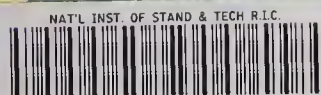


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Malcolm W. Chase and Joan C. Sauerwein, Editors

Standard Reference Data  
National Institute of Standards and Technology  
Gaithersburg, MD 20899

February 1992  
Supersedes NIST Special Publication 782, 1991 Edition



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## **ABSTRACT AND KEY WORDS**

The National Institute of Standards and Technology's (NIST) Standard Reference Data Program provides reliable, well-documented data to scientists and engineers for use in technical problem-solving, research, and development. This catalog lists published data compilations and current databases in the Standard Reference Database Series. This edition of the catalog contains many new databases and updates current ones. These data compilations have been subdivided into eight categories. Prices and ordering information are located at the back of the document.

Key words: atomic physics; chemistry; compilations; databases; evaluated data; materials; numeric data

## PREFACE

The formal existence of the National Standard Reference Data System dates from 1963, when the Federal Council for Science and Technology asked the then-National Bureau of Standards (now NIST) to assume primary responsibility in the Federal Government for promoting and coordinating the critical evaluation of numerical data in the physical sciences. The program was conceived as a decentralized national effort with financial support coming from a variety of government and private sources, but with NBS responsible for the overall planning and coordination. In 1968 Congress provided a specific legislative mandate for the program through passage of Public Law 90-396, the Standard Reference Data Act. This Act states the policy of Congress to make reliable reference data available to scientists, engineers, and the general public.

The Standard Reference Data Program has been providing evaluated, high-quality data for a wide range of applications to industry, government, and academic institutions for over twenty-eight years. Standard reference data has been utilized to improve design efficiency of chemical processes, identify potentially toxic substances in the environment, improve materials durability, and calculate performance of chemical reactors, to name but a few applications. With the present availability of the personal computer at every scientist's fingertips, standard reference data is even more accessible and will play an even more critical role in the future. With this, the third annual Standard Reference Data Products Catalog, we hope to make the scientific community more aware of our highly evaluated, high quality data in all of its many forms.



*The SRD Program provides evaluated data which are vital to industry.*







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## INTRODUCTION

The NIST Standard Reference Data (SRD) Program provides reliable, well-documented reference data to scientists and engineers for use in technical problem solving, research, and development.

Experts in the physical, chemical, and materials sciences critically evaluate data that result from experimental measurements, calculations, and theory. The evaluations are carried out through a network of data centers, projects, and cooperative programs that comprise the National Standard Reference Data System (NSRDS). Experienced researchers in each area assess the accuracy of the data, prepare compilations, and recommend best values. The outputs are widely distributed as publications and computer-readable databases.

Current activities in the Standard Reference Data Program are carried out in long-term data centers, located primarily at NIST, and numerous short-term projects, primarily at universities and industrial research centers. In addition, the Program maintains many long-term collaborations on cooperative data programs which draw support from both industry and other government programs.



*The Standard Reference Data booth appears at many scientific conferences and meetings.*

The activities concentrate in the following disciplines:

***Analytical Chemistry*** — mass spectral, surface analysis, crystallographic, and electron diffraction data for chemical identification.

***Atomic Physics*** — atomic energy levels, transition probabilities and collision data used for diagnostics, wavelengths, and modeling.

***Biotechnology*** — data on important groups of molecules, such as lipids, and biological macromolecules, such as proteins, nucleic acids, and viruses.

***Chemical Kinetics*** — rate data on gas-phase reactions.

***Materials Properties*** — structure and characterization of materials, performance properties, including tribology and mechanical corrosion, and phase equilibria.

***Molecular Structure and Spectroscopy*** — evaluated molecular data at microwave and infrared frequencies and, for transient molecules, vibrational and electronic energy levels.

***Thermodynamics and Thermochemistry*** — reliable, widely-used tables of organic and inorganic species.

***Thermophysical Properties of Fluids*** — thermophysical and transport properties of pure and mixed fluids, including refrigerants, that are of great importance to industry.

*Dr. Malcolm W. Chase is  
Chief of the Standard  
Reference Data Program.*





The data collections resulting from this work are disseminated in different ways:

***National Standard Reference Database Series*** — Databases on diskettes, magnetic tapes, and online systems.

***Journal of Physical and Chemical Reference Data*** — A bimonthly Journal published jointly with the American Chemical Society and the American Institute of Physics.

***Other publications*** — Journal and books published with technical society and private publishers.



*The Standard Reference Data Distribution Group (l to r) Cheryl Williams, Joan Sauerwein, and Sherena Johnson, market and distribute SRD databases.*

When ordering an SRD database, checks, purchase orders, Visa, and Mastercard are accepted. Orders can be placed by phone or FAX for quick turn-around. For further information on SRD databases, please contact:

**Joan Sauerwein  
Standard Reference Data  
National Institute of Standards and Technology  
Bldg. 221/Room A320  
Gaithersburg, MD 20899  
(301) 975-2208  
879-2208 (FTS)  
(301) 926-0416 (FAX)**

# STANDARD REFERENCE DATABASES

## ANALYTICAL CHEMISTRY

NIST/EPA/NIH Mass Spectral

NIST/EPA/NIH Mass Spectral: PC Version

NIST Mass Spectral Database of Common Compounds

NIST Crystal Data Identification

NIST/Sandia/ICDD Electron Diffraction

NIST X-Ray Photoelectron Spectroscopy

NIST/NIH Desktop Spectrum Analyzer Program and X-Ray Database

*The SRD Data Systems Development Group  
(seated l to r) Phoebe Fagan, Shari Young,  
(standing l to r) Dorothy Bickham, Gerry Dalton,  
and Mary Dal-Favero,  
programmers of SRD databases.*



## ATOMIC PHYSICS

NIST Electron and Positron Stopping Powers of Materials

NIST X-Ray and Gamma-Ray Attenuation Coefficients and Cross Sections

NIST Atomic Transition Probabilities Data Files

NIST Spectroscopic Properties of Atoms and Atomic Ions

## **STANDARD REFERENCE DATABASES *(continued)***

### **BIOTECHNOLOGY**

NIST/CARB Biological Macromolecule Crystallization

NIST Lipid Thermotopic Phase Transition

### **CHEMICAL KINETICS**

NIST Chemical Kinetics

### **MATERIALS PROPERTIES**

NACE/NIST Corrosion Performance

NIST Tribomaterials I (ACTIS)

NIST Structural Ceramics

Phase Diagrams for Ceramists

### **MOLECULAR STRUCTURES AND SPECTROSCOPY**

NIST Vibrational Electronic Energy Levels of Small Polyatomic Transient Molecules

### **THERMODYNAMICS AND THERMOCHEMISTRY**

NIST Chemical Thermodynamics

DIPPR Data Compilation of Pure Compound Properties

Student Version of DIPPR Data Compilation of Pure Compound Properties

NIST JANAF Thermochemical Tables

NIST Estimation of Thermodynamic Properties for Organic Compounds at 298.15 K  
Part I. Hydrocarbons

NIST Positive and Negative Ion Energetics

NIST Structures and Properties Database and Estimation Program

NIST Molten Salts

NIST Thermodynamic Properties of the Elements



## STANDARD REFERENCE DATABASES *(continued)*

### THERMOPHYSICAL PROPERTIES OF FLUIDS

NIST Thermophysical Properties of Hydrocarbon Mixtures

NIST Thermophysical Properties of Water

NIST Thermophysical Properties of Fluids

NIST Mixture Property Program

NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures



*The Bedford Composition Group — Judy Calabrese (l) and Connie Seymour, electronic typesetters for the Journal of Physical and Chemical Reference Data.*

### NIST Special Databases

NIST Binary Images of Printed Digits, Alphas, and Text

NIST Structured Forms Reference Set of Binary Images



## ANALYTICAL CHEMISTRY

In the field of analytical chemistry, the SRD Program provides a set of comprehensive, easy-to-use databases and printed data compilations that help the analytical chemist identify unknown materials, and in many cases, once identified, avoid the need to recharacterize a substance. SRD databases cover a wide range of analytical techniques, including mass spectrometry, x-ray spectrometry, surface analysis, and single crystal and electron diffraction.

To reach the greatest possible audience, the data collections are offered in several formats: as PC diskettes, on magnetic tape for inclusion in in-house laboratory systems, as incorporated into instruments themselves, and via online database systems.

In every case, the data have been fully evaluated using a variety of techniques. When appropriate, duplicate measurements have been included for completeness. All the databases are updated on a regular basis. The PC diskette versions of these databases include easy-to-use interfaces that can be mastered quickly and without having to resort to large manuals.

The NIST/EPA/NIH Mass Spectral Database continues to reach an ever-widening audience as it is improved and expanded and stands alone as the only database which fulfills EPA requirements for use in characterizing "tentatively identified compounds." This year it has undergone a major evaluation assessment program with an emphasis on including only the highest quality spectra in the database.

The brand-new NIST/NIH Desktop Spectrum Analyzer Program and X-Ray Database performs rapid yet detailed generation, interpretation, and analysis of x-ray spectra and is creating great interest in the microbeam analytical community.

## **SRD Analytical Chemistry Databases**

### **Mass Spectra**

NIST/EPA/NIH Mass Spectral Database

NIST/EPA/NIH Mass Spectral Database: PC Version

NIST Mass Spectral Database of Common Compounds

### **Surface Data**

NIST X-Ray Photoelectron Spectroscopy Database

### **Diffraction Data**

NIST/Sandia/ICDD Electron Diffraction Database

NIST Crystal Data Identification

### **Spectrum Analysis**

NIST/NIH Desktop Spectrum Analyzer Program and X-Ray Database

## **SRD Major Publications in Analytical Chemistry**

The Wiley/NBS Registry of Mass Spectral Data

Crystal Data Determinative Tables (6 vols.)

Elemental and Interplanar Spacing Index

# ANALYTICAL CHEMISTRY DATABASES

## 1. NIST/EPA/NIH Mass Spectral Database 1992 Version



**Sharon G. Lias**  
**Mass Spectrometry Data Center**  
**National Institute of Standards**  
**and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-2562**

The database contains ionization mass spectra of well over 60,000 different compounds. Each spectrum has a "quality index" associated with it, the Chemical Abstracts Service (CAS) name, synonyms, the molecular weight and formula, and the CAS Registry Number. Structures are included for 97 percent of the spectra. Categories of substances identified are steroids, alkaloids, drugs, derivatives, amino acids, metals, carbohydrates, fatty acids and lipids, pesticides, and primary pollutants. This is the only database which fulfills EPA requirements for use in characterizing "tentatively identified compounds."

This new updated version has undergone a major data evaluation assessment program with retention of only the highest quality spectra available. A new auxiliary file has been added with replicate spectra.

This database is available as a magnetic tape, both in an ASCII and a Binary Version. It is widely used in the mass spectrometers of many commercial instrument manufacturers.

**To order JPCRD issues, reprints, or monographs:**  
**Call (202) 872-4405**



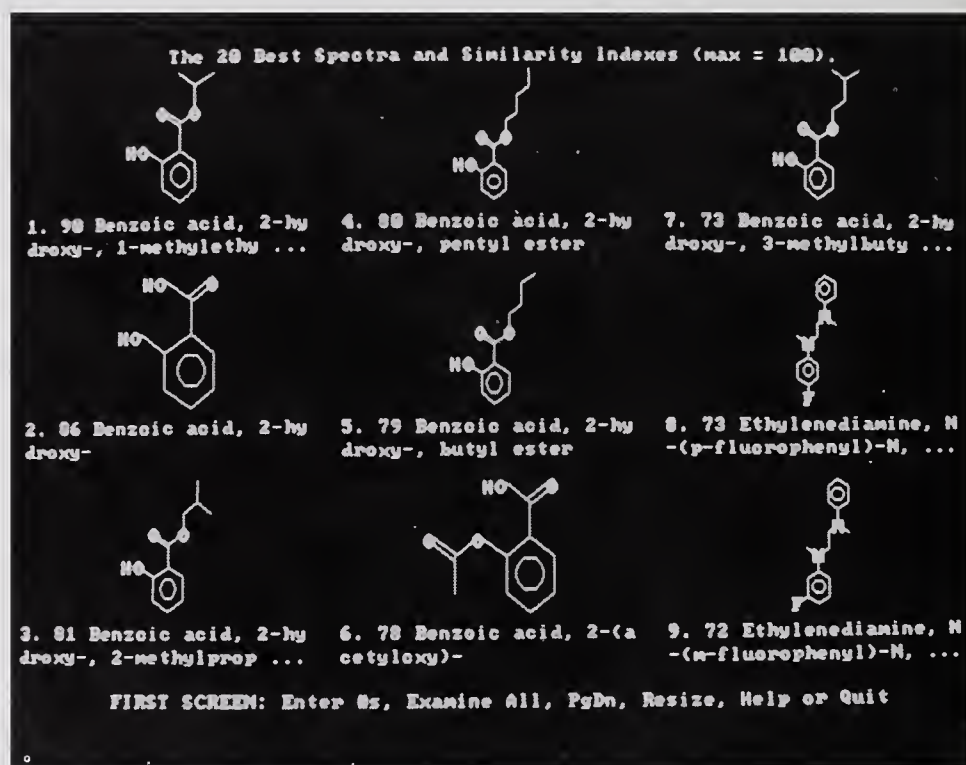
# 1A. NIST/EPA/NIH Mass Spectral Database PC Version 4.0



