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Vibrational Assignments and Rotational Isomerism of Dichloroethylmethylsilane and 2,2-Dichlorobutane

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The vibrational spectra of dichloroethylmethylsilane and 2,2-dichlorobutane have been measured. The vibrational assignments of these molecules have been made in relation to the rotational isomerism. The normal vibration calculations based on the modified Urey-Bradley force field have been carried out and have confirmed for both molecules that, in the liquid state, the *trans* and *gauche* isomers coexist, while the *trans* isomer alone persists in the crystalline state.

A number of studies concerning rotational isomerism around a C–C bond as an axis have been reported.[1] Recently, the existence of the rotational isomers around a C–Si bond in the homologous series of alkylsilanes has become apparent.[2] We have taken an interest in studying the rotational isomerism in the homologous series of alkylsilanes. In this paper, we will deal with the vibrational assignments and the rotational isomerism of dichloroethylmethylsilane and its analogues, *viz.*, 2,2-dichlorobutane.

Experimental

Dichloroethylmethylsilane was prepared from methyltrichlorosilane by adding C_2H_5MgBr.[3] 2,2-Dichlorobutane was prepared by the reaction of ethyl methyl ketone with PCl_5.[4]

The infrared spectra in the 250—4000 cm^{-1} region were recorded on a Perkin-Elmer instrument(Model 621). For the measurements in the crystalline state in this region, the vapor was condensed on a CsI window cooled with liquid nitrogen; the sample was then annealed near the melting point. For the spectra of dichloroethylmethylsilane in the 30—400 cm^{-1} region, a Hitachi Fis-3 far-infrared spectrometer equipped with a cell of polyethylene windows was used. The Raman spectra of dichloroethylmethylsilane in the liquid state were recorded on a JEOL Raman spectrometer (Model JRS-02AS), using an argon-ion laser(488.0 nm) for excitation.

Rotational Isomerism

Figure 1 shows the infrared and Raman spectra of $C_2H_5SiCl_2CH_3$ in the region below 900 cm^{-1}. The $SiCl_2$ stretching vibrations can be expected in the 400—600 cm^{-1} region from a comparison of the spectra with those of $(CH_3)_2SiCl_2$.[5] In the infrared spectra, the very-strong pair band at 546 and 530 cm^{-1} and the strong pair band at 471 and 467 cm^{-1} are observed in the liquid state. In the supercooled liquid state before annealing, the absorption intensities of both the higher-frequency bands of the pairs are weaker than the lower-frequency bands, while the reverse is true in the liquid state. In the crystalline state, both the lower-frequency bands of the two pairs persist, while the disappeared bands again appear with a rise in the temperature. These results indicate that rotational isomers exist in the liquid state, while one isomer persists in the crystalline state. On the other hand, in the Raman spectra, the very-strong pair counterpart at 460 and 470 cm^{-1} and the very-weak pair counterpart at 531 and 540 cm^{-1}, corresponding to the pair bands around 470 and 540 cm^{-1} respectively in the infrared spectra, are observed in the liquid state; they are, therefore, assigned to the $SiCl_2$ symmetric and antisymmetric stretching vibrations respectively.

On the other hand, Fig. 2 shows the infrared

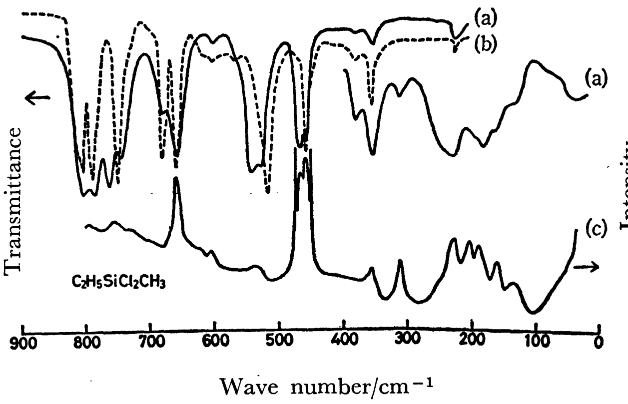

Fig. 1. The vibrational spectra of dichloroethylmethylsilane.
(a): the infrared spectra in the liquid state, (b): the infrared spectra in the crystalline state, (c): the Raman spectra in the liquid state.

