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Structural Studies of Antimony Tribromide and Its Molecular Complex with Benzene by Means of the ^{81}Br Nuclear Quadrupole Resonance

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The structures of α-antimony tribromide and its molecular complex with benzene $2SbBr_3 \cdot C_6H_6$ were investigated by studying the Zeeman effect on the nuclear quadrupole resonance (NQR) due to ^{81}Br at room temperature. The bond angles, ∠Br–Sb–Br, of α-antimony tribromide in its solid state were found to be 94°14′±4′, 94°31′±8′, and 98°27′±7′. The polar angles specifying the directions of the Sb–Br bonds with respect to the orthorhombic crystal axes are (60°0′±9′, 62°13′±7′), (59°10′±7′, −54°35′±8′), and (57°39′±17′, 180°0′±3′). These values are consistent with those of the X-ray analysis by Cushen *et al.* within about 1°. The asymmetry parameters at the three bromine atoms were 0.068±0.002, 0.049±0.002, and 0.080±0.004. On the other hand, the bond angles, ∠Br–Sb–Br, of the $SbBr_3$ molecule in the complex $2SbBr_3 \cdot C_6H_6$ were found to be 92°24′±11′, 97°7′±14′, and 97°40′±6′. The crystal has a monoclinic symmetry, and the three Sb–Br bonds have directions making angles of 29°4′±21′, 76°26′±9′ and 63°33′±11′ relative to the *b*-axis. The asymmetry parameters at the three bromine atoms in the complex were 0.169±0.001, 0.063±0.002, and 0.094±0.002. The largest value of the asymmetry parameters seems to be the result mostly of the intermolecular bonding. From the coupling constants, the Sb–Br bond characteristics in antimony tribromide and its molecular complex, $2SbBr_3 \cdot C_6H_6$, are considered to be almost the same.

It has long been known that antimony tribromide has two distinct crystal "habits," acicular and bipyramidal. When a warm carbon disulfide solution of antimony tribromide is cooled, needle-like crystals of α-antimony tribromide are obtained, contaminated with a few crystals of the β-form. The α-form is gradually transformed into the β-form at room temperature. When the β-form is melted, it can be reversed to the α-form.

Studies of the nuclear quadrupole resonance on antimony tribromide have been made by several authors.[1–3] All of them, however, used polycrystalline samples. The X-ray analyses of the α- and β-forms were carried out by Cushen[4] and Hulme[5] respectively. The α-form is orthorhombic, with the *c*-axis as the needle axis, and it has four molecules in the unit cell. The space group is $P2_12_12_1$. The β-form is orthorhombic, with the *a*-axis as the bipyramidal axis, and it has four molecules in the unit cell. The space group is *Pbnm*. The molecule in the gaseous state has been found to have a trigonal pyramidal form by the electron diffraction method. According to the latest report by Swingle[6] it has a bond angle of 97°±2° for ∠Br–Sb–Br and a bond distance of 2.51±0.02 Å for Sb–Br.

On the other hand, it is well known that antimony tribromide forms 1 : 1 and 2 : 1 molecular complexes with aromatic compounds. Studies of the nuclear quadrupole resonances for the powder of these complexes have already been reported,[1,3] but neither a Zeeman analysis of the resonances nor X-ray analysis has been done, so far as we know. Therefore we carried out a Zeeman analysis of the single crystals of α-antimony tribromide and its molecular complex with benzene, $2SbBr_3 \cdot C_6H_6$, in order to identify the ^{81}Br resonance lines and clarify the nature of the Sb–Br bonds as well as the shape of the $SbBr_3$ molecule.

Experimental

Antimony tribromide (mp 96°C) was synthesized by the reaction of bromine and antimony powder suspended in carbon disulfide; it was then refined by distillation. A 2 : 1 molecular complex of antimony tribromide with benzene was prepared by mixing molten antimony tribromide and a small excess of benzene. It was filtered

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[1] V. S. Grechiskin and I. A. Kyuntsel, *Zh. Struct. Khim.*, **5**, 53 (1964).

[2] S. Ogawa, *J. Phys. Soc. Jap.*, **13**, 618 (1958).