Stephen E. Stein  
Mass Spectrometry Data Center  
National Institute of Standards  
and Technology  
Gaithersburg, MD 20899  
(301) 975-2505

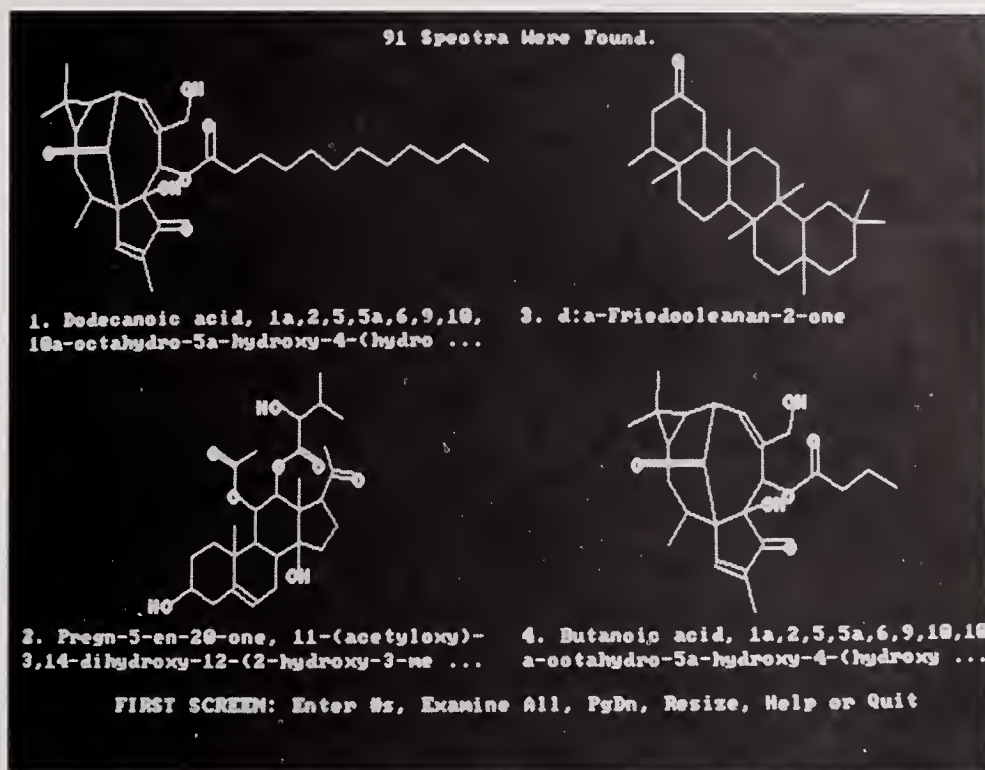
The PC Version of the NIST/EPA/NIH Mass Spectral Database was released in September 1987. Version 2.0 was released in December 1988, and Version 3.0 was released in June 1990. The new Version 4.0 consists of well over 60,000 electron ionization mass spectra (with structures for almost all compounds), various index files for rapid data retrieval, and related software for searching the database in various ways. A quickly-learned interface allows the database to be searched by:

- identification number
- CAS Registry Number
- chemical name  
(including tens of thousands of alternative names)
- molecular formula
- molecular weight
- any peaks (up to 10 peaks with an intensity range for each)
- major peaks (up to 3 ordered peaks)
- your spectrum (choose quick, standard, or extensive search options)
- neutral losses



*The 1992 version has undergone a major data evaluation program. Only the highest quality spectra are retained in the database.*





Various display features are available:

- masses of major peaks
- expand scale
- autoscale
- dump to laser or dot matrix printer
- difference plots
- spectrum scrolling

*The new version has well over 60,000 electron ionization mass spectra; almost all compounds have structures included.*

This important PC database provides a powerful tool for locating a particular spectrum or for identifying spectra of unknown compounds. Regular and frequent updates are planned. It comes on both 5¼" and 3½" high density diskettes. It can also be used on Macintosh computers which have a PC emulator program. A CD ROM version is available from Aldrich Chemical Company, Inc.

## 1B. NIST Mass Spectral Database of Common Compounds

Stephen E. Stein  
Mass Spectrometry Data Center  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-2505

This version has the same rapid, sophisticated search software as the full database, but contains a smaller number of spectra, thus requiring only a fraction of the disk space needed for the full version. The data set has 10,330 spectra for important commercial compounds, as well as compounds of environmental or pharmaceutical interest. It comes on both 5¼" and 3½" high density diskettes. It can also be used on Macintosh computers which have a PC emulator program.

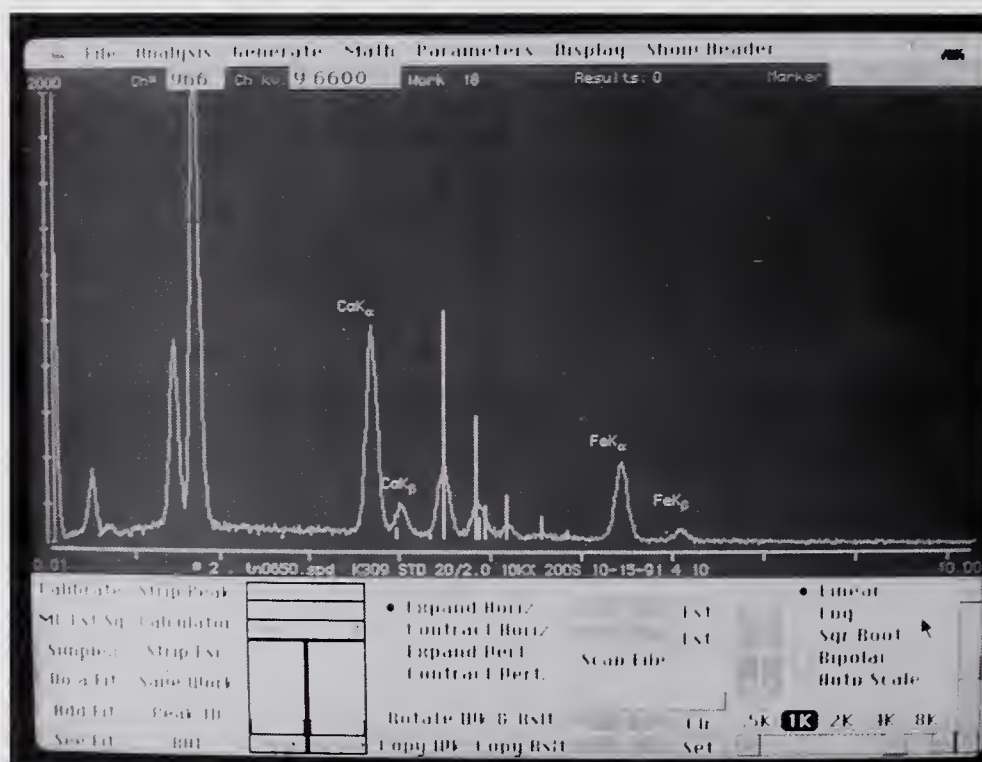
## 36. NIST/NIH Desktop Spectrum Analyzer Program and X-Ray Database



**Charles E. Fiori**  
**Surface and Microanalysis**  
**Sciences Division**  
**National Institute of Standards**  
**and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-3926**

This computer program performs rapid yet detailed generation, interpretation, and analysis of x-ray spectra.

The program provides all of the usual multichannel analyzer features, including extensive KLM markers, ten 8192 channel, real-valued, spectrum displays under operator control, and peak labeling with Siegbahn notation.



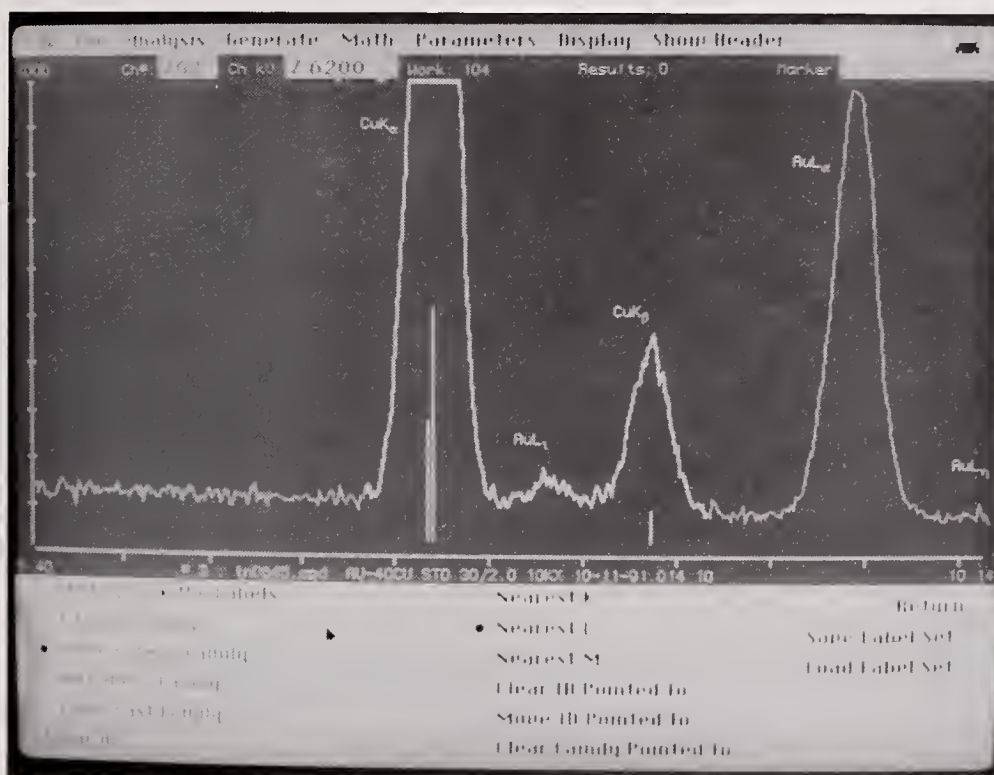
*The Desktop Spectrum Analyzer and X-Ray Database performs detailed analysis of a collection of spectra at one's desktop.*



Some features of the program:

- Processes commercial multi-channel analyzer spectra; many commercial data formats can be read directly into the program with spectra stored in internal format
- Spreadsheet output
- Conversion of WDS spectra to energy distribution with all DTSA procedures applicable to resulting spectra. Direct comparison with EDS spectra possible
- Linear and non-linear curve fitting procedures to extract peak intensities
- Qualitative analysis tools to find hidden peaks
- Automatic calibration
- Extensive spectrum calendar
- Extensive use of batch processing to support curve fitting, quantitation, and printing

**This database requires a basic Macintosh II class computer.**



*This program/database is  
a fully-functioning multi-  
channel analyzer.*

**Contact us for information on new and upcoming databases**  
**(301) 975-2208**

### **3. NIST Crystal Data**

**Alan D. Mighell  
Crystal Data and Electron Diffraction Center  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-6254**

This database contains chemical, physical, and crystallographic information useful to characterize more than 154,000 inorganic and organic crystalline materials. The data include the standard cell parameters, cell volume, space group number and symbol, the calculated density, and classification by chemical type, chemical formula, and chemical name. Each entry has an associated literature reference.

The database can be utilized as a practical analytical tool for compound identification because the lattice/formula combination uniquely characterizes a crystalline phase. The database is useful in conjunction with other data for materials design and properties prediction.

The file includes reliable data across the entire spectrum of the solid state including inorganics, organics, minerals, intermetallics, metals, alloys, drugs, antibiotics, and pesticides. Comprehensive chemical, crystallographic, and identification search software is provided with the database.

The database is available in magnetic tape and CD ROM formats. In addition, it may be searched interactively via CISTI's online international service. For further information, please contact International Centre for Diffraction Data, 1661 Park Lane, Swarthmore, PA 19081. Phone: (215) 328-9400.

### **15. NIST/Sandia/ICDD Electron Diffraction Database**

**Alan D. Mighell  
Crystal Data and Electron Diffraction Center  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-6254**

This database is designed for phase characterization obtained by electron diffraction methods. The database and associated software permit highly selective identification procedures for microscopic, as well as macroscopic, crystalline materials. The database contains chemical, physical, and crystallographic information on a wide variety of materials (over 70,000) including minerals, metals, intermetallics, and general inorganic compounds.



