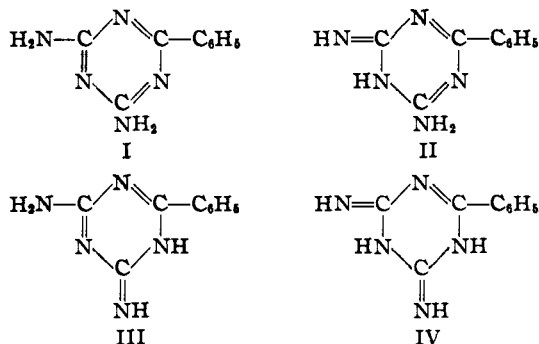


physico-chemical measurements have been made with compounds of this class.¹⁻⁷ Of these, only one group of absorption spectra has been reported,⁸ referring to cyanuric acid types, as well as at an early date. As a portion of some other investigations, the spectral characteristics of 4,6-diamino-2-phenyl-1,3,5-triazine 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}

Ultraviolet absorption spectra of 4,6-diamino-2-phenyl-1,3,5-triazine solutions shown in Fig. 1¹³ 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

(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) Böseken, *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 $C_8H_8N_6 \cdot HCl \cdot H_2O$; N, 28.98; Cl, 14.67. Found: N, 28.68; Cl, 14.82. Ostrogovich⁹ 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)].

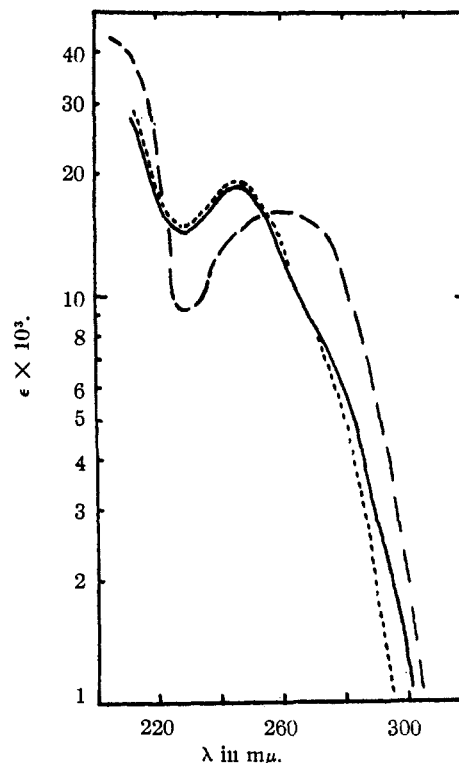


Fig. 1.—Spectrum of 4,6-diamino-2-phenyl-1,3,5-triazine monohydrochloride in — ethanol (95%) and in water, — — 0.01 N NaOH, ---- 0.01 N HCl.

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.

TABLE I

MAXIMA OF 4,6-DIAMINO-2-PHENYL-1,3,5-TRIAZINE		
Solvent	λ , in $m\mu$	$\epsilon \times 10^3$
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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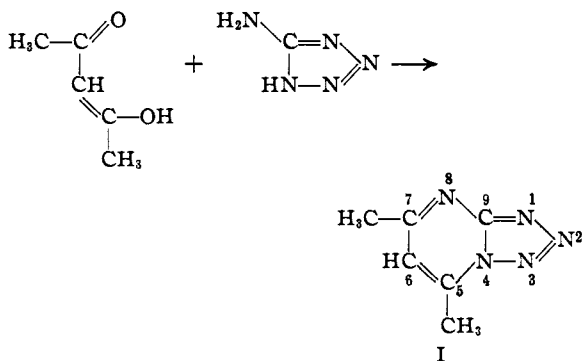
Absorption Spectra of 5,7-Dimethyltetrazolo(a)-pyrimidine

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.*, **43**, 4433 (1909).

ignated as above according to the system employed in the "Ring Index."² It has not been studied further since its preparation from 5-aminotetrazole and acetylacetone in the presence of piperidine, the method which was also employed in this work.³



From an examination of the spectra of 5,7-dimethyltetrazolo[a]pyrimidine shown in Fig. 1,⁴ a tremendous batho- and hyperchromic shift is to be noted in comparing the spectrum at pH 13 with that in neutral and acidic solutions. As the

