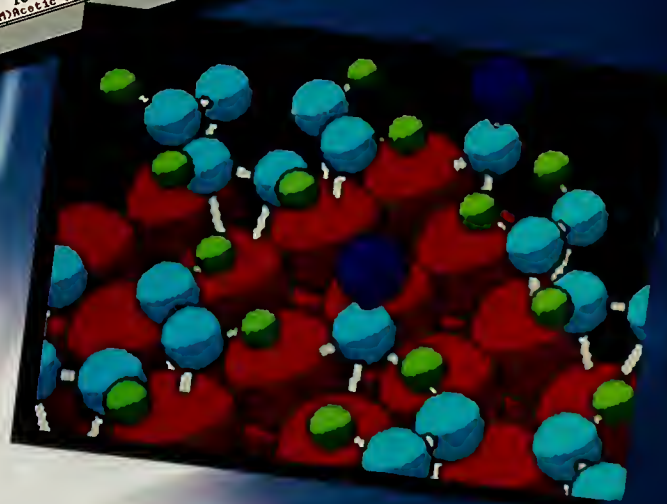
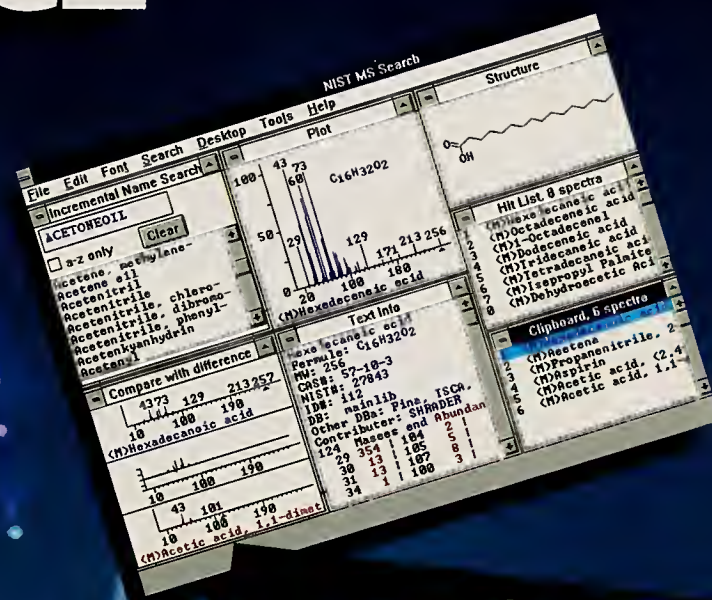




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NIST STANDARD REFERENCE DATA PRODUCTS CATALOG 1995-96

Joan C. Sauerwein, Editor

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

July 1995
Supersedes NIST Special Publication 782, 1994 Edition



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National Institute of Standards
and Technology
Special Publication 782,
1995-1996 Edition
Natl. Inst. Stand. Technol.
Spec. Publ. 782, 1995-1996 Ed.
133 pages (July, 1995)
CODEN: NSPUE3

U.S. Government Printing Office
Washington: 1995

For sale by the Superintendent of
Documents
U.S. Government Printing Office
Washington, DC 20402

The editor would like to acknowledge
Cheryl E. Williams: original design/layout
Jeanne R. Bride: proofreading
Warren Overman: printing coordination
Ernie Kunz: cover design.

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 current databases and published data in the National Standard Reference Database Series. This edition of the catalog contains many new databases and updates current ones. These data compilations have been subdivided into ten categories. Prices and ordering information are located at the back of the document.

Key words: character recognition; 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.

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. Users can now browse our catalog information on gopher and through Mosaic on the World Wide Web. With this, the sixth 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 their 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.



The SRD Program has provided valuable evaluated data to industry for over 30 years.

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ORDER FORM AND PRICE LIST

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. Now, in the mid-nineties, SRD is providing 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 and other technical areas 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 electronic 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 in cooperative data programs which draw support from both industry and other government and international programs.

The activities concentrate in the following disciplines:

Analytical Chemistry – mass spectral, FT-IR absorption spectra, and surface analysis, used for chemical identification.

Atomic and Molecular Physics – atomic energy levels and wavelengths, transition probabilities, and collisional data used for diagnostics and modeling. Also includes evaluated molecular data at microwave and infrared frequencies and, for transient molecules, vibrational and electronic energy levels.

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

Chemical and Crystal Structure - important collections of compounds with structural and crystallographic data.

Chemical Kinetics – rate data on gas-phase and solution reactions.

Industrial Fluids and Chemical Engineering – thermophysical and transport properties of pure and mixed fluids, including refrigerants, that are of critical importance to industry.

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

Surface Data - surface analysis, photoelectron and Auger spectral data.

Thermodynamics and Thermochemistry – reliable, widely used tables of organic and inorganic species.

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, 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 in Journal and Monograph form continues with Dr. Jean W. Gallagher, Editor.

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

If you have programmatic questions about Standard Reference Data, please contact John R. Rumble, Jr., Acting Chief, at (301) 975-2200 or Jean W. Gallagher at (301) 975-2204.

If you have questions or suggestions for improvements on the SRD Databases, please contact Dorothy Blakeslee at (301) 975-2524.

ORDERING INFORMATION

When ordering an SRD database, checks, purchase orders, VISA, and Mastercard are accepted. Orders can be placed by 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 (VOICE)

(301)926-0416 (FAX)

SRDATA@enh.nist.gov
(E-MAIL)

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.

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 reviewed by mass spectrometry experts, all spectra have been reevaluated on an individual basis. The database includes thousands of spectra of diverse compounds, such as pharmaceuticals, flavors and fragrances, and compounds of industrial and environmental interest. The new Version 4.5 for DOS was a significant enhancement of the software. Now SRD is proud to announce the new Microsoft® Windows™ Version of the NIST/EPA/NIH Mass Spectral Database.

The 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 DOS Version of the NIST/EPA/NIH 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 under electron bombardment. Version 2.0 adds many enhancements to the software.

Analytical Chemistry

SRD Analytical Chemistry Databases

Mass Spectra

NIST/EPA/NIH Mass Spectral

NIST/EPA/NIH Mass Spectral: PC Version

WindowsTM Version of the NIST/EPA/NIH Mass
Spectral Database

Spectrum Analysis

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

Infrared

NIST/EPA Gas-Phase Infrared

SRD Major Publications in Analytical Chemistry

Elemental and Interplanar Spacing Index

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1. NIST/EPA/NIH Mass Spectral Database

Sharon G. Lias

Mass Spectrometry Data Center

National Institute of Standards and Technology

Gaithersburg, MD 20899

(301) 975-2562

sgl@micf.nist.gov

This database contains ionization mass spectra of well over 62,000 different compounds. Each spectrum has a "quality index" associated with it, as well as 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 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 on diskettes in an ASCII Version and as a CD-ROM. It is widely used in the mass spectrometers of many commercial instrument manufacturers.

Analytical Chemistry Databases

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FAX (301) 926-0416

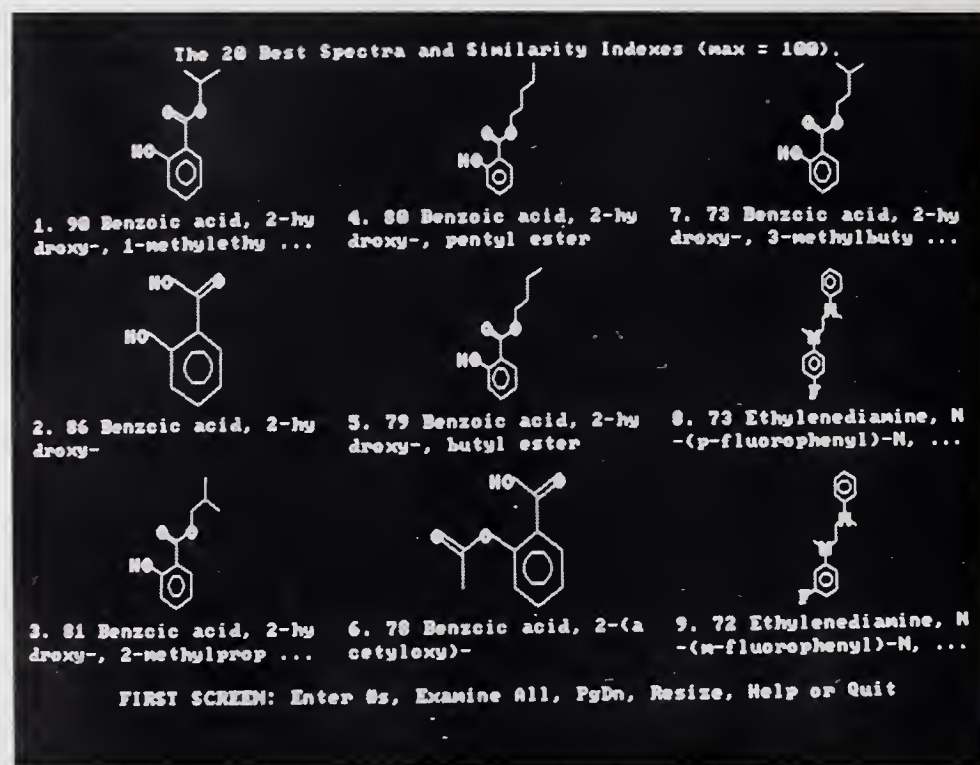
e-mail SRDATA@enh.nist.gov

Analytical Chemistry Databases

1A. NIST/EPA/NIH Mass Spectral Database: PC Version 4.5

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

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 enabling easy searching of this important database. The new Version 4.5 consists of electron ionization mass spectra for 62,235 compounds (with structures for almost all compounds), various added index files for more rapid data retrieval, and related software for searching the database.

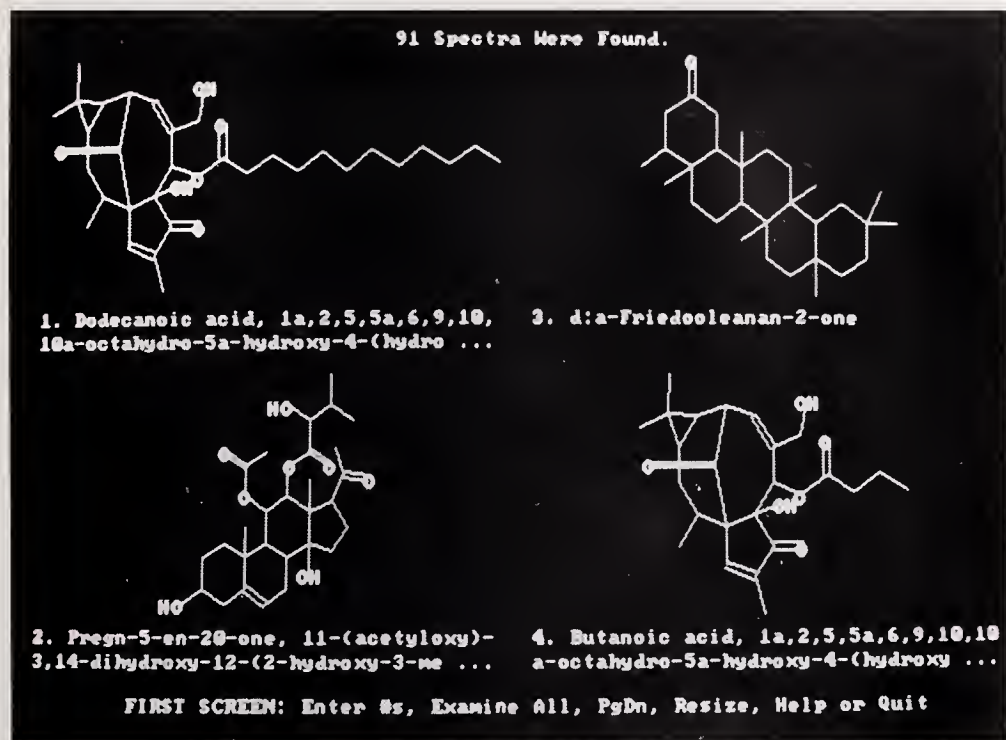


This collection consists of over 74,000 spectra of 62,235 compounds. You may also add your spectra to your personal library.

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e-mail SRDATA@enh.nist.gov

A quickly-learned interface allows the data to be searched by:

- CAS Registry Number
- incremental chemical name (including tens of thousands of alternative names)
- molecular formula
- any peaks (up to 10 peaks of 4 classes with an intensity range for each)
- user input spectrum (choose identity, similarity, or extensive search options)
- neutral losses
- rank



The database has spectra of diverse compounds such as pharmaceuticals, flavors, and fragrances, and compounds of industrial and environmental interest.

Various display features are available:

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

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 3½" high density disks and CD-ROM.

Analytical Chemistry Databases

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e-mail SRDATA@enh.nist.gov

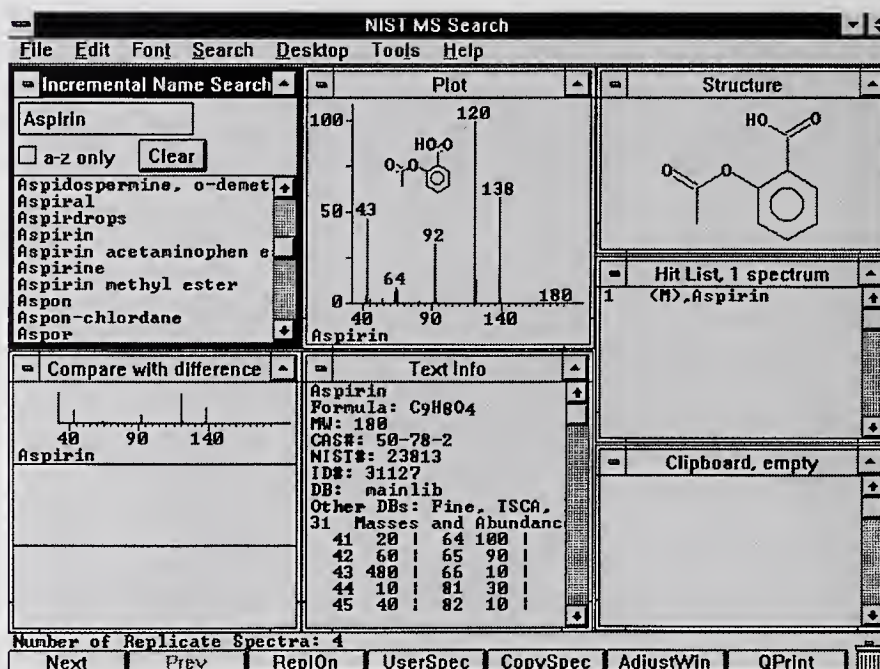
Analytical Chemistry Databases

1A. Windows™ Version of the NIST/EPA/NIH Mass Spectral Database



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

SRD is proud to announce an easy-to-use, full-featured program for the world's most widely-used mass spectral library that is now available for Microsoft® Windows™. This program allows easy performance of both routine and specialized tasks from a customized workspace. In addition to the 62,235 spectra, over 12,000 selected replicate spectra are included. Compounds are identified by chemical structure, molecular formula, CAS Registry Number or alternate chemical names. Users may also build or convert their own libraries within the program or use a separate utility.



