appear in both spectra. This is in complete disagreement with the data; all five frequencies in this region appear in both the Raman and infrared spectra.

It is clear that "cyclic" $C_3F_6$ is not hexafluorocyclopropane.

The Raman spectrum indicates a molecule which has either no symmetry or at most one element of symmetry, in which case all 21 fundamental modes of vibration would appear individually in both the Raman and infrared spectra. Molecules containing a double bond have their stretching fundamental at *ca.* 1650 cm.$^{-1}$[10] which is shifted in polyfluorinated ethylenes to *ca.* 1750 cm.$^{-1}$.[11,12] This corresponds to the Raman line found at 1790 cm.$^{-1}$ and the infrared band at 1798 cm.$^{-1}$. Thus the spectra indicate the structure $CF_3CF{=}CF_2$!

It is difficult to predict the character of the vibrations of this molecule because of the lack of symmetry restrictions and the complexity resulting from the large interactions between the fluorine atoms. An approximate description of them based upon the neglect of coupling between the groups is found in Table I. The correlation between the expected magnitudes[5–12] and the observations is good. No definite assignment of all the frequencies can be made yet. For example, it is not clear why only five lines are found in the region where the six C–F stretching vibrations are expected. Work now under way in this Laboratory on similar molecules should throw light on these matters, however. The correlation of Table I is given solely to show that the spectrum has the proper number of lines in the proper spectral region for such a model.

In order to conclusively demonstrate that "cyclic" $C_3F_6$ is in reality hexafluoropropylene, the infrared spectrum between 2 and 15$\mu$ of an authentic sample of $CF_3CF{=}CF_2$ is included in Table III, column 2. It is identical with that for "cyclic" $C_3F_6$. This spectrum was obtained and furnished by Mr. D. G. Weiblen of the Central Research Department, Minnesota Mining and Manufacturing Company, using material prepared by Lyle Hals of that laboratory.

It is now clear why the physical properties of $CF_3CF{=}CF_2$[13] are so close to those earlier reported for "cyclic" $C_3F_6$.

**Acknowledgment.**—The author is indebted to Dr. A. F. Benning who furnished the infrared spectrum and sample of $C_3F_6$. Thanks are also due to Mr. D. G. Weiblen for the infrared spectrum of hexafluoropropylene.

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[10] G. Herzberg, "Infrared and Raman Spectra of Polyatomic Molecules," D. Van Nostrand Company, Inc., New York, N. Y., 1945, p. 195.

[11] J. B. Hatcher and D. M. Yost, *J. Chem. Phys.*, **5**, 992 (1937).

[12] P. Torkington and H. W. Thompson, *Trans. Faraday Soc.*, **41**, 236 (1945).

[13] Henne and Waalkes, THIS JOURNAL, **68**, 496 (1946).

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# The Identification of $C_3F_6$[1]

BY F. A. M. BUCK AND R. L. LIVINGSTON

The compound $C_3F_6$, obtained by pyrolysis of polytetrafluoroethylene and by pyrolysis of monochlorodifluoromethane has been reported to be hexafluorocyclopropane[2,3] although some doubt as to its identity has been expressed.[4] Interpretation of electron diffraction photographs of this compound has led us to the conclusion that the compound is not hexafluorocyclopropane but is hexafluoropropene. This conclusion has been reached independently by other workers.[5,6]

The electron diffraction photographs[7] were prepared using an apparatus built by Professor H. J. Yearian of the Purdue Physics Department. The sample of $C_3F_6$ was kindly supplied by Drs. Young and Benning of the Jackson Laboratory of E. I. du Pont de Nemours and Company. Diffraction maxima were observable on the photographs out to $s = 33$ ($s = 4\pi/\lambda \sin \theta/2$). A radial distribution curve (Fig. 1) was calculated using essentially a method previously described.[8] The five prominent peaks of this curve at 1.32, 2.16,

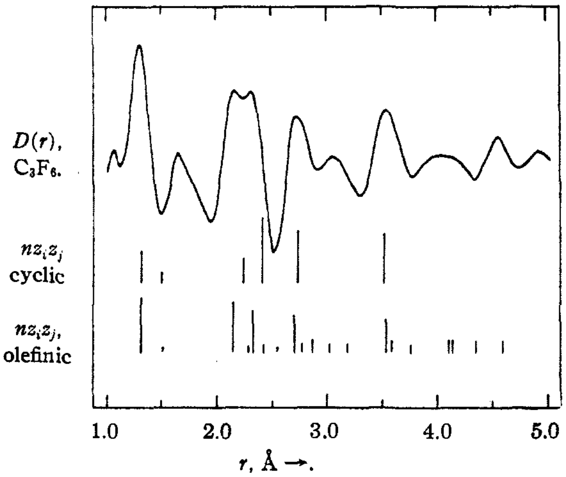

Fig. 1.—Radial distribution curve for $C_3F_6$. The lines under the curve correspond to bond distances in models of hexafluorocyclopropane and hexafluoropropene; the lengths of the lines indicate the relative weights, $nz_iz_j$, of the corresponding terms in the simplified intensity function.

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[1] From the Ph. D. thesis of F. A. M. Buck, duPont Fellow in Chemistry, Purdue University.

[2] A. F. Benning, F. B. Downing and J. D. Park, U. S. Patent 2,394,581 (February 12, 1946).

[3] J. D. Park, A. F. Benning, F. B. Downing, J. F. Laucius and R. C. McHarness, *Ind. Eng. Chem.*, **39**, 354 (1947).

[4] E. E. Lewis and M. A. Naylor, THIS JOURNAL, **69**, 1968 (1947).

[5] W. F. Edgell, *ibid.*, **70**, 2816 (1948). We appreciate the cooperation of Dr. Edgell in making his data available in advance of publication.

