Atomic Databases and Online Computational Tools at NIST

Yuri Ralchenko
National Institute of Standards and Technology
Gaithersburg, USA

Keldysh IAM, May 24 2011

Supported in part by the Office of Fusion Energy Sciences,
U.S. Department of Energy

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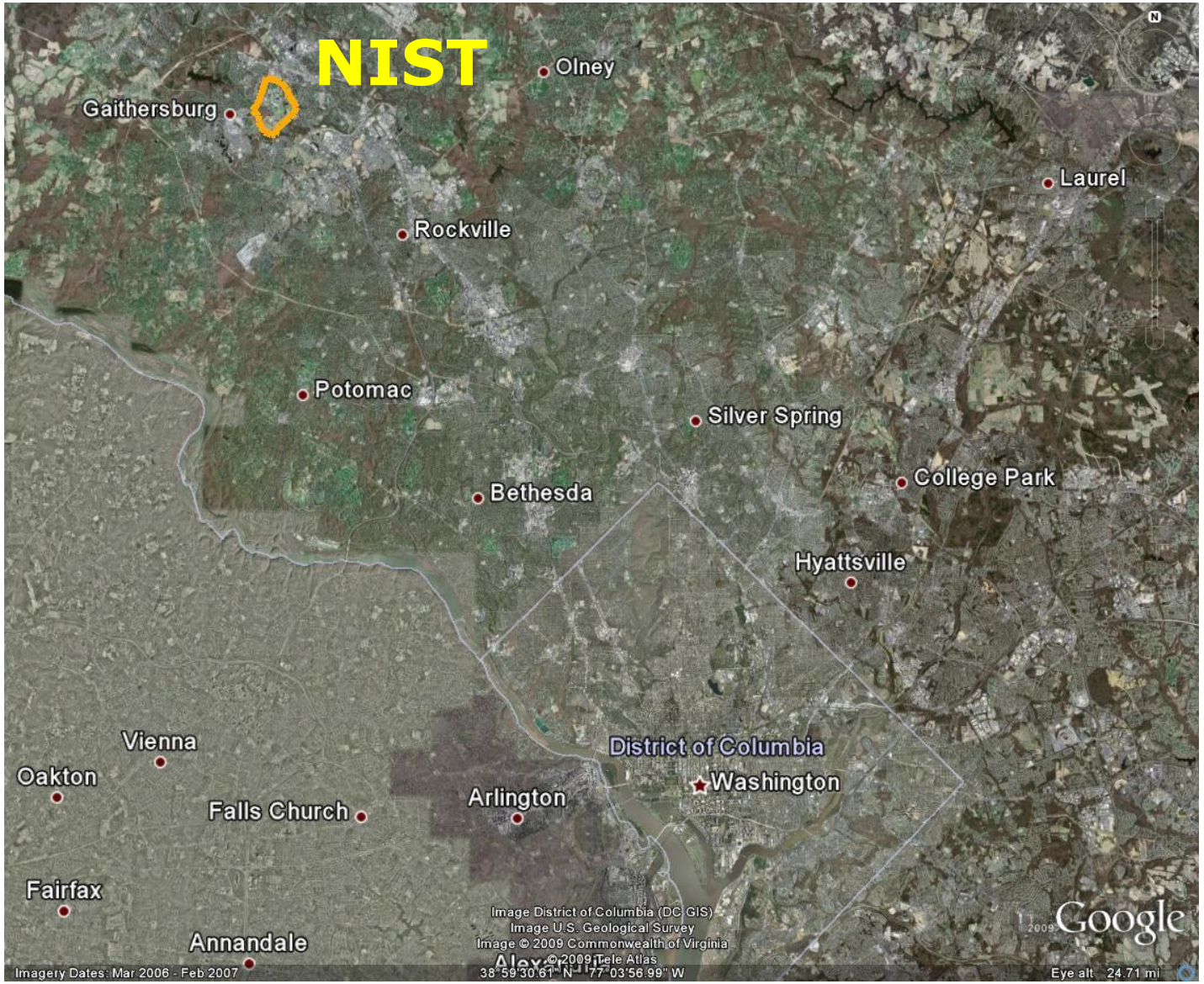
Collaborators

- A. Kramida
- J. Reader

- K. Olsen
- R. Dragoset

- Data Compilers
  - J. Sansonetti
  - E. Saloman
  - L. Podobedova
  - D. Kelleher
  - W. Wiese
  - J. Fuhr
  - A. Kramida
  - J. Reader



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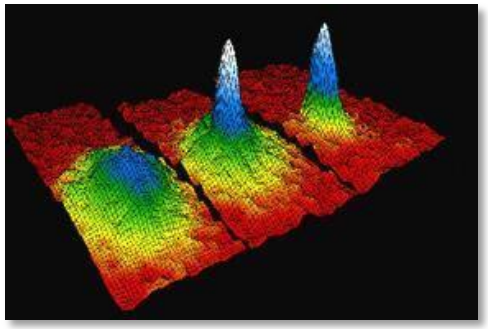

Est: 1901

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NIST Research Laboratories

- Material Measurement Laboratory
- Engineering Laboratory
- Information Technology Laboratory
- Center for Nanoscale Science and Technology
- Center for Neutron Research
- Physical Measurement Laboratory

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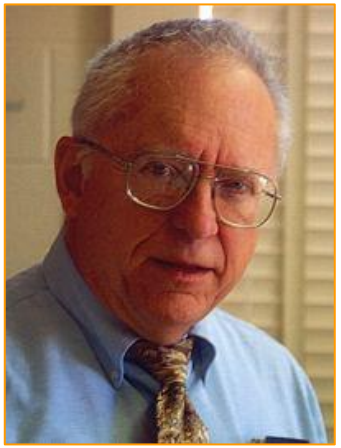
NIST Nobel Prize Winners (Physics)

W.D. Phillips
1997

Laser cooling

E. Cornell
2001

Bose-Einstein condensation



J.L. Hall
2005

Frequency combs

Physical Reference Data Program

NIST Time | NIST Home | About NIST | Contact Us
A-Z Site Index
Physical Measurement Laboratory
Search
About PML | Publications | Topic/Subject Areas | Products/Services | News/Multimedia | Programs/Projects | Facilities

NIST Home > PML > Physical Reference Data

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Physical Reference Data

Elemental Data Index

Provides access to the holdings of NIST Physical Measurement Laboratory online data organized by element.

Periodic Table: Atomic Properties of the Elements

Contains NIST critically-evaluated data on atomic properties of the elements.
Suitable for high-resolution color printing for desk or wall-chart display.

Physical Constants

Contains values of the fundamental physical constants and a related bibliographic database.

Atomic Spectroscopy Data

Contains databases for energy levels, wave
probabilities for atoms and ions and related

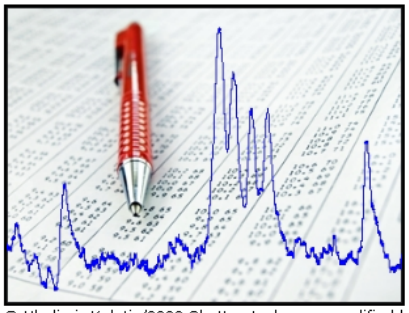
- Atomic Spectra Database
- Handbook of Basic Atomic Spectroscopic Data
- Energy Levels of Hydrogen and Deuterium
- Ground Levels and Ionization Energies
- Spectral Data for the Chandra X-ray Observatory
- NLTE Databases and Codes
- Ultraviolet Spectrum of Platinum Lamp
- Spectrum of Th-Ar Hollow Cathode Lamps
- X-ray Transition Energies
- Bibliographic Databases on Atomic Spectroscopy

Molecular Spectroscopic Dat

Includes databases containing spectroscopi
hydrocarbons, and interstellar molecules. In
publications containing equations and the u
spectroscopy.

