



# Spectroscopic Research Projects at NIST on Light Elements

**John J. Curry**

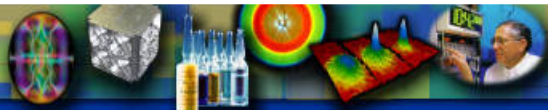
Atomic Spectroscopy Group

National Institute of Standards and Technology

USA

**NIST ATOMIC SPECTRA DATABASE**

[physics.nist.gov](http://physics.nist.gov)



## Participants

Experimental Research:

J. Reader, J. Tan, G. Nave, J. Gillaspay,  
C. Sansonetti, J. J. Curry, A. Tauheed\*

Theoretical Approaches:

Ch. Froese-Fischer\*, Y. Ralchenko\*,  
M. Ali\*, O. Zatsarrinny\*, J.-F. Wyart\*,

Data Assessment and  
Compilations:

J. Reader, E. Saloman\*, J. Fuhr\*, D. Kelleher\*,  
L. Podobedova\*, J. Sansonetti\*, A. Kramida\*,  
W. Wiese\*, C. Sansonetti, J. J. Curry, G. Nave

Database Development:

Y. Ralchenko\*, A. Kramida\*, R. Ibacache,  
A. Jackson, A. Zimmermann

\*contractors/Guest Researcher



## Projects on Light Elements

- A. Atomic Spectra Database
- B. H,D, and T
- C. He and Li
- D. Be and B
- E. Other Light Elements
- F. W
- G. Future Plans

**NIST ATOMIC SPECTRA DATABASE**

[physics.nist.gov](http://physics.nist.gov)



## A. ASD and Associated Databases

### Atomic Spectra Database –

Version 3.15 (4.0 coming)

950 spectra

144,000 transition wavelengths

77,000 energy levels

Auxiliary tools

Grotrian diagram

Saha-equil. radiation plot for arbitrary plasma parameters

Line ID plot

FLYCHK spectral modelling

50,000 queries per month

### Bibliographic Databases

EL and Wavelengths

Atomic transition probabilities

Line shapes and shifts

**NIST ATOMIC SPECTRA DATABASE**

[physics.nist.gov](http://physics.nist.gov)



## C. H, He, and Li

- **'Accurate atomic transition probabilities for hydrogen, helium, and lithium,'** Wiese and Fuhr, JPCRD 2009.
- **'Relativistic all-order and multi-configuration Hartree-Fock calculations of the 4d-4f energy separation in Li I,'** Safronova, Fischer, and Ralchenko, PRA 2007.
- **'Electron-impact excitation and ionization cross sections for ground state and excited state helium atoms,'** Ralchenko et al., At. Data and Nucl. Data Tables 2008.



## B. H, D, and T

Transition		Hydrogen			Deuterium		Tritium	
		$\lambda$ (nm)	$A_{\text{non-rel}}$	$A_{\text{relativ}}$	$\lambda$	$A_{\text{relativistic}}$	$\lambda$	$A_{\text{relativistic}}$
$L_{\alpha}$	1 – 2	121.567	4.699	4.6986	121.533	4.6999	121.523	4.7004
$L_{\beta}$	1 – 3	102.572	5.575e-1	5.5751e-1	102.544	5.5766e-1	102.535	5.5771e-1
$H_{\alpha}$	2 – 3	656.464	4.410e-1	4.4101e-1	656.29	4.4113e-1	656.23	4.4117e-1
$H_{\beta}$	2 – 4	486.270	8.419e-2	8.4193e-1	486.14	8.4216e-2	486.09	8.4224e-2



## B. H, D, and T

Hydrogen

Transition	Non-relativistic value	Relativistic values		
	Green et al. 1957	Baker 2008	Jitrik & Bunge 2004	Pal'chikov 1998
$1s - 2p$	6.265	6.2649		
$1s - 2p_{1/2}$		6.2649	6.2649	6.2649
$1s - 2p_{3/2}$		6.2648	6.2648	6.2648
$1s - 3p$	1.672	1.6725		
$1s - 3p_{1/2}$		1.6725	1.6725	1.6725
$1s - 3p_{3/2}$		1.6725	1.6725	1.6725
$1s - 4p$	0.6818	0.68186		
$1s - 4p_{1/2}$		0.68186	0.68186	0.68186
$1s - 4p_{3/2}$		0.68186	0.68186	0.68186



