The Atomic Spectroscopy Data Center at the National Institute of Standards and Technology (NIST)

Activities 2005 – 2007

Wolfgang L. Wiese
Atomic Physics Division, NIST
## The NIST Atomic Spectroscopy Data Center

<table>
<thead>
<tr>
<th>Data Center Area</th>
<th>Director</th>
<th>Staff</th>
</tr>
</thead>
<tbody>
<tr>
<td>a. Atomic Energy Levels and Wavelengths</td>
<td>J. Reader</td>
<td>E. Saloman, C. Sansonetti, W.C. Martin,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>J. Sansonetti, A. Kramida</td>
</tr>
<tr>
<td>c. Spectral Line Shapes and Shifts</td>
<td>W.L. Wiese</td>
<td>No permanent workforce;</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Occasional contractors, guest scientists,</td>
</tr>
<tr>
<td></td>
<td></td>
<td>collaborations</td>
</tr>
<tr>
<td>d. Database Design and Expansion</td>
<td>Y. Ralchenko, A. Kramida</td>
<td></td>
</tr>
<tr>
<td>e. Bibliographical Databases</td>
<td>A. Kramida</td>
<td>R. Ibacache</td>
</tr>
</tbody>
</table>

### Compilations of Numerical Data*

<table>
<thead>
<tr>
<th></th>
<th>Recent Work</th>
<th>In Progress</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelengths and Energy Levels</td>
<td>Be II, Ne II, III, VII, VIII, Ga, Rb, Xe, Ba I, II, W, Kr</td>
<td>He I, B, F, Na, Si I, Cl, Ar, K, Cs, Ba, W</td>
</tr>
<tr>
<td>Transition Probabilities</td>
<td>All Spectra of Na, Mg, Al, Si, Cl I, Ne II-IV, Fe I and Fe II, C I,II, N I, N II</td>
<td>H, D, He, Li, Be, B, S, Cl, Ar,</td>
</tr>
<tr>
<td>Line Shapes and Shifts</td>
<td>Stark Broadening Parameters for non-hydrogenic lines</td>
<td></td>
</tr>
<tr>
<td>Comprehensive Bibliographies</td>
<td>New unified bibliography DBs for wavelengths, energy levels, transition probabilities and line shapes</td>
<td>Upgraded, up-to-date bibliographies, seamlessly integrated with numerical databases</td>
</tr>
</tbody>
</table>

*If the chemical element symbol is given without roman numerals, all spectra are compiled.
NIST Databases on the World Wide Web
(address: http://physics.nist.gov)

1. **Annotated Bibliographic databases:**
   - Transition probabilities, 1914 – 2007
   - Energy levels and wavelengths 1908 – 2007 **NEW!**

2. **Numerical databases:**
   (a) Atomic Spectra Database (ASD), Version 3.1.3

   This is a new, greatly expanded database covering spectroscopic reference data for all chemical elements. Light elements up to Cu (Z = 29) are covered for most states of ionization, heavier elements are usually represented by neutral atoms and low stages of ionization.

<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>• 120,400 wavelengths</td>
<td>• 143,800 wavelengths</td>
</tr>
<tr>
<td>• 75,700 energy levels</td>
<td>• 77,100 energy levels</td>
</tr>
<tr>
<td>• 44,200 transition probabilities</td>
<td>• 60,500 transition probabilities</td>
</tr>
<tr>
<td>• 930 spectra</td>
<td>• 947 spectra</td>
</tr>
</tbody>
</table>
NIST Databases on the World Wide Web – Continued

(b) Handbook of Basic Atomic Spectroscopic Data (updated, including energy level diagrams)

(c) Spectral Data for the Chandra X-ray Observatory

(d) Ground Levels and Ionization Energies for the Neutral Atoms (updated)

(e) X-ray Transition Energies

(f) Electron-Impact Cross Sections for Ionization and Excitation (based on the binary encounter Bethe (BEB) model

(g) Energy Levels of Hydrogen and Deuterium

(h) FLYCHK Collisional – Radiative Code

(i) SAHA Plasma Population Kinetics Database
The NIST Reference Data Program

• The NIST Atomic spectroscopy Data Center puts considerable effort into critical assessment of the data.

