NIST STANDARD REFERENCE DATA PRODUCTS CATALOG 1993

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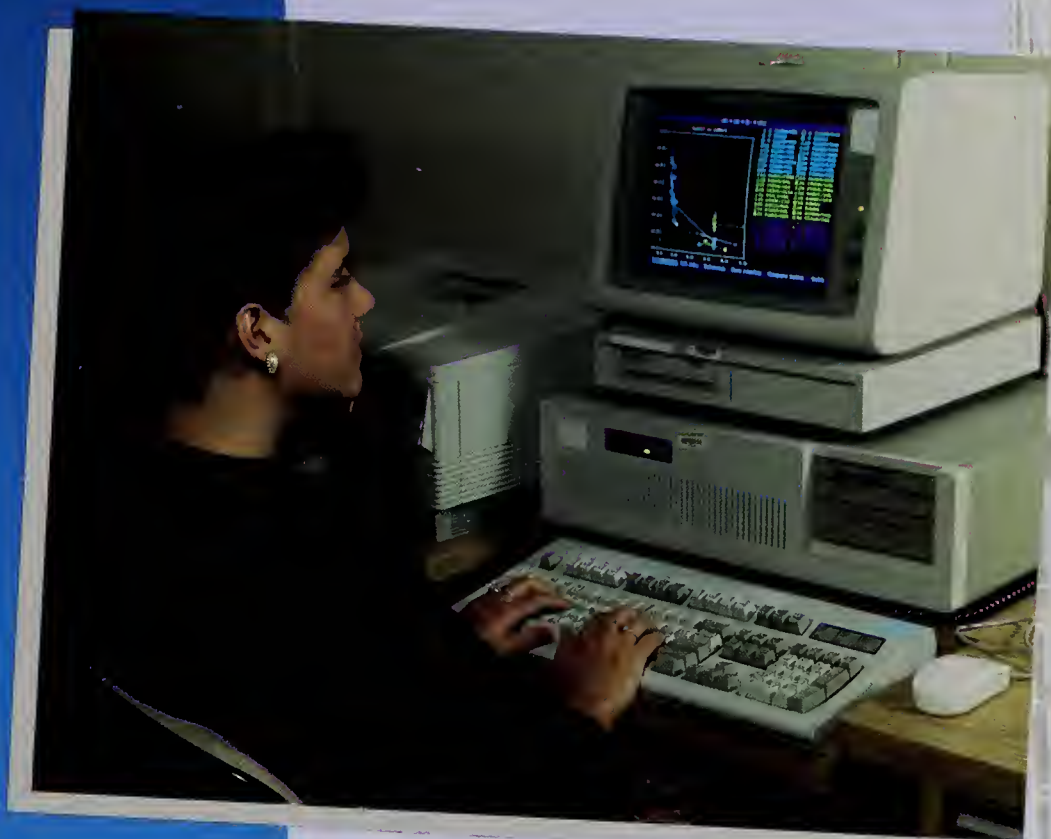
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U.S. DEPARTMENT OF COMMERCE
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NIST STANDARD REFERENCE DATA PRODUCTS CATALOG 1993

U.S. DEPARTMENT OF COMMERCE
Barbara Hackman Franklin, *Secretary*

Technology Administration
Robert M. White, *Under Secretary for Technology*

National Institute of Standards and Technology
John W. Lyons, *Director*

ACKNOWLEDGMENTS

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: chemistry; compilations; databases; evaluated data; materials; numeric data; physics

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 details the policy of Congress to make reliable, critically evaluated data compilations available to scientists, engineers, and the general public.

Fulfilling data needs for thirty years, the SRD Program provides evaluated data which are vital to industry.

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 30 years. Standard reference data have 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 are even more accessible and play a more critical role in technological advancement each year. With this, the fourth annual Standard Reference Data Products Catalog, we want to make the scientific community more aware of our highly evaluated, high-quality data in all of its many forms. *We value your comments on any of our products*. Please let us know how we can improve existing software and databases and what new areas to explore in order to fulfill your data needs and increase your productivity.

NIST SPECIAL SOFTWARE

1. NIST Scoring Package Release 1.0

NEW!

Michael Garris
National Institute of
Standards and Technology
Gaithersburg, MD 20899
(301) 975-2928

This software was used to score the results from the First Census Optical Character Recognition (OCR) System Conference sponsored by the Bureau of the Census and hosted by NIST. A User's Guide is provided which presents the concepts of scoring forms processing systems and character classifiers, discusses the concepts and the algorithm used for dynamic string alignment, defines the files and their formats required as input to the Scoring Package, and documents how the Scoring Package software is installed and invoked.

This software release has the following features:
- supports both form-based and character-based scoring
- applicable to a wide variety of structured forms
- can be used in conjunction with NIST Special Databases (SD1, SD2, SD3, SD6, & SD7)
- supports user-defined form structures
- includes scoring examples from forms and isolated characters

The NIST Scoring Package can be used to:
- determine if OCR technology is economically advantageous to deploy for a specific application
- determine which OCR product is best suited for a specific application
- choose from a large variety of diverse algorithmic approaches when developing OCR systems

The NIST Scoring Package has the following attributes and requirements:
- written in the 'C' progamming language and UNIX shell languages
- developed to run on a UNIX system running SunOS 4.1.1
- distributed on a 5.25" CD-ROM
- requires a CD-ROM drive with ISO-9660 format software
- utilizes 5 megabytes of magnetic disk storage upon installation and compilation

Order FORM & Price List

The following prices on databases represent one location use. For distributor agreements, online agreements, and more than one location pricing, please contact Standard Reference Data.

☐ I would like more information on the databases checked.

☐ I am ordering the databases checked.

☐ I am enclosing a check or purchase order payable to the National Institute of Standards and Technology.

☐ I am enclosing Visa or MasterCard information.

Number _____

Expiration Date _____

1. NIST/EPA/NIH Mass Spectral: ASCII Version	$ 1,200.00
1A. NIST/EPA/NIH Mass Spectral: PC Version 4.0	1,200.00
1B. NIST Mass Spectral Database of Common Compounds	350.00
2. NIST Chemical Thermodynamics	1,000.00
3. NIST Crystal Data[1]	2,000.00
4. NIST Thermophysical Properties of Hydrocarbon Mixtures	490.00
7. NIST Electron and Positron Stopping Powers of Materials	300.00
8. NIST X-Ray and Gamma-Ray Attenuation Coefficients and Cross Sections	400.00
10. NIST Thermophysical Properties of Water	300.00
11. DIPPR Data Compilation of Pure Compound Properties Verson 7.0	3,000.00
11A. Student DIPPR	75.00
12. NIST Thermophysical Properties of Pure Fluids Version 3.0 (with Source Code)	415.00 550.00
13. NIST JANAF Thermochemical Tables	1,200.00
14. NIST Mixture Property Program	400.00
15. NIST/Sandia/ICDD Electron Diffraction[1]	3,000.00
16. NACE/NIST Corrosion Performance COR*SUR 1[2] COR*SUR 2[2]	 270.00 240.00
17. NIST Chemical Kinetics Version 4.0	390.00
18. NIST Estimation of the Thermodynamic Properties for Organic Compounds at 298.15 K	215.00
19AB. NIST Positive and Negative Ion Energetics	130.00

INTRODUCTION

Since 1968, the NIST Standard Reference Data (SRD) Program has been providing reliable, well-documented reference data to scientists and engineers for use in technical problem-solving, research, and development. As we enter the mid-nineties, SRD is poised to provide a wide array of data compilations with sophisticated software. Our tradition of quality continues with a growing list of new and updated databases.

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 databases.

The Standard Reference Data booth appears at many scientific conferences and meetings. Please stop by to give us your comments on our 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 activities concentrate in the following disciplines:

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

Atomic Physics — atomic energy levels and wavelengths, transition probabilities, and collisional data used for diagnostics 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 and solution reactions.

Materials Properties — structure and characterization of materials, performance properties, including tribology and mechanical corrosion, and phase equilibria.
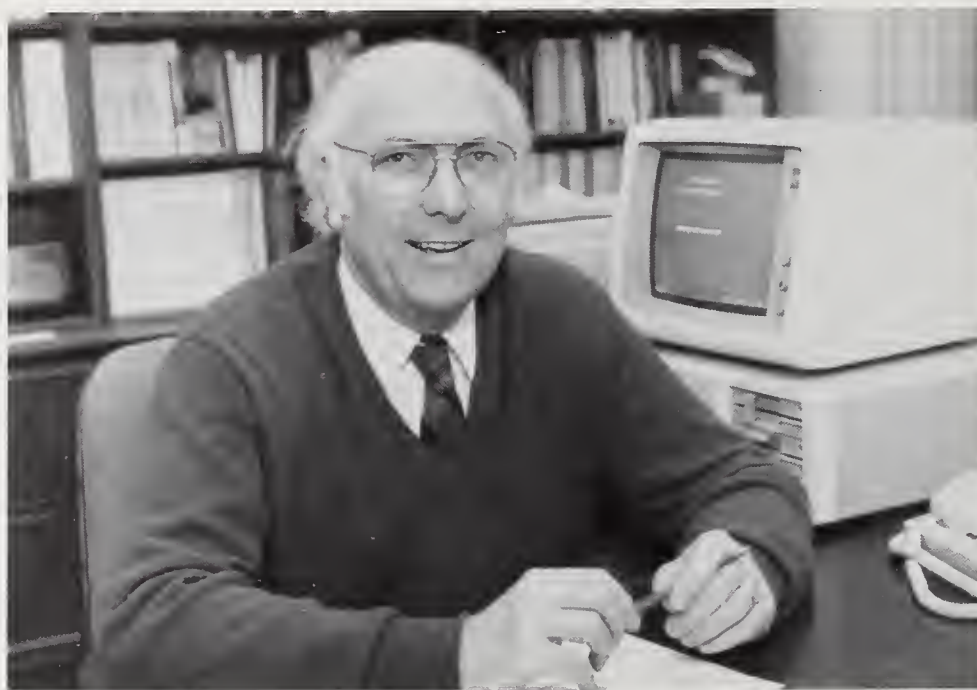
Dr. Malcolm W. Chase is Chief of the Standard Reference Data Program.

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 critical importance to industry.

