

Atomic Databases: General Ideas and Some Examples

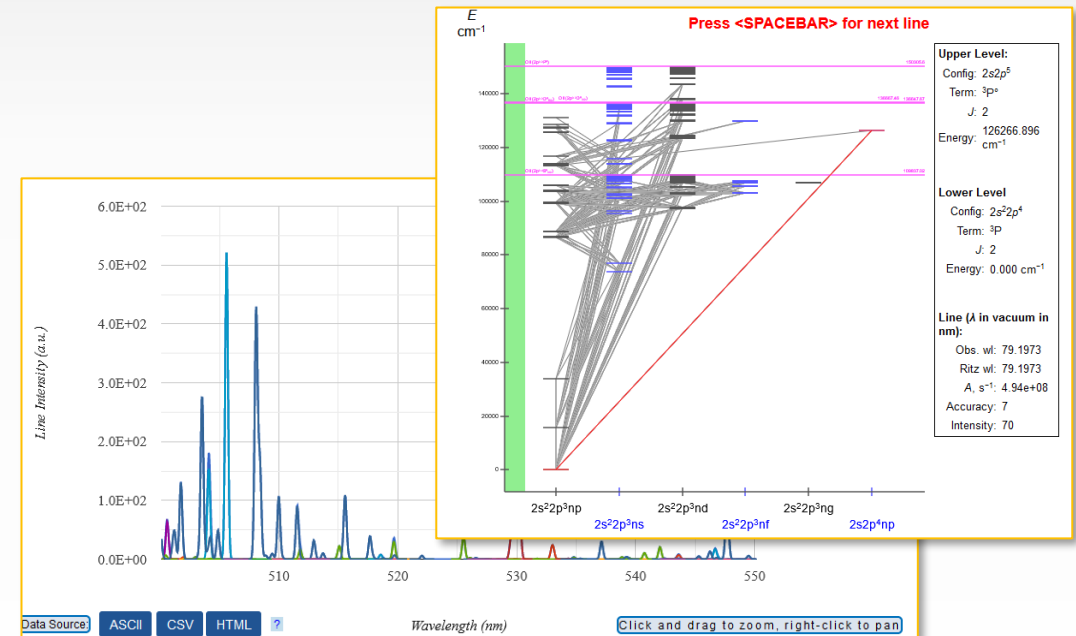
Yuri Ralchenko

University of Maryland, College Park, MD 20742

X-Ray Astrophysics Laboratory, NASA GSFC,
Greenbelt, MD 20771

CRESST II, NASA GSFC, Greenbelt, MD 20771

May 8, 2026



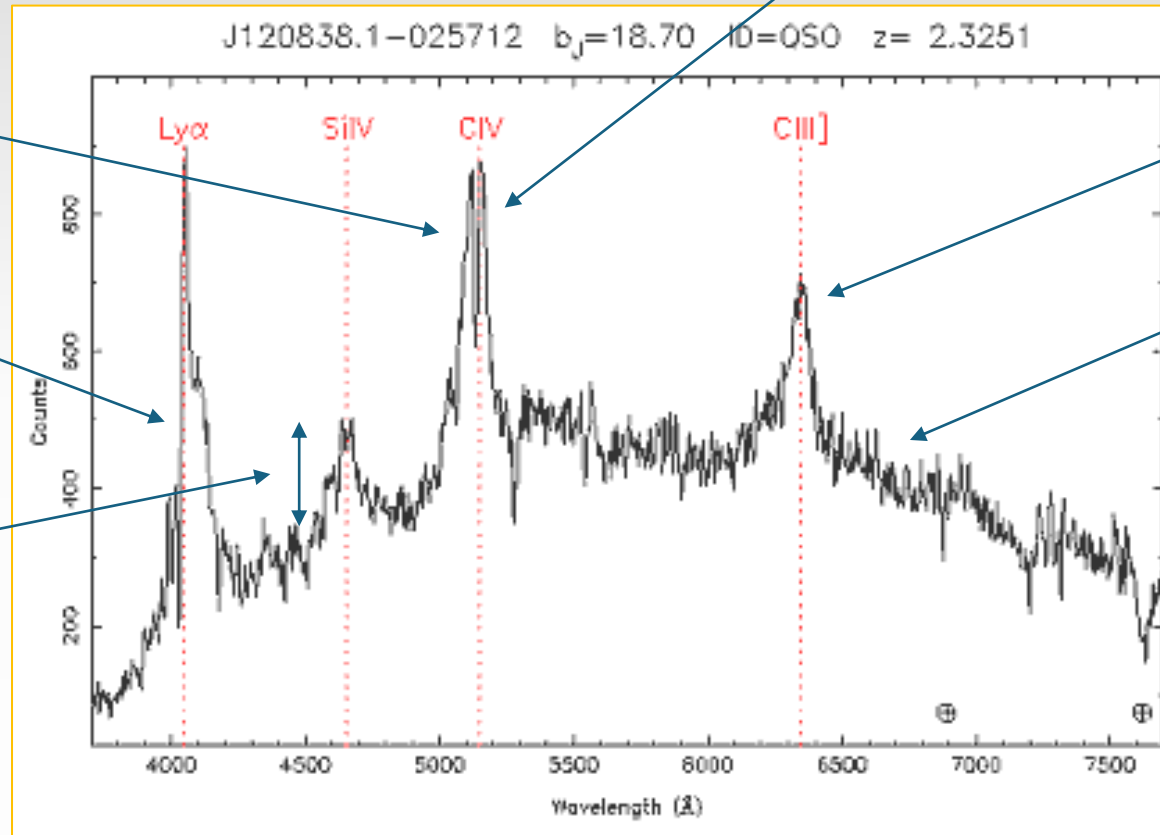
Spectral parameters

Line identification

Line splitting, EM fields

Line broadening

Line intensity



Wavelength, line shift

Background, continuum

Plus:

- Cross sections
- Rate coefficients
- ...