• Only one numerical value is presented for each quantity. This may be either from a single source, considered to be the most accurate one, or from an average of several sources of about equal reliability.

• For atomic transition probabilities (oscillator strengths), explicit accuracy ratings are given.

• NIST data tables are limited to REFERENCE data, i.e., data of a certain minimum quality.
Recently Completed Data Compilations
(during 2006 and 2007)
(on NIST website and/or published)

**Handbook of Basic Atomic Spectroscopic Data**

_J.E. Sansonetti and W.C. Martin_

This handbook covers all elements H through Es (Z=1-99) and includes wavelengths and intensities for some 11,000 strong lines, together with energy levels and transition probabilities for persistent lines of all neutral and singly-ionized spectra. The handbook is available on the Web and in electronic book (eBook) format. A printed book was published as JPCRD _34_, 1559 – 2259(2005)

---

**Atomic Transition Probabilities for Neutral and Singly Ionized Iron**

Recently Completed Data Compilations - Continued

**Spectral Data of Gallium**
*Ga I through Ga XXXI*

*T. Shirai, J. Reader, A.E. Kramida and J. Sugar*

Wavelengths, energy levels, ionization energies, line classifications, and intensities have been critically reviewed and tabulated for all stages of ionization, *J. Phys. Chem. Ref. Data* 36, 509-615 (2007)

**Updates for Bibliographies**

*J. R. Fuhr, A.E. Kramida, R. Ibacache*

The bibliographies on Atomic Transition Probabilities and Spectral Line Shapes (present versions are 8.1 and 2.0) and the new bibliography on energy levels and wavelengths (present version 1.0) are up-to-date and continuously updated.
## Major Data Compilations in Press or Nearing Completion

<table>
<thead>
<tr>
<th>Compilation</th>
<th>Authors</th>
<th>Journal</th>
<th>Year</th>
<th>Notes</th>
</tr>
</thead>
</table>
Search for Publications on Atomic Energy Levels and Spectra


<table>
<thead>
<tr>
<th>Spectra:</th>
<th>W I-III e.g., Fe I, or Na, or Mg+, or Al3+, or mg iv,vi-VIII, or Ne-like-S-like, or Ne-Fe I-III, or S-</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Word/Pattern in title:</th>
<th>Publication Year: From To</th>
</tr>
</thead>
<tbody>
<tr>
<td>Author(s):</td>
<td></td>
</tr>
</tbody>
</table>

**Publication Source:**
- JOURNALS
- COLLECTIONS
- BOOKS
- REPORTS
- THESES
- PREPRINTS
  - Acta Phys. Austriaca

**Method type**
- Experiment
- Theory
- Both

**Specific Subject**
- Energy Levels
- Ionization Potentials
- Series Formulae
- Wavelengths
- Classified Lines
- New Designations
- Hyperfine Structure
- Isotopic Shift

**General Interest Category**
1. Isoelectronic Sequences
2. Compilations
3. Reviews and Bibliographies
4. Additional Theoretical Papers
5. Other

Sort by: • published year, • first author's last name.

[Search for References] [Clear Form]
Publications on Atomic Energy Levels that include numerical data

Spectra included: W I, II, III

Included are only references with the following research subject:
  Ionization Potential

11 references found

Back to search form

LaTeX source code  BibTex source code  Show search results as pdf

Ionization Energies of Tungsten Ions: W^{2+} Through W^{71+},
  A. E. Kramida and J. Reader,
  DOI:10.1016/j.adt.2006.03.002

Compilation of Wavelengths, Energy Levels, and Transition Probabilities for W I and W II,
  A. E. Kramida and T. Shirai,
  DOI:10.1063/1.1836763

Handbook of Basic Atomic Spectroscopic Data,
  J. E. Sansonetti and W. C. Martin,
  DOI:10.1063/1.1800011

Systematic Calculation of Total Atomic Energies of Ground State Configurations,
  G. C. Rodrigues, P. Indelicato, J. P. Santos, P. Patté, and F. Parente,
Search for Publications on Atomic Transition Probabilities