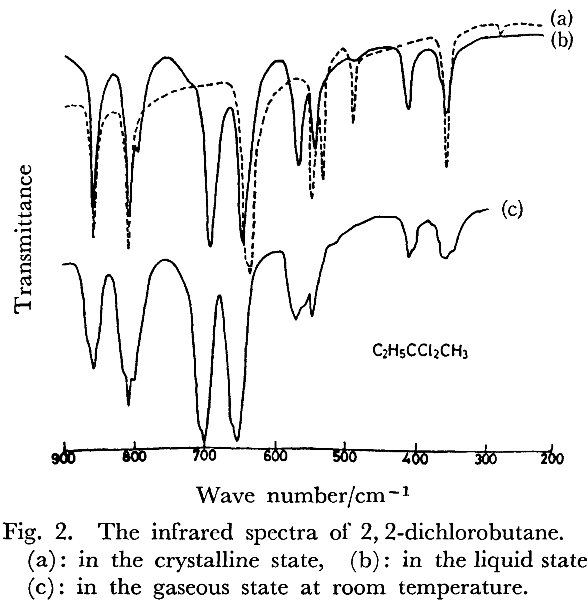

Fig. 2. The infrared spectra of 2, 2-dichlorobutane.
(a): in the crystalline state, (b): in the liquid state, (c): in the gaseous state at room temperature.

spectra of 2,2-dichlorobutane in the 250—900 cm^{-1} region. For alkyl chlorides, useful information about the rotational isomerism has been obtained from the C–Cl stretching and skeletal deformation vibrations.[1] In this molecule, the very-strong pair band at 692 and 645 cm^{-1} and the strong pair band at 567 and 544 cm^{-1} in the liquid state, clearly separated from each other, are observed; they are easily assigned to the CCl_2 antisymmetric and symmetric stretching vibrations respectively by reference to the spectra of 2,2-dichloropropane,[6] while both the higher-frequency bands of the pairs disappear in the crystalline state. In Fig. 2, the split pattern of the band at 544 cm^{-1} in the crystalline state may be due to the influence of the crystalline field because, in the supercooled liquid state before annealing, this pattern is not observed. The tendency of the CCl_2 stretching vibrations is the same as that of the $SiCl_2$ stretching vibrations. Therefore, it may be expected that, for both molecules, only one isomer with the same molecular form persists in the crystalline state, while two isomers coexist in the liquid state.

The results of the normal vibration calculations, which will be given in Tables 4 and 5, indicate that the antisymmetric and symmetric YCl_2 stretching vibrations (Y=C, Si) for the *gauche* isomer are higher in frequency than those for the *trans* isomer and that, among the skeletal deformation vibrations, the highest-frequency vibration for the *trans* isomer is higher in frequency than that for the *gauche* isomer. The conclusion regarding the molecular form obtained from the skeletal deformation vibration is consistent with that obtained from the YCl_2 stretching vibrations.

Energy Difference between Isomers. For 2,2-dichlorobutane, the relative intensities of the bands at 692 and 645 cm^{-1} assigned to the CCl_2 antisymmetric stretching vibration for the *gauche* and *trans* isomers respectively are measured in the gaseous state at ten different temperatures; in the crystalline state the former disappears, while the latter persists. Figure 3 shows some typical examples of the infrared bands at 301, 320, 343, 368, and 399 K. From the observed optical densities, the energy difference between the isomers is found to be *ca.* 0.5 kcal/mol, where the *trans* isomer is more stable than the *gauche* isomer. This value is in good agreement with the value estimated by means of the interactions of the atoms in the 1,3 positions lying on parallel bonds which has been presented by Štokr *et al.*[8] However, for dichloroethylmethylsilane, measurements of the relative intensities of the bands cannot

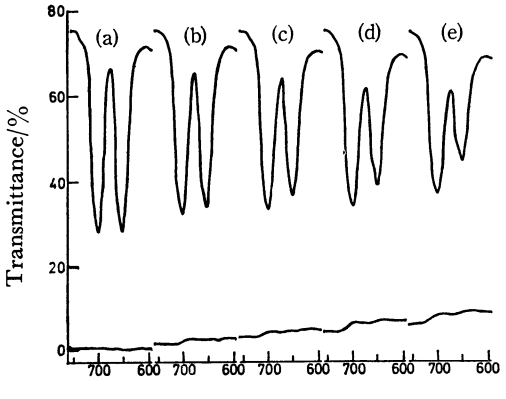

Fig. 3. The relative intensities of the infrared bands at 692 and 645 cm^{-1} in the gaseous state.
Upper: absorption spectra, Lower: base line; (a): at 301 K, (b): at 320 K, (c): at 343 K, (d): at 368 K, (e): at 399 K.

