

NOTES

The Absence of Hydrogen Bonding in Two Benzoic Acid Esters as Indicated by their Infrared Transmission

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An example of the well-known ortho effect is found in the compounds ethyl 2-methyl-5-isopropylbenzoate and ethyl 3-methyl-6-isopropylbenzoate, the former having about twice the reactivity¹ of the latter. One explanation of the effect ascribes the behavior of the benzoic acid esters to the possibility of hydrogen bonding either in the resting state² of the molecule or in the transition state.³ The availability of an infrared spectrometer made it convenient to check on the presence of hydrogen bonding in the resting state of the two molecules.

taken to observe any shift⁴ in the carbonyl frequency. However, this vibration appears to occur at the same wave length for both compounds, namely, 5.77 μ , and near the position customarily found. This we interpret as evidence of the absence of strong hydrogen bonding in the two compounds. In this connection a recent paper by Brown and Barbaras⁵ is of interest.

Experimental

Materials.—The two benzoic acid esters had been previously purified by Dr. C. T. Lester and Mr. Carroll Bailey¹ of the Department of Chemistry and to them we are indebted for the samples used.

Instrument.—The spectral measurements were made on a Perkin-Elmer infrared spectrometer Model 12-B using a Brown Instrument ink recorder. The data were obtained on a point by point basis from the ink trace which

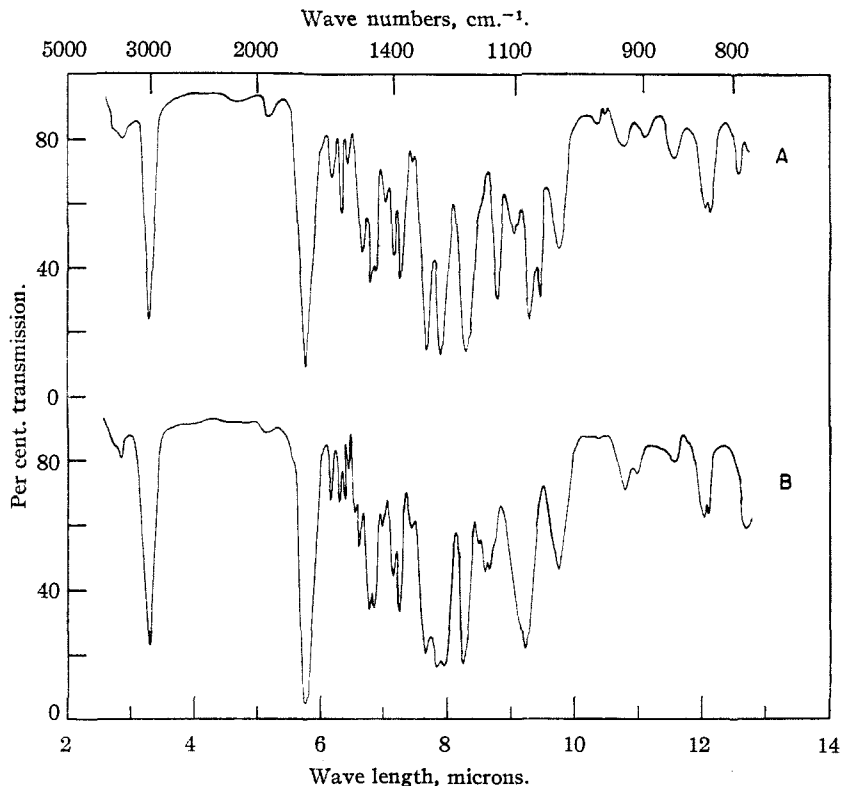


Fig. 1.—Infrared transmission curves: A, ethyl 3-methyl-6-isopropylbenzoate; B, ethyl 2-methyl-5-isopropylbenzoate.

The per cent. transmission of liquid films of the compounds about 0.002 cm. thick was measured from two to thirteen microns. The results are shown in Fig. 1. It is seen that the transmission curves are essentially alike. Particular care was

gave transmission with the sample out of the beam and transmission with the sample in the beam. At 6 microns data were also taken on a point by point basis using a galvanometer and scale method.

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EMORY UNIVERSITY, GEORGIA RECEIVED APRIL 28, 1948

(1) Lester and Bailey, *THIS JOURNAL*, **68**, 375 (1946).
(2) Sidgwick and Callow, *J. Chem. Soc.*, **125**, 527 (1924).
(3) Watson, "Modern Theories of Organic Chemistry," Oxford University Press, New York, N. Y., 1941.

(4) Gordy, *J. Chem. Phys.*, **8**, 518 (1940).

(5) Brown and Barbaras, *THIS JOURNAL*, **69**, 1137 (1947).