<table>
<thead>
<tr>
<th>Spectra:</th>
<th>Ar Ne-like</th>
<th>e.g., Fe I, or Na, or Mg+, or Al3+, or Mg iv,vi-VIII, or Fe ne-like-S-like, or Ne-Fe I-III, or S-</th>
</tr>
</thead>
<tbody>
<tr>
<td>Word/Pattern in title:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Author(s):</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Publication Source:</td>
<td>JOURNALS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>COLLECTIONS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>BOOKS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>REPORTS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>THESES</td>
<td></td>
</tr>
<tr>
<td></td>
<td>PREPRINTS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Acta Phys. Austriaca</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Acta Phys. Pol. A</td>
<td></td>
</tr>
<tr>
<td>Publication Year:</td>
<td>From</td>
<td>To</td>
</tr>
</tbody>
</table>

**Publication Source:**

- JOURNALS
- COLLECTIONS
- BOOKS
- REPORTS
- THESES
- PREPRINTS
  - Acta Phys. Austriaca
  - Acta Phys. Pol. A

**Method type**

- Experiment
- Theory
- Both

**Special \(A\)-value type**

- Forbidden Lines
- Relative \(A\)-values
- Both

**Specific Subject**

- EXPERIMENTAL
  - Absorption
  - Emission
  - Hook
  - Lifetime
  - Miscellaneous
    - THEORETICAL
    - Quantum

**General Interest Category**

1. Literature compilations
2. Review articles
3. Fundamental relationships and basic concepts
4. Detailed descriptions of experimental or theoretical methods
5. General Comments
6. Environmental influences on \(f\)-values

Sort by: ○ published year, ○ first author's last name.

[Search for References] [Clear Form]
Publications on Atomic Transition Probabilities that include numerical data

Spectrum included: Ar IX

Included are only references with the following methods: Quantum or Coulomb approximation or Estimation or Interpolation

Included are only references with data on absolute $A$-values for forbidden lines

6 references found

Back to search form

LaTeX source code  BibTex source code  Show search results as pdf

Electric-dipole, electric-quadrupole, magnetic-dipole, and magnetic-quadrupole transitions in the neon isoelectronic sequence,
U. I. Safronova, C. Namba, I. Murakami, W. R. Johnson, and M. S. Safronova,
DOI:10.1103/PhysRevA.64.012507

The 2p$^5$3l configurations of highly stripped Ne-like ions: possibility of X-ray laser emission,
T. K. Ghosh, A. K. Das, T. K. Mukherjee, and P. K. Mukherjee,

Proton collisional excitation among the 2p$^5$3s configuration levels in the Ne isoelectronic sequence ions Na II - Ni XIX,
D. A. Landman,

Atomic data and spectral line intensities for the neon isoelectronic sequence (Si V through Kr XXVII),
A. K. Bhatia, U. Feldman, and J. F. Seely,
At. Data Nucl. Data Tables 32, 435 (1985)

Wavelength predictions for lines of interest in the Ne I sequence,
S. O. Kastner,
Search for Publications on Atomic Line Broadening and Shifts


| Spectra: | Mg+ | e.g., Fe I, or Na, or Mg++, or Al3++, or mg iv, vi-VIII, or Fe ne-like-S-like, or Ne-Fc I-III, or S- |
| Word/Pattern in title: | | |
| Author(s): | | |
| Publication Year: | From | To |
| Publication Source: | JOURNALS | COLLECTIONS |
| | BOOKS | REPORTS |
| | THESIS | Acta Astrophys. Sinica |
| | | Acta Cienc. Venezolana |
| | | Acta Phys. Pol. A |
| Method type | Experiment | Theory | Both |
| Comment | Compilation |
| Mechanism | Doppler | Pressure | Resonance |
| | Stark | Zeeman | van der Waals by: |
| | | | Al |
| | | | Ar |
| General Interest Category | PRESSURE BROADENING... | Stark broadening and shifts... |
| | Hydrogen and hydrogen-like (overlapping) lines | Isolated lines of neutral spectra |
| | Isolated lines of ionic spectra | Topics of particular interest... |
| | Line wings | Effects of collective electric fields |

Sort by: ◦ published year, ◦ first author's last name.

