# Hyperfine Structure in the Rotational Spectrum of CuBr

J. Hoeft and K. P. R. Nair
Institut für Molekülphysik, Freie Universität Berlin

Z. Naturforsch. **34 a,** 1290 – 1295 (1979); received September 17, 1979

The hyperfine structure of the $J = 2 \leftarrow 1$ rotational transition of CuBr has been measured in the 12 GHz frequency region using a Stark modulated high temperature microwave spectrometer. The molecules were produced by the reaction of $Br_2$ vapour with copper in the heated zone of a splitted wave guide at a temperature of 800 °C. The analysis of the hyperfine structure yielded the following quadrupole coupling constants.

| | $B_0 + 8\,Y_{02}$ (MHz) | $e\,q_0\,Q$(Br) (MHz) | $e\,q_0\,Q$(Cu) (MHz) |
|---|---|---|---|
| $^{63}Cu^{79}Br$ | 3048.8893 (40) | +261.17 (20) | +12.76 (20) |
| $^{63}Cu^{81}Br$ | 3015.5213 (40) | +218.38 (20) | +12.72 (20) |

## Introduction

Microwave spectroscopy has provided large amounts of information on gas phase molecular structure and molecular interactions. In this concern, studies of diatomic molecules are of basic interest because of the significant variations in the bonding character causing remarkable changes and trends of molecular parameters such as electric dipole moments or nuclear quadrupole coupling constants which can be measured by microwave spectroscopy. Since the advent of high temperature microwave spectroscopy a number of high temperature diatomic molecules have been studied in this laboratory which have yielded informations regarding systematic variations in quadrupole hyperfine interactions and electric dipole moments in a series of compounds (see for example: Hoeft, Lovas, Tiemann, Törring [1], Nair, Hoeft, Tiemann [2, 3]). In the present paper we describe our studies on the hyperfine structure in the rotational spectrum of CuBr which has been produced at high temperatures inside a microwave absorption wave guide. Copper halides are of particular importance especially when they are compared with the I a halides for a discussion of chemical bonding. Moreover, recently copper halides have been found to show laser action [4 – 6], and hence their rotational spectrum is of basic interest.

The existence of the monomeric form of copper halides in the gas phase was evident from the analysis of band spectra in the optical region by Mullikan [7] and Ritschl [8]. Later high resolution experiments gave information about the rotational structure in these molecules [9 – 13]. Measurements of the pure rotational spectrum were done recently by Manson et al. in the mm wave region from which precise rotational and potential constants were derived [14 – 16]. They observed small hyperfine splittings in CuI and CuBr yielding a good estimation of the predominant halogen coupling constants. The hyperfine splitting due to the nuclear quadrupole interaction of Cu was unresolvable by them. Hence for further information on the quadrupole hyperfine structure we undertook the present studies on lower rotational transitions of copper halides in the X-band region of microwave spectroscopy. In low rotational transitions the quadrupole interactions of both nuclei should be observable with the typical resolving power of microwave spectroscopy.

We have recently reported the hyperfine structure in the rotational spectrum of CuF, CuCl and CuI [17 – 19], in which case a systematic trend in the quadrupole coupling constants of Cu nucleus is observed. We have now completed our work on the diatomic CuBr molecule, and the present paper deals with the hyperfine interactions in the $J = 2 \leftarrow 1$ rotational transition lying in the 12 GHz region.

---

Reprint requests to Professor Dr. J. Hoeft, Institut für Molekülphysik, Freie Universität Berlin, Boltzmannstr. 20, 1000 Berlin 33.

0340-4811 / 79 / 1100-1290 $ 01.00/0. — Please order a reprint rather than making your own copy.