## C. Helium and Lithium

He I, 128 lines → 2243 lines

Li I, 57 lines → 152 lines

Li II, 52 lines → 475 lines





## C. Helium and Lithium

Lithium

	Line Strengths	
	$2s\ ^2S - 2p\ ^2P^o$	$2p\ ^2P^o - 3d\ ^2D$
<b><i>THEORY:</i></b>		
Yan and Drake	32.9990726 (length) 32.9990681 (velocity)	77.00916742
Fischer et al.	33.0027	77.0068
Pestka and Woznicki	33.0093	76.9775
Qu et al.	33.0076	—
Peach et al.	33.023	—
<b><i>LIFETIME EXPTS.:</i></b>		
Schmitt et al.	33.02	76.99*
McAlexander et al.	33.005	—
Martin et al.	32.97	—



## D. Beryllium and Boron

- **‘Tables of Atomic Transition Probabilities for Be and B,’** Wiese and Fuhr, in progress.
- **‘A critical compilation of energy levels and spectral lines of neutral boron,’** Kramida and Ryabtsev, Phys. Scripta 2008.
- **‘Additions to the spectrum and energy levels and critical compilation of doubly-ionized boron, B II,’** Kramida, Ryabtsev, Ekberg, Kink, Mannervik, and Martinson, Phys. Scripta 2008.
- **‘Additions to the spectrum and energy levels and a critical compilation of helium-like and hydrogen-like boron, B IV and B V,’** Kramida, Ryabtsev, Ekberg, Kink, Mannervik, and Martinson, Phys. Scripta 2008.



## D. Beryllium and Boron

Be I

	<i>gf</i> -values			
	$2s^2\ ^1S - 2s2p\ ^1P^o$	$2s2p\ ^3P^o - 2p^2\ ^3P$	$2s2p\ ^1P^o - 2s3s\ ^1S$	$2s2p\ ^1P^o - 2s3d\ ^1D$
<b>CALCULATIONS:</b>				
Tachiev and Froese Fischer	1.380 (D=0.1 %)	4.005 (D=0.3 %)	0.3452 (D=2.6 %)	1.1934 (D=4.5 %)
Nam	1.383 (D=1.0 %)	4.047 (D=1.4 %)	0.3633 (D=0.8 %)	1.2306 (D=0.0 %)
Weiss	1.3755 (D=0.14 %)	4.0232 (D=0.15 %)	0.3559 (D=1.57 %)	1.2011 (D=1.89 %)
Jönsson et al.	1.3711 (D=0.12 %)	4.0178 (D=0.07 %)	—	—
Fleming et al.	1.375 (D=0.23 %)	—	—	—
<b>LIFETIME EXPTS.:</b>				
Irving et al.	$1.40 \pm 0.04$	—	—	—
Schnabel and Kock	$1.34 \pm 0.03$	—	—	—



## D. Beryllium and Boron

**BI**

	Experiments			Calculations	
Atomic Level	Lundberg <i>et al.</i>	O'Brian and Lawler		Tachiev and Froese Fischer	Fernley <i>et al.</i>
$2s2p^2\ ^2D$	—	$23.1\pm 1.2$		22.9	—
$2s^23s\ ^2S$	—	$4.0\pm 0.2$		4.00	—
$2s^23d\ ^2D$	—	$4.7\pm 0.2$		4.63	—
$2s^24s\ ^2S$	—	$8.7\pm 0.4$		—	9.09
$2s^24d\ ^2D$	$10.3\pm 0.5$	$10.0\pm 0.5$		—	9.39
$2s^25s\ ^2S$	$11.0\pm 0.6$	—		—	14.66



