

# **What's New at NIST: An Update on Web Resources Available from the National Institute of Standards and Technology**



**SLA Maryland Chapter  
Xtreme Reference: Navigating Government Data**

**October 21, 2010**

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Information Services Office**

# Presentation Overview



Free web resources available through NIST

- Background on data resources at NIST
- Updates on specific resources
- Some favorite data-rich NIST web sites

NIST Digital Archives (NDA)

- Images/information on NIST Museum artifacts
- Full-text PDF files of the *Journal of Research of National Institute of Standards and Technology*

NIST/NBS History

- Full-text PDF files of three-volume history set

# National Institute of Standards and Technology

## NIST's Mission:

“To promote U.S. innovation and industrial competitiveness by advancing measurement science, standards, and technology in ways that enhance economic security and improve our quality of life.”

- Non-regulatory agency within the US Department of Commerce.
- About 1500 scientists and 1800 guest researchers and post-doctoral students.



# Information Services Office (ISO)

## **Mission:**

*“To support and enhance the research activities of the NIST scientific and technological community through a comprehensive program of knowledge management.”*

## **Organizational Structure:**

- Research Library and Information Program
- Electronic Information and Publications Program
- NIST Museum and History Program

# NIST Standard Reference Data

Standard Reference Data: Data which has been extracted from the world's literature, assessed for reliability, and then evaluated to select the preferred values.


## **The Standard Reference Data Act**

Public Law 90-396. July 11, 1968

- “To provide for the collection, compilation, critical evaluation, publication and sale of standard reference data.”
- “The Congress hereby finds and declares that reliable standardized scientific and technical reference data are of vital importance to the progress of the Nation's science and technology. It is therefore the policy of the Congress to make critically evaluated reference data readily available to scientists, engineers, and the general public.”

# NIST Data Gateway: A Federated Search

<http://srdata.nist.gov/gateway/>

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## About: Standard Reference Data (SRD)

### Standard Reference Data Act of 1968 (PL 90-396)

[Standard Reference Data](#)  
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[NIST Online Databases List](#)  
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[Lista de Precios/Base de Datos En Linea](#)

[SRD Database Numbering System](#)

[NIST Databases Indexed by Discipline](#)  
[Analytical Chemistry](#)  
[Atomic and Molecular Physics](#)  
[Biometrics](#)  
[Biotechnology](#)  
[Chemical and Crystal Structure](#)


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[Chemical Kinetics](#)  
[Chemistry](#)  
[Communications](#)

## The NIST Data Gateway

NIST Data Gateway—provides easy access to many (currently over 80) of the NIST scientific and technical databases. These databases cover a broad range of substances and properties from many different scientific disciplines. The Gateway includes links to free online NIST data systems as well as to information on NIST PC databases available for purchase. To use the Gateway, select one of the following search options:

[Keyword](#)  
[Property](#)  
[Substance Name](#)



[Journal of Physical and Chemical Reference Data \(JPCRD\)](#) is published by the American Institute of Physics (AIP) for NIST. The objective of the Journal is to provide critically evaluated physical and chemical property data, fully documented as to the original sources and the criteria used for evaluation.

[Journal of Physical and Chemical Reference Data](#)  
[JPCRD Reprints](#)  
[JPCRD Monographs and Supplements](#)





[The National Standard Reference Data System \(NSRDS-NBS\)](#) provides access to the quantitative data of physical sciences, critically evaluated and compiled.

[National Standard Reference Data Series \(NSRDS\)](#)

Quick List:

[Atomic Spectra Database](#)  
[CODATA Fundamental Physical Constants](#)  
[NIST Ceramics WebBook](#)

## What's New in NIST Data

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[Chem-Blas: Gateway for PDB Ligands](#)

[NIST/EPA/NIH Mass Spectral Database NIST 08](#)

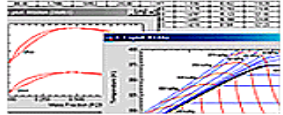
[Click here for a list of our distributors.](#)

[NIST Standard Reference Subscription Database 1NIST X-Ray Photoelectron Spectroscopy Database: Version 4.0](#)

[NIST Standard Reference Subscription Database 2Web Thermo Tables \(WTT\) - Lite Edition](#)

[NIST Standard Reference Subscription Database 3Web Thermo Tables \(WTT\) - Professional Edition](#)

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[NIST Reference Fluid Thermodynamic and Transport](#)

# NIST Standard Reference Databases

Select **List** under **NIST Online Databases** from the left menu on the home page of the NIST Data Gateway to see a complete list of NIST online databases.