For information or to order:
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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

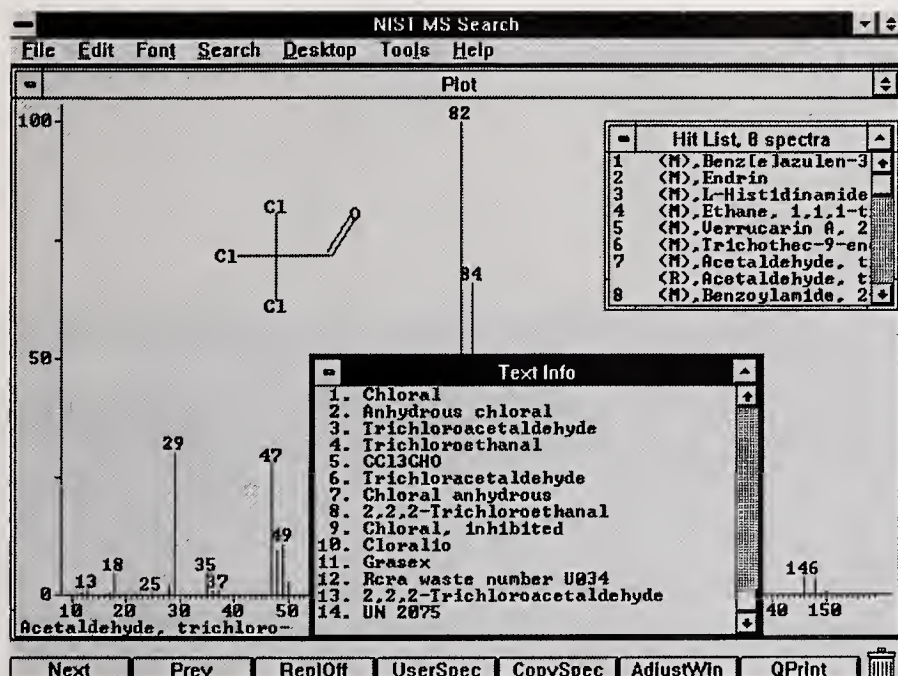
*Your workspace can be easily customized with the new
Windows™ Version of the NIST/EPA/NIH Mass Spectral
Database.*

Analytical Chemistry Databases

Seven different data windows can be customized and positioned in building a personal desktop. A new similarity search has been specially optimized for finding similar compounds if an unknown is not in the library. Also, four types of peaks may be combined in special "peak-oriented" searches:

- 1) normal peak
- 2) neutral loss peak
- 3) peak rank
- 4) maximum mass peak

This new program reads various spectral formats from commercial instrument systems. Also, extensive help is available at all times. This database comes on 3½" high density disks and CD-ROM.



Searching for unknowns is now easier than ever.

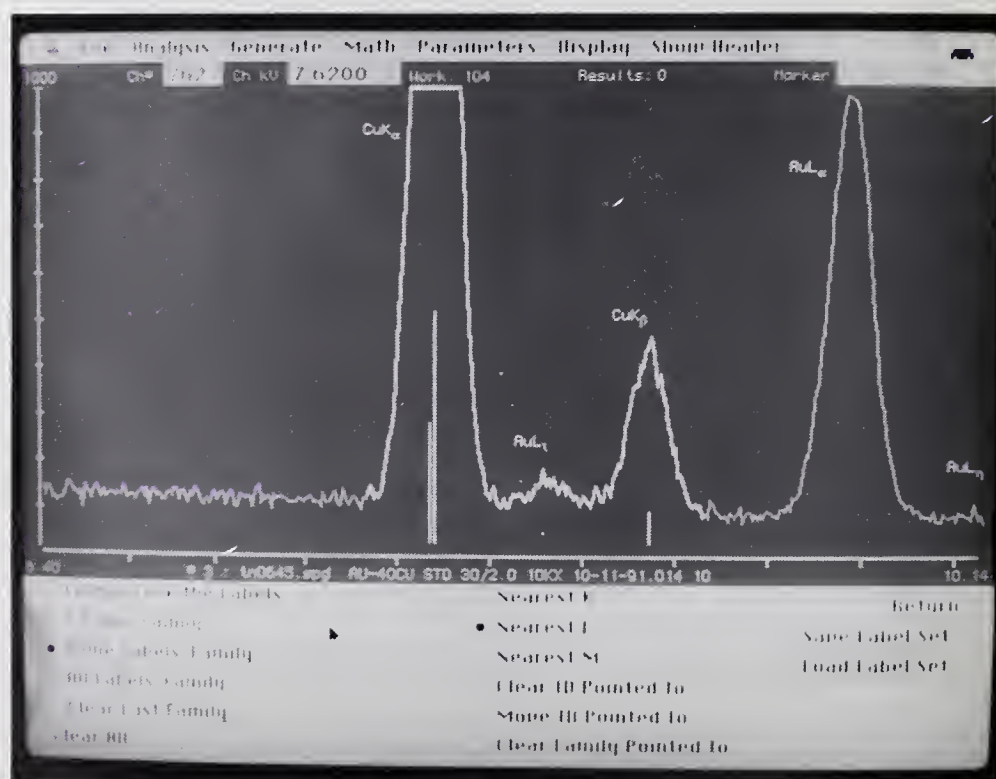
For information or to order:
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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Analytical Chemistry Databases

36. NIST/NIH Desktop Spectrum Analyzer Program and X-Ray Database Version 2.0

Robert L. Myklebust/Carol Thomas
Surface and Microanalysis Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3906/3926
myklebust@gapnet.nist.gov/swyt@micf.nist.gov

The NIST/NIH Desktop Spectrum Analyzer Program (DTSA) generates, interprets and analyzes x-ray spectra from specimens under electron bombardment. This remarkable software/database package simulates the experimental environment and emulates specimen properties to generate spectra reflecting the relevant physics, chemistry, and statistics of a real world application.



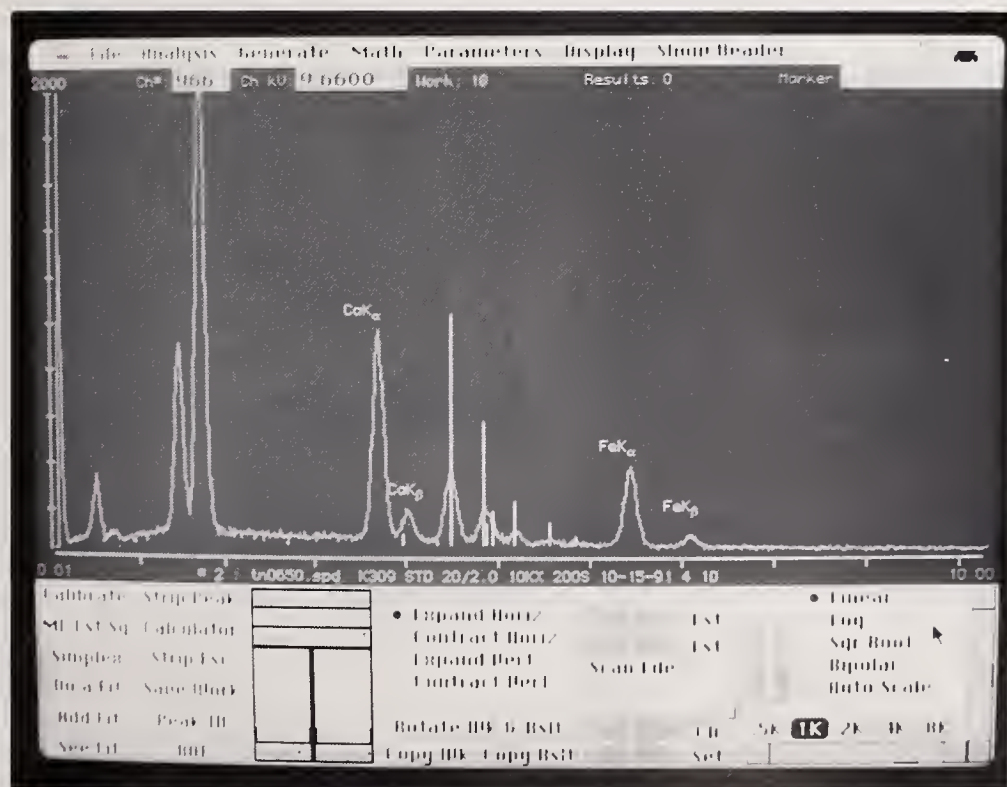
DTSA incorporates many widely accepted x-ray data analysis procedures developed over many years at NIST and NIH.

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Incorporating many widely accepted x-ray data analysis procedures developed over many years at the National Institute of Standards and Technology (NIST) and the National Institutes of Health (NIH), DTSA has many outstanding features:

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- New automatic peak identification
- New automatic peak region (ROI) setup
- New user database for compositions
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- Linear and non-linear curve-fitting
- KLM markers including edges, lines, escapes, satellites
- Composition conversion calculator
- Automatic spectrum calibration
- Siegbahn peak labeling
- Graphical output to printer
- Spectral calculator containing many mathematical functions
- First principles spectrum simulation, with all relevant physics and true counting statistics
- Thick and thin specimen options
- Ten 8192 channel displays
- Accurate MDL estimates
- Outputs to text files or spreadsheets

The package works on any Macintosh computer with 5 megabytes of memory and math coprocessor.



DTSA can perform a complete spectrum analysis at your desk.

Analytical Chemistry Databases

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FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Analytical Chemistry Databases

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
sstein@enh.nist.gov

Containing FT-IR absorption spectra for over 5,200 compounds, this significant database 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:

- direct comparison of up to 4 spectra
- use external FT-IR files for comparison plots
- context sensitive help

This database is available in 3½" and 5¼" disks. A flat file of the infrared data in JCAMP format is also available.

For information or to order:
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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Elemental and Interplanar Spacing Index

**International Centre for
Diffraction Data,
Newtown Square, 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 identify readily a material with the chemical and diffraction data routinely collected on most modern analytical electron microscopes.

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\$250.00 (set price).

Analytical Chemistry Publications

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e-mail SRDATA@enh.nist.gov

Atomic and Molecular 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. The SRD Program has also produced several important compilations of molecular data.

The Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules Database has been steadily updated to include more data and software enhancements. New this year is the NIST Database for Atomic Spectroscopy which has wavelengths and transition probabilities for most ionization stages of elements Hydrogen through Nickel. The Elastic-Electron Scattering Cross-Section Database provides values of differential cross-sections for elastic-electron scattering.

The NIST Atomic Spectroscopic Database (Beta Version) provides access and search capability to critically evaluated atomic spectroscopic data on energy levels. It is available on WWW: URL http://aeldata.phy.nist.gov/nist_atomic_spectra.html.

SRD Atomic and Molecular Physics Databases

- NIST Spectroscopic Properties of Atoms and Atomic Ions
- NIST Wavenumber Calibration Tables
- NIST Electron and Positron Stopping Powers of Materials
- NIST Form Factor, Attenuation, and Scattering Tables
- NIST X-Ray and Gamma-Ray Attenuation Coefficients and Cross Sections
- NIST Elastic-Electron-Scattering Cross-Section
- NIST Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules
- NIST Database for Atomic Spectroscopy

SRD Major Publications in Atomic and Molecular Physics

- Atomic Energy Levels Publications
- Atomic Transition Probabilities Publications

Atomic and Molecular Physics Databases

38. NIST Spectroscopic Properties of Atoms and Atomic Ions Database

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

Providing easy access to prominent emission wavelengths for all neutral atoms and their first four stages of ionization, the data in this interactive database 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.

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

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

39. NIST Wavenumber Calibration Tables Database

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

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 cm^{-1} 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 cm^{-1} 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 on $3\frac{1}{2}$ " and $5\frac{1}{4}$ " disks. They may also be used on Macintosh computers with PC emulator software.

Atomic and Molecular Physics Databases

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Atomic and Molecular Physics Databases

7. NIST Electron and Positron Stopping Powers of Materials Database



Stephen M. Seltzer
Photon and Charged Particle Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-5552
seltzer@enh.nist.gov

This database 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.

66. NIST Form Factor, Attenuation, & Scattering Tables (from $E=1\text{-}10\text{ eV}$ to $E=0.4\text{-}1.0\text{ MeV}$)



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

Tables for form factors and anomalous dispersion are widely used in the UV, x-ray and γ -ray communities, and have existed for a considerable period of time. In this data compilation, the primary interactions of x-rays with isolated atoms from ($Z=1\text{-}92$) are described and computed for energies from $E=1\text{-}10\text{ eV}$ and $400\text{-}1000\text{ KeV}$. The f_1 and f_2 components of the form factors, together with the photoelectric attenuation coefficient for the atom, ν , and the value for the K-shell, ν_K , are given as functions of energy and wavelength. Also provided are estimated correction factors, conversion factors, and the sum of the scattering contributions.

The data files are available in ASCII on diskette.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

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



Stephen M. Seltzer
Photon and Charged Particle Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-5552
seltzer@enh.nist.gov

This database 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.

Databases #7 and #8 have been adopted by the International Commission on Radiation Units and Measurements.

This database is available in PC diskette format.

Atomic and Molecular Physics Databases

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Atomic and Molecular Physics Databases

64. NIST Elastic-Electron- Scattering Cross-Section Database



Cedric Powell
Surface Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2534
cpowell@enh.nist.gov

This software package provides calculated values of differential cross sections for elastic-electron-scattering for elements with atomic numbers from 1 to 96 and for electron energies between 50 eV and 10,000 eV (in steps of 1 eV). The differential cross sections can be calculated using both relativistic and nonrelativistic approaches, and can be presented in three different coordinate systems. The software provides:

- graphical display of the calculated cross section in different coordinate systems;
- creation of files containing the cross sections for specified elements, energies, and coordinates;
- creation of random number generators providing the polar scattering angles to be used in Monte Carlo simulations of electron transport in solids; and
- tests of the random number generators.