[Search for References] [Clear Form]
Publications on Atomic Line Broadening and Shifts that include numerical data

Spectrum included: Mg II
Included are only references on the following broadening mechanism: Stark

16 references found

Plasma plume induced during laser welding of magnesium alloys,
J. Hoffinan, Z. Szymański, and V. Azharonok,

Mg II 448.1 nm spectral line Stark broadening parameters,
S. Djeniže, A. SrečkoVić, and S. Bukvić,
DOI:10.1143/JJAP.44.1450

Mg II spectral line broadening in helium, oxygen and argon-helium plasmas,
S. Djeniže, S. Bukvić, A. SrečkoVić, and M. Platiša,

Mg II h and k lines Stark parameters,
S. Bukvić, A. SrečkoVić, and S. Djeniže,

Electron-impact broadening of Mg II spectral lines for astrophysical and laboratory plasma research,
M. S. Dimitrijević and S. Sahal-Bréchot,

Stark widths and shifts predictions from regularities for higher members of several Mg I and Mg II spectral series,
J. Purić, V. Milosavljević, M. Milosavljević, and M. Ćuk,
Number of atomic-spectroscopy papers per element

- Years 1900-1980
- Years 1981-2006

Elements: He, Ne, Ar, Ca, Fe, Kr, Mo, Cd, Ba, Nd, Eu, Yb, W, Hg, Pb, Th, U

Z-axis: 0 to 120
Number of atomic-spectroscopy papers per isoelectronic sequence

Sequence number (1 = [H], 100 = [Fm])
Work in progress on bibliographic databases

1) Automation of retrieval of new papers
2) Enhancement of rendered content
3) Integration with Atomic Spectra Database
Some data for neutral and singly-charged ions are available in the [Handbook of Basic Atomic Spectroscopic Data](http://physics.nist.gov/asd3).

