peaks at 47 cm^{-1} was found in the E_g and F_{2g} vibrations.

It must be mentioned that only the positions but not the intensities of the observed and calculated peaks have been compared. An additional comparison of the intensities might be particularly useful if calculations based on different theoretical models were available. Then the various models could be judged how well they fit the experimental data. However, at present only the calculations of Benedek and Nardelli are available.

In conclusion it can be stated that the experimentally determined peaks in the scattering spectrum are fully explained on theoretical grounds.

We thank Prof. K. **Dransfeld** for his permanent interest in this work. Thanks are due to Prof. H. **Bilz** and Dr. D. **Strauch** for discussion and to the Deutsche Forschungsgemeinschaft for financial support.

	Experiment cm^{-1}	Theory [19] cm^{-1}	Ag^+ pair frequency [14] cm^{-1}
A_{1g}	—	124	
E_g	47		a
	85 (s)	87	
	137 (m)	137	
F_{2g}	47 (w)		47.5
	87 (m)	(80), b	
	112 (w)	117	
	135 (m)	140	
	155 (w)	155	
	171 (s)	174	

[a] The pair frequency of type E_g may be slightly different from $\omega_P = 47.5$ cm^{-1} (F_{2g}-type), see text.
[b] Strong peak at 85 cm^{-1} in E_g geometry, see text.

Table 1. Position of the peaks in the Raman spectra (1. column: Experiment) and in the density of states (2. column: Theory). The calculated Ag^+ pair frequency is listed in the 3. column. The observed Raman intensities are denoted by s (strong), m (medium) and w (weak).

Microwave Absorption Spectra of AlF, GaF, InF, and TlF

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Observation of various rotational transitions of four Group IIIa monofluoride allowed the Dunham coefficients Y_{01}, Y_{11}, Y_{21} and Y_{12} to be determined. From the hyperfine structure of the AlF, GaF and InF spectra, the nuclear electric quadrupole coupling constants, $e\,q_V\,Q$, and spin-rotation coupling constant, c_I, were obtained for several vibrational states, v:

$$e\,q_V\,Q\,(^{27}\text{Al}\,^{19}\text{F}) = -37{,}75\,(8) \quad +0{,}44\,(8) \quad (v+1/2)\ \text{MHz}\,,$$
$$e\,q_V\,Q\,(^{69}\text{Ga}\,^{19}\text{F}) = -107{,}07\,(8) \quad +1{,}09\,(7) \quad (v+1/2)\ \text{MHz}\,,$$
$$e\,q_V\,Q\,(^{71}\text{Ga}\,^{19}\text{F}) = -67{,}46\,(8) \quad +0{,}68\,(7) \quad (v+1/2)\ \text{MHz}\,,$$
$$e\,q_V\,Q\,(^{115}\text{In}\,^{19}\text{F}) = -727{,}06\,(20) +6{,}64\,(20) \quad (v+1/2)\ \text{MHz}\,.$$

Stark effect measurements on GaF and InF in the ground vibrational state resulted in the following electric dipole moments:

$$^{69}\text{Ga}\,^{19}\text{F}: \quad |\bar{\mu}_0| = 2{,}45\,(5)\ \text{D},$$
$$^{115}\text{In}\,^{19}\text{F}: \quad |\bar{\mu}_0| = 3{,}40\,(7)\ \text{D}.$$

Introduction

Microwave absorption studies of the Group IIIa monofluorides have resulted in improved rotational and hyperfine structure constants for AlF and InF and the first observation of the GaF spectrum. Previously, only the $v=0$ and 1 spectra of AlF [1] and InF [2] were reported, leaving the rather large Y_{21} $(=\gamma_e)$ rotational constant unknown, so that the reported Y_{01} and Y_{11} rotational constants are somewhat erroneous.

An additional goal of this work was to obtain more accurate hyperfine interaction constants, $e\,q\,Q$ and c_I, for the Al, Ga and In nuclei and to determine the molecular electric dipole moments of GaF and InF. The rotational constants [3], magnetic hyper-

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[1] David R. Lide, Jr., J. Chem. Phys. **38**, 2027 [1963]; **42**, 1013 [1965].

[2] F. J. Lovas and T. Törring, Z. Naturforsch. **24 a**, 634 [1969].

[3] H. G. Fitzky, Z. Physik **151**, 351 [1958]. — R. K. Ritchie and H. Lew, Can. J. Phys. **43**, 1701 [1965]. — A. H. Barrett and M. Mandel, Phys. Rev. **109**, 1572 [1958].

fine constant and dipole moment[4] of TlF have been determined from both microwave absorption and molecular beam electric resonance studies. In the present work TlF served as the Stark field standard, $\mu_0(\text{TlF}) = 4.2282(8)\ D$ from BOECKH et al.[4]. Since various rotational transitions of TlF were employed in these studies, an extensive study of the TlF spectrum was completed as a by-product of our Stark effect measurements.