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The data collections resulting from the work of the SRD Program are disseminated in different ways:

National Standard Reference Database Series
— Databases on diskettes, CD-ROM, 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. The 20 year-plus tradition of significant data compilations continues as Dr. Jean W. Gallagher succeeds Dr. David R. Lide as new Editor of the *Journal*.

Other Publications
— Journal articles and books published with technical society and private publishers.

Dr. Jean W. Gallagher is the new editor for the **Journal of Physical and Chemical Reference Data.**


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

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ORDERING INFORMATION

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

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

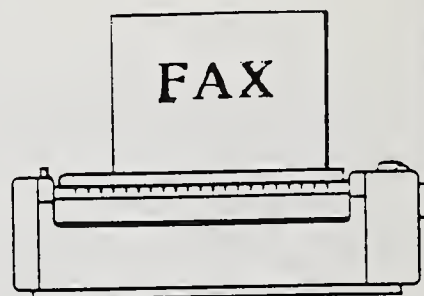# THREE EASY WAYS TO ORDER!
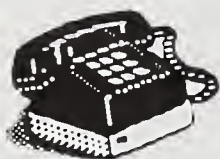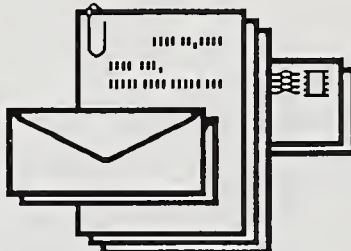
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STANDARD REFERENCE DATABASES

ANALYTICAL CHEMISTRY

NIST/EPA/NIH Mass Spectral

NIST/EPA/NIH Mass Spectral:
PC Version (UPDATED)

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

NIST/EPA Gas-Phase Infrared (NEW)

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

NIST Wavenumber Calibration Tables
(NEW)

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

STANDARD REFERENCE DATABASES *(continued)*

BIOTECHNOLOGY

NIST/CARB Biological Macromolecule
Crystallization **(UPDATED)**

CHEMICAL KINETICS

NIST Chemical Kinetics **(UPDATED)**

NDRL/NIST Solution Kinetics **(NEW)**

MATERIALS PROPERTIES

NACE/NIST Corrosion Performance

NIST Tribomaterials I (ACTIS)

NIST Structural Ceramics **(UPDATED)**

Phase Diagrams for Ceramists

NIST Surface Structure **(NEW)**

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

STANDARD REFERENCE DATABASES *(continued)*

MOLECULAR STRUCTURE AND SPECTROSCOPY

NIST Vibrational and Electronic Energy of Small Polyatomic Transient Molecules

THERMODYNAMICS AND THERMOCHEMISTRY

NIST Structures and Properties Database and Estimation Program

NIST Positive and Negative Ion Energetics

NIST JANAF Thermochemical Tables

NIST JANAF Shomate Coefficients (NEW)

NIST Molten Salts: Single Salts and Mixtures

THERMOPHYSICAL PROPERTIES OF FLUIDS

NIST Thermophysical Properties of Hydrocarbon Mixtures

NIST Thermophysical Properties of Water

NIST Thermophysical Properties of Pure Fluids (UPDATED)

NIST Mixture Property Program

NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures (UPDATED)

NIST Heat Capacities of Liquids (NEW)

The SRD Database series continues to grow at a rapid pace. We update and add several new databases each year.

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STANDARD REFERENCE DATABASES *(continued)*

NIST SPECIAL DATABASES

NIST Binary Images of Printed Digits, Alphas, and Text

NIST Structured Forms Reference Set of Binary Images

NIST Binary Images of Handwritten Segmented Characters (NEW)

NIST 8-Bit Gray Scale Images of Fingerprint Image Groups (NEW)

IVTANTHERMO (NEW)

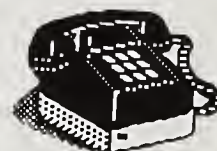NIST Structured Forms Reference Set of Binary Images 2 (NEW)

NIST Test Data 1: Binary Images of Handprinted Segmented Characters (NEW)

NIST Machine-Print Database of Gray Scale and Binary Images (NEW)
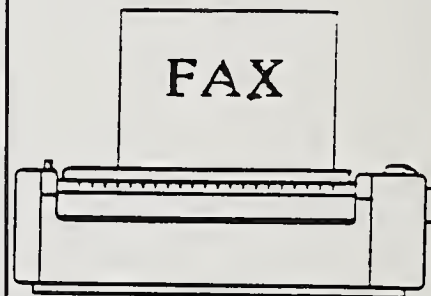
NIST SPECIAL SOFTWARE

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Contact us for information on new and upcoming databases
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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, single crystal and electron diffraction.

In every case, the data have been fully evaluated using a variety of techniques. When appropriate, duplicate measurements have been included for completeness. All databases are updated and expanded on a regular basis. The PC version of these databases has sophisticated software that enables a search that will take only seconds of your time.

The NIST/EPA/NIH Mass Spectral Database continues to reach an ever-widening audience. Meticulously evaluated by mass spectrometry experts, all spectra were recently reevaluated on an individual basis. It includes thousands of spectra of diverse compounds, such as pharmaceuticals, flavors and fragrances, and compounds of industrial and environmental interest.

The brand-new NIST/EPA Gas-Phase Infrared Database contains FT-IR absorption spectra for over 5,200 compounds and is a combined compilation of spectra from NIST and the Environmental Protection Agency. It has the same easy to use software as the Mass Spectral Database.

The 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.

Would you like to be on SRD's mailing list?
Call and let us know.

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

Infrared

NIST/EPA Gas-Phase Infrared

Surface Data

NIST X-Ray Photoelectron Spectroscopy

Diffraction Data

NIST/Sandia/ICDD Electron Diffraction

NIST Crystal Data Identification

Spectrum Analysis

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

SRD Major Publications in Analytical Chemistry

Crystal Data Determinative Tables (6 vols.)

Elemental and Interplanar Spacing Index

ANALYTICAL CHEMISTRY DATABASES

1. NIST/EPA/NIH Mass Spectral Database

UPDATED!

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

This 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 compounds. Categories of substances identified are steroids, alkaloids, drugs, derivatives, amino acids, metals, carbohydrates, fatty acids and lipids, pesticides, and primary pollutants.

This new updated version has undergone a major data evaluation assessment program with retention of only the highest quality spectra. 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 and as a CD-ROM. It is widely used in the mass spectrometers of many commercial instrument manufacturers.

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

UPDATED!

The first PC Version of the NIST/EPA/NIH Mass Spectral Database was released in September 1987. It was hailed at the time as an impressive, well-designed breakthrough designed to make searching this important database easy. 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. A quickly-learned interface allows the data to be searched by:
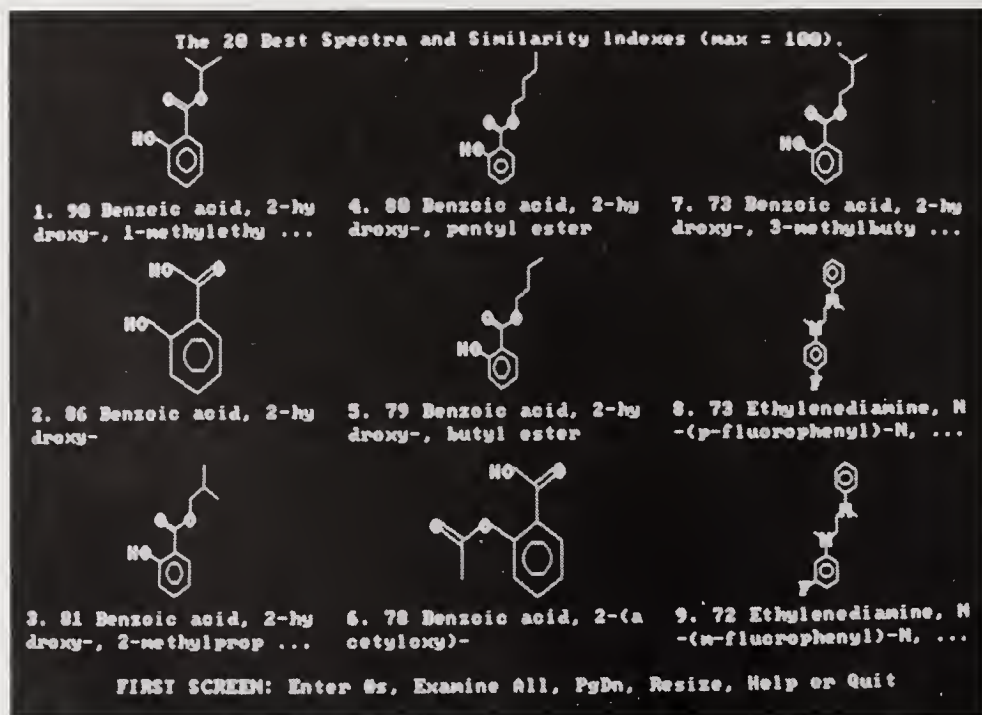
- identification number
- CAS Registry Number
- chemical name (including tens of thousands of alternative names)
- molecular formula
- any peaks (up to 10 peaks with an intensity range for each)
- major peaks (up to 3 ordered peaks)
- your spectrum (choose quick, standard, or extensive search options)
- neutral losses
- highest mass peak

This collection of over 62,000 different compounds is the only large mass spectrometric collection comprised almost entirely of complete spectra.