2dF Quasar Survey

Examples of atomic numerical databases

AtomDB (CfA-Harvard)

ADAS (UK)

ALADDIN (IAEA, Austria)

CollisionDB (IAEA, Austria)

BEAMDB (Serbia)

CAMDB (China)

CCC (Australia)

CHIANTI (NASA, USA, UK)

CLOUDY (Univ.Kentucky)

Kurucz database (Harvard)

NIFS (Japan)

NIST Atomic Databases

PEARL (Korea)

Spectr-W3 (Russia)

Stark-B (France/Serbia)

TIP/TOPbase (NASA, Venezuela, UK)

TOPS (LANL)

VALD (Austria, Sweden, Russia)

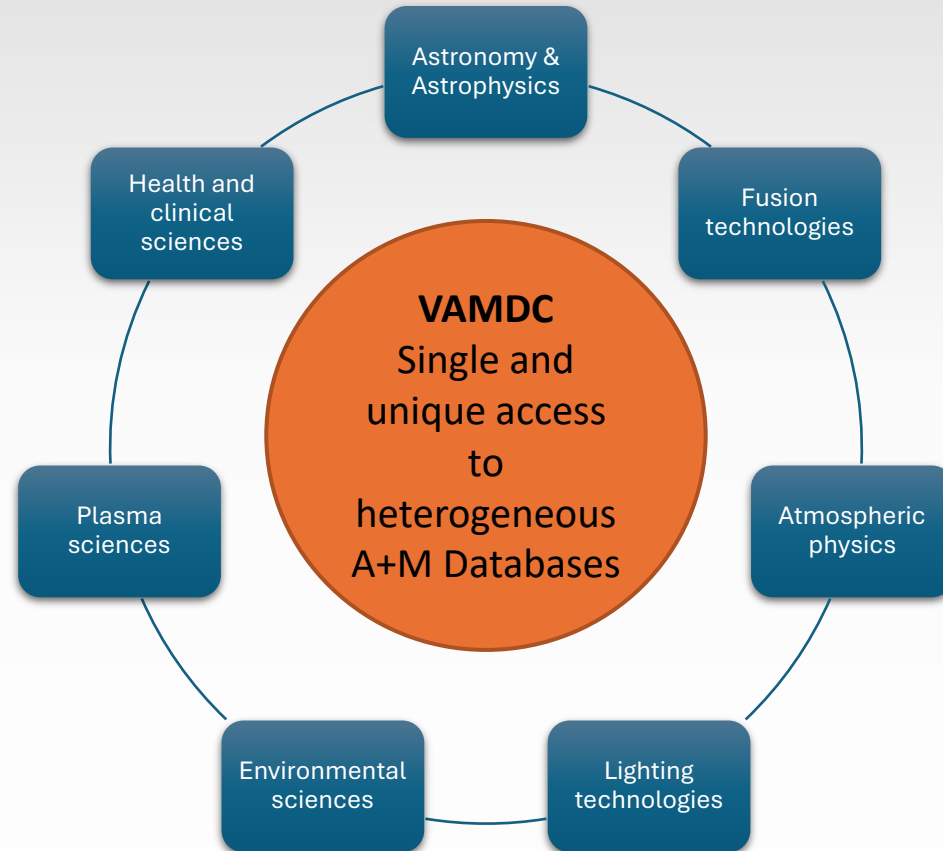
...and more...



The Virtual Atomic and Molecular Data Centre

<http://www.vamdc.org>

<http://vamdc.eu/>



- About 40 heterogeneous databases
- The “V” of VAMDC stands for Virtual in the sense that the e-infrastructure does not contain data. The infrastructure is a wrapping for exposing in a unified interoperable way a set of heterogeneous databases.
- High quality scientific data come from different Physical/Chemical Communities
- Provides data producers with a large dissemination platform
- Led by astronomers and astrophysicists

Why are these databases different?

- Different atomic parameters (structure/radiation, collisions)
- Coverage of data (species, ions,...)
- Completeness of information (quantum numbers etc)
- Sources of data
- Online tools and options
- **Critical evaluation of the data**

Critically-evaluated atomic databases

AtomDB (CfA-Harvard)

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...and more...

