Nuclear Quadrupole Resonance and Stereochemistry. Part 7.[1] The Axial and Equatorial Chlorine Atoms in Octahedral Complexes of Antimony Pentachloride, $SbCl_5L$ (L = Donor Ligand)

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Chlorine-35 and $^{121,123}Sb$ n.q.r. frequencies and their temperature dependencies for various octahedral complexes of antimony pentachloride, $SbCl_5L$ (L = donor ligand), are reported. Assignments of ^{35}Cl resonances to axial or equatorial chlorine atoms of the $SbCl_5$ fragment have been possible in some cases. There are no apparent systematic differences between the frequencies of the axial or equatorial chlorine atoms, such differences as there are being masked by crystal-field effects of similar magnitude.

In the octahedral complexes of antimony pentachloride, $SbCl_5L$, one of the five chlorine atoms is in an axial configuration with respect to the donor L while the other four atoms occupy the equatorial positions; the majority of ligands do not however possess symmetry axes of high order so that the four equatorial chlorine atoms are not equivalent. For ligands having a plane of symmetry two situations are common: (1) if the ligand plane lies in the plane bisecting an equatorial ClSbCl angle the equatorial chlorine atoms fall into two equivalent pairs: (2) alternatively the ligand plane coincides with the plane defined by the axial chlorine atom and two *trans*-equatorial chlorine atoms (which will in general be distinct) while the remaining two, above and below the symmetry plane, are equivalent. Both these residual symmetries may however be removed in the solid state. The configurational differences among the chlorine atoms are reflected in the Sb–Cl bond lengths, although the differences are not very great.[2-7] In the present context they give rise to different ^{35}Cl quadrupole coupling constants, but it is not always and indeed not often apparent which experimental resonance frequency should be attributed to which chlorine atom. Thus in attempts at correlating the ^{35}Cl quadrupole resonance frequencies with the donor properties of L the only possibility is to use the average resonance frequency.

For compounds of known crystal structure the observation of the n.q.r. Zeeman effect will in principle solve the problem of the attribution of the resonances to the different atoms. However, most of the present complexes are formed by precipitation and even when recrystallisation is possible the crystals are usually small and unsuitable for Zeeman studies. Their melting points are high and often melting is accompanied by decomposition, so the Bridgeman method of preparing large single crystals is inappropriate. We are therefore reduced to more indirect methods of solving this problem.

As we show below, observation of the temperature dependence of the resonance frequency often permits a distinction between axial and equatorial chlorine atoms. It then becomes possible to discover whether the frequencies of the axial chlorine atoms and the equatorial chlorine atoms are affected differently by the substituent, and how the frequency difference brought about by the positioning of the chlorine atoms compares with the frequency differences induced by other intra- or inter-molecular effects.

Experimental

The complexes were prepared by dropwise addition of a slight excess of a 10% solution of redistilled antimony pentachloride in methylene chloride to a 10% solution of the donor in the same solvent at 0 °C. The precipitated complex was washed with a little dry carbon tetrachloride and sealed in a glass ampoule for n.q.r. measurements. All operations were carried out under an atmosphere of dry nitrogen or argon.

N.q.r. spectra were measured on a Decca super-regenerative spectrometer, frequencies being compared to harmonics from an internal crystal-controlled oscillator. Temperatures were measured with a Hewlett Packard 2802A digital thermometer and varied between 77 K and room temperature by using a cryostat controlled with an Artronix 5301-E temperature controller.

Results and Discussion

Inorganic ^{35}Cl *Resonances.*—The ^{35}Cl resonance frequencies at 77 K of a variety of $SbCl_5$ complexes are shown in Table 1.

The structures of the $SbCl_5$ adducts of benzoyl chloride and *m*-toluoyl chloride [5] are similar in that they have a plane of symmetry which bisects equatorial ClSbCl bond angles so that the equatorial chlorine atoms form two equivalent pairs. The three resonance frequencies have relative intensities of 2 : 2 : 1 and thus the frequency of the axial chlorine atom is apparent.† However, at 77 K, whereas in the benzoyl chloride adduct the axial chlorine atom has the highest frequency, for the *m*-toluoyl complex it has the lowest frequency.