## Experimental

CuBr was produced by the reaction of $Br_2$ vapour with copper in the heated zone of a splitted wave guide (rectangular cross section), which is described in a former publication [20]. The production of molecules were essentially the same as in CuCl and CuI. Before each run the inner walls of the absorption cell were covered by a thin paste made of fine copper powder and methyl alcohol. During the measurement a continuous stream of $Br_2$ vapour passed the hot cell coming from a container outside the hot region. The reduction valve of the bromine container was kept at a slightly higher temperature than the room temperature in order to prevent bromine clotting at the valve. The excess of $Br_2$ was collected in a liquid nitrogen trap to avoid corosion in the pumping system. The gas flow rate of $Br_2$ could not be measured but the mean pressure in the hot region was estimated to be $10^{-1}$ Torr. The transitions were observed at a reaction temperature of about 800 °C.

We used a 100 kHz Stark modulation spectrometer for our measurements. Due to lack of intensity we restricted our measurements to the most abundant isotopic species $^{63}Cu^{79}Br$ (35%) and $^{63}Cu^{81}Br$ (34%) in their ground vibrational state of the $X^1\Sigma$ electronic ground state. The quadrupole coupling constants of other isotope $^{65}Cu$ can be evaluated from the results on $^{63}Cu$ using the ratio of the nuclear quadrupole moments which are known from the hyperfine structure studies of CuF [17], for instance. Because of the low signal to noise ratio the lines were recorded with a signal averager. Weak lines required integration times up to 40 minutes which have a sweeptime of 20 secs, time constant 100 msec at 6 dB/Octave. In the case of fully resolved lines the full half width of a hfs component was about 400 kHz. A typical part of the spectrum is shown in Figure 1.

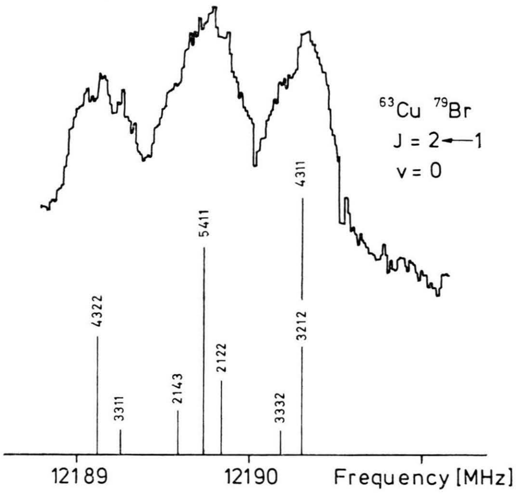

Fig. 1. Part of $J = 2 \leftarrow 1$ rotational transition of $^{63}Cu^{79}Br$. (For the quantum numbers refer Table I a.)

## Theory and Analysis

The theory for interpretation of rotational transitions of diatomic molecules with quadrupole coupling of two nuclei is compiled in [21, 22]. For the analysis of the spectra we estimated a value of the coupling constant $e q_0 Q$ of $^{63}Cu$ in CuBr from the known constants of other copper halides considering a systematic behaviour as in the case of alkali halides. From these estimations one expects a ratio of the interaction constants of the Cu nucleus of a factor of 1/20 as that of the Br nucleus. Therefore, the coupling of the angular momenta in CuBr may be described by the following scheme. The rotational angular momentum $\boldsymbol{J}$ couples with the nuclear spin $\boldsymbol{I}_1$ of bromine ($I_1 = 3/2$) giving the angular momentum $\boldsymbol{F}_1$ with the quantum number $\boldsymbol{F}_1$. $\boldsymbol{F}_1$ couples with the spin $\boldsymbol{I}_2$ of the copper nucleus ($I_2 = 3/2$) yielding the total angular momentum $\boldsymbol{F}$ with the quantum number $F$. For the assignment of the observed lines the hyperfine structure of the $J = 2 \leftarrow 1$ rotational transition was calculated using estimated coupling constants and the rotational constants measured by Manson et al. and by a direct diagonalisation of the energy matrix as described earlier [22]. According to the mentioned coupling scheme each energy level is characterised by the three quantum numbers $J$, $F_1$, and $F$. Very often, especially when two quadrupole couplings are of the same order, mixing of quantum numbers takes place and $F_1$ cannot be treated as a good quantum number. The only exact quantum number $F$ is given by the total angular momentum $\boldsymbol{F}$ which is the vector sum of $J$, $I_1$ and $I_2$. Because of the large rotational energy in comparison to the coupling energies the hyperfine structure levels can be definitely assigned to good quantum number $J$ characterising the rotational state of the molecule. The quantum number