Experimental Techniques

For the rotational transition measurements, both the hot cell and cold cell (pseudo molecular beam) spectrometers were employed, while Stark effect measurements were obtained in the hot cell spectrometer. Of the four monofluorides investigated, only TlF is commercially available. Thus, Al, Ga and In monofluorides were produced by means of a high temperature reaction-vaporization technique. Finely divided metal was mixed with AlF_3 or CaF_2 and heated to 900 – 1200 °C. The trifluorides of Ga and In, which are commercially available, are not suitable as reaction partners due to their high volatility.

During observations on GaF, vaporized from a mixture of Ga and AlF_3 at 900 °C in the cold cell spectrometer, it was found that the black condensate from this vapor could be revaporized at considerably lower temperatures (300° – 500 °C) and produced more than five times the absorption intensity. In a systematic study[5] of the reactions of Al, Ga and In metals with AlF_3 and CaF_3, we found that about 5% of the metal was converted to the corresponding monofluoride in each case and that the condensed black material contained 40 – 60% pure monofluoride. Since spectra of GaF, InF and TlF were observed at the same temperature, 300 °C, in the hot cell spectrometer, it appears that they have very similar vapor pressure. The condensed AlF required a temperature about 100 °C higher than the Al + AlF_3 mixture before resonances were observable. This high vaporization temperature (600° to 700 °C) for AlF made the measurements relatively difficult in comparison to the other monofluorides since all of these substances evidence dissociation reactions which are directly proportional to the cell temperature.

Theoretical Considerations

The molecular rotational constants were derived in the usual manner using the Dunham expansion of the molecular potential[6]. The hyperfine splittings were removed from the observed spectra to give a hypothetical pure rotational transition frequency which may be expressed in terms of the Dunham coefficients as:

$$\begin{aligned}\nu_{v,\,J\to J+1} = 2[&Y_{01} + Y_{11}(v+1/2) \\ &+ Y_{21}(v+1/2)^2 + \dots](J+1) \\ &+ 4[Y_{02} + \dots](J+1)^3 + \dots\end{aligned} \tag{1}$$

where

$$Y_{01} \sim 1/\mu_r\,,\quad Y_{11} \sim 1/\mu_r^{3/2},\quad \text{and}\quad Y_{21}\,, Y_{02} \sim 1/\mu_r^2$$
$$(\mu_r\text{: reduced mass}).$$

The expressions used for the hyperfine structure calculation are given in detail elsewhere[2, 7].

Although TAYLOR et al.[8] have reported a new set of fundamental physical constants recently, we have retained the value of h and amu used in previous reports[13] from this laboratory for the calculation of the internuclear distance:

$$r_e = \frac{h}{8\,\pi^2\,Y_{01}\,u\,\mu_r} = \frac{5.053750 \times 10^5}{Y_{01}\,\mu_r}\ \text{Å} \tag{2}$$

where Y_{01} is given in MHz and μ_r in amu. In terms of absolute error, Eq. (2) has 61 ppm error and the new constants would increase r_e by 16 ppm with an absolute error of 7 ppm.

The potential coefficients a_0 and a_1 may be calculated from the following relations:

$$a_0 = \omega_e^2/4\,Y_{01}\,, \tag{3}$$

$$a_1 = Y_{11}\,\omega_e/6\,Y_{01}^2 - 1 \tag{4}$$

where the value of ω_e reported from band spectra measurement was employed. The measured centrifugal stretching term, Y_{02} $(= -D_e)$, may be compared with that calculated from the relation:

$$Y_{02} = -4\,Y_{01}^3/\omega_e^2 \tag{5}$$

or ω_e may likewise be calculated with this expression from the measured Y_{02}.

In the case where measurements of the nuclear quadrupole coupling constant, $e\,q_v\,Q$, were obtained for several vibrational states, the equilibrium value and first order vibrational term were determined according to the following equation:

$$e\,q_v\,Q = e\,q_e\,Q + e\,q_I\,Q(v+1/2)\,. \tag{6}$$

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[5] J. HOEFT, F. J. LOVAS, E. TIEMANN, and T. TÖRRING, Z. Naturforsch. **25 b** [1970], im Erscheinen.

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[7] C. H. TOWNES and A. L. SCHAWLOW, Microwave Spectroscopy, McGraw-Hill Book Co. Inc., New York 1955.