The relative intensities shown in Table 1 are only approximate, particularly since in almost all cases the spectra have been measured with a super-regenerative spectrometer. However, Figures 1 and 2 show the temperature dependencies of these three resonances, measured from 77 K to room temperature for each of the two complexes. In both cases the two resonances which have been assigned to the equatorial chlorines fade out at around 170 K whereas the remaining resonance persists to 300 K and above. This parallel in behaviour increases our confidence in the above assignment; such a fade-out of resonances is moreover what might be expected for the equatorial chlorines as a consequence of high-amplitude librations or reorientations of the $SbCl_5$ group around the L–Sb–Cl axis. Since this movement does not affect the directions of the principal values of the field-gradient tensors of the axial chlorine or the antimony nuclei, whose asymmetry parameters would be zero in a complex of ideal C_{4v} symmetry, it will have no perceptible effect on their resonance frequencies, while the bulk of the ligand prevents an analogous movement around axes in the equatorial plane.

A number of the complexes shown in Table 1 also have three resonances in a 2 : 2 : 1 intensity ratio. Although the crystal

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† At 77 K the two resonances from the equatorial chlorine atoms of the benzoyl chloride complex accidentally overlap (see Figure 1).

Table 1. Chlorine-35 and ^{121,123}Sb resonance frequencies (MHz) of antimony pentachloride complexes at 77 K

		SbCl$_5$ Fragment				
			^{121}Sb		^{123}Sb	
Donor	Donor ^{35}Cl	^{35}Cl	$m = \frac{1}{2}\rightarrow\frac{3}{2}$	$m = \frac{3}{2}\rightarrow\frac{5}{2}$	$m = \frac{1}{2}\rightarrow\frac{3}{2}$	$m = \frac{3}{2}\rightarrow\frac{5}{2}$
PhCOCl	34.135	26.418,[a] 26.418,[a] 26.818	30.62		18.58	37.16
3-MeC$_6$H$_4$COCl	34.200	26.505, 26.825,[a] 26.852 [a]	31.847 [b]		19.336 [b]	
4-MeC$_6$H$_4$COCl	34.311	26.159, 26.311, 26.643, 26.803, 26.946				
PhCN	—	26.011,[a] 26.123,[a] 26.641	26.171 [b]	52.209 [b]	15.858 [c]	31.704 [c]
2-ClC$_6$H$_4$CN	36.734	25.889,[a] 26.425,[a] 27.475				
3-ClC$_6$H$_4$CN	36.065	25.129, 25.959, 26.282, 26.322, 26.630				32.185 [d]
4-ClC$_6$H$_4$CN	35.506, 35.659	25.766, 26.046,[a] 26.109,[a] 26.254, 27.125, 27.512				31.931 [d]
2-ClC$_5$H$_4$N	37.867	24.771, 25.387, 26.114, 26.178, 26.698				
3-ClC$_5$H$_4$N	37.058	24.901, 25.153, 25.192,[a] 25.542				
PhCOCH$_2$Cl	39.463	25.370, 25.460, 25.909, 26.367, 26.920				30.309 [d]
4-ClC$_6$H$_4$COMe	35.866	25.746, 26.186, 26.261				
CCl$_3$CHO	39.891, 40.048, 40.963	25.330, 25.593, 27.071, 27.791, 28.215	28.662	57.210	17.482	34.694 [e]
ClCOCH$_2$CH$_2$COCl	34.054	26.058, 26.616, 27.236, 27.481, 27.686				35.762 [d]
Et$_2$O	—	25.491, 25.734, 25.967, 26.099, 26.620	26.169		16.505	30.970

[a] Approximately twice the intensity of the other ^{35}Cl resonances in the same complex. [b] At 303 K. [c] At 119 K. [d] Tentative assignment. [e] ^{123}Sb ($\frac{5}{2}$—$\frac{7}{2}$) frequency is 52.120 MHz.

