

A black line drawing of an infrared spectrum is overlaid on the red background. It features several sharp absorption bands of varying widths and depths, characteristic of a complex organic molecule. The bands are distributed across the visible range of the spectrum.

**MOLECULAR FORMULA  
LIST**

**OF COMPOUNDS, NAMES,  
AND REFERENCES TO  
PUBLISHED  
INFRARED SPECTRA**

**AMD 31**



**AMERICAN SOCIETY FOR TESTING AND MATERIALS**

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

**An Index to 92,000 Published  
Infrared Spectra**

**AMD 31**

**List price \$50.00**



**AMERICAN SOCIETY FOR TESTING AND MATERIALS**

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## P R E F A C E

The Molecular Formula List of Compounds, Names, and References includes the 92,000 compounds whose infrared spectra have been indexed by the ASTM Spectral Data System as issued through the thirteenth supplement. The serial numbers provide a reference to the location of the original infrared spectra as published in the literature or in standard catalogs of spectra. Serial numbers are the same as those assigned by the several publishers, and the added letters have the following significance:

1. Final letters indicate the spectral range, thus:

A—Infrared, 2 to 16  $\mu$

G—Far Infrared, 11 to 36  $\mu$

2. Penultimate letters indicate the source of spectra, thus:

A—American Petroleum Institute, Research Project 44, Chemistry Department, Agricultural and Mechanical College of Texas, College Station, Texas. 77843

C—The Sadtler Research Laboratories, 3314-20 Spring Garden Street, Philadelphia, Pa. 19104

D—NRC-National Bureau of Standards Committee on "Spectral Absorption Data," National Bureau of Standards, Washington, D. C. 20234

E—Spectra abstracted from the literature.

F—Documentation of Molecular Spectroscopy, Butterworth Scientific Publications, London WC2.

G—Coblentz Society, Spectra available from the Sadtler Research Laboratories, 3314-20 Spring Garden Street, Philadelphia, Pa. 19104

H—Manufacturing Chemists Association Research Project, Chemistry Department, Agricultural and Mechanical College of Texas, College Station, Texas. 77843

J—Infrared Data Committee of Japan, Sanyo Shuppan Boeki Co., Inc., Hoyo Building, 8, 2-chome, Takaracho, Chuo-ku, Tokyo, Japan.

3. Prefix letters have special meanings assigned by the publishers. For those serial numbers issued by the Sadtler Laboratories, the prefix letters have the following significance:

A—Agricultural Chemicals

B—Polyols

C—Surface Active Agents

D—Monomers and Polymers, Resins and Gums, Pyrolyzates

E—Plasticizers

F—Perfumes and Flavors

G—Fats, Waxes, and Derivatives

H—Lubricants

J—Rubber Chemicals

K—Fibers

L—Solvents

M—Intermediates

P—Petroleum Chemicals

R—Pharmaceuticals

S—Steroids

T—Textile Chemicals

U—Food Additives

W—ATR's

X—Dyes, Pigments, and Stains

Y—Inorganics

Also, for those serial numbers issued by the Documentation of Molecular Spectroscopy, the prefix "A" is for inorganic compounds.

The names of the compounds are those provided by the authors. These have been rearranged to provide an index name according to the inversion naming system used by Chemical Abstracts. The printed listing is limited to standard IBM characters, digits, and letters. Among these, a slanting line serves as a parenthesis and bracket marks, and the letters PR indicate a prime mark. Greek letters are either spelled out or represented by English equivalents. Obvious abbreviations as C for Cis, T for Trans, O for Ortho, M for Meta, P for Para, D for Dextrorotary, L for Levorotary, N for Normal, etc. should offer no difficulties.

The book consists of three sections: the Molecular Formula List for Infrared and Far-Infrared Spectra; the Organic and Inorganic

Alphabetical List for Infrared and Far-Infrared Spectra; and the References for Abstracted Infrared and Far-Infrared Spectra. The infrared and far-infrared spectra are together in all sections.

The first section is arranged in numerical order according to the number of atoms in the molecular formula. Vertical columns of digits record the numbers of atoms involved in increasing numerical order. The series of digits on a given line indicates the numbers and kinds of atoms in the molecular formula of the compound listed on that same line. The positions of molecular formulae in the list are determined by the number of atoms of elements based on carbon and ordered from right to left in increasing number down the page. Elements other than those given are ignored. This includes Deuterium.

The second section contains a list of organic compounds with unknown molecular formulae (or whose formulae were not supplied by the authors) and inorganic compounds in alphabetical order.

The third section of the book contains a list, in serial number order, of the infrared and far-infrared spectra that have been abstracted from the general literature. These abstracted spectra are characterized by the penultimate letter "E" in their serial numbers. Journal or book references to the original published data are given in the right hand column.

Since the list indexes all published infrared and far-infrared spectra, there are many cases where several references for the same compound are given. This offers the user the opportunity of selecting the most readily available and reliable reference for the spectrogram of a compound or of selecting several spectra for comparative purposes.

The spectral and chemical data from which this list is prepared are coded by subcontractors and volunteer members of Subcommittee III on Reference Data of ASTM Committee E-13 on Molecular Spectroscopy.

Use has been made of CODEN\* for the journal references. This is a five letter code assigned to each journal title that permits a shortened reference designation. The complete titles and related CODEN used in this list are given at the back of this book or may be found in ASTM DS23, "CODEN for Periodical Titles", Volumes 1 and 2. Each CODEN is followed by a volume number, page number, and finally the last two digits of the year. Books are coded by the first eight letters of the author's name, followed by a code for the publisher, the page number, and then the last two digits of the year of publication.

Supplements to this publication will be issued periodically to cover new spectra added to the file. This book provides an excellent source of references to the published literature of infrared spectra and should find ready use in any infrared laboratory. Questions, comments, and reported errors should be directed to:

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ORDERS should be directed to:

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\*The CODEN was originated by Dr. Charles Bishop of the University of Buffalo, Department of Medicine, Buffalo, N. Y.