[6] E. G. Young and W. S. Murray, *ibid.*, **70**, 2814 (1948).

[7] For a general review of the method of electron diffraction, see L. O. Brockway, *Rev. Modern Phys.*, **8**, 231 (1936).

[8] R. Spitzer, W. J. Howell and V. Schomaker, THIS JOURNAL, **64**, 62 (1942).

2.34, 2.70, and 3.54 Å. are not compatible with any cyclic model having $D_{3h}$ symmetry. The bond distances in one cyclic model are indicated by vertical lines under the radial distribution curve; other cyclic models disagree with the curve to about the same extent or to a greater extent. Also the theoretical intensity curves for cyclic models are incompatible with the observed pattern.

We have succeeded in finding a model for hexafluoropropene which gives very good agreement with the prominent peaks on the radial distribution curve. This agreement is indicated under the curve by vertical lines representing bond distances in this model. In addition the theoretical intensity curve for this model agrees qualitatively with the photographs and the average of the $s_{\text{calcd.}}/s_{\text{obs.}}$ (for eleven features which may be confidently compared) is 0.999 with an average deviation of 0.006. Further work is necessary in order to determine the accuracy with which the various parameters in the molecule can be evaluated. The identity of the compound, however, seems clearly established.

We wish to thank Professor Yearian for the use of his diffraction apparatus and for many helpful discussions. We are also grateful to E. I. du Pont de Nemours and Company for the free grant fellowship which made this work possible.

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## Maxima in Vapor Pressure Curves

BY A. E. KORVEZEE AND P. DINGEMANS

Recently N. B. Keevil[1] has given the vapor pressures of aqueous solutions of a number of salts over an extensive temperature range. In case of highly soluble salts, maxima occur in the vapor pressure curves and the author stresses the point that the maxima lie at increasing temperatures with increasing melting point of the salts.

We have found analogous results for a series of salts with lower melting points. Moreover we have derived[2] the approximate expression

$$\frac{1}{T_{\max}} = \frac{1}{T_s} + 0.00021.$$

$T_s$ = melting point of the sale (absolute temperature)
$T_{\max}$ = absolute temperature of the maximum.

This expression is derived for ideal solutions, but it proves to give also fairly trustworthy results for the temperature of the pressure maxima even for our saturated salt solutions. The relation given is also valid for vapor pressure curves of solutions saturated with respect to two or more salts, in which case $T_s$ = the eutectic temperature of the salt mixture.[3] A number of examples are to be found in our publications.[4]

We have applied our formula to those of Keevil's curves, for which the temperature of the maximum and the melting point of the salt have been directly determined. The results are collected in Table I.

TABLE I

| Salt | Melting point, °C. | Temperature of the maximum, °C. measured | Temperature of the maximum, °C. calculated |
|---|---|---|---|
| NaCl | 804 | 600 | 606 |
| NaBr | 755 | 570 | 573 |
| KCl | 770 | 565 | 582 |

From the figures given it is clear that a fairly accurate estimation of the temperature of the maximum in the vapor pressure curve can be derived from melting point data with the aid of our formula.

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[1] N. B. Keevil, THIS JOURNAL, **64**, 841 (1942).

[2] A. E. Korvezee and P. Dingemans, *Rec. trav. chim.*, **62**, 653 (1943).

[3] A. E. Korvezee, P. Dingemans and L. L. Dijkgraaf, *ibid.*, **66**, 389 (1947); A. E. Korvezee, *ibid.*, **66**, 549 (1947).

[4] P. Dingemans, *et al.*, *Rec. trav. chim.*, **56**, 839 (1937); **58**, 574 (1939); **60**, 317 (1941); **61**, 605 (1942); **62**, 85 (1943); **62**, 625 and 639 (1943); **64**, 194 and 199 (1945); **65**, 477 (1946); **66**, 239 (1947).

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## The Preparation of Allyl Iodide[1]

BY R. L. LETSINGER AND JAMES G. TRAYNHAM

Reported methods for the preparation of allyl iodide involve the reaction of allyl alcohol or glycerol with either hydriodic acid or phosphorus and iodine.[2] We find that preparative quantities of allyl iodide may be obtained very conveniently by the action of sodium iodide on allyl chloride in acetone. This preparation is based on a reaction investigated kinetically by Conant, Kirner and Hussey.[3]

A mixture made of 0.6 mole (45.9 g.) of allyl chloride, 0.75 mole (113 g.) of sodium iodide, and 100 cc. of acetone was warmed on the steam-bath for three hours and then poured into 500 cc. of water. The organic layer was separated, washed with both a dilute sodium bisulfite solution and with water, dried over sodium sulfate, and distilled. The yield of allyl iodide (b. p. 101–102°, $d^{22}{}_4$ 1.8454, $n^{22}{}_D$ 1.5542) was 63.1 g. (62.6%). When the reflux time was increased to twenty-four hours and 200 cc. of acetone was used as solvent, the yield was increased to 76.7%.

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[1] This investigation was supported by a grant from the Abbott Fund of Northwestern University.

[2] McCullough and Cortese, THIS JOURNAL, **51**, 226 (1929); Norris, Watt and Thomas, *ibid.*, **38**, 1076 (1916); Datta, *ibid.*, **36**, 1005 (1914); Tollens and Henninger, *Ann.*, **156**, 156 (1870).

[3] Conant, Kirner and Hussey, THIS JOURNAL, **47**, 488 (1925).

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## Absorption Spectra of 4,6-Diamino-2-phenyl-1,3,5-triazine

BY FREDERICK C. NACHOD AND EDGAR A. STECK

Although 1,3,5-triazine derivatives have been the subject of many investigations, relatively few