

Other Sources of Data on the Web

NIST - National Institute of Standards and Technology

This web site contains a vast amount of data.

Chemistry

Mass Spectrometry (PC, GC/MS Instrument, Web)
Chemical Kinetics (PC, Web)
Fluid Properties (PC, Web)
Gas Phase Infrared Spectroscopy (Web)
Quantitative Infrared Spectroscopy (PC)
Ion Kinetics and Energetics (Web)
Critical Stability Constants (PC)
Alternative Refrigerants (PC, Web)
X-Ray Photoelectron Spectroscopy (Web)
Chemical Thermodynamics (Web)

Surface Science

X-Ray Photoelectron Spectroscopy (Web)
Surface Crystallization Structures (PC)

Biotechnology

Protein Data Bank (CD-ROM, Web)
Biomacromolecules/Crystallization (Web)
Lipid Thermotropic Phase Transitions (Web)
Thermodynamics of Enzyme-Catalyzed Reactions (Web)

Physics

X-Ray and Gamma-Ray Data (Web)
Fundamental Constants (Web)
Atomic Spectroscopy (Web)
Electron and Positron Stopping Powers (PC, Web)
Molecular Microwave Transitions (Web)
X-Ray Form Factors and Scattering (Web)
X-COM: Photon Cross Sections Database (Web)

Materials Properties

Crystallography and Electron Diffraction (PC)
Phase Equilibria Diagrams (PC)
Composite Reinforcement Permeability Values (Web)
Advanced Ceramics Performance (Web)
High Temperature Superconductors (Web)

Construction and Fire Science

Insulation Materials (Web)
Fire Test Database (PC)
Spectral UV-B Data (Future Web)
Refrigeration Engineering (PC)

Electronics

Plasma Modelling for Semiconductor Manufacturing (Web)

WEBSITES

PSIgate Physical Sciences Information Gateway

(<http://www.psigate.ac.uk>)

NIST Standard Reference Data Catalog

(<http://physics.nist.gov/data>)

NIST Data Gateway

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

NIST Chemistry WebBook

(<http://webbook.nist.gov>)

NIST Physical Reference Data

(<http://physics.nist.gov/PhysRefData/contents.html>)

NIST Atomic Spectra

(http://physics.nist.gov/cgi-bin/AtData/main_asd)

Isotopic Composition of Selected Atmospheric Constituents

(<http://deuterium.nist.gov/Index.html>)

Protein Data Bank

(<http://www.rcsb.org>)

Biological Macromolecule Crystallization Database

(<http://www.bmcd.nist.gov:8080/bmcd/bmcd.html>)

NIST Ceramics WebBook

(<http://www.ceramics.nist.gov/webbook/evaluate.htm>)

NIST Plasma Modeling Data

(<http://www.eeel.nist.gov/811/refdata/>)

Thermodynamics of Enzyme-Catalyzed Reactions

(<http://www.bmcd.nist.gov:8080/enzyme/enzyme.html>)

Polycyclic Aromatic Hydrocarbon Structure Index

(<http://ois.nist.gov/pah>)

X-Ray Photoelectron Spectroscopy Data

(<http://srdata.nist.gov/xps/>)

Composite Reinforcement Permeability Values

(<http://srdata.nist.gov/permeability/>)

CKMech

(<http://www.nist.gov/cstl/div836/ckmech/>)

Lipid Thermotropic Phase Transitions

(<http://www.lipidat.chemistry.ohio-state.edu/>)

CONTACT

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NIAIST - National Institute of Advanced Industrial Science and Technology

This web site contains a vast number of spectra for downloading and reproduction. It contains:

- (a) 47300 ir spectra;
- (b) 13700 ¹H-nmr spectra;
- (c) 11800 ¹³C-nmr spectra;
- (d) 20500 ms data;
- (e) 3500 Raman spectra;
- (f) 2000 esr spectra.

Access to the database and reproduction of the spectra are free of charge, but users are requested not to download more than 50 spectra per day.

To download spectra, go to the NIAIST web site <http://www.aist.go.jp/RIODB/SDBS/menu-e.html> and click on 'Integrated Spectra Data Base System for Organic Compounds (SDBS)'. Then click on 'Search Compounds/Search NMR & MS/Display Spectra'. A screen appears which invites you to input the compound for which you want spectral data. Help is available (<http://www.aist.go.jp/RIODB/SDBS/help-e.html>) if required. The box labelled 'Compound Name' is probably the least helpful of the options. It is less frustrating to search by molecular formula. For more complicated cases we recommend searching via a compound's CAS registry number. These are available in most chemical suppliers' catalogues.

To identify a compound from its spectra, go to the 'search' frame you used for obtaining spectra for a specific compound http://www.aist.go.jp/RIODB/SDBS/sdbs/owa/sdbs_sea.cre_frame_sea (The right hand side is used for searching (¹³C- and ¹H-nmr, and and ms data only).

EPA - Environmental Protection Agency - Analytical Methods

The EPA, www.epa.gov/ost/methods/ publishes laboratory analytical methods used by industries and municipalities to analyse the chemical and biological components of waste water, drinking water, sediment, and other environmental samples that are required by EPA regulations under the authority of the Clean Water Act and the Safe Drinking Water Act.

Chemfinder

Chemfinder, www.chemfinder.com indexes many hundreds of web sites that contain free chemical and spectroscopic data. It is possible to search the site using CAS Registry numbers, the most effective means of searching for any chemical substance.

Orbitron

The web site (<http://www.shef.ac.uk/chemistry/orbitra>) contains

Images representing orbitals

Animated plots of wave functions

Animated plots of electron density

'Dot-density' plots of electron density (Chime required for this feature)

Plots of radial distribution functions.

Databook web refs