Dipole Moments of Organosilicon Compounds

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Although organosilicon chemistry, which has made remarkable progress recently, has produced a large number of new compounds, their molecular configurations remain unknown. The present author has, therefore, been studying them by the determination of their dipole moments, and several of his results will be reported on here.

Experimental

The compounds which have been measured for the present work are:

(I)	Methoxytrimethylsilane	b.p. 56.1～57.3°C
(II)	Dimethoxydimethylsilane	b.p. 80.5°C
(III)	Trimethoxymethylsilane	b.p. 103.5°C
(IV)	Tetramethoxysilane	b.p. 121.5°C
(V)	Tetra-trimethylsiloxy-silane	
(VI)	Methoxytrichlorosilane	
(VII)	Dimethoxydichlorosilane	
(VIII)	Trimethoxychlorosilane.	

Of these compounds, tetra-trimethylsiloxy-silane (V) and three methoxychlorosilanes (VI, VII and VIII) were furnished to us by Mr. M. Yokoi of Shinshu University and Mr. H. Murata of Hiroshima University respectively. The others were prepared by the reactions of methyl alcohol upon the corresponding methylhalosilanes[1].

The dielectric constants and the specific volumes of the benzene solutions were measured at 25 and 50°C.

For the calculation of the molecular polarization of the solute at infinite dilution, $P_{2\infty}$, the following equations proposed by Halverstadt and Kumler[2] were used:

$$P_{2\infty}=M\left\{(v_0+\beta)\frac{\varepsilon_0-1}{\varepsilon_0+2}+\frac{3\alpha v_0}{(\varepsilon_0+2)^2}\right\}$$

$$\alpha=\frac{\varepsilon-\varepsilon_0}{w},\quad \beta=\frac{v-v_0}{w}$$

where M is the molecular weight, ε_0 and v_0 are the dielectric constant and the specific volume of the solvent respectively, ε and v are those of the solution, and w is the weight fraction of the solute in the solution.

For the calculation of the dipole moment, (P_A+P_E) is assumed to be 1.1 MR_D, as in the case of hexamethyldisiloxane[3], where P_A and P_E are the atomic polarization and the electronic polarization respectively, and MR_D is the molar refraction for the D line. The results are shown in Table I.

Results and Discussion

Assumed Bond Angles and Bond Moments.— To determine the configurations of the compounds, the bond angles and bond moments

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[1] Cf., for example, D. F. Peppard, W. G. Brown and W. C. Johnson, *J. Am. Chem. Soc.*, **68**, 73 (1946).

[2] I. F. Halverstadt and W. D. Kumler, ibid., **64**, 2988 (1942).

[3] Y. Kurita and M. Kondo, This Bulletin, **27**, 160 (1954).

TABLE I. THE OBSERVED VALUES OF THE COMPOUNDS

	Temp. °C	ε_0	v_0 cc./g.	α	β	$P_{2\infty}$ cc.	MR_D cc.	μ D
(I)	25	2.273	1.145	1.108	0.167	62.5	31.0	1.18
(II)	25	2.273	1.145	1.304	0.021	71.2	31.7	1.33
	50	2.223	1.180	1.103	0.022	68.2		1.33
(III)	25	2.273	1.145	1.765	−0.086	88.2	32.4	1.60
	50	2.223	1.181	1.580	−0.096	85.5		1.62
(IV)	25	2.273	1.145	1.986	−0.171	101.1	33.1	1.78
	50	2.223	1.181	1.775	−0.180	97.8		1.80
(V)	25	2.273	1.145	0.146	−0.010	140.7	105.4	1.10
	50	2.223	1.181	0.119	−0.017	138.8		1.10
(VI)	25	2.273	1.146	2.528	−0.390	116.1	29.6	2.02
	50	2.223	1.181	2.252	−0.402	111.4		2.04
(VII)	25	2.273	1.146	2.685	−0.316	121.3	30.8	2.04
	50	2.223	1.181	2.435	−0.327	117.8		2.08
(VIII)	25	2.273	1.146	2.576	−0.264	117.2	32.0	1.97
	50	2.223	1.181	2.364	−0.275	114.7		2.02

used for the calculations of the dipole moments were assumed as follows.

The bond angle of the silicon atom is tetrahedral, and angle SiOC is assumed to be 113° from the results of the electron diffraction study of tetramethoxysilane[4] and methoxytrichlorosilane[5]. Angle SiOSi for tetra-trimethylsiloxy-silane is assumed to be 140° from the results of the electron diffraction study[4].