## E. Other Light Elements

- **Improved critical compilations of selected transition probabilities for neutral and singly-ionized carbon and nitrogen,** Wiese and Fuhr, JPCRD 2007.
- **'MCDHF energies and transition probabilities for ... transitions in Ne II,'** Fisher and Ralchenko, Int. J. Mass Spec. 2008.
- **'Experimental study of weak intersystem lines and related strong persistent lines of Ne II,'** Bridges and Wiese, PRA 2007.
- **'Extended EUV and UV spectrum of Ne II,'** Kramida, Brown, Feldman, and Reader, Phys. Scripta 2006.
- **'The Ne II spectrum,'** Kramida and Nave, Eur. Phys. J. D 2006.
- **'New FTS measurements, optimized energy levels and refined VUV standards in the Ne III spectrum,'** Kramida and Nave, Eur. Phys. J. D 2006.
- **'Energy levels and spectral lines of Ne VIII,'** Kramida and Buchet-Poulizac 2006.
- **'Energy levels and spectral lines of Ne VII,'** Kramida and Buchet-Poulizac, Eur. Phys. J. D 2006.



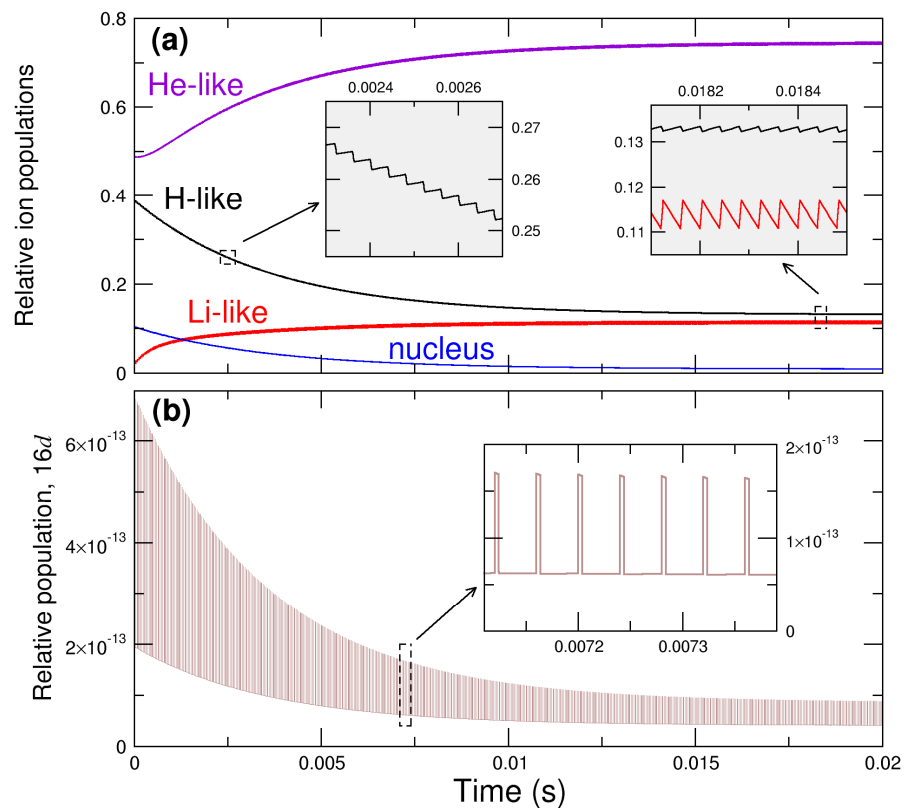
## E. Other Light Elements (Na → Ar)

- **'Atomic transition probabilities of sodium and magnesium: A critical compilation,'** Kelleher and Podobedova, JPCRD 2008.
- **'Atomic transition probabilities of aluminum: A critical compilation,'** Kelleher and Podobedova, JPCRD 2008.
- **'Atomic transition probabilities of silicon: A critical compilation,'** Kelleher and Podobedova, JPCRD 2008.
- **'Critically evaluated atomic transition probabilities for sulfur S I-XV,'** Podobedova, Kelleher, and Wiese, JPCRD 2009.
- **'Experimental transition probabilities for infrared lines of Cl I,'** Bridges and Wiese, PRA 2008.
- **'Kinetics of highly-excited states in Ar17+ charge-exchange recombination fusion plasma spectroscopy,'** Marchuk, Ralchenko, et al., J. Phys. B 2009.
- **'Kinetics of highly-excited states in Ar17+ charge-exchange recombination fusion plasma spectroscopy,'** Marchuk, Ralchenko, et al., J. Phys. B 2009.