TABLE 1. VIBRATIONAL FREQUENCIES OF DICHLOROETHYLMETHYLSILANE[a] (cm^{-1})

Infrared			Raman	Assignment
Liquid	Int.	Crystal Int.	Liquid Int.	
2970	s	2970 s	2975 s	C–H str.
2944	m	2944 m	2943 s	
2917	m	2917 w	2911 vvs	
2885	m	2888 s	2884 vs	
1468 sh	m	1466 m		CCH_3 asym. def.
1461	m	1455 m	1462 w	
1410	m	1408 m	1406 w	$SiCH_3$ asym. def.
1401 sh	m	1399 w		CH_2 sci.
1384	w	1376 w	1381 vw	CCH_3 sym. def.
		1366 vw		
1262 vs		1264 s	1261 vw	$SiCH_3$ sym. def.
1242	m	1246 m	1241 w	CH_2 wag.
1232	w	1232 w	1230 vw	CH_2 twist.
1087 b	w			
1021	m	1025 m	1019 w	C–C str.
1011	s	1015 vw	1011 mw	
974 sh	w	974 vw	973 w	CCH_3 rock.
965	m	959 m		
806	vs	807 vs	807 vw	$SiCH_3$ rock.
788	vs	792 vs		
767	vs	—	766 w	C–Si antisym. str.
748	s	754 vs	746 w	
		705 vw		
685	m	684 s		CH_2 rock.
662	s	663 vs	662 m	C–Si sym. str.
606	w	609 w	604 w	
		574 w		
		565 w	557 w	
543	vs	—	540 w	$SiCl_2$ antisym. str.
531	vs	518 vs	531 w	
		477 w		
470	s	—	470 vvs	$SiCl_2$ sym. str.
461	s	459 s	460 vvs	
427	vw		426 vw	
383	w	384 w	383 w	
356	m	356 m	357 mw	Skeletal def. or torsion
315	vw	—	314 m	
231	m	228 w	231 s	
			199 ms	
184	m		183 s	
167 sh	w		164 ms	
138	w		134 m	
			79 mw	

a) Int.=intensity; s, m, w=strong, medium, weak; v=very; sh=shoulder; and b=broad.

TABLE 2. VIBRATIONAL FREQUENCIES OF 2,2-DICHLOROBUTANE$^{a)}$ (cm^{-1})

Infrared						Raman$^{b)}$		Assignment
Gas	Int.	Liquid	Int.	Crystal	Int.	Liquid	Int.	
2996	vs			3001	w			C–H str.
2990		2980	vs	2973	s	2986	4b	
2987								
2951	vs							
2941		2944	s	2936	m	2936	6b	
2930		2930 sh	ms	2921				
2897 sh	w	2892	ms					
		2866	vw	2875	m			
2850 sh	w	2848	vw					CH$_3$ asym. def.
1465	s	1463	s	1465	s			
1460		1454	s	1453	s			
						1441	4b	
1452				1447				
1446		1443	s	1443	w			
1438	m	1427	mw	1436	s			CH$_2$ sci.
1432				1432				
1394 sh								
1389	s			1379	s			
1382	vs	1382	s	1376		1380	1	CH$_3$ sym. def.
1343	w	1342	w	1348	w			
1335	w	1332	w	1343	m	1329	0	
1287	m							
1280		1283 sh	m	1284	s			
1275		1279		1277		1272	1	CH$_2$ wag.
						1224	0	CH$_2$ twist.
		1185	w					
1172	m	1170	m	1174	s	1167	1	C–C str. or CH$_3$ rock.
1148 b	s	1146	s	—				
1128	vs			1136	m			
1123		1120	s	1122	s	1113	1	
				1111				
1102	vs							
1097		1091	s	—		1088	1	
1092				1087	vw			
				1075	vw			
1042	s	1042 sh	ms					
1037		1037		1034	s			
1030				1033		1020	1/2	
1007	m	1008	w	—				
998		999	w	998	s			
991								
982	m	982	m	—		977	1	
859	s	859	s	856	s	853	2	
854								
815	s							CH$_2$ rock.
809		808	s	808	s			
803		796	m	—		793	0	
708	vs							CCl$_2$ antisym. str.
701		692	vs	—		688	3	
696								
662	vs	645	vs	635	vs	642	3	
656								