Various display features are available:

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

The database has spectra of diverse compounds, such as pharmaceuticals, flavors and fragrances, and compounds of industrial and environmental interest. Virtually all compounds have structures included.
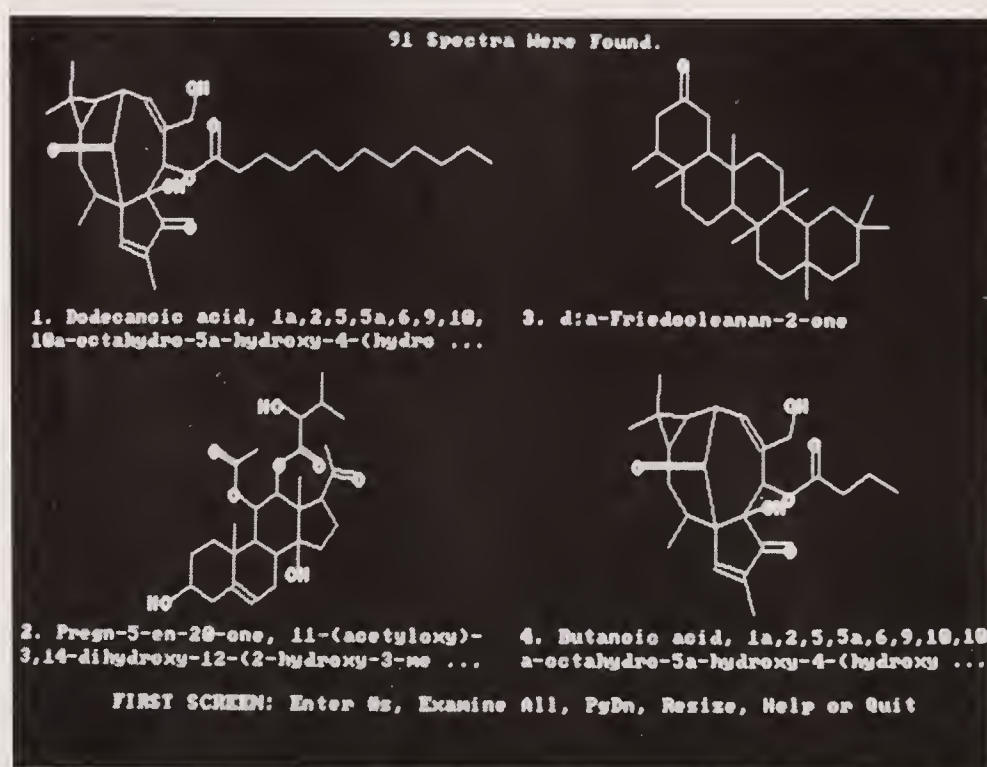
This important PC database provides a powerful tool for locating a particular spectrum or for identifying spectra of unknown compounds. It is regularly updated. It comes on both 5¼" and 3½" high density diskettes. It can also be used on Macintosh computers which have a PC emulator program. A CD-ROM version is planned.

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

Robert L. Myklebust/Carol Swyt
Surface and Microanalysis Sciences Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3926

This computer program, also called DTSA, 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 a detailed analysis of a collection of spectra at one's desktop.
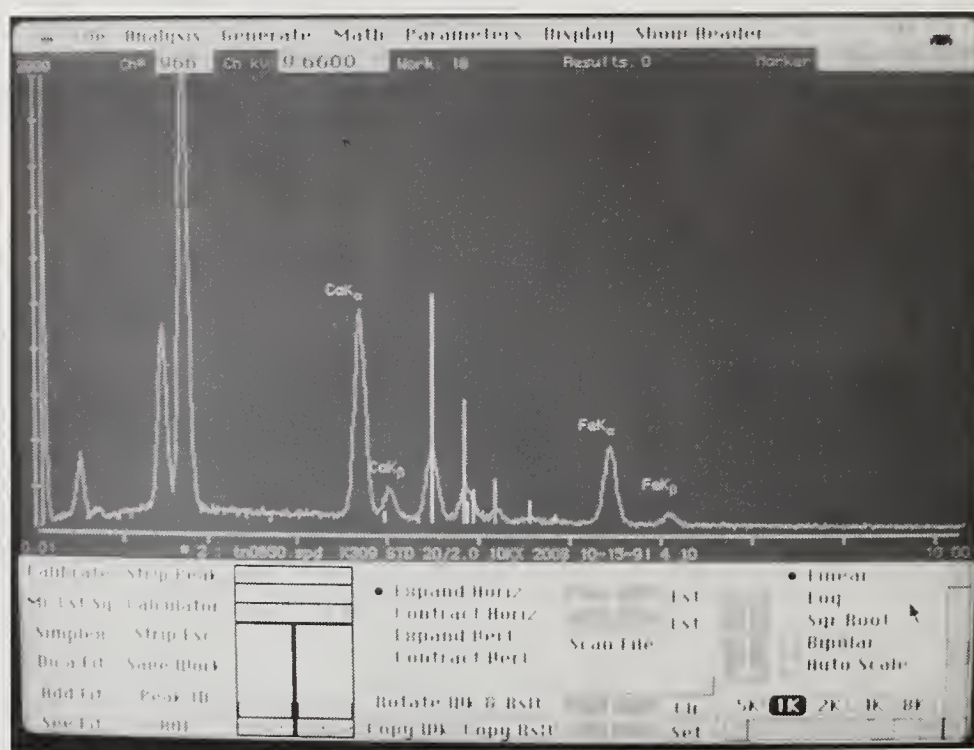
Some features of the program:

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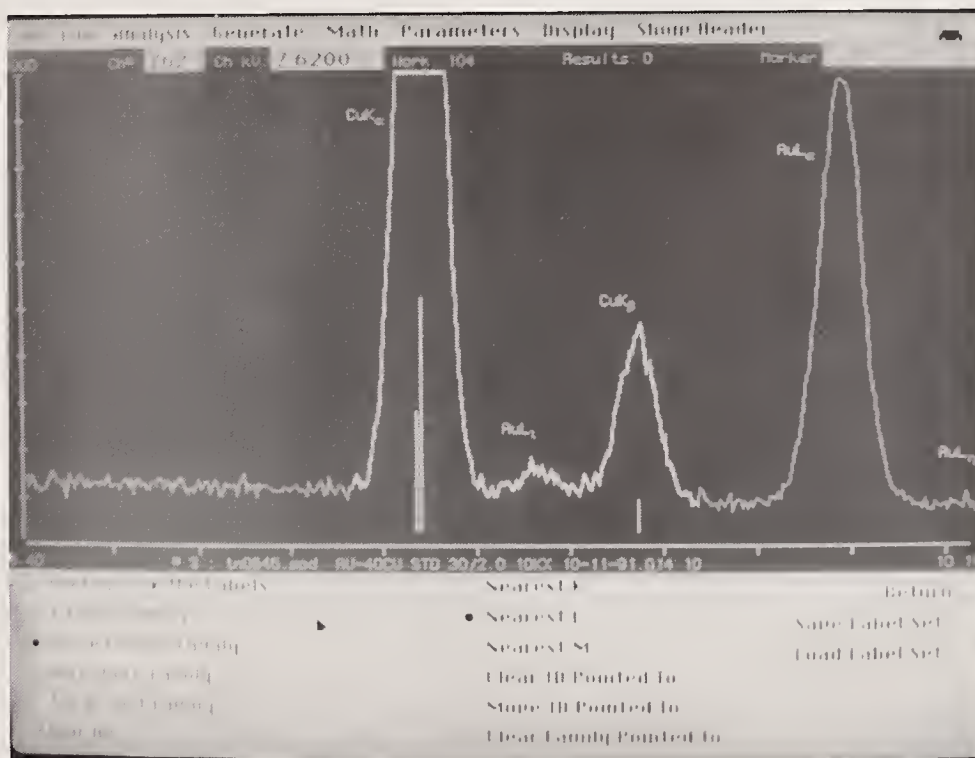
This program/database is a fully functioning multi-channel analyzer.

3. NIST Crystal Data

Alan D. Mighell
Crystal Data and Electron Diffraction Data 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 the Canada Institute for Scientific and Technical Information (CISTI's) online international service. For further information, please contact International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081. Phone: (215) 328-9400.

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

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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, 1601 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.

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

Each record in 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. Regular updates are scheduled. The program can be used on Macintosh computers which have a PC emulator program.

35. NIST/EPA Gas-Phase Infrared Database

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

NEW!

This significant new database contains FT-IR absorption spectra for over 5,200 compounds and represents a combined compilation of the National Institute of Standards and Technology and the Environmental Protection Agency. The spectra have been meticulously evaluated and low-quality spectra eliminated. This database has a modern intuitive user interface — built from the widely-used NIST/EPA/NIH Mass Spectral Database software.

Search Options
- up to 10 absorption maxima (wavelength and intensity)
- chemical name
- empirical formula

Additional Search Constraints
- name fragment
- molecular weight
- elemental composition
- presence in other specialized databases

More Features
- directly compare up to 4 spectra
- read external FT-IR files for comparison plots
- context sensitive help

This database is available in 5¼" and 3½" diskettes. A flat file of JCAMP raw data is also available.

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

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.

NIST Spectroscopic Properties of Atoms and Atomic Ions has reached a wide audience in the past year. This database provides easy access to prominent emission wavelengths for all neutral atoms and their first four stages of ionization. The new Wavenumber Calibration Tables Database contains the most accurate atlas available for the calibration of infrared spectrometers.

SRD Atomic Databases

NIST Spectroscopic Properties of Atoms and Atomic Ions

NIST Wavenumber Calibration Tables

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)

SRD Major Publications in Atomic Data

1986 CODATA Recommended Values of the Fundamental Physical Constants

Atomic Transition Probabilities Publications

Atomic Energy Levels Publications

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 interactive PC database provides easy access to prominent emission wavelengths for all neutral atoms and their first four stages of ionization. These data originally appeared in the well-known and widely-used NSRDS-NBS 68 — *Wavelengths and Transition Probabilities for Atoms and Atomic Ions. Part I. Wavelengths.*

Atomic masses, ground-state configurations, and terms and ionization potentials for the neutrals and ions are also included. For stable isotopes, abundances, nuclear spins, and dipole and quadrupole moments are also given. Wavelength line lists for individual elements may be written to external files.

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

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

39. NIST Wavenumber Calibration Tables

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

The information in this diskette package is a supplement to NIST Special Publication 821 — *Wavenumber Calibration Tables from Heterodyne Frequency Measurements*. This publication contains the most accurate atlas to date for the calibration of infrared spectrometers. Accuracy has been increased because data are based on frequency rather than wavelength measurement techniques for absolute references. The best Fourier transform measurements available were used for different frequency measurements. A description of the heterodyne frequency measurement techniques, details of the analysis including the Hamiltonians and least-squares-fitting and calculation procedures are also given. Intensities and lineshape parameters are included.

The primary calibration molecules are the linear triatomics, carbonyl sulfide (OCS) and nitrous oxide (N_2O), which cover portions of the infrared spectrum ranging from 488 to 3120 cm^{-1}. Some gaps in the coverage afforded by OCS and N_2O are partially covered by NO, CO, and CS_2. An additional region from 4000 to 4400 cm^{-1} based on CO is also included.