National Institute for Fusion Science, Japan

<https://dbshino.nifs.ac.jp>

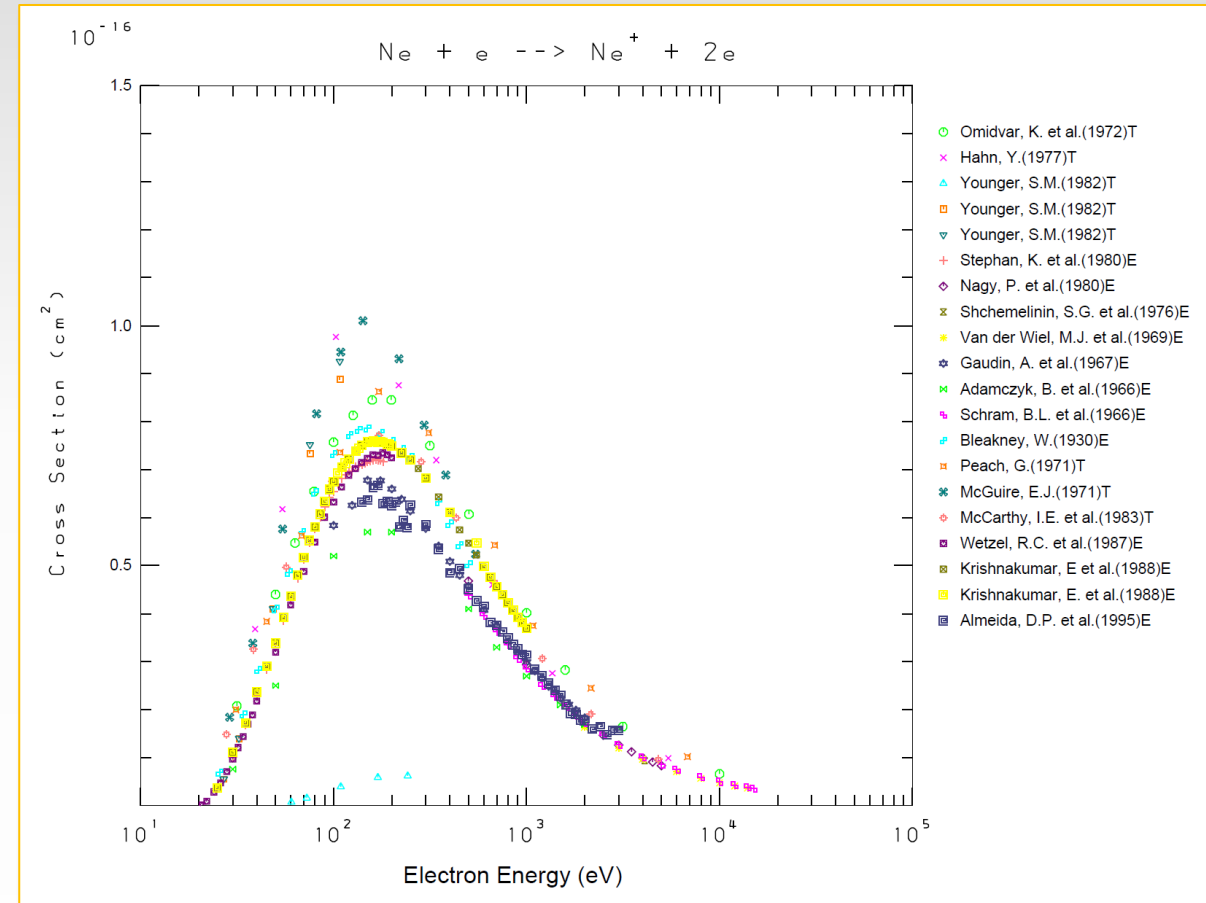
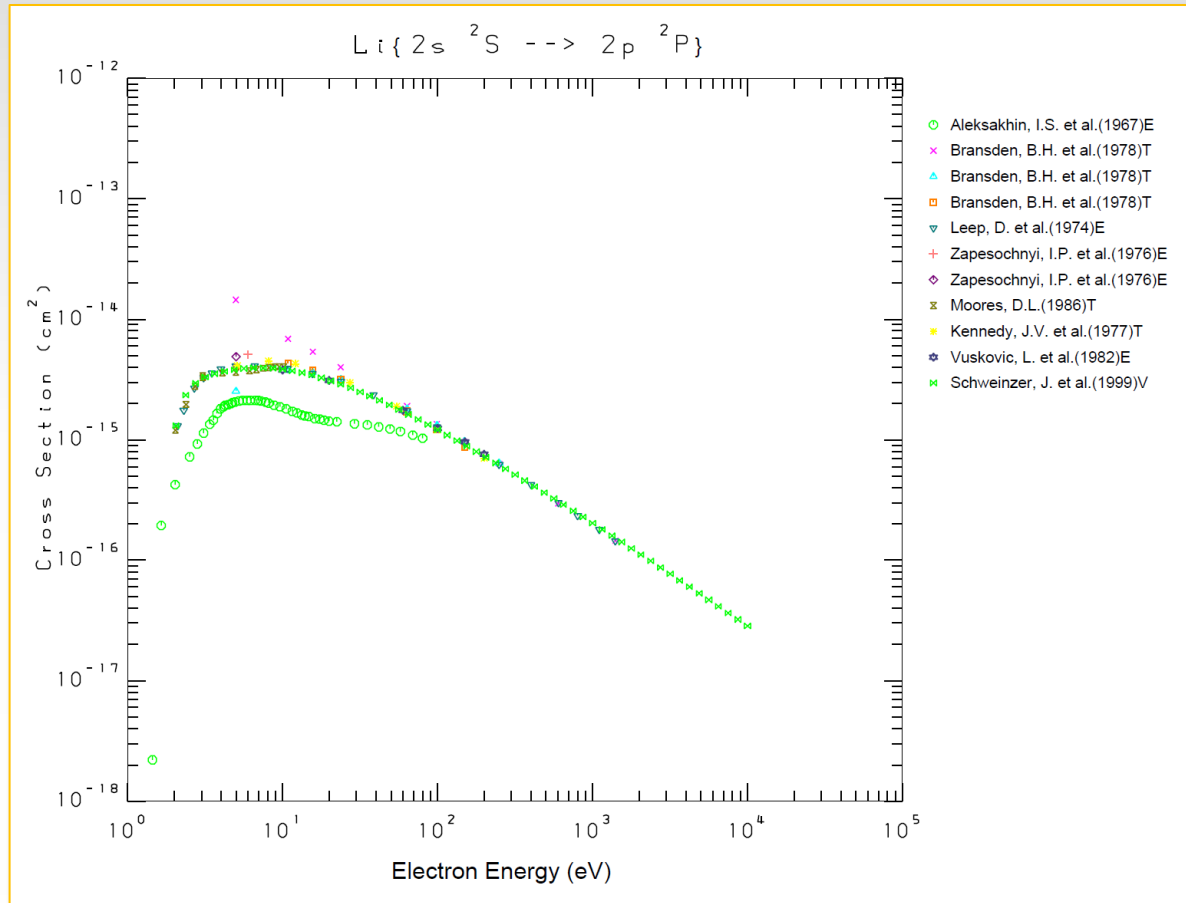
One of the most extensive collisional databases

Welcome to NIFS DATABASE

Please select the database. Atomic and Molecular Research Center, NIFS is making the Atomic and Molecular Numerical databases for various collisional processes and the Bibliographic Databases. You can access the databases only which you applied for at the registration. Information on each database will be found from [i](#) .

Atomic and Molecular Numerical Databases i					Simple search				
AMDIS i	EXC i	ION i	REC i	DIO i		EXC	ION	REC	DIO
CHART i	AMOL i		CMOL i		CHART	AMOL		CMOL	
BACKS i	SPUTY i		CURVE i		BACKS	SPUTY			
Bibliographic Database i									
					ORNL i				

NIFS Database output



NIST NASA Atomic Databases and Tools

- [Atomic Spectra Database](#)
- [Handbook of Basic Atomic Spectroscopic Data](#)
- [Laser Induced Breakdown Spectroscopy \(LIBS\)](#)
- [Energy Levels of Hydrogen and Deuterium](#)
- [Ground Levels and Ionization Energies](#)
- NLTE Databases and Codes
 - [NIST-LANL Lanthanide Opacity Database](#)
 - [FLYCHK Collisional-Radiative Code](#)
 - [SAHA Plasma Population Kinetics Database](#)
 - [NLTE4 Plasma Population Kinetics Database](#)
- [Spectrum of Platinum Lamp for Ultraviolet Spectrograph Calibration](#)
- [Spectrum of Th-Ar Hollow Cathode Lamps](#)
- [X-ray Transition Energies](#)
- [Atomic Spectra Bibliographic Databases](#)



NIST LIBS Database ?