The CH_3O group moment, 1.15D, is calculated from the dipole moment of methyl ether, 1.29 D[6], and its angle COC, 111.5°[7]. For the group moment of $(CH_3)_3SiO$, Kurita and Kondo obtained 0.95 D[3] from the dipole moment of hexamethyldisiloxane, 0.80D, assuming that angle SiOSi is 130°[4]. However, the $(CH_3)_3SiO$ group moment is assumed to be 1.05D, assuming that angle SiOSi is 135°[*]. Therefore, 1.65D is obtained for the SiO bond moment and 0.60D for the CH_3Si group moment.

The SiCl bond moment 2.94D is calculated from the dipole moment study of methoxytrichlorosilane in this report, as will be shown below.

Assumed Configurations.—Using the above bond angles and bond moments, the present author calculated the dipole moments of the compounds, assuming the following models:

1) Fundamental Models (trans and gauche Models).—The CH_3 groups of the CH_3O groups and the $(CH_3)_3Si$ groups of the $(CH_3)_3SiO$ groups are at trans or gauche positions with regard to the nonbonding oxygen atoms. The cis models were rejected because of their instability.

The trans and gauche positions are shown in Figs. 1—3; $a_1, b_1, c_1 \cdots\cdots$ are the positions of the CH_3 groups in Figs. 1 and 2, and of the CH_3 groups or $(CH_3)_3Si$ groups in Fig. 3.

2) The Free Rotation Model.—The CH_3 groups and the $(CH_3)_3Si$ groups are rotating around the SiO bonds freely.

The calculated dipole moments for these models, 1) and 2), are shown in Tables II, IV, VI, VIII, X and XII. Moreover, as it has been known that the bond angle of an oxygen atom in organosilicon compounds shows various values, the angles SiOC and SiOSi are calculated from the observed dipole moments which are shown in the third columns of these tables.

3) The Vibration Models and the Staggered Models.—The CH_3–O bonds and the Si–O bonds

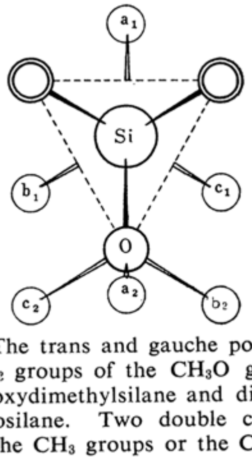

Fig. 1. The trans and gauche positions of the CH_3 groups of the CH_3O groups of dimethoxydimethylsilane and dimethoxydichlorosilane. Two double circles indicate the CH_3 groups or the Cl atoms.

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4) M. Yokoi, ibid., **30**, 100 (1957); K. Yamasaki, A. Kotera, M. Yokoi and Y. Ueda, *J. Chem. Phys.*, **18**, 1414 (1950).

5) J. Kakinoki, H. Murata, K. Katayama and K. Shimizu, *Annual Rep. of the Inst. for Fiber Research, Osaka Univ.*, **7**, 14 (1953).

6) R. J. W. Le Fèvre, "Dipole Moments", Methuen & Co., London (1953).

[*] Mr. M. Yokoi kindly suggests to us in private communication that angle SiOSi may be larger than 130°; C. M. Lucht obtained 137±7°, which figure is yet unpublished.

7) K. Kimura and M. Kubo, *J. Chem. Phys.*, **30**, 151 (1959).

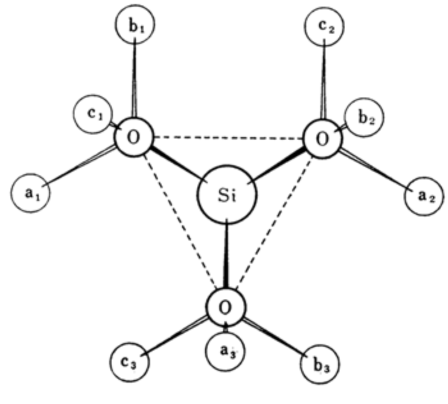

Fig. 2. The trans and gauche positions of the CH_3 groups of the CH_3O groups of trimethoxymethylsilane and trimethoxychlorosilane.