Statistically determined and documented uncertainties for the listed transitions are given as well as a discussion of the intensity calculations and pressure shifts, and a bibliography of frequency and intensity measurements.

The data files are available in 5¼" and 3½" disks. They can be used on Macintosh computers which have a PC emulator program.

7. NIST Electron and Positron Stopping Powers of Materials

Stephen 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 calculations 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.

The 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

Stephen 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 enables the user to obtain data by entering chemical formulas or other defining 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.
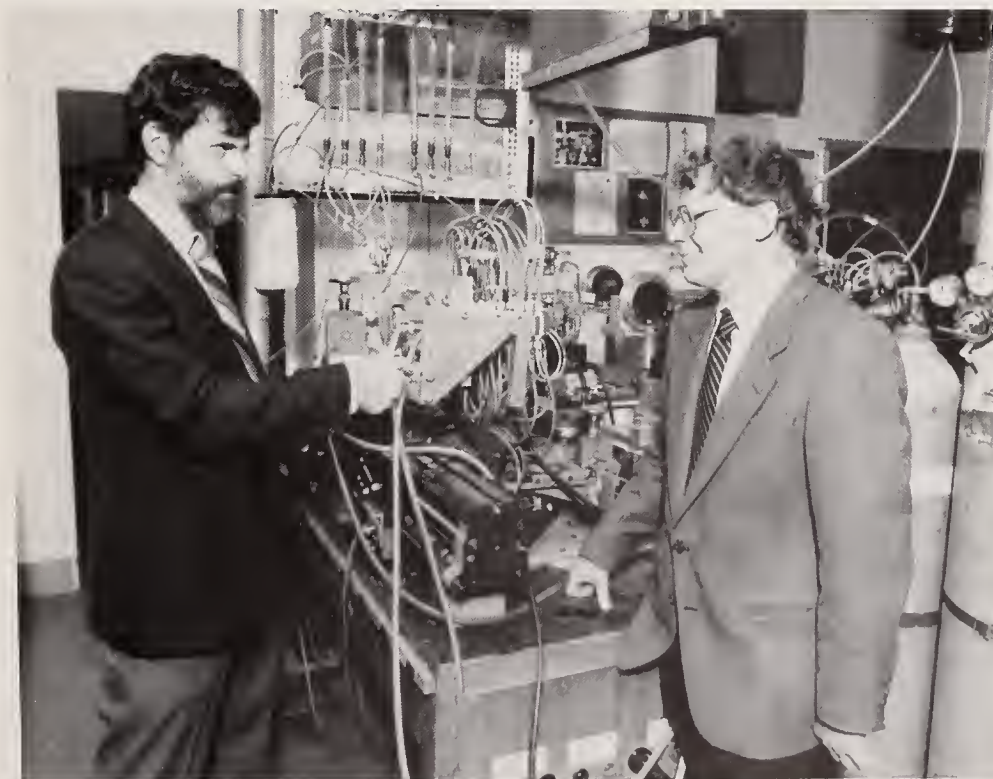
The user may request data to be tabulated at the fixed energies stored in the database, or at an arbitrary set of user-specified energies, or at a combination of both. The tabulated results include the individual contributions and the total mass attenuation coefficient, both with and without coherent 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 in modeling programs.

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.

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

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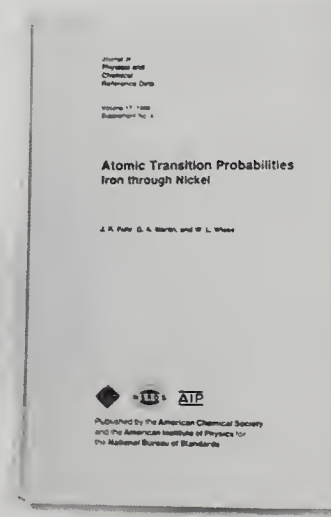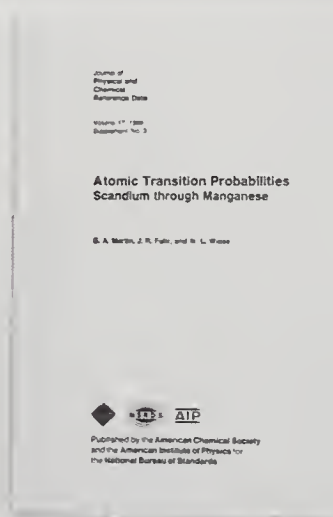
Atomic Energy Levels of the Iron-Period Elements: Potassium through Nickel — J. Sugar and C. Corliss. Journal of Physical and Chemical Reference Data **14**, Supplement 2 (1985).

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	**$50.00**
Abroad	**$58.00**
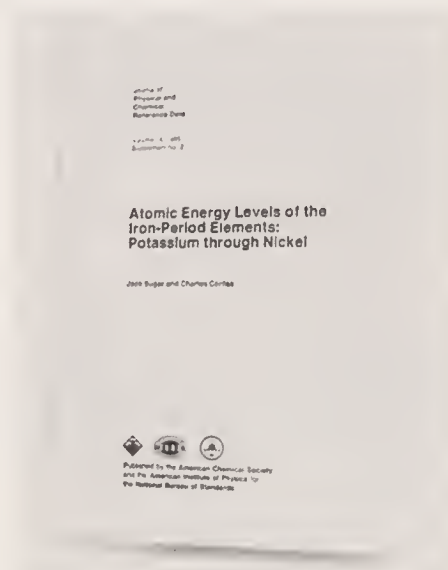
Atomic Weights of the Elements 1989 — J.R. de Laeter. Journal of Physical and Chemical Reference Data **20** (1991).

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, JPCRD Reprint 429, $10.00

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

Spectral Data and Grotrian Diagrams for Highly Ionized Cobalt, Co VIII through Co XXVII — Toshizo Shirai, Alberto Mengoni, Yohta Nakai, Jack Sugar, Wolfgang L. Wiese, Kazuo Mori, and H. Sakai. Journal of Physical and Chemical Reference Data **21**, 23 (1991).

Recommended wavelengths, energy levels, and transition probabilities for highly ionized cobalt ions are tabulated. Grotrian diagrams are also presented to give an overview of the spectra.
Available from the American Chemical Society, JPCRD Reprint 433, $22.00

Spectral Data and Grotrian Diagrams for Highly Ionized Vanadium, V VI through V XXIII — Toshizo Shirai, Toshiaki Nakagaki, Jack Sugar, and Wolfgang L. Wiese. Journal of Physical and Chemical Reference Data **21**, 273 (1992).

Recommended wavelengths, energy levels, and transition probabilities for highly ionized vanadium ions are tabulated. Grotrian diagrams are also presented to give an overview of the spectra.
Available from the American Chemical Society, JPCRD Reprint 437, $24.00

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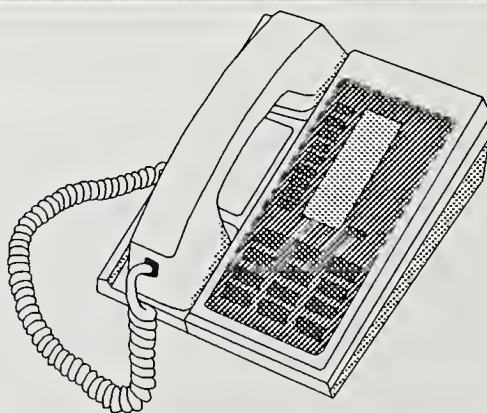
BIOTECHNOLOGY

Standard Reference Data has developed new databases for the burgeoning new biotechnology field which are proving to be valuable research tools for biochemists. A significant new upgrade to the NIST/CARB Biological Macromolecule Crystallization Database. This provides convenient sources of existing knowledge and eliminate tedious time at the library. Regular updates are planned.

SRD Biotechnology Databases

NIST/CARB Biological Macromolecule Crystallization

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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 database contains crystal data and the crystallization conditions of 1,476 crystal forms of 930 biological macromolecules. The data have been extracted from the scientific literature through 1989.

This system provides a fast and convenient method of searching the crystallization data for any of the parameters listed below:

Macromolecule
1. Macromolecule name
2. Biological source
3. Molecular weight
4. Subunit composition
5. Prosthetic group
6. Multiple crystal forms

Crystal Data
7. Space group
8. Unit cell dimension
9. Z
10. Crystal density

Crystallization Conditions
11. Crystallization method
12. Macromolecule concentration
13. Temperature of crystallization
14. pH of crystallization
15. Crystal growth time
16. Chemical additions to crystallization solution

Reference
17. Author
18. Year reported
19. Journal

The system provides a convenient method for verifying whether or not a particular biological macromolecule has been crystallized and, if so, provides the details for reproducing the crystallization procedure. Multiparameter searches can be done easily. The search results can be displayed in a number of different formats and stored in user files.

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

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.

The best-selling NIST Chemical Kinetics Database is currently on Version 4.0. Updated every year, it allows scientists instant access to reaction rate data, as well as supporting information. This year, we will see an excellent complement to the Chemical Kinetics Database — the NDRL/NIST Solution Kinetics Database. This database is derived from the well-known data evaluations of the Radiation Chemistry Data Center at the University of Notre Dame.

SRD Chemical Kinetics Databases

NIST Chemical Kinetics Database

NDRL/NIST Solution Kinetics: Reactive Intermediates Database

SRD Major Publications in Chemical Kinetics

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

Evaluated Kinetic Data for Combustion Modeling

Biweekly List of Papers on Radiation Chemistry and Photochemistry

CHEMICAL KINETICS DATABASES

17. NIST Chemical Kinetics Database Version 4.0

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

UPDATED!

