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

Data Center Area	Director	Staff
a. Atomic Energy Levels and Wavelengths	J. Reader	E. Saloman, C. Sansonetti, W.C. Martin, J. Sansonetti, A. Kramida
b. Atomic Transition Probabilities	W.L. Wiese	D.E. Kelleher, L. Podobedova, J.R. Fuhr
c. Spectral Line Shapes and Shifts	W.L. Wiese	No permanent workforce; Occasional contractors, guest scientists, collaborations
d. Database Design and Expansion	Y. Ralchenko, A. Kramida	
e. Bibliographical Databases	A. Kramida	R. Ibacache
Compilations of Numerical Data*	**Recent Work**	**In Progress**
Wavelengths and Energy Levels	Be II, Ne II, III,VII, VIII, Ga, Rb, Xe, Ba I, II, W, Kr	He I, B, F, Na, Si I, Cl, Ar, K, Cs, Ba, W
Transition Probabilities	All Spectra of Na, Mg, Al, Si, Cl I,Ne II-IV, Fe I and Fe II, C I,II, N I, N II	H, D, He, Li, Be, B, S, Cl, Ar,
Line Shapes and Shifts	Stark Broadening Parameters for non-hydrogenic lines	
Comprehensive Bibliographies	New unified bibliography DBs for wavelengths, energy levels, transition probabilities and line shapes	Upgraded, up-to-date bibliographies, seamlessly integrated with numerical databases

*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

   Line Widths and Shifts, 1992 – 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.

Version 3.0.2 (2005)	Version 3.1.3 (2007)
•120,400 wavelengths •75,700 energy levels •44,200 transition probabilities • 930 spectra	•143,800 wavelengths • 77,100 energy levels • 60,500 transition probabilities • 947 spectra

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

J.R. Fuhr and W.L. Wiese, J. Phys. Chem. Ref. Data 35 ,1669-1809 (2007)

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

Compilation of Wavelengths, Energy Levels and Transition Probabilities for W I and W II

A.E. Kramida and T. Shirai, J. Phys. Chem. Ref. Data, 35,, 423-683 (2006)

Atomic Transition Probabilities of Sodium and Magnesium, A Critical Compilation

D.E. Kelleher and L.I. Podobedova, J. Phys. Chem. Ref. Data, in press
(Already part of ASD)

Atomic Transition Probabilities of Aluminum and of Silicon, A Critical Compilation

D.E. Kelleher and L.I. Podobedova, submitted to J. Phys. Chem. Ref. Data
(Already part of ASD)

Critically Evaluated Atomic Transition Probabilities for Sulfur, S I through S XV

L.I. Podobedova, D.E. Kelleher, and W.L. Wiese submitted to J. Phys. Chem. Ref. Data
(Already part of ASD)

Physics Laboratory
Physical Reference Data

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Search for Publications on Atomic Energy Levels and Spectra

Help on search

The database presently contains 10549 references dating from 1908 to 2007. Last updated on September 11, 2007.

Spectra: W I-III

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-

Word/Pattern in title:

Author(s):

Publication Year: From / To

Publication Source:

JOURNALS
COLLECTIONS
BOOKS
REPORTS
THESES
PREPRINTS
Acta Phys. Acad. Sci. Hung.
Acta Phys. Austriaca
Acta Phys. Hung.
Acta Phys. Pol.

Method type	**Specific Subject**	**General Interest Category**
☐ Experiment ☐ Theory ☐ Both	Energy Levels Ionization Potentials Series Formulae Wavelengths Classified Lines New Designations Hyperfine Structure Isotopic Shift	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]

NIST
National Institute of Standards and Technology
Physics Laboratory

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,
At. Data Nucl. Data Tables **92**, 457–479 (2006)
DOI:10.1016/j.adt.2006.03.002

Click to open the article in the journal online archive

Compilation of Wavelengths, Energy Levels, and Transition Probabilities for W I and W II,
A. E. Kramida and T. Shirai,
J. Phys. Chem. Ref. Data **35**, 423–683 (2006)
DOI:10.1063/1.1836763

Handbook of Basic Atomic Spectroscopic Data,
J. E. Sansonetti and W. C. Martin,
J. Phys. Chem. Ref. Data **34**(4), 1559–2259 (2005)
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,
At. Data Nucl. Data Tables **86**, 117–233 (2004)

Physics Laboratory
Physical Reference Data

NIST National Institute of Standards and Technology

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Search for Publications on Atomic Transition Probabilities

Help on search

The database presently contains 7463 references dating from 1914 to 2007. Last updated on September 11, 2007.

Spectra: Ar Ne-like

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-

Word/Pattern in title:

Author(s):

Publication Year: From | To

Publication Source:

JOURNALS
COLLECTIONS
BOOKS
REPORTS
THESES
PREPRINTS
Acta Phys. Acad. Sci. Hung.
Acta Phys. Austriaca
Acta Phys. Pol.
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

NIST National Institute of Standards and Technology Physics Laboratory

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

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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,
Phys. Rev. A **64**, 012507 (2001)
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,
Astrophys. J. **452**, 949 (1995)

Proton collisional excitation among the $2p^5 3s$ configuration levels in the Ne isoelectronic sequence ions Na II - Ni XIX,
D. A. Landman,
J. Quant. Spectrosc. Radiat. Transfer **34**, 365 (1985)

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,
J. Opt. Soc. Am. **70**, 1550 (1980)

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Physical Reference Data

NIST National Institute of Standards and Technology

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Search for Publications on Atomic Line Broadening and Shifts

Help on search

The database presently contains 3666 references dating from 1961 to 2007. Last updated on September 11, 2007.