Atomic and Molecular Data

Contains databases on electron-impact cross sections (of atoms & molecules) and potential energy surfaces of group II dimers.



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The use of International Units and the expression of uncertainty in measurement is critical to all data activities. For information on these topics, see guidelines for evaluating and expressing measurement uncertainty, and information on the International System of Units

data and databases are being
or this Web site.

ne 1994

nformation:
200 Telephone
038 Facsimile

100 Bureau Drive, M/S 8400
Gaithersburg, MD 20899-8400

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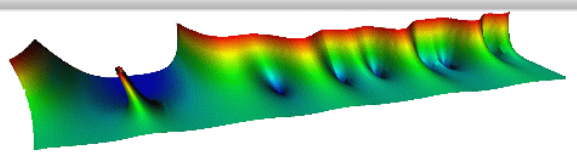

NIST Digital Library of Mathematical Functions

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*

http://dlmf.nist.gov

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Atomic Spectra Database v.4.1.0

Version History & Citation Information | Disclaimer
Help for Users with Text Browsers

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NIST Atomic Spectra Database

Version 4

Welcome to the NIST Atomic Spectra Database, NIST Standard Reference Database #78. The spectroscopic data may be selected and displayed according to wavelengths or energy levels by choosing one of the following options:

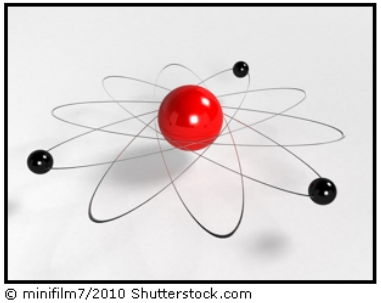
Lines — Spectral lines and associated energy levels displayed in wavelength order with all selected spectra intermixed or in multiplet order. Transition probabilities for the lines are also displayed where available.

Levels — Energy levels of a particular atom or ion displayed in order of energy above the ground state.

Additional information about the database may be obtained through the following links:

Introduction	Introduction to the Atomic Spectra Database.
List of Spectra	Overview of data contained in the database.
Ground States and Ionization Energies	Table of Ground States and Ionization Energies for Neutral Atoms.
Bibliography	Bibliography of data sources used for this database.
Help	On-line help in using the database.

This database provides access and search capability for NIST critically evaluated data on atomic energy levels, wavelengths, and transition probabilities that are reasonably up-to-date. The Atomic Energy Levels Data Center and Data Center on Atomic Transition Probabilities and Line Shapes have carried out these critical compilations. Both Data Centers are located in the Physical Measurement Laboratory at the National Institute of Standards and Technology (NIST).



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NIST ASD Team

Principal Developers (Currently Active):
Yu. Ralchenko,[1] A.E. Kramida,[1] and J. Reader[1]

Data Compilers (Currently Active):
Atomic Energy Levels and Wavelengths:
A.E. Kramida,[1] E.B. Saloman,[1] J.E. Sansonetti,[1] and J.J. Curry[1]

Atomic Transition Probabilities:
D.E. Kelleher,[1] A.E. Kramida,[1] J.R. Fuhr,[1] L. Podobedova,[1] and W.L. Wiese[1]

Database Developers (Currently Active):
Database Management:
Yu. Ralchenko,[1] A.E. Kramida,[1] and K. Olsen[2]

World Wide Web Interface:
Yu. Ralchenko[1]

Past Contributors:
G.R. Dalton,[3] R. Dragoset,[2] F.-C. Jou,[1] W.C. Martin,[1] P.J. Mohr,[1] A. Musgrove,[1] C.J. Sansonetti,[1] and G. Wiersma[2]

[1]Atomic Physics Division

MySQL
Perl
Java

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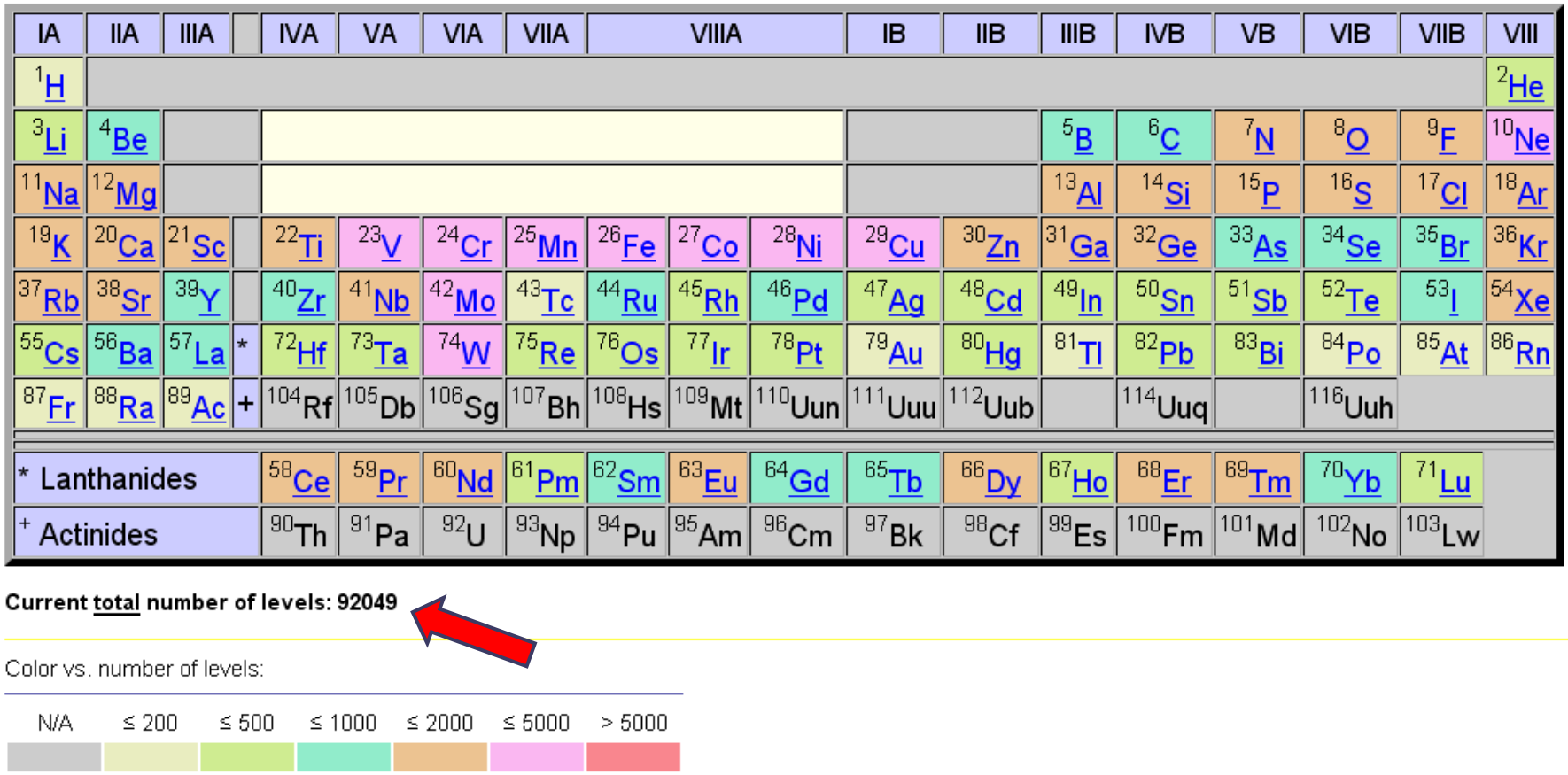
NIST Atomic Spectra Database - Levels Holdings