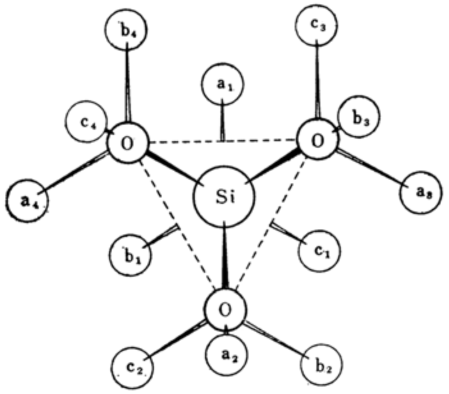

Fig. 3. The trans and gauche positions of the CH_3 groups of tetramethoxysilane, and of the $(CH_3)_3Si$ groups of tetra-trimethylsiloxy-silane.

of $(CH_3)_3SiO$ groups are vibrating about given "equilibrium" positions, trans or gauche positions respectively, or staggering from these positions. The amplitude or the staggered angles are denoted by θ. In the case of the staggered model, if CH_3 or $(CH_3)_3Si$ groups are staggered and situated at θ counterclockwise from the given "equilibrium" positions when viewed from the centered Si atom, these staggered angles may be defined $+\theta$.

The calculated angle θ, giving the observed dipole moments, are shown in Tables III, V, VII, IX, XI and XIII; in every case the "equilibrium" model means that one of the trans and gauche models with the smallest dipole moment.

(I) Methoxytrimethylsilane.—The moment is measured only at 25°C, because of its low boiling point.

The observed value, 1.18D, is in coincidence with the dipole moment of ethoxytrimethylsilane, 1.18D8). The observed value is consistent with the calculated value, 1.22D. Hence, the assumed bond angle SiOC, 113°, and the $(CH_3)_3SiO$ group moment, 1.05D, seem reasonable.

As to the molecule of this type, it should be noticed that it is impossible to determine the precise position of the CH_3 group by only the dipole moment data.

(II) Dimethoxydimethylsilane.—The observed value, 1.33D, is also in good agreement with that of diethoxydimethylsilane, 1.36D8).

The facts that the calculated dipole moments for various models in Table II are not consistent with the observed value, and that the observed dipole moment is independent of the temperature, suggest that the molecule is in the free rotational state.

When it is assumed that the two CH_3 groups rotate with each other freely, the observed moment is well consistent with the calculated moment, provided that angle SiOC is taken

TABLE II. THE CALCULATED MOMENTS OF DIMETHOXYDIMETHYLSILANE (see Fig. 1)

Model	μ (D)	< SiOC
b_1-b_2, c_1-c_2	0.16	
a_1-b_2, a_1-c_2	1.72	129°
b_1-a_2, c_1-a_2	1.72	129°
b_1-c_2, c_1-b_2	1.85	>145°
a_1-a_2	2.40	
Free rotation	1.63	128.5°
(observed 25°C	1.33)	
(observed 50°C	1.33)	

TABLE III. THE VIBRATION MODEL (V) AND THE STAGGERED MODEL (S) OF DIMETHOXYDIMETHYLSILANE

θ show the vibrational amplitudes of the C-O bonds of CH_3O groups for (v), and the staggered angles for these bonds for (s), and, + and − are the signs of θ which is positive if the C-O bonds stagger counterclockwise.

	Equilibrium model	θ
	(b_1-b_2)	
(v)		110°
(s)	++	172°
	−−	51°
	+−	60.5°
	−+	60.5°
	(a_1-a_2)	
(v)		>180°
(s)	++	69°
	−−	69°
	+−	150°
	−+	150°

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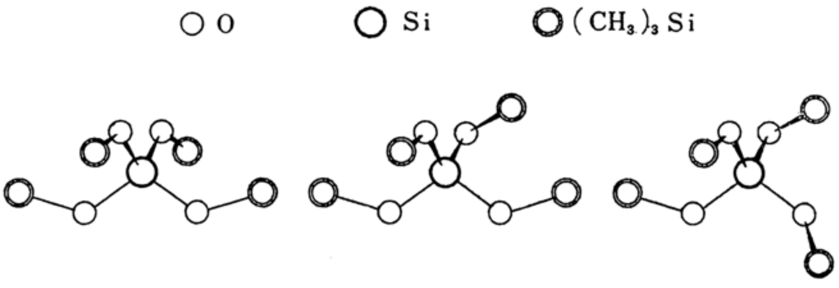
8) H. Freiser, M. V. Eagle and J. Speier, *J. Am. Chem. Soc.*, **75**, 2824 (1953).