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-Fe I-III, or S-

Word/Pattern in title:

Author(s):

Publication Year: From | To

Publication Source:

JOURNALS
COLLECTIONS
BOOKS
REPORTS
THESES
Acta Astrophys. Sinica
Acta Cient. Venezolana
Acta Fac. Rerum Nat. Univ. Comenianae, Phys.
Acta Phys. Hung.
Acta Phys. Pol. A

Method type | **Mechanism** | **General Interest Category**

- Experiment
- Theory
- Both
- Comment
- Compilation

Doppler
Pressure
Resonance
Stark
Zeeman
van der Waals by:
Al
Ar

Combine mechanisms by
- OR
- AND

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

NIST National Institute of Standards and Technology Physics Laboratory

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

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Plasma plume induced during laser welding of magnesium alloys,
J. Hoffman, Z. Szymański, and V. Azharonok,
in *Plasma 2005, AIP Conf. Proc. 812*, 469-472 (Edited by M. J. Sadowski, M. Dudeck, H.-J. Hartfuss, and E. Pawelec, AIP Press, Melville, NY, 2006)

Mg II 448.1 nm spectral line Stark broadening parameters,
S. Djeniže, A. Srećković, and S. Bukvić,
Jpn. J. Appl. Phys. **44**, 1450–1451 (2005)
DOI:10.1143/JJAP.44.1450

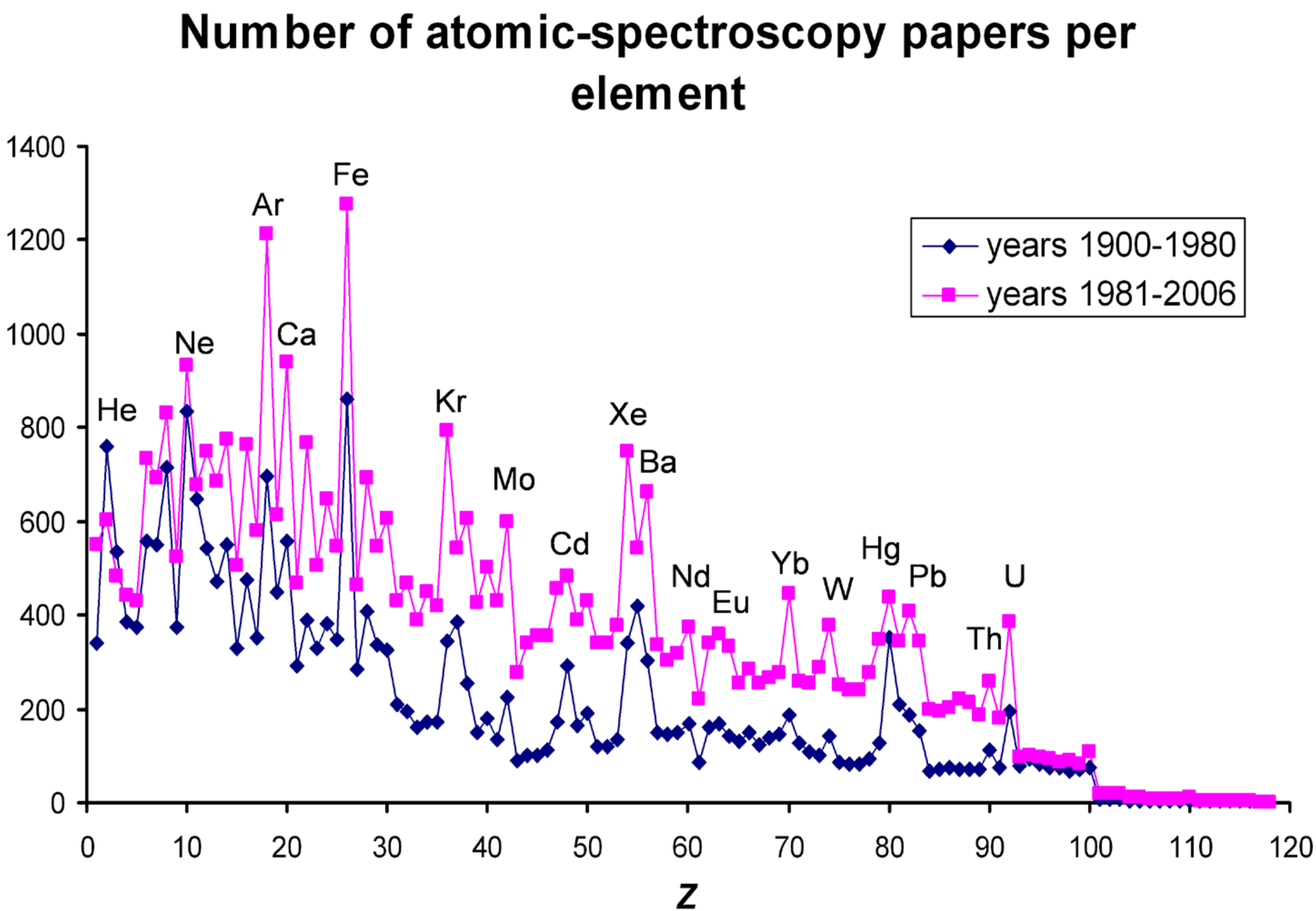
Mg II spectral line broadening in helium, oxygen and argon-helium plasmas,
S. Djeniže, S. Bukvić, A. Srećković, and M. Platiša,
Astron. Astrophys. **424**, 561–564 (2004)