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 4.0 contains over 20,000 records on over 6,900 reactant pairs and for over 3,500 compounds which are reactants or products. It is current through 1991.
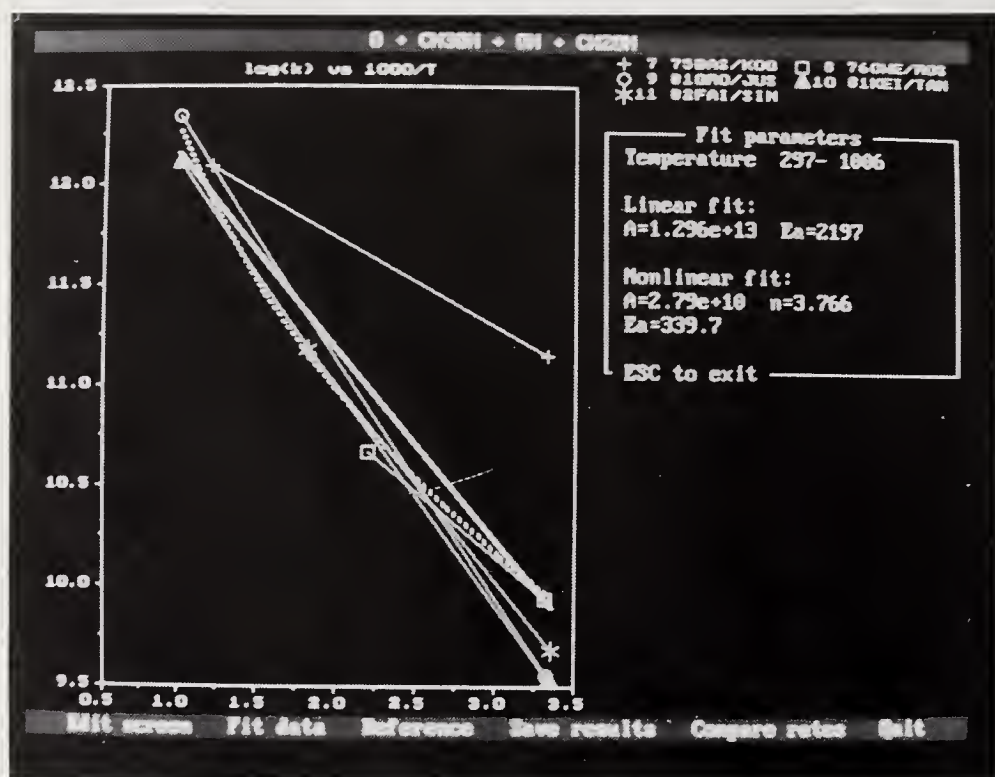
Arrhenius graphs of rate constants in the NIST Chemical Kinetics Database.

Display Options

- up to 5 least square fits
- A T^n or $A(T/298)^n$ and activation energies in kcal/mol or kJ/mol, 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 comparisons
- 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
- product
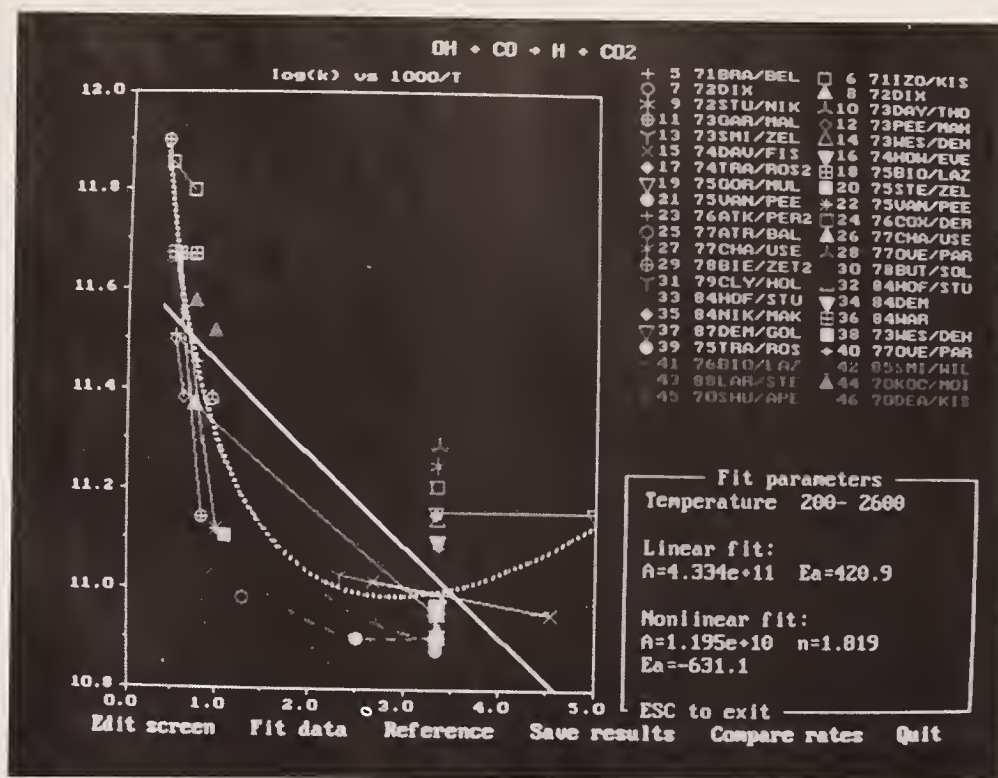
Updated every year, user input has been incorporated into enhancements of this database.

Version 4.0 has now included reactions of excited states of atoms and molecules. 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.

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40. NDRL/NIST Solution Kinetics

NEW!

Alberta B. Ross
Radiation Chemistry Data Center
University of Notre Dame
Notre Dame, IN 46556
(219) 239-6527

This database provides rapid access to rate constants for radical processes involving inorganic radicals in aqueous solution and organic peroxyl radicals in various solvents. Searches may be made for reactant pairs, for all reactions of a single reactant, for reactions of species containing a particular element, and for reactions generating a particular product. You may also search by author and generate files for output. The database contains over 10,000 entries for over 7,500 reactions; searches may be made for over 6,000 chemical species which are reactants or products. This database was developed from the well-known and widely-used data evaluations published in the *Journal of Physical and Chemical Reference Data* with additions of data from the literature through 1990.
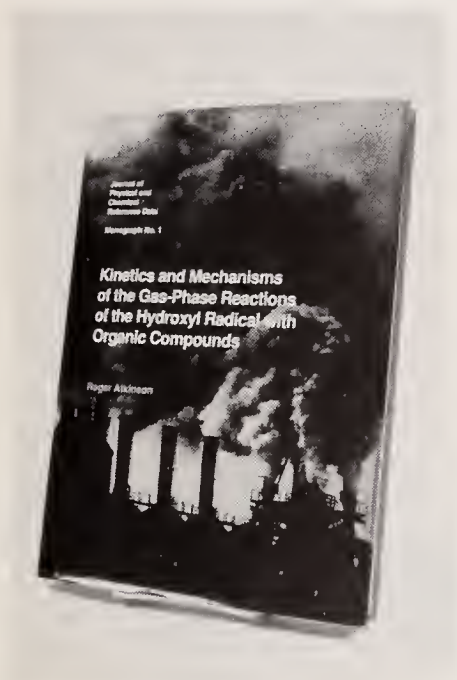
This database is available in 5¼" and 3½" diskettes.

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

Evaluated Kinetic Data for Combustion Modelling — D.L. Baulch, C.J. Cobos, R.A. Cox, C. Esser, P. Frank, Th. Just, J.A. Kerr, M.J. Pilling, J. Troe, R.W. Walker, and J. Warnatz. Journal of Physical and Chemical Reference Data **21**, 411 (1992).

This is a compilation of recommended data for nearly 200 elementary gas-phase chemical reactions which play an important part in combustion of simple hydrocarbons. Each data sheet presents the relevant thermodynamic data, rate coefficient measurements, reliability assessments, and recommended rate constants. The reasons for each choice of recommended values are discussed, and full references are given.
Available from the American Chemical Society, JPCRD Reprint 438, $70.00

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 Sheets for High-Temperature Reactions. Part II — N. Cohen and K.R. Westberg. Journal of Physical and Chemical Reference Data **20**, 1211 (1991).

Kinetic data on over 50 reactions of interest in combustion and atmospheric chemistry have been evaluated. Results are presented in tabular and graphical form in a series of data sheets. Uncertainty limits and the basis of the recommendations are discussed.
Available from the American Chemical Society, JPCRD Reprint 428, $22.00

Kinetics and Mechanisms of the Gas-Phase Reactions of the NO_3 Radical with Organic Compounds — Roger Atkinson. Journal of Physical and Chemical Reference Data **20**, 459 (1991).

Kinetics and mechanisms of the gas-phase reactions of the NO_3 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_3 are discussed.
Available from the American Chemical Society, JPCRD Reprint 413, $8.00

Gas-Phase Tropospheric Chemistry of Organic Compounds — Roger Atkinson. Journal of Physical and Chemical Reference Data **21**, (1992).

The gas-phase reactions of selected classes of organic compounds (alkanes, alkenes (including isoprene and monoterpenes), alkynes, aromatic hydrocarbons and oxygen-continuing organic compounds and their degradation products) under tropospheric conditions are reviewed and evaluated.
Available from the American Chemical Society, JPCRD Reprint 447

MATERIALS PROPERTIES

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

Several materials performance property databases are now available. Version 2.0 of the NIST Structural Ceramics Database was recently released. This database contains state-of-the-art materials property data for both research and commercial grades of silicon carbides and silicon nitrides with the addition of many new properties. 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.

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 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 DATABASES

30. NIST Structural Ceramics Database Version 2.0

Ronald Munro
Ceramics Division
National Institute of
Standards and Technology
Gaithersburg, MD 20899
(301) 975-6118

Version 2.0 contains thermal, mechanical, and corrosion properties of silicon carbides and silicon nitrides in a stand-alone, user-friendly database system that operates on DOS-based personal computers. Searches of the data are conducted by means of SCD's unique combination of menus, query-by-example technique, and computer-assisted entries. Users may search for properties of a selected ceramic or find ceramics satisfying specified property values. This database contains state-of-the-art materials property data for both research and commercial grades of silicon carbides and silicon nitrides.

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

Mechanical Properties

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

Corrosion Properties

- Oxidation Rate
- Oxidation Activation Energy
- Oxidation Diffusivity

Measurement Methods

- Specimen Preparation
- Apparatus
- Procedures

Bibliography

Complete Documentation of Data Sources through 1991

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

16. NACE-NIST Corrosion Performance Database

Richard Ricker
Corrosion Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-6023

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

The 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. Phone: (713) 492-0535.

FAX your order to SRD
(301) 926-0416

22. NIST Tribomaterials I (ACTIS) Database

William 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. Phone: (302) 998-8240.

A flat ASCII file on tribomaterials is also available from ACTIS. Please contact (302) 998-8240 for more information.

31. Phase Diagrams for Ceramists Database

Stephen Freiman
Phase Diagrams for Ceramists Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-6119

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 and is available from the American Ceramic Society, 735 Ceramic Place, Westerville, OH 43081. Phone: (614) 890-4700.