(a) $a_1-a_2-a_3-a_4$ (b) $a_1-a_2-a_3-b_4$ (c) $a_1-b_2-a_3-c_4$

Fig. 4. The configurations of tetra-trimethylsiloxy-silane.

as 128.5°. In this case the $CH_3 \cdots\cdots CH_3$ distance is 2.9 Å; it is a little larger than the sum of the covalent radii of a carbon atom and a hydrogen atom, which makes the free rotation possible.

The value of angle SiOC, 128.5°, is larger than the observed value, 113°, which is obtained by the electron diffraction study of tetramethoxysilane, but it is comparable to the values of angle SiOSi, 130±10° and 137±7° in hexamethyldisiloxane, and 140±5° in tetra-trimethylsiloxy-silane, which values are obtained by electron diffraction studies; therefore, the value obtained here may not be unreasonable.

Next, in explanation of the observed value, a vibration or fixed staggered model for this molecule, with the b_1-b_2 model as the equilibrium model, was assumed. The calculated results are shown in Table III. In the staggered models two cases are considered; a) two CH_3 groups are staggering from the given equilibrium positions, b_1 and b_2, in the same direction by angle $+\theta$ or $-\theta$ ($++$ and $--$ in Table III), and b) they are staggering in different directions, one by angle $+\theta$ and the other by $-\theta$ ($+-$ and $-+$ in the same table).

The large amplitude and the staggered angle θ's shown in Table III are difficult to interpret in terms of the intramolecular potential of the molecule. For example, the model with the staggered angle 51° from the b_1-b_2 (gauche) model makes a form almost identical to the cis form. Therefore, it is unsuitable to use these models to explain the experimental results. When the c_1-c_2 model is taken as the equilibrium model, similar relations are obtained.

On the other hand, when the trans (a_1-a_2) model is taken as the equilibrium model, the staggered model, in which one CH_3 group staggers by +150° and the other by −150°, is obtained. This is identical with the case in which the b_1-c_2 model or the c_1-b_2 model is taken as the equilibrium model. That is, for example, if the b_1-c_2 model is chosen as the equilibrium model, the CH_3 group placed at the b_1 position staggers by +30° and the CH_3 group placed at the c_2 position staggers by −30°. This model is considered the most reasonable one, if one ignores the fact that the most stable model, with the smallest dipole moment, is taken as the fundamental equilibrium model.

The third possibility to explain the observed data lies in the consideration of the molecule consisting of a mixture of the various configurations. As there are many configurations which can be mixed with the b_1-b_2 model and the c_1-c_2 model to make the calculated moment fit the observed moment, it is desirable to use the other physical method to determine its details.

(III) Trimethoxymethylsilane.—As is shown in Table IV, these observations can be made about the trans and gauche models and the free rotation model as well as about dimethoxydimethylsilane.

When the $a_1-a_2-a_3$ model or the $a_1-b_2-b_3$ model is chosen as the equilibrium model for

TABLE IV. THE CALCULATED MOMENTS OF TRIMETHOXYMETHYLSILANE (see Fig. 2)

Model type*	μ (D)	<SiOC
$a_1-a_2-a_3$	1.22	<90°
$a_1-b_2-b_3$	1.22	<90°
$a_1-b_2-a_3$	1.39	
$a_1-c_2-b_3$	2.10	128°
$a_1-b_2-c_3$	2.20	136°
$c_1-b_2-a_3$	2.39	148.5°
$a_1-a_2-b_3$	2.79	143°
Free rotation	1.93	128°
(observed 25°C	1.60)	
(observed 50°C	1.62)	

* All of the other trans and gauche models are classified into one of the above models.

Table V. The vibration model (v) and the staggered model (s) similar to Table III but for trimethoxymethylsilane

	Equilibrium model	θ	
	($a_1-a_2-a_3$)		
(v)		80°	
(s)	+++	—	
	−−−	—	
	++−	—	
	−−+	—	
	+−+	32°	
	+−−	32°	
	−+−	29°	
	−++	29°	
	($a_1-b_2-b_3$)		
(v)		80.5°	
(s)	+++	32°	168°
	−−−	29°	110°
	++−	75°	165°
	−−+	15°	104°
	+−+	17°	148°

the vibration model and the staggered models, the calculated angles, θ's, are shown in Table V. The large amplitude, 80°, shows that the vibration model must be rejected upon considering the intramolecular potential. Of all the staggered forms, the models staggering by 15, 17, 29 and 32° from the given equilibrium positions seem reasonable models.