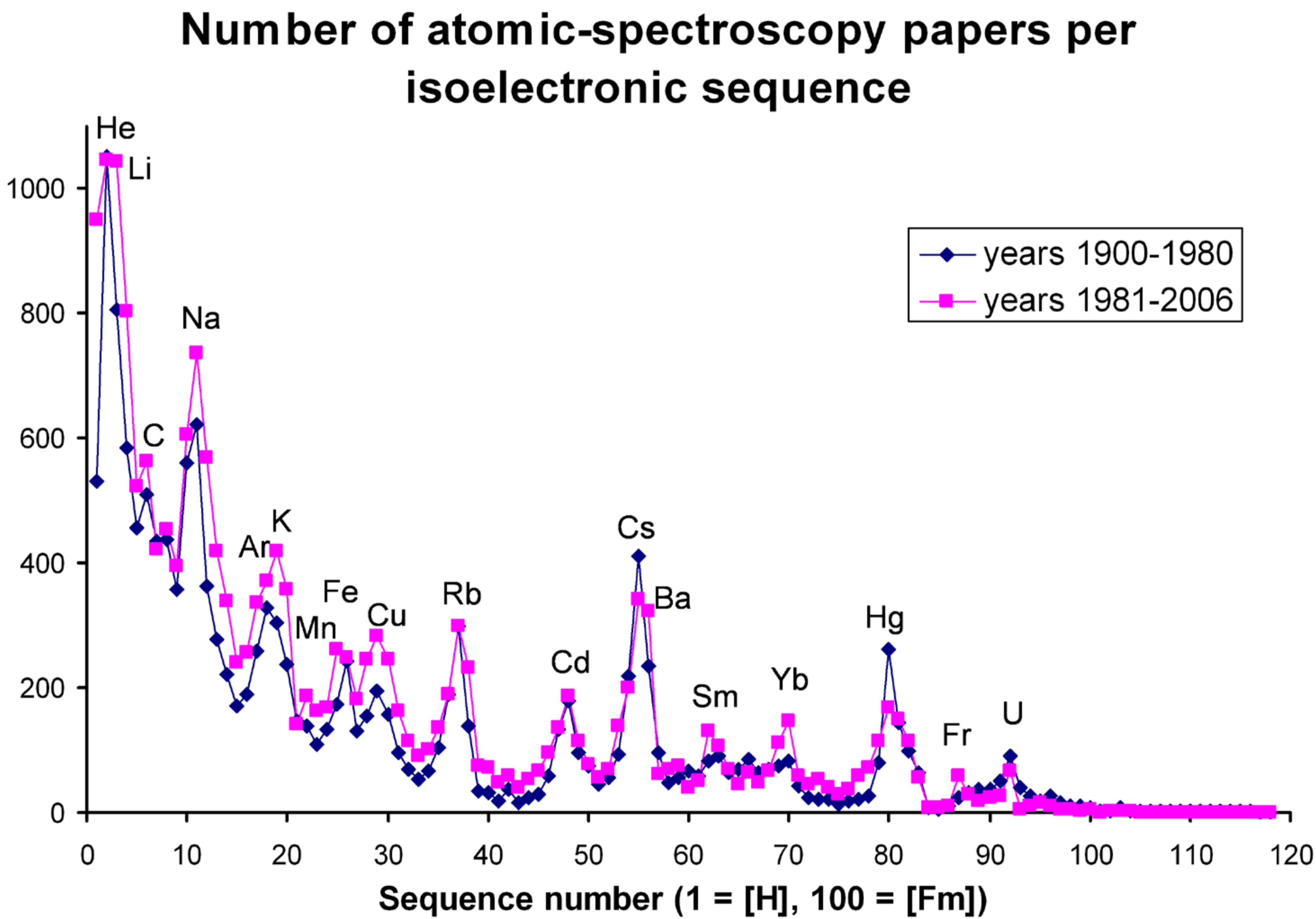
Click to open the journal's online archive

