.

Theoretical dipole moments envisaged for individual conformations were calculated within the framework of bond and group moments scheme[36]. The following moments were used, including always the conjugation with the benzene nucleus (in 10^{-30} C m): C_{ar}—H 0, C_{ar}—Br $5·23$, two C_{ar}—Br bonds in an *ortho* position $6·33$, C≡N $13·2$, OCH_3 $4·2$ at an angle of 74° to the O—C_{ar} bond (according to ref.[37] and essentially in agreement with previous estimates[12,13,15,21]), COOR $6·23$ (64° to the C_{ar}—C bond, ref.[38]), CHO $9·9$ (39° to the C_{ar}—C bond, ref.[13]). The extra-

-conjugation of the CN and OCH_3 groups in the *para* position was expressed by a mesomeric moment of 1·2 inferred from the experimental dipole moment of 4-methoxybenzonitrile[39]. This value is reduced if the methoxy group is not strictly coplanar. On the other hand, we have neglected a possible effect of the rotation of the methoxy group on its group moment itself or on the angle C—O—C. The calculated dipole moments for the adopted, most probable conformation are listed in Table I, last column, the remaining ones are shown only in the Figs 1—5.

TABLE I

Polarization and dipole moments of benzene 1,2-dimethoxy and 1,2,3-trimethoxy derivatives (benzene, 25°C)

No	Compound	M.p. °C	α^a β^b	P_0 cm^3 $R_D{}^b$	$\mu(5)^c$ $\mu(15)^c$	$\mu_{calc}{}^d$
I	1,2-$(CH_3O)_2C_6H_4$	—	—	—	4·4^e	4·3
				39·64^f	—	
II	1,2-$(CH_3O)_2$-4-BrC_6H_3 (ref.[29])	^{g}	1·44 −0·484	101·5 47·5	5·3 5·1	6·2^h
III	1,2-$(CH_3O)_2$-4,5-Br$_2C_6H_2$ (ref.[30])	91	1·95 −0·610	155·6 55·3	7·3 7·1	7·0
IV	1,2-$(CH_3O)_2$-4-CNC_6H_3 (ref.[31])	68	11·49 −0·246	395·8 45·0	13·8 13·7	14·1^h
V	1,2,3-$(CH_3O)_3C_6H_3$	—	—	159·1^i 46·0^i	7·8^i —	7·5
VI	1,2,3-$(CH_3O)_3$-5-CNC_6H_2 (ref.[32])	92	5·64 −0·328	251·7 51·3	10·4 10·3	10·7
VII	1,2,3-$(CH_3O)_3$-5-CHOC_6H_2	75	3·78 −0·314	187·9 52·0	8·5 8·4	9·4
VIII	1,2,3-$(CH_3O)_3$-5-COOCH$_3C_6H_2$ (ref.[32])	82	2·67 −0·348	167·2 57·5	7·6 7·4	8·4
IX	1,2,3-$(CH_3O)_3$-5-COOC$_2H_5C_6H_2$ (ref.[33])	55	2·83 −0·316	187·1 62·2	8·2 7·9	8·4
X	1,2,3,5-$(CH_3O)_4$-C_6H_2	—	—	—	9·0^i —	9·1

^{a} Slopes of the plots ε_{12} *vs* w_2 and d^{-1}_{12} *vs* w_2, respectively; ^{b} calculated from increments, see Experimental; ^{c} units 10^{-30} C m, correction for the atomic polarization 5% or 15% of the R_D value, respectively; ^{d} units 10^{-30} C m, calculated for a 40 : 60 mixture of conformers *IA* (180°, 0°) and *IC* (90°, 0°) in the case of 1,2-dimethoxy derivatives, and for the conformation (165°, 90°, 15°) in the case of 1,2,3-trimethoxy derivatives; ^{e} ref.[21], in agreement with previous data[39] and with measurements in decalin[20] or tetrachloromethane[10,24]; ^{f} ref.[22]; ^{g} b.p. 141°C/1·8 kPa; ^{h} the two possible conformations *IC* assumed equally populated which is not quite true, see Discussion; ^{i} ref.[13], the dipole moment in agreement with ref.[12]; ^{j} ref.[12].