[3] H. Negita, T. Okuda and M. Kashima, *J. Chem. Phys.*, **45**, 1076 (1966).

[4] D. W. Cushen and R. Hulme, *J. Chem. Soc.*, **1964**, 4162.

[5] D. W. Cushen and R. Hulme, *ibid.*, **1962**, 2218.

[6] S. M. Swingle, *Structure Reports*, **13**, 421 (1950).

and dried in a vacuum desiccator. The melting point of the product was 93°C, whereas the literature value[1] is 92.5°C. The single crystals of these substances were obtained by a melting method. They were 15 mm in diameter and 40 mm in length. The single crystal obtained for antimony tribromide was the α-form, because a melting method was used.

An externally-quenched super-regenerative spectrometer with Lecher wires was used for the detection of the resonance absorption lines, which were displayed on an oscilloscope. The resonance frequency was measured by a frequency meter, TS-175 C/U. The single crystal was set on a goniometer equipped with a Helmholtz electro-magnet, and the magnetic field was applied on the sample from all directions in order to obtain the zero-splitting patterns. Several kinds of Zeeman fields ranging from 150 to 300 gauss were used in order to avoid misreading of the spurious signal. The crystal could be rotated about a fixed axis of the crystal, and its angle, Φ, could be measured to within 0.1°. On the other hand, the magnetic field could be rotated on a horizontal plane, and its angle, Θ, could be measured to within 1′. All of the measurements were carried out at about 20°C.

Results and Discussion

In a previous paper[3] we reported the ^{81}Br nuclear quadrupole resonance frequencies of antimony tribromide and its complexes. The ^{81}Br quadrupole resonance lines of α-antimony tribromide have been observed at 135.11, 135.32, and 140.35 MHz, with an intensity ratio of 1 : 1 : 1, at room temperature (19.5°C), as may be seen in Fig. 1 (a). In the case of β-antimony tribromide, the resonance lines have been observed at 135.96 and 141.49 MHz, with an an intensity ratio of 2 : 1, at room temperature (20.5°C), as may be seen in Fig. 1 (b). The resonance frequencies of α- and β-antimony tribromides are slightly different from one another. This fact reflects the delicate difference in the crystal fields surrounding the resonant nuclei in these modifications.

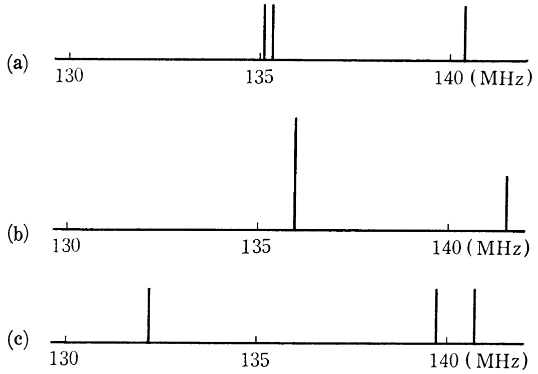

Fig. 1. Resonance spectra of antimony tribromide and its complex with benzene.
(a) α-$SbBr_3$, (b) β-$SbBr_3$, (c) $2SbBr_3 \cdot C_6H_6$

The quadrupole resonances of two modifications of antimony tribromide were reported by Ogawa.[2] Her synthesized antimony tribromide (1) corresponds to α-antimony tribromide, but her purchased antimony tribromide (2) is different from β-antimony tribromide. We could not obtain a sample like her second one.

As for the ^{81}Br resonance lines of $2SbBr_3 \cdot C_6H_6$, we have reported two resonance lines in a previous paper.[3] Through reexamination, however, we found a new resonance line, at about 8 MHz, below these two lines. Finally, then, three resonance lines with the same intensity have been observed; the frequencies are 132.14, 139.70, and 140.69 MHz at room temperature (21.5°C), as may be seen in Fig. 1 (c). The resonance lines in the complex are more widely spread than those of antimony tribromide, and two of them are closely spaced on the higher-frequency side. The grouping of the resonance lines is reversed from those of α- and β-antimony tribromides. We may say, however, that all resonance lines of the three samples are in nearly the same frequency regions. Thus, it can be assumed that there is no essential difference in the nature of the Sb–Br bonds, and that the shape of $SbBr_3$ molecule in its own crystal is retained in the complex.