[8] B. N. TAYLOR, W. H. PARKER, and D. N. LANGENBERG, Rev. Mod. Phys. **41**, 375 [1969].

Aluminum Monofluoride

The microwave absorption spectrum of $^{27}Al^{19}F$ was reported by LIDE[1] for the ground and first excited vibrational state. In his first report on AlF, Lide indicated that more accurate measurements should be possible; however, no improved spectrum has as yet been reported. We have undertaken the present study in order to obtain more accurate molecular constants for AlF, and especially to determine the Dunham constant, Y_{21}, which could not be obtained from Lide's data.

The $J=0 \rightarrow 1$ rotational transitions were measured in both the hot and cold cell spectrometers for the $v=0$ and 1 vibrational states, whereas the $v=2$ transitions could be obtained only in the more sensitive hot cell spectrometer. The AlF vapor was produced by heating a mixture of Al and AlF_3 to 580° – 700 °C. It was found that revaporization of the condensed AlF required a temperature about 100 °C higher than the mixture and resulted in weaker transition intensities. The observed line widths were between 200 and 400 kHz. The measured transition frequencies are listed in Table 1 for $^{27}Al^{19}F$. The rotational and hyperfine structure constants derived from this data are shown in Table 2 along with Lide's constants, corrected for Y_{21}. The nuclear electric quadrupole coupling constants were calculated according to Eq. (6) rather than deriving them for each vibrational state separately. For the $v=0$ state Lide obtained $e\,q_0\,Q(\mathrm{Al}) = -37.6(10)$ MHz which agrees very well with the present value of $-37.53(12)$ MHz.

$J \rightarrow J'$	$F \rightarrow F'$	v	ν (MHz)	$\Delta\nu$ (MHz)
		$^{27}Al^{19}F$		
$0 \rightarrow 1$	$5/2 \rightarrow 3/2$	0	32981,827 (40)	0,002
	$5/2 \rightarrow 7/2$	0	32978,500 (20)	0,000
	$5/2 \rightarrow 5/2$	0	32970,592 (30)	– 0,001
	$5/2 \rightarrow 3/2$	1	32684,963 (50)	0,003
	$5/2 \rightarrow 7/2$	1	32681,688 (30)	– 0,012
	$5/2 \rightarrow 5/2$	1	32673,825 (50)	0,034
	$5/2 \rightarrow 3/2$	2	32390,198 (70)	0,068
	$5/2 \rightarrow 7/2$	2	32387,048 (50)	– 0,032
	$5/2 \rightarrow 5/2$	2	32379,263 (70)	0,028

Table 1. The $J=0 \rightarrow 1$ rotational transition frequencies of $^{27}Al^{19}F$. The differences between the calculated and observed line frequencies are shown in the last column. The nuclear spin of the Al nucleus is 5/2.

Molecular Constants for $^{27}Al^{19}F$

	Present	*Lide*[a]	
Y_{01}	16562,969 (15)	16562,97 (5)	MHz
Y_{11}	– 149,483 (15)	– 149,48 (5)	MHz
Y_{21}	+ 0,541 (20)		MHz
$Y_{02}\,(=-4B_e^3/\omega_e^2)$	– 30,5[b]	– 30[b]	kHz
eq_eQ (Al)	– 37,75 (8)		MHz
eq_IQ (Al)	+ 0,44 (8)		MHz
c_{Al}	+ 8 (6)		kHz

[a] See Ref. [1]. Lide's rotational constants, $B_e=16\,562.56(10)$ and $\alpha_e=148.40(10)$ MHz, should not be directly compared with the present values since Lide's were derived by neglecting the γ_e (or Y_{21}) constant. The constants shown in the table have been corrected with our measured Y_{21}.

[b] See Table 13 for the ω_e values used in computation Y_{02}.

Table 2. The derived rotational and hyperfine structure constants for $^{27}Al^{19}F$. After this work was submitted for publication, another microwave study of AlF appeared (F. C. WYSE, W. GORDY, and E. F. PEARSON, J. Chem. Phys. **52**, 3887 [1970]). There is a slight discrepancy between their Y_{01} and Y_{11} and our values. Although the origin of this discrepancy is not obvious, it might be attributable in part to the fact that WYSE et al. made no corrections for the unresolved hyperfine structure in their lower observed rotational transitions, e. g. $J=5 \rightarrow 6$. The strongest lines of their $J=2 \rightarrow 3$ and $J=3 \rightarrow 4$ transitions also show an unsatisfactory fit.