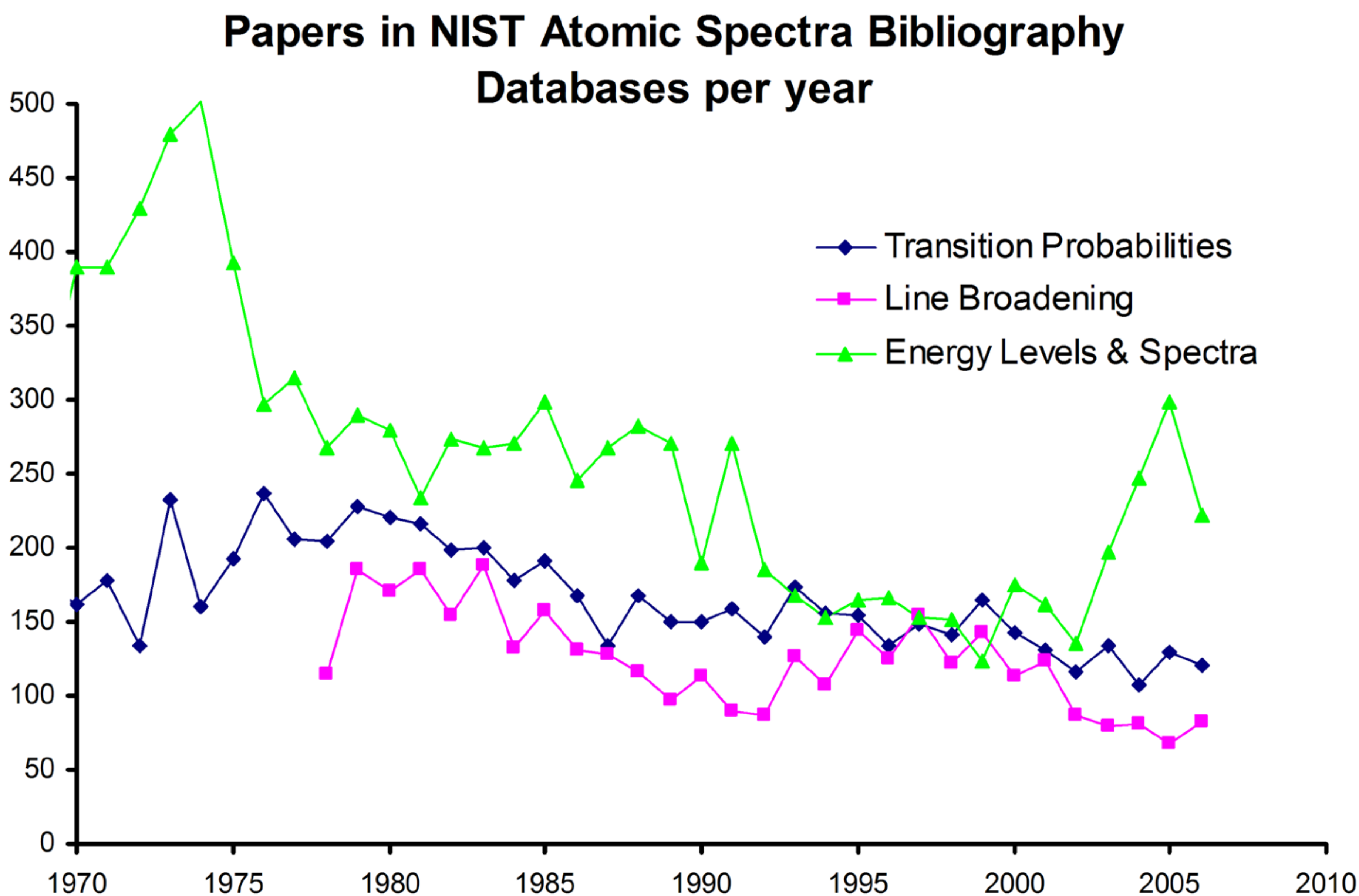
Mg II h and k lines Stark parameters,
S. Bukvić, A. Srećković, and S. Djeniže,
New Astron. **9**, 629-633 (2004)

Electron-impact broadening of Mg II spectral lines for astrophysical and laboratory plasma research,
M. S. Dimitrijević and S. Sahal-Bréchot,
Phys. Scr. **58**, 61 (1998)

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,
Publ. Astron. Obs. Belgrade, No. 53, 143 (1996)


Number of atomic-spectroscopy papers per element
1400
1200
1000
800
600
400
200
0
0
10
20
30
40
50
60
70
80
90
100
110
120
Z
years 1900-1980
years 1981-2006
He
Ne
Ar
Ca
Fe
Kr
Mo
Cd
Xe
Ba
Nd
Eu
Yb
W
Hg
Pb
Th
U


Number of atomic-spectroscopy papers per isoelectronic sequence
He
Li
Na
C
Ar
K
Mn
Fe
Cu
Rb
Cd
Cs
Ba
Sm
Yb
Hg
Fr
U
years 1900-1980
years 1981-2006
0
200
400
600
800
1000
0
10
20
30
40
50
60
70
80
90
100
110
120
Sequence number (1 = [H], 100 = [Fm])



Papers in NIST Atomic Spectra Bibliography Databases per year
500
450
400
350
300
250
200
150
100
50
0
1970
1975
1980
1985
1990
1995
2000
2005
2010
Transition Probabilities
Line Broadening
Energy Levels & Spectra

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

NIST Atomic Spectra Database Lines Data

Example of how to reference these results:
Ralchenko, Yu., Jou, F.-C., Kelleher, D.E., Kramida, A.E., Musgrove, A., Reader, J., Wiese, W.L., and Olsen, K. (2007). *NIST Atomic Spectra Database* (version 3.1.3), [Online]. Available: http://physics.nist.gov/asd3 [2007, September 12]. National Institute of Standards and Technology, Gaithersburg, MD.