The results of the Zeeman analyses of ^{81}Br resonance lines of α-antimony tribromide and its molecular complex with benzene $2SbBr_3 \cdot C_6H_6$ will be described below.

(a) α-Antimony Tribromide. Let us label the three resonance lines of ^{81}Br as ν_1, ν_2, and ν_3 from the lower to the higher. Then, from the number and their intensity ratio, these lines can be ascribed to three kinds of bromine atoms, Br_1, Br_2, and Br_3, in one molecule. The zero-splitting patterns of the Zeeman effect on the resonance lines are shown in Fig. 2. For the resonance lines, ν_1, ν_2, and ν_3, four, four, and two loci were obtained respectively. These loci are contributed by the Br_{1A}, Br_{1B}, Br_{1C}, and Br_{1D} atoms, the Br_{2A}, Br_{2B}, Br_{2C}, and Br_{2D} atoms, and the Br_{3A} and Br_{3B} atoms respectively. The direction of the principal z-axis of the field gradient on the bromine atom can be obtained from the zero-splitting pattern. The z-axis is usually parallel to the direction of the Sb–Br bond; the angle between any two Sb–Br bonds can thus be deduced. These angles are listed in Table 1, where the angle in parenthesis is the supplementary angle of the other. Since the gas molecule of $SbBr_3$ has been found to be a trigonal pyramid, one may expect that this molecule is nearly a trigonal pyramid in the solid state.

Taking the molecular shape and the bond angle, 97°, in the gaseous state into consideration, we find from Table 1 that each of the groups—Br_{1A}, Br_{2A}, Br_{3A}; Br_{1B}, Br_{2B}, Br_{3B}; Br_{1C}, Br_{2C}, Br_{3A}, and Br_{1D}, Br_{2D}, Br_{3B}, belongs to the same molecule. The directions of the symmetry axes of the crystal, a, b,

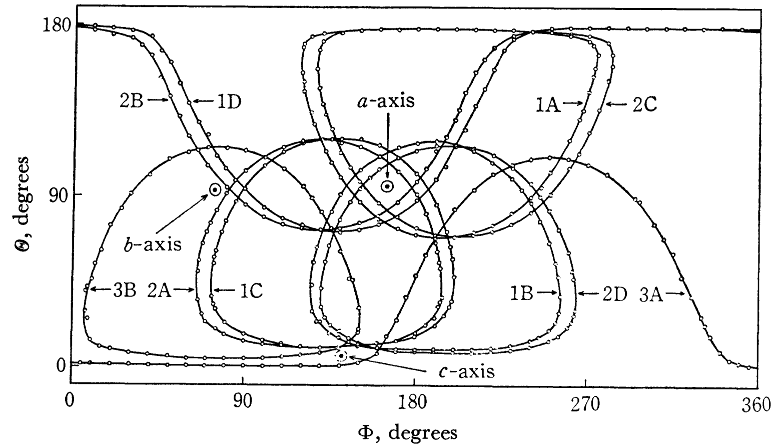

Fig. 2. Zero-splitting patterns of Zeeman lines of α-$SbBr_3$.
Θ and Φ are polar angles with respect to the orthogonal coordinate axes XYZ fixed to the sample.
1A, 1B, *etc.*, represent the zero-splitting directions of Zeeman lines at the nuclei Br_{1A}. Br_{1B}, *etc.*, respectively.

