The Moment of Inertia of CF3CH3
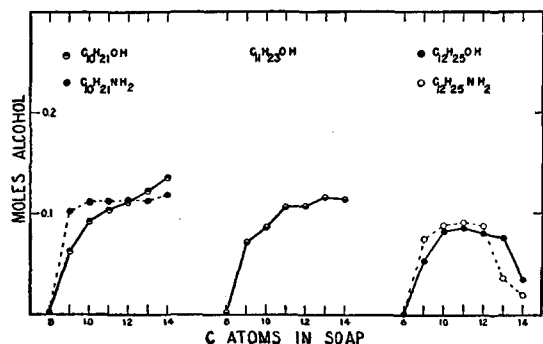
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FIG. 3.

amine, etc., since in this case also the activity of the compound decreases rapidly with chain length. However, most of the relations are complex, and there is evidence that what may be described as molecular fitting enters, especially if the lengths of the soap chain and that of the polar-non-polar-non-ionic chain are not too different. For example, the solubility of the 11-C atom alcohol is in general higher than that which corresponds to the solubility of the 10- and 12-C atom alcohols.

Substances which enter the micelle by film penetration lower the critical micelle concentration. The rate of lowering with film concentration increases with extreme rapidity with the length of the molecule.[2] Substances which enter by solubilization have little effect upon the critical micelle concentration.

[1] W. D. Harkins, R. W. Mattoon, and R. Mittelmann, J. Chem. Phys. 15, 763 (1947).
[2] M. L. Corrin and W. D. Harkins, J. Chem. Phys. 10, 640 (1946), and later work with higher alcohols.

The Moment of Inertia of CF_3CH_3

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August 25, 1948

THE C—C bond distance in polyfluorinated compounds is a subject of much interest. On the basis of electron diffraction measurements Brockway, Secrist, and Lucht[1] reported a distance of 1.45A in C_2F_6. On the other hand, nearly normal hydrocarbon bond distances for both the single and double bond in hexafluoropropene—namely, 1.52 and 1.31A, were found by Buck and Livingston[2] in their electron diffraction study. As an initial step in determining the bond distances and angles in CF_3CH_3 we have made a preliminary study of its microwave spectrum near 1.5-cm wave-length. The absorption cell was a five-foot section of standard 1.25-cm wave guide, used as a Hughes-Wilson[3] Stark effect spectrometer.

Two lines were found. The first had a frequency of $20,741\pm2$ megacycles and had an absorption coefficient of the order of 2×10^{-6} cm^{-1}. It is due to the $J=1$ to $J=2$ transitions (for $K=0$ and $K=1$) in the ground state. Both linear and quadratic Stark effects were observed. The second line at $20,710\pm2$ megacycles appeared with an intensity of about half that of the first line, and is probably caused by the same rotational transition in a low lying, excited vibrational state. A second-order Stark effect was observed.

These data permit the calculation of the moment of inertia perpendicular to the threefold axis. Using Birge's[4] values for the fundamental constants,

$$I_B = 161.80\pm0.07\times10^{-40} \text{ g cm}^2$$

in the ground state; for the unidentified excited state,

$$I_B = 162.04\pm0.07\times10^{-40} \text{ g cm}^2.$$

It is not possible to determine bond distances from these data alone, yet it is interesting to note several combinations which are in harmony with the observations. The electron diffraction measurements of Shand and Spurr[5] yield $C-C = 1.52\pm0.02$A, $C-F = 1.37\pm0.02$A, $<C-C-F = 112° 10'\pm2°$, $<F-C-F = 107° 32'\pm2°$ when a tetrahedral methyl group with $C-H = 1.09$A was assumed. The moment of inertia[5] calculated from these values, $I_B = 166.7\pm5.8\times10^{-40}$, while in agreement within the stated limits with the microwave value, does not represent the best choice of the distances and angles.

Before beginning the search for the microwave spectrum, a calculation of the microwave line positions was made with the following parameters: $C-C = 1.54$A, $C-F = 1.33$A, $C-H = 1.093$A, $F-F = 2.16$A, $<H-C-H = 109° 28'$, $H = 1.008$, $C = 12.01$, $F = 19.00$, and $N = 6.0228\times10^{23}$. These lead to $I_B = 161.9\times10^{-40}$, the close agreement with experiment probably being fortuitous. A shorter $C-C$ distance of 1.45A with all other distances and angles as listed immediately above gives $I_B = 154.7\times10^{-40}$. Such a distance requires compensation elsewhere; for example, $I_B = 161.7\times10^{-40}$ when $C-C = 1.45$A and $C-F = 1.38$A, the other distances and all angles remaining as before.

If recent work[2,6] may be interpreted as favoring the shorter $C-F$ bond distance and angles which are nearly tetrahedral, the present results would favor a $C-C$ distance in CF_3CH_3 more nearly like that in ethane than like that reported for C_2F_6.[1]

Work is planned on the preparation of isotopic molecules from which these distances may be determined unambiguously, within the limits imposed by zero-point vibration corrections.

[1] L. O. Brockway, J. H. Secrist, and C. M. Lucht, Abstracts, American Chemical Society Meeting, Buffalo, New York, 1942.
[2] F. A. M. Buck and R. Livingston, J. Am. Chem. Soc., in press. Thanks are due these authors for permission to use their data in advance of publication.
[3] R. H. Hughes and E. B. Wilson, Jr., Phys. Rev. 71, 562 (1947).
[4] R. T. Birge, Rev. Mod. Phys. 13, 233 (1941).
[5] W. Shand and R. A. Spurr, quoted by H. Russell, Jr., D. R. V. Golding, and D. M. Yost, J. Am. Chem. Soc. 66, 16 (1944).
[6] H. J. Bernstein and G. Herzberg, J. Chem. Phys. 16, 30 (1948).