### NIST Atomic Spectra Database Lines Data

**Example of how to reference these results:**

**Query NIST Bibliographic Databases for Ga I (new window):**
- Wavelengths
- Transition Probabilities

### Ga I: 342 Lines of Data Found

**Wavelength in:** vacuum below 2000 Å, air between 2000 and 20000 Å, vacuum above 20000 Å

**Highest relative intensity:** 100


<table>
<thead>
<tr>
<th>Observed Wavelength Vac (Å)</th>
<th>Ritz Wavelength Vac (Å)</th>
<th>Rel. Int. (?!)</th>
<th>Aki (s⁻¹)</th>
<th>Acc.</th>
<th>E_i (cm⁻¹)</th>
<th>E_k (cm⁻¹)</th>
<th>Configurations</th>
<th>Terms</th>
<th>J_i - J_k</th>
<th>g_i - g_k</th>
</tr>
</thead>
<tbody>
<tr>
<td>571.3</td>
<td>571*</td>
<td>2a</td>
<td>0</td>
<td>-175 10</td>
<td>150</td>
<td>0</td>
<td>3d₁⁰4s²4p - 3d₈(2D)4s²4p²(1S)</td>
<td>2P⁰ - 2D</td>
<td>1/2 - 3/2</td>
<td>2 - 4</td>
</tr>
<tr>
<td>574.2</td>
<td>574*</td>
<td>0a</td>
<td>826.190</td>
<td>175 10</td>
<td>150</td>
<td>0</td>
<td>3d₁⁰4s²4p - 3d₈(2D)4s²4p²(1S)</td>
<td>2P⁰ - 2D</td>
<td>3/2 - 3/2</td>
<td>4 - 4</td>
</tr>
<tr>
<td>584.9</td>
<td>585*</td>
<td>3a</td>
<td>826.190</td>
<td>171 790</td>
<td>0</td>
<td>-166 050</td>
<td>3d₁⁰4s²4p - 3d₈(2D)4s²4p²(1D)</td>
<td>2P⁰ - 2D</td>
<td>3/2 - 5/2</td>
<td>4 - 6</td>
</tr>
<tr>
<td>601.3</td>
<td>602*</td>
<td>7a</td>
<td>826.190</td>
<td>166 050</td>
<td>0</td>
<td>-166 050</td>
<td>3d₁⁰4s²4p - 3d₈(2D)4s²4p²(1D)</td>
<td>2P⁰ - 2D</td>
<td>3/2 - 3/2</td>
<td>4 - 4</td>
</tr>
<tr>
<td>606.1</td>
<td>605*</td>
<td>14a</td>
<td>826.190</td>
<td>166 050</td>
<td>0</td>
<td>-166 050</td>
<td>3d₁⁰4s²4p - 3d₈(2D)4s²4p²(1D)</td>
<td>2P⁰ - 2D</td>
<td>3/2 - 3/2</td>
<td>4 - 4</td>
</tr>
<tr>
<td>609.8</td>
<td>610*</td>
<td>15a</td>
<td>826.190</td>
<td>163 930</td>
<td>0</td>
<td>-163 930</td>
<td>3d₁⁰4s²4p - 3d₈(2D)4s²4p²(1D)</td>
<td>2P⁰ - 2P</td>
<td>1/2 - 1/2</td>
<td>2 - 2</td>
</tr>
<tr>
<td>613.3</td>
<td>613*</td>
<td>13a</td>
<td>826.190</td>
<td>163 930</td>
<td>0</td>
<td>-163 930</td>
<td>3d₁⁰4s²4p - 3d₈(2D)4s²4p²(1D)</td>
<td>2P⁰ - 2P</td>
<td>3/2 - 1/2</td>
<td>4 - 2</td>
</tr>
<tr>
<td>616.1</td>
<td>616*</td>
<td>7a</td>
<td>826.190</td>
<td>163 140</td>
<td>0</td>
<td>-163 140</td>
<td>3d₁⁰4s²4p - 3d₈(2D)4s²4p²(1D)</td>
<td>2P⁰ - 2D</td>
<td>3/2 - 5/2</td>
<td>4 - 6</td>
</tr>
</tbody>
</table>
Y.-K. Kim, K.K. Inikura, M.E. Rudd, M.A. Ali, and P.M. Stone

1: National Institute of Standards and Technology, Physics Laboratory, Atomic Physics Division
2: NIST, Chemical Science and Technology Laboratory, Physical and Chemical Properties Division
3: University of Nebraska-Lincoln, Department of Physics and Astronomy, Lincoln, NE 68588-0111
4: Howard University, Department of Chemistry, Washington, DC 20059
5: NIST, Physics Laboratory, Office of Electronic Commerce in Scientific and Engineering Data

This is a database primarily of total ionization cross sections of molecules by electron impact. The database also includes cross sections for some atoms and energy distributions of ejected electrons for H, He, and H₂. The cross sections were calculated using the Binary-Encounter-Bethe (BEB) model, which combines the Mott cross section with the high-incident energy behavior of the Bethe cross section. Selected experimental data are included. Electron-impact excitation cross sections are also included for some selected atoms.

Introduction and References

Access the Database: Atoms & Molecules

Contributions of the following colleagues are gratefully acknowledged:
W. M. Huo, NASA Ames Research Center, Moffet Field, CA 94035-1000
W. Hwang, Samsung Electronics, Suwon, Korea
Electron-Impact Cross Section Database
(http://physics.nist.gov/ionxsec)

M. A. Ali, K. K. Irikura, Y.-K. Kim, P. M. Stone

Already in the database:
1. Total ionization cross sections of neutral atoms and molecules, singly charged molecular ions (about 100)
2. Differential ionization cross sections of H, He, H₂
3. Excitation cross sections of light atoms

New results to be added by summer, 2007:
4. Total ionization cross sections (direct + excitation-autoionization) of Mo, Mo⁺, W, W⁺ (joint work with KAERI, see graphs)—BEB model plus BE/E scaling of Born cross sections [Mo/Mo⁺ in Kwon, Rhee & Kim, Int. J. Mass Spectrometry, 245, 26 (2005)]
5. Excitation cross sections of H₂ (see graphs)—BE scaling of Born cross sections
6. Ionization cross sections of Si, Ge, Sn, Pb, Cl, Br, I, Cl₂, Br₂, I₂