The Electron Diffraction Database has been designed to include all the data required to identify materials using computerized d-spacing/formula matching techniques. The data for each entry include the conventional cell, reduced cell, lattice type, space group, calculated or observed d-spacings, chemical name, chemical and empirical formula, material class indicators, references, and other parameters.

This database and search software are available in magnetic tape format and in CD ROM format. For further information, please contact International Centre for Diffraction Data, 1661 Park Lane, Swarthmore, PA 19081. Phone: (215) 328-9400.

## **20. NIST X-Ray Photoelectron Spectroscopy Database Version 2.0**



**Cedric Powell  
Surface Data Center  
National Institute of Standards  
and Technology  
Gaithersburg, MD 20899  
(301) 975-2534**

The new version of the NIST X-Ray Photoelectron Spectroscopy (XPS) Database gives easy access to photoelectron and Auger spectral data. The database contains over 13,000 line positions, chemical shifts, and splittings resulting from a critical evaluation of the published literature by Dr. Charles Wagner. Version 2.0 has a major interface improvement with powerful new searching software, including chemical nomenclature, and new sort and print options.

Graphics have been added for "Wagner plots." Users can easily identify unknown measured lines by matching to all previous measurements.

Each record on the database contains:

- Element and chemical compound, including names and formulas
- Line type, i.e., photoelectron, Auger, Auger parameter, chemical shift, doublet splitting, other splittings
- Line energy or energy difference
- Experimental details such as calibration, charge reference, and physical state
- Reference citation

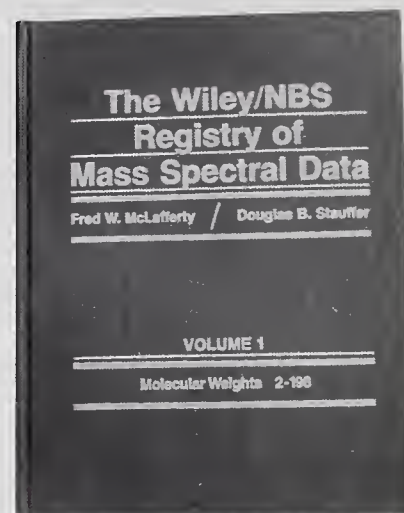
This database is available on both 5¼" and 3½" high density diskettes. Updates are regularly scheduled. It can also be used on Macintosh computers which have a PC emulator program.

## ANALYTICAL CHEMISTRY PUBLICATIONS

### **The Wiley/NBS Registry of Mass Spectral Data**

— F. McLafferty and D. B. Stauffer. Wiley-Interscience, New York, 1988.

This 7-volume work combines mass spectra from the NIST/EPA/MSDC Mass Spectral Database and Wiley's Registry of Mass Spectral Data. It includes spectra of over 112,275 compounds, with structures for over 89,903 compounds. Substance names (CAS and common), molecular weights, empirical formula, and CAS Registry Numbers are provided. Spectra are arranged by ascending molecular weight, elemental composition, and type of compound. In addition, complete indexing is given. Available from Wiley-Interscience, New York. (212) 850-6000, \$700.00 (set price)



**Crystal Data Determinative Tables, Third Edition** — 6 vols., International Centre for Diffraction Data, Swarthmore, PA.

The NIST Crystal Data Determinative Tables are the largest collection of crystallographic data available. These volumes contain data on over 43,000 organic and organometallic compounds, as well as 27,000 inorganic, metallic, and mineral compounds. Produced and edited by the NIST Crystal Data Center, these reference books are well-indexed by crystallographic system and determinative number. The data for each entry are comprehensive and include cell dimensions, space group or diffraction aspect, measured and calculated density, name, and literature reference.

Available from the International Centre for Diffraction Data, Swarthmore, PA. (215) 328-9400, \$379.00 (set price, individual volumes available)

**Elemental and Interplanar Spacing Index**, International Centre for Diffraction Data, Swarthmore, PA.

The Elemental and Interplanar Spacing Index (EISI) is designed to be used independently or in conjunction with a computer database for phase characterization using electron or x-ray diffraction. The EISI Index is arranged to enable the diffractionist to readily identify a material with the chemical and diffraction data routinely collected on most modern analytical electron microscopes.

Available from the International Centre for Diffraction Data, Swarthmore, PA. (215) 328-9400, \$250.00 (set price)



# ATOMIC PHYSICS

The Standard Reference Data Program has worked together with the world-famous NIST Atomic Physics Program to produce the most comprehensive set of reliable atomic data available anywhere. The NIST collection of atomic energy levels, transition probabilities, and collision data is widely used by groups for characterizing and modeling all types of gaseous systems, including plasmas, planetary atmospheres, and astrophysical media, and for health physics applications. Databases and publications make these data easy to find and easy to use.

In recent years, two important databases, one on electron and positron stopping powers and one on x-ray and gamma-ray attenuation, have become widely used. The first computer file of NIST Atomic Transition Probability Data has been made available, and this year a new database on Spectroscopic Properties of Atoms and Atomic Ions is being announced.

The SRD Fundamental Constants Data Center is responsible for work on revision of the fundamental constants, including release of the latest revision of 1986.

## SRD Atomic Databases

NIST Electron and Positron Stopping Powers of Materials

NIST X-Ray and Gamma-Ray Cross Section and Attenuation Coefficients

NIST Atomic Transition Probabilities Data Files (Scandium through Nickel)

NIST Spectroscopic Properties of Atoms and Atomic Ions

## SRD Major Publications in Atomic Data

1986 CODATA Recommended Values of the Fundamental Physical Constants

Atomic Transition Probabilities

Atomic Energy Levels Publications



# **ATOMIC PHYSICS DATABASES**

## **7. NIST Electron and Positron Stopping Powers of Materials**

**S.M. Seltzer  
Photon and Charged Particle Data Center  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-5552**

This database (also known as EPSTAR) provides rapid calculation of stopping powers (collisional, radiative, and total), CSDA ranges, radiation yields and density effect corrections for incident electrons or positrons with kinetic energies from 1 keV to 10 GeV, and for any chemically defined target material. The interactive database allows the user to specify an incident particle, an energy range, the target material and density, and for a gas, temperature and pressure. Clear instructions make the calculations easy to perform. Results can be saved to an external file for future use.

This database is available in PC diskette format. It can also be used on Macintosh computers which have a PC emulator program.

## **8. NIST X-Ray and Gamma-Ray Attenuation Coefficients and Cross Sections**

**S.M. Seltzer  
Photon and Charged Particle Data Center  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-5552**

This database (called XGAM) provides photon cross sections (interaction coefficients) and attenuation coefficients for any substance. An interactive database is provided which enables the user to obtain data by entering chemical formulas or other measures of composition for a mixture of component materials. The user may also select the energy range over which data are desired.

The system operates from a database of cross sections for coherent and incoherent scattering, photoionization, and pair production for the elements  $Z = 1$  to 100 at energies from 1 keV to 100 GeV. These data were obtained by a critical data analysis combining theoretical and experimental results.

The user may request data to be tabulated at the fixed energies stored in the database, or at an arbitrary set of user-specified energies, or at a combination of both. The tabulated results include the individual contributions and the total mass attenuation coefficient, both with and without coherent scattering.

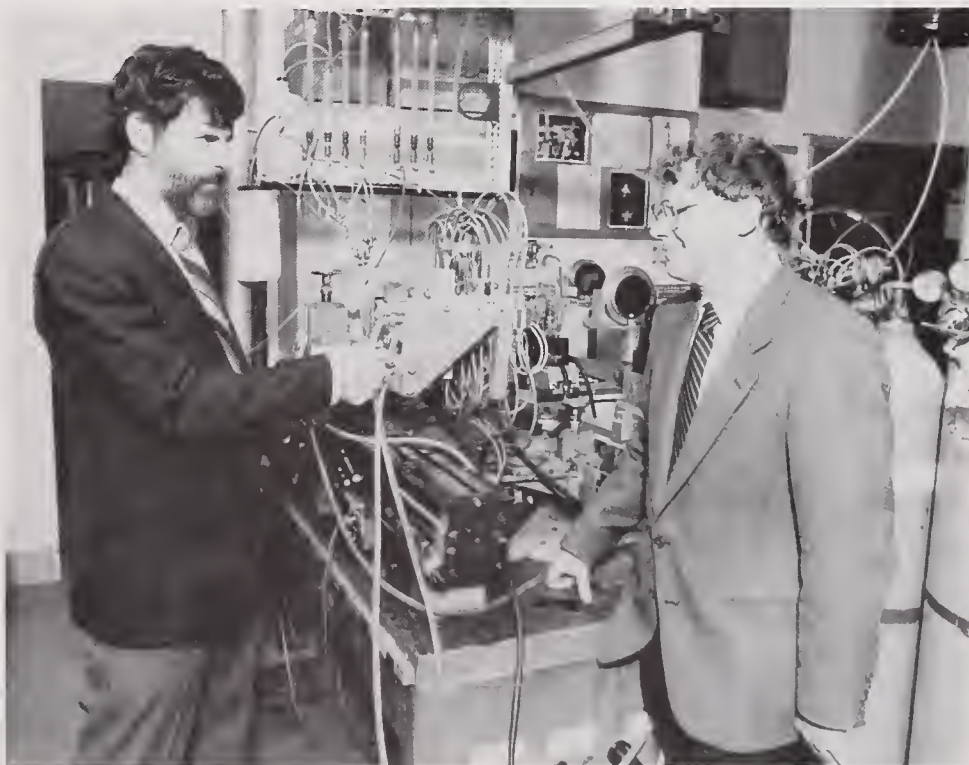
This database is available in PC diskette format. It can also be used on Macintosh computers which have a PC emulator program.

## **24. NIST Atomic Transition Probabilities Data Files (Scandium through Nickel)**

**Jeffrey Fuhr**  
**Atomic Transition Probabilities Data Center**  
**National Institute of Standards and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-3204**

This diskette package provides computer access to the numerical data given in "Atomic Transition Probabilities, Scandium Through Manganese" and "Atomic Transition Probabilities, Iron Through Nickel," which were published as Supplements 3 and 4 to Volume 17 (1988) of the *Journal of Physical and Chemical Reference Data*. The diskettes contain two types of files: the numeric files containing the transition probabilities and related data and the bibliographic files of references pertaining to the numeric tables. There are separate numeric and bibliographic files for each of the eight elements from scandium through nickel. Within each element, the data files are ordered by the ionization stage. The numeric data files are suitable for direct use by modeling programs.

This database is available on both 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.



*Jeffrey Fuhr and Dr. Wolfgang Wiese measure atomic transition probabilities with a wall-stabilized arc.*



## 38. NIST Spectroscopic Properties of Atoms and Atomic Ions



Jean W. Gallagher  
Standard Reference Data  
National Institute of Standards  
and Technology  
Gaithersburg, MD 20899  
(301) 975-2204

This is an interactive, menu-driven PC database containing wavelengths and ionization potentials for all neutral elements and the first four stages of ionization. The data originally appeared in NSRDS-NBS 68 — *Wavelengths and Transition Probabilities for Atoms and Atomic Ions. Part I. Wavelengths*. Additional information includes atomic masses, isotopic abundances, nuclear spins, and dipole and quadrupole moments.

This database comes on both 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.

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### ATOMIC PHYSICS PUBLICATIONS

**The 1986 CODATA Recommended Values of the Fundamental Physical Constants** — E. Richard Cohen and Barry N. Taylor. *Journal of Physical and Chemical Reference Data* 17, 1795 (1988).

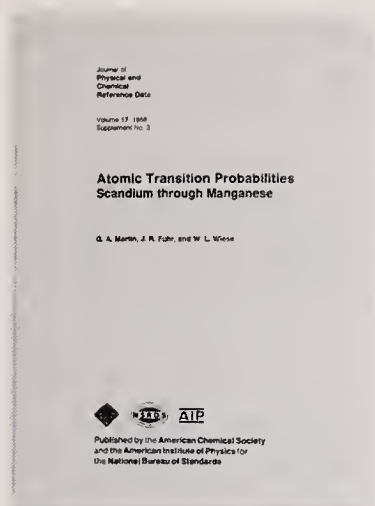
This article presents values of the basic constants and conversion factors of physics and chemistry resulting from the 1986 least-squares adjustment of the fundamental physical constants as recommended for international use by the CODATA (Committee on Data for Science and Technology) Task Group on Fundamental Constants. The 1986 CODATA set of values replaces the 1973 set also developed by CODATA.

Available from the American Chemical Society, Reprint 354, \$5.00

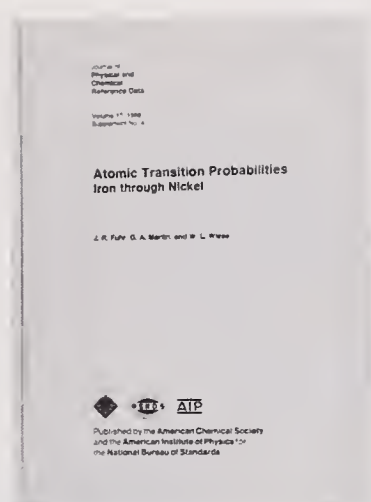
**Atomic Transition Probabilities, Scandium Through Manganese** — G.A. Martin, J.R. Fuhr, and W.L. Wiese. *Journal of Physical and Chemical Reference Data* 17, Supplement 3 (1988).