Current total number of levels: 92049

Color vs. number of levels:

N/A	≤ 200	≤ 500	≤ 1000	≤ 2000	≤ 5000	> 5000

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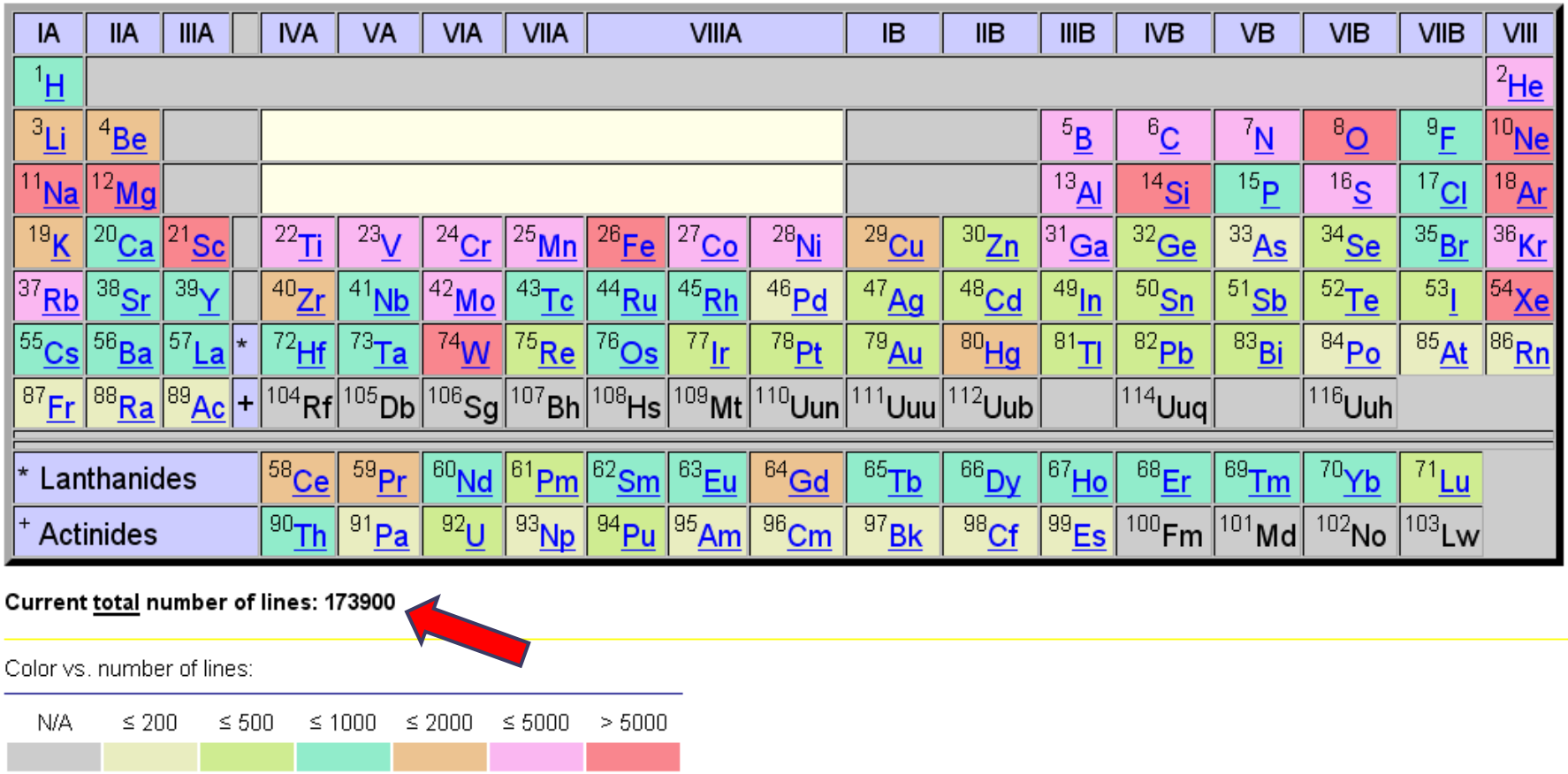
NIST Atomic Spectra Database - Lines Holdings



Current total number of lines: 173900

Color vs. number of lines:

N/A	≤ 200	≤ 500	≤ 1000	≤ 2000	≤ 5000	> 5000

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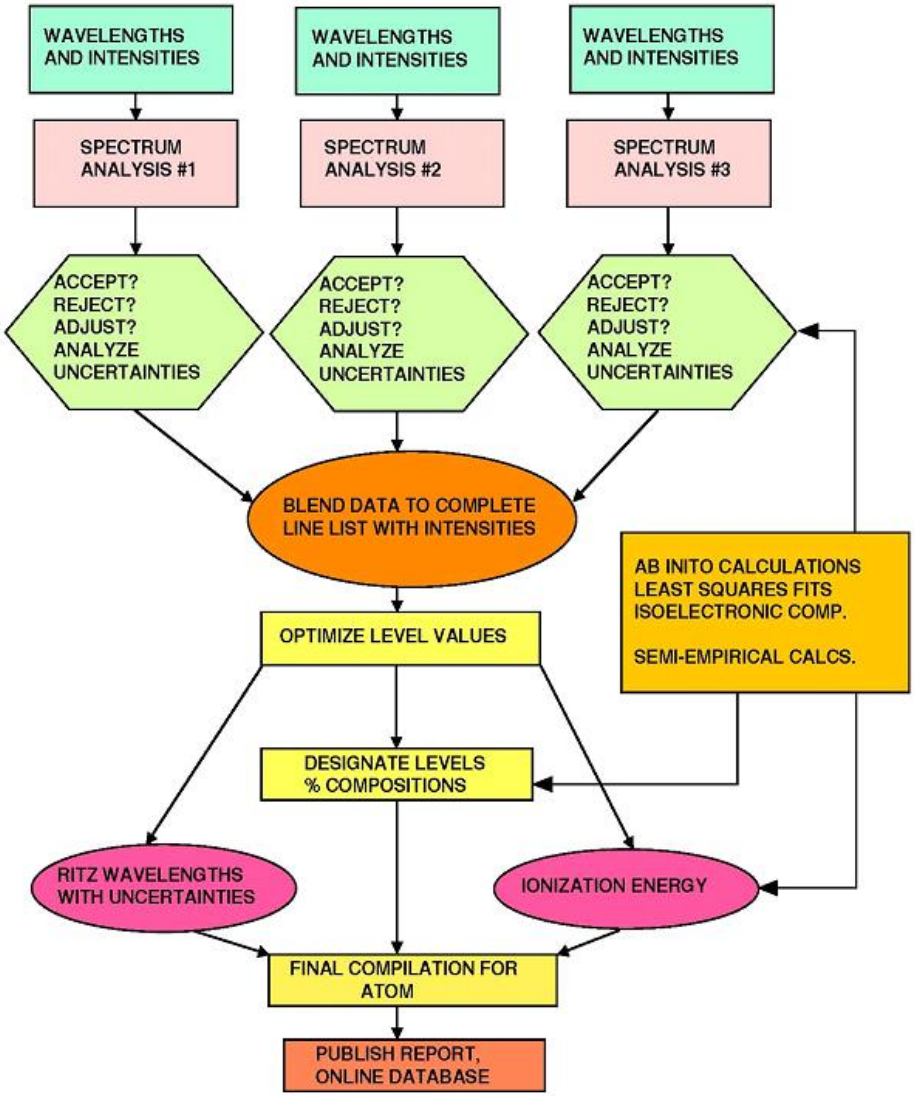
Compilation scheme