Simulations of elastic-electron-scattering effects in solids are important in the development of improved models for quantitative surface analysis by Auger-electron spectroscopy and x-ray photoelectron spectroscopy. This software package is designed for such simulations but can be used in other applications where detailed knowledge of electron transport at similar energies is required.

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

**26. NIST Vibrational and
Electronic Energy Levels of
Small Polyatomic Transient
Molecules Database
Version 4.0**



**Marilyn E. Jacox
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2547
jacoxm@tiber.nist.gov**

This program provides rapid access to experimental data on:

- the ground-state vibrational fundamentals of transient molecules with from 3 to 16 atoms and
- 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.

Over 1,775 molecules are included in VEEL4, an increase of over 200 molecules from the previous version. In addition, data for the fully deuterium-substituted counterparts of these molecules are included, where available.

The database may be searched by:

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

Searches may be restricted to:

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

Literature references are from the widely-known Monograph [M.E. Jacox, Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules, J. Phys. Chem. Ref. Data, Monograph 3 (1994)] and from more recently published work concerned with more than 400 molecules. This database is available on both 3½" and 5¼" disks. It may also be used on Macintosh computers with PC emulator software.

**Atomic and
Molecular Physics
Databases**

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Atomic and Molecular Physics Databases

61. NIST Database for Atomic Spectroscopy



Daniel E. Kelleher
Atomic Transition Probabilities
Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3202
kelleher@enh.nist.gov

This new database contains wavelengths, transition probabilities, and levels for most ionization stages of elements Hydrogen through Nickel ($Z=1-28$). DAS includes about 27,000 lines (from 1 to 200,000 Angstroms) and 45,000 levels.

The transition probabilities are taken from the NIST critical compilations of W.L. Wiese, et al. The atomic energy levels are taken from the compilation of the NIST Atomic Energy Levels Data Center (where available) and R.L. Kelly.

The self-contained menu-driven database has full search and select capabilities. Users may change default options for units, output, etc.

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Atomic Weights of the Elements 1993

International Union of Pure and Applied Chemistry, Inorganic Chemistry Division, Commission on Atomic Weights and Isotopic Abundances
Journal of Physical and Chemical Reference Data (in press).

The Commission on Atomic Weights and Isotopic Abundances reviewed the literature over the previous two years and evaluated the published data on atomic weights and isotopic compositions on an element-by-element basis.

Available from the American Chemical Society (in press).

Atomic Transition Probabilities of Carbon, Nitrogen and Oxygen: A Critical Data Compilation

W.L. Wiese, J.R. Fuhr, and T.M. Deters.
Journal of Physical and Chemical Reference Data Monograph 7 (1995).

This monograph is a critical compilation for approximately 13,000 spectral lines of the three elements carbon, nitrogen, and oxygen (nuclear charges $Z = 6-8$), based on all available theoretical and experimental literature sources in all stages of ionization. The data are presented in separate tables for each element and ion and as a multiplet table in ascending lower and upper excitation energy order. Also included is a discussion of evaluation methods and principal criteria for judgments.

Available from the American Chemical Society, JPCRD Monograph 7 (1995).

Atomic and Molecular Physics Publications

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Atomic and Molecular Physics Publications

Atomic Weights of the Elements 1989

J.R. de Laeter and
K.G. Heumann.

Journal of Physical
and Chemical Reference
Data 20, 1313 (1991).

The Commission on Atomic
Weights and Isotopic
Abundances monitored the
literature over the past two
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

Spectral Data and Grotrian Diagrams for Highly Ionized Chromium, Cr V through Cr XXIV

Toshizo Shirai, Yohta Nakai,
Toshiaki Nakagaki, Jack
Sugar, and Wolfgang L.
Wiese.

Journal of Physical and
Chemical Reference Data
22, 1279 (1993).

Wavelengths, energy levels,
ionization energies, line
classifications, oscillator
strengths, and atomic
transition probabilities for Cr
V to Cr XXIV are tabulated. A
short review of the line
identifications and
wavelength measurements is
given for each stage of
ionization, along with
Grotrian diagrams.

Available from the
American Chemical Society,
JPCRD Reprint 461, \$28.00

Spectral Data and Grotrian Diagrams for Highly Ionized Manganese, Mn VII through Mn XXV

Toshizo Shirai, Toshiaki
Nakagaki, Kiyohiko Okazaki,
Jack Sugar and Wolfgang L.
Wiese.

Critically evaluated wave-
lengths, energy levels,
ionization energies, line
classifications, oscillator
strengths, and atomic
transition probabilities for
Mn VII to Mn XXV are
tabulated. A short review of
the line identifications and
wavelength measurements is
given for each stage of
ionization, along with
Grotrian diagrams.

Available from the
American Chemical Society,
JPCRD Reprint 471, \$24.00

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

**A Compilation of
Energy Levels and
Wavelengths for the
Spectrum of Singly-
Ionized Oxygen (O II)**

W.C. Martin, Victor
Kaufman, and Arlene
Musgrove.

Journal of Physical and
Chemical Reference Data 22,
1179 (1993).

A complete list of the most
accurately measured
wavelengths for all classified
lines of O II is presented.
Relevant astrophysical
wavelength measurements,
appropriately weighted, were
included in the level-
optimization calculations.

Available from the
American Chemical Society,
JPCRD Reprint 459, \$14.00

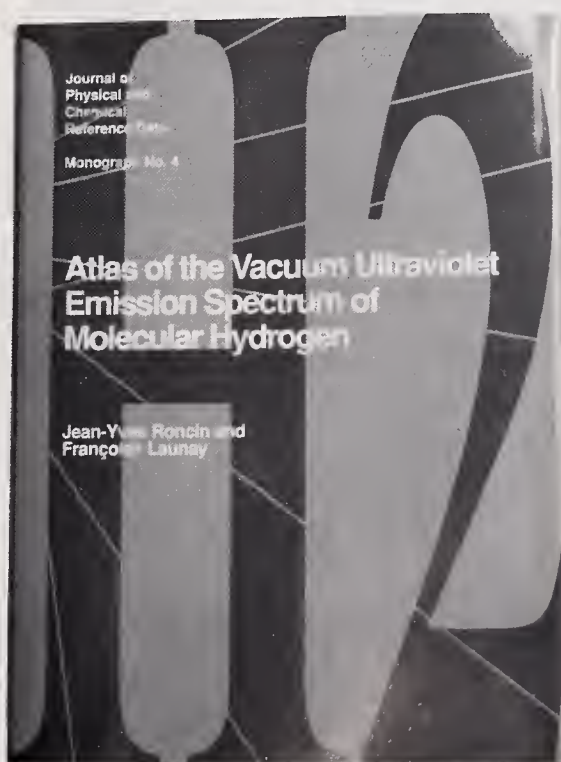
**Atlas of the Vacuum
Ultraviolet Emission
Spectrum of Molecular
Hydrogen**

Jean-Yves Roncin and
Francoise Launay.

Journal of Physical and
Chemical Reference Data
Monograph
no. 4(1994).

Vacuum ultraviolet emission
lines of H₂ have been studied
and compiled. Detailed
analysis of the Lyman and
Werner bands is included.

Available from the
American Chemical Society,
\$140.00



**Atomic and
Molecular Physics
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FAX (301) 926-0416

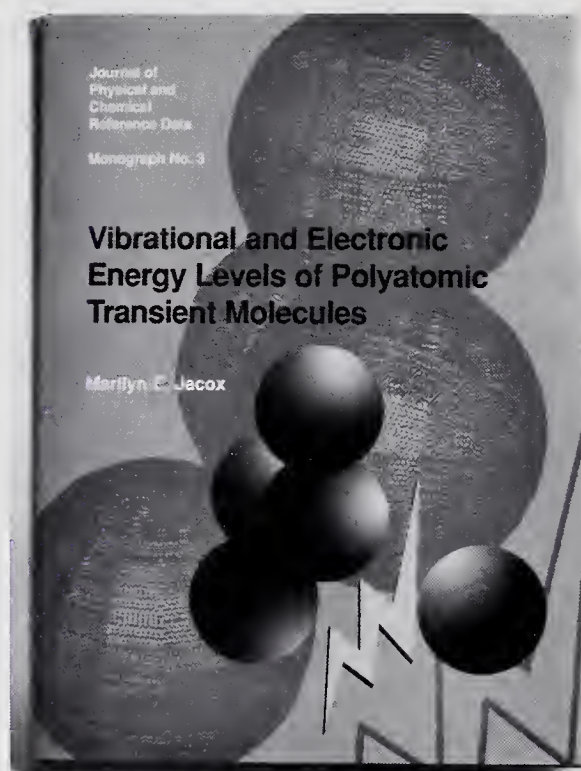
e-mail SRDATA@enh.nist.gov

Atomic and Molecular Physics Publications

Vibrational and Electronic Energy Levels of Polyatomic Transient Molecules

Marilyn E. Jacox.
Journal of Physical and
Chemical Reference Data
Monograph 3 (1994).

A critical evaluation and summary of the experimentally determined vibrational fundamentals and electronic band origins of more than 1550 neutral and ionic transient molecules possessing from three to sixteen atoms is presented.



Data are included for species containing the heavy elements. 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 \$140.00

Energy Levels of Germanium, Ge I through Ge XXXII

Jack Sugar and Arlene
Musgrove.
Journal of Physical and
Chemical Reference Data
22, 1213 (1993).

Atomic energy levels of germanium have been compiled for all stages of ionization for which experimental data are available. Experimental g-factors and leading percentages for calculated eigenvectors of levels are given. A value for the ionization energy, either experimental when available or theoretical, is included for the neutral atom and each ion. Available from the American Chemical Society, JPCRD Reprint 460, \$18.00

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Standard Reference Data has developed new databases for the exciting new biotechnology field. These are providing valuable research tools for biochemists. A significant new upgrade to the NIST/NASA/CARB Biological Macromolecule Crystallization Database is now available. The new updated Lipid Thermotropic Phase Transitions Database provides a convenient source of information on an increasingly important group of molecules.

Biotechnology data are available via the Internet: URL:
<http://ibm4.carb.nist.gov:4400/carb.html>
<http://ibm4.carb.nist.gov:4400/bmcd/bmcd.html>

SRD Biotechnology Databases

NIST/NASA/CARB Biological Macromolecule
Crystallization
Lipid Thermotropic Phase Transitions

Biotechnology

Biotechnology Databases

21. NIST/NASA/CARB Biological Macromolecule Crystallization Database Version 3.0



Gary L. Gilliland/Jane E. Ladner
Center for Advanced Research in Biotechnology
National Institute of Standards and Technology
9600 Gudelsky Drive
Rockville, MD 20850
(301) 738-6272
gary@iris8.carb.nist.gov

The database contains crystal data and the crystallization conditions of over 2,100 crystal forms of about 1,500 biological macromolecules. The data have been extracted from the scientific literature through 1993.

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

Macromolecule

- Macromolecule name
- Biological source
- Molecular weight
- Subunit composition
- Prosthetic group
- Multiple crystal forms

Crystallization Conditions

- Crystallization method
- Macromolecule concentration
- Temperature of crystallization
- pH of crystallization
- Crystal growth time
- Chemical additions to crystallization solution

Crystal Data

- Space group
- Unit cell dimension
- Z
- Crystal density

Reference

- Author
- Year reported
- Journal
- Database cross reference

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, printed or spooled to a file in a number of different formats.

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

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

34. Lipid Thermotropic Phase
Transitions: LIPIDAT2
Version 2.0



Biotechnology
Databases

Martin Caffrey
Chemistry Department
The Ohio State University
Columbus, OH 43210-1063
(614) 292-8437
mcaffrey@magnus.acs.ohio-state.edu

LIPIDAT2 is a convenient, sophisticated, and centralized source of data on one of the most diverse and important groups of molecules which is currently the subject of intensive research. This database provides thermodynamic data on complex polar lipids.

LIPIDAT2 contains:

- thermodynamic data on over 900 lipids – enthalpies and transition temperatures
- complete literature referencing and list of authors through January 1993
- data for partially- and fully-hydrated lipids
- data on the effects of various other additives, such as proteins, drugs, etc.
- over 15,000 records

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

This category describes databases that are becoming valuable tools for today's chemists, physicists, and materials scientists. These databases identify compounds or look for insights into material structures.

The NIST Crystal Database now covers the entire spectrum of well-characterized crystalline compounds, with 210,403 inorganic and organic compounds.

The widely-used Structures and Properties Database enables a user to obtain information on a molecule's thermochemical properties simply by drawing its structure or substructure. If data are not available the program calculates enthalpies of formation, vapor pressures, and boiling points from the well-known Benson's method.

SRD Chemical and Crystal Structure Databases

NIST Crystal Data

NIST/Sandia/ICDD Electron Diffraction

NIST Structures and Properties Database and
Estimation Program

SRD Major Publication in Chemical and Crystal Structure

Crystal Data Determinative Tables, 3rd Edition

Chemical and Crystal Structure Databases

3. NIST Crystal Data



Alan D. Mighell/
Vicky Lynn Karen

Crystal Data and Electron Diffraction Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899

(301) 975-6255

mighela@tiber.nist.gov/karen@tiber.nist.gov

NIST Crystal Data contains chemical, physical, and crystallographic information useful to characterize more than 210,403 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 range of solid state materials 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, Newtown Square Corporate Campus, 12 Campus Blvd., Newtown Square, PA 19073-3273. Phone (610) 325-9810.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

15. NIST/Sandia/ICDD
Electron Diffraction Database



Alan D. Mighell/
Vicky L. Karen

Crystal Data and Electron Diffraction Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-6255
mighela@tiber.nist.gov/karen@tiber.nist.gov

Designed for phase characterization using data obtained by electron diffraction methods, this 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 81,534) 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 PC format. For further information, please contact International Centre for Diffraction Data, Newtown Square Corporate Campus, 12 Campus Blvd., Newtown Square, PA 19073-3273. Phone: (610) 325-9810.