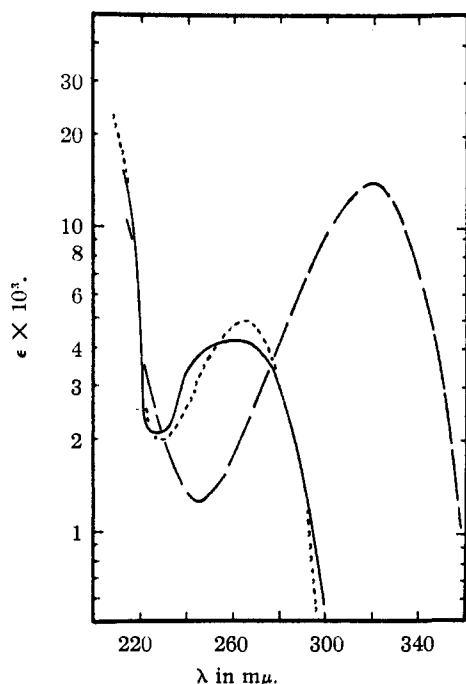


Fig. 1.—Spectra of 5,7-dimethyltetrazolo[a]pyrimidine in — ethanol (95%), ---- 0.01 *N* HCl, — 0.01 *N* NaOH.

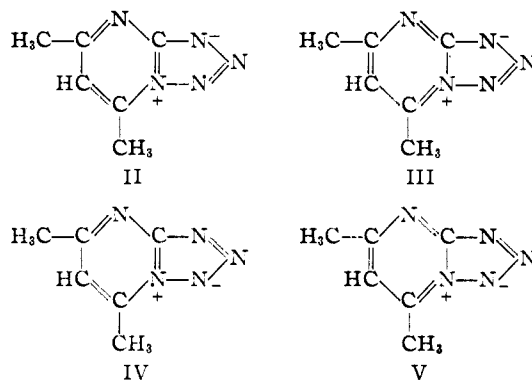
nitrogen atoms do not bear any hydrogen [atoms], a classical picture on the basis of tautomeric

(2) Patterson and Capell, "The Ring Index," Reinhold Publishing Corp., New York, N. Y., 1940.

(3) The authors wish to express their appreciation to Miss R. Pauline Brundage for her preparation of the compound.

(4) All spectral determinations were made with a Beckman quartz spectrophotometer, Model DU, Serial No. D-377, as in earlier work [cf. Ewing and Steck, *THIS JOURNAL*, **66**, 2181 (1946)].

shifts cannot be developed. However, if one admits ionic structures,⁵ this behavior can apparently be explained satisfactorily. The dipolar ions ("Zwitterions") shown in (II) to (V) contribute to the arrangement of the compound in acid, and, to a somewhat lesser extent, in neutral solution. These considerations would lead one to expect that the resulting spectrum, with respect to the position of the maximum, should be similar to that of a benzenoid ring with a conjugated double bond. Indeed, a measure of similarity to the spectra of styrene,⁶ indole,⁷ benzotriazole⁸ and even benzoxazole⁹ is observable. In alkaline medium, however, this polarization tendency, due to the addition of protons in position 1 or 3, disappears and the structure (I) is the only one remaining. Such a spectrum should more closely resemble that of a polyene and shift the absorption maximum toward the visible range. This is borne out by the similarity of the spectrum of 5,7-dimethyltetrazolo[a]pyrimidine in alkali with that of 1,3,5,7-octatetraene which was studied by Kovner¹⁰ and Hausser.¹¹ Both of the compounds have four conjugated double bonds and a "maximum extinction coefficient" beyond 300 $m\mu$.



(5) The authors are grateful to Dr. Elmer J. Lawson for his helpful discussion on the formation of dipolar ions.

(6) Elliott and Cook, *Ind. Eng. Chem., Anal. Ed.*, **16**, 20 (1944); Rodebush and Feldman, *THIS JOURNAL*, **68**, 896 (1946).

(7) Johnson, Bruce and Dutcher, *ibid.*, **66**, 2005 (1943).

(8) Specker and Gawrosch, *Ber.*, **75B**, 1338 (1942).

(9) Ramart-Lucas and Vantu, *Bull. soc. chim.*, [5] **146**, 1165 (1936).

(10) Kovner, *Acta Physicochim. (U.R.S.S.)*, **19**, 385 (1944). Cf. also Ferguson and Branch, *THIS JOURNAL*, **66**, 1467 (1944).

(11) Hausser, *Z. techn. Physik*, **15**, 10 (1934).

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Remarks on the Physico-Chemical Mechanism of Muscular Contraction and Relaxation

BY JACOB RISEMAN AND JOHN G. KIRKWOOD

The physico-chemical processes underlying the contraction and relaxation of muscle have been the subject of much speculation. Recently significant analogies between the elastic behavior of muscle and that of rubber and synthetic elastomers have