- Energy levels added for **Ac III, Ag III, At I, Bi III-VI, Cd I-IV, Cs I-II, Hf I-II, I I-VIII, I XII-XIII, In I-V, Ir I-II, Nb I-VII, Nb XV, Os I-II, Pb I-II, Pd I-III, Po I, Pt I-II, Ra I-II, Re I-II, Rh I-III, Rn I-II, Ru I-III, Sb I-VI, Sn I-VI, Sr I-V, Sr XI-XII, Ta I-II, Tc I-II, Te I-VII, Tl I-II, Y I-V, Y XII-XIII, Zr I-II, Zr V-VI, Zr XIV.**
- Energy levels updated for **^{198}Hg I, Ac I, Ag II, Ar II-III, Ar VII-XVII, Au I, Mo VI, W XIV, W XXIX, W XLI-LXXII.**
- Spectral lines added for **Ar XII, Ar XV-XVIII, W LII, W LIV, W LVI-LXXII**
- Spectral lines updated for **^{198}Hg I, Ar II-XI, Ar XIII-XIV, Mo VI, Sr I, W XIV, W XXIX, W XLIII-LI, W LV-LXIII, W LXV**.

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NIST Atomic Spectra Database Levels Form

Best viewed with the latest versions of Web browsers and JavaScript enabled

This form provides access to NIST critically evaluated data on atomic energy levels.

Spectrum: W I **e.g.,** Fe I

Default Values | Retrieve Data

Level Units: cm-1
Format output: HTML (formatted)
Display output: in its entirety
Page size: 15
Term ordered ◉ term energy ☐
Energy ordered ○
Level information: ☑ Principal configuration ☑ Principal term ☑ Level ☑ J ☑ Lande-g ☑ Leading percentages
Bibliographic references: ☑
Level splitting: ☐
Partition function for T_e (eV):

Update Criteria **Optional Search Criteria** for **W I**
(total **509** levels, highest energy = **63 532.78** cm^{-1})

Upper bound of energy: cm^{-1}
Parity: both
Configuration: All / 5d4.6s2 / 5d5.(6S).6s / 5d5.(4G).6s — or configuration's first symbols: — or configuration's last symbols:
Term: All / 5D / 7S / 3P2 — or term's first symbols: — or term's last symbols:
J-value: e.g., 3/2 or 2

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ASD | Data: Lines Levels | Information: List of Spectra, Ground States & Ionization Energies, Bibliography, Help

NIST Atomic Spectra Database Lines Form

Best viewed with the latest versions of Web browsers and JavaScript enabled

Spectrum [ ] e.g., Fe I or Na, Mg , Al or mg i-iii

Lower Wavelength: [ ] or Upper Wavenumber (in cm^{-1}) [ ]

Upper Wavelength: [ ] or Lower Wavenumber (in cm^{-1}) [ ]

Units: Å

Reset input | Retrieve Data

Dynamic Plots

Line Identification Plot: ○

Saha-LTE Spectrum: ○

Doppler Broadening Parameters

Electron Temperature T_e(eV): [ ]

Electron Density N_e(cm^{-3}): [ ]

Number of points: [ ] (≤ 20000)

Ion Temperature T_i(eV): [ ] (if $T_i \neq T_e$)

Grotrian Diagram

Java subwindow size:
○ 640 x 640 ○ 800 x 640 ◉ 1024 x 768 ○ 1280 x 1024

☐ Group by configurations | [ ] Term multiplicity

☐ Show only radiatively linked levels

Make Grotrian Diagram (requires Java2)

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Output Options

Format output: HTML (formatted)

No JavaScript ☐

Energy Level Units: cm-1

Display output: in its entirety

Page size: 15

Output ordering: ◉ Wavelength ○ Multiplet

Optional Search Criteria

Maximum lower level energy: (e.g., 100000)

Maximum upper level energy: (e.g., 400000)

Transition strength bounds will apply to: Aki

Minimum transition strength: (e.g., 1.2e+05)

Maximum transition strength: (e.g., 2.5e+12)

Accuracy minimum: (e.g., C+)

Relative intensity minimum: (e.g., 1.2e-03)

Additional Criteria

Lines: ◉ All ○ Only with transition probabilities ○ Only with energy level classifications ○ Only with observed wavelengths

Bibliographic Information: ☑ TP references, Line references

Wavelength Data: ☑ Observed ☑ Ritz ☐ Observed - Ritz (difference) ☐ Wavenumber (in cm^{-1})

Wavelengths in: ○ Vacuum (< 2,000 Å) Air (2,000 - 10,000 Å) Wavenumber (> 10,000 Å) ○ Vacuum (< 10,000 Å) Wavenumber (> 10,000 Å) ◉ Vacuum (< 2,000 Å) Air (2,000 - 20,000 Å) Vacuum (> 20,000 Å) ○ Vacuum (all wavelengths) ○ Air (all wavelengths) ○ Wavenumber (all wavelengths)

Transition strength: ◉ A_{ki} ○ g_kA_{ki} ☐ in units of 10^8 s^{-1}

☐ f_{ik} ☐ S_{ik} ☐ log(gf)

☑ Relative Intensity

Transition Type: ☑ Allowed (E1) ☑ Forbidden (M1,E2,...)

Level information: ☑ Configurations ☑ Terms ☑ Energies ☑ J ☑ g

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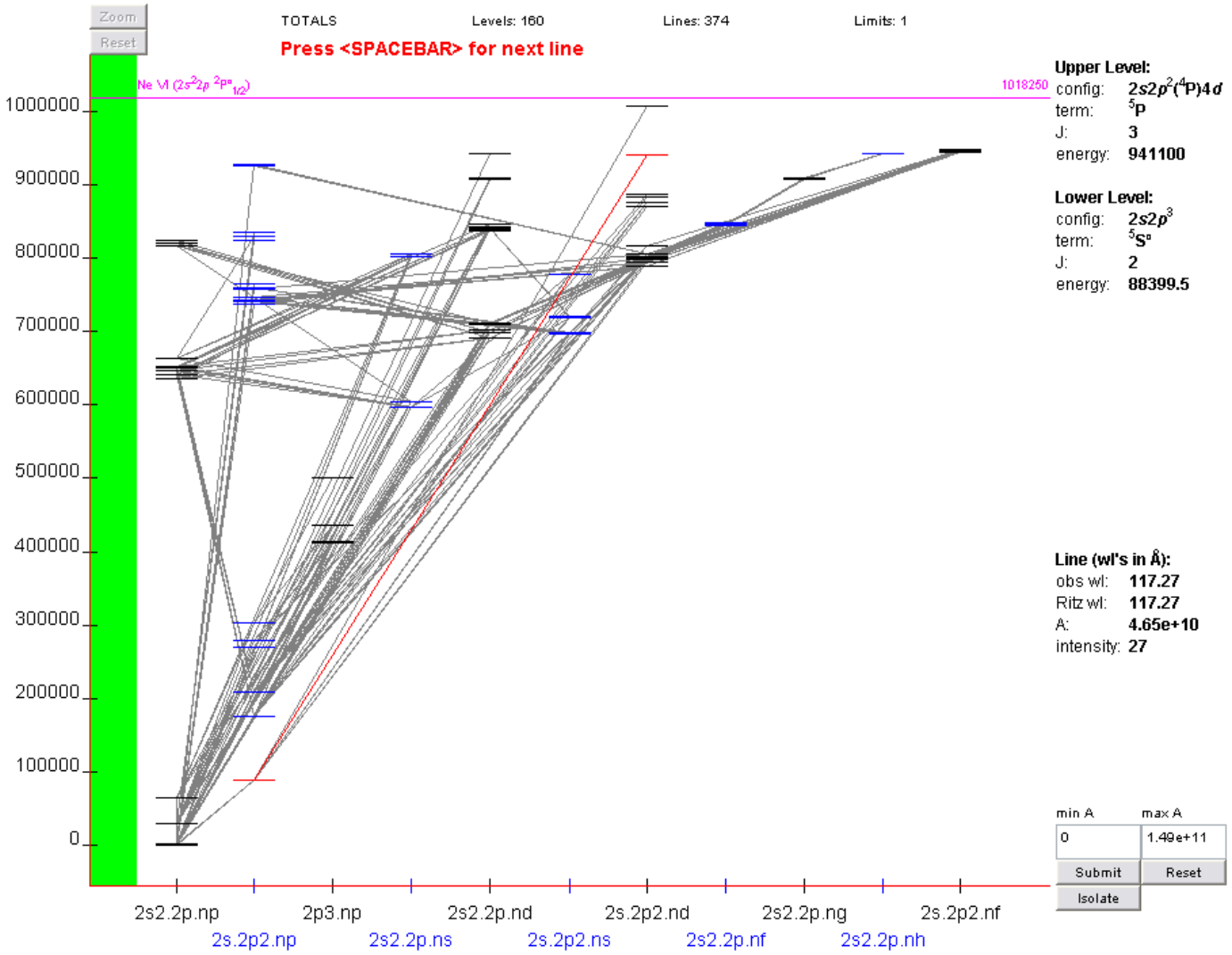
Dynamic Grotrian Diagrams