Table 2. Continued

Infrared						Raman[b)] Liquid		Assignment
Gas	Int.	Liquid	Int.	Crystal	Int.		Int.	
572 560	m	567	m	—		566	4	CCl_2 sym. str.
548	m	544	m	545 529	s	544	4	
		490	vw	488	m	486	0	Skeletal def. or torsion
418 413 406	m	413	m	—		410	2	
375 368 365	m	367 sh	m	—				
357 353	m	358	m	356	s	362	4	
				281	vw	276	2	
						252	2	
						202	2	

a) See a) of Table 1. b) See Ref. 18.

be made because of the overlapping of the bands assigned to the $SiCl_2$ stretching vibrations in the gaseous state.

Vibrational Assignments

The *trans* form of dichloroethylmethylsilane and 2,2-dichlorobutane may have C_s symmetry. The 36 normal modes are reduced by group theory to 21 modes of the A′ species and 15 of A″. The *gauche* form belongs to the trivial point group C_1. All of the 36 modes are of the same symmetry species. All of the fundamental vibrations of the *trans* and *gauche* forms are infrared and Raman-active. The observed frequencies are given in Tables 1 and 2, together with the brief vibrational assignments.

Dichloroethylmethylsilane. It is expected that the vibrations of the $SiCH_3$ group are considerably lower in frequency than the corresponding vibrations of the CCH_3 group because of the difference in the electronegativity of the adjacent atom. Actually, these vibrations of the CCH_3 and $SiCH_3$ groups are observed at different frequencies clearly separated from each other. The infrared spectra of dichloroethylmethylsilane in the 800—1500 cm^{-1} region are not so different in the liquid and crystalline states, and they are close to the superposition of the spectra of ethyltrichlorosilane[9)] and methyltrichlorosilane.[10)] The infrared spectra in the 400—800 cm^{-1} region are also similar to those of dimethyldichlorosilane.[5)] Therefore, the vibrational assignments in the 400—1500 cm^{-1} region can easily be made by a comparison of the spectra with those of analogues. The bands in the region below 400 cm^{-1} may be assigned to the skeletal deformation or torsional vibrations. However, the vibrational assignments in this region cannot be made easily, for a large mode mixing among the several skeletal deformation vibrations must be expected; they are tentatively assigned in Table 4 on the basis of the results of the normal vibration calculations.

2,2-Dichlorobutane. In the infrared spectra in the 300—1500 cm^{-1} region, as too many bands for a unique molecular form are observed in the liquid state and as several bands vanish in the crystalline state, it may be concluded that rotational isomers coexist in the liquid state, while only one isomer persists in the crystalline state. The infrared spectra show that most of the vibrations of the two CH_3 groups may be coincident with each other, because the presence of one CH_3 group is sufficient to account for the number of observed bands. Therefore, the infrared spectra in the 1200—1500 cm^{-1} region can easily be assigned on the basis of a comparison of the spectra with those of analogues, such as CH_3CCl_3[11)] and CH_3CH_2X.[12)] The bands in the 800—1200 cm^{-1} region may be assigned to the C–C stretching or CH_3 rocking vibrations, but three C–C stretching and four CH_3 rocking vibrations are expected for a unique molecular form and may mix with each other in the same symmetry species. Therefore, the vibrational assignments in this region are made from the results of the normal vibration calculations. On the other hand, the strong infrared bands at 796 and 808 cm^{-1} and the weak Raman counterpart at 793 cm^{-1} are assigned to the CH_2 rocking vibrations. The very-strong pair band around 670 cm^{-1} and the strong pair band around 550 cm^{-1} are easily assigned to the CCl_2 stretching vibrations, as has already been mentioned. The infrared bands in the region below 500 cm^{-1} may be assigned to the skeletal deformation or torsional vibrations. These bands are assigned on the basis of the results of the normal vibration calculations, because large mixings of the modes are expected.

