

NIST Atomic and Molecular Databases on the World Wide Web

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The Physics Laboratory of the National Institute of Standards and Technology is using the World Wide Web to disseminate the physical reference data it has been producing and/or evaluating. Each Web database developed has an interface specially designed for its user community. The databases currently available are: 1) CODATA Recommended Values of the Fundamental Physical Constants; 2) Fundamental Constants Bibliographic Database; 3) Atomic Spectroscopic Database; 4) Platinum Lamp Spectrum, 113 nm to 443 nm; 5) Bibliographic Database of Atomic Transition Probabilities; 6) Infrared Spectrometer Calibration Tables; 7) Rest Frequencies for Observed Interstellar Microwave Transitions; 8) Electron-Impact Ionization Cross Section Database; 9) Tables of X-ray Mass Attenuation Coefficients; 10) Bibliographic Database of X-ray Attenuation Coefficient Measurements; 11) X-Ray Form Factor, Attenuation, and Scattering Tabulation; 12) Radionuclide Half-Life Measurements Made at NIST; and 13) Atomic Model Data for Electronic Structure Calculations. The Web versions of these databases represent the work of many people — from the compilers and evaluators of the data to the designers and programmers of the web interfaces. Work continues to add new databases and to improve those currently provided. The databases may be obtained from the Web at the URL <http://physics.nist.gov/> by selecting the link Physical Reference Data.

The 13 databases currently on the Web are divided into seven categories:

1 Physical Constants, Units, and Measurement Uncertainty

Fundamental Physical Constants

by E. Richard Cohen and Barry N. Taylor

This database gives values of the basic constants and conversion factors of physics and chemistry resulting from the 1986 least-squares adjustment of the fundamental physical constants as published by the CODATA Task Group on Fundamental Constants and recommended for international use by CODATA.

Fundamental Constants Bibliographic Database

by Peter J. Mohr and Barry N. Taylor

This searchable database gives the citations for the most important theoretical and experimental publications relevant to the fundamental physical constants and closely related precision measurements published since the mid 1980s. Earlier papers of particular interest are also included. The database is regularly updated through the addition of papers from the current literature and made more comprehensive through the addition of earlier papers.

2 Atomic Spectroscopic Data

Atomic Spectroscopic Database

by J. R. Fuhr, W. C. Martin, A. Musgrove, J. Sugar, and W. L. Wiese

This database includes most of the existing critically evaluated NIST data on atomic energy levels, transition probabilities, and wavelengths that are reasonably up-to-date. This interactive database has energy level data for over 500 spectra, transition probabilities for Sc through Ni, and wavelength data for spectra of several elements.

Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibration

by J. E. Sansonetti, J. Reader, C. J. Sansonetti, and N. Acquista

An atlas of the spectrum of a platinum/neon hollow-cathode reference lamp in the region 1130 Å to 4330 Å is given, with the spectral lines marked and their intensities, wavelengths, and classifications listed. Graphical figures of the spectrum are included.

Bibliographic Database on Atomic Transition Probabilities

by J. R. Fuhr and H. R. Felrice

This interactive database contains references on atomic transition probabilities (oscillator strengths, line strengths, and radiative lifetimes). Both theoretical and experimental papers are listed.

3 Molecular Spectroscopic Data

Wavenumber Tables for Calibration of Infrared Spectrometers

by Arthur G. Maki and Joseph S. Wells

This database is an atlas of molecular spectra and associated tables of wavenumbers from heterodyne frequency measurements for the calibration of infrared spectrometers. Five molecules are included in the atlas: CO, OCS, N₂O, NO, and CS₂. The spectra cover the 488 cm⁻¹ to 3120 cm⁻¹ and 4000 cm⁻¹ to 4400 cm⁻¹ regions.

Frequencies for Interstellar Molecular Microwave Transitions

by Frank J. Lovas

This database contains critically evaluated transition frequencies for molecular transitions detected in interstellar and circumstellar clouds recommended by NIST for reference in future astronomical observations in the microwave and millimeter wavelength regions.

4 Ionization Data

Electron-Impact Ionization Cross Section Database

by Y.-K. Kim and M. E. Rudd

This is a database of total ionization cross sections of various molecules by electron impact. The cross sections were calculated using the Binary-Encounter-Bethe (BEB) model, which combines the Mott cross section with the high- T behavior of the Bethe cross section. Selected experimental data are included.

5 X-Ray and Gamma-Ray Data

X-Ray Attenuation and Absorption for Materials of Dosimetric Interest

by J. H. Hubbell and S. M. Seltzer

Tables and graphs of computed photon mass attenuation coefficients and mass energy-absorption coefficients from 1 keV to 20 MeV are presented for all of the elements ($Z = 1$ to 92) and for 48 compounds and mixtures of radiological interest. These coefficients are basic quantities used in calculations of the penetration and the energy deposition by photons (x-ray, gamma-ray, bremsstrahlung) in biological, shielding, and other materials.

Bibliography of Photon Attenuation Measurements

by J. H. Hubbell

This bibliography contains papers (1907-1995) reporting absolute measurements of photon (XUV, x-ray, gamma-ray, bremsstrahlung) total interaction cross sections or attenuation coefficients for the elements and some compounds used in a variety of medical, industrial, defense, and scientific applications. The energy range covered is from 10 eV to 13.5 GeV.

X-Ray Form Factor, Attenuation and Scattering Tabulation

by C. T. Chantler

The primary interactions of x rays with isolated atoms from $Z = 1$ (hydrogen) to $Z = 92$ (uranium) are described and computed within a self-consistent Dirac-Hartree-Fock framework. The results are provided over the energy range from either 1 eV or 10 eV to 433 keV, depending on the atom. Self-consistent values of the f_1 and f_2 components of the atomic scattering factors are tabulated, together with the photoelectric attenuation coefficient for the atom, μ , and the value for the K-shell, μ_K , as functions of energy and wavelength.

6 Nuclear Physics Data

Radionuclide Half-Life Measurements Made at NIST

by M. P. Unterweger, D. D. Hoppes, and F. J. Schima

This database is a table of the half lives of 56 important radionuclides measured with ionization chambers by the Radioactivity Group of NIST. The included half lives range from 1.8 hours to 31.5 years.

7 Condensed Matter Physics Data

Atomic Model Data for Electronic Structure Calculations

by Svetlana Kotochigova, Zachary Levine, Eric Shirley, Mark Stiles, and Charles Clark

This database consists of evaluated data for use in total-energy calculations of electronic structure by density-functional theory. It contains total energies and orbital energy eigenvalues for all atoms from hydrogen to uranium, with micro-Hartree uncertainty in the total energy, as computed in the local-density approximation (LDA), the local-spin-density approximation (LSD), the relativistic local-density approximation (RLDA), and the scalar-relativistic local-density approximation (ScRLDA).

Conclusion

There are several new or improved databases currently being prepared for dissemination on the Web to meet the needs of the atomic and molecular data community. In particular, a description of the extended version of the Atomic Spectroscopic Database under development is included in this NIST Special Publication in the paper "NIST Atomic Spectroscopic Database," by G. R. Dalton, et al. All Physics Laboratory databases can be accessed from the Web at <http://physics.nist.gov/> by selecting the link Physical Reference Data.