TABLE 1. THE ANGLES BETWEEN Sb–Br BONDS IN α-$SbBr_3$

∠Br–Sb–Br	Br_{1A}	Br_{1B}	Br_{1C}	Br_{1D}	Br_{2A}	Br_{2B}	Br_{2C}	Br_{2D}	Br_{3A}
Br_{1B}	119°54′ (60° 6′)*								
Br_{1C}	100° 3′ (79°57′)	47°31′ (132°29′)							
Br_{1D}	47°44′ (132°16′)	99°58′ (80° 2′)	120° 5′ (59°55′)						
Br_{2A}	**94°22′** (85°38′)	63°19′ (116°41′)	6°53′ (173° 7′)	118°49′ (61°11′)					
Br_{2B}	54° 1′ (125°59′)	**94°15′** (85°45′)	118°40′ (61°20′)	6°51′ (173° 9′)	118°19′ (61°41′)				
Br_{2C}	6°26′ (173°34′)	118°43′ (61°17′)	**94°45′** (85°15′)	53°41′ (126°19′)	88°51′ (91° 9′)	59°47′ (120°13′)			
Br_{2D}	118°45′ (61°15′)	6°23′ (173°37′)	53°25′ (126°35′)	**94°43′** (85°17′)	59°37′ (120°23′)	88°47′ (91°13′)	118°22′ (61°38′)		
Br_{3A}	**94°23′** (85°37′)	52°23′ (127°37′)	**94° 5′** (85°55′)	52°35′ (127°25′)	**98°28′** (81°32′)	45°51′ (134° 9′)	**98°46′** (81°14′)	46° 8′ (133°52′)	
Br_{3B}	52°27′ (127°33′)	**94°10′** (85°50′)	52°36′ (127°24′)	**94°17′** (85°43′)	45°52′ (134° 8′)	**98°19′** (81°41′)	46° 9′ (133°51′)	**98°14′** (81°46′)	115°18′ (64°42′)

* The value in parenthesis is supplementary angle.

and c, can easily be found from the symmetry distributions of the z-axes. These directions are shown in Fig. 2.

The values of the asymmetry parameters can be determined from the distortion of the zero-splitting loci by the following equation:⁽⁷⁾

$$\eta = 3(\sin^2\theta_{\max}-\sin^2\theta_{\min})/(\sin^2\theta_{\max}+\sin^2\theta_{\min}) \quad (1)$$

where $\theta_{\max}$ and $\theta_{\min}$ are the maximum and minimum zero-splitting angles, corresponding to $\phi=0°$ and 90° respectively. Consequently, the quadrupole coupling constant can be calculated by substituting the value of η in the following relation:

$$\nu = (eQq_{zz}/2)(1+\eta^2/3)^{1/2} \quad (2)$$

The values of η and eQq_{zz} derived in this way are listed in Table 2.

All of the asymmetry parameters are relatively small. In the antimony trichloride, which has the same crystal structure as β-antimony tribromide and

TABLE 2. RESONANCE FREQUENCIES (ν), ASYMMETRY PARAMETERS (η) AND QUADRUPOLE COUPLING CONSTANTS (eQq_{zz}) OF ^{81}Br ATOMS IN α-$SbBr_3$ AT 19.5°C

Compound	ν,	MHz	η, %	eQq_{zz}, MHz
α-$SbBr_3$	ν_1	135.11	6.8±0.2	270.01
	ν_2	135.32	4.9±0.2	270.53
	ν_3	140.35	8.0±0.4	280.40

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7) C. Dean, *Phys. Rev.*, **96**, 1053 (1954).

TABLE 3. THE ORIENTATIONS (Θ', Φ') OF Sb–Br BONDS WITH RESPECT TO THE CRYSTAL AXES IN α-$SbBr_3$

Bond	$Sb–Br_1$	$Sb–Br_2$	$Sb–Br_3$
NQR	(60°0′±9′, 62°13′±7′)	(59°10′±7′, −54°35′±8′)	(57°39′±17′, 180°0′±3′)
X-Ray	(59°28′, 62°16′)	(57°52′, −55°4′)	(58°49′, 181°18′)

which exhibits a similar pattern of NQR lines, the value of η is 15.3%[8] for the chlorine atom corresponding to the lower line, which has an intensity twice as strong as the higher. This large asymmetry parameter has been ascribed by Peterson[9] to the intermolecular bonding between the chlorine and antimony atoms.