$F_1$ is replaced by the number $X$ which counts the hyperfine sublevels of each system $(J,\ F)$ in increasing order of energy. The measured frequencies are given in Table 1. The relative intensities shown are normalized to the sum of all hyperfine structure components of $J=2 \leftarrow 1\ (=100\%)$. Only lines with more than 0.8% intensity are given in the table. In most cases the observed lines contain two or more overlapping components and hence the line frequencies were corrected, by taking into account the intensities as weighting factors, for a least squares fit. The differences between the corrected frequencies $\nu_{\text{meas, corr}}$ and single lines of the calculated spectrum are given in the last column of Table 1. The standard deviation of the least squares fit was 29 kHz for both isotopic species. This is within the estimated accuracy of 40 kHz for the measured frequencies.

Table 2 shows the result of the fit to the three parameters $e\,q_0\,Q$ (Cu), $e\,q_0\,Q$ (Br), and $B_0+2\,Y_{02}(J+1)^2=B_0+8\,Y_{02}$ for both molecular species. The "effective" rotational constant

$$B_0+8\,Y_{02}+\cdots=Y_{01}+\frac{1}{2}\,Y_{11}+\frac{1}{4}\,Y_{21}+\frac{1}{8}\,Y_{31}+\cdots+8\,Y_{02}+\cdots$$

($Y_{lk}$: Dunham coefficients) is compared with the results of Manson et al. in the same table. A test fit

Table 1 a. Calculated and observed frequencies of the hyperfine structure components of $J=2 \leftarrow 1$ rotational transition of $^{63}$Cu$^{79}$Br in the ground vibrational state.