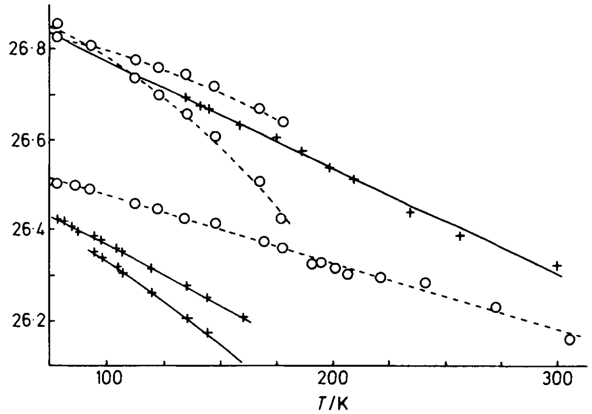

Figure 1. Temperature dependence of the ^{35}Cl resonance frequencies of the antimony pentachloride fragment in the complexes with benzoyl chloride (+) and *m*-toluoyl chloride (○). The symbols mark the experimental points while the solid and broken lines were constructed from the quadratic equations $\nu = A + BT + CT^2$ by which the experimental data were fitted by least squares

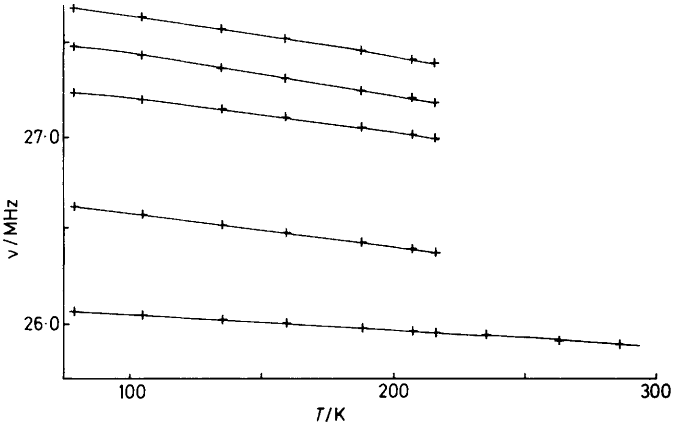

Figure 2. Temperature dependence of the ^{35}Cl resonance frequencies of the antimony pentachloride fragment in the complex with succinyl chloride. The symbols mark the experimental points and the lines were constructed from the quadratic equations $\nu = A + BT + CT^2$

structures of these compounds have not been determined it is reasonable to suppose that the resonance of unit relative intensity arises from the axial chlorine. We have measured the temperature dependence for the benzonitrile complex and its behaviour is very similar to that of the benzoyl chloride derivative, although the fade-out temperature is somewhat higher, around 200 K. Two other complexes, those of acetophenone[8] and of nitrobenzene,[8] which show three 2 : 2 : 1 resonances at 77 K, are reported to have only one resonance at room temperature with a frequency corresponding to that of the line of lowest intensity. For all these compounds the assignment of the axial chlorine atom seems beyond doubt.

The structure of the succinyl chloride 1 : 2 adduct with SbCl$_5$ is such that all five chlorine atoms bonded to antimony are inequivalent[4] and five distinct ^{35}Cl resonances may be observed. Their temperature dependence is shown in Figure 2: four of the resonances fade out around 220 K while one remains at room temperature and above. On the basis of what has gone before we may again conclude that this resonance arises from the axial chlorine atom. The behaviour of the 3-chlorobenzonitrile complex is similar, the fade-out temperature being around 200 K.

Some of the complexes showing three chlorine resonances with a 2 : 2 : 1 intensity ratio do not show this differential

Table 2. Temperature dependencies and temperature coefficients at 150 K of the ^{35}Cl resonance frequencies of $SbCl_5$ complexes. The resonance frequencies have been fitted by the quadratic $\nu = A + BT + CT^2$