Chemical and Crystal Structure Databases

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Chemical and Crystal Structure Databases

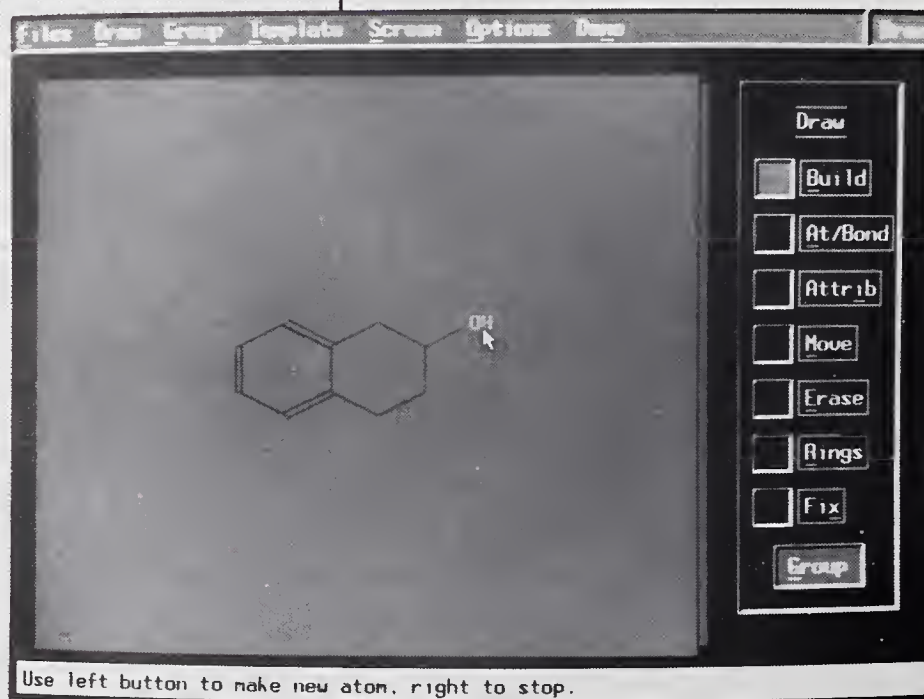
25. NIST Structures and Properties Database and Estimation Program

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

This unique product combines a database of properties and structures, a data prediction engine, and structural drawing module in an integrated system for finding and estimating chemical property data. The database contains structural drawings, names and Chemical Abstracts Registry Numbers for approximately 11,000 compounds, and experimental enthalpies for formation and entropies for 5,000 compounds. In this update, the product has been combined with Standard Reference Database 19A, NIST Positive Ion

Energetics, and therefore also contains a database of 22,000 measurements of ionization and appearance energies.

The database allows estimation of automatic perception of rings and long-range interactions.



The structure drawing module is linked to a

complete implementation of Benson's Group Additivity estimation method for gas-phase heats of formation, entropies, and heat capacities, so that properties of molecules drawn on the screen are automatically estimated without a need for the user to have any knowledge of such estimation methods. Also included is a structure-based method for estimating vapor pressures and boiling points.

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

**Crystal Data
Determinative Tables,
Third Edition, 6 vols.**

International Centre for
Diffraction Data, Newtown
Square, PA

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.
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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.
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Newtown Square, PA
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\$370.00 (set price,
individual volumes
available).

**Chemical and
Crystal Structure
Publication**

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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov



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 systems 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 6.0. Updated every year, it allows scientists instant access to reaction rate data, as well as supporting information. SRD has made available 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

NDRL/NIST Solution Kinetics

SRD Major Publications in Chemical Kinetics

Gas-Phase Tropospheric Chemistry of Organic
Compounds

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

Evaluated Kinetic Data for Combustion Modelling

Biweekly List of Papers on Radiation Chemistry and
Photochemistry

Chemical Kinetic Data Sheets for High-Temperature
Reactions. Part II

Kinetics and Mechanisms of the Gas-Phase Reactions
of the NO₃ Radical with Organic Compounds

Evaluated Kinetic and Photochemical Data for
Atmospheric Chemistry

Chemical Kinetics Databases

17. NIST Chemical Kinetics Database Version 6.0

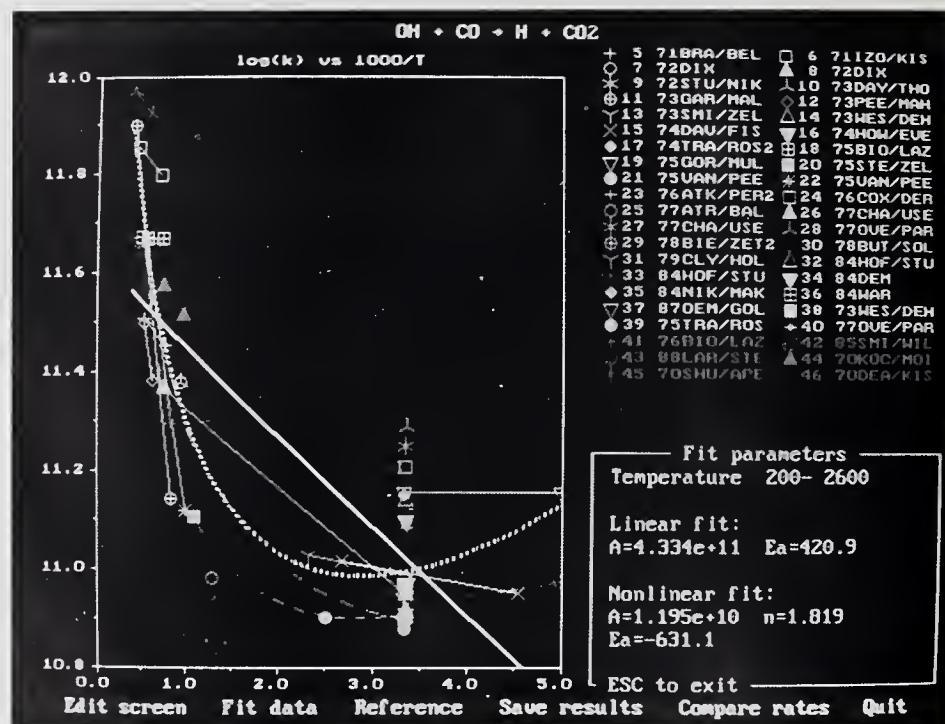


W. Gary Mallard
Chemical Kinetics Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2564
gmallard@enh.nist.gov

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 6.0 contains 29,200 rate constants, 9,200 reactions, 4,400 compounds, and 7,500 literature references. It is current through 1993.

Searching Modes:

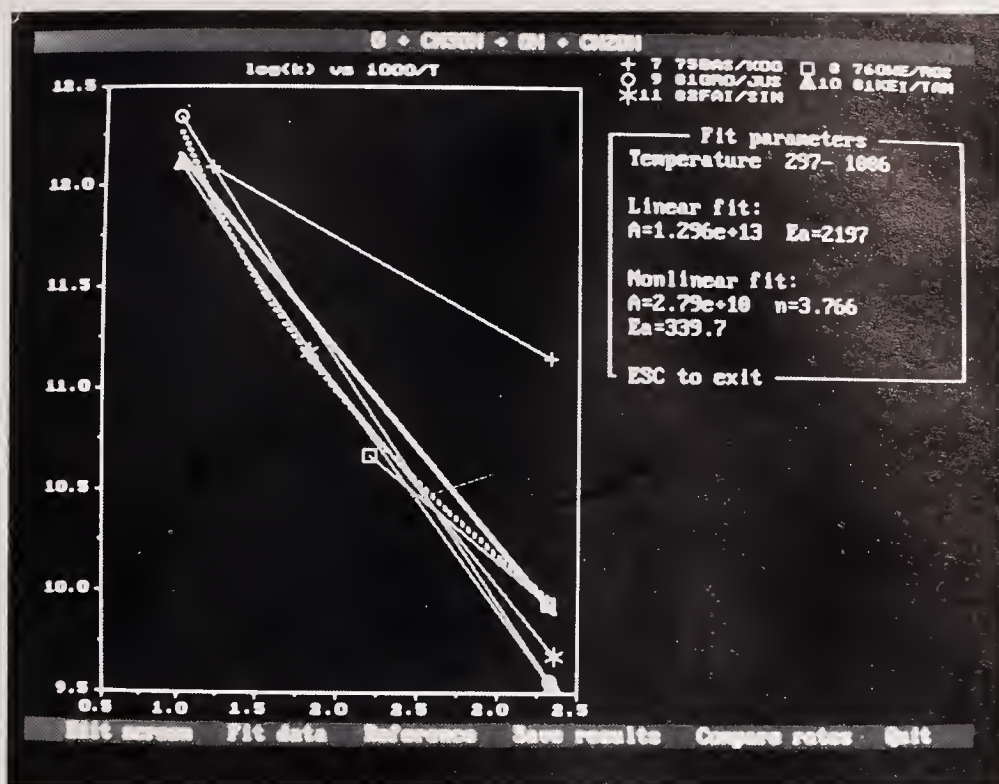
- by reactants, including various logical screens
- by author – all authors in a given paper are included
- for reactions in a particular paper
- for all reactions producing a given product



Arrhenius graphs of rate constants of NIST Chemical Kinetics Database.

For information or to order:
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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Chemical Kinetics Databases



Updated every year, user input has been incorporated into enhancements of the database.

Reactant Search Modes:

- specific reactant pairs
- reaction of compounds containing a single element
- Boolean restrictions on reactants
- elemental restrictions on reactants

Data Output:

- Individual abstracts or citations may be saved in a format suitable for use in word processors or may be printed directly.
- User selected sets of rate data may be fit to Arrhenius equations using least squares fitting. The resulting fits may be saved to a file.

This database is available on 3½" and 5¼" disks. It may also be used on Macintosh computers with PC emulator software. This database is updated regularly.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Chemical Kinetics Databases

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

40. NDRL/NIST Solution Kinetics Database Version 2.0

Alberta B. Ross
Radiation Chemistry Data Center
Radiation Laboratory
University of Notre Dame
Notre Dame, IN 46556
(219) 631-6527
ross@rcdvax.rad.nd.edu

Version 2.0 includes chemical kinetic data for free radical processes involving primary radicals from water, inorganic radicals and carbon-centered radicals in aqueous solution, and organic peroxy radicals in various solvents. Data from the literature through the end of 1992 have been compiled and evaluated at the Radiation Chemistry Data Center (Notre Dame Radiation Laboratory); recommended values of rate constants are designated for certain reactions. The database programs use the same sophisticated software as the widely-used database for gas-phase reactions - The NIST Chemical Kinetics Database. The database allows the user to quickly find previously determined rate constants, and to add data or append notes on specific reactions.

Data

- 14,000 rate determinations
- 10,800 reactions
- 7,800 chemical species for which there are data as reactants or products

Searching

- all reactions of a chemical species
- all reactions of species containing a particular element
- all reactions generating a particular product
- subsets of reactions of a particular species
- author - all authors on each paper indexed
- citation - showing all reactions from a particular paper
- chemical name fragment
- collection of acid-base forms of a particular species

Additional Features

- user input of data and user-added notes

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

Gas-Phase Tropospheric Chemistry of Organic Compounds

Roger Atkinson.

Journal of Physical and
Chemical Reference Data,
Monograph 2 (1994).

The gas-phase reactions of selected classes of organic compounds such as alkanes, alkenes (including isoprene and monoterpenes), alkynes, aromatic hydrocarbons and oxygen-containing organic compounds and their degradation products under tropospheric conditions are reviewed and evaluated.

Available from the
American Chemical Society,
\$120.00

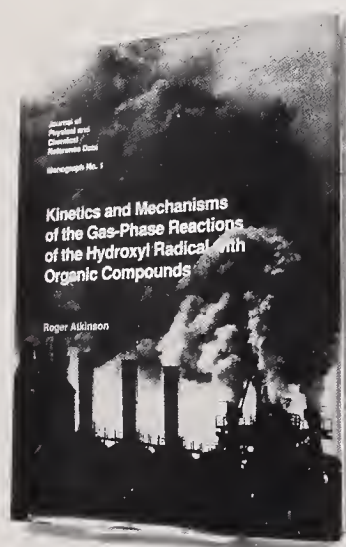
Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds

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 K 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
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Chemical Kinetics Publications

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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
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Radiation Laboratory,
University of Notre Dame,
Notre Dame, IN 46556
\$52.00/year

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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

**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 NO₃ 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
NO₃ radical in the gas-phase
are reviewed and
recommended rate constants
are presented. Reactions with
organic compounds are
covered. Needs for additional
data on NO₃ are discussed.

Available from the
American Chemical Society,
JPCRD Reprint 413, \$16.00

**Chemical
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Publications**

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Chemical Kinetics Publications

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry. Supplement IV. IUPAC

Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry

R. Atkinson, D.L. Baulch,
R.A. Cox, R.F. Hampson, Jr.,
J.A. Kerr (Chairman) and
J. Troe.

Journal of Physical and
Chemical Reference Data 21
1125 (1992).

The Subcommittee on Gas Kinetic Data Evaluation of the International Union of Pure and Applied Chemistry presents its latest recommendations on reaction rate constants and other kinetic and photochemical data needed as input to calculations which model atmospheric chemistry. Data sheets on 489 reactions are included, giving a summary of the experimental data and the basis for selection of the preferred value and assessment of its accuracy. Summary tables of the recommended rate constants and associated thermodynamic data are given. Available from the American Chemical Society, JPCRD Reprint 446, \$70.00

For information or to order:

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Industrial Fluids and Chemical Engineering

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 generate 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. REFPROP continues to be a timely and valuable tool for refrigeration engineers, chemical and equipment manufacturers, and others who use chlorofluorocarbons. Version 5.0 now provides data on 40 pure refrigerants and refrigerant mixtures. The new CYCLE_D Database will be a valuable tool for refrigeration engineers since it can simulate vapor compression refrigeration cycles using the same refrigerants as in REFPROP.

SRD Industrial Fluids and Chemical Engineering Databases

- CYCLE_D: NIST Vapor Compression Cycle Design Program
- NIST Thermophysical Properties of Pure Fluids
- NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures
- NIST Thermophysical Properties of Hydrocarbon Mixtures
- NIST Mixture Property
- NIST Thermophysical Properties of Water
- PICT/NIST Heat Capacities of Liquid Hydrocarbons
- GRI/NIST Orifice Meter Discharge Coefficient

SRD Major Publications in Industrial Fluids and Chemical Engineering

- International Equations for the Pressure along the Sublimation Curve of Ordinary Water Substance
- Thermophysical Properties of Ethane
- An International Standard Equation of State for the Thermodynamic Properties of Refrigerant 123...

