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(*Terms expire June 30, 1953*)

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Punched-Card Bibliography of Infrared Spectra

ONE of the newer developments in the field of chemistry is the widespread application of the techniques of infrared spectroscopy to chemical problems. Not only are the infrared spectra of chemical compounds useful analytical tools, but they also provide important information on the molecular forces that determine chemical properties.

With the rapid growth of information on the infrared absorption of chemical compounds, workers in the field have been faced with the problem of quickly gaining access to the results obtained by others. About 500 papers a year are now being added to the already large supply of available literature on the subject. In general, this literature is widely scattered, because papers dealing with instrumental advances, calculation of structure, techniques of sample handling, and analytical procedures appear in separate journals. Yet, because of its incidental application as a special technique in many fields, the presence of infrared in a publication often fails to be indicated in any index.

Moreover, each laboratory that uses infrared techniques requires a large library of infrared spectra as an aid in qualitative identification and empirical determination of structure. This has caused a vast duplication of effort, particularly in the collection and purification of the chemical compounds involved. And, once the data have been obtained, the charts produced by automatic recording spectrometers are so large as to require special indexing and storage facilities.

To meet these problems, a comprehensive punched-card catalogue of all available data on the infrared spectra of organic and inorganic compounds is being set up by the National Bureau of Standards under the sponsorship of the National Research Council's Committee on Spectral Absorption Data. The card catalogue not only fills the pressing need for a general reference library of infrared spectra but also provides a survey of the literature on each compound, abstracts of the papers covered, and other useful data. By means of the punched cards, the reported spectra of many compounds can be quickly found, the more important chemical linkages associated with a given spectral line can be determined, the work of any given author can be quickly assembled, and the properties of a compound that will aid in its identification can be located without loss of time.

The use of punched cards as an indexing medium has several advantages. In addition to an enormous capacity for storing data, they are well adapted to cross-indexing. Two kinds of cards are available: the machine-sorted and the edge-punched, hand-sorted type. Each of these may be used to supplement the other. Thus, a set of edge-punched cards may serve as a small "working file" containing all the spectra normally encountered in a given laboratory; this file can be kept close at hand and readily sorted with a needle. On the other hand, a larger "reference file" of the more unusual compounds can be more easily handled—especially if it is voluminous—by using machine-sorted cards of the type recently designed by L. E. Kuentzel, of Wyandotte Chemicals Corporation.

A bibliography of between 9000 and 10,000 infrared references has been contributed by the National Bureau of Standards and is being kept current with the aid of a group of volunteer abstracters. A search of approximately half these references has yielded a file of about 7500 compounds. As infrared spectra are contributed by cooperating laboratories, the applicable literature references accumulated to date are tabulated on the cards, which are then printed, slotted, and sold at cost. (Detailed instructions for ordering may be obtained from the National Bureau of Standards, Washington 25, D. C.) Efforts are now being made to extend the present coverage to the visible and ultraviolet regions, as well as to the infrared.

E. CARROLL CREITZ

NRC Committee on Spectral Absorption Data
National Bureau of Standards

SCIENCE, founded in 1880, is published each Friday by the American Association for the Advancement of Science at the Business Press, 10 McGovern Ave., Lancaster, Pa. Entered as second-class matter at the Post Office at Lancaster, Pa., January 13, 1948, under the Act of March 3, 1879. Acceptance for mailing at the special rate postage provided for in the Act of February 28, 1925, embodied in Paragraph (d-2) Section 34.40 P. L. & R. of 1948.

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Annual subscriptions, $7.50; single copies, $.25; foreign postage, outside the Pan-American Union, $1.00; Canadian postage, $.50. Special rates to members of the AAAS.

The AAAS also publishes THE SCIENTIFIC MONTHLY. Subscription and advertising rates on request.

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