**Atomic Transition Probabilities, Iron Through Nickel** — J.R. Fuhr, G.A. Martin, and W.L. Wiese. *Journal of Physical and Chemical Reference Data* 17, Supplement 4, (1988).





These two supplements to the *Journal of Physical and Chemical Reference Data* contain almost 18,000 atomic transition probabilities. With over 1,000 pages of tables and critical discussion, it is the first and most comprehensive reference source for the transition probabilities of the eight transition metals, scandium through nickel. The data in these two volumes are



presented by element and spectrum. Finding lists are provided to facilitate transition location. The tables include spectroscopic classification, wavelengths of the transitions, the lower and upper energy levels, and their statistical weights. For each line an uncertainty estimate, the result of careful, critical evaluation, is given.

**Both available from the American Chemical Society**

**U.S. and Canada \$65.00 each**

**Abroad \$78.00 each**

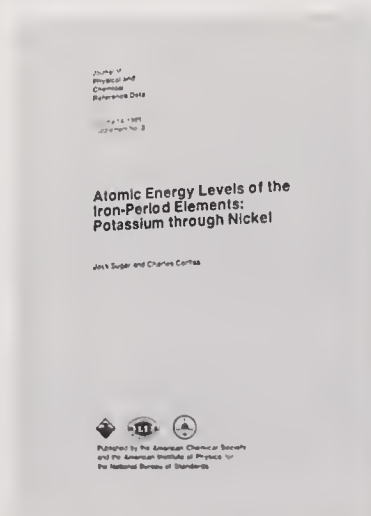
### **Atomic Energy Levels of the Iron-Period Elements: Potassium Through Nickel — J. Sugar and C. Corliss. *Journal of Physical and Chemical Reference Data* 14, Supplement 2 (1985).**

This supplement is a compilation of atomic energy levels of the iron-period elements, potassium through nickel, in all stages of ionization. The result of a critical evaluation of all literature published through 1985, it gives for each energy level the position relative to the ground state, configuration, term designation, J-value, and, where available, the g-value and the two leading percentages of the eigenvector composition in the most appropriate coupling scheme. This is an invaluable research tool for atomic, molecular, plasma, and astronomical scientists.

**Available from the American Chemical Society**

**U.S. and Canada \$65.00 each**

**Abroad \$58.00 each**



**Spectral Data and Grotrian Diagrams for Highly Ionized Copper, Cu X - Cu XXIX** — Toshizo Shirai, Toshiaki Nakagaki, Yohta Nakai, Jack Sugar, Keishi Ishii, and Kazuo Mori. *Journal of Physical and Chemical Reference Data* **20**, 1 (1991).



Wavelengths, energy levels, level classifications, intensities, and transition probabilities for the copper spectra Cu X to Cu XXIX are compiled. The data are critically compiled and best results quoted. Grotrian diagrams are also presented. Available from the American Chemical Society, Reprint 405, \$10.00

*The Atomic Energy Levels Data Center (l to r — William C. Martin, Arlene Robey, and Jack Sugar) have produced numerous data compilations on energy levels and spectral lines of atoms and atomic ions.*

**Wavelengths and Energy Level Classifications of Magnesium Spectra for All Stages of Ionization (Mg I through Mg XII)** — V. Kaufman and W. C. Martin. *Journal of Physical and Chemical Reference Data* **20**, 83 (1991).

Wavelengths and their classifications are compiled for the spectra of magnesium. All classifications have been verified with predictions made by differencing the energy levels. In addition to the spectra ordered by ionization stage, two finding lists are included. Available from the American Chemical Society, Reprint 406, \$9.00

**Atomic Weights of the Elements 1989** — J. R. de Laeter. *Journal of Physical and Chemical Reference Data* **20** (1991).

The Commission on Atomic Weights and Isotopic Abundances monitored the literature over the past 2 years and evaluated the published data on atomic weights and isotopic compositions on an element-by-element basis. Available from the American Chemical Society, Reprint 429



## **BIOTECHNOLOGY**

Standard Reference Data has developed new databases for the burgeoning new biotechnology field which will prove to be valuable research tools for biochemists. A major new database on lipids called LIPIDAT is being released, along with an upgrade to the important NIST/CARB Biological Macromolecule Crystallization Database. Both provide convenient data sources of existing knowledge and eliminate tedious library time. Regular updates are planned for both.

### **SRD Biotechnology Databases**

NIST/CARB Biological Macromolecule Crystallization

NIST Lipid Thermotopic Phase Transition

**Questions on the SRD Program?  
(301) 975-2208**



## BIOTECHNOLOGY DATABASES

### 21. NIST/CARB Biological Macromolecule Crystallization Database Version 2.0



Gary L. Gilliland  
Center for Advanced Research  
in Biotechnology  
National Institute of Standards  
and Technology  
9600 Gudelsky Drive  
Rockville, MD 20850  
(301) 251-2244

The NIST/CARB Crystallization database contains crystallization conditions and unit-cell parameters of crystals of biological macromolecules which have been reported in the literature. The biological macromolecules include proteins, nucleic acids, protein:protein complexes, nucleic acid:nucleic acid complexes, protein:nucleic acid complexes, and viruses. This database provides a convenient method for verification that a particular biological macromolecule has been crystallized and the details for reproducing the crystallization procedure. Version 2.0 adds approximately 400 new crystal forms and updates the literature through 1989.

The general information compiled for each macromolecule includes the name(s), molecular weight, sub-unit composition, and the presence of prosthetic group(s).

The description of the crystallization procedures consists of the macromolecular concentration, temperature, pH, and growth time. If there are unique aspects to the crystallization procedure, they are described in detail. The crystal data include the space group, unit cell dimensions, Z, crystal density, crystal habit, and size.

This database was developed at the Center for Applied Research in Biotechnology (CARB) and is available on both 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.

## 34. NIST Lipid Thermotopic Phase Transition Database



**Martin Caffrey**  
**Department of Chemistry**  
**Ohio State University**  
**Columbus, OH 43210-1173**  
**(614) 292-8437**

This database, also known as LIPIDAT, is a convenient, sophisticated, and centralized source of data on one of the most diverse and important groups of molecules. LIPIDAT provides thermodynamic data on mesomorphic and polymorphic transition temperatures and enthalpy changes for synthetic and biologically-derived complex polar lipids.



*Dr. Jacky Hogan demonstrates her new database on lipids.*

LIPIDAT contains:

- Thermodynamic data on over 800 lipids — enthalpies and transition temperatures
- Complete literature referencing and list of authors
- Data for partially and fully-hydrated lipids
- Data on the effects of various other additives, such as proteins, drugs, etc.
- Over 10,000 records
- Bibliographic information complete through January 1990

LIPIDAT was developed at Ohio State University and is available on both 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.



# CHEMICAL KINETICS

The NIST Program on Chemical Kinetics has long been a source of reliable, critically evaluated data on gas-phase reactions. Over the years, data provided by the program have been instrumental in modeling and predicting many important scientific problems such as combustion chemistry, atmospheric changes related to ozone depletion and warming, plasmas, and free-radical chemistry.

Recently, a comprehensive, easy-to-use PC database on over 2,000 gas-phase reactions has been widely distributed allowing scientists quick access to reaction rate data, as well as supporting information. In addition, the Radiation Chemistry Data Center at the University of Notre Dame provides a biweekly literature current awareness service on kinetics of ions and free-radicals.

## **SRD Chemical Kinetics Database**

NIST Chemical Kinetics Database

## **SRD Major Publications in Chemical Kinetics**

Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds

Biweekly List of Papers on Radiation Chemistry and Photochemistry

**Comments on our databases?  
Call us and give your input.**



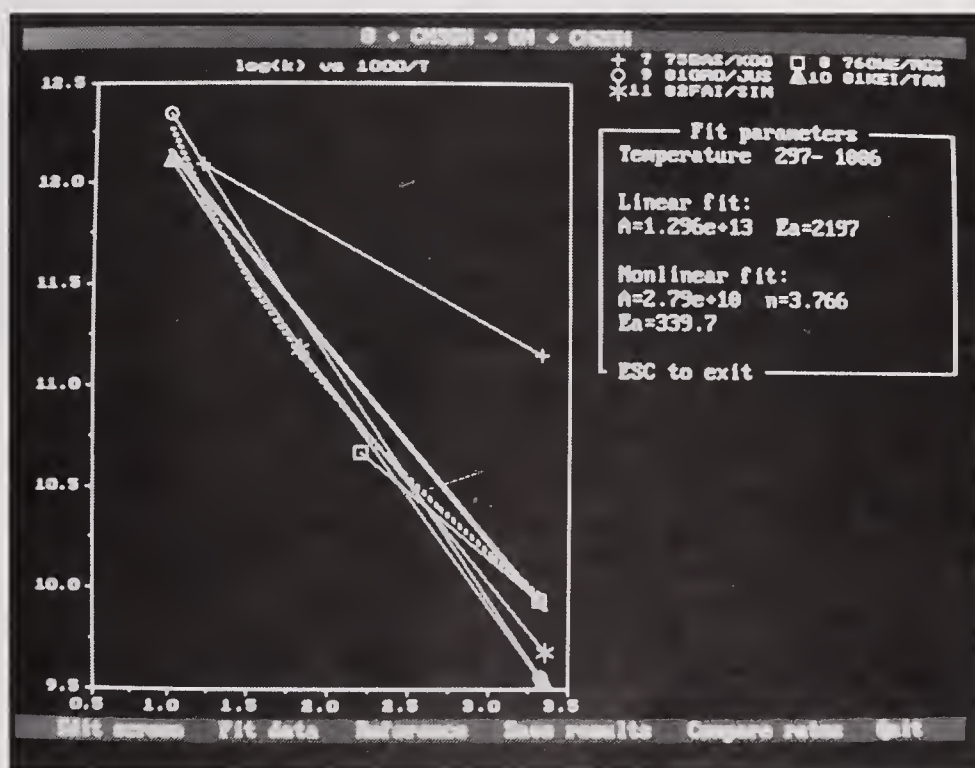
# CHEMICAL KINETICS DATABASE

## 17. NIST Chemical Kinetics Database Version 3.0



W. Gary Mallard  
Chemical Kinetics Data Center  
National Institute of Standards  
and Technology  
Gaithersburg, MD 20899  
(301) 975-2564

The NIST Chemical Kinetics Database is designed to provide rapid access to kinetics data for gas-phase reactions. Searches provide a summary of all of the literature on a particular reaction, all of the reactions of a specific species, subsets of all of the reactions, and the data available from a given paper. Version 3.0 contains over 16,000 records on over 5,000 reactions and for over 2,800 compounds which are reactants or products.