On the basis of X-ray data, let us ascertain whether or not there are unbound Sb–Br distances which are smaller than the sum of the van der Waals radii, 4.15 Å, as preparation for discussing the effect of the intermolecular bonding in antimony tribromide. In β-antimony tribromide there are short unbound Sb–Br distances, 3.66 and 3.85 Å, for the bromine atom, which contributes to the lower NQR line. The value of 3.66 Å seems evidently to be ascribable to the intermolecular bonding, and it is thought that the bromine atom corresponding to the lower NQR line has an asymmetry parameter as large as 15.3% in antimony trichloride. On the other hand, in α-antimony tribromide there are short unbound Sb–Br distances, 3.81 and 3.84, 3.75 and 4.10, and 3.78 Å for Br_1, Br_2, and Br_3 atoms respectively. These values are, however, larger than that of 3.66 Å in β-antimony tribromide. Therefore, we consider that the intermolecular bonding in α-antimony tribromide is less considerable than in antimony trichloride and β-antimony tribromide.

Gordy[10] proposed, on the basis of an extensive study using the equation of Schomaker-Stevenson,[11] that the tendency to form a double bond by using *d* orbitals falls off rapidly in descending rows in the periodic table, essentially vanishing for such fifth-row elements as Sn and Sb. In the case of $SbBr_3$, the bond length, Sb–Br, calculated by means of the Shomaker-Stevenson equation is in good agreement with the experimental value calculated by means of the electron diffraction. Therefore the possibility of double-bond formation is thought to be negligibly small, so that the ionicity of the Sb–Br bond, *i*, may be obtained from the following equation:

$$U_p = (1-i)(1-s) \tag{3}$$

where *s* is the *s* electron character and where U_p is the number of unbalanced *p* electrons. Usually *s* is assumed to be 0.15,[12] and U_p is evaluated from the observed quadrupole coupling constant:

$$U_p = (eQq_{zz})_{obs}/(eQq_{zz})_{atom} \tag{4}$$

where $(eQq_{zz})_{atom}$ is 643.0 MHz.[13] From the mean value of $(eQq_{zz})_{obs}$, 273.65 MHz, one obtains the values of $U_p=42.5\%$ and $i=50.0\%$.

The values of (Θ', Φ') specifying the direction of the Sb–Br bonds with respect to the crystal axes are listed in Table 3, together with those values obtained from X-ray analysis. In this table, the direction of $\Theta'=0°$ is chosen to be along the *c*-axis, and the plane of $\Theta'=0°$ is taken as the *bc* plane. The bond angles obtained from the Zeeman and X-ray analyses[4] are listed in Table 4, together with the bond angles of the β-form obtained from X-ray analysis.[5] Our values are consistent with those obtained from X-ray analysis to within about 1°. The direction of the $Sb–Br_3$ bond obtained from the Zeeman analysis lies on the *bc* plane, whereas that from X-ray analysis deviates from the *bc* plane by about 1°. According to the X-ray analysis, there must be four nonequivalent directions of $Sb–Br_3$ bonds, in each of which two directions are situated close together. However, for the Br_3 atom, which is responsible for the ν_3 line, we could observe only two loci and could not resolve either of them into two closely situated loci, even when a field of 350 gauss was used. At this stage we can not determine whether the present result and/or those obtained by the X-ray analysis are correct.

TABLE 4. THE BOND ANGLES $\angle$Br–Sb–Br IN α-AND β-$SbBr_3$

α-$SbBr_3$	$\angle Br_1–Sb–Br_2$	$\angle Br_2–Sb–Br_3$	$\angle Br_3–Sb–Br_1$
NQR	94°31′±8′	98°27′±7′	94°14′±4′
X-ray	93°38′	97°23′	95°28′

β-$SbBr_3$	$\angle Br_1–Sb–Br_2$	$\angle Br_2–Sb–Br_3$	$\angle Br_3–Sb–Br_1$
X-ray	92°48′	97°37′	97°37′

(b) The Molecular Complex $2SbBr_3 \cdot C_6H_6$. Let us label the three resonance lines of ^{81}Br as before. Again, from the number and the intensity ratio of the resonance lines, these lines can be ascribed to the three kinds of bromine atoms, Br_1,

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[8] T. Okuda, A. Nakao, M. Shiroyama and H. Negita, This Bulletin, **41**, 61 (1968).

[9] G. E. Peterson, Thesis, Pittsburgh, 1962.