The screenshot shows the NIST Standard Reference Database Online Database List page. The header includes the NIST logo and navigation links: NIST Time, NIST Home, About NIST, Contact Us, A-Z Site Index, and a search bar. Below the header is a blue banner for Technology Services with links to About TS, Products/Services, Publications, News/Events, Training/Education, and Virtual Library. The main content area is titled "NIST Online Database List" and features a left sidebar with "Topic Areas" and a main list of databases. The "Topic Areas" sidebar lists various fields such as Analytical Chemistry, Atomic and Molecular Physics, Biometrics, Biotechnology, Chemical and Crystal Structure, Chemical Kinetics, Chemistry, Communications, Construction, Environmental Data, Fire, Fluids, International Trade, Law Enforcement, Materials Properties, Mathematical Databases, Software and Tools, and Optical Character Recognition. The main list includes databases like AnthroKids - Anthropometric Data of Children, Algorithms and Data Structures Database, Atlas of the Spectrum of a Platinum/Neon Hollow-Cathode Lamp in the Region 1130-4330 Å, Atomic Energy Levels and Wavelengths, Periodic Table: Atomic Properties of the Elements, Atomic Reference Data for Electronic Structure Calculations, NIST Atomic Spectra Database (ASD), Atomic Spectral Line Broadening Bibliographic Database, Atomic Transition Probability Bibliographic Database, Atomic Weights and Isotopic Compositions, Basic Linear Algebra Computations in Java (JAMA), Bibliography of Photon Total Cross Section (Attenuation Coefficient) Measurements, NIST Biofuel Database, Biological Macromolecule Crystallization Database, Ceramics WebBook, NIST Chemical Kinetics Database, NIST Chemistry WebBook, and Chem-Blast Gateway for PDB Ligands. A "SHARE" button with social media icons is located at the top right of the database list.

NIST  
Technology Services  
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NIST Home > TS > Measurement Services > Standard Reference Data > NIST Standard Reference Database Online Database List

Topic Areas

- Analytical Chemistry
- Atomic and Molecular Physics
- Biometrics
- Biotechnology
- Chemical and Crystal Structure
- Chemical Kinetics
- Chemistry
- Communications
- Construction
- Environmental Data
- Fire
- Fluids
- International Trade
- Law Enforcement
- Materials Properties
- Mathematical Databases, Software and Tools
- Optical Character Recognition

NIST Online Database List

AnthroKids - Anthropometric Data of Children

Algorithms and Data Structures Database

Atlas of the Spectrum of a Platinum/Neon Hollow-Cathode Lamp in the Region 1130-4330 Å

Atomic Energy Levels and Wavelengths

Periodic Table: Atomic Properties of the Elements

Atomic Reference Data for Electronic Structure Calculations

NIST Atomic Spectra Database (ASD)

Atomic Spectral Line Broadening Bibliographic Database

Atomic Transition Probability Bibliographic Database

Atomic Weights and Isotopic Compositions

Basic Linear Algebra Computations in Java (JAMA)

Bibliography of Photon Total Cross Section (Attenuation Coefficient) Measurements

NIST Biofuel Database

Biological Macromolecule Crystallization Database

Ceramics WebBook

NIST Chemical Kinetics Database

NIST Chemistry WebBook

Chem-Blast Gateway for PDB Ligands

SHARE



# NIST Standard Reference Databases

Select a **Topic Area** from left menu to view list of databases in that area.

Note the format(s) of the database. “Online” code represents a free online system.

NIST Standard Reference Databases: Biotechnology - Windows Internet Explorer

http://www.nist.gov/ts/msd/srd/biotech.cfm

card game court wist

File Edit View Favorites Tools Help

Information Services Division... NIST Standard Reference...

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Technology Services

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NIST Home > TS > Measurement Services > Standard Reference Data > NIST Standard Reference Databases: Biotechnology

Topic Areas

- Analytical Chemistry
- Atomic and Molecular Physics
- Biometrics
- Biotechnology**
- Chemical and Crystal Structure
- Chemical Kinetics
- Chemistry
- Communications
- Construction
- Environmental Data
- Fire
- Fluids

Biotechnology

NIST has developed several databases in the rapidly-growing field of biotechnology.

The codes in the list below have the following meanings:

PC	PC product, most available for purchase, some are free
Online	Free online system
DG	Inclusion in the NIST Data Gateway - a portal providing access to many NIST scientific and technical databases. It is searchable by keyword, property, or substance name.
*	Product contains data that have undergone rigorous critical evaluation by experienced researchers who recommend best values.
Online Subscription	Product is a yearly subscription web product.