| $F' \leftarrow F$ | $X' \leftarrow X$ | relative intensity (%) | $\nu_{\text{calc}}$ (MHz) | $\nu_{\text{meas}}$ (MHz) | $\nu_{\text{meas corr}}$ (MHz) | $\nu_{\text{meas corr}}-\nu_{\text{calc}}$ (kHz) |
|---|---|---|---|---|---|---|
| $2 \leftarrow 1$ | $3 \leftarrow 3$ | 1.0 | 12143.006 | | | |
| $2 \leftarrow 3$ | $3 \leftarrow 2$ | 1.0 | 12143.047 | 12143.066 | | |
| $3 \leftarrow 3$ | $2 \leftarrow 2$ | 3.6 | 12143.065 | | 12143.080 | +15 |
| $2 \leftarrow 2$ | $3 \leftarrow 3$ | 1.4 | 12145.088 | | 12145.095 | + 7 |
| $1 \leftarrow 2$ | $2 \leftarrow 3$ | 1.0 | 12145.106 | 12145.105 | | |
| $3 \leftarrow 2$ | $2 \leftarrow 3$ | 1.1 | 12145.106 | | | |
| $1 \leftarrow 0$ | $3 \leftarrow 1$ | 1.4 | 12186.569 | | | |
| $2 \leftarrow 2$ | $2 \leftarrow 2$ | 1.2 | 12187.674 | | | |
| $1 \leftarrow 1$ | $3 \leftarrow 3$ | 1.1 | 12188.529 | | | |
| $4 \leftarrow 3$ | $2 \leftarrow 2$ | 7.8 | 12189.115 | 12189.161 | 12189.139 | +24 |
| $3 \leftarrow 3$ | $1 \leftarrow 1$ | 1.6 | 12189.247 | | | |
| $2 \leftarrow 1$ | $4 \leftarrow 3$ | 2.9 | 12189.582 | | | |
| $5 \leftarrow 4$ | $1 \leftarrow 1$ | 13.8 | 12189.731 | 12189.736 | 12189.733 | + 2 |
| $2 \leftarrow 1$ | $2 \leftarrow 2$ | 4.9 | 12189.834 | | | |
| $3 \leftarrow 3$ | $3 \leftarrow 2$ | 1.4 | 12190.173 | | | |
| $3 \leftarrow 2$ | $1 \leftarrow 2$ | 7.1 | 12190.295 | 12190.265 | | |
| $4 \leftarrow 3$ | $1 \leftarrow 1$ | 10.1 | 12190.303 | | 12190.277 | −26 |
| $2 \leftarrow 2$ | $4 \leftarrow 3$ | 1.4 | 12191.665 | 12191.649 | 12191.649 | −16 |
| $3 \leftarrow 2$ | $3 \leftarrow 3$ | 4.9 | 12192.214 | 12192.236 | 12192.218 | + 4 |
| $4 \leftarrow 4$ | $1 \leftarrow 1$ | 1.1 | 12192.313 | | | |
| $2 \leftarrow 1$ | $1 \leftarrow 1$ | 2.7 | 12195.565 | | | |
| $1 \leftarrow 2$ | $1 \leftarrow 1$ | 2.7 | 12195.593 | 12195.564 | 12195.561 | −32 |
| $2 \leftarrow 2$ | $1 \leftarrow 1$ | 2.5 | 12195.634 | | | |
| $3 \leftarrow 3$ | $3 \leftarrow 1$ | 1.7 | 12254.724 | 12254.723 | 12254.723 | − 1 |
| $2 \leftarrow 2$ | $4 \leftarrow 2$ | 1.1 | 12255.222 | 12255.235 | 12255.235 | +13 |
| $4 \leftarrow 4$ | $2 \leftarrow 1$ | 3.1 | 12255.675 | 12255.702 | 12255.702 | +27 |
| $1 \leftarrow 1$ | $3 \leftarrow 2$ | 0.9 | 12256.329 | 12256.379 | 12256.379 | +50 |
| $2 \leftarrow 1$ | $3 \leftarrow 1$ | 1.3 | 12261.098 | | | |
| $1 \leftarrow 1$ | $2 \leftarrow 1$ | 1.3 | 12261.116 | 12261.088 | | |
| $2 \leftarrow 2$ | $3 \leftarrow 1$ | 1.3 | 12261.168 | | | |
| $3 \leftarrow 2$ | $2 \leftarrow 1$ | 3.6 | 12261.185 | | 12261.118 | −67 |

Table 1 b. Calculated and observed frequencies of the hyperfine structure components of $J = 2 \leftarrow 1$ rotational transition of $^{63}$Cu$^{81}$Br in the ground vibrational state.