# E. Ar

Charge-exchange recombination spectroscopy with heavy impurities (Ar)





## F. Tungsten

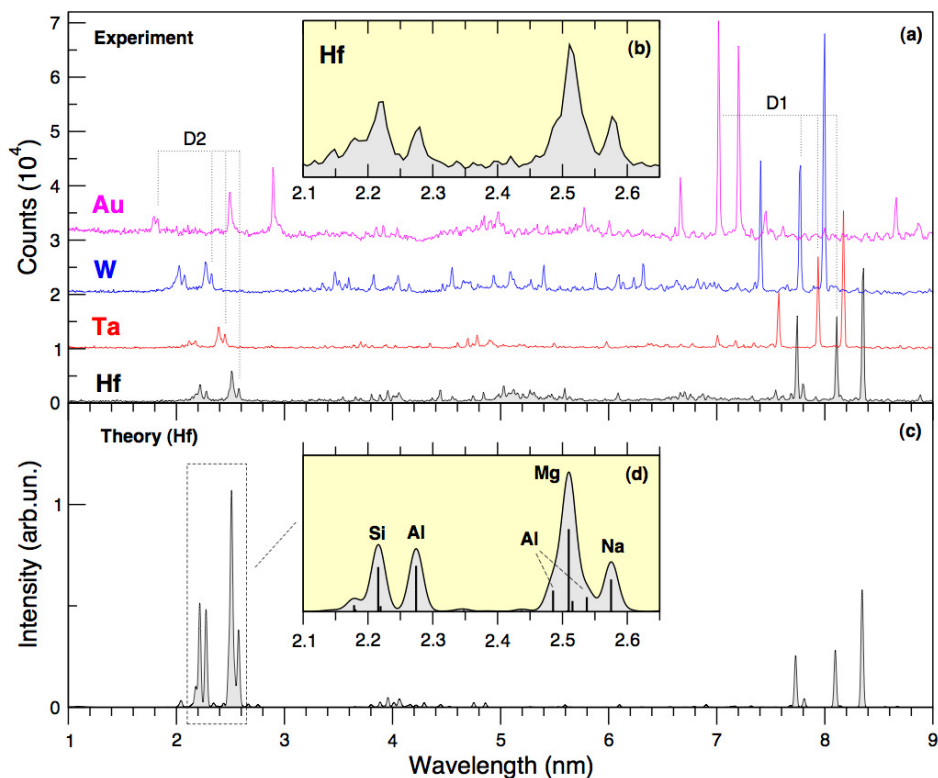
- **'Energy levels and spectral lines of tungsten, W III through W LXXIV,'** Kramida and Shirai, At. Data and Nuc. Data Tables 2009.
- **'Ionization energies of tungsten ions: W<sup>2+</sup> through W<sup>71+</sup>,** Kramida and Reader, At. Data and Nuc. Data Tables 2006.
- **'Compilation of wavelengths, energy levels, and transition probabilities for W I and W II,'** Kramida and Shirai, JPCRD 2006.
- **'Measurement of the D-line doublet in high-Z highly-charged sodium-like ions,'** Gillaspay et al., PRA 2009.
- **'Bright EUV lines emitted by highly-ionized tungsten ions as diagnostic indicators of the tungsten transport in ITER core plasmas,'** Feldman et al., Nuc. Fus. 2008.
- **'EUV spectra of highly-charged ions W<sup>54+</sup> - W<sup>63+</sup> relevant to ITER diagnostics,'** Ralchenko et al. J Phys. B 2008.
- **'Spectra of W<sup>39+</sup> - W<sup>47+</sup> in the 12 – 20 nm region observed with an EBIT light source,'** Ralchenko et al., J. Phys. B 2007.
- **'Density dependence of the forbidden lines in Ni-like tungsten,'** Ralchenko, J. Phys. B 2007.
- **'Accurate modeling of benchmark x-ray spectra from highly-charged ions of tungsten,'** Ralchenko et al., PRA 2006.