[10] W. Gordy, W. V. Smith and R. F. Trambarulo, "Microwave Spectroscopy," John Wiley & Sons, Inc., New York (1953), p. 313.

[11] V. Schomaker and D. P. Stevenson, *J. Amer. Chem. Soc.*, **63**, 37 (1941).

[12] C. H. Townes and B. P. Dailey, *J. Chem. Phys.*, **17**, 782 (1949).

[13] J. G. King and V. Jaccarino, *Phys. Rev.*, **94**, 1610 (1954).

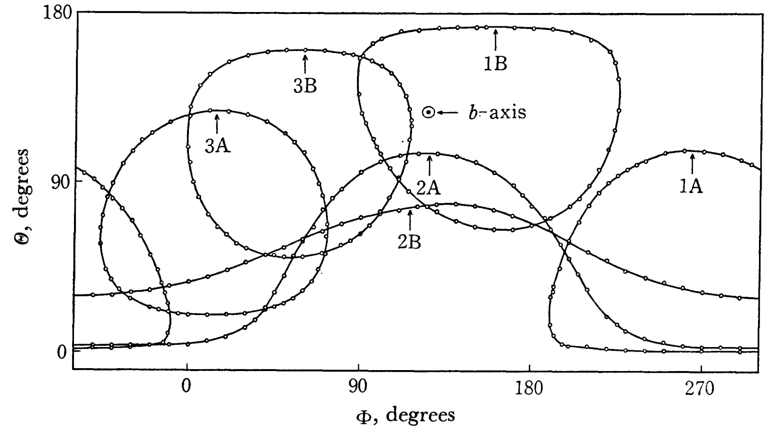

Fig. 3. Zero-splitting patterns of Zeeman lines of the complex $2SbBr_3 \cdot C_6H_6$. Θ and Φ are polar angles with respect to the orthogonal coordinate axes XYZ fixed to the sample.
1A, 1B, *etc.*, represent the zero-splitting directions of Zeeman lines at the nuclei Br_{1A}, Br_{1B}, *etc.*, respectively.

Br_2, and Br_3, in one molecule. The zero-splitting patterns obtained for these lines are shown in Fig. 3. For each of these lines, two loci of the zero-splitting were obtained; these loci are contributed by the atoms, Br_{1A} and Br_{1B} atoms, the Br_{2A} and Br_{2B} atoms, and the Br_{3A} and Br_{3B} atoms respectively. The angles between the Sb–Br bonds (z-axes) thus obtained are listed in Table 5.

TABLE 5. THE ANGLES BETWEEN Sb–Br BONDS IN THE COMPLEX $2SbBr_3 \cdot C_6H_6$

∠Br–Sb–Br	Br_{1A}	Br_{1B}	Br_{2A}	Br_{2B}	Br_{3A}
Br_{1B}	58° 7′ (121°53′)*				
Br_{2A}	82°15′ (**97°45′**)	73°37′ (106°23′)			
Br_{2B}	105°46′ (74°14′)	**97°34′** (82°26′)	27° 9′ (152°51′)		
Br_{3A}	87°26′ (**92°34′**)	144°56′ (35° 4′)	**97°21′** (82°39′)	85° 1′ (94°59′)	
Br_{3B}	34°41′ (145°19′)	**92°13′** (87°47′)	85°13′ (94°47′)	**96°53′** (83° 7′)	52°55′ (127° 5′)

* The value in parenthesis is the supplementary angle.

Considering that the antimony tribromide molecule may retain a trigonal pyramid and take the value of the bond angle near to 97°, we find from Table 5 that each of the groups, Br_{1A}, Br_{2A}, and Br_{3A}, and Br_{1B}, Br_{2B}, and Br_{3B}, belongs to the same molecule.

Because each line has two nonequivalent z-axes (zero-splitting loci), we conclude that this complex crystal has a monoclinic symmetry.[14] However, it is impossible to distinguish between C_s, C_2, and C_{2h} on the basis of the Zeeman analysis, which always introduces the center of symmetry to the crystal. The relative orientations of the $Sb–Br_1$, $Sb–Br_2$, and $Sb–Br_3$ bonds with respect to the b-axis are 29°4′±21′, 76°26′±9′, and 63°33′±11′ respectively. The bond angles obtained from Table 5 are listed in Table 6. The shape of the $SbBr_3$ molecule in the complex is similar to that of β-antimony tribromide as established by X-ray analysis.