| $F' \leftarrow F$ | $X' \leftarrow X$ | relative intensity (%) | $\nu_{\text{calc}}$ (MHz) | $\nu_{\text{meas}}$ (MHz) | $\nu_{\text{meas corr}}$ (MHz) | $\nu_{\text{meas corr}} - \nu_{\text{calc}}$ (kHz) |
|---|---|---|---|---|---|---|
| $2 \leftarrow 1$ | $3 \leftarrow 3$ | 0.9 | 12017.997 | | | |
| $2 \leftarrow 3$ | $3 \leftarrow 2$ | 1.0 | 12018.046 | 12018.030 | | |
| $3 \leftarrow 3$ | $2 \leftarrow 2$ | 3.5 | 12013.060 | | 12018.044 | −16 |
| $2 \leftarrow 2$ | $3 \leftarrow 3$ | 1.4 | 12020.081 | | 12020.092 | +11 |
| $1 \leftarrow 2$ | $2 \leftarrow 3$ | 1.0 | 12020.095 | 12020.100 | | |
| $3 \leftarrow 2$ | $2 \leftarrow 3$ | 1.0 | 12020.095 | | | |
| $1 \leftarrow 0$ | $3 \leftarrow 1$ | 1.4 | 12054.037 | | | |
| $2 \leftarrow 2$ | $2 \leftarrow 2$ | 1.2 | 12055.092 | | | |
| $1 \leftarrow 1$ | $3 \leftarrow 3$ | 1.1 | 12055.976 | 12055.988 | 12055.988 | +12 |
| $4 \leftarrow 3$ | $2 \leftarrow 2$ | 7.6 | 12056.559 | 12056.589 | 12056.568 | + 9 |
| $3 \leftarrow 3$ | $1 \leftarrow 1$ | 1.5 | 12056.682 | | | |
| $2 \leftarrow 1$ | $4 \leftarrow 3$ | 2.6 | 12057.027 | | | |
| $5 \leftarrow 4$ | $1 \leftarrow 1$ | 13.5 | 12057.164 | 12057.224 | 12057.219 | +55 |
| $2 \leftarrow 1$ | $2 \leftarrow 2$ | 4.8 | 12057.265 | | | |
| $3 \leftarrow 3$ | $3 \leftarrow 2$ | 1.4 | 12057.617 | | | |
| $3 \leftarrow 2$ | $1 \leftarrow 2$ | 6.9 | 12057.706 | 12057.713 | | |
| $4 \leftarrow 3$ | $1 \leftarrow 1$ | 9.9 | 12057.736 | | 12057.735 | − 1 |
| $2 \leftarrow 2$ | $4 \leftarrow 3$ | 1.4 | 12059.111 | 12059.095 | 12059.095 | −16 |
| $3 \leftarrow 2$ | $3 \leftarrow 3$ | 4.8 | 12059.652 | 12059.659 | 12059.644 | − 8 |
| $4 \leftarrow 4$ | $1 \leftarrow 1$ | 1.1 | 12059.732 | | | |
| $2 \leftarrow 1$ | $1 \leftarrow 1$ | 2.6 | 12062.094 | | | |
| $1 \leftarrow 2$ | $1 \leftarrow 1$ | 2.6 | 12062.127 | 12062.089 | 12062.084 | −43 |
| $2 \leftarrow 2$ | $1 \leftarrow 1$ | 2.5 | 12062.176 | | | |
| $3 \leftarrow 3$ | $3 \leftarrow 1$ | 1.6 | 12111.465 | 12111.460 | 12111.460 | − 5 |
| $2 \leftarrow 2$ | $4 \leftarrow 2$ | 1.1 | 12111.949 | 12111.929 | 12111.929 | −20 |
| $4 \leftarrow 4$ | $2 \leftarrow 1$ | 3.0 | 12112.403 | 12112.411 | 12112.411 | + 8 |
| $1 \leftarrow 1$ | $3 \leftarrow 2$ | 0.8 | 12113.071 | 12113.131 | 12113.131 | +60 |
| $2 \leftarrow 1$ | $3 \leftarrow 1$ | 1.2 | 12116.870 | | | |
| $1 \leftarrow 1$ | $2 \leftarrow 1$ | 1.3 | 12116.885 | 12116.885 | | |
| $2 \leftarrow 2$ | $3 \leftarrow 1$ | 1.3 | 12116.952 | | | |
| $3 \leftarrow 2$ | $2 \leftarrow 1$ | 3.5 | 12116.967 | | 12116.920 | −47 |

Table 2. Molecular constants of CuBr in the ground vibrational state given in MHz from measurements on hfs of $J = 2 \leftarrow 1$, $v = 0$ of the ground electronic state. [a] Ref. [16].

| | $^{63}$Cu$^{79}$Br | | $^{63}$Cu$^{81}$Br | |
|---|---|---|---|---|
| | This work | Manson et al. [a] | This work | Manson et al. [a] |
| $B_0 + 8\,Y_{02}$ | 3048.8893 (40) | 3048.8896 (6) | 3015.5213 (40) | 3015.5285 (6) |
| $e\,q_0\,Q$ (Br) | +261.17 (20 | – | +218.38 (20) | +221 (8) |
| $e\,q_0\,Q$ (Cu) | + 12.76 (20) | – | + 12.72 (20) | – |

with an additional magnetic spin rotation parameter of the bromine nucleus gave no statistical evidence for this parameter.

