

Ramsay D A. Intensities and shapes of infrared absorption bands of substances in the liquid phase. *J. Amer. Chem. Soc.* 74:72-80, 1952.
[Division of Chemistry, National Research Council, Ottawa, Canada]

Three methods are described for determining the true integrated absorption intensity of an infrared absorption band of a liquid using a spectrometer with moderate resolving power. Assuming a Lorentz curve for the true band shape and a triangular slit function, tables are presented to assist the experimental application of these methods. [The SC1[®] indicates that this paper has been cited in over 575 publications since 1961.]

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"This paper and its companion¹ were essentially the last papers I wrote on infrared spectra before switching my activities in 1949 to high resolution studies of the electronic spectra of simple molecules and free radicals.

"The work commenced in 1947 when I arrived at the National Research Council in Ottawa, Canada, from the University of Cambridge, England. I had just completed my doctoral thesis under the supervision of G.B.B.M. Sutherland (later Sir Gordon). I started work in the Division of Chemistry with R. Norman Jones who had an interesting project on the infrared spectra of steroids. Norman, together with many others, had obtained the infrared spectra of about 400 steroids and had shown that the stretching frequency of the carbonyl group was characteristic of the position of this group in the steroid ring system.² This work was part of a collaborative project with Konrad

Dobriner of the Sloan-Kettering Institute for Cancer Research in New York. The steroid fractions of urine samples from cancerous and noncancerous patients were separated by chromatographic columns and were analysed by infrared spectroscopy. The resulting histograms were correlated in the hope that some clue might be found concerning the origin of cancer.

"I was impressed by the specificity of the carbonyl correlations and wondered if intensities might add any useful information. Measurements of infrared intensities in the gas phase by different workers at that time frequently yielded values for a given band differing by an order of magnitude. These discrepancies were largely caused by the use of spectral slit widths which were much larger than the individual line widths. Wilson and Wells³ had just produced an interesting paper suggesting that these difficulties could be minimized by pressure-broadening the lines and using certain extrapolation procedures.

"I studied the shapes of infrared bands of liquids and solutions and satisfied myself that the rotational structure was quenched and that isolated bands could be fitted by Lorentz curves. Since the slit widths which I used were still comparable to the widths of the bands under study, corrections had to be made for the use of finite resolving power. I adopted a triangular slit function and constructed tables by which 'true' Lorentz curves could be obtained from 'apparent' Lorentz curves, knowing the experimental parameters. All these calculations were performed using a hand calculating machine.

"Like many other authors, I do not consider that this paper is my most important contribution to the literature. Its popularity is presumably connected with the fact that it discusses general methods and contains useful tables. It was interesting to read it again after a lapse of 30 years."

1. Jones R N, Ramsay D A, Keir D S & Dobriner K. The intensities of carbonyl bands in the infrared spectra of steroids. *J. Amer. Chem. Soc.* 74:80-8, 1952.
2. Jones R N, Humphries P & Dobriner K. Studies in steroid metabolism. IX. Further observations on the infrared absorption spectra of ketosteroids and steroid esters. *J. Amer. Chem. Soc.* 72:956-61, 1950.
3. Wilson E B, Jr. & Wells A J. The experimental determination of the intensities of infra-red absorption bands. I. Theory of the method. *J. Chem. Phys.* 14:578-80, 1946. (Cited 160 times.)