Industrial Fluids and Chemical Engineering Databases

49. CYCLE_D: NIST Vapor Compression Cycle Design Program



Piotr A. Domanski
Building Environment Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-5877
pad@tiber.nist.gov

The CYCLE_D database package simulates the vapor compression refrigeration cycles using the 38 pure fluids and mixtures covered by the well-known and widely-used NIST Standard Reference Database 23 - NIST Thermodynamic Properties of Refrigerants and Refrigerant Mixtures (REFPROP). Using the Carnahan-Starling-DeSantis equation of state for all fluids except ammonia, the model can simulate both a reversed Rankine cycle and a cycle with a liquid-line/suction-line heat exchanger. The high-accuracy formulation developed by Haar and Gallagher is used for ammonia. CYCLE_D operates in a user-friendly Windows™ environment to facilitate evaluating the performance of selected working fluids at different operating conditions.

The system simulated by CYCLE_D consists of a compressor, discharge line, condenser, expansion device, evaporator, compressor suction line, and an optional liquid-line/suction-line heat exchanger. The compressor can be represented by either compressor efficiency or compressor maps provided by the user. The user of the program specifies the refrigerant and the above hardware components except the expansion device (the expansion process is assumed to be isenthalpic). The user can also input the parasitic power of the indoor fan, outdoor fan, and the control unit of the system.

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

12. NIST Thermophysical
Properties of Pure Fluids
Database
Version 4.0



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

This database, recently updated, includes thermodynamic surfaces for benzene, methanol, and toluene. Like the previous version, this new database 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 is also available, enabling users to incorporate properties directly into design, simulation, or other property-dependent software.

The fluids now available in this database are:

- Argon
- Benzene
- Butane (Iso)
- Butane (Normal)
- Carbon dioxide
- Carbon monoxide
- Deuterium
- Ethane
- Ethylene
- Helium (including superfluid states)
- Hydrogen (Normal)
- Hydrogen(Para)
- Methane
- Methanol
- Nitrogen
- Nitrogen trifluoride
- Oxygen
- Propane
- Toluene
- Xenon

Industrial Fluids
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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Industrial Fluids and Chemical Engineering Databases

The database provides equilibrium thermodynamic properties for each fluid in addition to transport properties (viscosity and thermal conductivity) and the dielectric constant for many of the fluids over broad ranges of temperature and pressure. Most of the thermodynamic surfaces are based on a 32-term modified Benedict-Webb-Rubin equation of state, but the recently included surfaces for benzene, methanol, and toluene are based on alternative NIST formulations published in the *Journal of Physical and Chemical Reference Data*.

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

23. NIST Thermodynamic
Properties of Refrigerants and
Refrigerant Mixtures
Database (REFPROP)
Version 5.0



Mark McLinden
Fluid Mixtures Data Center
National Institute of Standards and Technology
Boulder, CO 80303
(303) 497-3580
markm@bldrdoc.gov

NIST REFPROP calculates thermodynamic and transport properties of pure refrigerants and refrigerant mixtures. The package enables the user to evaluate 41 pure refrigerants and refrigerant mixtures (with up to five components) including the new environmentally acceptable HFC refrigerants. Version 5.0 is a significant enhancement of this important database.

The database includes the following fluids:

| | | |
|-------|---------|-------------------|
| R11 | R123a | R245cb |
| R12 | R124* | R290 (Propane)* |
| R13 | R125* | E134 |
| R13B1 | R134 | RC270 |
| R14 | R134a* | Butane * |
| R21 | R141b | Isobutane * |
| R22 | R142b | Pentane * |
| R23 | R143 | Isopentane* |
| R32 * | R143a * | Ammonia |
| R113 | R152a * | RC318 |
| R114 | R218 | E245 |
| R115 | R227ea | Carbon Dioxide* |
| R123* | R236ea | R245ca (NEW) |
| | | R236fa (NEW)* |
| | | R1270 (Propylene) |

Industrial Fluids
and Chemical
Engineering
Databases

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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Industrial Fluids and Chemical Engineering Databases

New in Version 5.0 is the option of calculating all mixture properties with an extended corresponding states (ECS) model. This model, previously available only for pure fluids, gives more accurate results than the CSD equation of state. (The CSD equation of state is still included in the database). The mixture interaction parameter required for mixture calculations is based on experimental data, when available, or calculated with an estimation algorithm to allow the calculation of virtually any mixture of the 41 pure fluids. For 14 pure fluids (indicated by a * on the above list) the thermodynamic properties may be calculated with a high-accuracy MBWR equation of state. New MBWR equations are included for R143a, R152a and R1270; in addition, the MBWR equations for R32, R123, and R125 have been updated and improved since Version 4.0. Ammonia properties are calculated with a special, high-accuracy equation of state. Fourteen properties are available, including enthalpy, entropy, viscosity, and thermal conductivity, and the user may choose which of these to display. FORTRAN source code is also included for those wishing to access the property routines from their own applications.

The database is available on 3½" and 5¼" disks. A Macintosh version is under development - inquire as to availability.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

4. NIST Thermophysical Properties of Hydrocarbon Mixtures Database



Marcia Huber
Fluid Mixtures Data Center
National Institute of Standards and Technology
Boulder, CO 80303
(303) 497-5252
huber@boulder.nist.gov

This powerful database (also known as 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. Liquid natural gases can easily be modeled. SUPERTRAPP performs phase equilibria calculations and gives the thermodynamic properties of all phases and the feed. These results include:

Equilibrium properties

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

Transport properties

- viscosity
- thermal conductivity

Commands are available 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
- add (and remember) a new component not in the current database
- enter data from the keyboard or from data files
- save results in a file

The database comes on 3½" and 5¼" high and low density disks.

Industrial Fluids and Chemical Engineering Databases

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Industrial Fluids and Chemical Engineering Databases

14. NIST Mixture Property Database



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

The NIST Mixture Property Database calculates 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 CO₂-rich mixtures), but results for other properties and mixtures are also accurate.

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. 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.

NIST14 provides the following properties for any specified mixture:

- bubble point pressure and temperature
- dew point pressure and temperature
- 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" disks.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

10. NIST Thermophysical Properties of Water Database



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

This database consists of an interactive program that 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 database will be revised, as appropriate, when a new formulation is adopted by this organization.

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.

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

- pressure – temperature
- density – temperature
- entropy – temperature
- enthalpy – temperature
- enthalpy – pressure

A 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.

Industrial Fluids and Chemical Engineering Databases

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Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Industrial Fluids and Chemical Engineering Databases

The range approved by IAPS for this formulation includes temperatures from 0 °C to 1000 °C and pressures up to 1500 MPa. The range over which usable results are obtainable 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 (1984).



For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

41. PICT/NIST Heat Capacities of Liquid Hydrocarbons Database



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

Developed at the Prague Institute of Chemical Technology, this database 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 an estimate of the overall percent error of the equation values
- tables of heat capacities in a specified temperature interval
- enthalpy and entropy difference between two specified temperatures

Selected data are displayed and can optionally be directed to an output device or disk file. The database can 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.

Industrial Fluids and Chemical Engineering Databases

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Industrial Fluids and Chemical Engineering Databases

45. GRI/NIST Orifice Meter Discharge Coefficient Database



Jennifer Scott
Process Measurements Division
National Institute of Standards and Technology
Boulder, CO 80303
(303) 497-3684
jscott@bldrdoc.nist.gov

Sponsored by the Gas Research Institute (GRI), Chicago, Illinois, the database contains orifice meter research data compiled at the National Institute of Standards and Technology at Gaithersburg and Boulder and at Southwest Research Institute in San Antonio.

The database will contain nitrogen gas data for the nominal 2", 4", and 6" orifice meter and water data for the 2" orifice meter.

Information available will include:

- meter tube
size
- Flow conditioning
None
Sprenkle, Zanker, etoile, or tube bundle
- Reference system
Primary
Secondary

A choice between SI and engineering units will be provided. Every data point in the database will include:

- Pipe Reynolds number
- ANSI/API 2530 equation values (1985 and 1992 version)
- Fluid properties (pressure, temperature, and density)

At the completion of a search of the database, the user can plot discharge coefficient vs. pipe Reynolds number and/or save the data found to an ASCII file to analyze as desired. Future versions will include orifice meter data from facilities both inside and outside the United States.

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

International Equations for the Pressure along the Sublimation Curve of Ordinary Water Substance

W. Wagner, A. Saul, and A. Pruss.

Journal of Physical and Chemical Reference Data 23, 515 (1994).

Correlation equations for the pressure along the melting curve of the various modifications of ice as well as for the pressure along the sublimation curve are presented in order to define the phase boundary between the solid phase (ice) and the fluid phase (liquid and gas) of ordinary water substance in pressure-temperature coordinates.

Available from the American Chemical Society, JPCRD Reprint 477, \$10.00

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 K - 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

Industrial Fluids and Chemical Engineering Publications

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e-mail SRDATA@enh.nist.gov

Industrial Fluids and Chemical Engineering Publications

An International Standard Equation of State for the Thermo- dynamic Properties of Refrigerant 123 (2,2-Dichloro-1,1,1- Trifluoroethane)

Ben A. Younglove and
Mark O. McLinden.
*Journal of Physical and
Chemical Reference Data* 23,
731 (1994).

A modified Benedict-Webb-Rubin (MBWR) equation of state has been developed for Refrigerant 123 based on recently measured thermodynamic property data and data available from the literature. Single-phase pressure-volume-temperature (*PVT*), heat capacity, and sound speed data, second virial, vapor pressure, and saturated liquid and saturated vapor density data, were used with multiproperty linear least squares fitting techniques to fit the 32 adjustable coefficients of the MBWR equation.

Available from the
American Chemical Society,
JPCRD Reprint 480, \$18.00

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e-mail SRDATA@enh.nist.gov

The NIST Materials Data Program provides evaluated data on phase equilibria, structure and characterization, and performance for a wide variety of engineering materials.

Several materials performance property databases are now available, including the new NIST High Temperature Superconductors Database, a database of evaluated property data for oxide superconductors. Version 2.0 of the NIST Structural Ceramics Database contains 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 High Temperature Superconductors

- 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)

- NIST Tribo-Ceramic Materials

- Phase Diagrams for Ceramists

SRD Major Publications in Materials Properties

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

- Binary Alloy Phase Diagrams, 2nd edition

- Phase Diagrams for Ceramists

- Critical Compilation of Surface Structures Determined by Ion Scattering Methods

- Critical Compilation of Surface Structures Determined by Surface Extended X-Ray Absorption Fine Structure (SEXAFS) and Surface Extended Electron Energy Loss Spectroscopy (SEELFS)

Materials Properties Databases

62. NIST High Temperature Superconductors Database



R.G. Munro

Ceramics Division

National Institute of Standards and Technology

Gaithersburg, MD 20899

(301) 975-6127

munro_rg@enh.nist.gov

The database of materials properties for high temperature superconductors provides evaluated property data for oxide superconductors. The range of materials covers the many series of compounds derived from the Y-Ba-Cu-O, Bi-Sr-Ca-Cu-O, Tl-Sr-Ca-Cu-O, and La-Cu-O chemical families, along with numerous other variants of the cuprate and bismate materials that are known to have superconducting phases. The materials are described by specification and characterization information that includes processing details and chemical compositions. Physical characteristics such as density and crystal structure are given in numeric tables. The material properties include superconducting characteristics (T_c , j_c , H_{c1} , H_{c2} , etc.), thermal properties (conductivity, expansion, specific heat) mechanical properties (elasticity, strength, toughness), and crystallography (cell parameters, atomic coordinates), methods, procedures, and conditions. In all cases, the sources of the data (papers published in the years 1987-1993) are fully documented in a comprehensive bibliography.

The database has a WindowsTM interface. It is available on 3½" and 5¼" disks.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

30. NIST Structural
Ceramics Database
Version 2.0



Ronald Munro
Ceramics Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-6127
munro_rg@enh.nist.gov

Version 2.0 contains thermal, mechanical, and corrosion properties of silicon carbides and silicon nitrides in a self-contained database system. Searches of the data are conducted by means of SCD's powerful combination of menus, query-by-example technique, and computer-assisted entries. Users may search for properties of a selected ceramic or use specified property values to identify required ceramics. This database contains state-of-the-art 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
- Knoop Hardness
- Fracture Toughness
- Fracture Energy
- Weibull Modulus
- Creep Exponent
- Creep Rate
- Creep Activation Energy

Materials
Properties
Databases

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e-mail SRDATA@enh.nist.gov

Materials Properties Databases

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 3½" and 5¼" high and low density disks. It may also be used on Macintosh computers with PC emulator software.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

16. NACE/NIST Corrosion Performance Databases

Charles Sturrock
Corrosion Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-6027
sturrock@enh.nist.gov

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.

Materials Properties Databases

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Materials Properties Databases

22. NIST Tribomaterials I (ACTIS) Database



John R. Rumble, Jr.
Standard Reference Data Program
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2200
rumble@enh.nist.gov

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 contacts. This new Version 2.0 includes a new, friendlier data management system (using a sort/eliminate process), along with graphical capability for either line or X-Y plots using the data of interest to the user.

The database is available in 3½" and 5¼" disks.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

47. NIST Tribo-Ceramic Materials Database



John R. Rumble, Jr.
Standard Reference Data Program
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2200
rumble@enh.nist.gov

NIST Tribo-Ceramic Materials Database is the most extensive tribology database on ceramics presently available. With data gathered from NIST research activities, selected published data, and national and international round-robin measurement programs, the database contains almost 370 records covering seven different ceramic materials in 36 combinations. Focusing on ceramics with high industrial importance and for which data availability has been poor, it includes wear data, friction data, lubricated sliding data, and mechanical and physical design data.

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

Materials Properties Databases

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Materials Properties Databases

31. Phase Diagrams for Ceramists Database Version 2.0



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

This PC WindowsTM-based CD-ROM 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 1-10, Annual Volumes for 1991-93, and the Superconductor Monograph in the PDFC series are included. 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, conversion from mole % to weight % and vice versa. In addition, all bibliographic references and chemical systems from volumes of the PDFC series are available.