## Discussion

The ratio of the quadrupole moment $Q$ of $^{79}$Br and $^{81}$Br can be calculated from the present $e\,q\,Q$ values of both isotopic species, which give a value

$$Q(79)/Q(81) = 1.1959(20).$$

This value is in very good agreement with the value obtained for free bromine atoms by atomic beam experiments of Brown and King [23], $Q(79)/Q(81) = 1.1970636(10)$. This supports our analysis.

In Table 3 we have collected the quadrupole coupling constants in I a and I b halides. The coupling constant of $^{63}$Cu changes from 21.95 (10) MHz in CuF to 8.14 (20) MHz in CuI. This ratio is comparable in magnitude to the isovalent potassium halides. The halogen coupling constants are comparatively large in I b halides compared to I a halides. This clearly indicates the importance of d electrons in I b atoms in forming the chemical bond. (The electronic configurations of K and Rb atoms are (Ar) $4\,s^1$ and (Kr) $5\,s^1$, respectively, and those of Cu and Ag are (Ar) $3\,d^{10}\,4\,s^1$ and (Kr) $4\,d^{10}\,5\,s^1$, respectively.) Again the ratio of the halogen coupling $e\,q_0\,Q$ (Cu X)/$e\,q_0\,Q$ (Ag X) is a constant in all cases of Cu X and Ag X, namely 0.88, which is not the case with the I a halides where such a relation is not possible. This is another indication of the predominant role played by the d electron of I b atoms in the quadrupole coupling.

Another remarkable observation is the systematic variation of the quadrupole coupling constants of metal atoms with the internuclear distances. Figure 2 shows such a diagram. Similar behaviour has been observed in other groups of diatomic molecules (see for example [3]). From the quadrupole coupling, the ionic character $i_c$ of the bond can be calculated using the relation [24]

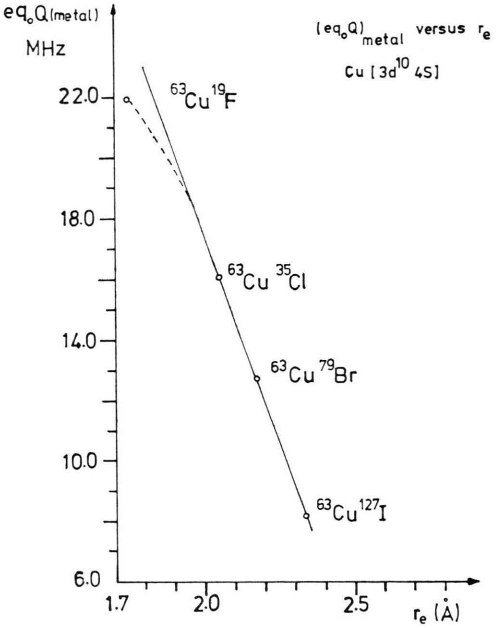

Fig. 2 a. Quadrupole coupling constant $e\,q_0\,Q$ versus internuclear distance $r_e$ in Copper halides.

$$i_c = 1 + \chi_z / e\,q_{n10}\,,$$

Table 3. Quadrupole coupling constants ($\chi_0 = e\,q\,Q$) for the ground vibrational state and internuclear distances $r_e$ in I b and I a halides.