(IV) Tetramethoxysilane.—As is shown in Table VI, of all the trans and gauche models the $a_1-a_2-a_3-b_4$ type models and the $a_1-b_2-a_3-c_4$ type models have the most suitable calculated values to fit the observed dipole moment. Therefore, it is possible to consider that the molecule consists of a mixture of, or one of, these models.

On the other hand, by electron diffraction study[4], the configuration of this molecule is found to be the staggered model in which four CH_3 groups stagger against nonbonding oxygen atoms.

Table VI. The calculated moments of tetramethoxysilane (see Fig. 3)

Model type*	μ (D)	<SiOC
$a_1-a_2-a_3-a_4$	0	
$a_1-b_2-b_3-a_4$	0	
$a_1-a_2-a_3-b_4$	1.83	115°
$a_1-b_2-a_3-c_4$	1.83	115°
$a_1-a_2-b_3-b_4$	2.59	140°
$a_1-a_2-b_3-c_4$	3.18	148.5°
Free rotation	2.12	128.5°
(observed 25°C	1.78)	
(observed 50°C	1.80)	

* All of the other trans and gauche models are classified into one of the above models.

Table VII. The vibration model (v) and the staggered model (s) similar to Table III but for tetramethoxysilane

	Equilibrium model	θ
	($a_1-a_2-a_3-a_4$)	
(v)		105°
(s)	++++	—
	−−−−	—
	+++−	58°
	+−−−	58°
	+−+−	37°
	++−−	—
	($a_1-b_2-b_3-a_4$)	
(v)		105°
(s)	++++	37°
	−−−−	37°
	+++−	58°
	++−+	58°
	++−−	58°
	+−+−	58°
	+−−+	—

As is shown in Table VII, of all the staggered models assuming the $a_1-a_2-a_3-a_4$ model or the $a_1-b_2-b_3-a_4$ model as the equilibrium model, the staggered models with the staggered angle of 37° are considered to be most suitable to explain the configuration of the molecule.

Moreover, Asbuzov and Shavsha[9] measured the dipole moment for this molecule and obtained 1.61D, their calculated moment with the free rotation model being 1.7D. From this, they concluded that the free rotation model is reasonable. However, as their report is not available and the details are not known exactly, their results cannot be discussed in the present report.

Configuration of Methoxymethylsilanes and Tetramethoxysilane.—As has been mentioned above, throughout four compounds, three methoxymethylsilanes and tetramethoxysilane, it can be considered first that the configurations for these molecules are in the free rotational state, as the observed dipole moments are independent of temperature, and it has been known in general that organosilicon compounds have a low intramolecular potential barrier as compared with carbon compounds. In methoxytrimethylsilane the observed moment is consistent with the calculated moment, assuming 113° for angle SiOC, while in dimethoxydimethyl-, trimethoxymethyl- and tetramethoxysilane, the angle SiOC must open wider by 15° to make the calculated moments fit the observed moments. These features of the angle may be possible, but it seems difficult

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9) B. A. Asbuzov and T. G. Shavsha, *Doklady Akad. Nauk. S. S. S. R.*, **68**, 859 (1949); *Chem. Abstr.*, **44**, 886 (1950).

to accept the free rotation for the configuration of compounds, so long as the bond angles of an oxygen atom are assumed to be the same in these molecules belonging to a series.

As was seen in the conclusion of the electron diffraction study for tetramethoxysilane, some of the staggered models in which the CH_3 groups stagger about each given equilibrium positions seem to be suitable.

The third possibility to explain the configurations of these compounds lies in the assumption that these compounds consist of a mixture of various trans and gauche models. The temperature dependence is expected to appear as more or less in this case.

(V) Tetra-trimethylsiloxy-silane. — The observed moment is independent of temperature. The free rotation model seems preferable. The calculated moment is consistent with the observed moment if angle SiOSi is taken to be 148.5°. This value of the angle is in agreement comparatively with 140±5° according to the results of the electron diffraction study for this compound. But if angle SiOSi is assumed to be 148.5°, the distance between one CH_3 group belonging to one of four $(CH_3)_3Si$ groups and one CH_3 group belonging to another amounts to 1.16 Å. The distance between the two above-mentioned CH_3 groups is too small to make the $(CH_3)_3Si$ groups rotate freely, so that the free rotation model is impossible.