Donor	Line	A/MHz	B/kHz K^{-1}	C/Hz K^{-2}	$10^{-4}[(1/\nu)(\delta\nu/\delta T)]_{150}$
PhCOCl	1	26.605	−2.185	−1.929	−1.054
	2	26.622	−2.467	−4.660	−1.478
	3	27.018	−2.448	0.178	−0.898
	Organic	34.455	−3.964	−0.703	−1.234
$3\text{-}MeC_6H_4COCl$	1	26.637	−1.64	0.361	−0.580
	2	26.864	0.079	−7.673	−0.832
	3	26.924	0.336	−17.44	−1.842
	Organic	34.480	−3.107	−2.763	−1.159
$4\text{-}MeC_6H_4COCl$	1	26.176	0.272	−6.412	−0.633
	2	26.158	3.733	−2.278	1.144
	3	26.709	−0.453	−4.578	−0.688
	4	27.224	−6.897	19.188	−0.428
	5	26.971	−0.523	−10.748	−1.408
	Organic	34.462	−1.126	−9.075	−1.129
PhCN	1	26.224	−2.580	−1.680	−1.19
	2	26.319	−2.208	−3.625	−1.27
	3	27.043	−5.313	4.430	−1.512
$2\text{-}ClC_6H_4CN$	1	26.043	−1.503	−5.524	−1.23
	2	26.550	−1.096	−5.487	−1.04
	3	27.740	−3.213	−1.069	−1.298
	Organic	37.007	−3.1232	−4.275	−1.209
$3\text{-}ClC_6H_4CN$	1	25.379	−3.080	1.047	−1.109
	2	26.066	−1.1928	−1.868	−0.678
	3	26.437	−1.739	−2.373	−0.938
	4	26.439	−1.179	−3.723	−0.877
	5	26.837	−2.520	−0.531	−1.013
	Organic	36.263	−1.422	−13.648	−1.543
$4\text{-}ClC_6H_4CN$	1	25.854	−0.9225	−2.154	−0.611
	2	26.181	−1.640	−0.437	−0.683
	3	26.191	−0.846	−2.032	−0.559
	4	26.314	−0.583	−2.309	−0.487
	5	27.206	−0.8339	−2.810	−0.621
	6	27.632	−1.3057	−2.605	−0.762
	Organic	35.642	−1.4272	−3.085	−0.665
	Organic	35.816	−1.7352	−2.693	−0.716
$2\text{-}ClC_5H_4N$	1	24.907	−1.5929	0.181	−0.624
	2	25.503	−1.4236	0.729	−0.476
	3	26.304	−2.3356	1.264	−0.753
	4	26.298	−1.455	0.569	−0.492
	5	26.839	−1.709	0.545	−0.581
	Organic	38.065	−2.193	−2.529	−0.783
$3\text{-}ClC_5H_4N$	1	24.491	−0.2636	−2.655	−0.427
	2	25.233	−0.8759	−1.872	−0.574
	3	25.274	−0.923	−1.549	−0.553
	4	25.628	−1.0139	−1.280	−0.549
	Organic	37.162	−1.0205	−3.517	−0.562
$PhCOCH_2Cl$	1	25.491	−1.206	−3.199	−0.858
	2	25.533	−0.722	−2.072	−0.529
	3	26.070	−1.872	−0.939	−0.836
	4	26.486	−1.478	−0.895	−0.858
	5	27.129	−2.458	−1.711	−1.112
	Organic	39.732	−2.711	−7.937	−1.301
$4\text{-}ClC_6H_4COMe$	1	25.582	−0.211	−13.263	−1.324
	2	26.288	0.672	−23.375	−1.897
	3	26.419	−0.175	−21.344	−2.031
	Organic	36.138	−3.103	−1.868	−1.028
CCl_3CHO	1	25.283	0.7238	−1.520	0.106
	2	25.690	−1.3496	1.910	−0.304
	3	27.077	0.4344	−7.860	−0.710
	4	27.854	−0.3785	−5.917	−0.778
	5	28.172	1.2986	−11.876	−0.806
	Organic	40.210	−2.248	−23.927	−2.396
	Organic	40.227	−0.182	−27.366	−2.120
	Organic	41.094	0.5767	−29.956	−2.076
$ClCOCH_2CH_2COCl$	1	26.123	−0.8563	−0.094	−0.340
	2	26.747	−1.624	−0.590	−0.680
	3	27.341	−1.167	−2.144	−0.667
	4	27.638	−1.188	−1.113	−0.813
	5	27.832	−1.698	−1.681	−0.780
	Organic	34.247	−1.761	−9.415	−1.358

Table 2 (*continued*)