| Molecule | $r_e$ (Å) | $\chi_0$ (MHz) (metal) | $\chi_0$ (MHz) (halogen) | $\chi_0$ (CuX) / $\chi_0$ (AgX) | Ref. |
|---|---|---|---|---|---|
| $^{63}$CuF | 1.7449508 (17) | 21.95 (10) | — | | a |
| $^{63}$Cu$^{35}$Cl | 2.051177 (8) | 16.08 (20) | − 32.25 (15) | 0.88 | b |
| $^{63}$Cu$^{79}$Br | 2.173435 (6) | 12.76 (20) | + 261.17 (20) | 0.88 | c |
| $^{63}$Cu$^{127}$I | 2.338317 (1) | 8.14 (20) | − 938.07 (20) | 0.88 | d |
| $^{107}$AgF | 1.983203 (1) | | — | | |
| $^{107}$Ag$^{35}$Cl | 2.2808190 (2) | | − 36.50 (10) | | e |
| $^{107}$Ag$^{70}$Br | 2.393138 (3) | | + 297.10 (15) | | e |
| $^{107}$Ag$^{127}$I | 2.544651 (3) | | −1062.17 (40) | | e |
| $^{39}$KF | 2.1714777 (2) | − 7.93387 (80) | — | | |
| $^{39}$K$^{35}$Cl | 2.6666830 (7) | − 5.6684 (3) | + 0.0585 (8) | | |
| $^{39}$K$^{79}$Br | 2.820809 (3) | − 5.0151 (9) | + 10.2383 (7) | | |
| $^{39}$K$^{127}$I | 3.0478801 (11) | − 4.12 (10) | − 86.79 (10) | | |
| $^{85}$RbF | 2.2703609 (8) | −70.341 (1) | — | | |
| $^{85}$Rb$^{35}$Cl | 2.7867690 (14) | −52.675 (5) | + 0.744 (9) | | |
| $^{85}$Rb$^{79}$Br | 2.9447792 (12) | −47.11 (17) | + 3.50 (29) | | |
| $^{85}$Rb$^{127}$I | 3.1769183 (45) | −40.40 (30) | − 59.89 (30) | | f |

a) Ref. [17]. b) Ref. [19]. c) Present. d) Ref. [18]. e) Ref. [25]. f) Ref. [26] other references from F. J. Lovas and E. Tiemann, J. Phys. and Chem. Ref. Data **3**, 609–770 (1974).

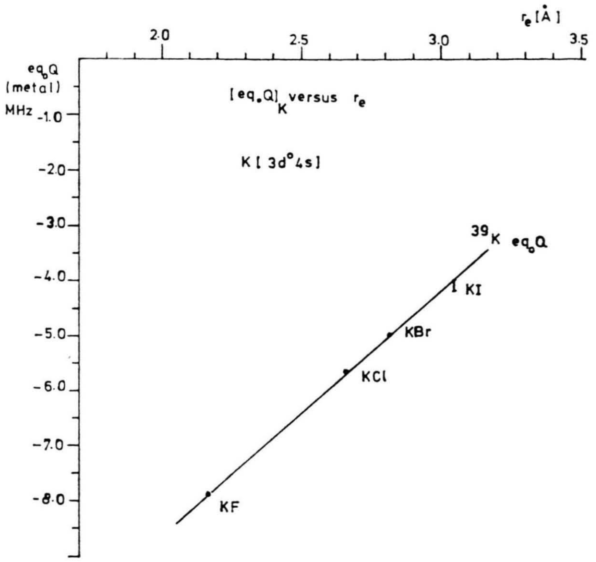

Fig. 2 b. Quadrupole coupling constant $e\,q_0\,Q$ versus internuclear distance $r_e$ in Potassium halides.

where $\chi_z$ is the quadrupole coupling constant $e\,q\,Q$ of the molecule and $e\,q\,Q_{n10}$ is that of the atom. If we take $e\,q\,Q_{n10} = -769.76$ for $^{79}$Br and $e\,q\,Q_{n10} = -643.04$ MHz for $^{81}$Br, the relation gives a value of $i_c = 0.66$ from measurements of $e\,q\,Q$ in both the isotopic molecular species.