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

Primary data source: **T. Shirai, J. Reader, A. E. Kramida, and J. Sugar, J. Phys. Chem. Ref. Data 36(2), 509 (2007)**

Observed Wavelength Vac (Å)	Ritz Wavelength Vac (Å)	Rel. Int. (?)	A_{ki} (s^{-1})	Acc.	E_i (cm^{-1})		E_k (cm^{-1})	Configurations	Terms	J_i - J_k	g_i - g_k
571.3	571*	2a			0	-	175 010	$3d^{10}4s^24p$ - $3d^9(^2D)4s^24p^2(^1S)$	$^2P°$ - ^2D	1/2 - 3/2	2 - 4
574.2	574*	0a			826.190	-	175 010	$3d^{10}4s^24p$ - $3d^9(^2D)4s^24p^2(^1S)$	$^2P°$ - ^2D	3/2 - 3/2	4 - 4
584.9	585*	3a			826.190	-	171 790	$3d^{10}4s^24p$ - $3d^9(^2D)4s^24p^2(^1S)$	$^2P°$ - ^2D	3/2 - 5/2	4 - 6
601.3	602*	7a			0	-	166 050	$3d^{10}4s^24p$ - $3d^9(^2D)4s^24p^2(^1D)$	$^2P°$ - ^2D	1/2 - 3/2	2 - 4
606.1	605*	14a			826.190	-	166 050	$3d^{10}4s^24p$ - $3d^9(^2D)4s^24p^2(^1D)$	$^2P°$ - ^2D	3/2 - 3/2	4 - 4
609.8	610*	15a			0	-	163 930	$3d^{10}4s^24p$ - $3d^9(^2D)4s^24p^2(^1D)$	$^2P°$ - ^2P	1/2 - 1/2	2 - 2
613.3	613*	13a			826.190	-	163 930	$3d^{10}4s^24p$ - $3d^9(^2D)4s^24p^2(^1D)$	$^2P°$ - ^2P	3/2 - 1/2	4 - 2
616.1	616*	7a			826.190	-	163 140	$3d^{10}4s^24p$ - $3d^9(^2D)4s^24p^2(^1D)$	$^2P°$ - ^2D	3/2 - 5/2	4 - 6

Electron-Impact Cross Sections for Ionization and Excitation

Y.-K. Kim,[1] K.K. Irikura,[2] M.E. Rudd,[3] M.A. Ali,[4] and P.M. Stone[1]
J. Chang,[5] J.S. Coursey,[5] R.A. Dragoset,[5] A.R. Kishore,[5] K.J. Olsen,[5] A.M. Sansonetti,[5] G.G. Wiersma,[5] D.S. Zucker,[5] and M.A. Zucker,[5]

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 H_2. 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)

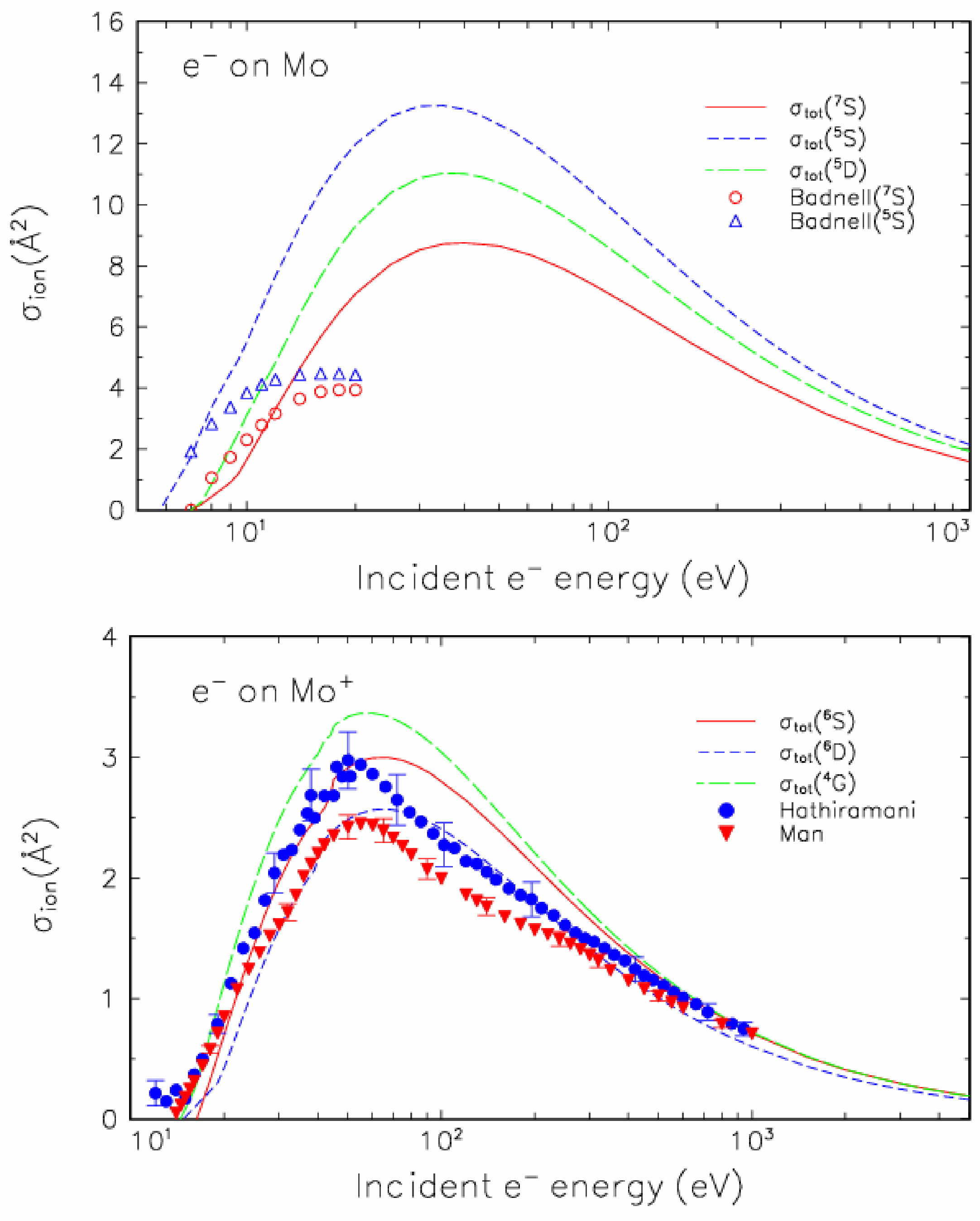
M. A. Ali, K. K. Irikura, Y.-K. Kim, P. M. Stone