RESULTS AND DISCUSSION

For the conformation of two *ortho*-standing methoxy groups the dipole moments of compounds *I* and *III* are most telling and will be discussed first. If the two bromine atoms in *III* are taken as a single substituent, its moment is oriented symmetrically with respect to the two equivalent methoxy groups and the number of possible conformers is reduced. There is only one complication with substitution of this type that the substituent moment cannot be calculated as the vector sum of standard bond moments but has to be derived directly from the experiment on 1,2-dibromobenzene[39], as given in Experimental. Comparison[27] of calculated and experimental dipole moments is shown in Fig. 1. In addition to the planar conformation *IA* and *IB* we have taken into consideration non-planar conformations of two kinds: either one methoxy group is rotated while the other keeps the *anti* position (full line in Fig. 1), or the two methoxy groups are rotated simultaneously, whether in the same direction or in opposite directions (broken lines). The experimental dipole moments are compatible with any of the following hypotheses: *a*) one non-planar unsymmetrical conformation with the dihedral angles (110°, 0°), *b*) one non-planar symmetrical C_s conformation with dihedral angles (145°, 35°), *c*) a mixture of planar conformers *IA* and *IB* in the ratio 70 : 30, *d*) a mixture of the planar conformers *IA* and non-planar *IC* in the ratio 40 : 60. The last possibility seems most probable to us, in particular
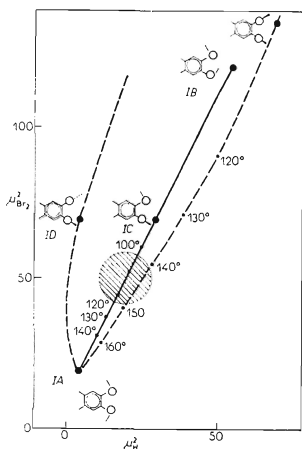

Fig. 1

Comparison of squared dipole moments of 1,2-dimethoxybenzene (*I*) (*x*-axis) and its 4,5-dibromo derivative *III* (*y*-axis). Full points — calculated for individual conformations, hatched circle — experimental; full lines represent rotation of one methoxy group, dashed lines of two methoxy groups simultaneously

with respect to a shoulder observed[14] in the PE spectrum and to further reasoning given[14] in favour of a non-planar conformation. Equilibrium of two conformers also accords with the temperature dependence of dipole moments[20,21,25] while the conformation ad b) seems improbable in virtue of the electrostatic repulsion of lone electron pairs (compare this effect in the molecule of acetals[40]). Of course, we cannot warrant that the energy minimum of *IC* is just at 90°, in any case the potential energy curve must be rather flat.

Essentially the same result as above was obtained from the monobromo derivative *II*, except that the two methoxy groups are no more equivalent and a more complex pattern is obtained (Fig. 2). The preferred conformation ad *d*) has to be specified in such a manner that it is either the methoxy group in the position 1 (*para* to the bromine atom) which takes a non-planar position, or that this form is at least more populated than the second form with the non-planar methoxy group in position 2. The latter formulation is more cautious; although it does not follow immediately from Fig. 2, it is in better agreement with the results on 4-cyano derivative *IV* (Fig. 3). When constructing Fig. 3, attention had to be paid to the extra-conjugation of the cyano group with the methoxy group in *para* position, which increases the dipole moment. The necessary correction was formally expressed as an additional mesomeric moment in the direction of the $C \equiv N$ bond, its value was derived from the experi-
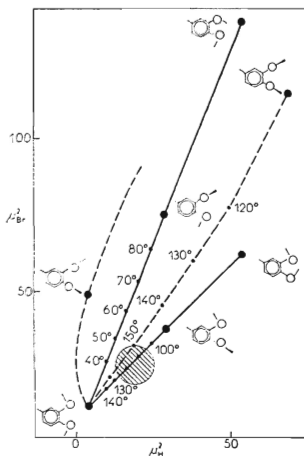

Fig. 2

Comparison of squared dipole moments of 1,2-dimethoxybenzene (*I*) (*x*-axis) and its 4-bromo derivative *II* (*y*-axis) with the same symbols as in Fig. 1

mental dipole moment[39] of 4-methoxybenzonitrile. If the coplanarity of the *para*-standing methoxy group is impaired in any conformation, the mesomeric moment is reduced appropriately and becomes zero for the perpendicular position. The named corrections modify the shape of the curves in Fig. 3 as compared to Fig. 2. Nevertheless, the final result is the same: the conformation with the 1-methoxy group out of plane is slightly preferred. In Table I, last column, the dipole moments were calculated with the assumption that either methoxy group can be non-planar with the same probability, hence the values are somewhat low for compounds *II* and *IV*.