Donor	Line	A/MHz	B/kHz K^{-1}	C/Hz K^{-2}	$10^{-4}[(1/\nu)(\delta\nu/\delta T)]_{150}$
Et_2O	1	25.533	−0.0337	−3.706	−0.450
	2	25.784	−0.408	−3.206	−0.534
	3	25.991	−0.7687	−6.197	−1.021
	4	26.133	−1.4828	−1.910	−0.795
	5	26.608	1.642	−9.699	−0.476

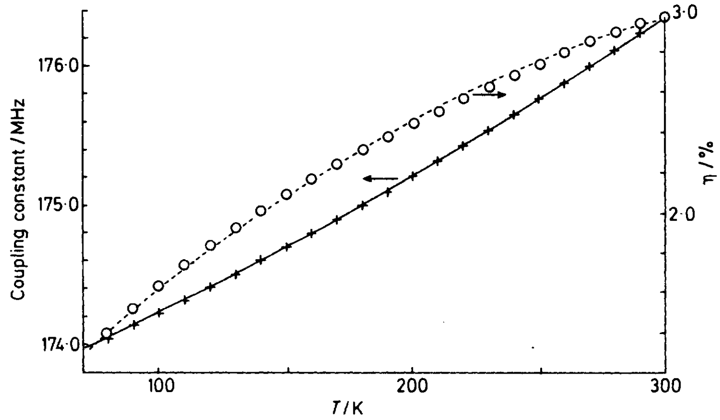

Figure 3. Temperature dependence of the ^{121}Sb coupling constant (+) and asymmetry parameter (○) of the antimony pentachloride fragment of the complex with benzonitrile. The symbols represent the experimental points and the solid or dotted lines were constructed from the cubic equations $\nu(\eta) = A + BT + CT^2 + DT^3$

Table 3. Temperature dependencies of the principal values of the quadrupole coupling tensor. The tensor components were fitted by the cubic equation $\nu = A + BT + CT^2 + DT^3$ in the range 77—300 K; their signs are only relative

Component	A/MHz	B/kHz K^{-1}	C/Hz K^{-2}	D/Hz K^{-3}
(*a*) CCl_3CHO				
e^2Qq_{xx}	−91.878	7.288	8.907	—
e^2Qq_{yy}	−99.450	7.623	−126.93	0.3350
e^2Qq_{zz}	191.36	−15.655	122.64	−0.3438
(*b*) PhCN				
e^2Qq_{xx}	−86.573	12.827	−46.434	0.050 57
e^2Qq_{yy}	−87.065	−15.491	10.248	0
e^2Qq_{zz}	173.40	7.421	8.120	0
(*c*) Et_2O				
e^2Qq_{xx}	−83.041	−239.8	1 331.6	−2.5125
e^2Qq_{yy}	−84.605	173.63	−987.7	1.9065
e^2Qq_{zz}	167.65	66.166	−343.94	0.6061

fading out. Thus for the 2-chlorobenzonitrile complex the resonances are not very intense and all of them disappeared around 175 K; the 4-chloroacetophenone complex behaves similarly. The assignment of the axial chlorine resonance for these two compounds is thus based only on the relative intensities, but since these relative intensities are more or less independent of the spectrometer variables such as the quenching frequency and the radiofrequency power the assignment is probably fairly reliable. Three other complexes, of acetonitrile,[9] cyanogen chloride,[10] and of trimethyl phosphate,[8] have intensity ratios which allow the assignments of the axial resonance.

There remain a number of complexes where neither the relative intensities nor the temperature dependence provides any evidence as to the assignment of the frequency of the axial chlorine atom. Thus the $POCl_3$ adduct has a structure in which the phosphorus atom lies in a symmetry plane containing two of the equatorial chlorine atoms and the axial chlorine atom. The remaining equatorial chlorine atoms are equivalent.[9] The intensity of their resonances is twice that of the other three, but on raising the temperature it is the resonances of the PCl_3 group which begin to fade. The complexes of trichloroacetaldehyde and of diethyl ether studied here both have five distinct resonances for the ^{35}Cl nuclei of the $SbCl_5$ fragment, and for neither is there a fade-out of the resonances which would permit an assignment to the axial chlorine atom. The ether complex shows evidence of a phase change at around 100 K, while the temperature dependencies of the two lowest frequencies of the trichloroacetaldehyde complex are anomalous in that one has a positive slope and the other a positive second derivative. In this complex the resonances of the CCl_3 group fade out at 180 K showing that here the CCl_3 is the more mobile fragment. None of these facts however leads to an assignment of the resonances.

