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.

CONTRIBUTION FROM THE
PURDUE RESEARCH FOUNDATION AND THE
DEPARTMENT OF CHEMISTRY
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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	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).

DEPARTMENT OF CHEMISTRY
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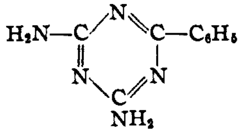
Absorption Spectra of 4,6-Diamino-2-phenyl-1,3,5-triazine

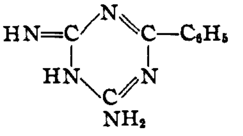
BY FREDERICK C. NACHOD AND EDGAR A. STECK

Although 1,3,5-triazine derivatives have been the subject of many investigations, relatively few physico-chemical measurements have been made with compounds of this class.[1-7] Of these, only one group of absorption spectra has been reported,[6] referring to cyanuric acid types, as well as at an early date. As a portion of some other investigations, the spectral characteristics of 4,6-diamino-2-phenyl-1,3,5-triazine became of interest. The compound (I) was prepared by the reaction of benzonitrile with dicyandiamide in the presence of piperidine,[8] being an improvement over earlier work.[9,10]

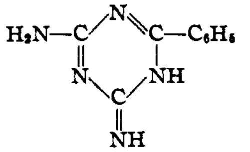
The tautomeric states possible in 4,6-diamino-2-phenyl-1,3,5-triazine are indicated in the structures I–IV. The two mono-imino forms (II and III) are twice as likely of being the more probable structures of the compound because only one diamino and only one di-imino structure can be formulated (I and IV). This may also account for the fact that only monohydrochlorides are formed in this type.[11,12]



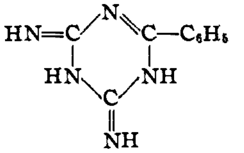
I



II



III



IV

Ultraviolet absorption spectra of 4,6-diamino-2-phenyl-1,3,5-triazone solutions shown in Fig. 1[13] clearly indicate that at pH 7 and 13 essentially the same maxima and minima are attained. On passing to pH 1, however, a marked batho- and hypochromic shift is to be observed. This indicates that the degree of conjugation is diminished and Table I, which lists the actual values for the maxima obtained, further emphasizes the differences in spectra. The shifting could easily be interpreted as the result of a favoring of structure (IV) in strongly acidic solution as the preferential form. However, in the crystallization of the hydrochloride, the more probable forms (II) and (III) are predominant. Although the structures (II) and (III) are not equivalent, presumably they do have nearly the same energy content and may be present in a solid solution or hydrogen-bonded condition in the solid state.

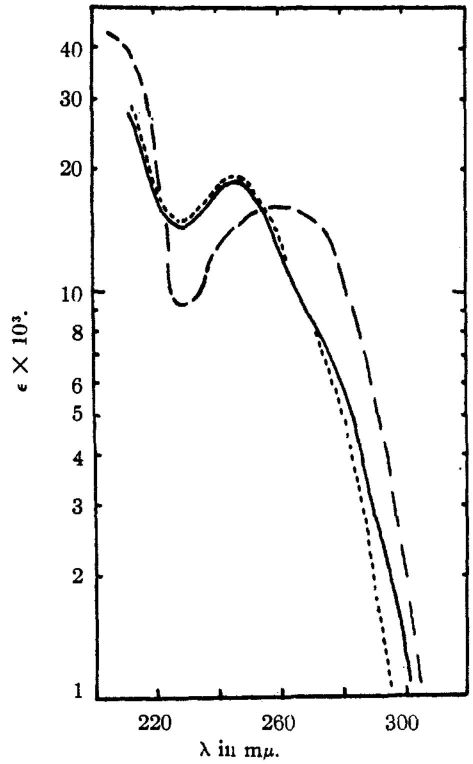


Fig. 1.—Spectrum of 4,6-diamino-2-phenyl-1,3,5-triazine monohydrochloride in — ethanol (95%) and in water, — — 0.01 N NaOH, ---- 0.01 N HCl.

TABLE I

MAXIMA OF 4,6-DIAMINO-2-PHENYL-1,3,5-TRIAZINE

Solvent	λ, in mμ	ε × 10³
95% Ethanol	244	18.6
Water	244	18.6
0.01 N NaOH	247	19.2
0.01 N HCl	255–261	16.2

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[1] Lemoult, *Compt. rend.*, **121**, 352 (1895); **125**, 822 (1897); *Ann. chim.*, [7] **16**, 348, 372, 410 (1899); *Bull. soc. chim.*, [3] **13**, 1024 (1895).

[2] Hantzsch, *Ber.*, **39**, 145 (1906).

[3] Wightman and Jones, THIS JOURNAL, **39**, 1752 (1917).

[4] Böeseken, *Rec. trav. chim.*, **37**, 147 (1917).

[5] Wood, *J. Chem. Soc.*, **83**, 576 (1903).

[6] Hartley, *ibid.*, **41**, 48 (1882); Hartley, Dobbie and Lauder, *ibid.*, **79**, 848 (1901).

[7] Kahovec, *Monatsh.*, **72**, 364 (1939).

[8] Zerweck and Brunner, U. S. Patent 2,302,162.

[9] Ostrogovich, *Atti reale accad. Lincei*, [5] **20**, I, 182, 251 (1911).

[10] Rackmann, *Ann.*, **376**, 181 (1910).

[11] The compound was purified and used as the monohydrochloride monohydrate, needles from aqueous alcohol, m. p. 246–247°, dec. *Anal.* Calcd. for $C_9H_9N_5 \cdot HCl \cdot H_2O$; N, 28.98; Cl, 14.67. Found: N, 28.68; Cl, 14.82. Ostrogovich[9] reported this compound but gave no melting point.

[12] Ostrogovich and Gheorghiu, *Gazz. chim. ital.*, **60**, 648 (1930).

[13] The spectra were determined with a Beckman quartz spectrophotometer, Model DU, Serial No. D-377, as in our earlier studies [*e. g.*, Ewing and Steck, THIS JOURNAL, **68**, 2181 (1946)].

Absorption Spectra of 5,7-Dimethyltetrazolo(a)-pyrimidine

BY FREDERICK C. NACHOD AND EDGAR A. STECK

The interest in the absorption spectral behavior of 5,7-dimethyltetrazolo[a]pyrimidine resulted from certain aspects of related heterocyclic studies. The compound, named 5,7-dimethyl-1,-2,3,4-tetraazaindolizine by Bülow,[1] is now des-

[1] Bülow, *Ber.*, **42**, 4433 (1909).