Electronic Spectra of Mono-, Di- and Tri-Azines of the Naphtalene Series.

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Summary. — The electronic absorption spectra of quinoline, isoquinoline, quinoxaline, phtalazine, quinazoline and cinnoline were taken. The bands are assigned to the different electronic transitions and for the $\pi - \pi^*$ transitions the experimental results for position and intensity were compared with values from theoretical calculation, to which they closely agreed.

The ultraviolet spectra of quinoline, isoquinoline and benzodiazines have been described by different authors (1) in different solvents, but a complete comparison of the spectra of all these molecules in the same conditions is still lacking. In the present paper the spectra in cyclohexane and in methanol of quinoline, isoquinoline, phtalazine, quinoxaline, quinazoline and cinnoline are presented, the bands are assigned to electronic transitions and the results are compared with positions and intensities predicted for the same electronic transitions by the Pariser and Parr's theory.

1. - Experimental procedure and results.

Materials: quinoline and isoquinoline were pure Eastman Kodak products purified by repeated distillation under vacuum; quinoxaline was a pure "Fluka".

product, m.p. 27.5 °C; all the other azines were prepared and purified in our laboratory; quinazoline from o-nitrobenzaldehyde according to J. D. Riedel (2) (m.p. 48.5 °C); phtalazine from o-phtalic aldehyde, according to Gabriel and Pinkus (3) (m.p. 91 °C); cinnoline according to Drake and Peck (4) (m.p. 38 °C). Eastman Kodak cyclohexane and methanol were used as solvent.

Spectra were obtained by the standard technique (5); the data are plotted in Fig. 1 to 6, as the log of the molar extinction versus wave length (in Å).

Wave lengths and molar extinctions of the observed bands are collected in Table I; the band origin is also indicated.


The Pariser and Parr approximation of the SCF LCAO MO method has proved to be useful in the interpretation and prediction of electronic absorption spectra of azines (2, 6). To test the soundness of our band assignment to electronic transitions a Pariser and Parr treatment was performed for all the molecules studied. The details of the calculations are not reported here, as the scheme followed was the same as in a previous work (5). Also the values for all the parameters were already known. The geometry of the molecules was assumed from data for pyridine, pyrimidine and pyrazine by Pariser and Parr (6), on the assumption that in our molecules the benzene ring is a regular hexagon with C-C bond distance equal to 1.39 Å. As starting orbitals naphtalene LCAO molecular orbitals were used (5).

Results are summarized in Table II.

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(2) P. Friedländer: *Fortschritte der Teerfarbenfabrikation*, 8, 1238 (1907).
(3) S. Gabriel and G. Pinkus: *Ber.*, 26, 2210 (1893).