*Arrhenius graphs of rate constants in the NIST Chemical Kinetics Database.*

## Display Options

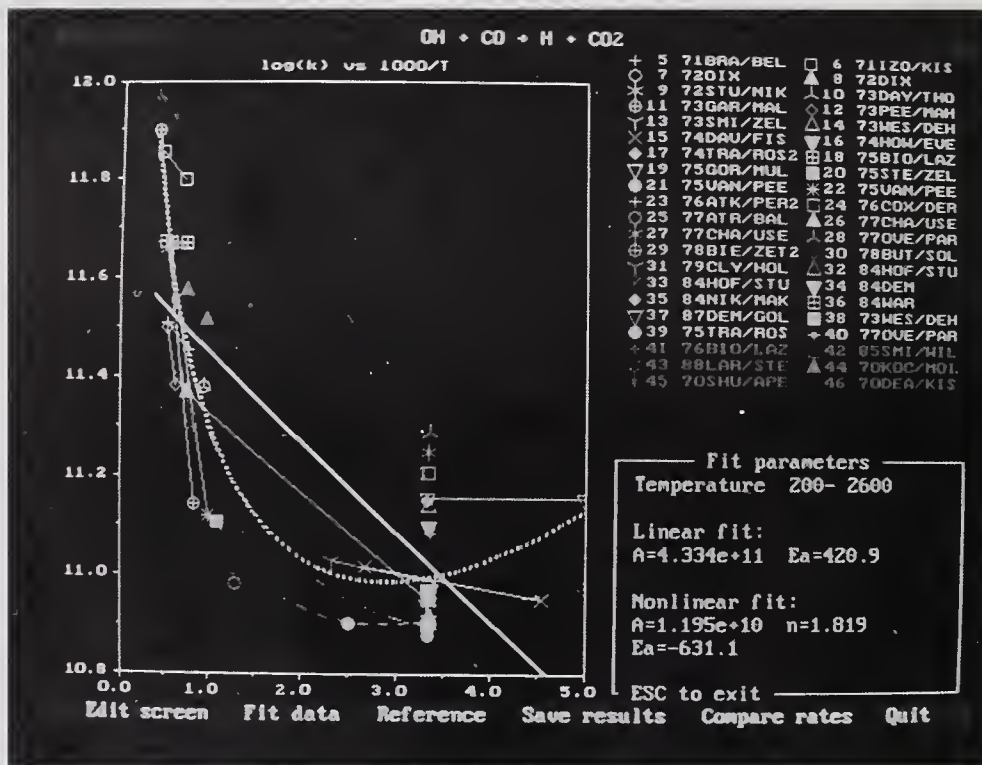
- up to 5 least square fits
- $A T^n$  or  $A(T/298)^n$  and activation energies in kcal/mol or kJ/mole, as well as K
- rate at a single temperature displayed in summary sheets for instant comparison of data
- simultaneous display of abstracts and graphics
- user settings for the axis to allow data comparison
- context sensitive help screens, including graphics

## User Input

- user can add data to be plotted and fit
- user can add extensive comments

## Searching Options

- all reactions of a species
- all reactions of a species containing a specific item
- reactions of a species with molecular subsets
- author
- citation



*User input has been incorporated into enhancements of this database.*

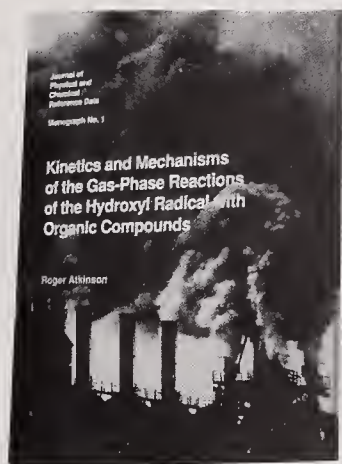
Version 3.0 has new printer/plotter options.

This database is available on 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers with PC emulator software. This database is updated yearly.



## CHEMICAL KINETICS PUBLICATIONS

**Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds** — Roger Atkinson. *Journal of Physical and Chemical Reference Data*, Monograph 1 (1989).



This monograph reviews the entire literature through 1988 concerning the kinetics and mechanisms of gas-phase reactions of the hydroxyl radical with organic compounds and evaluates the data. Rate data for temperatures ranging from 220 to over 2000 K are included. Recommended rate expressions are given. Each recommendation is accompanied by text discussion, the available data, and the rationale behind the recommendation of best values. Also included are the estimated uncertainties in the recommended rate expression and discussions concerning the reaction mechanisms.

Available from the American Chemical Society  
U.S. and Canada \$55.00  
Abroad \$65.00

**Biweekly List of Papers on Radiation Chemistry and Photochemistry** — Radiation Chemistry Data Center, Notre Dame, IN.

This is a current-awareness publication with special emphasis on the kinetics and other properties of transient ions, radicals, and the excited species. Papers are included on the radiation chemistry and photochemistry of chemically-defined systems containing organic and inorganic compounds, biological molecules, and polymers, with references to ESR and luminescence studies. The references listed are obtained from scanning 60 current journals, as well as Chemical Abstracts, INIS Atomindex, and other publications.

Available from Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Notre Dame, IN 46556 \$42.00/year

**Chemical Kinetic Data Base for Combustion Chemistry. Part 2. Methanol** — Wing Tsang. *Journal of Physical and Chemical Reference Data* 16, 471 (1987).

This publication contains evaluated and estimated data on the kinetics of reactions involving methanol and hydroxymethyl radicals and various small inorganic and organic species which are of importance for methanol combustion or pyrolysis.

Available from the American Chemical Society, Reprint 327, \$7.00



**Chemical Kinetic Data Base for Combustion Chemistry. Part 3. Propane**  
— Wing Tsang. *Journal of Physical and Chemical Reference Data* 17, 887 (1988).

With evaluated and estimated data on the kinetics of reactions involving propane, isopropyl radical, n-propyl radical, and various small inorganic and organic species, this publication is important for propane pyrolysis and combustion.

Available from the American Chemical Society, Reprint 344, \$9.00

**Chemical Kinetic Data Base for Combustion Chemistry. Part 4. Isobutane**  
— Wing Tsang. *Journal of Physical and Chemical Reference Data* 19, 1 (1990).

This publication contains evaluated and estimated data on the kinetics of reactions involving isobutane, t-butyl radical, and isobutyl radical and various small inorganic and organic species which are of importance for the proper understanding of isobutane combustion and pyrolysis.

Available from the American Chemical Society, Reprint 374, \$9.00

**Chemical Kinetic Data Base for Combustion Chemistry. Part V. Propene —**  
Wing Tsang. *Journal of Physical and Chemical Reference Data* 20, 221 (1991).

This paper adds data on propene reactions to the series of compilations of rate constants and other data relevant to the modeling of combustion systems. Recommended kinetic and thermodynamic data are given for 57 reactions involving propene and the allyl radical with various organic and inorganic species.

Available from the American Chemical Society, Reprint 409, \$8.00

**Kinetics and Mechanisms of the Gas-Phase Reactions of the NO<sub>3</sub> Radical with Organic Compounds** — Roger Atkinson. *Journal of Physical and Chemical Reference Data* 20, 459 (1991).

Measurements on reactions of the NO<sub>3</sub> radical in the gas-phase are reviewed and recommended rate constants are presented. Reactions with organic compounds are covered. Needs for additional data on NO<sub>3</sub> are discussed.

Available from the American Chemical Society, Reprint 413, \$8.00

## **MATERIALS PROPERTIES**

The NIST Materials Data Program provides evaluated data on phase equilibria, structure and characterization, and performance properties.

The NIST/American Ceramics Society Program for Phase Diagrams for Ceramists has for many years published the authoritative sources for these data and has added a new database to supplement its nine-volume series. The Binary Alloy Phase Diagram Program jointly sponsored by NIST and ASM International has completed its work to evaluate all binary alloy phase diagrams. A major new compendium has just been published.

Several materials performance property databases are available. The revised NIST Structural Ceramics Database contains the most current data for various silicon carbides and silicon nitrides. It is the first structural ceramics database publicly available. Corrosion data (in conjunction with the National Association of Corrosion Engineers) and tribology data (together with ACTIS, Inc.) have been evaluated, and several databases produced by these programs have gained wide acceptance.

Crystallographic, electron diffraction, and surface analysis databases are also available and described in more detail under Analytical Chemistry.

### **NIST Materials Properties Databases**

NIST Structural Ceramics

NACE-NIST Corrosion Performance Databases

COR\*SUR 1 - Corrosion Rate Data for Metals

COR\*SUR 2 - Corrosion Rate Data for Non-Metals

NIST Crystal Data

NIST/Sandia/ICDD Electron Diffraction

NIST X-Ray Photoelectron Spectroscopy

NIST Tribomaterials I (ACTIS)

Phase Diagrams for Ceramists

### **SRD Major Publications in Materials Properties**

Journal of Phase Equilibria (formerly Bulletin of Alloy Phase Diagrams)

Phase Diagrams for Ceramists

Binary Alloy Phase Diagrams, 2nd edition

# MATERIALS PROPERTIES DATABASES

## 30. NIST Structural Ceramics Database

**Ronald Munro/E.F. Begley**  
**Ceramics Division**  
**National Institute of Standards and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-6118**

This unique database contains thermal and mechanical properties of silicon carbides and silicon nitrides in a stand-alone, user-friendly system that operates on PCs.

Primary properties in the Structural Ceramics Database:

### *Materials Specification*

- Name
- Formula
- Chemical Composition
- Fabrication
- Physical Properties
- Microstructural Information
- Processing

### *Thermal Properties*

- Conductivity
- Diffusivity
- Expansion
- Specific Heat
- Shock Resistance

### *Bibliography*

- Complete documentation of data sources through 1990

### *Mechanical Properties*

- Elastic Modulus
- Poisson's Ratio
- Flexural Strength
- Tensile Strength
- Compressive Strength
- Vicker's Hardness
- Knopp Hardness
- Fracture Toughness
- Fracture Energy
- Weibull Modulus
- Creep Exponent

### *Measurement Methods*

- Specimen Preparation
- Apparatus
- Procedures

This database comes on both 5¼" high density diskettes and 3½" high and low density diskettes. It will run on a Macintosh with PC emulator software.



## **16. NACE-NIST Corrosion Performance Database**

**David Anderson  
Corrosion Data Center  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-6026**

The corrosion databases developed under the NACE-NIST Corrosion Data Program give users reference data for general guidance on the performance of engineering materials in corrosive environments. COR\*SUR 1 includes data for 25 common metals for exposures in over 1,000 corrosive environments at various temperatures and concentrations. COR\*SUR 2 provides similar data for 36 nonmetallic materials (elastomers, polymers, composites, thermoplastics, etc.) in over 850 environments. Data can be retrieved from both programs by:

- tabular listing of materials exhibiting a specified range of corrosion rates in selected environments
- graphic presentation of corrosion rate ranges for a given material in a matrix of environment, concentration, and temperature
- tabular listing of corrosion rate data for a specified material in a corrosive environment as a function of temperature and concentration

Programs are derived from the Corrosion Data Survey publications produced by the National Association of Corrosion Engineers (NACE) and are available in diskette form for use on IBM or compatible personal computer systems and are available from NACE, P.O. Box 218340, Houston, TX 77218. (713) 492-0535.

**NIST Crystal Data — see page 14**

**NIST/Sandia/ICDD Electron Diffraction — see page 14**

**NIST X-Ray Photoelectron Spectroscopy — see page 15**

## **NIST Tribomaterials I (ACTIS) Database**

**Bill Ruff  
Tribology Data Center  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-6010**

This database contains property data for 261 materials commonly used in tribology applications. The data cover a wide range of properties including basic physical and mechanical as well as tribology properties for both lubricated and unlubricated wear. This user-friendly PC database is available from ACTIS, 118 Highgate Road, Wilmington, DE 19808. (302) 998-8240.

## **31. Phase Diagrams for Ceramists Database**



**Ronald Munro  
Phase Diagrams for Ceramists  
Data Center  
National Institute of Standards  
and Technology  
Gaithersburg, MD 20899  
(301) 975-6127**

This PC package provides computer access to the well-known and widely-distributed *Phase Diagrams for Ceramists* (PDFC). The software permits searches for diagrams by chemical system, author, or year of publication. All diagrams from volumes 5-8 in the PDFC series are included. After identifying figure numbers in a search, diagrams can be plotted on a screen. The graphics software permits diagram manipulation, such as magnification of selected regions, overlay of related diagrams, lever rule calculations, display of the cursor position in real units, and selection of the temperature scale. In addition, all bibliographic references and chemical systems from volumes 1-8 of the PDFC series are available.

This database comes on both 5¼" and 3½" diskettes.

## **MATERIALS PROPERTIES PUBLICATIONS**

**Journal of Phase Equilibria (formerly the Bulletin of Alloy Phase Diagrams)** — ASM International, Metals Park, OH.

The Bulletin was retitled in 1991. It has been expanded to include original research on the generation and application of data to attain or prevent phase equilibria. It presents theoretical and experimental research on the determination of phase diagrams and provides critical phase diagram evaluations authored by international experts for scientifically and industrially important alloy systems and updates of systems previously published.

**Available from ASM International, Metals Park, OH (216) 338-5151**

**Binary Alloy Phase Diagrams, Second Edition, 3 vols.** — ASM International, Metals Park, OH.

This is the most thorough alloy reference available. All systems published in the original set have been updated. This set contains 2,925 critical evaluations with key references, plus additional related citations.

**Available from ASM International, Metals Park, OH (216) 338-5151, \$583.00**

**Phase Diagrams for Ceramists**, American Ceramic Society, Columbus, OH.

This publication series has become the definitive source of ceramic phase diagrams in the scientific community. These nine volumes contain commentaries and binary, ternary and higher order phase diagrams of oxide, metals-oxide, and metal-oxygen systems, halide, and other ceramic systems.

**Available from the American Ceramic Society, Columbus, OH (614) 268-8645, \$125.00/vol./Annual volume \$69.00**

**Critical Compilation of Surface Structures Determined by Ion Scattering Methods** — Philip R. Watson. *Journal of Physical and Chemical Reference Data* 19, 85 (1990).

This review critically compiles all surface structures derived by ion scattering techniques. These investigations cover all types of surfaces including clean and adsorbate-covered metal, semiconductor, and other nonmetallic substrates. The important experimental and theoretical aspects of such investigations have been extracted into easily understood tabular form supplemented by figures and ancillary tables and complete references.

