

Infrared Absorption Spectrum of Heavy Acetic Acid

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Infrared Absorption Spectrum of Heavy Acetic Acid

The infrared absorption spectrum of acetic acid-*d* (CH_3COOD) vapor has been investigated in the region 1–15.5 μ by means of a rocksalt spectrometer, previously described in the literature.¹ This investigation was undertaken with the aim of bringing out the hydrogen bond frequency by a deuterium substitution. It is well known that acetic acid vapor at room temperature exists mostly as double molecules, the bonding occurring through the mechanism of "hydrogen bridges." According to current ideas,² the hydrogen bonded O–H frequency is shifted from 2.75 μ into the region of the C–H valence vibrations at 3.3 μ and cannot be clearly discerned. In heavy acetic acid this frequency will be shifted approximately by a factor of $\sqrt{2}$ and will lie in a region usually unoccupied by absorption bands (4.3 μ). That this is so, is clearly brought out by the curves in Fig. 1, and Table I which gives the

TABLE I.

3079 \pm 40 cm^{-1}	1389 \pm 10 cm^{-1}	1000 \pm 5 cm^{-1}
2325 \pm 20	1317 \pm 10	840 \pm 5
2105 \pm 15	1250 \pm 10	667 \pm 20
1725 \pm 15	1056 \pm 5	

positions of the band centers. It is of interest to note that the C–H valence frequency appears only weakly. This fact suggests a possible interpretation of the broad and deep absorption at 3.25 μ in light acetic acid as being chiefly due to the hydrogen bond vibration.

Raman spectra of liquid CH_3COOD ^{3,4} show no lines in the region 1655 to 2940 cm^{-1} , thus making impossible a complementary study in the Raman effect.

Our sample of heavy acetic acid was prepared by reacting

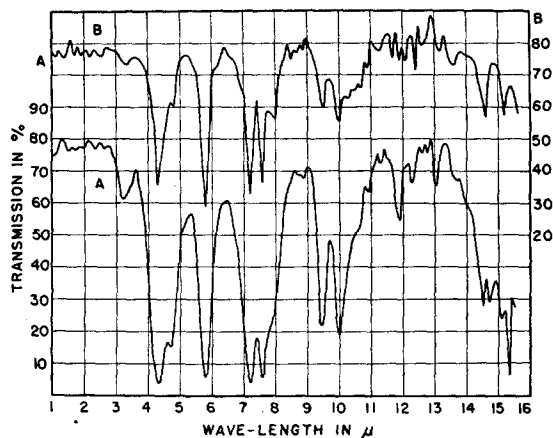


FIG. 1. Absorption spectra of CH_3COOD . Curve A, pressure 15.5 mm, temperature 24°C; curve B, pressure 4 mm, temperature 24°C. Absorption cells 15 cm in length.

pure acetyl chloride with 99.6 percent heavy water by a method previously employed by Engler.⁴

Further experiments are now in progress to determine how association through the deuterium bond is affected by temperature.

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Princeton University,
Princeton, New Jersey,
December 17, 1937.

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R. HOFSTADTER

¹ Barnes, Brattain and Seitz, *Phys. Rev.* **48**, 582 (1935).

² Badger and Bauer, *J. Chem. Phys.* **5**, 839 (1937).

³ W. R. Angus, A. H. Leckie and C. L. Wilson, *Proc. Roy. Soc. Lond.* **155**, 183 (1936).

⁴ W. Engler, *Zeits. f. physik. Chemie* **B32**, 471 (1936).