TABLE VIII. THE CALCULATED MOMENTS OF TETRA-TRIMETHYLSILOXY-SILANE (see Fig. 3)

Model type*	μ (D)	<SiOSi
$a_1-a_2-a_3-a_4$	0	
$a_1-b_2-b_3-a_4$	0	
$a_1-a_2-a_3-b_4$	1.17	143°
$a_1-b_2-a_3-c_4$	1.17	143°
$a_1-a_2-b_3-b_4$	1.65	154.5°
$a_1-a_2-b_3-c_4$	2.02	159.5°
Free rotation	1.35	148.5°
(observed 25°C	1.10)	
(observed 50°C	1.10)	

* All of the other trans and gauche models are classified into one of the above models.

TABLE IX. THE VIBRATION MODEL (V) AND THE STAGGERED MODEL (S) SIMILAR TO TABLE III BUT FOR TETRA-TRIMETHYLSILOXY-SILANE

	Equilibrium model	θ
	$(a_1-a_2-a_3-a_4)$	
(v)		98°
(s)	++++	—
	----	—
	+++-	54.5°
	+---	54.5°
	+-+-	35°
	++--	—
	$(a_1-b_2-b_3-a_4)$	
(v)		98°
(s)	++++	35°
	----	35°
	+++-	54.5°
	++-+	54.5°
	++--	54.5°
	+-+-	54.5°
	+--+	—

On the other hand, of all the trans and gauche models in Table VIII, the calculated dipole moments of the $a_1-a_2-a_3-b_4$ type models and the $a_1-b_2-a_3-c_4$ type models are most consistent with the observed one. The features of these two models are shown in Figs. 4 (b) and (c). Therefore, it is considered that the configuration of this molecule is identical with one of, or a mixture of, these two types of models.

Considering the resembrance of the structural formula between this molecule and tetramethoxysilane, it is possible that the configuration of the molecule fits any staggered model. For example, when the $a_1-a_2-a_3-a_4$ model or the $a_1-b_2-b_3-a_4$ model is taken as the equilibrium model, the calculated angle of amplitude and the staggered angles are as shown in Table IX. The vibration model is impossible because of its large amplitude, while it seems that, of all the staggered models shown in Table IX, the models having the staggered angle 35° are most suitable as the configuration for the molecule.

According to the conclusion of the electron diffraction study⁴⁾, this molecule has a configuration in which two $(CH_3)_3Si$ groups belonging to the different W-shaped chains shown in Fig. 4 (a) are twisted by 60° from each other. The calculated dipole moment of this model is identical with those of the $a_1-a_2-a_3-b_4$ type models and the $a_1-b_2-a_3-c_4$ type models; that is, it is consistent with the observed moment. Little consideration has been given to this model, however, as it is identical with the case in which the two twisted $(CH_3)_3Si$ groups take cis positions against the respective nonbonding oxygen atoms.

(VI) Methoxytrichlorosilane.—The observed dipole moment is independent of temperature. In order to calculate the dipole moment for this molecule, it is necessary to have the value of the SiCl bond moment. The value, 2.67D, is obtained for the SiCl bond moment from the dipole moment of triethylchlorosilane, 2.07D¹⁰⁾, assuming the SiC_2H_5 group

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10) C. Curran, D. M. Witucki and P. A. McCusker, *J. Am. Chem. Soc.*, **72**, 4471 (1950).

moment, 0.60D. Using this bond moment, the calculated moment for this molecule is 1.81D. This value is too small as compared with the observed value.

Using the observed dipole moment, the Cl_3SiO group moment is calculated as 1.29D. From this value, the SiCl bond moment 2.94D is obtained, provided that the SiO bond moment is 1.65D. This SiCl bond moment, 2.94D, is larger than that obtained from the dipole moment study of triethylchlorosilane, 2.67D.

Of this tendency of the SiCl bond moment, the following argument seems to be the most suitable among the various considerations.

It has generally been known that the SiCl bonds in chlorosilane and ethylchlorosilane have the $Cl^+{=}Si^-$ double bond structure in spite of the fact that the electronegativities of a silicon atom and a chlorine atom are quite different[10,11], and that in many other silane derivatives, such as those containing a phenyl group, there is a so-called "reverse halogen effect" +  $=Si^-$ [12]. In the ClSiO bond of the molecule, it must be considered that the contribution of the structure $Cl^+{=}Si^-{-}O$ decreases and the contribution of the $Cl^-Si{=}O^+$ type structure rather increases, leading one to the conclusion that the $Si^-{=}O^+$ double bond structure contributes appreciably to the normal state of the SiO bond.