**Available from the American Chemical Society, Reprint 376, \$6.00**



**Coupled Phase Diagram/Thermodynamic Analysis of the 24 Binary Systems,  $A_2CO_3$ -AX and  $A_2SO_4$ -AX where A = Li, Na, K and X = Cl, F,  $NO_3$ , OH — Yves Dessureault, James Sangster, and Arthur D. Pelton. Journal of Physical and Chemical Reference Data 19, 1149 (1990).**

A complete bibliographic search for all thermodynamic and phase diagram data on the 24 binary systems was carried out. A computer-assisted simultaneous evaluation of all data was performed in order to obtain optimized equations for the thermodynamic properties of the phases. These are considered to be the best evaluated phase diagrams which can be deduced from the data currently available.

**Available from the American Chemical Society, Reprint 398, \$6.00**

**FAX your order to SRD  
(301) 926-0416**

# **MOLECULAR STRUCTURE AND SPECTROSCOPY**

Building upon the renowned NIST research on molecular spectroscopy and structure, the SRD Program has produced several important compilations of molecular data. Numerous comprehensive microwave spectra for astrophysically interesting molecules have been published and are widely used in radio astronomy. In addition, several comprehensive compilations of microwave spectral tables are now available.

The database on vibrational and electronic lines has been updated to include more data.

## **SRD Molecular Structure and Spectroscopy Database**

NIST Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules

## **SRD Molecular Structure and Spectroscopy Publications**

Microwave Spectral Tables III. Hydrocarbons  
Electronic Energy Levels of Small Polyatomic Transient Molecules

Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules

**All SRD databases have complete, easy-to-use user manuals.**

# MOLECULAR STRUCTURE AND SPECTROSCOPY DATABASE

## 26. NIST Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules Version 2.0



**Marilyn Jacox**  
**National Institute of Standards  
and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-2547**

This database (also called VEEL) is designed to give rapid access to experimental data on vibrational and electronic energy levels of natural and transient molecules with from 3 to 6 atoms. There is a 25 percent increase in data in Version 2.0, making a total of approximately 1,240 molecules included in the database. In addition, where data are available for the fully deuterium-substituted counterparts of these molecules, those data are also included. Searches can be made for a particular molecule, for a specific wavenumber, by electronic band origin, and by wavelength range for a transition.



*Dr. Marilyn Jacox, developer of the VEEL database.*

Searches can also be restricted 1) to molecules containing a specified chemical element; 2) to either the ground or excited electronic states; 3) to observations in the gas-phase or in a specified inert solid matrix; or 4) to data obtained using a specific technique. Provision is made for the display of references to the original literature pertinent to each line of the compilation or of all references associated with the molecule of interest.

This database is available on both 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.



## MOLECULAR STRUCTURE AND SPECTROSCOPY PUBLICATIONS

**Microwave Spectral Tables III. Hydrocarbons, CH to C<sub>10</sub>H<sub>10</sub>** — F.J. Lovas and R.D. Suenram. *Journal of Physical and Chemical Reference Data* **18**, 1245 (1989).

All of the rotational spectral lines observed and reported in the open literature for 91 hydrocarbon molecules have been tabulated. The isotopic molecular species, assigned quantum numbers, observed frequency, estimated measurement uncertainty, and references are given for each transition reported. The derived molecular properties, such as rotational and centrifugal distortion constants, hyperfine structure constants, electric dipole moments, and rotational g-factors are listed.

**Available from the American Chemical Society, Reprint 369, \$22.00**

**Electronic Energy Levels of Small Polyatomic Transient Molecules** — Marilyn E. Jacox. *Journal of Physical and Chemical Reference Data* **17**, 269 (1988).

The experimentally determined electronic energy levels of approximately 500 neutral and ionic transient molecules possessing from 3 to 6 atoms are tabulated, together with the associated vibrational structure, the radiative lifetime, the principal rotational constants, and references to the present literature. Vibrational and rotational data for the ground state are also given. Observations in the gas-phase, in molecular beams, and in rare-gas and nitrogen matrices are included.

**Available from the American Chemical Society, Reprint 342, \$20.00**

**Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules. Supplement 1** — Marilyn E. Jacox. *Journal of Physical and Chemical Reference Data* **19** (1990).

New information on the experimentally determined vibrational and electronic energy levels of approximately 470 neutral and ionic transient molecules possessing from 3 to 16 atoms has been evaluated and added to the previous established database for these species. Electronic spectral data are also given for a number of transient molecules which possess more than six atoms. Radiative lifetimes and the principal rotational constants are included. Observations in the gas-phase, in molecular beams, and in rare-gas and nitrogen matrices are evaluated.

**Available from the American Chemical Society, Reprint 403, \$14.00**

# **THERMODYNAMICS AND THERMOCHEMISTRY**

NIST has a long history as the source for reliable thermochemical data starting with the International Critical Tables from the 1920's. The tradition continues as new SRD databases on thermochemical properties of inorganic and small organic molecules gain acceptance.

The NIST Standard State Thermochemical Tables are recognized as the internationally authoritative source of standard state data for inorganics. The JANAF Thermochemical Tables contain the most complete compilations of evaluated temperature-dependent thermodynamic data for inorganic species. The new Structures and Properties Database is gaining wide acceptance as it allows chemists and engineers to draw structures or substructures which locate chemicals in the database with the same molecular fragment.

NIST thermochemical databases are available both in convenient PC formats and as online systems.

## **SRD Thermochemical Databases**

NIST Structures and Properties

NIST Chemical Thermodynamics

NIST Thermophysical Properties of Water

NIST JANAF Thermochemical Tables

DIPPR Data Compilation of Pure Compound Properties

NIST Positive Ion Energetics

NIST Negative Ion Energetics

NIST Estimation of Thermodynamic Properties for Organic Compounds at 298.15 K

NIST Molten Salts

NIST Thermophysical Properties of the Elements

## **SRD Major Publications in Thermochemistry**

NBS Tables of Chemical Thermodynamic Properties

JANAF Thermochemical Tables

Gas-Phase Ion and Neutral Thermochemistry

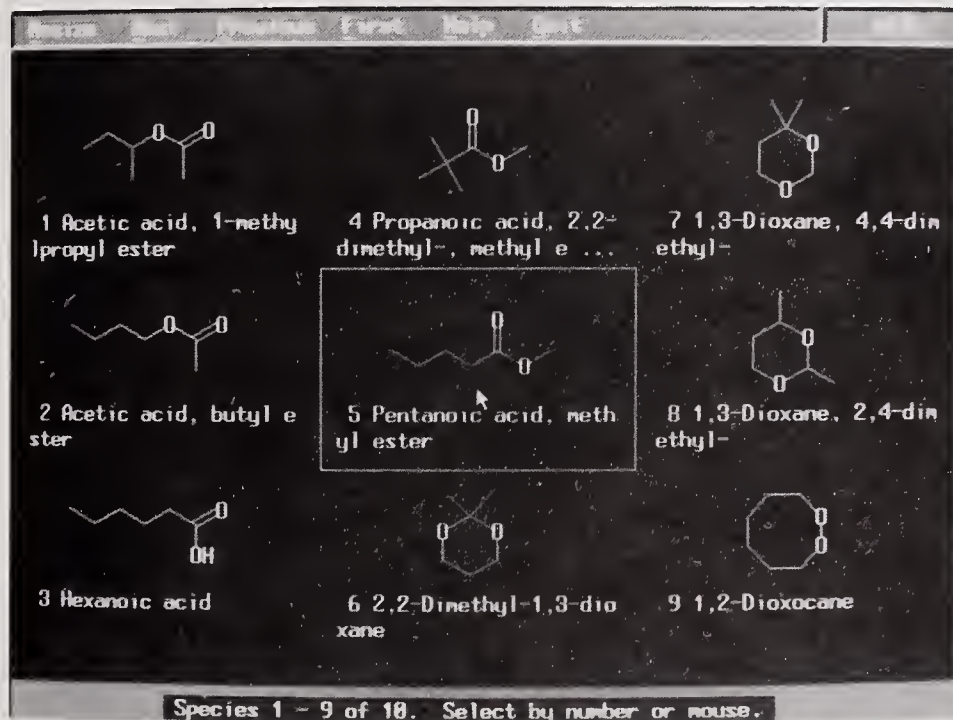


# THERMODYNAMIC AND THERMOCHEMICAL DATABASES

## 25. NIST Structures and Properties Database and Estimation Program

Stephen E. Stein  
Chemical Kinetics and Thermodynamics Division  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-2505

This unique product is based on a new approach for accessing chemical data. It combines a database of properties and structures, a data prediction engine, and structural drawing module into an integrated system for finding and estimating chemical property data. This database



*NIST Structures and Properties has many versatile graphics capabilities.*

points. Properties are estimated solely from structures drawn with an integrated, easy-to-use drawing module. Alternatively, all compounds containing drawn substructures may be located. No knowledge of estimation methods is required.

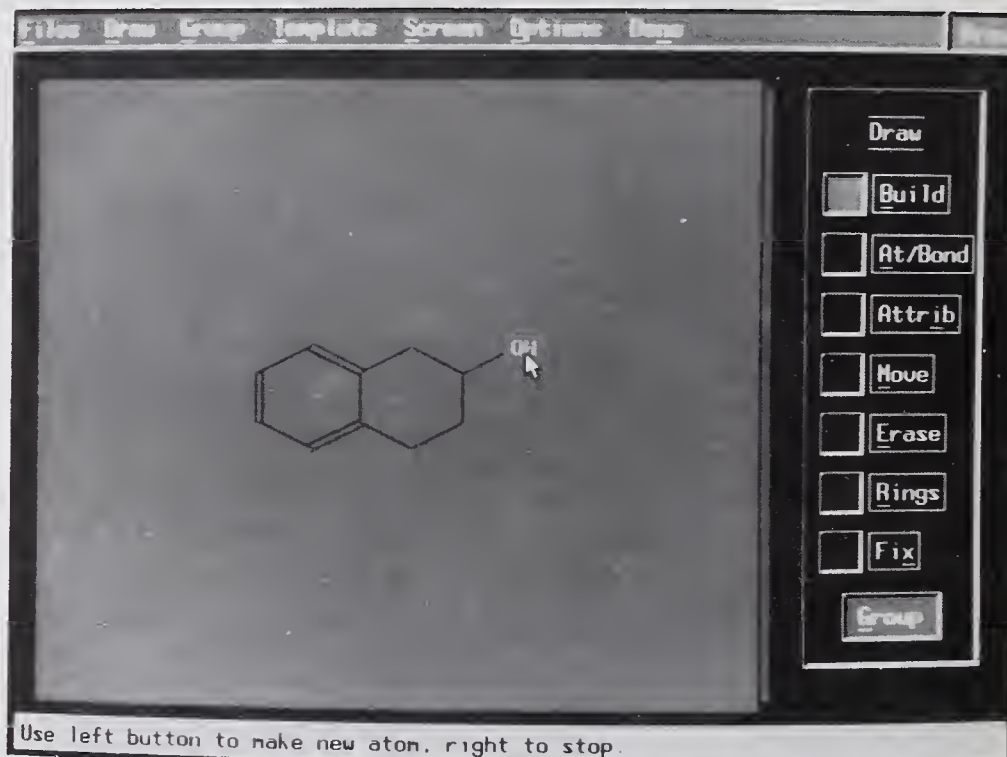
contains thermochemical data for nearly 5,000 compounds from three widely-accepted Standard Reference Databases - NIST Positive Ion Energetics Database, NIST Chemical Kinetics Database, and NIST JANAF Thermochemical Tables. It also features a complete implementation of Benson's Group Additivity estimation method for gas-phase heats of formation, entropies, and heat capacities as well as a structure-based method for estimating vapor pressures and boiling



Some special features are:

- Automatic perception of rings and long-range interactions
- Determination of symmetry number correction — even for complex ring systems
- Computation of equilibrium constants for user-created chemical reactions
- Inclusion of 50 new group values and 80 new ring corrections derived from recent literature data

*NIST Structures and Properties has an easy-to-use drawing module.*



Search for data by:

- Name
- CAS Registry Number
- Formula (complete or partial)
- Substructure

The database is available on both 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.

**SRD accepts VISA and MasterCard**

## 2. NIST Chemical Thermodynamics Database

David Neumann  
Chemical Thermodynamics Data Center  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-2525

This database contains recommended values for selected thermodynamic properties of more than 15,000 inorganic substances. These properties include the following:

### Standard state properties at 298.15 K and 1 bar

- enthalpy of formation from the elements in their standard state
- Gibbs energy of formation for the elements in their standard state
- enthalpy  $H^\circ(298.15\text{ K}) - H^\circ(0\text{ K})$
- heat capacity at constant pressure
- entropy

### Properties at 0 K

- enthalpy of formation

The database is available in a magnetic tape format and online through STN and CIS.

## 13. NIST JANAF Thermochemical Tables

Malcolm W. Chase  
Standard Reference Data  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-2200

The JANAF Thermochemical Tables provide a compilation of critically evaluated thermodynamic properties of approximately 1800 substances over a wide range of temperatures. Recommended temperature-dependent values are provided for inorganic substances and for organic substances containing only one or two carbon atoms.