Gallium Monofluoride

BARROW and coworkers[9] have reported a rotational analysis of $^{69}Ga^{19}F$ from absorption band spectra produced by heating a mixture of Ga and AlF_3 to 1000 °C. The $J=1 \rightarrow 2$ microwave absorption spectrum of GaF was first observed in the cold cell spectrometer using a similar mixture heated to 850° – 1000 °C. Subsequently the spectrum was obtained at 500° – 550 °C from the GaF condensed during runs with mixtures of Ga and AlF_3 or CaF_2. The $J=0 \rightarrow 1$ spectrum was measured in the hot cell spectrometer at 300° – 350 °C with this black condensate containing GaF.

The $J=0 \rightarrow 1$ and $1 \rightarrow 2$ transition frequencies for $^{69}Ga^{19}F$ (60.1%) and $^{71}Ga^{19}F$ (39.9%) are tabulated in Tables 3 and 4, respectively. The $J=0 \rightarrow 1$ lines had line widths at half-maximum of 150 kHz, while the $J=1 \rightarrow 2$ line widths were 250 kHz. The rotational and hyperfine structure constants derived from these measurements are shown in Table 5. The experimentally determined ratio of the nuclear quadrupole moment,

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[9] R. F. BARROW, P. G. DODSWORTH, and P. B. ZEEMAN, Proc. Phys. Soc. London A **70**, 34 [1957].

$J \rightarrow J'$	$F \rightarrow F'$	v	ν (MHz)	$\Delta\nu$ (MHz)
		$^{69}Ga^{19}F$		
$0 \rightarrow 1$	$3/2 \rightarrow 1/2$	0	21496,874 (15)	0,002
	$3/2 \rightarrow 5/2$	0	21475,627 (15)	− 0,005
	$3/2 \rightarrow 3/2$	0	21448,957 (15)	0,004
	$3/2 \rightarrow 1/2$	1	21326,060 (15)	0,029[a]
	$3/2 \rightarrow 5/2$	1	21305,063 (15)	− 0,011
	$3/2 \rightarrow 3/2$	1	21278,657 (15)	0,006
	$3/2 \rightarrow 1/2$	2	21156,518 (15)	0,004
	$3/2 \rightarrow 5/2$	2	21135,705 (15)	− 0,003
	$3/2 \rightarrow 3/2$	2	21109,575 (15)	0,008
	$3/2 \rightarrow 1/2$	3	20988,173 (20)	0,000
	$3/2 \rightarrow 5/2$	3	20967,561 (20)	0,010
	$3/2 \rightarrow 3/2$	3	20941,725 (20)	0,000
$1 \rightarrow 2$	$3/2 \rightarrow 3/2$	0	42961,445 (30)	0,025
	$5/2 \rightarrow 7/2$ $3/2 \rightarrow 5/2$	0	42942,484 (30)	0,003
	$1/2 \rightarrow 1/2$	0	42940,147 (30)	0,006
	$5/2 \rightarrow 5/2$	0	42915,785 (30)	0,025
	$1/2 \rightarrow 3/2$	0	42913,545 (30)	0,010
	$5/2 \rightarrow 7/2$ $3/2 \rightarrow 5/2$	1	42601,434 (35)	− 0,008
	$5/2 \rightarrow 7/2$ $3/2 \rightarrow 5/2$	2	42262,832 (40)	− 0,021

[a] Overlaps $^{71}Ga^{19}F$ $v=0$, $F=3/2 \rightarrow 3/2$ transition.

Table 3. The $J=0 \rightarrow 1$ and $1 \rightarrow 2$ rotational transition frequencies for $^{69}Ga^{19}F$. The nuclear spin, I, for ^{69}Ga is 3/2. The last column shows the differences between the calculated and observed line frequencies.

$J \rightarrow J'$	$F \rightarrow F'$	v	ν (MHz)	$\Delta\nu$ (MHz)
		$^{71}Ga^{19}F$		
$0 \rightarrow 1$	$3/2 \rightarrow 1/2$	0	21356,510 (15)	− 0,005
	$3/2 \rightarrow 5/2$	0	21343,148 (15)	0,002
	$3/2 \rightarrow 3/2$	0	21326,322 (15)	0,005
	$3/2 \rightarrow 1/2$	1	21187,373 (15)	− 0,002
	$3/2 \rightarrow 5/2$	1	21174,155 (15)	− 0,003
	$3/2 \rightarrow 3/2$	1	21157,493 (15)	0,006
	$3/2 \rightarrow 1/2$	2	21019,460 (30)	− 0,019
	$3/2 \rightarrow 5/2$	2	21006,363 (30)	− 0,005
	$3/2 \rightarrow 3/2$	2	20989,868 (30)	0,007
	$3/2 \rightarrow 5/2$	3	20839,742 (50)	0,026
$1 \rightarrow 2$	$5/2 \rightarrow 7/2$ $3/2 \rightarrow 5/2$	0	42680,665 (50)	− 0,030
	$1/2 \rightarrow 1/2$	0	42679,188 (50)	− 0,048
	$5/2 \rightarrow 5/2$	0	42663,805 (50)	− 0,006
	$1/2 \rightarrow 3/2$	0	42662,414 (50)	0,023
	$5/2 \rightarrow 7/2$ $3/2 \rightarrow 5/2$	1	42342,680 (100)	0,013