Normal Vibration Calculation

The normal vibrations were calculated on the basis of the modified Urey-Bradley force field in order to determine the molecular forms and the vibrational assignments. The force constants were transferred from those of $CH_3CH_2SiH_3$[13)] and $(CH_3)_2SiCl_2$[5)] for C_2H_5-$SiCl_2CH_3$ and from those of $CH_3CHClCHClCH_3$[14)]

TABLE 3. FORCE CONSTANTS FOR DICHLOROETHYLMETHYLSILANE AND 2,2-DICHLOROBUTANE[a)]

$C_2H_5SiCl_2CH_3$			
K(C-H)	4.297	Y(C-C)	0.109
K(C-C)	2.400	Y(C-Si)	0.052
K(C-Si)	1.991	p(C-H)	−0.070
K(Si-Cl)	2.590 (2.226)	p(Si-Cl)	(0.174)
H(C-C-H), CH_3	0.164	F(C·C·H), CH_3	0.470
H(H-C-H), CH_3	0.370	F(H·C·H), CH_3	0.200
H(C-C-Si)	0.087	F(C·C·Si)	0.540
H(Si-C-H)	0.123	F(Si·C·H)	0.271
H(C-C-H), CH_2	0.278	F(C·C·H), CH_2	0.540
H(H-C-H), CH_2	0.331	F(H·C·H), CH_2	0.200
H(C-Si-C)	0.110	F(C·Si·C)	0.040
H(C-Si-Cl)	0.085	F(C·Si·Cl)	0.162
H(Cl-Si-Cl)	0.059	F(Cl·Si·Cl)	0.290
$\kappa(CCH_3)$	0.008	$\kappa(SiCl_2)$	0.130
$\kappa(CH_2)$	−0.040	$\kappa(SiCH_3)$	−0.050
$C_2H_5CCl_2CH_3$			
K(C-H)	4.350	Y(C-C)	0.109
K(C-C)	2.750	p(C-H)	−0.086
K(C-Cl)	1.697 (1.353)	p(C-Cl)	(−0.090)
H(C-C-H), CH_3	0.186	F(C·C·H), CH_3	0.470
H(H-C-H), CH_3	0.370	F(H·C·H), CH_3	0.200
H(C-C-C)	0.275	F(C·C·C)	0.335
H(C-C-H), CH_2	0.186	F(C·C·H), CH_2	0.470
H(H-C-H), CH_2	0.343	F(H·C·H), CH_2	0.200
H(C-C-Cl)	0.087	F(C·C·Cl)	0.747
H(Cl-C-Cl)	0.062	F(Cl·C·Cl)	0.697
$\kappa(CH_2)$	0.100	$\kappa(CH_3)$	0.008

a) All the force constants are transferred from ethylsilane[13)] and dimethyldichlorosilane[5)] for dichloroethylmethylsilane and from 2,3-dichlorobutane[14)] and dichloromethane[15)] for 2,2-dichlorobutane. The adjusted force constants are given in brackets. The units of the force constants are in mdyn/Å for stretching, K; bending, H; repulsion, F; and bond-interaction, p; and in mdyn·Å for intramolecular tension, k; and internal rotation, Y.

and CH_2Cl_2[15)] for $C_2H_5CCl_2CH_3$. The following assumptions were made for the force field: 1) the bond-interaction constant, p(C–H), was added in order to reproduce the observed C–H stretching frequencies, 2) the torsional force constant, Y(C–C), was assumed to be the value (3.49 kcal/mol) obtained from the reported far-infrared band for the CH_3 torsion of ethyl chloride[16)] and the Y(C–Si) constant was assumed to be the value(1.65 kcal/mol) of dimethylsilane determined by microwave study,[17)] and 3) for $C_2H_5SiCl_2CH_3$, the force constants, H(H–C–H) and F(H·C·H), were assumed to be the same values for the CCH_3 and $SiCH_3$ groups, while for $C_2H_5CCl_2CH_3$, the force constants, H(H–C–H), H(C–C–H), F(H·C·H) and F(C·C·H), were assumed to be the same values for both the CH_3 groups.