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, $1053.00

Phase Diagrams for Ceramists — American Ceramic Society, Westerville, 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, Westerville, OH (614) 890-4700, $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 clear 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, JPCRD 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, JPCRD Reprint 398, $6.00

Critical Compilation of Surface Structures Determined by Surface Extended X-Ray Absorption Fine Structure (SEXAFS) and Surface Extended Electron Energy Loss Spectroscopy (SEELFS) — Philip R. Watson. Journal of Physical and Chemical Reference Data **21**, 123 (1992).

This review critically compiles all surface structures derived by the technique of surface extended x-ray absorption fine-structure spectroscopy (SEXAFS) and surface electron energy loss fine-structure spectroscopy (SEELFS) reported in the refereed literature prior to January 1990, They are compared with the extensive low-energy electron diffraction and ion scattering databases Watson has previously reported.
Available from the American Chemical Society, JPCRD Reprint 434, $14.00

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
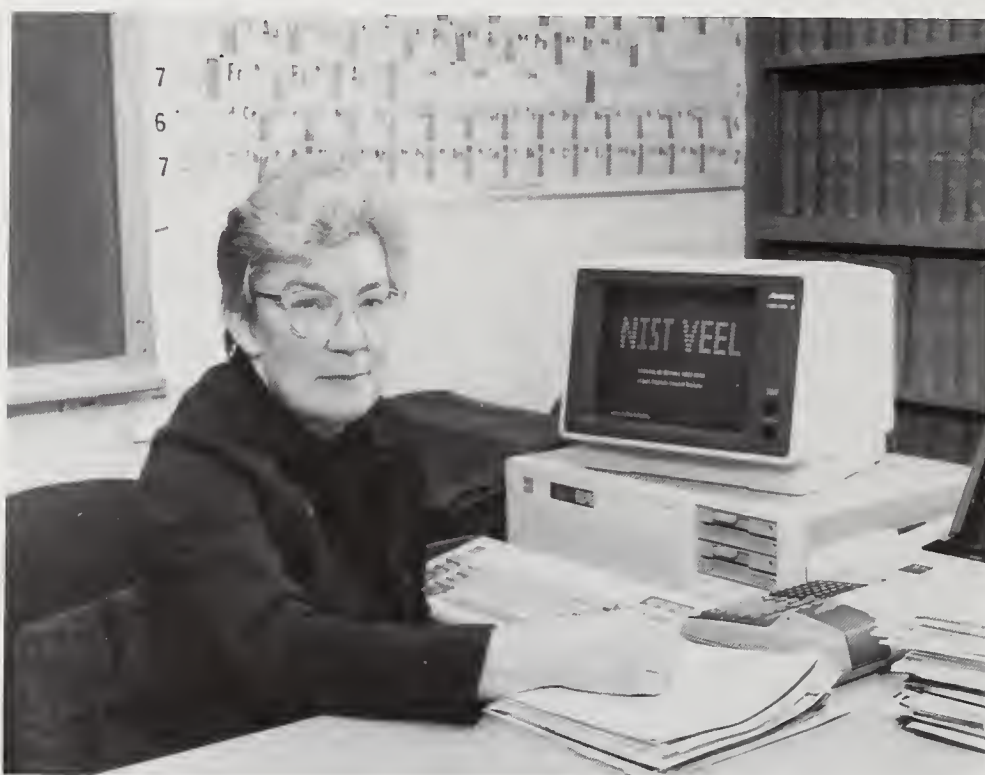
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MOLECULAR STRUCTURE AND SPECTROSCOPY DATABASE

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) provides rapid access to experimental data on:

- the ground-state vibrational fundamentals of transient molecules with from 3 to 16 atoms
- the electronic energy levels of excited-state vibrational fundamentals of transient molecules with from 3 to 6 atoms and of selected transient molecules with from 7 to 16 atoms.

Version 2.0 represents a 30% increase in data; 1,327 molecules are now included. In addition, data for the fully deuterium-substituted counterparts of these molecules are now included, where available.

The database can be searched by:

- molecule
- wavenumber
- wavelength range in which an electronic transition appears

Dr. Marilyn Jacox, developer of the VEEL Database.

Searches may be restricted to:

- molecules containing a specified chemical element
- the ground or excited electronic states
- observations in the gas phase or a specified inert solid matrix
- data obtained using a specific technique

Searching speed has also been significantly increased in Version 2.0. All literature references from the published tables are included in the database.

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 $C_{10}H_{10}$ — 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, JPCRD 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, JPCRD 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**, 1387 (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, JPCRD Reprint 403, $14.00

Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions — 1991 Revision — Frank J. Lovas. Journal of Physical and Chemical Reference Data **21**, 181 (1992).

Observation of molecular microwave transitions in interstellar clouds have been critically reviewed and transition frequencies compiled. A complete list of recommended rest frequencies for all transitions is presented. Other information on the transitions, as well as full references, is included.
Available from the American Chemical Society, JPCRD Reprint 436, $20.00

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

THERMODYNAMICS AND THERMOCHEMISTRY

NIST has a long history as the source for reliable thermochemical data starting from the 1920's with the International Critical Tables. 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 to locate chemicals in the database with the indicated molecular fragment.

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

SRD Thermochemical Databases

NIST Structures and Properties

NIST Positive and Negative Ion Energetics

NIST JANAF Thermochemical Tables

NIST JANAF Shomate Coefficients

NIST Molten Salts

NIST Chemical Thermodynamics

DIPPR Data Compilation of Pure Compound Properties

Student DIPPR

NIST Estimation of Thermodynamic Properties for Organic Compounds at 298.15 K

IVTANTHERMO — see page 70

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 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 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.
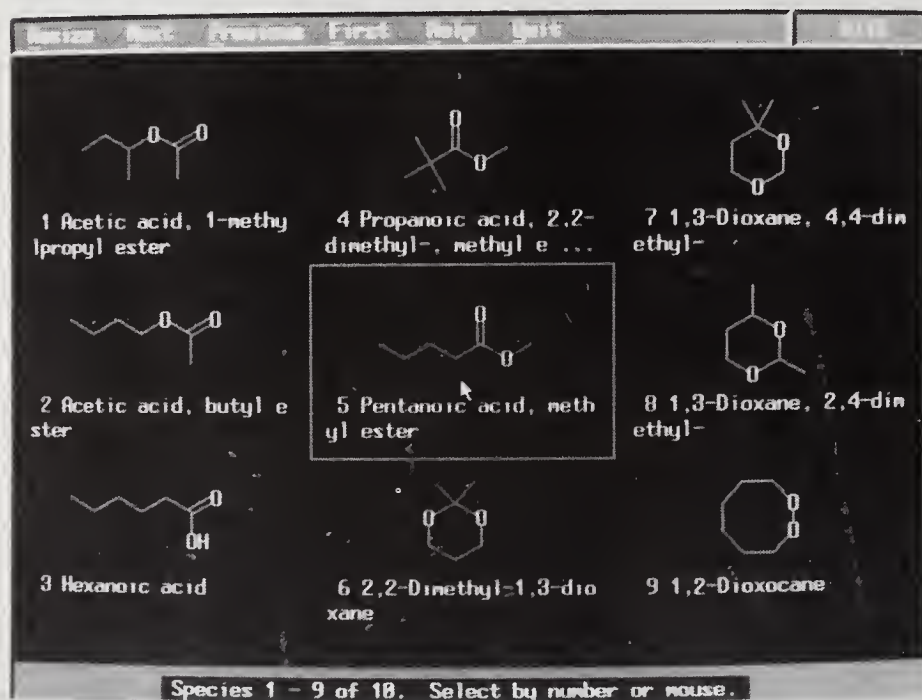
NIST Structures and Properties has many versatile graphics capabilities.

48

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

Search for data by:

- Name
- CAS Registry Number (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.

NIST Structures and Properties has an easy-to-use drawing module.
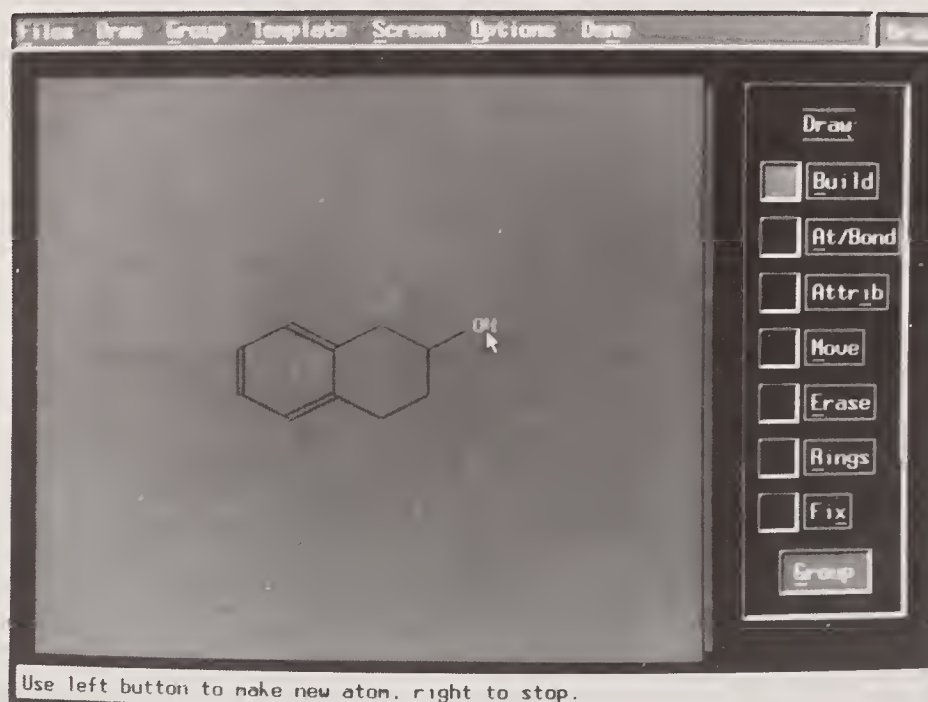
Any questions about our products?

?

Feel free to call and inquire.

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

This database is available in magnetic tape format, on diskette, and online through STN and CIS.