This database comes on CD-ROM and runs under Microsoft[®] WindowsTM 3.1 and is available from the American Ceramic Society, 735 Ceramic Place, Westerville, OH 43081. Phone: (614) 890-4700.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

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

ASM International, Metals
Park, OH.

The Bulletin was retitled in 1991 and 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 complete reference on alloy phase information 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, \$1290.00

**Materials
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Publications**

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FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Materials Properties Publications

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 volumes contain commentaries and binary, ternary and higher order phase diagrams of oxide, metals-oxide, and metal-oxygen systems, halide, superconductor 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 clean and adsorbate-covered metal, semiconductor, and other nonmetallic substrates. The important experimental and theoretical aspects of such investigations have been extracted into easily understood tabular form supplemented by figures and ancillary tables and complete references.

Available from the
American Chemical Society,
JPCRD Reprint 376, \$12.00

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

**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

**Materials
Properties
Publications**

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FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov



This new category highlights two databases which allow surface scientists, tribologists, and analytical chemists to analyze surfaces of materials. The NIST X-Ray Photoelectron Spectroscopy Database has long been a valuable tool for determining wear, friction, and resistance to corrosion. The NIST Surface Structure Database provides 3-dimensional graphics to allow researchers to analyze quickly the surface structures of crystal surfaces of the atomic scale.

SRD Surface Structures Databases

NIST Surface Structure

NIST X-Ray Photoelectron Spectroscopy

SRD Surface Structures Publication

Atlas of Surface Structures

Surface Databases

42. NIST Surface Structure Database Version 2.0



Philip R. Watson
Department of Chemistry
Oregon State University
Corvallis, OR 97331-4003
(503) 737-2081
watsonp@ccmail.orst.edu

The Surface Structure Database (SSD) is the only complete critical compilation of reliable crystallographic information now available on surfaces and interfaces. SSD brings instant access to detailed *text and graphical* displays of about 800 experimentally determined atomic-scale structural analyses. Using the powerful, yet easy-to-use capabilities of SSD, scientists in physics, chemistry, and materials science can quickly and easily find the answer to such questions as:

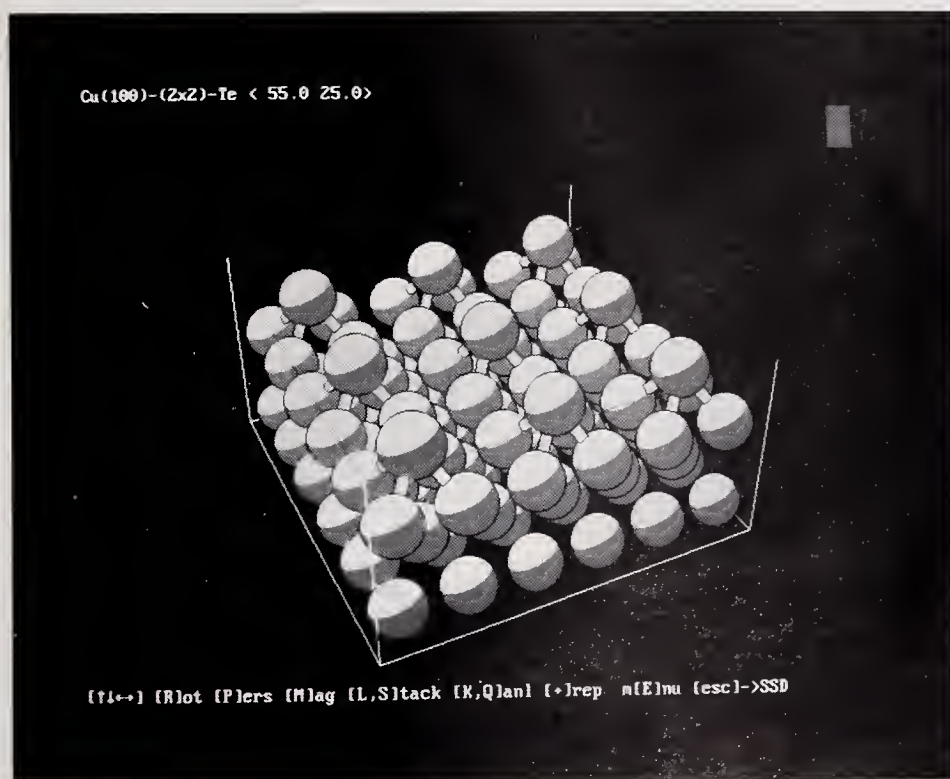
- what adatom structures on compound semiconductors have been solved?
- what are the coordinates of the atoms at the CoSi_2/Si interface?
- how many studies on Ag surfaces have appeared since 1980?
- do C-C bond lengths vary in adsorbed hydrocarbons?
- how do different surfaces of Si reconstruct?
- has the Al/GaAs (110) system been studied with LEED?

Searching needed information has been made as painless as possible, and context-sensitive on-line help is available at all times. Searches involve simply filling in the blanks with each criterion of interest and clicking the mouse - *No arcane and repetitive search procedures*. If you are not sure of the spelling or would like some suggestions, simply double-click the mouse to see a list of possibilities for that criterion. You can search for specific items (e.g., Si substrate, (111) crystal face, Al adsorbate), or for classes of materials or structures (e.g., metallic substrates, molecular adsorbates, reconstructions).

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

The database provides a wealth of information for each structure using five data screens:

| | |
|----------------------|---|
| <i>Summary</i> | full reference and brief summary of the surface structure |
| <i>Technique</i> | details of sample preparation, experimental technique, dataset and theoretical analysis |
| <i>2D Unit Cells</i> | complete description of the bulk and surface unit cell(s) |
| <i>Coordinates</i> | scrollable list of coordinates, with error bars, for surface or interface atoms |
| <i>Bonds</i> | scrollable list of important bond lengths and angles |



The powerful graphics of SSD allow detailed assessment of atomic scale structures of surfaces.

Surface Databases

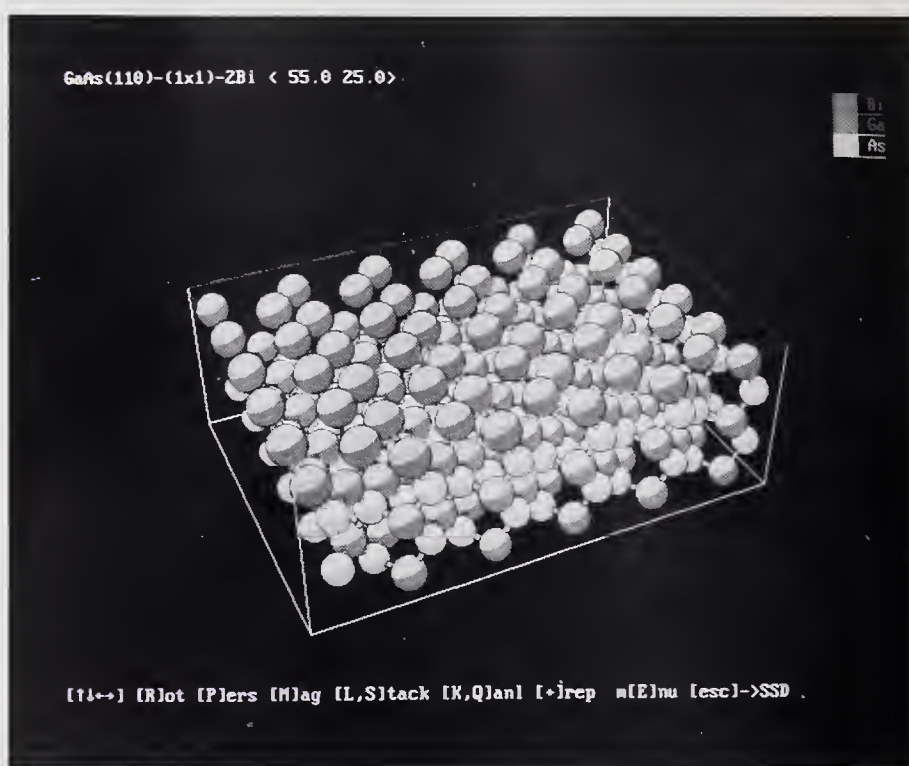
For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Surface Databases

Any or all of this information can be printed out in a convenient form suitable for reports.

However, SSD is more than a critical compilation of data. This database contains integrated 3D VGA or EGA color graphics that allow you to view all surface structures including:

- rotation, magnification and choice of perspective
- display of atoms as circle, disks, shaded spheres, etc.
- color or gray-scale publication-quality Postscript output
- full-color or red/blue stereo modes
- storage and comparison of related structures
- choice of colors for atoms, bonds and background



The data output includes printout of any numerical and textual data and on-screen 3-D visualization.

The visualization capabilities of SSD extend beyond display to interactive analysis of structural relationships - interatomic distances, bond angles, number and distance of neighbors and much more.

The database is available in 3½" and 5¼" disks.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

**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
cpowell@enh.nist.gov**

XPS gives easy access to photoelectron and Auger spectral data. Resulting from a critical evaluation of the published literature, the database contains over 13,000 line positions, chemical shifts, and splittings. A highly interactive program allows the user to search by element, line type, line energy, and many other variables. Users can easily identify unknown measured lines by matching to all previous measurements.

This version contains new data, especially polymers, and software enhancements to make data searching and display more convenient and efficient for the user. Pull-down menus are now available to:

- Initiate searches for the identification of unknown lines
- Retrieve data on photoelectron lines (core-level binding energies), Auger parameters, and doublet splittings for selected elements
- Retrieve data on chemical shifts for selected elements based on direct measurements or on calculations with respect to elemental reference energies
- Initiate searches of the database for selected groups of elements based on or for specified classes of materials
- Display Wagner plots
- Search for specified fields of the database

In addition, users can sort the displayed data in order to make the presentation more suitable for their needs. Displayed information can also be printed.

The database is available on both 3½" and 5¼" disks. It may also be used on Macintosh computers with PC emulator software.

Surface Databases

**For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov**

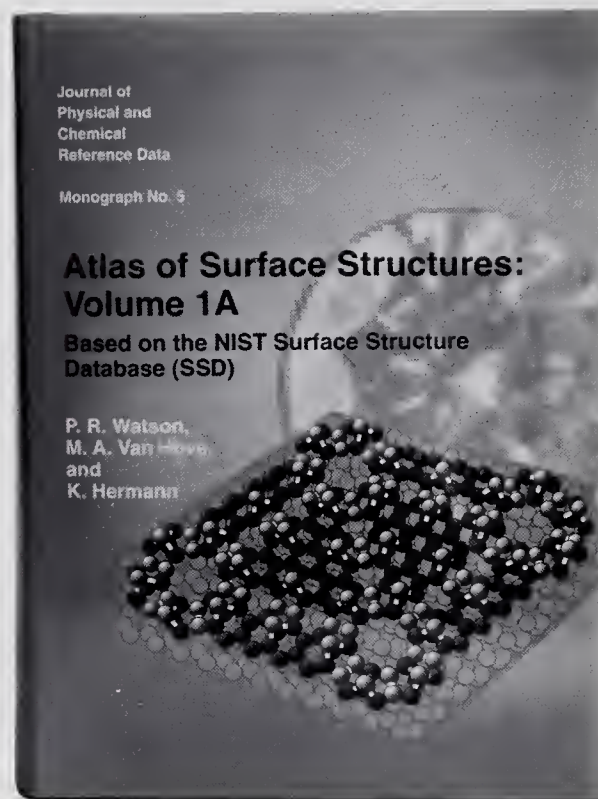
Surface Data Publication

Atlas of Surface Structures: Volume 1A (1994) Based on the NIST Surface Structure Database (SSD)

P.R. Watson, M.A. Van
Hove, and K. Hermann.
Journal of Physical and
Chemical Reference Data
Monograph 5 (1994).

These volumes contain listings of crystallographic information on nearly 600 surface structures contained in the NIST Surface Structure Database (SSD). Prefaced by explanatory text and combined with computer-generated views of the surface, the listings include references, statements on experimental and theoretical methods used, bulk and surface unit cells, and a complete list of atomic coordinates.

Available from the
American Chemical Society
\$145.00



For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

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 JANAF Thermochemical Tables contain the most complete compilations of evaluated temperature-dependent thermodynamic data for inorganic species. The Positive and Negative Ion Energetics Database now has the sophisticated Structures and Properties software.

The DIPPR® Data Compilation of Pure Compound Properties continues to represent an increasing number of chemicals of high industrial priority and provides 39 different properties to the user.

A new Special Database is available – IVTANTHERMO. This important collection of reference data developed for Soviet rocket-space technology is now readily accessible with thermodynamic properties of nearly 2300 compounds.

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

Thermodynamics and Thermochemistry

Thermodynamics and Thermochemistry

SRD Thermochemical Databases

NIST Critically Selected Stability Constants of
Metal Complexes
NIST Chemical Thermodynamics
NIST JANAF Thermochemical Tables
DIPPR® Data Compilation of Pure Compound
Properties
DIPPR® Data Compilation Access Program II –
Student DIPPR®
NIST Positive Ion Energetics with Structures and
Properties Software and NIST Negative Ion Energetics
NIST Estimation of the Thermodynamic Properties for
Organic Compounds
NIST Molten Salts
NIST JANAF Thermochemical Tables –
Shomate Coefficients
NIST JANAF Thermochemical Tables –
NASA-Lewis Coefficients
DIPPR®/NIST Activity and Osmotic Coefficients in
Aqueous Solutions Database
NIST ITS-90 Thermocouple Database

SRD Major Publications in Thermochemistry

JANAF Thermochemical Tables
Gas-Phase Ion and Neutral Thermochemistry
Physical and Thermodynamic Properties of Pure
Chemicals
Thermodynamic Properties of Individual Substances
Thermodynamic Properties of the Group IA Elements
Thermodynamic Properties of the Group IIA Elements

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

46. NIST Critically Selected Stability Constants of Metal Complexes Database

A.E. Martell
Department of Chemistry
Texas A&M University
College Station, TX 77843-3255
(409) 845-2011

This significant database provides comprehensive coverage of interactions for aqueous systems of organic and inorganic ligands with protons and various metal ions. Based on the six-volume Critical Stability Constants by Martell and Smith, the data in this database have been thoroughly reexamined and critically evaluated and new material added. It enables quick location of a needed equilibrium constant or associated heat of reaction with complete references. Every ligand possesses a structural formula for quick identification. The database has the following features:

For nearly 4000 ligands:

- metal stability constants and related equilibrium constants
- thermodynamic constants
- a complete bibliography
- structural formulas
- empirical formulas and type of ligand
- protonation constants under specified conditions of temperature and ionic strength
- heats of protonation
- entropies of protonation

For an additional 1000 ligands:

- metal ions studied
- bibliographic citations

A three-part searching system provides quick visual recognition. The metal-ligand data and optional bibliographic information for each ligand-metal system are shown in one of two standard display screens.