These tables cover the thermodynamic properties with single phase and multi-phase tables for the crystal, liquid, and ideal gas multi-phase states. The properties tabulated are heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound from the elements in their standard reference states. This database is consistent with the Third Edition of the JANAF Thermochemical Tables published as Supplement No. 1 to Volume 14 of the *Journal of Physical and Chemical Reference Data*.

This database is available as a magnetic tape with a PC product in preparation. It is currently available on-line through STN.



## **11. DIPPR Data Compilation of Pure Compound Properties**

**T.E. Daubert and R.P. Danner  
Penn State University  
133 Fenske Laboratory  
University Park, PA 16802  
(814) 863-4638**

The DIPPR database contains data on 39 properties for 1,212 chemical compounds of high industrial priority. Thermodynamic, physical, transport, and environmental property data are given. The database was prepared by Pennsylvania State University for the Design Institute for Physical Property Data, a cooperative project sponsored by 50 major chemical manufacturers and related companies under the auspices of the American Institute of Chemical Engineers.

For each chemical compound included, values are given for 26 single-valued property constants and for 13 properties as functions of temperature, calculated from correlation coefficients. The database also includes estimates of the accuracy of each property value and references to the sources of measured or predicted data which were used in selecting the recommended values. The database includes numeric values as well as interactive software which allows access to specific properties of the compounds included, in any specified set of units.

This database is available in magnetic tape and diskette format. It is available on-line through STN.

### **11A. DIPPR Data Compilation Access Program II — Student DIPPR**

The student version of NIST Standard Reference Database 11 — DIPPR Data Compilation of Pure Compound Properties — contains data for 100 compounds. For each compound, values are given for 26 single-valued property constants and for 13 properties as functions of temperature. The user can construct a list of compounds of interest from the available database, select any unit system, select the type of output device, and then plot or tabulate the properties of interest. An invaluable teaching tool, this database is available in diskette and magnetic tape format.



## **19A. NIST Positive Ion Energetics Database**

**Sharon G. Lias**  
**Chemical Kinetics and Thermodynamics Division**  
**National Institute of Standards and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-2562**

This database provides rapid access to evaluated ionization potentials, enthalpies of formation of ions, enthalpies of formation of the corresponding neutral species, and all references to these data. The initial source of the database is the positive ion table in "Gas-Phase Ion and Neutral Thermochemistry," *Journal of Physical and Chemical Reference Data*, Volume 17, Supplement 1, 1988. Evaluated proton affinity values can also be retrieved. The database has a highly interactive interface that allows the user to retrieve data through three different search options: by empirical formula, by name, and by proton affinity.

## **19B. NIST Negative Ion Energetics Database**

**John E. Bartmess**  
**University of Tennessee**  
**Knoxville, TN 37996**  
**(615) 974-6578**

Providing easy access to gas-phase electron affinities, acidities, negative-ion affinities to neutral species, negative-ion enthalpies of formation, and the literature references for the primary sources of the data, this database includes data on 2,000 negative ions. The species covered include all organic and inorganic atoms, molecules, and radicals for which pertinent data were found in the literature through the end of 1988. Designed to accompany the NIST Positive Ion Energetics Database, this database also uses the *Journal of Physical and Chemical Reference Data*, Volume 17, Supplement 1, 1988 as an initial source.

Both databases come in PC diskette format. They can be used on Macintosh computers which have a PC emulator program.

## 37. NIST Thermophysical Properties of the Elements



**Malcolm W. Chase  
Standard Reference Data  
National Institute of Standards  
and Technology  
Gaithersburg, MD 20899  
(301) 975-2200**

This new prototype database contains thermodynamic data on the condensed phases of Group II elements (Be, Sr, Mg, Ca, Ba). The properties available include:

- summary of results, including fusion temperature, transformation temperatures, Cp/H data measured or smoothed
- fitting equations for Cp/H data in different temperature ranges
- methods of measurement
- comment on accuracy of data
- Cp/H data measured or smoothed and temperature
- bibliographic information

The database may be searched by author, transitions, and Cp/H. Data may also be plotted. Further updates are to include all available elements. This database is available on both 5¼" and 3½" high or low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.

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## 18. NIST Estimation of the Thermodynamic Properties for Organic Compounds at 298.15 K — Hydrocarbons Version 2.0



**Eugene S. Domalski**  
**Chemical Kinetics and**  
**Thermodynamics Division**  
**National Institute of Standards**  
**and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-2529**

This database (also called THERM/EST) is an estimation algorithm which calculates thermodynamic properties at 298.15 K and contains a database with experimental and estimated values for approximately 429 hydrocarbon compounds. The thermodynamic properties calculated are:

- enthalpy of formation
- heat capacity
- entropy
- entropy of formation
- Gibbs energy of formation
- equilibrium constant for the formation reaction

The thermodynamic properties have been developed for the gas, liquid, and solid phases. The lists of the hydrocarbon compounds and their properties are divided into the following files:

- straight-chain aliphatic hydrocarbons
- branched aliphatic hydrocarbons/tertiary carbon branching
- branched aliphatic hydrocarbons/quaternary carbon branching
- straight-chain alkene hydrocarbons
- substituted alkene hydrocarbons
- alkyne hydrocarbons
- aromatic hydrocarbons
- alicyclic hydrocarbons

A feature of the new version is conversion of energy units from joules to calories.

THERM/EST is available on both 5 ¼" or 3 ½" high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.



## **27. NIST Molten Salts Database Single Salts and Mixtures Database Version 2.0**



**George Janz  
Molten Salts Data Center  
Rensselaer Polytechnic Institute  
Department of Chemistry  
Troy, NY 12181  
(518) 276-6344**

This database provides easy and rapid access to the properties of inorganic salts in the molten state. This is the culmination of a long-term data evaluation project at RPI. The database allows calculation of the following properties of single salt systems and multi-component systems (which are primarily binary):

- density
- surface tension
- viscosity
- electrical conductance

Some data for more complex salt mixtures are also given. Data can be extracted by chemical formula or the user can browse through the database to find the system of choice. All property value calculations display:

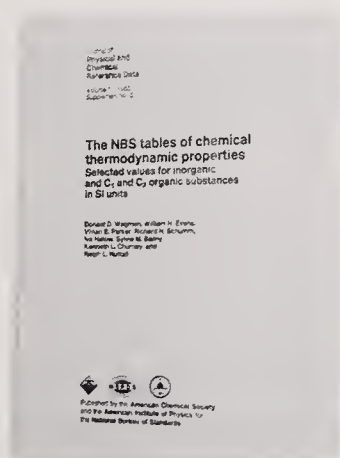
- the salt system
- temperature measurement limits
- correlation equation
- accuracy estimates
- reliability statements
- results in a single temperature or range of temperatures in S/I units

This database is available on both 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers with PC emulator software.

# THERMODYNAMIC AND THERMOCHEMICAL PUBLICATIONS

## The NBS Tables of Chemical Thermodynamic Properties. II. Selected Values for Inorganic and C<sub>1</sub> and C<sub>2</sub> Organic Substances in SI Units —

Donald D. Wagman, William H. Evans, Vivian B. Parker, Richard H. Schumm, Iva Halow, Sylvia M. Bailey, Kenneth L. Churney, and Ralph L. Nuttall. *Journal of Physical and Chemical Reference Data* 11, Supplement 2 (1982).



This publication provides the chemical thermodynamic properties of inorganic substances and organic substances usually containing only one or two carbon atoms. Where available, values are given for the enthalpy of formation, Gibbs energy of formation, entropy and heat capacity at 298.15 K, the enthalpy difference between 298.15 and 0 K, and the enthalpy of formation at 0 K. All values are given in SI units and are for a standard state pressure of 100,000 pascal. Gaseous, liquid, and crystalline substances, solutions in water, and mixed aqueous and organic solutions are given values. This publication supersedes the National Bureau of Standards Technical Note 270 series.

Available from the American Chemical Society  
U.S. and Canada \$40.00  
Abroad \$48.00

## JANAF Thermochemical Tables. Third Edition — M.W. Chase, Jr., C.A.

Davies, J.R. Downey, Jr., D.J. Frurip, R.A. McDonald and A.N. Syverud. *Journal of Physical and Chemical Reference Data* 14, Supplement 1 (1985).

These updated volumes contain thermodynamic properties for more than 1,800 substances over a wide temperature range. All tables are in SI units and the notation has been made consistent with current international recommendations. There are single-phase and multi-phase tables in the crystal, liquid, and ideal gas states. The properties tabulated are heat capacity, entropy, Gibbs energy function, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound. Each tabulation is accompanied by a critical evaluation of the literature upon which the thermochemical table is based and literature references are given.

Available from the American Chemical Society  
U.S. and Canada \$130.00  
Abroad \$156.00

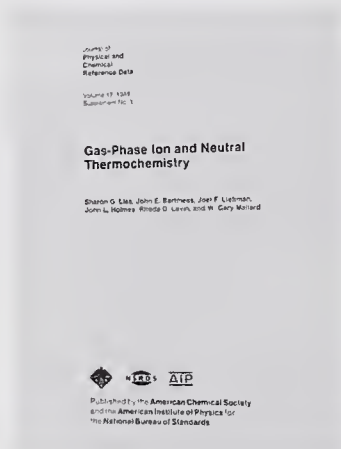


**CODATA Thermodynamic Tables. Selections for Some Compounds of Calcium and Related Mixtures: A Prototype Set of Tables** — D. Garvin, V.B. Parker, and H.J. White, Jr. (editors). Hemisphere, NY, 1987.

Prepared as the first of a series of cooperative, ongoing international projects, this volume presents recommended values for chemical thermodynamic properties of selected compounds of calcium and their mixtures. Forty-one tables of thermal functions (heat capacity, entropy, enthalpy, and Gibbs energy functions) are given for those compounds of magnesium, calcium, and potassium for which the properties have been evaluated in this work. Twenty-four tables of thermal functions are given for auxiliary substances.

Available from Hemisphere Press, NY, (800) 821-8312, \$77.00

**Gas-Phase Ion and Neutral Thermochemistry** — S.G. Lias, J.E. Bartmess, J.L. Holmes, R.D. Levin, J.F. Liebman, and W.G. Mallard. Journal of Physical and Chemical Reference Data 17, Supplement 1 (1988).



This volume includes evaluated ionization energies of 4,000 atoms and molecules and proton affinities of 1,000 compounds, as well as electron affinities and gas-phase acidities of approximately 3,000 species. The thermochemistry of the related neutral species is also provided.

Available from the American Chemical Society	
U.S. and Canada	<b>\$70.00</b>
Abroad	<b>\$84.00</b>

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**Physical and Thermodynamic Properties of Pure Chemicals** — T. E. Daubert and R. P. Danner. Hemisphere Press, NY, 1989. **Supplement 1**. Hemisphere Press, NY, 1991.

This 4-volume looseleaf set offers an encyclopedic guide to pure chemical properties and contains more than 2,000 pages of recommended physical, thermodynamic, and transport property data for 900 of the most common chemicals. Approved by the AIChE and NIST Standard Reference Data Program, this compilation contains critically evaluated, internally consistent data that follow the laws of physical chemistry.

Supplement 1 contains data on 121 additional chemicals and includes a synonyms list, references, errata for property constants, errata for references, tables for new compounds, and replacement tables for acids.

**Available Hemisphere Press, NY, (800) 821-8312, \$305.00, Supplement 1, \$95.00**

**Thermodynamic Properties of Individual Substances** — Edited by L. V. Gurvich, I. V. Veyts, and C. B. Alcock, Two volumes in two parts. Hemisphere Press, NY, 1990.

This important resource, recently updated, contains thermodynamic properties of about 1,100 condensed and gaseous substances formed by 50 elements. The first volume studies 15 elements (O, H (D, T), F, Cl, Br, I, He, Ne, Ar, Kr, Xe, Rn, S, N, P) and has numerical values in tabular format for heat capacity, entropy, Gibbs energy function, enthalpy, and equilibrium constant.

Volume 2 deals with the properties of 5 elements (carbon, silicon, germanium, tin, and lead) and their compounds with oxygen, hydrogen, halogens, sulfur, and nitrogen.

**Available Hemisphere Press, NY, (800) 821-8312, Vol. 1 \$200.00, Vol. 2 \$249.00**

# **THERMOPHYSICAL PROPERTIES OF FLUIDS**

The complexity of providing reliable data on the thermophysical properties of fluid mixtures has been the focus of considerable attention of the SRD Program. Over the years, a set of combined theoretical and empirical predictive techniques have been developed that firmly rest on evaluated data. These techniques have been tested and incorporated into interactive computer programs that will provide a large variety of properties based upon the specified composition and the appropriate state variables.