SRD 21 The Biological Macromolecule Crystallization Database, Online, DG, \*

SRD 74 Thermodynamics of Enzyme Catalyzed Reactions, Online, DG, \*

SRD 130 Short Tandem Repeat DNA Internet Database, Online, DG \*

SRD 102 HIV Protease Database, Online, \*

Mito Analyzer, free download \*

SRD 131 Human Mitochondrial Protein Database, Online \*

SRD 153 NIST Biofuel Database, Online, DG, \*

SRD 155 Chem-Blast Gateway for PDB Ligands, Online, DG \*

Local intranet 100%

start

Desktop My Documents My Computer My Network Places

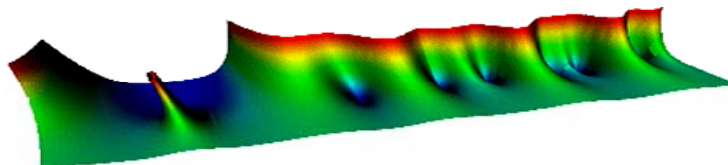
Search Desktop

12:31 PM Tuesday 9/14/2010



# NIST Digital Library of Mathematical Functions

<http://dlmf.nist.gov/>



## NIST Digital Library of Mathematical Functions

companion to the [NIST Handbook of Mathematical Functions](#)

### Project News


2010-05-11 [Handbook published and DLMF goes public](#)

2010-05-06 [Firefox 3.6 slow on Windows](#)

• [More news](#)

- Preface
- Mathematical Introduction
- 1 Algebraic and Analytic Methods
- 2 Asymptotic Approximations
- 3 Numerical Methods
- 4 Elementary Functions
- 5 Gamma Function
- 6 Exponential, Logarithmic, Sine, and Cosine Integrals
- 7 Error Functions, Dawson's and Fresnel Integrals
- 8 Incomplete Gamma and Related Functions
- 9 Airy and Related Functions
- 10 Bessel Functions
- 11 Struve and Related Functions
- 12 Parabolic Cylinder Functions
- 13 Confluent Hypergeometric Functions
- 14 Legendre and Related Functions
- 15 Hypergeometric Function
- 16 Generalized Hypergeometric Functions and Meijer  $G$ -Function
- 17  $q$ -Hypergeometric and Related Functions
- 18 Orthogonal Polynomials
- 19 Elliptic Integrals
- 20 Theta Functions
- 21 Multidimensional Theta Functions
- 22 Jacobian Elliptic Functions
- 23 Weierstrass Elliptic and Modular Functions
- 24 Bernoulli and Euler Polynomials
- 25 Zeta and Related Functions
- 26 Combinatorial Analysis
- 27 Functions of Number Theory
- 28 Mathieu Functions and Hill's Equation
- 29 Lamé Functions
- 30 Spheroidal Wave Functions
- 31 Heun Functions
- 32 Painlevé Transcendents
- 33 Coulomb Functions
- 34  $3j, 6j, 9j$  Symbols
- 35 Functions of Matrix Argument
- 36 Integrals with Coalescing Saddles
- Bibliography
- Index
- Notations
- Software

# Digital Library of Mathematical Functions (DLMF)



- The definitive reference work on applied mathematics' "special functions"
- Print companion: *NIST Handbook of Mathematical Functions*
- More than 8,000 equations and almost 500 figures

# NIST Chemistry WebBook

<http://webbook.nist.gov>



- Contains thermochemical data, reaction thermochemistry data, spectra (IR, mass, UV/Vis, electronic/vibrational), ion energetics data
- Latest major revision in June 2005
- Incremental revisions since June 2005
  - Improved display of site on handheld devices (smart phones).
  - Updated vibrational and electronic energy levels.
  - Update to thermochemical data.
  - Added support for permanent links to individual species using IUPAC InChI.
  - Added formula browser.