Summarizing, the evidence from solution dipole moments is in accord with the conclusions of Anderson and coworkers[14], *viz.* better with the PE spectra than with
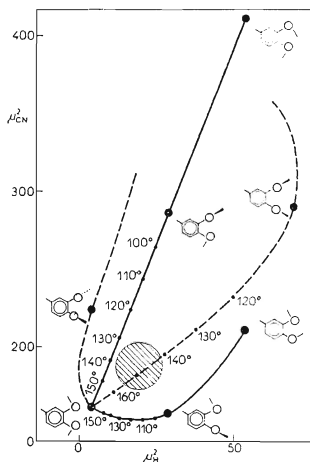

FIG. 3

Comparison of squared dipole moments of 1,2-dimethoxybenzene (*I*) (*x*-axis) and its 4-cyano derivative *IV* (*y*-axis) with the same symbols as in Fig. 1
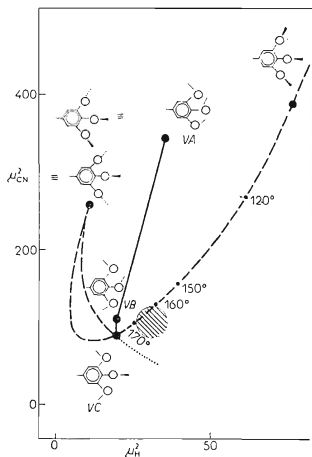
FIG. 4

Comparison of squared dipole moments of 1,2,3-trimethoxybenzene (*V*) (*x*-axis) and its 5-cyano derivative *VI* (*y*-axis). The same symbols are used as in Fig. 1, the dotted line represents reduction of the mesomeric moment of the methoxy groups

STO-3G calculations. The conformation[14] _ID_, or others with a C_2 symmetry[18,23], were clearly disproved. The result is interesting from the general point of view concerning the conformation around two equivalent bonds[1]. As mentioned in the introduction, one cannot expect that the conformation of _ortho_ derivatives should conform with that of corresponding mono derivatives. However, the case of 1,2-dimethoxybenzene is exceptional in that the conformation on two equivalent bonds is different. The explanation may be either sought in some interactions of the lone electron pairs, or more probably in the mere form of the potential energy function for one methoxy group. If this function exhibits a secondary minimum[7,10], a large rotation of one group is evidently more favourable than simultaneous smaller rotation of both groups.

With 1,2,3-trimethoxybenzene we have to do with a greater variety of possible conformations so that the consideration must be restricted to the more probable ones, possessing some degree of symmetry. We calculated the anticipated dipole moments for the two planar forms _VA_ and _VB_ and the transitory non-planar forms between them, for the preferred[12,14] non-planar symmetrical C_s form _VC_, and for further forms arising from _VC_ by simultaneous rotation of the two outer methoxy groups either in the same directions or in opposite directions. All these calculations are confronted with the experimental results in Fig. 4 which refers to the symmetrical molecules of _V_ and _VI_. The calculations with the _para_ cyano group had again to account for the extra-conjugation but the reliability of necessary corrections has been already tested on compound _IV_ (Fig. 3). In any case these corrections are not of decisive importance. Fig. 4 reveals that none of the conformations _VA_–_VC_ is in agreement with experiments. The only acceptable hypothesis is a distorted form _VC_ in which even the outer methoxy groups are slightly out of plane (effective dihedral angles approximately 15°). Such a conformation is to be regarded merely as an effective one, representing the mean position of oscillating groups. Such cases are rather common, but surprising is the finding that in this mean conformation all three methoxy groups should be displaced towards one side of the benzene ring plane, compare the high energy calculated[14] for the conformation of 1,2-dimethoxybenzene with the two methoxy groups on one side. Instead of the distorted conformation we still took into consideration that conjugation of the methoxy groups could be reduced due to their accumulation in the molecule. However, this effect would account for the enhanced dipole moment of _V_ but not of _VI_ (the dotted line in Fig. 4). Of course, the accuracy of our approach must not be overestimated. The dashed circles in Figs 1–5 should represent approximately the combined uncertainty, arising merely from the imperfect additivity of group moments than from the experimental error alone. Accordingly, the deviation from the conformation _VC_ is just close to the limit of reliability, nevertheless it is confirmed by the results on compounds _VII_–_IX_. The use of axially unsymmetrical substituents CHO and COOR is made possible by the fact that the most important conformations of the functional group are symmetrical. It follows that

although the degeneracy of some forms is removed and their number increased, this does not affect the final conclusion. The result is shown in Fig. 5 for the substituents COOCH$_3$ and COOC$_2$H$_5$ (the calculated values are equal) and in Table I, last column for substituents CHO and OCH$_3$, the experimental value for the latter being taken from the literature[12]. Figs 4 and 5 can serve as a good example of how important is a proper substitution in dipole moment work: it grants these diagrams the second dimension and allows to arbitrate cases undistinguishable on the basis of one compound alone.

