

Die Abb. 8 liefert folgendes Gesetz  $\mu_p \sim T^{-0,92}$ . Für die Beweglichkeit der Elektronen ergeben sich für die In-dotierten Proben folgende Werte bei Zimmertemperatur:

Probe	P 10	P 11	P 15	P 19
$\mu_n[\text{cm}^2/\text{Vs}]$	124	218	137	266

Tab. 2.

Berechnung der effektiven Masse  $m^*$  aus der Thermokraft

$$\alpha = (k/e)[r + 2 + \ln\{2(2\pi m^* k T)^{3/2}/h^3 n\}]$$

liefert unter der Annahme akustischer Gitterschwingungen, d.h.  $r = 0$ , für die Defektelektronen  $m_p^*/m \approx 0,7$  und für die Elektronen der Proben P 10, P 11 und P 19 einen Durchschnittswert von

$m_n^*/m \approx 0,8$ . Diese Werte liegen aber wahrscheinlich etwas zu hoch, da  $r$  sicher größer als Null ist, wie schon aus der Steigung in Abb. 8 hervorgeht.

Auch das negative Vorzeichen des transversalen Nernst-Ettingshausen-Effektes spricht nicht für Streuung an akustischen Gitterschwingungen, wobei allerdings parabolische Bandstruktur vorausgesetzt wäre. Für die Kurven ergibt sich ein Maximum für  $Q^\perp$  beim Übergang vom p- zum n-Leitungsmechanismus, d.h. im Gebiet gemischter Leitung, wenn Elektronen und Defektelektronen im Temperaturgradienten ohne zu große Thermogegegenspannung in gleicher Richtung diffundieren und vom Magnetfeld in verschiedene Richtung abgelenkt werden.

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## Microwave Rotational Spectrum of Indium Monofluoride

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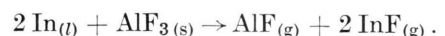
The rotational transitions  $J = 1 \rightarrow 2$  and  $2 \rightarrow 3$  were measured in  $^{115}\text{In}^{19}\text{F}$ . From these spectra the following molecular parameters have been determined: the Dunham-coefficients  $Y_{01}$ ,  $Y_{11}$  and  $Y_{02}$ , the quadrupole coupling constants, eqQ, in the  $v = 0$  and  $v = 1$  vibrational states as well as the spin-rotation coupling constant  $c_{\text{In}}$ .

Rotational spectra of the indium monohalides, with the exception of the monofluoride, have been observed by BARRETT and MANDEL<sup>1</sup> and other workers<sup>2</sup>. The lack of the observation of the InF spectra might be attributed to the necessity of using a rather high temperature (750—1000°C) which is aggravated by the problem of chemical reaction of the fluorides with the hot wave guide and vacuum enclosure of the typical high temperature microwave absorption spectrometer. This difficulty has been eliminated in the spectrometer used in the present study. Details of the construction of this spectrometer are to be published elsewhere, so only a brief outline will be given here.

The source is a metal oven (Ta or Mo) heated by resistance heating and located directly below the

absorption cell which has an opening to allow the vapor to pass through. Since the cell is water cooled, most of the evaporated material condenses in the absorption cell and on the STARK modulation electrode. Due to attenuation resulting from this condensed material the effective running time is limited. In the present study of InF it was about three-quarters to one hour. Thus, the spectrometer was designed so that rapid disassembly and cleaning are possible.

Since InF is not commercially available, a mixture of In metal filings and  $\text{AlF}_3$  was used to produce a reaction of the following type:



Condensed material from the cell was mixed with fresh mixture and better results were usually ob-

<sup>1</sup> A. H. BARRETT and M. MANDEL, Phys. Rev. **109**, 1572 [1958].

<sup>2</sup> J. HOEFT, Z. Physik **163**, 262 [1961]. — G. A. L. DELVIGNE and H. W. DE WIJN, J. Chem. Phys. **45**, 3318 [1966].



tained, probably due to the presence of powdered In rather than to InF. The strongest absorption line first appeared at 700°C but rather quickly decreased in intensity. Thus, the oven temperature was periodically increased during each run up to 1000°C

at which point the evaporation of AlF<sub>3</sub> becomes predominant.