Databases are now available for hydrocarbon mixtures, including natural gas, as well as a number of pure and mixed fluids of industrial importance. The database REFPROP has proven to be a valuable tool for refrigeration engineers, chemical and equipment manufacturers, and others who use chlorofluorocarbons.

## **SRD Fluids Properties Databases**

NIST Thermophysical Properties of Hydrocarbon Mixtures

NIST Thermophysical Properties of Fluids

NIST Mixture Property Program

NIST Thermophysical Properties of Refrigerants and Refrigerant Mixtures

**Contact us for information on new and upcoming databases  
(301) 975-2208**

# THERMOPHYSICAL PROPERTIES OF FLUIDS DATABASES

## 4. NIST Thermophysical Properties of Hydrocarbon Mixtures

Marcia Huber  
Fluid Mixtures Data Center  
National Institute of Standards and Technology  
Boulder, CO 80303  
(303) 497-5252

This powerful database (also called SUPERTRAPP) is an interactive program for predicting thermodynamic properties of pure fluids and fluid mixtures of up to 20 components. The components are selected from a database of 116 components, mostly hydrocarbons. SUPERTRAPP performs phase equilibria calculations and gives the thermodynamic properties of all phases and the feed. These results include:

### *Equilibrium properties*

- density
- compressibility factor
- enthalpy
- entropy
- $C_p$
- $C_p/C_v$
- sound speed
- Joule-Thomson coefficient

### *Transport properties*

- viscosity
- thermal conductivity

SUPERTRAPP features commands that allow you to:

- perform bubble point pressure calculations
- perform dew point pressure calculations
- perform isothermal flash calculations
- obtain properties of pure components along the saturation boundary
- produce tables of properties along isobars or isotherms
- change units
- learn (and remember) a new component not in the current database
- enter data from the keyboard or from data files
- save results in a file

SUPERTRAPP comes on both 5¼" and 3½" high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.



## **12. NIST Thermophysical Properties of Fluids**

**Daniel G. Friend  
Fluid Mixtures Data Center  
National Institute of Standards and Technology  
Boulder, CO 80303  
(303) 497-5424**

This interactive database (called MIPROPS) computes thermophysical properties of 12 important industrial pure fluids: helium, argon, parahydrogen, oxygen, nitrogen, nitrogen trifluoride, ethylene, methane, ethane, propane, isobutane, and normal butane. The database provides prompting for selection of several options including choice of fluid, choice of units, and choice of single phase or liquid vapor phase calculations.

Properties are computed for the single phase region from input of two of the following variables: temperature, pressure, and density. Values on the liquid-vapor boundary are computed for either a given temperature or a given pressure. The database returns values for pressure, temperature, density, internal energy, enthalpy, entropy, specific heats at constant volume, pressure, and sound velocity. Viscosity, thermal conductivity, and dielectric constants are given for five of the fluids.

This database is available in PC diskette and magnetic tape format. It can also be used on Macintosh computers which have a PC emulator program.

## **14. NIST Mixture Property Database**

**Daniel G. Friend  
Fluid Mixtures Data Center  
National Institute of Standards and Technology  
Boulder, CO 80303  
(303) 497-5424**

The NIST Mixture Property Database (also called DDMIX) is a database which calculates various thermodynamic and transport properties of mixtures of fluids selected from any of 17 possible pure components. The emphasis of the database is on density prediction (especially for CO<sub>2</sub>-rich mixtures), but it will provide accurate results for other properties and mixtures.

All phase equilibrium calculations are performed with the Peng-Robinson equation of state, and co-existing phase properties are calculated with the NIST extended corresponding states model (DDMIX). Mixtures formed from any of 17 pure components (including hydrocarbons, nitrogen, oxygen, argon, carbon monoxide, carbon dioxide, and hydrogen sulfide) are handled by the database.

DDMIX provides the following outputs for any specified mixture:

- bubble point pressure
- dew point pressure
- saturation properties
- tables of density, enthalpy, entropy, and heat capacity as functions of T or P
- isothermal flash calculation yielding density, enthalpy, entropy, heat capacity, viscosity, and thermal conductivity of feed and vapor

This database is available in PC diskette format. It can also be used on Macintosh computers which have a PC emulator program.

### **23. NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures Version 3.0**



**John Gallagher**  
**Thermophysics Division**  
**National Institute of Standards**  
**and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-2455**

The refrigerants whose properties can be calculated from this program include:

R11	R14	R114	R125	R142b
R12	R22	R115	R134	R152a
R13	R23	R123	R134a	RC270
R13B1	R113	R124		

The program allows for the calculation of the properties of up to five mixtures. Version 3.0 adds two additional properties — viscosity and thermal conductivity — and has a “canned” rule for estimating interaction parameters for mixtures. This rule predicts the existence of 65 azeotropic mixtures, which may be used as alternative refrigerants.

REFPROP Version 3.0 provides equilibrium parameters for seven additional pure fluids:

E134	R218	R21	R290
R141b	RC318	R143	

This database is available on both 5¼” and 3½” high and low density diskettes. It can also be used on Macintosh computers which have a PC emulator program.



## 10. NIST Thermophysical Properties of Water

**John S. Gallagher**  
**Thermophysics Division**  
**National Institute of Standards and Technology**  
**Gaithersburg, MD 20899**  
**(301) 975-2455**

This database consists of an interactive program which calculates the thermodynamic properties of fluid  $\text{H}_2\text{O}$  (liquid and vapor) using the formulation as approved by the International Association for the Properties of Steam (IAPS) at its Tenth International Conference in 1984.

The interactive FORTRAN 77 program consists of three parts. The first part contains a package of subroutines to calculate the thermodynamic and transport properties of fluid  $\text{H}_2\text{O}$ . The other parts are main programs which call these routines to generate properties of  $\text{H}_2\text{O}$  interactively.

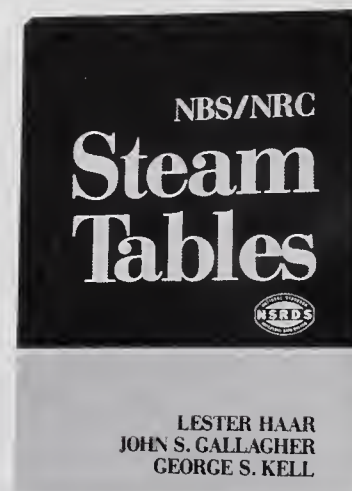
The main program allows the calculation and display of all properties at a single pair of independent variables:

pressure — temperature  
density — temperature  
entropy — temperature  
enthalpy — temperature  
enthalpy — pressure

The second main program allows the generation of tables of properties along isotherms, isobars, or isochores. To keep the tabular form compact, the user may choose which properties are to be displayed.

The range approved by IAPS for this formulation includes temperatures from 0 to 1000 °C and pressures up to 1500 MPa. The range over which usable results will be obtained extends to 2500 K and to 3000 MPa. This database is available in both magnetic tape and PC diskette versions. It can also be used on Macintosh computers which have a PC emulator program.

The printed version of this database, which includes a description of the data selection and evaluation procedures, is found in NBS/NRC Steam Tables — L. Haar, J.S. Gallagher, and G.S. Kell, Hemisphere Press, Washington, DC 1984.





## **THERMOPHYSICAL PROPERTIES OF FLUIDS PUBLICATIONS**

**Evaluation of Solubility Data of the System CO<sub>2</sub>-H<sub>2</sub>O from 273 K to the Critical Point of Water** — Rosa Crovetto. *Journal of Physical and Chemical Reference Data* **20**, 590 (1991).

Measurement on the solubility of carbon dioxide in water in the range of 273-647 K are reviewed and evaluated. Recommended values of the solubility are presented in the form of Henry's constants as a function of temperature and density.

**Available from American Chemical Society, Reprint 416, \$5.00**

**Thermophysical Properties of Ethane** — Daniel G. Friend, Hepburn Ingham, and James F. Ely. *Journal of Physical and Chemical Reference Data* **20**, 275 (1991).

Data on the thermodynamic and transport properties of ethane have been reevaluated and correlated using a new set of functions. A new equation of state is presented, which is accurate in the range of 90-625 K at pressures up to 70 MPa. Tables of recommended thermophysical properties are also provided.

**Sixteen Thousand Evaluated Experimental Thermodynamic Property Data for Water and Steam** — H. Sato, K. Watanabe, J. M. H. Levelt Sengers, J. S. Gallagher, P. G. Hill, J. Straub, and W. Wagner. *Journal of Physical and Chemical Reference Data* **20**, 1023 (1991).

As part of the activities of the International Association for the Properties of Water and Steam, all reliable sources of experimental data on the thermodynamic properties of ordinary (light) water and steam have been collected and converted to common temperature, pressure, volume, mass, and heat scales. Properties include the volume, enthalpy, heat capacities, sound velocity, internal energy, and Joule-Thomson and related coefficients.

**Available from American Chemical Society, Reprint 424**

# **NIST SPECIAL DATABASES**

## **1. NIST Binary Images of Printed Digits, Alphas, and Text**

**Charles Wilson  
National Institute of Standards and Technology  
Gaithersburg, MD 20899  
(301) 975-2080**

The NIST handprinted character database consists of 2,100 pages of bilevel, black and white image data of hand printed numerals and text with a total character count of over 1,000,000 characters. This database totals approximately 3 gigabytes of image data with 273,000 numerals and 707,700 alphabetic characters. With the sample taken from the Bureau of Census field staff and also geographically sampled, the database has the following features:

- over 1,000,000 character images
- 300 pixel/inch resolution
- images of full pages of data
- images of numbers with 2, 3, 4, 5, and 6 digits
- images of full alphabets
- images of unconstrained text

Suitable for both character recognition system research, development, and evaluation, the data set can be used for:

- field isolation: locating the text on the page
- character segmentation: separating the text into characters
- character recognition: identifying specific characters

The database is also a valuable tool for measurement of system performance and system comparison.

The system requirements are a CD-ROM drive with software to read ISO 9660 format.

## **2. NIST Structured Forms Reference Set of Binary Images**



**Charles Wilson  
National Institute of Standards  
and Technology  
Gaithersburg, MD 20899  
(301) 975-2080**

The NIST structured forms database consists of 5,590 pages of binary, black and white images of synthesized documents. The documents in this database are 12 different tax forms from the IRS 1040 Package X for the year 1988. These include Forms 1040, 2106, 2441, 4562, and 6251 together with Schedules A, B, C, D, E, F, and SE. Eight of these forms contain two pages or form faces; therefore, there are 20 different form faces represented in the database. The document images in this database appear to be real forms prepared by individuals, but the images have been automatically derived and synthesized using a computer. There are 900 simulated tax submissions represented in the database averaging 6.2 form faces per submission. This significant new database totals approximately 5.9 gigabytes of uncompressed image data including image format documentation and example software. The database has the following features:

- 900 simulated tax submissions
- 5,590 images of completed structured form faces
- 300 pixel/inch resolution
- 5,590 text files containing entry field answers
- 20 tables of entry field types and contexts
- image format documentation and example software

This database is a valuable tool for measurement of system performance and system comparison on complex forms.

The system requirements are a CD-ROM drive with software to read ISO-9660 format.





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Phone: (215) 328-9400

<sup>2</sup>Available from NACE, P.O. Box 218340, Houston, TX 77218. Phone: (713) 492-0535

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To obtain a FREE NIST Standard Reference Materials Catalog call the SRM sales office (301) 975-6776, or write to the address below.

Standard Reference Materials Program  
National Institute of Standards and Technology  
Building 202, Room 204  
Gaithersburg, MD 20899

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## NEW CALIBRATIONS USERS GUIDE

The National Institute of Standards and Technology (NIST) Calibration Services Users Guide provides detailed descriptions of currently available NIST calibration services, measurement assurance programs, and special-test services. The following measurement areas are covered: (1) dimensional; (2) mechanical, including flow, acoustic and ultrasonic; (3) thermodynamic; (4) optical radiation; (5) ionizing radiation; and (6) electromagnetic, including dc, ac, rf, and microwave. A separate Fee Schedule is issued annually, providing current prices for the services offered, updates on points-of-contact, and information on measurement seminars.

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The physical measurement services of the National Institute of Standards and Technology (NIST) are designed to help the makers and users of precision instruments achieve the highest possible levels of measurement quality and productivity. The hundreds of individual services you will find listed and described in this Users Guide constitute the highest order calibration services available in the United States. They directly link a customer's precision equipment or transfer standards to national measurement standards. These services are offered to public and private organizations and individuals alike.

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This Users Guide is designed to make the task of selecting and ordering an appropriate calibration service and quick and easy as possible. Nevertheless, questions will arise. When they do, we urge you to call or write for immediate clarification. Address general questions and lengthy inquiries to:

Calibration Program  
National Institute of Standards and Technology  
Building 411, Room A104  
Gaithersburg, MD 20899-0001  
Telephone: (301) 975-2002  
Telefax: (301) 975-2128



# **NIST** *Technical Publications*

## ***Periodical***

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