Already in the database:

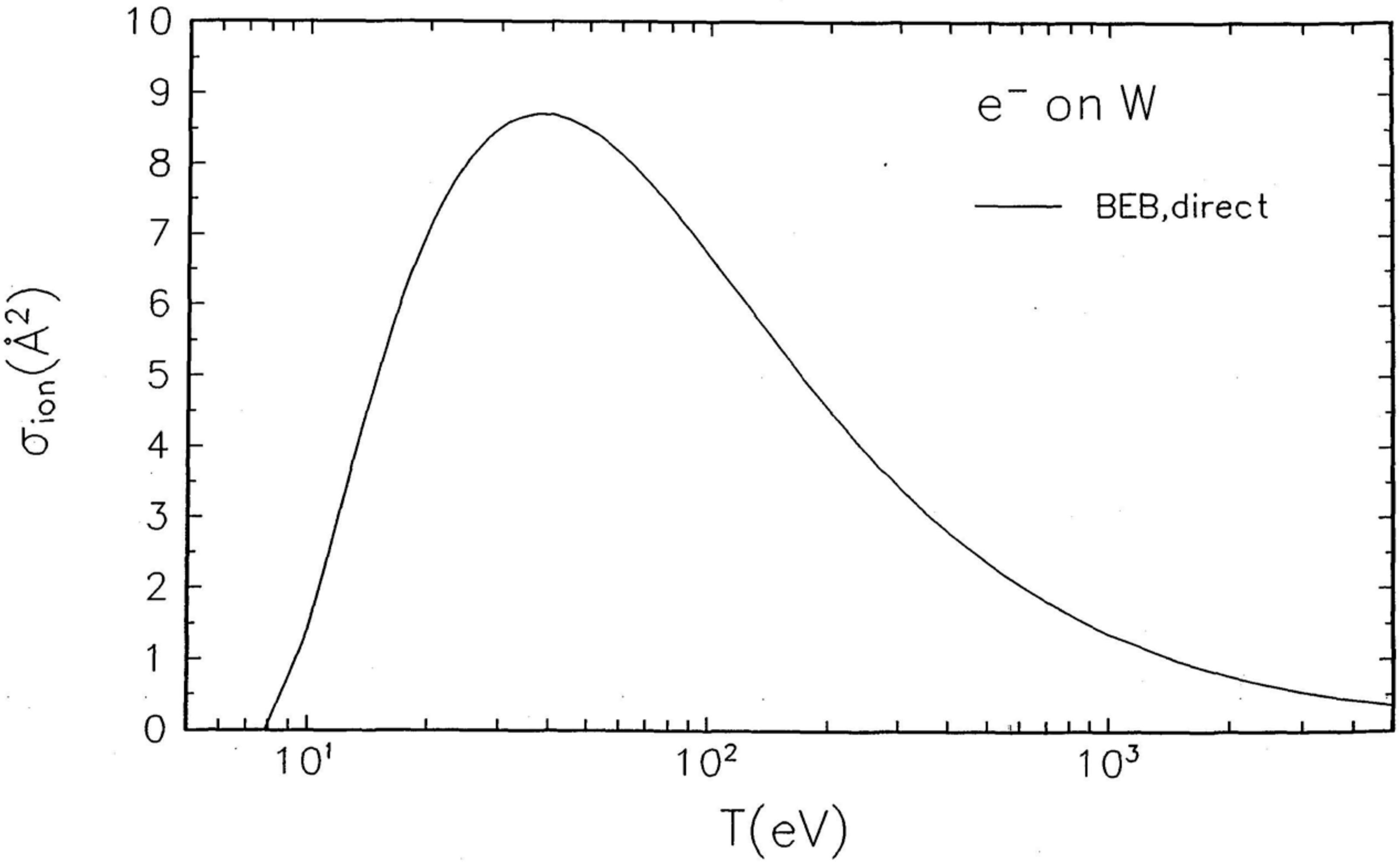
1. Total ionization cross sections of neutral atoms and molecules, singly charged molecular ions (about 100)
2. Differential ionization cross sections of H, He, H_2
3. Excitation cross sections of light atoms

New results to be added by summer, 2007:

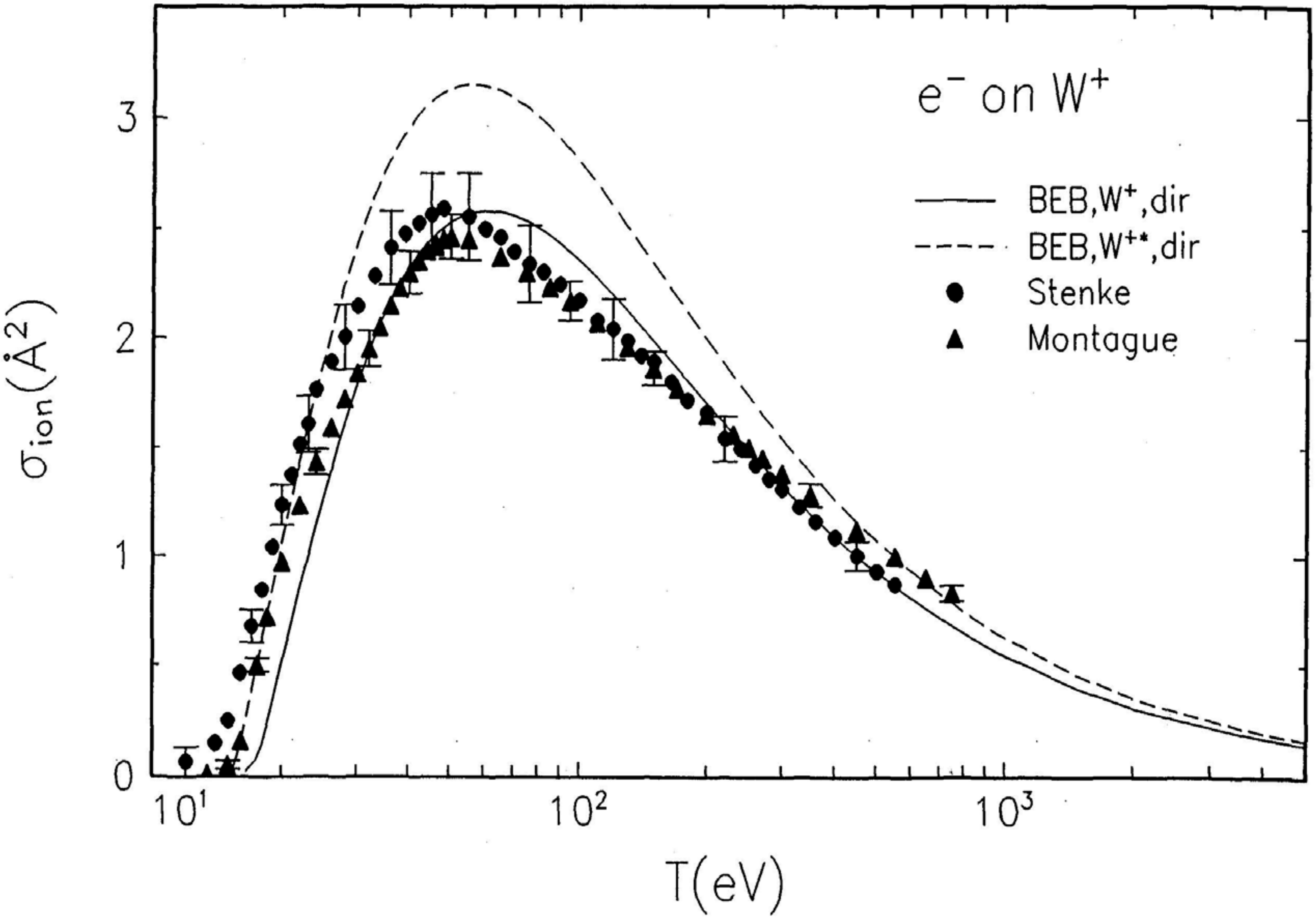
4. Total ionization cross sections (direct + excitation-autoionization) of Mo, Mo^+, W, W^+ (joint work with KAERI, see graphs)—BEB model plus BE/E scaling of Born cross sections [Mo/Mo^+ in Kwon, Rhee & Kim, Int. J. Mass Spectrometry, **245**, 26 (2005)]
5. Excitation cross sections of H_2 (see graphs)—BE scaling of Born cross sections
6. Ionization cross sections of Si, Ge, Sn, Pb, Cl, Br, I, Cl_2, Br_2, I_2