A. Kramida, K. Olsen, and Yu. Ralchenko

NIST-LANL Lanthanide Opacity Database

FLYCHK

**Atomic Energy Levels and
Spectra Bibliographic Database**

<https://www.nist.gov/pml/atomic-spectroscopy-databases>

Workflow of critical evaluation of data



Contents lists available at [ScienceDirect](https://www.sciencedirect.com)

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

Atomic Data and Nuclear Data Tables 149 (2023) 101548

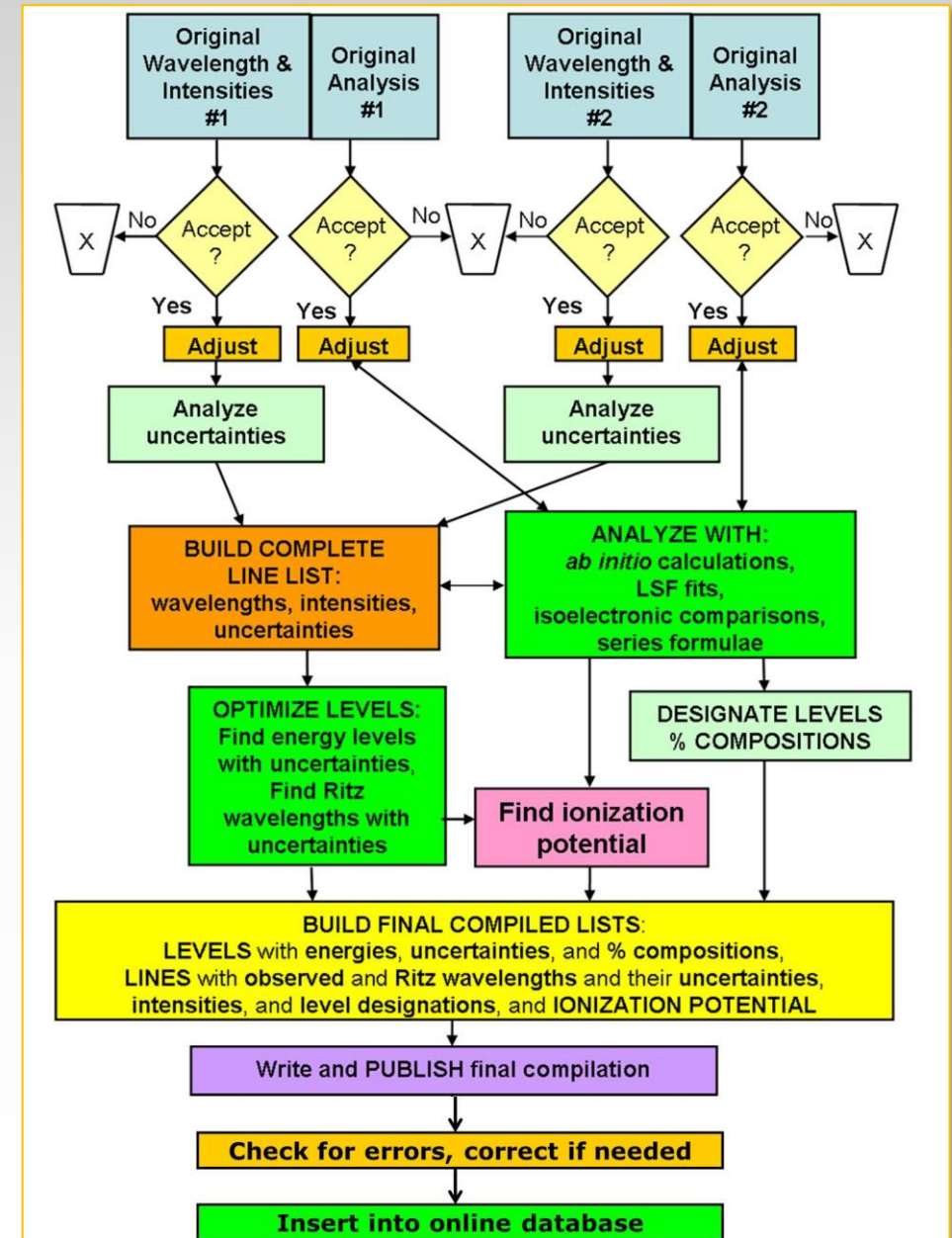
A critical compilation of experimental data on the $1s2l2l'$ core-excited states of Li-like ions from carbon to uranium

V.I. Azarov ^{a,*}, A. Kramida ^{b,**}, Yu. Ralchenko ^b

^a Associate, National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

^b National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

For the 16 energy levels of the $1s2l2l'$ core-excited configurations of Li-like ions, **999** absolute and **35** relative experimental energy-level measurements from **101** publications have been collected and analyzed. Modern statistical theory methods (e.g., “dark uncertainty”) were applied to derive the final uncertainties.



A. Kramida

Fus. Sci. Tech. **63**, 313 (2013)

ASD v.5.12 (Dec 2024)

<https://physics.nist.gov/asd>

Spectral lines

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H																	2 He
3 Li	4 Be								5 B	6 C	7 N	8 O	9 F	10 Ne			
11 Na	12 Mg								13 Al	14 Si	15 P	16 S	17 Cl	18 Ar			
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	+	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
* Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu		
* Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr		

Color vs. number of lines:



Energy levels

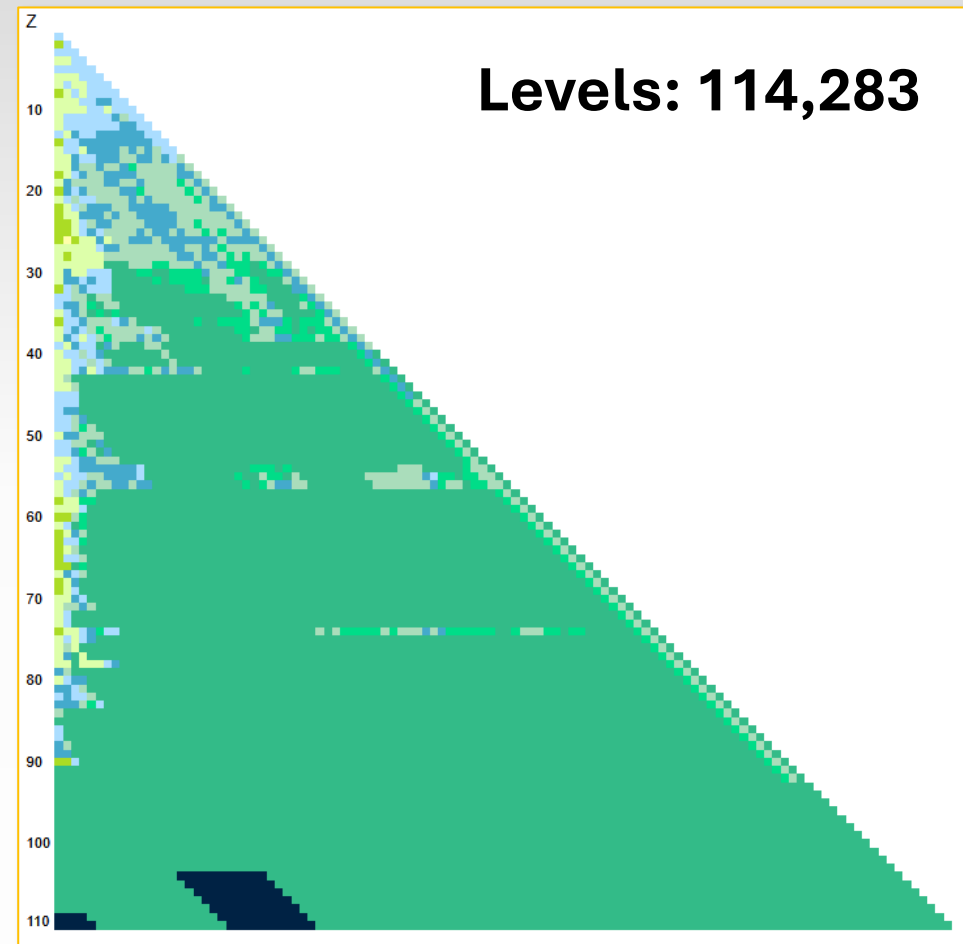
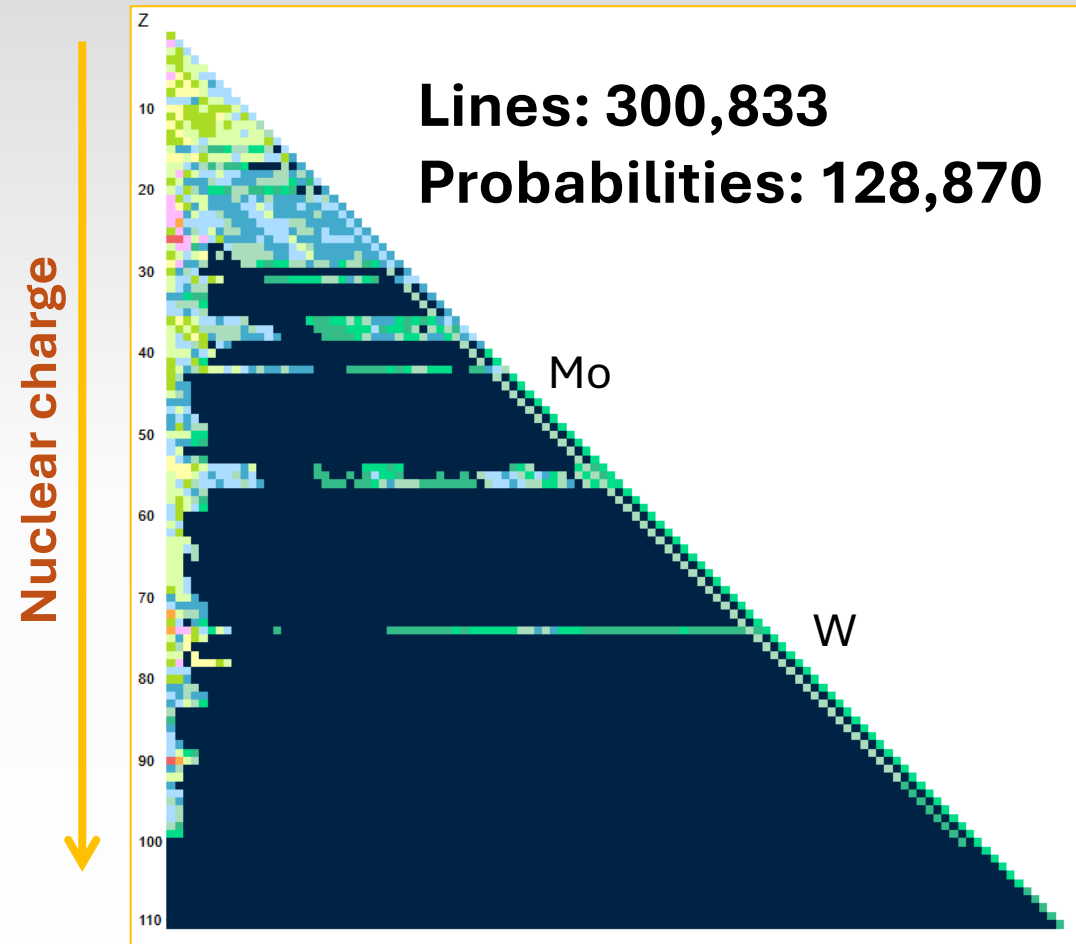
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
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19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	+	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
* Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu		
* Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr		

Color vs. number of levels:



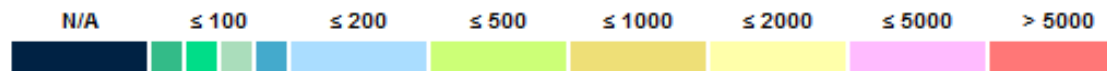
ASD v.5.12 (Dec 2024)

<https://physics.nist.gov/asd>



Ion charge

Color vs. number of lines:



ASD Output

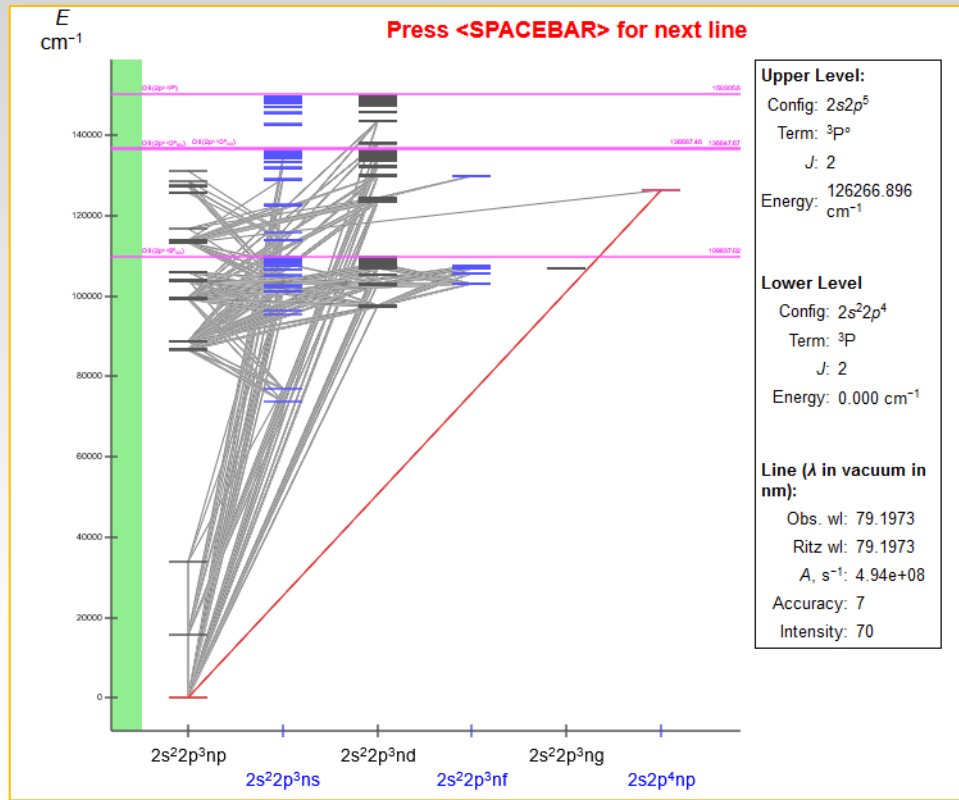
- Data tables in different formats (HTML, ASCII, XSAMS, csv,...)
- Uncertainties!!!**

Primary data sources			Query NIST Bibliographic Databases for Ar II (new window)
Energy Levels:	Saloman 2010	All energy level values from this compilation have been decreased by 0.0002 cm ⁻¹ to make the ground state energy equal to zero.	Ar II Energy Levels
Lines:	Saloman 2010		Ar II Line Wavelengths and Classification
Transition Probabilities:	Wiese et al. 1969		Ar II Transition Probabilities

Ar⁺

Observed Wavelength Vac (nm)	Unc. (nm)	Ritz Wavelength Vac (nm)	Unc. (nm)	Rel. Int. (?)	A _{ki} (s ⁻¹)	Acc.	E _i (cm ⁻¹)	E _k (cm ⁻¹)	Lower Level Conf., Term, J	Upper Level Conf., Term, J	Type	TP Ref.	Line Ref.
71.8091	0.0003	71.8089852	0.0000004	4	9.5e+08	D	0.0000 - 139 258.3389	139 258.3389	3s ² 3p ⁵ 2p ^o 3/2	3s ² 3p ⁴ (3P)4s 2p 1/2		T997	L16202
72.3361	0.0003	72.3360560	0.0000004	5	2.3e+09	D	0.0000 - 138 243.6444	138 243.6444	3s ² 3p ⁵ 2p ^o 3/2	3s ² 3p ⁴ (3P)4s 2p 3/2		T997	L16202
72.5550	0.0003	72.5548530	0.0000004	4	1.9e+09	D	1 431.5831 - 139 258.3389	139 258.3389	3s ² 3p ⁵ 2p ^o 1/2	3s ² 3p ⁴ (3P)4s 2p 1/2		T997	L16202
73.09300	0.00003	73.0929708	0.0000004	5	4.5e+08	D	1 431.5831 - 138 243.6444	138 243.6444	3s ² 3p ⁵ 2p ^o 1/2	3s ² 3p ⁴ (3P)4s 2p 3/2		T997	L1317
73.7457	0.0003	73.7453699	0.0000005	1	3.8e+06	E	0.0000 - 135 601.7336	135 601.7336	3s ² 3p ⁵ 2p ^o 3/2	3s ² 3p ⁴ (3P)4s 4p 1/2		T997	L16202