The database is available on 3½" and 5¼" disks. It may also be used on Macintosh computers with PC emulator software.

Thermodynamic and Thermochemical Databases

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Thermodynamic and Thermochemical Databases

2. NIST Chemical Thermodynamics Database



Malcolm W. Chase
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3692
chase@micf.nist.gov

This database contains recommended values for selected thermodynamic properties of more than 15,000 inorganic substances and organic substances containing only one or two carbon atoms. These properties include the following:

Standard state properties at 298.15 K and 1 bar

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

Properties at 0 K

- enthalpy of formation

The data files are available on diskette, and online through STN and CIS.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

13. NIST JANAF Thermochemical Tables Database



Malcolm W. Chase
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3692
chase@micf.nist.gov

The NIST 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.

The data files are available on 3½" and 5¼" disks. It is also currently available online through STN.

Thermodynamic and Thermochemical Databases

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Thermodynamic and Thermochemical Databases

11. DIPPR® Data Compilation of Pure Compound Properties Database



T.E. Daubert/R.P. Danner
The Pennsylvania State University
133 Fenske Laboratory
University Park, PA 16802-4400
(814) 863-4638
rpd@psuvm.psu.edu

The 1995 version of the DIPPR® database contains data on 39 properties for 1,458 chemicals of high industrial priority. Thermodynamic, physical, transport, and flammability property data are given. The database was prepared by The Pennsylvania State University with support from 22 members of the Design Institute for Physical Property Data (DIPPR)®, a sponsored research organization under the auspices of the American Institute of Chemical Engineers.

For each chemical included, values are given for 26 single-valued property constants and for 13 properties from correlation coefficients as functions of temperature. The database also includes estimates of the accuracy of each property value and references to the sources of measured or predicted data that 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. Output can be in the form of calculated tabular data or plots.

This database is a set of ASCII files available on diskette. It is also available online through STN.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

The Design Institute for Physical Property Data and the acronym DIPPR® are registered trademarks of the American Institute of Chemical Engineers (AIChE).

11A. DIPPR® Data Compilation Access Program II – Student DIPPR® Database

The student version of NIST Standard Reference Database 11 – DIPPR® Data Compilation of Pure Compound Properties – contains data for 100 chemicals. For each chemical, 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 on diskettes.

The Design Institute for Physical Property Data and the acronym DIPPR® are registered trademarks of the American Institute of Chemical Engineers (AIChE).

Thermodynamic and Thermochemical Databases

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Thermodynamic and Thermochemical Databases

19A. NIST Positive Ion Energetics Database Version 2.0 with Structures and Properties Software

Sharon G. Lias/Rhoda D. Levin
Chemical Kinetics and Thermodynamics Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2562
sgl@micf.nist.gov

Joel F. Liebman (Univ. of Maryland Baltimore County)
and Sherif A. Kafafi (Johns Hopkins Univ.)

This database provides rapid access to experimental data for ionization and appearance energies, enthalpies of formation of ions and the corresponding neutral species, and a complete bibliography. The powerful Structures and Properties software by Stephen E. Stein (Standard Reference Database 25) used with Version 2.0 permits the user to (1) locate all species having an ionization energy equal or close to a pre-selected value, and (2) search by structure or sub-structure. The software also can perform additivity-type estimations of thermochemical data for neutral molecules and carry out on-screen calculations of enthalpies of reaction. Data from more than 22,000 measurements of ionization and appearance energies pertaining to about 11,000 molecules are included.

Species covered are all atoms and organic and inorganic molecules, including radicals for which ionization energy or appearance energy data have been reported in the literature in the time period 1971-1991 plus data for a few selected species published before 1971.

The original source of the database was the positive ion table from "Gas-Phase Ion and Neutral Thermochemistry," J. Phys. Chem. Ref. Data 17 Suppl. 1, 1988 (the so-called GIANT Tables). Version 2.0 is an update of that publication and also includes enthalpies of formation and entropies taken from the NIST Chemical Kinetics Database (Standard Reference Database 17) and the NIST JANAF Thermochemical Tables.

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

19B. NIST Negative Ion Energetics Database

John E. Bartmess
University of Tennessee
Knoxville, TN 37996
(615) 974-6578
bartmess@utkvt.utm.edu

Gas-phase electron affinities, acidities, negative ion affinities to neutral species, negative ion enthalpies of formation and a complete bibliography are provided in this database. Data from approximately 4,100 measurements pertaining to 2,600 negative ions are included. The initial source of the database was the negative ion table from "Gas-Phase Ion and Neutral Thermochemistry," J. Phys. Chem. Ref. Data 17 Suppl. 1, 1988. This version includes corrections to that publication, subsequent data appearing through approximately the end of 1991, plus some additional data from 1992.

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

Thermodynamic and Thermochemical Databases

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Thermodynamic and Thermochemical Databases

18. NIST Estimation of the
Thermodynamic Properties for
Organic Compounds at 298.15 K
– Compounds Containing the
Elements C,H,N,O,S, and
Halogens



Eugene S. Domalski
Chemical Thermodynamics Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2529
domal@enh.nist.gov

This product (also called THERM/EST) provides a semi-automated means of carrying out additivity-type estimation schemes for thermodynamic properties of organic molecules at 298.15 K in the gas, liquid, and solid phases. A database with experimental data for approximately 1512 compounds is included. 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. Data are provided for compound types; alcohols, diols, triols, phenols, linear, branched and cyclic ethers, aldehydes; ketones, etc.

The user is offered the option of retrieving data in energy units of joules, calories, or British Thermal Units. Other features are the capacity to search the database by compound name or formula and a bibliography containing nearly 1000 references.

THERM/EST is available on 3½" or 5¼" disks. It may also be used on Macintosh computers with PC emulator software.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

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



Thermodynamic
and
Thermochemical
Databases

Malcolm W. Chase
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3692
chase@micf.nist.gov

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

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Thermodynamic and Thermochemical Databases

50. NIST JANAF Thermochemical Tables – Shomate Coefficients Database



Malcolm W. Chase
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3692
chase@micf.nist.gov

This database is a representation of the JANAF Thermochemical Tables in an equation format consistent with use in the China Lake equilibrium package (often referred to as PEP – the propellant evaluation program, developed at the Naval Weapons Center in China Lake, CA). These tabulations are represented by one or more sets of coefficients, which are derived from the following equation:

$$C_p = a + bT + cT^2 + eT^3 + d/T^2.$$

If possible, one set of coefficients is used to represent the entire thermochemical tabulation. Typically, however, two sets of coefficients are necessary with the temperature ranges being 298 K - 1000 K and 1000 K - 6000 K. The selected coefficients can be written to a file for use with the PEP program.

This database is available in both DOS and WindowsTM versions and is available on 3½" and 5¼" disks.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

51. NIST JANAF
Thermochemical Tables –
NASA-Lewis Coefficients
Database



Malcolm W. Chase
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3692
chase@micf.nist.gov

This database is a representation on the JANAF Thermochemical Tables in an equation format consistent with use in the NASA-Lewis equilibrium code (often referred to as CEC – the chemical equilibrium calculation, which was developed at the NASA-Lewis Research Center in Cleveland, OH). These tabulations are represented by one or more sets of coefficients, which are derived from the following equation:

$$C_p = a + bT + cT^2 + dT^3 + eT^4.$$

If possible, one set of coefficients is used to represent the entire thermochemical tabulation. Typically, however, two sets of coefficients are necessary with the temperature ranges being 298 K - 1000 K and 1000 K - 6000 K. The selected coefficients can be written to a file for use with the CEC program.

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

Thermodynamic
and
Thermochemical
Databases

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Thermodynamic and Thermochemical Databases

44. DIPPR®/NIST Activity and Osmotic Coefficients in Aqueous Solutions Database

David Neumann
Chemical Thermodynamics Data Center
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2525
neumann@enh.nist.gov

The DIPPR®/NIST Activity and Osmotic Coefficients in Aqueous Solutions Database calculates the activity and osmotic coefficients, the activity of water, and excess Gibbs energies for single and mixed electrolyte solutions from 25 °C to 200 °C and concentrations up to 12 molal and higher.

The database contains equation parameters and coefficients for approximately 350 single electrolytes and a large fraction of their mixtures. For many of the salts more than one equation exists in the system, making a total of 900 representations accessible. Resulting from the well-known DIPPR® Project 861-DIPPR® Electrolyte Database Project, this software includes the capability to calculate, tabulate, and graphically display activity coefficients of solutes and the osmotic coefficient of the solvent for aqueous solutions of pure and mixed electrolytes. The database permits several different modes of output, single points, tables or plots.

The database is available in 3½" and 5¼" disks.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

60. NIST ITS-90
Thermocouple Database



Dean Ripple
Process Measurements Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-4801
deanr@tiber.nist.gov

This database fully reproduces the tables of NIST Monograph 175, "Temperature-Electromotive Force Reference Functions and Tables for the Letter-Designated Thermocouple Types Based on the ITS-90," by Burns, Scroger, Strouse, Croarkin, and Guthrie. These reference functions have been adopted as standards by the American Society for Testing and Materials and the International Electrotechnical Committee. All temperatures in the database are given on the International Temperature Scale of 1990 (ITS-90).

Features of the database include:

- creation of tables with temperature as a function of voltage or voltage as a function of temperature
- interactive calculations at temperature or emf values selected by the user
- conversion of temperature or electromotive force data from a computer file
- calculations using customized thermocouple functions supplied by the user
- flexible units conversion
- output of reference function coefficients in a choice of units

The database is available on 3 1/2" and 5 1/4" disks.

Thermodynamic
and
Thermochemical
Databases

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

Thermodynamic and Thermochemical Publications

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
\$260.00

Journal of
Physical and
Chemical
Reference Data

Volume 17, 1988
Supplement No. 1

Gas-Phase Ion and Neutral Thermochemistry

Sharon G. Lias, John E. Bartmess, Joel F. Liebman,
John L. Holmes, Rocco D. Levin, and W. Gary Mallard

Published by the American Chemical Society
and the American Institute of Physics for
the National Bureau of Standards

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
\$140.00

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

Physical and Thermodynamic Properties of Pure Chemicals

T.E. Daubert and
R.P. Danner.
Taylor and Francis,
Bristol, PA, 1989.

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 the NIST Standard Reference Data Program, this compilation contains critically evaluated, internally consistent data that follow the laws of physical chemistry. The data were developed on a project supported by the Design Institute for Physical Property Data (DIPPR)[®].

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.

Supplement 2 provides data on 191 additional chemicals.

Supplement 3 contains data on 72 additional chemicals.

Supplement 4 contains data on 67 additional chemicals.

Supplement 5 contains data on 54 additional chemicals.

Available from Taylor and Francis,
Bristol, PA, (800) 821-8312.

Core Set, 900 chemicals, 1989
\$362.00

Supplement 1, 121 chemicals, 1991
\$110.00

Supplement 2, 191 chemicals, 1992
\$150.00

Supplement 3, 72 chemicals, 1993
\$125.00

Supplement 4, 67 chemicals, 1994
\$140.00

Supplement 5, 54 chemicals, 1995
\$140.00

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Thermodynamic and Thermochemical Publications

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 \$262.00, Vol. 2
\$310.00

Thermodynamic Properties of the Group IA Elements

C.B. Alcock, M.W. Chase, and V.P. Itkin.
Journal of Physical and Chemical Reference Data 23, 385 (1994).

This review describes thermodynamic properties of condensed phases of the alkali metal except francium. The properties included are: heat capacities from 0 K to 1600 K, temperatures and enthalpies of fusion and martensitic transformation in Li and Na, Debye temperature and electronic heat capacity coefficient at absolute zero temperature.

Available from the American Chemical Society, JPCRD Reprint 474, \$24.00

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**Thermodynamic
Properties of the
Group IIA Elements**

C.B. Alcock, M.W. Chase,
and V. Itkin

Journal of Physical and
Chemical Reference Data 22,
1 (1993).

The thermodynamic
properties of the alkaline
earth metals in the condensed
state have been critically
reassessed, and recommended
values for all of the relevant
thermodynamic properties are
given. Properties considered
are: temperatures and
enthalpies of phase
transformations and fusion,
heat capacities from 0 K to
2000 K, the Debye
temperatures, and electronic
heat capacity coefficients at
absolute zero temperature.

Available from the
American Chemical Society,
Reprint 447, \$20.00

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

Charles Wilson
Advanced Systems Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2080
wilson@magi.ncsl.nist.gov

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

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.

NIST Special Databases

2. NIST Structured Forms Reference Set of Binary Images (SFRS)

Charles Wilson
Advanced Systems Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-2080
wilson@magi.ncsl.nist.gov

SFRS 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.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

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

Craig Watson
Advanced Systems Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-4402
craig@magi.ncsl.nist.gov

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 is 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.

NIST Special Databases

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e-mail SRDATA@enh.nist.gov

NIST Special Databases

5. IVTANTHERMO-PC

Malcolm W. Chase
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Gaithersburg, MD 20899
(301) 975-3692
chase@micf.nist.gov

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 temperature range. 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 synthesis of refractory materials and microelectronic materials
- 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

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e-mail SRDATA@enh.nist.gov

The software provides a choice of formats, temperature scales, and energy units.

The methodology of the evaluation process of IVTANTHERMO is described in Volume 1 of the hard copy series Thermodynamic Properties of Individual Substances which is available from CRC Press, Inc. The data contained in this database will be included in a series of publications (5 volumes) available from CRC Press, Inc.

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

NIST Special Databases

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

NIST Special Databases

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

**Darrin Dimmick
Advanced Systems Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-4147
dld@magi.ncsl.nist.gov**

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 representation 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

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FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

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. System requirements are a 5¼" CD-ROM drive with software to read ISO-9660 format.