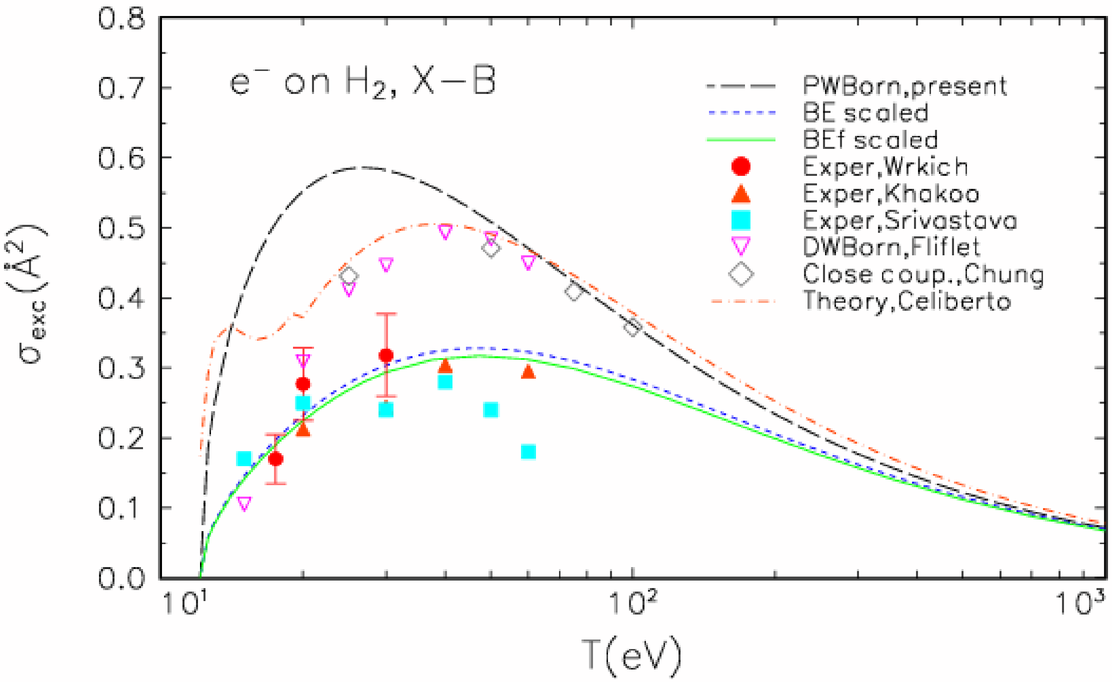
e⁻ on Mo
$\sigma_{tot}(^7S)$
$\sigma_{tot}(^5S)$
$\sigma_{tot}(^5D)$
Badnell(^{7}S)
Badnell(^{5}S)
$\sigma_{ion}(\text{Å}^2)$
Incident e⁻ energy (eV)
e⁻ on Mo⁺
$\sigma_{tot}(^6S)$
$\sigma_{tot}(^6D)$
$\sigma_{tot}(^4G)$
Hathiramani
Man
$\sigma_{ion}(\text{Å}^2)$
Incident e⁻ energy (eV)



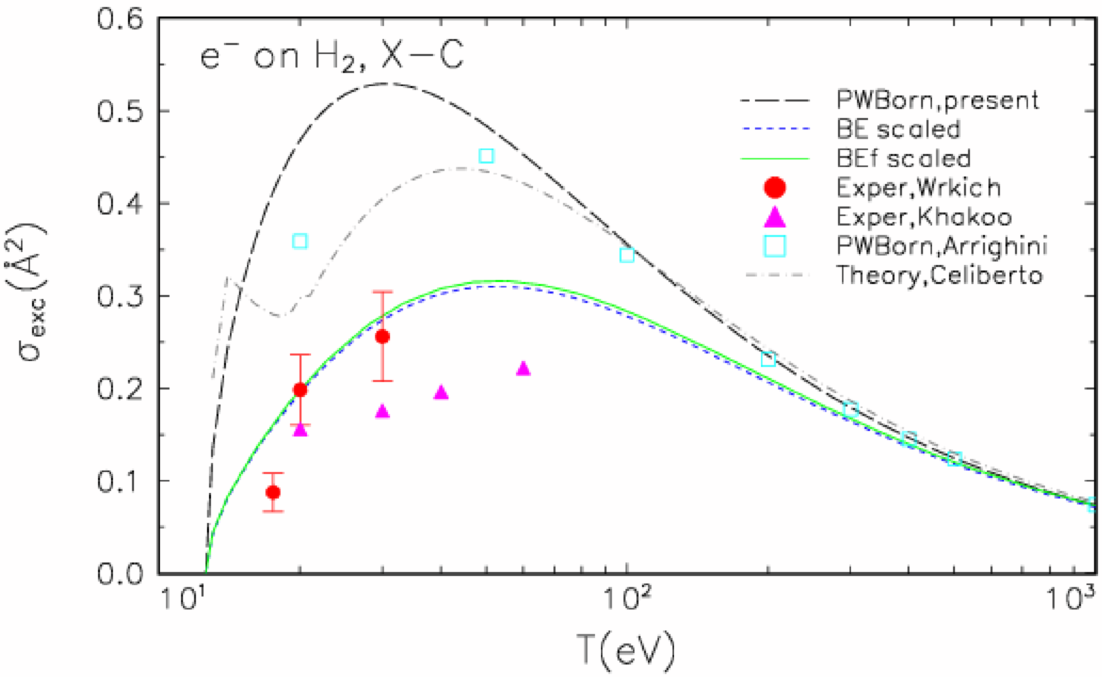
e⁻ on W
BEB,direct
σ_ion(Å²)
T(eV)
0
1
2
3
4
5
6
7
8
9
10
10¹
10²
10³



e⁻ on W⁺
BEB,W⁺,dir
BEB,W⁺*,dir
Stenke
Montague
σ_ion(Å²)
T(eV)
0
1
2
3
10¹
10²
10³



e^- on H_2, X−B
PWBorn,present
BE scaled
BEf scaled
Exper,Wrkich
Exper,Khakoo
Exper,Srivastava
DWBorn,Fliflet
Close coup.,Chung
Theory,Celiberto
$\sigma_{exc}(Å^2)$
T(eV)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
10^1
10^2
10^3



e^- on H_2, X−C
PWBorn,present
BE scaled
BEf scaled
Exper,Wrkich
Exper,Khakoo
PWBorn,Arrighini
Theory,Celiberto
$\sigma_{exc}(Å^2)$
T(eV)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
10^1
10^2
10^3