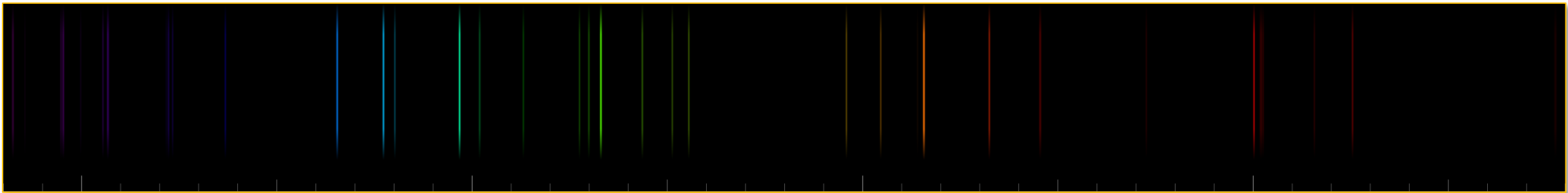
<https://physics.nist.gov/asd>



ASD: rich graphical options

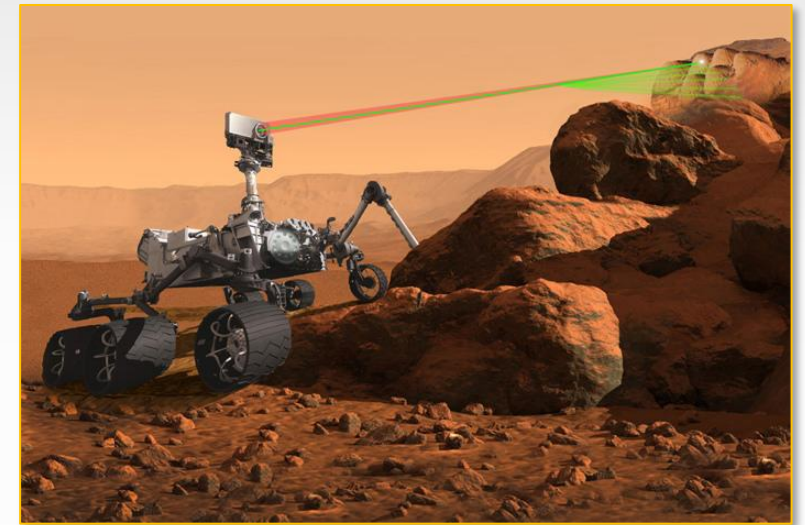
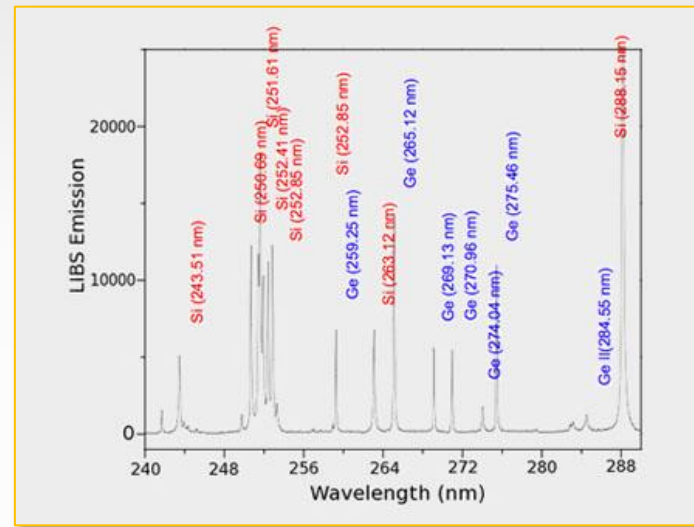
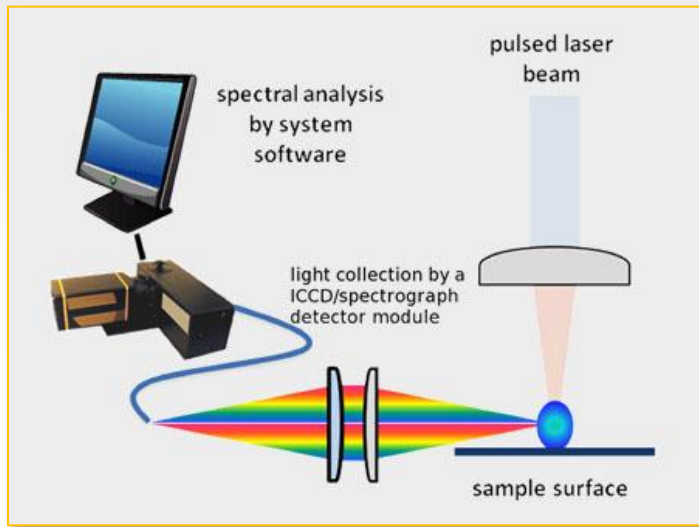
O I
 614 levels
 910 lines

O I
 174 lines, 380-780 nm



NIST LIBS Database: Laser Induced Breakdown Spectroscopy

<https://physics.nist.gov/LIBS>



© Applied Spectra

Numerous terrestrial and extra-terrestrial applications
(Curiosity and Perseverance rovers)

NIST LIBS Database

Low temperature, high density: Saha-LTE!

Element: Si
Percentage: 20
Element [Remove]: C
Percentage: 80
Lower Wavelength: 200
Upper Wavelength: 600
Wavelengths in: Vacuum (< 200 nm) Air (200 - 2000 nm) Vacuum (> 2000 nm)
 Vacuum (all wavelengths)
Units: nm
Resolution: 1000
Te (eV): 1
Ne (cm⁻³): 1e17
Advanced Options
Retrieve Data Reset Input

