
**FIRST SUPPLEMENT TO
MOLECULAR FORMULA LIST OF
COMPOUNDS, NAMES, AND
REFERENCES TO
PUBLISHED INFRARED SPECTRA**



**Published by the
AMERICAN SOCIETY FOR TESTING AND MATERIALS
1916 Race St., Philadelphia 3, Pa.**

ASTM Special Technical Publication No. 331 A

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Indexed by the Wyandotte-ASTM (Kuentzel) Punched-Card Index



Reg. U.S. Pat. Off.

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This book is the first in a series of supplements to STP No. 331, "Molecular Formula List of Compounds, Names, and References to Published Infrared Spectra." It is designed to keep abreast of the increasing number of published infrared spectra. This issue lists the compounds whose spectra were included in the Tenth Supplement to the Infrared Data Index of the Wyandotte-ASTM Punched-Card Index; it also covers all compounds whose near-infrared and far-infrared spectra have been so indexed. Of the 13,942 spectra listed, 2221 are near-infrared and 2055 are far-infrared.

All codes and conventions used in STP 331 apply to this supplement. The final letter of the serial number designates the spectral range of the spectrum involved, thus;

- A—Regular infrared, 2 to 16 μ
- H—Near-infrared, 0.7 to 3.6 μ
- G—Far-infrared, 11 to 36 μ

The penultimate letter indicates the source of the spectra as listed in STP 331, except that the following, which were inadvertently omitted originally, should be added:

- E—Abstracted from the literature by ASTM-sponsored groups. Journal and book references for these spectra will be found in an appendix to this book (page 101).

Also, for near-infrared spectra only, final letter H, the following penultimate letters and sources apply:

- C—Anderson Physical Laboratories, 609 South Sixth Street, Champaign, Illinois
- N—Sadler Research Laboratories, 1517 Vine Street, Philadelphia 2, Pa.

Additions to the categories of commercial spectra published by the Sadler Research Laboratories, serial number letters CA, make it necessary to expand the list of prefix codes as

assigned by the publisher. Following are the code letters and categories currently being used:

- A—Agricultural chemicals
- B—Polyols
- C—Surface-active agents
- D—Monomers and polymers
- E—Plasticizers
- F—Perfumes and flavors
- G—Waxes and derivatives
- J—Elastomers and rubbers
- K—Fibers
- L—Solvents
- M—Intermediates
- N—Inorganic
- P—Petroleum chemicals
- Q—Natural resins and gums
- R—Pharmaceuticals
- S—Steroids
- T—Textiles
- U—Food additives
- X—Pigments, dyes, stains
- Y—Rubber chemicals

Molecular formula listings connected with regular infrared, near-infrared and far-infrared spectra appear in separate sections of this book. Listings for regular infrared spectra, final letter A, begin on page 1, for near-infrared spectra, final letter H, the listing begins on page 74 and for far-infrared spectra, final letter G, the list begins on page 87. At the end of each section are listed, in alphabetical order of the names, those organic compounds for which no molecular formulas were available; inorganic compounds are also noted. For all compounds with penultimate letter E in the serial number of their spectra (abstracted spectra), one may find journal and book references to the original published data in an appendix beginning on page 101. Here again, serial number lists for regular infrared, near-infrared and far-infrared spectra are separate. Serial number reference lists for regular

infrared spectra begin on page 102, far-infrared spectra on page 105 and near-infrared spectra on page 107.

With this supplement, the total number of infrared spectra now included in the molecular formula listings is 57,442. However, the actual number of infrared spectra in the current complete Wyandotte-ASTM Punched-Card Index (including ten supplements) is only 55,655. The discrepancy arises because of the deletion of a sizeable number of spectra (and cards) from the system at the request of publishers and the fact that a block of Sadtler infrared spectra was included both in STP No. 331 and STP No. 331A. This was done purposely so that this supplement could list everything in the *Tenth Supplement to the Infrared Data Index*, even though some of the spectra were included in the first publication. When supplements to this molecular formula list are eventually combined with the parent

issue and a new combined listing made available, these discrepancies will be eliminated.

Material for this book was processed at the Wyandotte-ASTM Punched-Card Project, Wyandotte Chemicals Corp., Wyandotte, Mich. and acknowledgment is made of the donation, by the Corporation, of computer time for this purpose. Errors found in the listing should be reported to:

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Orders for index books and punched cards should be directed to:

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