The force constants used in the calculation are given in Table 3. The vibrational frequencies in the region below 1200 cm^{-1} depend more conspicuously upon the azimuthal angle of internal rotation. Therefore, the observed and calculated frequencies in this region are given in Tables 4 and 5, together with the predominant symmetry coordinates in the potential energy distributions. Set I of the calculation in Tables 4 and 5 shows the calculations using all the transferred force constants given in Table 3. A fair agreement is obtained between the observed and calculated frequencies, except for a few vibrations. Especially, the calculated frequencies of the YCl_2 stretching (Y=C, Si) and the highest-frequency skeletal deformation vibrations indicate that, for both dichloroethylmethylsilane and 2,2-dichlorobutane, the bands persisting in the crystalline state are attributable to the *trans* form, while the bands disappearing in the crystalline state are attributable to the *gauche* form. However, as the calculated YCl_2 stretching frequencies indicate that the values of both the force constants, K(C–Cl) and K(Si–Cl), have to be smaller than the transferred values, only these constants, K(C–Cl) and K(Si–Cl), are adjusted in order to reproduce the observed frequencies. We still cannot reproduce the separations between the YCl_2 antisymmetric and symmetric stretching frequencies satisfactorily. Therefore, the bond-interaction constants, p(C–Cl) and p(Si–Cl), are introduced.

The results of the calculations obtained in this modification are given in Set II of the calculation in Tables 4 and 5. The values of the adjusted force constants are K(C–Cl)=1.353, p(C–Cl)=−0.090, K(Si–Cl)=2.226, and p(Si–Cl)=0.174 mdyn/Å. It is inter-

TABLE 4. OBSERVED AND CALCULATED FREQUENCIES OF DICHLOROETHYLMETHYLSILANE (cm^{-1})[a)]

	Trans form				*Gauche* form			
	Obsd	Calcd			Obsd	Calcd		PED
		Set I	Set II			Set I	Set II	
A′	1021	1020	1020	A	1011*	1022	1022	ν(C-C)
	974	968	968		974	968	968	$r(CCH_3)$
	806	798	797		806	798	797	$r(SiCH_3)$
					767*	749	748	ν_a(C-Si), $r(CH_2)$
	748	729	729					ν_a(C-Si)
	662	682	679		662	667	663	ν_s(C-Si)
	461	471	460		470*	481	469	$\nu_s(SiCl_2)$
	356	342	342					δ(CCSi), $w(SiCl_2)$
					315*	319	316	δ(CCSi)
	231	220	220		231	234	234	δ(CCSi), $w(SiCl_2)$
					231	223	223	$w(SiCl_2)$, $r(SiCl_2)$
	184	184	184					$s(SiCl_2)$, $w(SiCl_2)$
					167	176	176	$s(SiCl_2)$, $\tau(SiCH_3)$
	138	134	134					$w(SiCl_2)$, $s(SiCl_2)$, δ(CSiC)
A″	965	967	967		965	967	967	$r(CCH_3)$
	788	796	793		788	795	792	$r(SiCH_3)$
	685	727	725					$r(CH_2)$
					685	708	707	$r(CH_2)$, ν_a(C-Si)
	531	585	531		543*	602	549	$\nu_a(SiCl_2)$
	—	241	241		—	240	240	$\tau(CCH_3)$
	231	233	232					$r(SiCl_2)$
					199	196	196	$r(SiCl_2)$, $t(SiCl_2)$
	184	188	188					$t(SiCl_2)$
					—	154	154	$\tau(SiCH_3)$, δ(CSiC), $s(SiCl_2)$
	—	152	152					$\tau(SiCH_3)$, $t(SiCl_2)$
					138	134	134	$t(SiCl_2)$
	—	56	56		79	58	58	τ(skel)

a) The observed infrared frequencies in the liquid state are listed, where asterisks indicate the bands disappearing in the crystalline state. The vibrational frequencies below 1200 cm^{-1} are included. Potential energy distributions are shown for the internal symmetry coordinates, where only contributions greater than 20% are included. ν, δ, s, w, t, r, and τ denote the stretching, deformation, scissoring, wagging, twisting, rocking, and torsional modes and a and s denote the antisymmetric and symmetric modes, respectively.