Therefore, it is better to assume the SiCl bond moment to be about 2.94D for methoxytrichlorosilane.

The configuration of this molecule cannot be decided only from the dipole moment data, whereas in the results of the electron diffraction study, the CH_3O group is placed at the trans position against one of three chlorine atoms[5].

(VII) Dimethoxydichlorosilane.—Among the fixed trans and gauche models in Table X, the calculated dipole moment of the a_1-b_2 type models is almost consistent with the observed moment. However, the dependence on temperature of the observed moment makes it difficult to select the particular configuration of the molecule.

The next possibility of explaining the observed data lies in the assumption that the molecule consists of a mixture of the various fixed models. That is, the a_1-a_2 model in Table X, where the two CH_3O groups are in the trans position with regard to each other as the most stable configuration, and many other models in Table X which are stable configurations at higher temperatures, are mixed. In this case, it is also expected that the temperature dependence will appear more or less.

TABLE X. THE CALCULATED MOMENTS OF DIMETHOXYDICHLOROSILANE (see Fig. 1)

Model type*	μ (D)
a_1-a_2	0.28
a_1-b_2	2.04
b_1-b_2	2.87
b_1-c_2	3.41
Free rotation	2.51
(observed 25°C	2.04)
(observed 50°C	2.08)

* All of the other trans and gauche models are classified into one of the above models.

TABLE XI. THE VIBRATION MODEL (V) AND THE STAGGERED MODEL (S) SIMILAR TO TABLE III BUT FOR DIMETHOXYDICHLOROSILANE

Equilibrium model		θ 25°C	θ 50°C
	(a_1-a_2)		
(v)		132.5°	136°
(s)	++	91°	92.5°
	−−	91°	92.5°
	+−	56°	57°

According to the electron diffraction study[5], the trans model seems to be the most reasonable one for the molecule, but this conclusion cannot explain the present experimental data.

(VIII) Trimethoxychlorosilane. — The configuration of this molecule is considered to be a mixture of the various trans and gauche models shown in Table XII, similar to the case of dimethoxydichlorosilane.

Configuration of Methoxychlorosilanes. — As has been mentioned above, from the results of the measurement for methoxytrichlorosilane, it is concluded that the SiCl bond moment

TABLE XII. THE CALCULATED MOMENTS OF TRIMETHOXYCHLOROSILANE (see Fig. 2)

Model type*	μ (D)
$a_1-c_2-b_3$	0.24
$a_1-a_2-b_3$	1.85
$a_1-a_2-a_3$	2.04
$a_1-b_2-b_3$	2.04
$a_1-b_2-c_3$	2.74
$a_1-b_2-a_3$	3.71
$c_1-b_2-a_3$	4.73
Free rotation	2.53
(observed 25°C	1.97)
(observed 50°C	2.02)

* All of the other trans and gauche models are classified into one of the above models.

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[11] L. O. Brockway and I. E. Coop, *Trans. Faraday Soc.*, **34**, 1429 (1938); E. L. Reilly, C. Curran and P. A. McCusker, *J. Am. Chem. Soc.*, **76**, 331 (1954).

[12] H. Freiser, M. V. Eagle and J. Speier, *J. Am. Chem. Soc.*, **75**, 2821 (1953).

TABLE XIII. THE VIBRATION MODEL (V) AND THE STAGGERED MODEL (S) SIMILAR TO TABLE III BUT FOR TRIMETHOXYCHLOROSILANE

Equilibrium model		θ	
	$(a_1-c_2-b_3)$	25°C	50°C
(v)		116.5°	120.5°
(s)	+++	146°	145°
	−−−	26°	25°
	++−	122°	121°
	+−+	122°	121°
	−++	122°	121°
	+−−	64°	61°
	−+−	64°	61°
	−−+	64°	61°

should be 2.94D, which corresponds to the contribution of the $Cl^-Si=O^+$ structure to the ClSiO bond.

Of the configurations of dimethoxydichloro- and trimethoxychloro-silane, it seems most suitable to suggest that these compounds consist of a mixture of various trans and gauche models, and not of one particular model, including the free rotation model and the vibration model, on condition that the observed moments depend on temperature.

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