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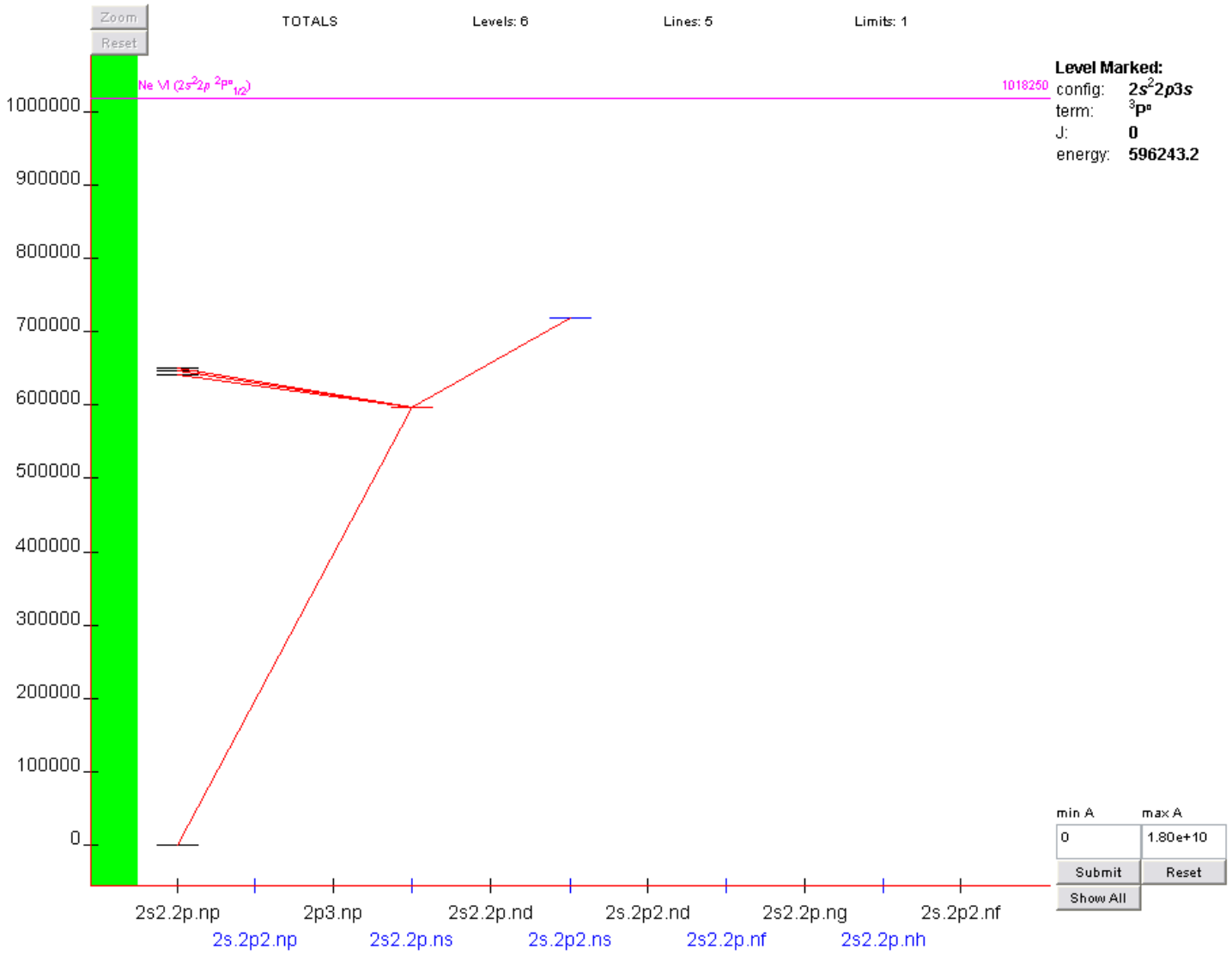

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ASD DATA — LINES LEVELS — INFORMATION — LIST OF SPECTRA GROUND STATES & IONIZATION ENERGIES BIBLIOGRAPHY HELP

NIST Atomic Spectra Database Lines Data

Fe X-XV: 117 Lines of Data Found

Wavelength range: 300 - 500 Å
Wavelength in: vacuum below 2000 Å, air between 2000 and 20000 Å, vacuum above 20000 Å
Highest relative intensity: 440

Query NIST Bibliographic Databases for **Fe X-XV** (new window)

Fe X-XV Energy Levels
Fe X-XV Line Wavelengths and Classification
Fe X-XV Transition Probabilities

Transition Probabilities Reference for Fe XV - Mozilla Firefox

File Edit View History Bookmarks Tools Help

http://physics.nist.gov/cgi-bin/ASBib1/get_ASBib_ref.cgi?db=tp&db_id=3154&comment_code=&element=Fe&sp

NIST Transition Probabilities Bibliographic Reference # 3154

Extra data for NIST internal use: Abstract PDF

Excitation energies and line strengths in the Mg isoelectronic sequence,
K.-T. Cheng and W. R. Johnson,
Phys. Rev. A **16**, 263 (1977)
DOI:10.1103/PhysRevA.16.263

Get all bibliography on Fe XV transition probabilities (new window)