esting to note that the value of p(C–Cl) is negative, while that of p(Si–Cl) is positive. It is also noticeable that the frequency differences of the YCl_2 stretching vibrations between the antisymmetric and symmetric modes and between the *trans* and *gauche* forms for $C_2H_5SiCl_2CH_3$ are smaller than those for $C_2H_5CCl_2CH_3$. This may be because, for the nonlinear YX_2-type molecule, the off-diagonal element of the **G**-matrix between the stretching modes is cos $\alpha\mu_y$ (μ_y is the reciprocal of the mass of the atom, Y).[7)] Therefore, the separation frequency between the antisymmetric and symmetric modes of the YCl_2 stretching may be mainly affected by the mass of the atom, Y, though the quite reverse influence of the corresponding off-diagonal element of the **F**-matrix containing only the repulsive force constant, F(Cl·Y·Cl), in the simple Urey-Bradley force field($F'=-0.1F$) can be expected, and though the couplings of the YCl_2 stretching modes with the other modes are not taken into account. In order to predict well the observed YCl_2 stretching frequencies, the bond-interaction constant, p(Y–Cl), is necessary.

On the other hand, the frequency separation of the YCl_2 stretching modes between the different molecular forms may be mainly influenced by the vibrations of the adjacent groups, which, in combination with the YCl_2 stretching modes, give the off-diagonal **G**-matrix elements containing the azimuthal angle, such as the Y–C–C bending and CH_2 rocking modes for $C_2H_5YCl_2CH_3$ (Y=C, Si). The larger couplings are expected from the perturbation theory[7)] when the vibrational frequencies come close to one another. The separations of the YCl_2 stretching modes with both the CH_2 rocking and Y–C–C bending modes for $C_2H_5CCl_2CH_3$ are smaller than those of $C_2H_5SiCl_2CH_3$. Therefore, it can be expected that the separations of the YCl_2 stretching vibrations between the different molecular forms for $C_2H_5CCl_2CH_3$ are larger than those for $C_2H_5SiCl_2CH_3$. This is supported by the results of the potential energy distributions of the modes, given in Tables 4 and 5.

Table 5. Observed and calculated frequencies of 2,2-dichlorobutane (cm^{-1})[a)]

	Trans form				*Gauche* form			
	Obsd	Calcd			Obsd	Calcd		PED
		Set I	Set II			Set I	Set II	
A′	1170	1156	1153	A				ν(C-C)
					1146*	1154	1150	ν(C-C), t(CH$_2$)
	1120	1112	1108					ν(C-C)
					1091*	1103	1100	ν(C-C), r(CH$_3$), r(CH$_2$)
	1037	1048	1047		1042*	1074	1072	ν(C-C)
	999	989	989		982*	985	985	r(CH$_3$)
	859	876	874		859	873	871	r(CH$_3$), ν(C-C)
					567*	597	568	ν_s(CCl$_2$), δ(CCC)
	544	576	547					ν_s(CCl$_2$)
	490	481	479					w(CCl$_2$), δ(CCC)
					413*	416	409	w(CCl$_2$)
					367*	377	374	δ(CCC), w(CCl$_2$)
	358	347	345					δ(CCC)
	276	265	265		252	257	257	s(CCl$_2$)
	202	190	190		202	190	190	δ(CCC), t(CCl$_2$), r(CCl$_2$)
A″	1037	1076	1075					r(CH$_3$), r(CH$_2$)
					1008*	1026	1021	r(CH$_3$), ν(C-C)
	999	997	996		982*	996	995	r(CH$_3$)
	808	860	859					r(CH$_2$), r(CH$_3$)
					796*	839	837	r(CH$_2$), r(CH$_3$), ν(C-C)
					692*	719	691	ν_a(CCl$_2$), r(CCl$_2$), δ(CCC)
	645	665	632					ν_a(CCl$_2$), r(CCl$_2$)
	358	366	364					r(CCl$_2$)
					358	359	357	r(CCl$_2$), w(CCl$_2$)
	276	302	301		276	302	302	t(CCl$_2$)
	—	240	240		—	240	240	τ(CH$_3$)
	—	222	222		—	228	228	τ(CH$_3$)
	—	81	81		—	86	87	τ(skel)

a) See a) of Table 4.

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