In conclusion, we have proven the conformation of 1,2,3-trimethoxy derivatives of benzene in solution which accords with that in the crystalline phase[14], supposed equilibrium[13] of the planar forms VA and VB has been clearly disproved. Whether the outer methoxyl groups in VC are exactly coplanar or slightly rotated out, in any case the conformation is governed by the general rule[1] that symmetrically located groups tend to adopt symmetrical conformations; the conformation of the outer methoxy groups is essentially the same as in monofunctional compounds, that of the inner methoxy group is changed in virtue of the strong steric hindrance. From the examples of 1,2-dimethoxy as well as of 1,2,3-trimethoxy benzenes we can confirm that the quoted rules[1] have a broad validity even when there are exceptions; in any
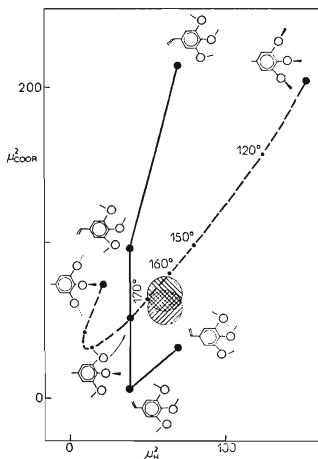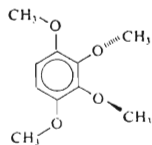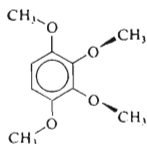

FIG. 5

Comparison of squared dipole moments of 1,2,3-trimethoxybenzene (V) (x-axis) and its 5-methoxycarbonyl and 5-ethoxycarbonyl derivatives $VIII$ and IX (y-axis) with the same symbols as in Fig. 1

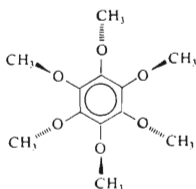case they can serve as starting point when discussing the conformation of more complex compounds.
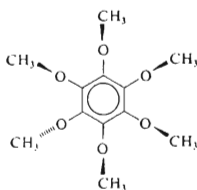

(180, 90, 270, 0)

XI A

(180, 90, 90, 0)

XI B

(90, 270, 90, 270, 90, 270)

XII A

(90, 90, 90, 90, 90, 270)

XII B

TABLE II

Possible conformations of hexamethoxybenzene

Methoxy groups situated on the same side of the ring		Statistical weight	Calculated μ (10^{-30} C m)
1, 2, 3, 4, 5, 6		2	24·2
1, 2, 3, 4, 5	(*XIIB*)	12	16·1
1, 2, 3, 4		12	8·1
1, 2, 3, 5		12	8·1
1, 2, 4, 5		6	8·1
1, 2, 3		6	0
1, 2, 4		12	0
1, 3, 5	(*XIIA*)	2	0
		weighted mean	9·9

With the experience gained we can attempt to estimate the conformation of benzene derivatives with more methoxy groups in vicinal positions. For 1,2,3,4-tetramethoxybenzene the conformations XIA and XIB come into consideration. Their statistical weights are equal, energetically XIB should be somewhat disfavoured in virtue of the repulsion of the two inner methoxy groups as discussed with the compounds I and V. The calculated values of dipole moments for XIA and XIB are 6·0 and 10·1, for their 50 : 50 mixture 8·3. The experimental value[12] of 8·8 suggests either a slight predominance of XIB contrary to the expectation, or an out-of-plane deviation of the outer methoxyl groups like in V. The methoxy groups of hexamethoxybenzene should adopt effectively perpendicular positions. Eight conformations are possible, each characterized by the position of the methyl groups situated on the same side of the ring plane; see Table II, where also the statistical weights and anticipated dipole moments are given. The experimental value[11,12] of 6·8 or 6·7 is now lower than the weighted mean of calculated values (9·9), suggesting a greater population of forms with methoxy groups in alternating positions (e.g. XIIA) than of those with several neighbouring methoxy groups on the same side (e.g. XIIB).

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Translated by the author (O. E.).