13. NIST JANAF Thermochemical Tables

Malcolm W. Chase
Standard Reference Data Program
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 stages. 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 online 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 1993 Version of the DIPPR database contains data on 39 properties for 1,336 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 over 40 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 online 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 on 3½" and 5½" disks. They can be used on Macintosh computers which have a PC emulator program.

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

Eugene S. Domalski
Chemical Thermodynamics Data Center
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

One feature of this database is the capability to convert energy units from joules to calories.

THERM/EST is available on both 5¼" or 3½" 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. As the culmination of a long-term data evaluation project at Rensselaer Polytechnic Institute, this database allows calculation of the following properties of approximately 320 single-salts and 4,000 multi-component systems (primarily binary).

- density
- surface tension
- viscosity
- electrical conductance

Not all properties are given for all salts.

Data can be extracted by chemical formula search or via a browse routine. For the salt system searched, results displayed are:

- temperature range of validity
- correlation equation
- accuracy estimates and reliability statements

A calculation routine lists properties at a single temperature or over a range of temperatures and does units conversions.

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

43. NIST JANAF Shomate Coefficients Database

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

This database is a representation of the JANAF Thermochemical Tables in an equation format consistent with use in the China Lake chemical equilibrium package (often referred to as PEP). The JANAF Thermochemical Tables are represented by one or more TL set(s) of coefficients necessary for the reproduction of each table. The selected coefficients can be written to a file for uploading into PEP. An easy regeneration of the thermochemical tables is possible. This database is available in 5¼" and 3½" diskette format.

THERMODYNAMIC AND THERMOCHEMICAL PUBLICATIONS

The NBS Tables of Chemical Thermodynamic Properties. II. Selected Values for Inorganic and C_1 and C_2 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.
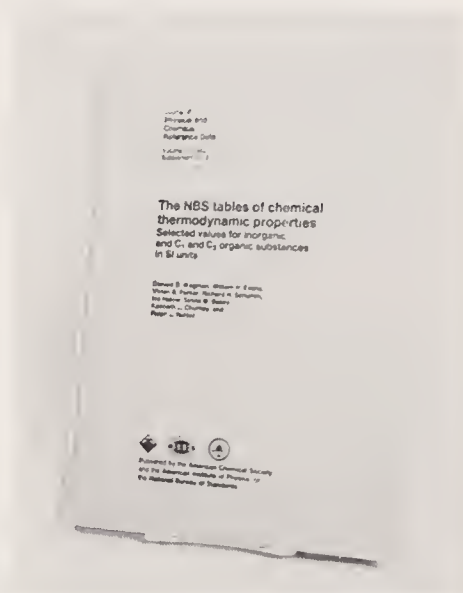
Available from the American Chemical Society

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.

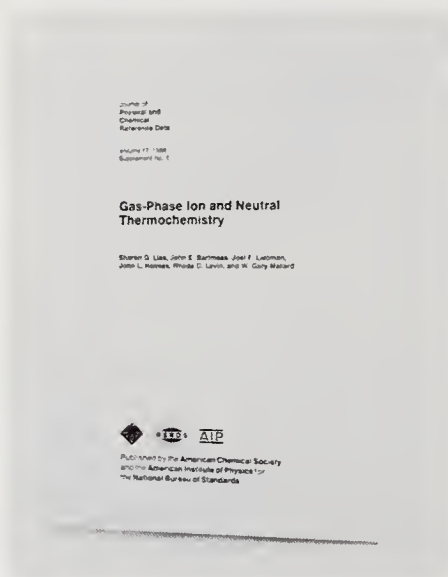**Available from the American Chemical Society**

U.S. and Canada	**$130.00**
Abroad	**$156.00**

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 $70.00
Abroad $84.00

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 from Taylor and Francis, Bristol, PA, (800) 821-8312, $315.00, 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 from Taylor and Francis, Bristol, PA, (800) 821-8312, Vol. 1 $200.00, Vol. 2 $249.00

Heat Capacities and Entropies of Organic Compounds in the Condensed Phase — Eugene S. Domalski, William H. Evans, and Elizabeth D. Hearing. Journal of Physical and Chemical Reference Data **13**, Supplement 1 (1984).

Heat capacities and entropies have been compiled for approximately 1400 organic compounds in the liquid and solid phases. Values for the enthalpies and entropies of phase transitions — solid state, fusion, and vaporization — which were encountered as part of this evaluation and tabulation are included. Articles begin at approximately 1925. The data given for each compound in the tabulation are: empirical formula, physical state, reference code, compound name(s), heat capacity, entropy, and, where available, phase-transition data, Wiswesser Line Notation for the compound, formula weight, and a rating which indicates the estimated overall quality of the reported data.
Available from the American Chemical Society
U.S. and Canada $40.00
Abroad $48.00

Heat Capacities and Entropies of Organic Compounds in the Condensed Phase, Volume II — Eugene S. Domalski and Elizabeth D. Hearing. Journal of Physical and Chemical Reference Data **19**, 881 (1990).

This paper supplements the data on heat capacities and entropies previously published in this journal. Data are presented on approximately 1300 organic compounds. Properties tabulated include heat capacity and entropy at 298.15 K and changes in the thermodynamic quantities for solid-solid, solid-liquid, solid-gas, and liquid-gas transitions.
Available from the American Chemical Society, Reprint 393, $15.00

THERMOPHYSICAL PROPERTIES OF FLUIDS

The complexity of providing reliable data on the thermophysical properties of fluid mixtures has been a primary area of focus of the SRD Program. A set of combined theoretical and empirical predictive techniques have been developed that rest firmly 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 continues to be a timely and valuable tool for refrigeration engineers, chemical and equipment manufacturers, and others who use chlorofluorocarbons.

The new NIST Thermophysical Properties of Pure Fluids has undergone a major update -now including 34 thermophysical properties of 17 pure fluids.

SRD Fluids Properties Databases

NIST Thermophysical Properties of Hydrocarbon Mixtures

NIST Thermophysical Properties of Pure Fluids

NIST Mixture Property Program

NIST Thermophysical Properties of Refrigerants and Refrigerant Mixtures

NIST Thermophysical Properties of Water

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

THERMOPHYSICAL PROPERTIES OF FLUIDS DATABASES

12. NIST Thermophysical Properties
of Pure Fluids
Version 3.0

UPDATED!

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

This database is a major update of NIST Standard Reference Database 12 — NIST
Interactive FORTRAN Programs to Calculate Thermophysical Properties of Fluids —
MIPROPS. Like the previous version, this new update computes thermophysical properties
according to the extremely accurate and wide-ranging NIST Standard Reference correlations.
This version provides great flexibility in the choice of units, output parameters, and input
parameters. Properties at the desired state points or tabular information, in the form of
isochores, isobars, isotherms, and isentropes may be displayed and saved in a file for further
use. The FORTRAN source code may also be provided, enabling users to incorporate
properties directly into design, simulation, or other property-dependent software.
The fluids available in this database are:

- Argon
- Butane (Iso)
- Butane (Normal)
- Carbon dioxide
- Carbon monoxide
- Deuterium
- Ethane
- Ethylene
- Helium (including superfluid states)

- Hydrogen (Normal)
- Hydrogen (Para)
- Methane
- Nitrogen
- Nitrogen trifluoride
- Oxygen
- Propane
- Xenon

The database provides equilibrium thermodynamic properties (based on a 32-term modified
Bennedict-Webb-Rubin (MBWR) equation of state) for each fluid in addition to transport
properties (viscosity and thermal conductivity) and dielectric constants for most of the fluids.
There are a total of 34 thermophysical properties included in this database.

This database is available on 5¼" and 3½" diskettes.

23. NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures Version 4.0

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

This database (also known as REFPROP) is designed to calculate thermodynamic properties of 27 pure refrigerants and refrigerant mixtures. The package enables the user to assess environmentally acceptable ethane-based refrigerants and refrigerant mixtures of up to five components as replacements for currently-used refrigerants. This important database has been significantly enhanced with the following features:

Increased Data: Carnahan-Starling-DeSantis-Morrison coefficients are included for 27 fluids:

R11	R23	R125	R152a
R12	R32	R134	R218
R13	R113	R134a	R290
R13B1	R114	R141b	RC270
R14	R115	R142b	RC318
R21	R123	R143	E134
R22	R124	R143a	

Based upon new measurements and a new method for the estimation of the binary interaction parameter for those pairs of fluids where measurements are not available, reliable estimates of the properties of all mixtures can be obtained.

New Properties: Fourteen properties are now available, including viscosity and thermal conductivity, and the user may choose which of these to display. Version 4.0 has a new equation of state.

Easier to Use: The user may now store the responses to oft-repeated questions to shorten the dialogue process before calculation begins.

This database is available on 5¼" and 3½" disks.

4. NIST Thermophysical Properties of Hydrocarbon Mixtures

Marcia Huber
Fluid Mixtures Data Center
National Institute of Standards and Technology
Boulder, CO 80303
(301) 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
- Cp
- Cp/Cv
- 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.

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_2-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 coexisting 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 predicts 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 on 5¼" and 3½" diskettes. It can also be used on Macintosh computers which have a PC emulator program.

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

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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 H_2O (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 H_2O. The other parts are main programs which call these routines to generate properties of H_2O 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

NBS/NRC
Steam Tables

LESTER HAAR
JOHN S. GALLAGHER
GEORGE S. KELL

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 a PC diskette version. 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, Taylor and Francis, Bristol, PA.

41. NIST Heat Capacities of Liquids

E.S. Domalski
Chemical Thermodynamics Data Center
National Institute of
Standards and Technology
Gaithersburg, MD 20899
(301) 975-2529

This database, developed at the Prague Institute of Chemical Technology, provides rapid and convenient access to critically assessed data on heat capacities of liquid hydrocarbons. The database provides:

- parameters of a correlating equation accompanied by the temperature interval to which the parameters relate and by the overall percent error of the data
- tables of heat capacities in a specified temperature interval
- enthalpy and entropy difference between two specified temperatures

The selected data are displayed on the screen and can optionally be directed to an output device or disk file.

The database may be searched by:
- chemical class
- molecular formula
- Chemical Abstracts Service Registry Number
- serial number

The hydrocarbon compounds are subdivided into:
- saturated aliphatic hydrocarbons
- saturated cyclic hydrocarbons
- unsaturated aliphatic hydrocarbons
- aromatic and unsaturated cyclic hydrocarbons

This database is available on 5¼" and 3½" disks. It can be used on Macintosh computers which have PC emulator software.