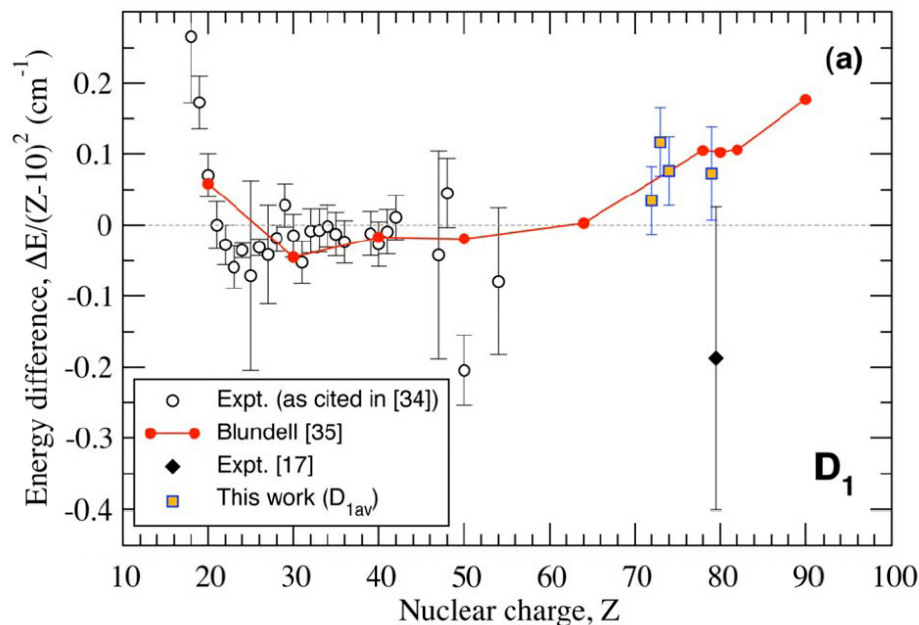


# F. Tungsten

Highly-ionized Hf, Ta, W, Au observed in the range of 2-20 nm, for range of electron impact energies