Ion	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	Type	TP Ref.	Line Ref.
Fe XIV		301.286		4.1e+08	E	475 202	-	807 113	$3s^23d$ - $3s3p(^3P°)3d$	^2D - $^2P°$	$^5/_2$ - $^3/_2$	6 - 4		T7228	L11926
Fe XV	302.334	302.33+	140	6.9e+09	C	233 842	-	564 602	$3s3p$ - $3p^2$	$^3P°$ - ^3P	0 - 1	1 - 3		T3154	L11926
Fe XIII		303.355		1.2e+09	D	0	-	329 647	$3s^23p^2$ - $3s3p^3$	^3P - $^3P°$	0 - 1	1 - 3		T4830	
Fe XV		303.494		6.4e+00	C	351 911	-	681 416	$3s3p$ - $3s3d$	$^1P°$ - ^3D	1 - 3	3 - 7	M2	T4668	
Fe XIV	303.573	303.57+				703 393	-	1 032 802	$3s3p(^3P°)3d$ - $3p^2(^1D)3d$	$^4D°$ - ^2D	$^7/_2$ - $^5/_2$	8 - 6			L11926
Fe XV	304.894	304.9*	400	1.3e+10	D	253 820	-	581 803	$3s3p$ - $3p^2$	$^3P°$ - ^3P	2 - 2	5 - 5		T3154	L11926
Fe XV		304.998		3.0e+07	E	351 911	-	679 785	$3s3p$ - $3s3d$	$^1P°$ - ^3D	1 - 2	3 - 5		T4668	
Fe XV	305.15	305.15+	1			1 074 887	-	1 402 592	$3p3d$ - $3d^2$	$^1P°$ - ^1D	1 - 2	3 - 5			L11926
Fe XV		305.889		2.6e+07	E	351 911	-	678 772	$3s3p$ - $3s3d$	$^1P°$ - ^3D	1 - 1	3 - 3		T4668	
Fe XIV	307.403	307.37+				651 946	-	977 283	$3s3p(^3P°)3d$ - $3p^2(^3P)3d$	$^4F°$ - ^4F	$^7/_2$ - $^7/_2$	8 - 8			L11926
Fe XV	307.730	307.7*	220	4.91e+09	C	239 660	-	564 602	$3s3p$ - $3p^2$	$^3P°$ - ^3P	1 - 1	3 - 3		T3154	L11926
Fe XIV	307.73	307.73+				645 988	-	970 948	$3s3p(^3P°)3d$ - $3p^2(^3P)3d$	$^4F°$ - ^4F	$^5/_2$ - $^5/_2$	6 - 6			L11926

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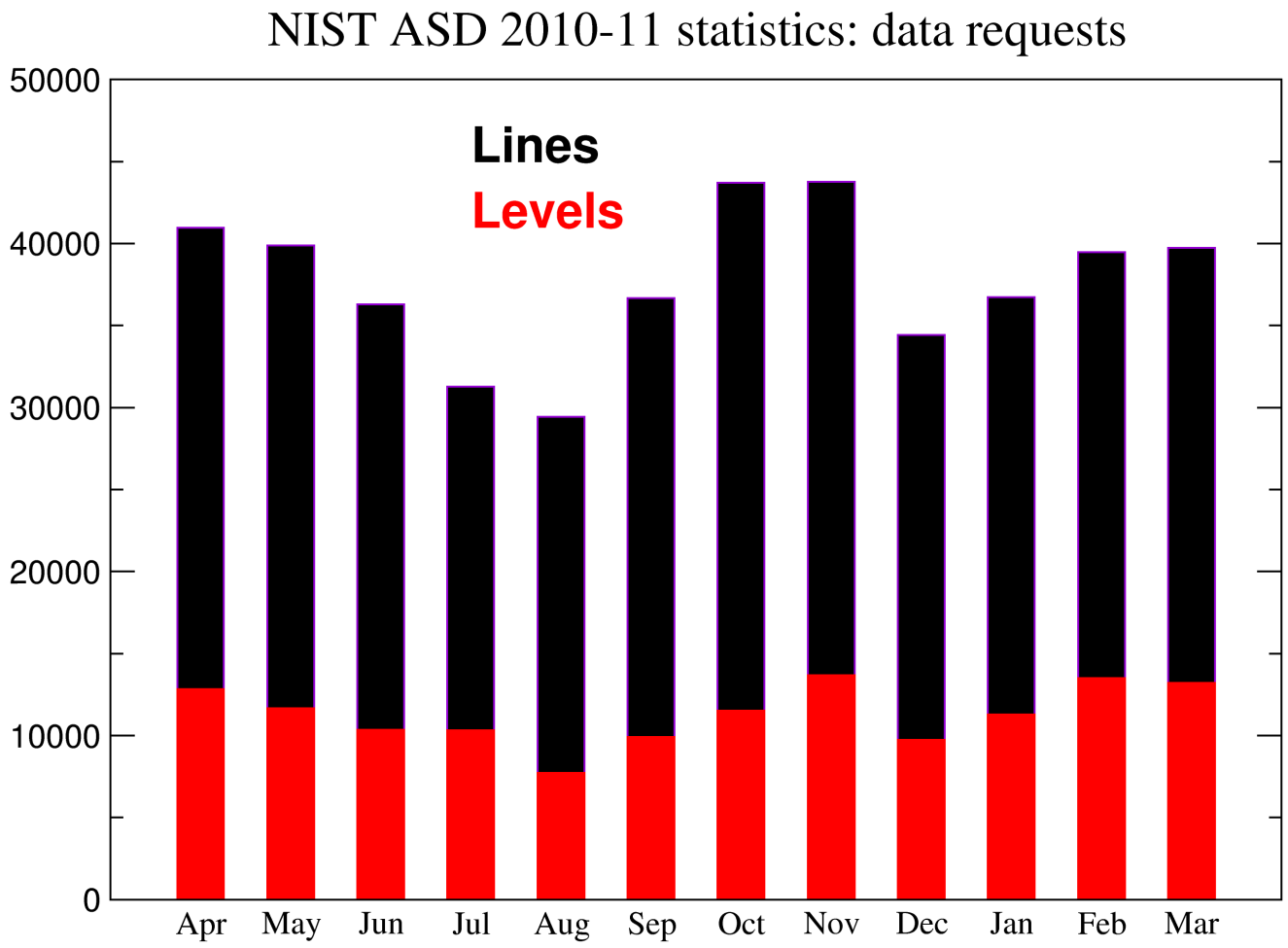
NIST ASD 2010-11 statistics: data requests
Lines
Levels
50000
40000
30000
20000
10000
0
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec
Jan
Feb
Mar

ome > PML > Physical Reference Data > Bibliographies on Atomic Spectroscopy

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NIST Atomic Spectra Bibliographic Databases

Welcome to the NIST Atomic Spectra Bibliographic Databases. References to publications may be selected and displayed after choosing one of the following three databases.

Atomic Transition Probability Bibliographic Database

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

Atomic Spectral Line Broadening Bibliographic Database

This interactive database contains references on atomic spectral line broadening (line shapes and shifts). Both theoretical and experimental papers are listed.

Atomic Energy Levels and Spectra Bibliographic Database

This interactive database contains references on atomic energy levels and wavelengths. Preference is given to experimental papers.

These databases provide access and search capability for NIST bibliography databases on atomic energy levels, wavelengths, transition probabilities, and line broadening and shapes. The Atomic Energy Levels Data Center and Data Center on Atomic Transition Probabilities and Line Shapes have implemented these databases, which are the main bibliography source for the NIST critical compilations. Both Data Centers are located in the Physical Measurement Laboratory at the National Institute of Standards and Technology (NIST).

These databases were funded [in part] by NIST's Standard Reference Data Program (SRDP) and by NIST's Systems Integration for Manufacturing Applications (SIMA) Program.