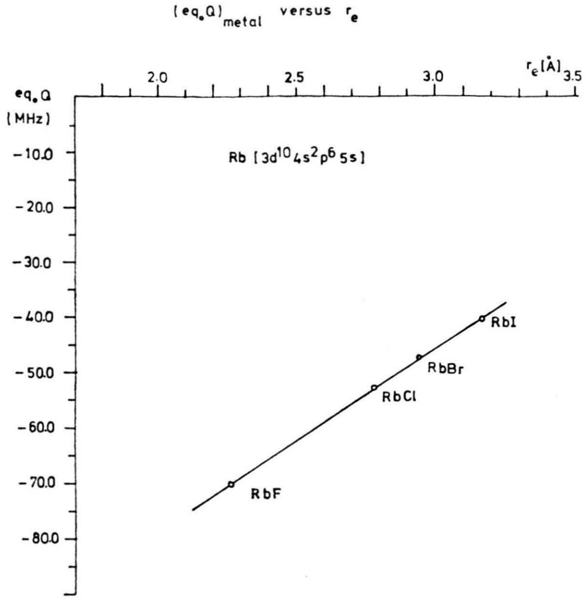

Fig. 2 c. Quadrupole coupling constant $e\,q_0\,Q$ versus internuclear distance $r_e$ in Rubidium halides.

## *Acknowledgements*

This work has been performed within the research program of Sonderforschungsbereich 161 "Hyperfine Interactions" which is supported by Deutsche Forschungsgemeinschaft.

[1] J. Hoeft, F. J. Lovas, E. Tiemann, and T. Törring, J. Chem. Phys. **53,** 2736 (1970).
[2] K. P. R. Nair, J. Hoeft, and E. Tiemann, Chem. Phys. Lett. **60,** 253 (1979).
[3] K. P. R. Nair, J. Hoeft, and E. Tiemann, J. Mol. Spectry (in press).
[4] N. N. Nerheim, A. A. Vetter, and G. R. Russell. J. Appl. Phys. **49,** 12 (1978).
[5] L. A. Cross, R. S. Jenkins, and M. C. Grokay, J. Appl. Phys. **49,** 453 (1978).
[6] O. Kafri and E. Bar-Ziv, Phys. Lett. A, **71,** 332 (1979).
[7] R. S. Mullikan, Phys. Rev. **26,** 1 (1925).
[8] R. Ritschl, Z. Physik **42,** 172 (1927).
[9] P. R. Rao and J. K. Brody, J. Chem. Phys. **35,** 776 (1961).
[10] P. R. Rao, R. K. Asundi, and J. K. Brody, Can. J. Phys. **40,** 412 (1962).
[11] K. P. R. Nair and K. N. Upadhya, Can. J. Phys. **44,** 1267 (1966).
[12] K. P. R. Nair and D. K. Rai, Can. J. Phys. **45,** 2810 (1967).
[13] P. R. Rao and K. V. S. R. Apparao, Can. J. Phys. **45,** 2805 (1967).
[14] E. L. Manson, F. C. De Lucia, and W. Gordy, J. Chem. Phys. **62,** 1040 (1975).
[15] E. L. Manson, F. C. De Lucia, and W. Gordy, J. Chem. Phys. **62,** 4796 (1975).
[16] E. L. Manson, F. C. De Lucia, and W. Gordy, J. Chem. Phys. **63,** 2724 (1975).
[17] J. Hoeft, F. J. Lovas, E. Tiemann, and T. Törring, Z. Naturforsch. **25 a,** 35 (1970).
[18] K. P. R. Nair, E. Tiemann, and J. Hoeft, Z. Naturforsch. **32 a,** 1053 (1977).
[19] E. Tiemann and J. Hoeft, Z. Naturforsch. **32 a,** 1477 (1977).
[20] J. Hoeft, F. J. Lovas, E. Tiemann, and T. Törring, Z. Angew. Physik **31,** 265 (1971).
[21] B. Schenk, E. Tiemann, and J. Hoeft, Z. Naturforsch. **25 a,** 1927 (1970).
[22] K. P. R. Nair, J. Hoeft, and E. Tiemann, Chem. Phys. Lett. **58,** 153 (1978).
[23] H. H. Brown and J. G. King, Phys. Rev. **142,** 53 (1966).
[24] W. Gordy and R. L. Cook, Microwave Molecular Spectra, Interscience Publications (1970).
[25] J. Hoeft, F. J. Lovas, E. Tiemann, and T. Törring, Z. Naturforsch. **26 a,** 240 (1971).
[26] E. Tiemann and J. Hoeft, Z. Naturforsch. **31 a,** 236 (1976).