THERMOPHYSICAL PROPERTIES OF FLUIDS
PUBLICATIONS

Evaluation of Solubility Data of the System CO_2-H_2O from 273 K to the Critical Point of Water — Rosa Crovetto. Journal of Physical and Chemical Reference Data **20**, 590 (1991).

Measurements 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 the American Chemical Society, JPCRD 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.
Available from the American Chemical Society, JPCRD Reprint 410, $18.00

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 the American Chemical Society, JPCRD Reprint 424, $12.00

NIST SPECIAL DATABASES

1. NIST Binary Images of Printed Digits, Alphas, and Text (HWDB)

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 handprinted 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

The NIST Special Database Series on CD-ROM is creating wide interest.

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 (SFRS)

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.

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

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3. NIST Binary Images of Handwritten Segmented Characters (HWSC)

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

The NIST database of handwritten segmented characters contains 313,389 isolated character images segmented from the 2,100 full-page images distributed with NIST Special Database 1. The database includes the 2,100 pages of binary, black-and-white, images of handprinted numerals and text. This significant new database contains 223,125 digits, 44,951 upper-case, and 45,313 lower-case character images. Each character image has been centered in a separate 128-by-128 pixel region and has been assigned a classification which has been manually corrected so that the error rate of the segmentation and assigned classification is less than 0.1%. The uncompressed database totals approximately 2.75 gigabytes of image data and includes image format documentation and example software.

NIST Special Database 3 has the following features:
- 313,389 isolated character images including classifications
- 223,125 digits, 44,951 upper-case, and 45,313 lower-case character images
- 2,100 full-page images
- 12 pixel per millimeter resolution
- image format documentation and example software

Suitable for automated hand-print recognition research, the database can be used for:
- algorithm development
- system training and testing

The database is a valuable tool for training recognition systems on a large statistical sample of handprinted characters. The system requirements are a 5¼" CD-ROM drive with software to read ISO-9660 format.

☎ (301) 975-2208

4. NIST 8-Bit Gray Scale Images of Fingerprint Image Groups

Craig Watson
National Institute of
Standards and Technology
Gaithersburg, MD 20899
(301) 975-4402

The NIST database of fingerprint images contains 2000 8-bit gray scale fingerprint image pairs. Each image is 512-by-512 pixels with 32 rows of white space at the bottom and classified using one of the five following classes: A=Arch, L=Left Loop, R=Right Loop, T=Tented Arch, W=Whirl. The database is evenly distributed over each of the five classifications with 400 fingerprint pairs from each class. The images are compressed using a modified JPEG lossless compression algorithm and require approximately 636 megabytes of storage compressed and 1.1 gigabytes uncompressed (1.6:1 compression ratio). The database also includes format documentation and example software.

NIST Special Database 4 has the following features:

- 2000 8-bit gray scale fingerprint image pairs including classifications
- 400 fingerprint pairs from each of the five classifications Arch, Left and Right Loops, Tented Arch, Whirl
- each of the fingerprint pairs are two completely different rollings of the same fingerprint
- 19.6850 pixels per millimeter resolution
- image format documentation and example software

Suitable for automated fingerprint classification research, the database can be used for:

- algorithm development
- system training and testing

The database is a valuable tool for evaluating fingerprint systems on a statistical sample of fingerprints which is evenly distributed over the five major classifications. The system requirements are a 5¼" CD-ROM drive with software to read ISO-9660 format.

5. IVTANTHERMO-PC (Version 1.0)

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

IVTANTHERMO is a computerized system providing information on the thermodynamic properties of about 2,300 substances (containing 85 elements and the electron) in the standard state over a wide range of temperature. It was developed by scientists at the Institute of High Temperatures in Moscow. The software permits the calculation of thermodynamic parameters of chemical reactions and the composition of chemical systems. All recommended values are cited with a reliability assessment.

This database is capable of thermodynamic analysis of:

- new high-temperature processes, including combustion processes
- the optimization of chemical processes, including combustion processes
- stability of materials at high temperatures and in various media
- chemical processes occurring in power-generating facilities, including nuclear plants
- the optimization of raw materials; use and waste management
- the emissions of incinerators and industrial exhaust gases into the atmosphere

The database contains the following information on each substance:

- substance name and chemical formula
- accuracy of thermodynamic properties
- isobaric heat capacity; entropy; change of enthalpy; Gibbs energy function
- equation(s) fitting tabulated values of Gibbs energy function
- enthalpy of formation; equilibrium constant

The database is available on 5¼" and 3½" diskettes. It can also be used on Macintosh computers which have PC emulator software.

6. NIST Structured Forms Reference
Set of Binary Images II (SFRS2)

Darrin Dimmick
National Institute of
Standards and Technology
Gaithersburg, MD 20899
(301) 975-4147

The second NIST Database of structured forms contains full page images of simulated tax forms completed using handprinting. The structured forms used in this database are 12 different forms from the 1988, IRS 1040 Package X. 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 making a total of 20 form faces represented in the database.

Each image is stored in bi-level black-and-white raster format. The images in this database appear to be real forms prepared by individuals, but the images have been automatically derived and synthesized using a computer and contain no "real" tax data. The entry field values on the forms have been automatically generated by a computer in order to make the data available without the danger of distributing privileged tax information.

In addition to the images, the database includes answer files, one for each image. Each answer file contains an ASCII represenatation of the data found in the entry fields on the corresponding image. Image format documentation and example software are also provided.

SFRS2 has the following features:
- full-page images of completed structured form faces
- answer files
- 12 pixel per millimeter resolution
- 20 tables of entry field types and context
- image format documentation and example software

Suitable for both document processing and automated data capture research, development and evaluation, the database can be used for:
- forms identification
- field isolation: locating entry fields on the form
- character segmentation: separating entry field values into characters
- character recognition: identifying specific handprinted characters.

The database is a valuable tool for measurement of system performance and system comparison on complex forms. The system requirements are a 5¼" CD-ROM drive with software to read ISO-9660 format.

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7. NIST Test Data 1: Binary Images of Handprinted Segmented Characters (TST1)

Jon Geist
National Institute of
Standards and Technology
Gaithersburg, MD 20899
(301) 975-2066

The NIST database contains almost 83,000 binary, black-and-white images of handprinted numerals and letters segmented from 500 forms of the same type used for NIST Special Database 3 — NIST Binary Images of Handwritten Segmented Characters. However, the forms were filled out by a very different writer population than the Bureau of Census field workers who filled out the 2,100 forms used for that database. NIST Test Data 1 is the database that was used for testing in the First Census OCR Systems Conference in May, 1992.

NIST Test Data 1 has the following features:
5¼" CD-ROM
- approximately 83,000 isolated character images without classifications
- approximately 59,000 digits and 24,000 upper-case and lower-case images
- 12 pixel per millimeter resolution

5¼" floppy disk
- keyed classifications for all character images on CD-ROM
- keyed index to 500 writers

This database is suitable for use in testing OCR systems against the results obtained by over 40 systems in the First Census OCR Systems Conference, and for use as a database for training OCR systems. The system requirements are a 5¼" CD-ROM drive with software to read ISO-9660 format and a 5¼" floppy drive with the software to read high-density MS-DOS format.

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

8. NIST Machine-Print Database of Gray Scale and Binary Images (MPDB)

Allen Wilkinson
National Institute of
Standards and Technology
Gaithersburg, MD 20899
(301) 975-3383

The NIST machine-printed database contains gray scale and binary images of machine printed pages. There are 360 digitized pages on three CD-ROM discs. There are a total of 3,063,168 characters in the set which is an average of 8509 characters per page. A reference file is included for each page. These reference files are the ASCII text pages that were used to generate the original hardcopy that was digitized. This database is being distributed for use in the development and testing of Optical Character Recognition (OCR) systems on a common set of images. This allow vendors to report results with respect to this common image set. The database has the following features:

- 3 font styles; Bold, Italics, and Normal
- 6 font types; Courier, Helvetica, New Century Schoolbook, Optima, Palatino, and Times Roman
- 10 point sizes; 4, 5, 6, 7, 8, 10, 11, 12, 15, 17, and 20
- randomly generated order and sequential ordered pages
- 360 unique pages each having a gray scale and binary representation
- 12 pixels/mm resolution
- 360 text files containing page reference answers
- image format documentation and example software

Suitable for automated machine print research, development, and evaluation, the data set can be used for:

- algorithm development
- system training and testing
- character segmentation: separating full page image into characters
- character recognition: identifying specific machine-printed characters

The database is a valuable tool for measurement and comparison of system performance on machine-print pages.

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

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[1]Available from the JCPDS-International Centre for Diffraction Data, 1601 Park Lane, Swarthmore, PA 19081. Phone: (215) 328-9400

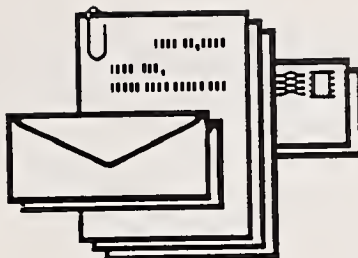[2]Available from NACE, P.O. Box 218340, Houston, TX 77218. Phone: (713) 492-0535

[3]Available from ACTIS Inc., 118 Highgate Rd., Wilmington, DE 19808. Phone: (302) 998-8240

[4]Available from the American Ceramic Society, 735 Ceramics Place, Westerville, OH 43214. Phone: (614) 890-4700
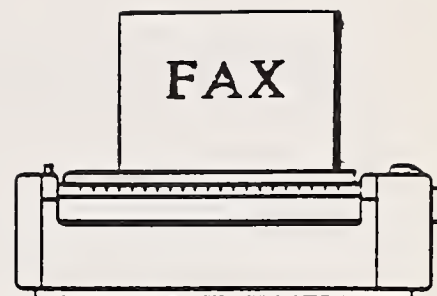
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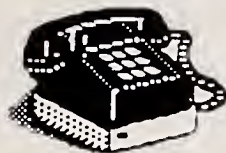
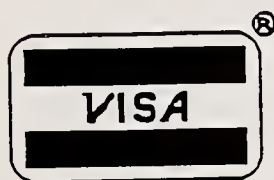| PHONE	MAIL	FAX

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Australia
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