NIST Special Databases

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Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

NIST Special Databases

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

Allen Wilkinson

Advanced Systems Division

National Institute of Standards and Technology

Gaithersburg, MD 20899

(301) 975-3383

urt@jaguar.ncsl.nist.gov

M PDB contains gray scale and binary images of machine-printed pages. There are 360 digitized pages on three CD-ROM disks. 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 allows 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-printed pages. The system requirements are a CD-ROM drive with software to read ISO-9660 format.

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

9. NIST 8-Bit Gray Scale Images of Mated Fingerprint Card Pairs (MFCP) – Volumes 1-5

Craig Watson
Advanced Systems Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-4402
craig@magi.ncsl.nist.gov

Five volumes of the NIST database of mated fingerprint card pairs have been released. Each volume is a 3-disk set with each CD-ROM containing 90 mated card pairs of segmented 8-bit gray scale fingerprint images (900 fingerprint image pairs per CD-ROM). Each segmented image is 832 by 768 pixels and classified using the National Crime Information Center (NCIC) classes given by the FBI. The images are compressed using a modified JPEG lossless compression algorithm. Each CD-ROM requires approximately 630-660 megabytes of storage compressed and 1.0 gigabytes - 1.2 gigabytes uncompressed (1.8:1 average compression ratio). The database also includes example software which was written on a SUN 4/470 SPARCserver. The software is the same code used with NIST Special Database 4.

NIST Special Database 9 has the following features:

- Each volume has 270 mated card pairs of segmented 8-bit gray scale fingerprint images
- NCIC classifications given by the FBI
- Cards selected randomly thus approximating a natural horizontal slice of the NCIC classifications
- Resolution of approximately 11.0 line pairs per millimeter resolution. Scanned at 19.6850 pixels per mm
- Image format documentation and example software (written on a SUN 4/470 SPARCserver)
- Software is the same code used with NIST Special Database 4

Suitable for automated fingerprint classification research, the database can be used for algorithm development and system training and testing.

The database is a valuable tool for evaluating fingerprint systems using a statistical sample of fingerprints which approximate a natural horizontal slice of the NCIC classifications.

NIST Special Databases

For information or to order:
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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

NIST Special Databases

10. NIST Supplemental Fingerprint Card Data (SFCD) (for Special Database 9 – 8-Bit Gray Scale Images)

**Craig Watson
Advanced Systems Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-4402
craig@magi.ncsl.nist.gov**

The NIST database of supplemental fingerprint card data provides a larger sample of fingerprint patterns that have a low natural frequency of occurrence and transitional fingerprint classes in NIST Special Database 9. The data in NIST Special Database 10 are a 3-disk set with the first CD-ROM containing 2160 images and the last two CD-ROMs containing 1680 images each. Each segmented image is 832 by 768 pixels and classified using the National Crime Information Center (NCIC) classes given by the FBI. The images are compressed using a non-standard implementation of the JPEG lossless compression algorithm. The first CD-ROM requires approximately 690 megabytes of storage and the second and third CD-ROM require approximately 590 megabytes of storage compressed and 1.4 and 1.1 gigabytes uncompressed (1.9:1 average compression ratio). The database also includes example software which was written on a SUN SPARCserver. The software is the same code used with NIST Special Databases 4 and 9.

NIST Special Database 10 has the following features:

- 552 non-mated cards of supplemental data concentrating on arches, tented arches, low ridge count loops, and whorls
- NCIC classifications given by the FBI
- Resolution of approximately 11.0 line pairs per millimeter resolution. Scanned at 19.6850 pixels per mm.
- Image format documentation and example software (written on a SUN SPARC server)
- Software is the same code used with NIST Special Databases 4 and 9.

**For information or to order:
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FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov**

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

- algorithm development
- system training or testing

The database is a valuable tool for evaluating fingerprint systems using a sample of fingerprints which provides more examples of low natural occurrence classes and transition NCIC classifications.

NIST Special Databases

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FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

NIST Special Databases

14. NIST Mated Fingerprint Card Pairs 2 (MFCP2)

Craig Watson
Advanced Systems Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-4402
craig@magi.ncsl.nist.gov

NIST Special Database 14 is being distributed for use in development and testing of automated fingerprint classification and matching systems on a set of images which approximate a natural horizontal distribution of the National Crime Information Center (NCIC) fingerprint classes and were compressed using an implementation of the wavelet scalar quantization (WSQ) compression specification. The database consists of three CD-ROM disks, each containing 9,000 image pairs and requiring approximately 670 megabytes of storage compressed and 11.5 gigabytes uncompressed (18.0:1 average compression ratio). Each segmented image is 832 by 768 pixels and classified using the NCIC classes given by the FBI. The database also includes example software which was written on a SUN SPARCserver.

NIST Special Database 14 has the following features:

- 27,000 pairs of segmented 8-bit gray scale fingerprint images
- Images compressed with an implementation of the WSQ compression specification
- NCIC classifications given by the FBI
- Cards selected randomly thus approximating the natural horizontal distribution of the NCIC classifications.
- Resolution of approximately 11.0 line pairs per millimeter resolution. Scanned at 19.6850 pixels per mm.
- Image format documentation and example software (written on a SUN SPARCserver)
- The first 13,500 fingerprint images are the same as the images losslessly archived in NIST Special Database 9, Volumes 1-5.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

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 using a statistical sample of fingerprints which approximate a natural horizontal distribution of the NCIC classifications and were compressed with an implementation of the WSQ compression specification.

NIST Special Databases

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NIST Special Databases

15. COMAR: International Data Bank on Reference Materials



Carmelita S. Davis
Standard Reference Materials
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-6439
carmen@micf.nist.gov

This database has its roots in the late 1970s when the Reference Materials Service of the Laboratoire Nationale d'Essais proposed an index CODE of Reference Materials to catalog the various characteristics of Certified Reference Materials (CRM) and Reference Materials (RMs) in a form easily understood and accessible to the international community. Standard Reference Materials are extremely critical because every measurement, particularly chemical analyses or testing of materials, involves the application of standards or references to establish the calibration and verify the accuracy of the measurement. The establishment of COMAR as an international data bank is an effective and efficient means of tracking the continuing development of CRMs, their application and properties.

The Data Bank provides:

- Basic area of application (classified into eight categories and then broken down further into ten sub-categories)
- Certified or reference properties, such as:
 - chemical composition physical properties
 - molecular composition conventional properties
- Form, shape of samples
- Country of origin
- Producer
- Producer CRM

The interrogation software used in the Data Bank makes searching simple by displaying the CRMs that the user has chosen by indicating various qualitative and quantitative criteria. Some of these criteria are the area and sub-area of utilization, the nature and amount of the major element, and the nature and amount of the certified elements.

For non-U.S. orders, contact Laboratoire National d'Essais, phone: 33 1 40 43 37 50, FAX: 33 1 40 43 37 37.

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FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

**16. CHETAH: Chemical
Thermodynamic and Energy
Release Program: Version 7.0**



**Malcolm W. Chase
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 975-3692
chase@micf.nist.gov**

CHETAH 7.0 is a unique tool for predicting both thermochemical properties and certain "reactive chemical" hazards associated with chemicals and their reactions. Approved by ASTM's Committee E37 on Hazardous Potential of Chemicals, CHETAH is designed to conveniently and accurately calculate properties such as:

- heat capacity
- enthalpy
- entropy and
- Gibbs energy of reactions as a function of temperature.

The output of the "Energy Release Evaluation" option provides information about the ability of a material to decompose with violence if subjected to a severe impact. This significant new release has a number of enhancements, including the ability to predict the lower flammable limit (LFL) for a substance and increased user-friendliness.

In addition to its accurate estimation of important thermochemical properties, CHETAH will have wide utility in the Reactive Chemicals Evaluation Programs of all personnel responsible for ensuring safe operations at research, process development or manufacturing sites.

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The following are some of the functions performed using CHETAH:

- calculation of the heat of combustion of compound mixtures
- calculation of the thermochemical properties for reactions: $\Delta_{\text{rxn}} C_p$, $\Delta_{\text{rxn}} H$, $\Delta_{\text{rxn}} S$, $\Delta_{\text{rxn}} G$, $\log K$
- calculation of the thermochemical properties for compounds: C_p , S , $\Delta_f H$, $\Delta_f G$, $\log K_f$, Gibbs Energy function $(G-H)/T$, $H(T)-H(298)$
- build compounds from user-entered library groups, gases or solid crystals
- build crystals from ionic groups
- private thermochemical data (Benson's groups, gases, or crystals)
- classification of a material or mixtures on its ability to decompose with violence when subjected to severe impact
- classification of mixtures for flammability and estimate LFL

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

For information or to order:

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e-mail SRDATA@enh.nist.gov

17. Automatic Link
Establishment (ALE) Clean
Tones for Testing
Interoperability of Federal
Standards 1045A and 1046/1



Dave Wortendyke
Institute for Telecommunication Sciences
National Telecommunications and Information
Administration
Boulder, CO 80303-3328
(303) 497-5241
davew@its.bldrdoc.gov

This database is a comprehensive selection of computer-generated audio modem tones for testing the interoperability of Automatic Link Establishment (ALE) High Frequency (HF) radios that have been built to the Specification of Federal Standards (FED-STD) 1045A and 1046/1. The database has been recorded on a single 47 minute audio compact disc (CD) in 62 tracks. The CD also contains a narrative on the purpose and use of the data, and a set of calibration tones for aligning the system under test. The database tones on the CD are perfect representations of the calls required by the referenced Federal Standards because the tones were generated in a computer mathematically in the digital domain. A high density floppy disk is included with the CD package. It contains instructions and documentation for each of the test tracks and information on how to perform the tests.

The ALE Clean Tone Audio CD has the following features:

- introductory and calibration tracks
- nine tracks of SOUNDS with and without noise
- one hundred quick SOUNDS with a variety of addresses
- ALLCALLS, and selective ALLCALLS
- INDIVIDUAL calls
- star NET and GROUP calls
- ANYCALLS and WILDCARD calls
- special purpose calls

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NIST Special Databases

The 3½" floppy contains:

- all the protocol files used to generate the ALE audio modem tones
- the test plan to conduct the interoperability tests
- data log sheets keyed to each track on the CD, to record the test data
- software to generate ALE audio sound files from the protocol files
- documentation on the entire package and how to use it

For information or to order:

Phone (301) 975-2208

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e-mail SRDATA@enh.nist.gov

18. NIST Mugshot Identification Database



Craig Watson
Advanced Systems Division
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craig@magi.ncsl.nist.gov

This database is being distributed for use in development and testing of automated mugshot identification systems. The database consists of three CD-ROMs, containing a total of 3248 images of variable size, compressed with lossless compression. Each CD-ROM requires approximately 530 megabytes of storage compressed and 1.2 gigabytes uncompressed (2.2:1 average compression ratio). There are images of 1573 individuals (cases) 1495 male and 78 female. The database contains both front and side (profile) views when available. Separating front views and profiles, there are 131 cases with two or more front views and 1418 with only one front view. Profiles have 89 cases with two or more profiles and 1268 with only one profile. Cases with both fronts and profiles have 89 cases with two or more of both fronts and profiles, 27 with two or more fronts and one profile, and 1217 with only one front and one profile. Decompression software, which was written in C on a SUN workstation is included with the database.

This NIST Special Database has the following features:

- 3248 segmented 8-bit gray scale mugshot images (varying sizes) of 1573 individuals
- 1333 cases with both front and profile views
- 131 cases with two or more front views and 89 cases with two or more profiles
- images scanned at 19.6850 pixels per mm
- image format documentation and example software

Suitable for automated mugshot identification research, the database can be used for:

- algorithm development
- system training and testing

The system requirements are a CD-ROM drive with software to read ISO-9660 format and the ability to compile C source code written on a SUN workstation.

NIST Special Databases

For information or to order:

Phone (301) 975-2208

FAX (301) 926-0416

e-mail SRDATA@enh.nist.gov

NIST Special Databases

19. NIST Handprinted Forms and Characters Database



Patrick Grother
Advanced Systems Division
National Institute of Standards and Technology
Gaithersburg, MD 20899
(301) 974-4157
patrick@magi.ncsl.nist.gov

Special Database 19 contains NIST's entire corpus of training materials for handprinted document and character recognition. It publishes Handprinted Sample Forms from 3600 writers, 810,000 character images isolated from their forms, ground truth classifications for those images, reference forms for further data collection, and software utilities for image management and handling. It supersedes NIST Special Databases 3 and 7.

The features of this database are:

- "Final" accumulation of NIST's handprinted sample data
- Full-page HSF forms from 3600 writers
- Separate digit, upper and lower case, and free text fields
- Over 800,000 images with hand-checked classifications
- Binary images scanned at 11.8 dots per mm (300 dpi)
- Updated CCITT IV Compression Source Code
- Database management utilities

The database is NIST's largest and probably final release of images intended for handprinted document processing and OCR research. The full-page images are the default input to the *NIST FORM-BASED HANDPRINT RECOGNITION SYSTEM*, a public domain release of end-to-end recognition software. The images of Special Database 19 form a superset of the images of two previous releases: NIST Databases 3 and 7, which are now discontinued.

Special Database 19 is available as a 5.25 inch CD-ROM in the ISO-9660 format.

For information or to order:
Phone (301) 975-2208
FAX (301) 926-0416
e-mail SRDATA@enh.nist.gov

20. NIST Scientific and Technical Document Database



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patrick@magi.ncsl.nist.gov

Special Database 20 contains 23,468 high resolution binary images obtained from copyright-expired scientific and technical journals and books. The images contain a very rich set of graphic elements such as graphs, tables, equations, two column text, maps, pictures, footnotes, annotations, and arrays of such elements. No ground truthing or original typesetting information is available. The images contain predominantly machine-printed English, although three French and German documents are included.

The features of the database are:

- 104 articles, books and journals
- 23,468 full page binary images
- high resolution 15.75 dots per mm (400 dpi)
- 4 compact discs each containing about 500 Mb
- updated CCITT IV Compression Source Code
- a structural statistics file for each image
- page rotation estimates
- software utilities

The database is available as a four 5 1/4" CD-ROM set in the ISO 9660 format.

NIST Special Databases

For information or to order:
Phone (301) 975-2208
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1. NIST Scoring Package Release 1.0

Michael Garris
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National Institute of Standards and Technology
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mdg@magi.ncsl.nist.gov

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 whether 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" programming 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



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