Table 4. The $J=0 \rightarrow 1$ and $1 \rightarrow 2$ rotational transition frequencies for $^{71}Ga^{19}F$. The nuclear spin of ^{71}Ga is 3/2. The last column shows the differences between the calculated and observed line frequencies.

$$\frac{Q(^{69}\mathrm{Ga})}{Q(^{71}\mathrm{Ga})} = \frac{e\, q_e\, Q(^{69}\mathrm{Ga})}{e\, q_e\, Q(^{71}\mathrm{Ga})} = 1.5871(10)$$

is in excellent agreement with the more precise ratio[10] determined from the $^2P_{3/2}$ state of Ga, i. e. 1.586904(3).

	$^{69}Ga^{19}F$		$^{71}Ga^{19}F$	
	Present	*Earlier*[9]	*Present*[a]	
Y_{01}	10778,023 (8)	10764	10712,379 (8)	MHz
Y_{11}	− 85,868 (8)	− 85	− 85,084 (8)	MHz
Y_{21}	+ 0,305 (8)		+ 0,301 (8)	MHz
Y_{02}	− 15,0 (15)		− 14,8 (15)	kHz
eq_0Q (Ga)	− 106,52 (6)		− 67,12 (6)	MHz
eq_1Q (Ga)	− 105,43 (6)		− 66,44 (6)	MHz
eq_2Q (Ga)	− 104,35 (6)		− 65,76 (10)	MHz
eq_3Q (Ga)	− 103,26 (8)		− 65,07 (20)	MHz
eq_eQ (Ga)	− 107,07 (8)		− 67,46 (8)	MHz
eq_IQ (Ga)	+ 1,09 (7)		+ 0,68 (7)	MHz
c_{Ga}	+ 14 (5)		+ 18 (5)	kHz

[a] Dunham coefficients calculated with isotope relations from^{69} GaF.

Table 5. The derived rotational and hyperfine structure constants for $^{69}Ga^{19}F$ and $^{71}Ga^{19}F$.

Stark effect measurements on ^{69}GaF were carried out in the hot cell spectrometer on the $J=0 \rightarrow 1$, $v=0$, $F=|M_F|=3/2 \rightarrow 5/2$ transition. The TlF transitions J, $|M_J|=0,0 \rightarrow 1,1$ and $1,1 \rightarrow 2,2$ served as standards for determining the electrode spacing. Although both GaF and TlF produce very intense spectra when studied separately, it was found when they were evaporated simultaneously from separate sample holders that absorption intensities were greatly reduced. A metallic coating of the absorption cell occurred in this case also, indicating that a decomposition reaction had occurred. However, Stark effect measurements were still obtained in several runs with the internal standardization technique. These measurements agreed very well with other runs in which the electrode spacing was fixed by a quartz spacer and standardized with TlF measurements previous or subsequent to the GaF

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[10] NORMAN F. RAMSEY, Molecular Beams, Oxford University Press, London 1956, p. 313.

measurement. In these cases the absorption cell was not dismantled or cleaned between runs. For GaF Stark shifts of 0.85 to 3.8 MHz were observed at electric field strengths of 225 to 485 V/cm. The dipole moments derived from these measurements are listed in Table 6, and all values lie well within the estimated error of the average value.

μ_0(D)	μ_0(D)	μ_0(D)	μ_0(D)
2,48	2,44	2,46	2,44
2,47	2,46	2,46	2,43
2,48	2,46	2,46	2,43
2,48	2,45	2,44	2,42
2,48	2,46	2,46	
2,48	2,45	2,45	
$\lvert \bar{\mu}_0 \rvert = 2{,}45 \pm 0{,}05$ D			

Table 6. The electric dipole moment of $^{69}Ga^{19}F$. The measurements were made in the hot cell spectrometer on the *J, F,* $\lvert M_F \rvert = 0, 3/2, 3/2 \rightarrow 1, 5/2, 5/2$ transition. All values are given in Debye.