# Clathrate Hydrate Physical Property Database

<http://gashydrates.nist.gov/>



- Free online collection of data on the properties of gas hydrates
- Includes phase equilibria and thermophysical property information such as thermal conductivity
- Potential database users
  - Climate modelers
  - Petroleum industry

# **Cryogenic Materials Properties Database**



- Free online database on the properties of solid materials at temperatures ranging from cryogenic to room temperature
- Covers wide range of materials from stainless steels to fiberglass epoxy
- Applications include medicine, energy storage, electronics, transportation, space exploration, environmental research, weather forecasting, and defense

**Physics Data: Elemental Data Index**  
[physics.nist.gov/PhysRefData/Elements/](https://physics.nist.gov/PhysRefData/Elements/)

NIST Physics Laboratory Holdings by Element

1 H																	2 He					
3 Li	4 Be															5 B	6 C	7 N	8 O	9 F	10 Ne	
11 Na	12 Mg															13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr					
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe					
55 Cs	56 Ba		72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn					
87 Fr	88 Ra		104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo					
			57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu					
			89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr					
No Frames   EDI Home																						
NIST	Physics Laboratory	Download Table										Physical Reference Data										

## 1 Hydrogen H

Atomic Weight: 1.00794(7)

*Ionization Energy:* 13.5984 eV

Ground-state Level:  $^2S_{1/2}$

Ground-state Configuration:  $1s$

Click a database icon to retrieve data on **Hydrogen**:

Atomic Spectroscopic Data ?

[LINES](#)
[LEVELS](#)
[Handbook](#)
[HDEL](#)

Atomic and Molecular Data 

Bibliographic Databases on Atomic Spectroscopy ?

Trans Shapes Levels

X-Ray and Gamma Ray Data ?



Radiation Dosimetry Data ?

*estar*   *astar*   *pstar*

Nuclear Physics Data 



**HALF-LIFE** Isotopic

Condensed Matter Physics Data ?

127.492  
641.6

# HIV Structural Database

## <http://xpdb.nist.gov/hivsdb/hivsdb.html>

HIV protease 	HIV Structural Database and Chem-BLAST <b>HIV Structural Database &amp; Chem-BLAST</b>	NIST 
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[HIV 2-D database](#) [HIV RT database](#) [CCR5](#) [Integrase](#) [Publications](#) [Deposit Structure](#) [Animation of enzyme inhibitor interactions](#)

### HIV Structural Reference Database (102) and Chem-BLAST

Biotechnology Division, National Institute of Standards and Technology Gaithersburg, MD 20899 U.S.A.

In citing this work please use the following publications:

- 1.Prasanna, M.D., Vondrasek, J., Wlodawer, A., Ehat, T.N. Application of InChI to curate, index and query 3-D structures. *PROTEINS: Structure, Function, and Bioinformatics* **60**, 1-4 (2005).
- 2.Prasanna M.D, Vondrasek J, Wlodawer A, Rodriguez H, Bhat T.N. Chemical compound navigator: a web-based Chem-BLAST, chemical taxonomy-based search engine for browsing compounds. *Proteins* **63**(4), 907-917(2006).

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**Information is available on the following topics:**

- [Chem-BLAST Gateway to PDB Ligands](#) (Includes all ligands in the PDB and many more diseases)
- [Show credits](#)
- [Accessibility Requirements](#)
- [Background](#)
- [How to Use This Database \(Help\)](#)
- [Advanced Inhibitor Searches Using Data-tree](#): Search inhibitors using chemical compound tree, Chem-BLAST [?](#)
- [Chem-BLAST Using Semantic Concepts](#) Search structures (needs Java enabling) using Semantic Concepts and Chem-BLAST **NEW**
- [General Text Search](#): Search on citation, abstract, inhibitor name, preamble to Chem-BLAST... [?](#)
- [Inhibitor Search](#): View inhibitors in 2-D using search on citation, abstract, inhibitor name, preamble to Chem-BLAST ... [?](#)
- [Picture gallery](#): Show pre-computed pictures [?](#)
- [View slides](#): AIDS Structural Meeting presentation 2004



# NIST Digital Archives (NDA)

- NIST Museum artifacts
  - Selected images of artifacts, including the first NIST laser, a quartz crystal time standard, gage blocks, and calorimeters, to name a few
- *Journal of Research of NIST*
  - Flagship publication of NIST
  - Published since 1904 under various titles
  - Full text PDF files available from 1996 – present

# NIST/NBS History

## NIST/NBS History Volumes

- Highlights NIST accomplishments from 1901 to 1993
- Three-volume set as searchable PDF files on NVL (<http://nvl.nist.gov>)
  - *Measures for Progress*
  - *A Unique Institution*
  - *Responding to National Needs*
- NIST history appendices (1994-2009)
  - Updates appendices in latest history volume

# Questions?

A thick, horizontal yellow brushstroke with a textured, painterly appearance, extending across the width of the slide below the title.

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**Note: The identification of any commercial product or trade name does not imply endorsement or recommendation by the National Institute of Standards and Technology.**