An approach to this general problem which has been applied on several occasions is to assume that the temperature dependence of the resonance frequencies is determined only by rigid-body librations of the whole molecule.[11] If the normal co-ordinates and frequencies of these librations were known the temperature coefficients of the resonance frequencies of the various quadrupolar nuclei could be deduced simply from the orientations of the various field-gradient tensors. The difficulty is of course that the normal co-ordinates are often not known and assumptions must thus be made. The simplest one is that there are three librational modes which occur about the three mutually perpendicular axes of the inertial tensor of the isolated molecule: this assumption is unfortunately probably almost always incorrect. It is thus almost certainly a waste of time to attempt this approach unless the crystal structure and the normal lattice modes are known.

Table 4. Chlorine-35 resonance frequencies (MHz) of axial and equatorial chlorine atoms and ^{121}Sb coupling constants (MHz) of the $SbCl_5$ fragment of octahedral antimony pentachloride complexes

	^{35}Cl		^{121}Sb		
Donor	axial	equatorial	e^2Qq	η	Ref.
PhCOCl	26.818	26.418 26.418	204.1	0.0	8, *a*, *b*
3-MeC_6H_4COCl	26.505	26.825 26.852	212.3	0.009	*a*
$ClCOCH_2CH_2COCl$	26.058	26.616 27.736 27.481 27.686	—	—	*a*
PhCOMe	26.528	25.294 25.904	157.7	0.028	8, *b*
4-ClC_6H_4COMe	26.261	25.746 26.186	—	—	*a*, *b*
PhCN	26.641	26.011 26.123	174.0	0.012	*a*
2-ClC_6H_4CN	27.475	25.899 26.425	—	—	*a*
3-ClC_6H_4CN	25.129	25.959 26.282 26.322 26.630	—	—	*a*
MeCN	24.99	26.37	216.3	0	9
ClCN	25.425	26.392 26.895	236.4	0	10
$PhNO_2$	27.030	26.295 26.839	189.4	0.01	8
$(CH_3O)_3PO$	25.64	24.81 25.14	—	—	8

[a] This study. [b] S. Ardjomande, Thesis, Université de Geneve, 1974.

In the present context, even though we do not in general have any of this information, we can make a number of observations about the possible validity of such an approach. Thus in the first place the four equatorial chlorine atoms are made up of two collinear Sb–Cl fragments and, even if the two chlorine nuclei are not equivalent and thus do not have identical resonance frequencies, their field-gradient principal axes are almost certainly parallel. Apart from the effect of internal rotation about the L–Sb axis discussed above, which in any case affects all four equatorial halogens equally, the rigid-molecule librations would affect such collinear pairs to the same extent and their temperature coefficients would be the same. Some of the molecules discussed above, such as the benzoyl chloride complex, have structures such that adjacent equatorial atoms are equivalent. In such cases, whatever the normal co-ordinates of the lattice vibrations may be, all four equatorial chlorine atoms would have the same temperature dependence if the model of rigid-molecule libration superimposed upon internal libration of the $SbCl_5$ group were correct. Reference to Figures 1 and 2 and to the numerical values of the slopes of the temperature dependencies at 150 °C given in Table 2 show that this is by no means the case for either the benzoyl chloride complex or the *m*-toluoyl chloride complex. The complexes of benzonitrile and 2-chlorobenzonitrile probably have structures which are similar to these; the temperature dependencies of the equatorial chlorine atoms are here much more alike.