The Hamiltonian applicable to a diatomic molecule containing one nucleus with a quadrupole moment and significant spin-rotation interaction is:

$$\hat{H} = \hat{H}_{J,v} - e q_{(v)} Q \frac{3(\hat{I} \cdot \hat{J})^2 + 3/2(\hat{I} \cdot \hat{J}) - I^2 J^2}{2I(2I-1)(2J-1)(2J+3)} + c(\hat{I} \cdot \hat{J}). \quad (1)$$

The first term in this Hamiltonian represents the energy of the vibrating rotor which is expressed in the DUNHAM<sup>3</sup> form as:

$$E_{J,v} = \sum_{l,j} Y_{l,j}(v+1/2)^l J^j (J+1)^j. \quad (2)$$

The frequency of a transition  $J \rightarrow J+1$ ,  $\Delta v = 0$  is then:

$$\nu = 2 Y_{01}(J+1) + 2 Y_{11}(v+1/2)(J+1) + 4 Y_{02}(J+1)^3 + \dots \quad (3)$$

where the  $Y_{l,j}$ 's correspond to the band spectroscopic constants in the following manner:

$$Y_{01} \approx B_e, \quad Y_{11} \approx -\alpha_e, \quad Y_{02} \approx -D_e.$$

Here  $B_e$  corresponds to a rigid rotor with  $r = r_e$  and

$$B_e = h/8\pi^2 \mu r_e^2 \quad (4)$$

where  $\mu$  is the reduced mass.

The second term in Eq. (1) represents the interaction between the quadrupole moment,  $Q$ , of the In nucleus with the electric field gradient,  $q_{(v)}$ , present at that nucleus. First order perturbation theory gives for this interaction:

$$E_Q^{(1)} = -e q_{(v)} Q \cdot f(I, J, F) \quad (5)$$

where  $f(I, J, F)$  is CASIMIR's function, which is tabulated in a number of places<sup>4</sup>. When the quadrupole interaction constant,  $e q Q$ , is large, as in the case of InF, the second order terms must also be included. BARDEEN and TOWNES<sup>5</sup> have derived the second order expression:

$$E_Q^{(2)} = \sum_J (IJFM_F | H_Q | IJ'FM_F)^2 / (E_J - E_{J'}) \quad (6)$$

where  $J' = J \pm 2$  and

$$\begin{aligned} (IJFM_F | H_Q | I, J+2, FM_F)^2 &= \left\{ \frac{3eqQ}{16I(2I-1)(2J+3)} \right\}^2 \\ &\times \frac{1}{(2J+1)(2J+5)} (F+I+J+3)(F+I+J+2)(I-F+J+2)(I-F+J+1) \\ &\times (F-I+J+2)(F-I+J+1)(F+I-J)(F+I-J-1). \end{aligned} \quad (7)$$

The tables of this second order interaction in Ref.4 are not evaluated for  $I = 9/2$ , so these values were obtained directly from the above equation.

The last term in the Hamiltonian, the magnetic coupling of the In nucleus to  $J$ , was evaluated from the following expression:

$$c_{\text{In}}(\hat{I} \cdot \hat{J}) = c_{\text{In}} \cdot \frac{F(F+1) - J(J+1) - I(I+1)}{2}. \quad (8)$$

It shows up as a small additional shift of all lines. The coupling of the  $F$  nucleus to the molecular

rotation was not taken into account. It will exhibit itself in a small splitting of the lines which is not observable in the present experiment.

The selection rules for the transitions are  $\Delta F = 0, \pm 1$  and  $\Delta J = \pm 1$ . Table I lists the calculated and measured line frequencies for the  $J = 1 \rightarrow 2$  and  $2 \rightarrow 3$  observations. Since observation of  $v = 2$  resonances was not possible, we were not able to measure  $Y_{21} = \gamma_e$ . However, it is expected to be quite small and will not have a significant effect on the other constants derived. The DUNHAM co-

<sup>4</sup> C. H. TOWNES and A. L. SCHAWLOW, *Microwave Spectroscopy*, p. 499ff.; McGraw-Hill Book Co., Inc., New York 1955. — W. GORDY, W. V. SMITH, and R. F. TRAMBARULO, *Microwave Spectroscopy*, p. 374ff.; John Wiley and Sons, Inc., New York 1953.