Indium Monofluoride

The $J=1 \rightarrow 2$ and $2 \rightarrow 3$ microwave absorption spectra of $^{115}In^{19}F$ were reported by LOVAS and TÖRRING [2] for the $v=0$ and 1 vibrational states. We have subsequently found that improved spectra may be obtained by employing the black condensate from the quenched vapor over $In + AlF_3$ or $In + CaF_2$. The new measurements were obtained in the hot cell spectrometer, and were undertaken in order to determine the Y_{21} rotational constant and the electric dipole moment.

Like GaF and TlF, the InF spectra were observed at 300° – 350 °C. About 0.4 g of InF, i. e. approximately 0.9 g of the impure condensate, allowed measurements with maximum line intensities for a period of one hour. The $^{115}In^{19}F$ (95.7%) $J=0 \rightarrow 1$, $v=0$, 1, 2 and 3 transitions and $^{113}In^{19}F$ (4.3%) $v=0$ transitions were observed and are listed in Table 7. The derived rotational and hyperfine structure constants are shown in Table 8. The measurements from the earlier work [2] were used in deriving these constants. This produced little change in the original agreement of calculated and observed line frequencies, with the exception of the $J=1 \rightarrow 2$, $v=1$, $F=7/2 \rightarrow 7/2$ transition which now deviates by -0.20 MHz from the calculated frequency. Line widths in the present study were 150 – 200 kHz compared with 450 kHz previously. The ratio of the In nuclear quadrupole moment determined here is,

$$\frac{Q(^{115}\mathrm{In})}{Q(^{113}\mathrm{In})} = \frac{e\,q_0\,Q(^{115}\mathrm{In})}{e\,q_0\,Q(^{113}\mathrm{In})} = 1.0139(4)$$

$J \rightarrow J'$	$F \rightarrow F'$	v	ν (MHz)	$\Delta\nu$ (MHz)
		$^{115}In^{19}F$		
$0 \rightarrow 1$	$9/2 \rightarrow 7/2$	0	15738,701 (15)	0,006
	$9/2 \rightarrow 11/2$	0	15708,668 (15)	– 0,009
	$9/2 \rightarrow 9/2$	0	15575,879 (15)	0,000
	$9/2 \rightarrow 7/2$	1	15625,980 (15)	0,004
	$9/2 \rightarrow 11/2$	1	15596,218 (15)	– 0,005
	$9/2 \rightarrow 9/2$	1	15464,654 (15)	– 0,003
	$9/2 \rightarrow 7/2$	2	15513,847 (15)	0,010
	$9/2 \rightarrow 11/2$	2	15484,366 (15)	– 0,003
	$9/2 \rightarrow 9/2$	2	15354,011 (15)	0,008
	$9/2 \rightarrow 7/2$	3	15402,330 (20)	– 0,005
	$9/2 \rightarrow 11/2$	3	15373,100 (20)	0,009
	$9/2 \rightarrow 9/2$	3	15243,981 (20)	0,003
		$^{113}In^{19}F$		
$0 \rightarrow 1$	$9/2 \rightarrow 7/2$	0	15777,109 (25)	– 0,007
	$9/2 \rightarrow 11/2$	0	15747,428 (25)	0,042
	$9/2 \rightarrow 9/2$	0	15616,498 (25)	0,017

Table 7. The $J=0 \rightarrow 1$ measured rotational transition frequencies for $^{115}In^{19}F$ and $^{113}In^{19}F$. The nuclear spin of both In isotopes is 9/2. The differences between the calculated and observed line frequencies are shown in the last column.

	$^{115}In^{19}F$		$^{113}In^{19}F$	
	Present	*Earlier* [2]	*Present* [b]	
Y_{01}	7864,279 (5)	7864,283 (8) [a]	7884,042 (6)	MHz
Y_{11}	– 56,354 (5)	– 56,358 (9) [a]	– 56,567 (6)	MHz
Y_{21}	+ 0,149 (5)		+ 0,150 (6)	MHz
Y_{02}	– 7,5 (4)		– 7,5 (5)	kHz
eq_0Q (In)	– 723,74 (15)	– 723,74 (23)	– 713,79 (20)	MHz
eq_1Q (In)	– 717,10 (15)	– 717,95 (39)		MHz
eq_2Q (In)	– 710,46 (15)			MHz
eq_3Q (In)	– 703,81 (20)			MHz
eq_eQ (In)	– 727,06 (20)			MHz
eq_IQ (In)	+ 6,64 (20)			MHz
c_{In}	+ 17 (4)	+ 15 (5)	+ 17 (6)	kHz

[a] Earlier value corrected with present Y_{21}.
[b] Dunham coefficients calculated with isotope relations from ^{115}InF.