TABLE 6. THE BOND ANGLES ∠Br–Sb–Br IN THE COMPLEX $2SbBr_3 \cdot C_6H_6$

Bond angle	$\angle Br_1–Sb–Br_2$	$\angle Br_2–Sb–Br_3$	$\angle Br_3–Sb–Br_1$
NQR	97°40′±6′	97°7′±14′	92°24′±11′

The values of the asymmetry parameter obtained from the zero-splitting loci using Eqs. (1) and the values of eQq_{zz} calculated from Eqs. (2) are listed in Table 7. The value of η at the Br_1 atom, 16.9%, is considerably larger than the remaining ones and those in α-$SbBr_3$; it is almost the same as the largest value in $SbCl_3$, which amounts to 15.3%. As we excluded the possibility of a double bond, this large value of η must be ascribed to the intermolecular bonding. Two cases of intermolecular bonding

TABLE 7. RESONANCE FREQUENCIES (ν), ASYMMETRY PARAMETERS (η) AND QUADRUPOLE COUPLING CONSTANTS (eQq_{zz}) OF ^{81}Br ATOMS IN THE COMPLEX $2SbBr_3 \cdot C_6H_6$ AT 21.5°C

Complex	ν,	MHz	η, %	eQq_{zz}, MHz
$2SbBr_3 \cdot C_6H_6$	ν_1	132.14	16.9±0.1	263.04
	ν_2	139.70	6.3±0.2	279.23
	ν_3	140.69	9.4±0.2	280.98

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[14] K. Shimomura, *J. Phys. Soc. Jap.*, **12**, 652 (1957).

may be thought of. One is the bonding between the Br atom and the benzene ring, this bonding being formed by charge transfer. The other is the intermolecular Sb–Br bonding among neighboring $SbBr_3$ molecules. Since the bonding by charge transfer is weak,15) the former is not likely to be responsible for the large value of η. On the contrary, the latter case seems reasonable.

The lowest line in the complex is lower by about 3 MHz than the lowest line of antimony tribromide itself. It has been thought that the charge transfer from the benzene to the bromine atom may cause the lowering of the resonance frequency. It has been found, however, that this lowering is very small.15,16) Thus, the relatively large frequency lowering in the complex can be considered to be caused primarily by the intermolecular Sb–Br bonding. On the other hand, the spacing of the resonance lines of this complex, as may be seen in Fig. 1 (c), resembles that of aluminum tribromide. One of the three lines is situated apart from the two closely-spaced lines on the higher-frequency side. This appearance is characteristic of the halides of the third-group elements which form the dimer.17) The lowest line is attributed to the bridging Br atom; it is lower by about 15 MHz than those of the upper pair in aluminum tribromide.18) The corresponding lowering in the present molecular complex is about 8 MHz.

Therefore, we consider that there exist predominantly interacting partner molecules of $SbBr_3$ in the complex crystal, and that the Br_1 atom in one molecule is bound to the Sb atom in a partner molecule to some extent. It must, however, be remembered that a slight deviation of the direction of the z-axis of the field gradient from the bond axis occurs because of moderate intermolecular covalent bonding.

At this stage, it is not evident whether the benzene ring is bound to the Br or the Sb atom in the complex. Meanwhile, Hulme and Szymański19) have proposed, on the basis of their X-ray analysis of the complex $2SbCl_3 \cdot C_{10}H_8$ that the aromatic ring is bound to the Sb atom; they based their proposal on the distance between the Sb atom and the aromatic ring

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15) H. O. Hooper, *J. Chem. Phys.*, **41**, 599 (1964).

16) D. F. R. Gilson and C. T. O'Konski, *ibid.*, **48**, 2767 (1968).

17) R. G. Barnes and S. L. Segel, *ibid.*, **25**, 180 (1956).

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19) R. Hulme and J. T. Szymański, *Acta Crystallogr.*, **B25**, 753 (1969).