As of May 17, 2011:

8435, 1914-2011

6599, 1889-2011

16574, 1802-2011

Updated almost daily
Automated system of article collection

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ASD | Data: Lines Levels | Information: List of Spectra, Ground States & Ionization Energies, Bibliography, Help

NIST Atomic Spectra Database Lines Form

Best viewed with the latest versions of Web browsers and JavaScript enabled

Spectrum [ ] e.g., Fe I or Na, Mg , Al or mg i-iii

Lower Wavelength: [ ] or Upper Wavenumber (in cm^{-1}) [ ]

Upper Wavelength: [ ] or Lower Wavenumber (in cm^{-1}) [ ]

Units: Å

Reset input | Retrieve Data

Dynamic Plots

Line Identification Plot: ○

Saha-LTE Spectrum: ○

Doppler Broadening Parameters

Electron Temperature T_e(eV): [ ]

Electron Density N_e(cm^{-3}): [ ]

Number of points: [ ] (≤ 20000)

Ion Temperature T_i(eV): [ ] (if $T_i \neq T_e$)

Grotrian Diagram

Java subwindow size:
○ 640 x 640 ○ 800 x 640 ◉ 1024 x 768 ○ 1280 x 1024

☐ Group by configurations | [ ] Term multiplicity

☐ Show only radiatively linked levels

Make Grotrian Diagram (requires Java2)

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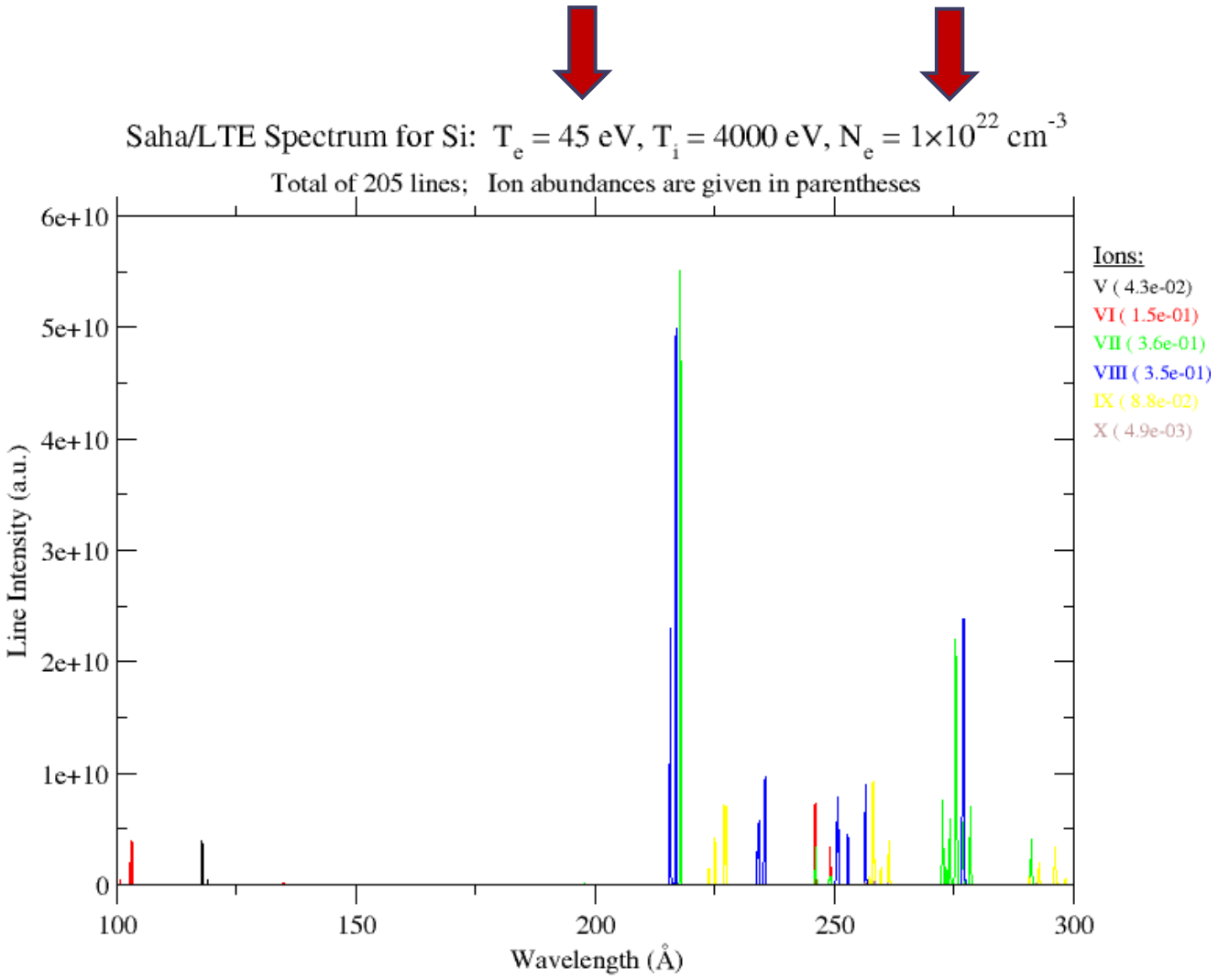
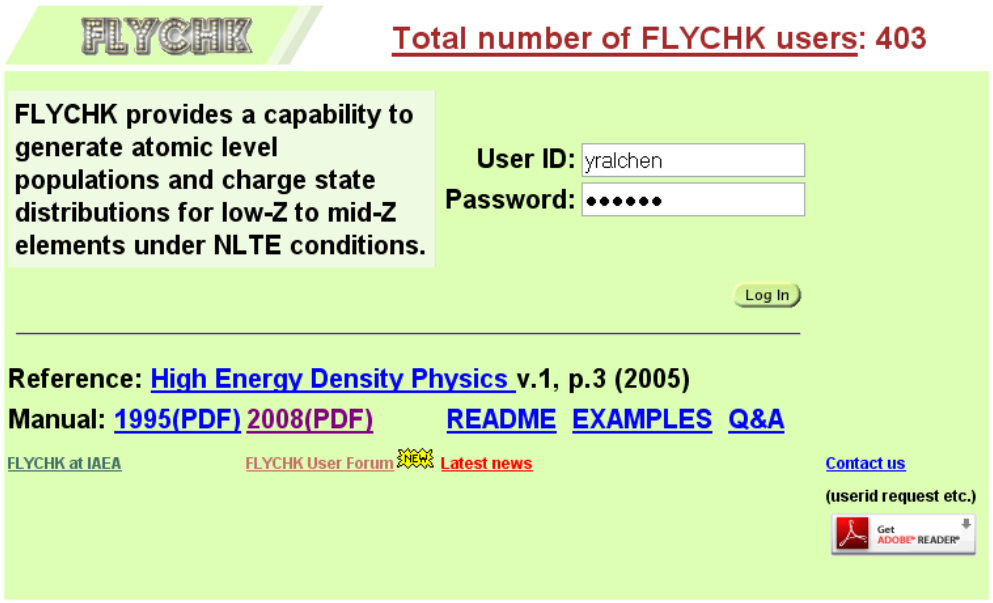
Saha/LTE Spectrum for Si V-X



NLTE Databases

- NLTE Code Comparison Workshops
  - Since 1996
  - NLTE-7: Vienna, Dec 2011
  - NLTE-3 and NLTE-4 results available
    - http://nlte.nist.gov/NLTE3, http://nlte.nist.gov/NLTE4
    - Ionization distributions, mean ion charge, radiative power losses, effective rated
    - Elements: C, Al, Ar, Sn, W, Au….

Collisional-Radiative Code FLYCHK



http://nlte.nist.gov/FLY

>>>> The latest version of Firefox (Windows) seems to confict with Java codes which may affect plotting in FLYCHK. The Linux version as well as Internet Explorer were found to work well (Apr 24, 2009).

>>>> As of March 2009, the FLYCHK code utilizes more accurate sets of auto-ionization rates, collisional excitation cross-sections and photoionization cross-sections for super-configuration levels, that is for ions with more than 3 electrons. Users may find a noticeable change in average charge states for M-shell or N-shell ions of high Z atoms. Though the new version has been thoroughly tested to our capacity, the authors would be greatly thankful for a feedback on any potential errors in the code.