Table 8. The derived rotational and hyperfine structure constants for $^{115}In^{19}F$ and $^{113}In^{19}F$.

while the same ratio[10] determined from atomic In is 1.01456(10).

Stark effect measurements on ^{115}InF were performed in the hot cell spectrometer on the $J=0\to 1$, $v=0$, $F=|M_F|=9/2\to 11/2$ transition. As was the case with GaF, the transition intensities of InF and TlF were greatly reduced when observed simultaneously. In this case a simultaneous standardization was not possible. The quartz spacer was used to give a stable Stark cell geometry and standardization with the TlF $J=1\to 2$ transition was performed before and after measurements on InF without dismantling the absorption cell. The TlF standardization showed a 1% increase in the electrode spacing as compared to mechanical measurement of the quartz spacer. Stark shifts of 2.5 to 6.4 MHz with electric field strengths of 240 to 385 V/cm were observed with line widths of 300 kHz at maximum shift. The dipole moments derived from several runs are listed in Table 9.

μ_0(D)	μ_0(D)
3,39	3,39
3,37	3,40
3,39	3,41
3,40	3,40
3,40	
$\lvert\bar{\mu}_0\rvert = 3{,}40 \pm 0{,}07$ D	

Table 9. The electric dipole moment of ^{115}In^{19}F in the ground vibrational state. The J, F, $|M_F|=0$, 9/2, $9/2\to 1$, 11/2, 11/2 transition of InF was observed in these measurements.

Thallium Monofluoride

The thallium monofluoride rotational spectra were observed in the hot cell spectrometer by heating commercially available TlF to 300° – 400 °C. All but the $J=0\to 1$ transition frequencies shown in Table 10 were measured in this laboratory. Since the $J=0\to 1$ spectrum reported by RITCHIE and LEW[3] was very accurately measured, these lines were included in the calculation of the rotational constants, and are listed in Table 10 also. Observed line widths were 350 kHz for the $J=1\to 2$ and $2\to 3$ transitions and about 700 kHz for the $J=3\to 4$ lines. Due to this relatively large line width, the magnetic hyperfine splitting from the Tl nucleus was not resolvable.

$J\to J'$	v	ν (MHz)	$\Delta\nu$ (MHz)	ν (MHz)	$\Delta\nu$ (MHz)
		^{203}Tl^{19}F		^{205}Tl^{19}F	
$0\to 1^a$	0	13 345,818 (5)	0,003	13 334,686 (5)	– 0,004
	1	13 255,916 (7)	0,007	13 244,894 (7)	0,003
	2	13 166,391 (10)	0,007	13 155,481 (10)	0,003
$1\to 2$	0	26 691,513 (25)	– 0,003	26 669,236 (25)	– 0,002
	1	26 511,717 (25)	– 0,006	26 489,686 (25)	– 0,026
	2	26 332,656 (25)	0,002	26 310,885 (25)	– 0,054
	3	26 154,362 (30)	0,003	26 132,798 (30)	– 0,037
	4	25 976,819 (35)	0,030	25 955,484 (35)	– 0,018
$2\to 3$	0	40 036,903 (50)	0,035	40 003,566 (50)	– 0,042
	1	39 767,257 (50)	– 0,026	39 734,153 (50)	0,001
	2	39 498,599 (70)	0,043	39 465,891 (70)	0,011
	3	—	—	39 198,741 (70)	0,047
$3\to 4$	0	53 381,902 (60)	0,070	53 337,445 (60)	– 0,024
	1	53 022,347 (60)	0,000	52 978.272 (60)	– 0,026
	2	52 664,255 (80)	– 0,043	52 620,521 (60)	0,038
	3	52 307,631 (80)	– 0,032	52 264,345 (80)	0,047
	4	—	—	51 909,743 (80)	0,032
	5	—	—	51 556,768 (100)	– 0,030

[a] Transition frequencies from RITCHIE and LEW[3].

Table 10. The measured rotational transition frequencies of ^{203}Tl^{19}F and ^{205}Tl^{19}F. The differences between calculated and observed line frequencies are shown in the columns labled $\Delta\nu$.