When no symmetry element exists, and all four equatorial chlorine atoms are distinct, the rigid-molecule treatment predicts that the pairs of *trans* atoms should have similar temperature coefficients. Inspection of the data in Table 2 for the complexes for which we have been able to distinguish the axial from the equatorial chlorine atoms as discussed above shows no clear evidence of such a grouping of the temperature coefficients, nor is there usually anything to distinguish them from that of the axial chlorine atom. We conclude that these molecules are by no means rigid, even allowing for internal rotation of the $SbCl_5$ fragment, and that the temperature coefficients are at least in part determined by low-frequency intramolecular vibrations. An approach based on rigid-molecule librations is thus not likely to cast any light on the problem of the assignment of the resonance frequencies to the various chlorine atoms in these molecules.

Organic ^{35}Cl *Resonances.*—A number of the complexes studied here have chlorine atoms attached to the organic fragment. As expected, complexation always increases the resonance frequency; in general, the magnitude of the effect decreases as the chlorine substituent becomes more remote from the centre of complex formation and only the phenacyl chloride complex calls for any comment in this respect. For this complex the chlorine atom is separated by three bonds from the oxygen-donor atom while the resonance frequency has been increased by 3.6 MHz. This is comparable with the shifts produced in benzoyl chloride (4.2 MHz) and 2-chloropyridine (3.7 MHz) where the chlorine atom is only separated by two bonds from the donor site, and very different from other molecules such as 3-chloropyridine (1.8 MHz) where the chlorine atom is separated by three bonds.

The ^{121}Sb *and* ^{123}Sb *Resonances.*—For only one of the complexes studied here, that formed by trichloroacetaldehyde, were we able to observe all five resonances due to the antimony nuclei. For two other complexes (benzonitrile and diethyl ether) a sufficient number of resonances were detected to permit unambiguous assignments, while for the remainder only one or two resonances at the most could be observed and thus only tentative assignments were possible. For the three complexes in which the antimony resonances were unambiguously assigned the asymmetry parameters are small, as expected, and the temperature dependence of the coupling tensor could be determined over the whole range. The temperature dependence has been fitted to a cubic equation and the coefficients are shown in Table 3, while Figure 3 shows the complete temperature dependence for the benzonitrile complex. It will be remembered that, in the absence of large intermolecular contributions to the field gradient, the increased amplitude of rigid-molecule librations brought about by a rise in temperature can only decrease the magnitude of the coupling constant and asymmetry parameter; two of the compounds discussed here show marked positive temperature coefficients for their coupling constants, while the trichloroacetaldehyde complex has a negative temperature coefficient for its coupling constant and a positive temperature coefficient for the asymmetry parameter. This behaviour can only be ascribed to intramolecular deformations which of course can both increase or decrease the quadrupole coupling parameters as this amplitude increases. We thus have clear additional evidence that the rigid-body approach cannot lead to correct assignments of the chlorine resonances for these molecules.

Correlations.—In Table 4 are collected the ^{35}Cl resonance frequencies for the $SbCl_5$ fragment for those molecules for which we have succeeded in clearly distinguishing the axial from the equatorial chlorine atoms. Also included when available are the ^{121}Sb parameters. A glance suffices to convince one that there is no clear trend as far as the relative values of the axial and equatorial frequencies are concerned: of the twelve compounds shown seven have the axial chlorine at a higher frequency. Closely related sets of molecules (the two benzoyl chlorides, the five nitrile derivatives) show both higher and lower frequencies for the axial chlorine atom. However, while the overall range of axial frequencies is very similar to the overall range of equatorial frequencies, it is remarkable that for all twelve complexes the individual axial resonance frequency never falls within the range of the individual equatorial resonances. It is either the lowest or the highest frequency even when the total spread of the equatorial resonances is greater than 1 MHz.

Of these twelve compounds seven have well determined ^{121,123}Sb parameters. Again no clear correlation with the ^{35}Cl resonance frequencies, either collectively or taking into account the axial/equatorial differences, can be discerned. It is possible that if data for a more extensive series of similar donors were available, nitriles for example, then a correlation between the antimony and chlorine parameters would become apparent, but it is equally likely that the antimony coupling constants are far too susceptible to small deformations of the ideal local C_{4v} geometry. On the whole the antimony pentachloride system, either from the point of view of the ^{35}Cl resonances or from the ^{121}Sb resonances, does not seem well adapted to providing information about the nature of the donor molecule.

Acknowledgements

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