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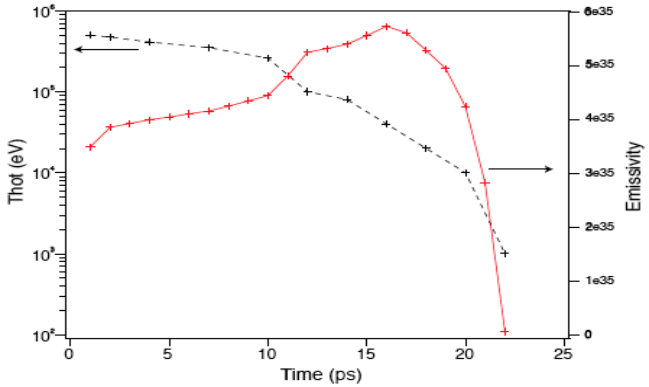
FLYCHK Model : *simple, but complete*

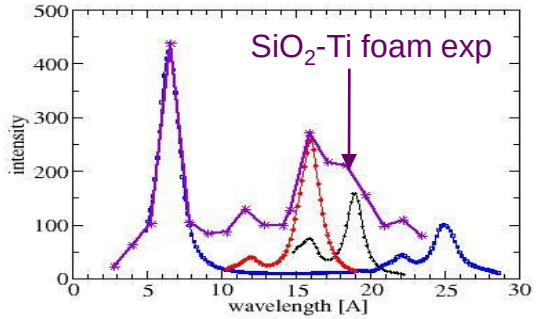
- Screened hydrogenic energy levels with relativistic corrections
- Relativistic Hartree-Slater oscillator strengths and photoionization cross-sections
- Fitted collisional cross-section to PWB approximation
- Semi-empirical cross-sections for collisional ionization
- Detailed counting of autoionization and electron capture processes
- Continuum lowering (Stewart-Pyatt)

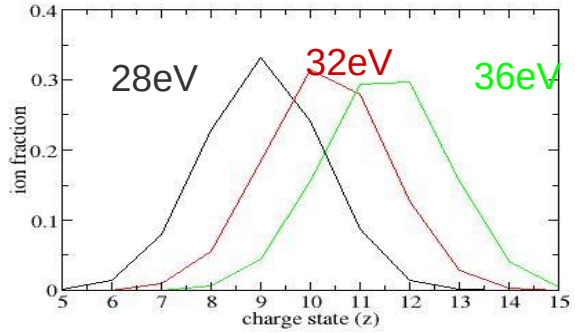
H.-K. Chung et al., HEDP **1**, 3 (2005)

Applications to Plasma Research

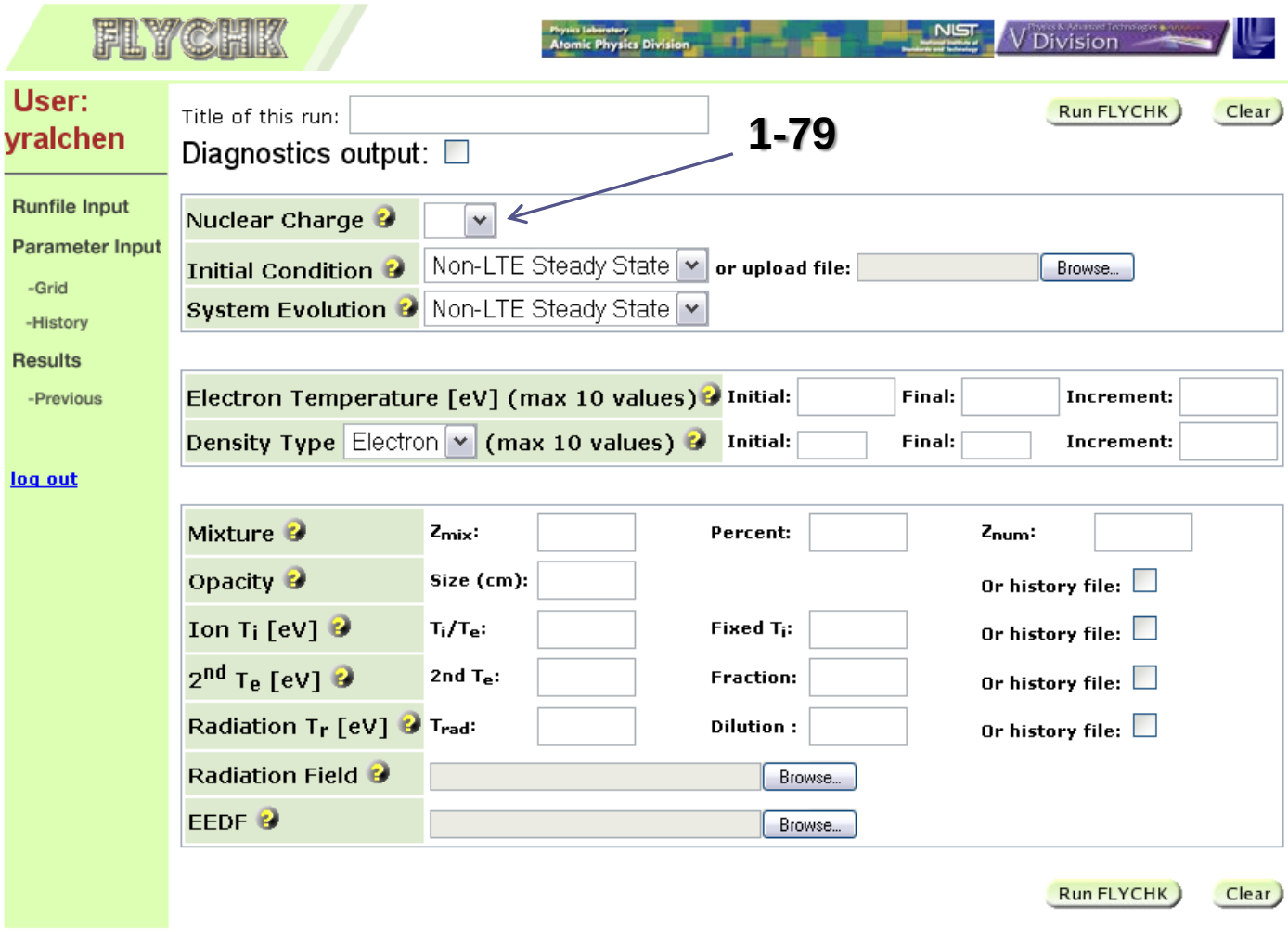
- **Short-pulse laser-produced plasmas**
  - Arbitrary electron energy distribution function
  - Time-dependent ionization processes
  - K-α shifts and broadening: diagnostics
- **Long-pulse laser-produced plasmas**
  - Average charge states
  - Spectra from a uniform plasma
  - Gas bag, Hohlraum (H0), Underdense foam
- **Z-pinch plasmas**: photoionizing plasmas
- **Proton-heated plasmas**: warm dense matter
- **EBIT**: electron beam-produced plasmas
- **EUVL**: Sn plasma ionization distributions
- **TOKAMAK**: High-Z impurities







FLYCHK: steady-state input



FLYCHK at NIST is developed and managed by H.-K. Chung, M. Chen and R. W. Lee at LLNL and Yu. Ralchenko at NIST. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under Contract No. W-7406-Eng-48

Conclusions

- NIST actively develops a well-established program on atomic data collection, evaluation and dissemination
- Development of atomic databases is an important part of this program
- Online tools include CR code FLYCHK, dynamic Grotrian diagrams, Saha-LTE plotting
- More tools to follow in the future