The computation of the rotational constants was performed by computer according to Method II described in Ref[11]. It was found that an improved least squares fit is obtained when several higher order terms were included in Eq. (1), i. e.

$$\nu_{v,J\to v,J+1} = \text{Eq. (1)} + 2\,Y_{31}(v+1/2)^3(J+1) + 4\,Y_{12}(v+1/2)(J+1)^3$$

where Y_{31}, $Y_{12} \sim 1/u_{\mathrm{r}}^{5/2}$. The rotational constants shown in Table 11 were obtained by fitting both the ^{203}TlF and ^{205}TlF lines by means of the isotopic

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[11] J. HOEFT and E. TIEMANN, Z. Naturforsch. **23 a**, 1034 [1968].

	$^{205}Tl^{19}F$	
Y_{01}	6689,8668 (32)	MHz
Y_{11}	− 45,0747 (61)	MHz
Y_{21}	0,0901 (30)	MHz
Y_{02}	− 5,38 (14)	kHz
Y_{31}	0,64 (40)	kHz
Y_{12}	− 0,144 (69)	kHz

Table 11. Molecular constants for $^{205}Tl^{19}F$.

	$^{203}Tl^{19}F$	$^{205}Tl^{19}F$	
	Ritchie and Lew		
Y_{01}	6695,467 (3)	6689,874 (2)	MHz
B_e	6695,509 (7)	6689,916 (7)	MHz
Y_{11}	− 45,139 (5)	− 45,085 (4)	MHz
Y_{21}	0,094 (2)	0,095 (2)	MHz
$D_e (= 4\,B_e^3/\omega_e^2)$	5,916	5,903	kHz
r_e	2,08442 (9)	2,08442 (9)	Å
	Barrett and Mandel		
B_e		6689,97 (6)	MHz
$-\alpha_e$		− 44,97 (8)	MHz
r_e		2,0844 (1)	Å
	Fitzky		
B_e	6695,46 (6)	6689,71 (5)	MHz
$-\alpha_e$	− 45,11 (6)	− 44,83 (4)	MHz
γ_e		0,130 (45)	MHz
r_e	2,0843 (1)	2,0843 (1)	Å

Table 12. Molecular constants for TlF reported previously. See Ref. [3].

dependence of these constants. For comparison, the values reported by other workers are listed in Table 12. The present analysis resulted in values slightly different than Ritchie and Lew's, due to inclusion of the higher order terms here and to the measurement of Y_{02} which deviates considerably from that calculated according to Eq. (5) with ω_e from band spectra measurements (see Table 13).

In Table 13 are listed those molecular constants derived from the rotational constants, e. g. potential coefficients, vibrational constants, centrifugal distortion constant and equilibrium internuclear distance. The nuclear masses used throughout this report were taken from Ref. [12] and the natural constants from COHEN and DUMOND [13]. The absolute error in r_e is that discussed in the Introduction, although the error from the measurements is several orders of magnitude lower. The a_0 and a_1 constants were calculated from Eqs. (3) and (4) using the ω_e value from band spectra except in the case of TlF, where the ω_e value determined here was employed.

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	^{27}AlF	^{69}GaF	^{115}InF	^{205}TlF	
Y_{02}		− 15,0 (15)	− 7,5 (4)	− 5,38 (14)	kHz
Y_{02}^{a}	− 30,48	− 14,40	− 7,553	− 5,903	kHz
ω_e		610 (60)	537 (30)	498 (7)	cm^{-1}
ω_e	814,5 [b]	622,2 [c]	535,35 [d]	475,00 [b]	cm^{-1}
a_0	3,002	2,692	2,731	2,776 (73)	$10^5\ cm^{-1}$
a_1	− 3,218	− 3,230	− 3,437	− 3,505 (33)	
μ_r	11,148474	14,893274	16,302861	17,386873	amu
r_e	1,6543601	1,7743619	1,9853883	2,0844302	Å
μ_0	1,53 (10) [e]	2,45 (5)	3,40 (7)	4,2282 (8) [f]	D

[a] Calculated from Eq. (5).
[b] G. HERZBERG, Spectra of Diatomic Molecules, D. Van Nostrand Co., New York 1950.
[c] Ref. [9].
[d] R. F. BARROW, D. V. GLASER, and P. B. ZEEMAN, Proc. Phys. Soc. London A **68**, 962 [1955].
[e] Ref. [1].
[f] Ref. [4].

Table 13. The dipole moments and molecular constants derived from the rotational constants of the Group IIIa monofluorides.

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[12] J. H. E. MATTAUCH, W. THIELE, and A. H. WAPSTRA, Nucl. Phys. **67**, 1 [1965].

[13] E. R. COHEN and J. W. M. DUMOND, Rev. Mod. Phys. **37**, 537 [1965]. Here the constants $h = 6.62559(16) \times 10^{-27}$ erg sec and $u = 1.66043(2) \times 10^{-24}$ gram were used.