- D-lines of Na-like Tungsten





## F. Tungsten

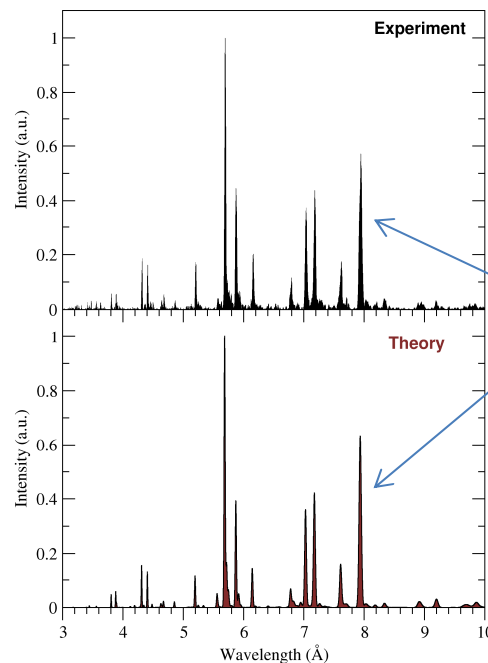
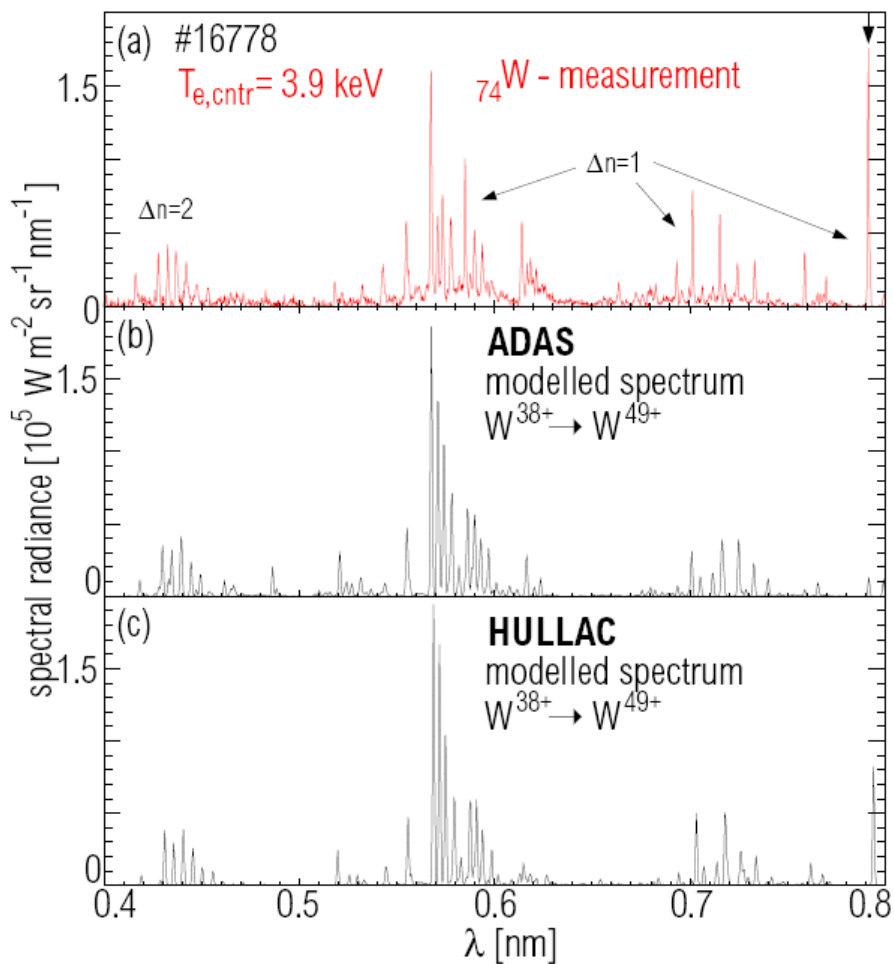
Many lines have been measured and identified for Hf, Ta, W, and Au

- **Hf, Ta, and Au:** 627 lines measured,  
152 identified,  
115 observed for the first time.
- **W:** several hundred lines are currently under analysis.

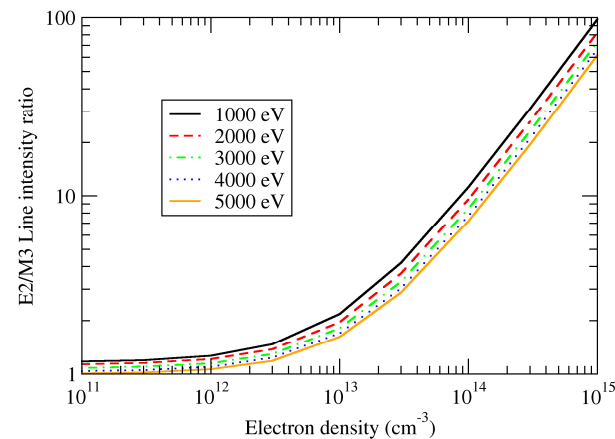


R. Neu et al, Nuclear Fusion  
45, 209 (2005)

# F. Tungsten



7.93 Å line:  
E2 + M3





## G. Future Plans

### Compilations

- H, D, T – Energy levels and Wavelengths (Kramida)
- F and Ne – Transition Probabilities (Wiese and Fuhr)
- Ar – Energy levels and Wavelengths (Saloman and Sansonetti)
- Cl – (Podobedova)

### Measurements

- Mg (Reader, Feldman, and Brown)



# Support

## External support

- U.S. Department of Energy, Office of Fusion Energy Sciences
- U.S. National Aeronautics and Space Administration

**NIST ATOMIC SPECTRA DATABASE**

[physics.nist.gov](http://physics.nist.gov)