<sup>5</sup> J. BARDEEN and C. H. TOWNES, *Phys. Rev.* **73**, 627, 1204 [1948].

<sup>3</sup> J. L. DUNHAM, *Phys. Rev.* **41**, 721 [1932].

$J = 1 \rightarrow 2$ $F \rightarrow F'$	Vibrational state $v = 0$			Vibrational state $v = 1$		
	Computed	Weighted average	Measured	Computed	Weighted average	Measured
9/2 $\rightarrow$ 7/2	31445,10		31445,09			
9/2 $\rightarrow$ 11/2	31380,59	31380,68	31380,64	31156,06	31156,15	31156,14
9/2 $\rightarrow$ 9/2	31380,78			31156,25		
7/2 $\rightarrow$ 5/2	31372,71			31148,25		
11/2 $\rightarrow$ 13/2	31359,95	31247,85	31247,84	31135,59	31024,39	31024,48
7/2 $\rightarrow$ 7/2	31282,27			31058,53		
11/2 $\rightarrow$ 11/2	31247,82			31024,36		
11/2 $\rightarrow$ 9/2	31248,01			31024,54		
7/2 $\rightarrow$ 9/2	31217,94					
$J = 2 \rightarrow 3$						
11/2 $\rightarrow$ 13/2	47036,20		47036,19			
5/2 $\rightarrow$ 3/2	47031,75	47031,89	47031,97			
11/2 $\rightarrow$ 9/2	47032,14					
9/2 $\rightarrow$ 9/2	47031,95					
13/2 $\rightarrow$ 15/2	47024,73		47024,75			

Table 1. Calculated and measured rotational lines of  $^{115}\text{In}^{19}\text{F}$  [MHz].

	Present <sup>a</sup>	Earlier <sup>b</sup>
$\omega_e$		535,3 <sub>5</sub> cm <sup>-1</sup>
$\omega_e x_e$		2,6 <sub>35</sub> cm <sup>-1</sup>
$Y_{01}$	7864,170 (8) MHz	7868,7 MHz
$Y_{11}$	- 56,059 (9) MHz	- 55,8 MHz
$Y_{02}$	- 7,55 kHz	- 7,5 kHz
$e q_0 Q_{\text{In}}/\hbar$	- 723,74 (23) MHz	
$e q_1 Q_{\text{In}}/\hbar$	- 717,95 (39) MHz	
$c_{\text{In}}$	15 (5) kHz	
$r_e$	1,985403 (20) Å	1,984 <sub>7</sub> Å
$\mu$	16,3028 amu	16,3081 amu

<sup>a</sup> The constants  $\hbar$  and amu are taken from Ref. 7 and the atomic masses from Ref. 8.

<sup>b</sup> Ref. 6.

Table 2. Derived constants for  $^{115}\text{In}^{19}\text{F}$ .

efficients  $Y_{01}$ ,  $Y_{11}$ , and the hyperfine constants were determined by the method of least-squares adjustment in which  $Y_{02} = -4 B_e^3/\omega_e^2$  was used. The vibrational frequency,  $\omega_e$ , was taken from Ref. 6. In Table II these derived molecular constants are presented along with those obtained by others from band spectra.

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<sup>6</sup> R. F. BARROW, D. V. GLASER, and P. B. ZEEMAN, Proc. Phys. Soc. London **68A**, 962 [1955].

<sup>7</sup> E. R. COHEN and J. W. M. DUMOND, Rev. Mod. Phys. **37**, 537 [1965].

<sup>8</sup> J. H. E. MATTAUCH, W. THIELE, and A. H. WAPSTRA, Nucl. Phys. **67**, 1 [1965].