$$I = N_0 \frac{g_i}{g_0} e^{-E/T} \cdot A$$

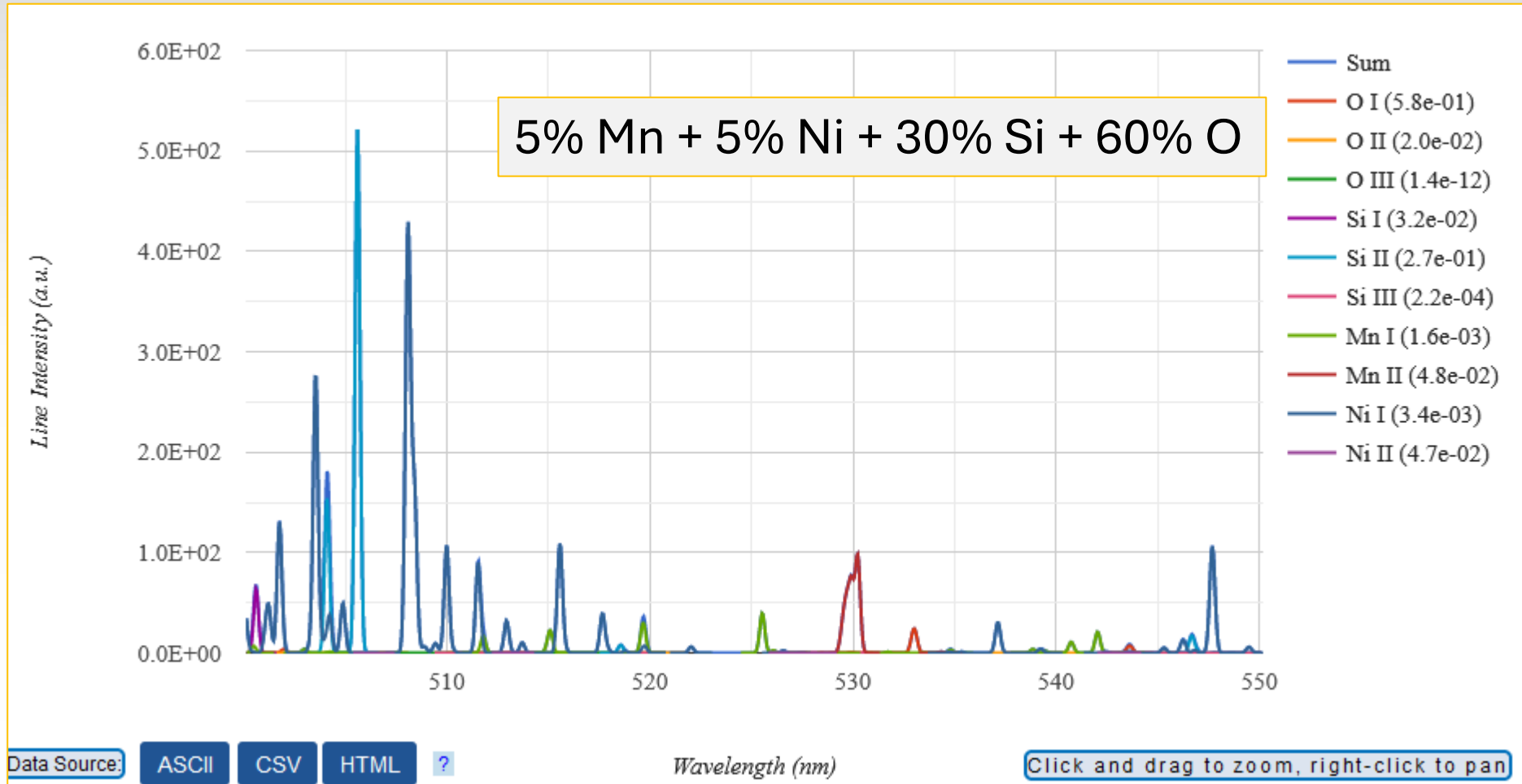
All needed data are already in ASD

- Calculation of Saha/LTE spectra for any element or combination thereof in ASD
- Arbitrary plasma parameters (but Saha/LTE!) and spectrum resolution
- ASD-based
- Graphical services
- Problem: not all ions, A's

<https://physics.nist.gov/LIBS>

NIST LIBS Database

<https://physics.nist.gov/LIBS>



$$T_e = 1 \text{ eV}$$

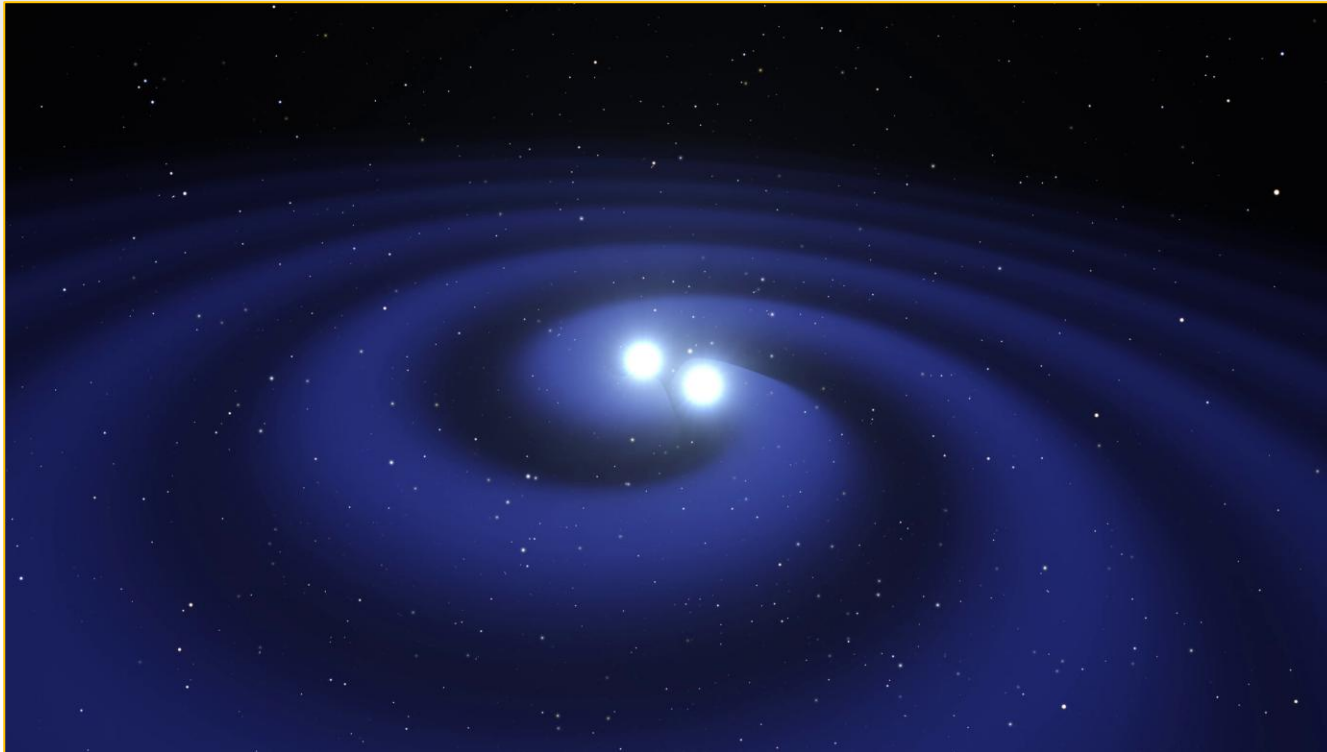
$$N_e = 10^{17} \text{ cm}^{-3}$$

$$R = 3000$$

Direct comparison
with measured data

New NIST-LANL Opacity Database

K. Olsen, C.J.Fontes, C.L.Fryer, A.L. Hungerford, R.T. Wollaeger, O. Korobkin, Yu. Ralchenko



©ESO/L. Calçada

- Neutron star merger
- Kilonova event
- Rich EM spectrum in addition to GW
- $Z = 57-71$ ($4f$ shell) and $Z = 89-102$ ($5f$ shell)
- Lanthanide/actinide opacities are critically important for kilonova analysis

NIST-LANL Lanthanide/Actinide Opacity Database

<https://nlte.nist.gov/OPAC>

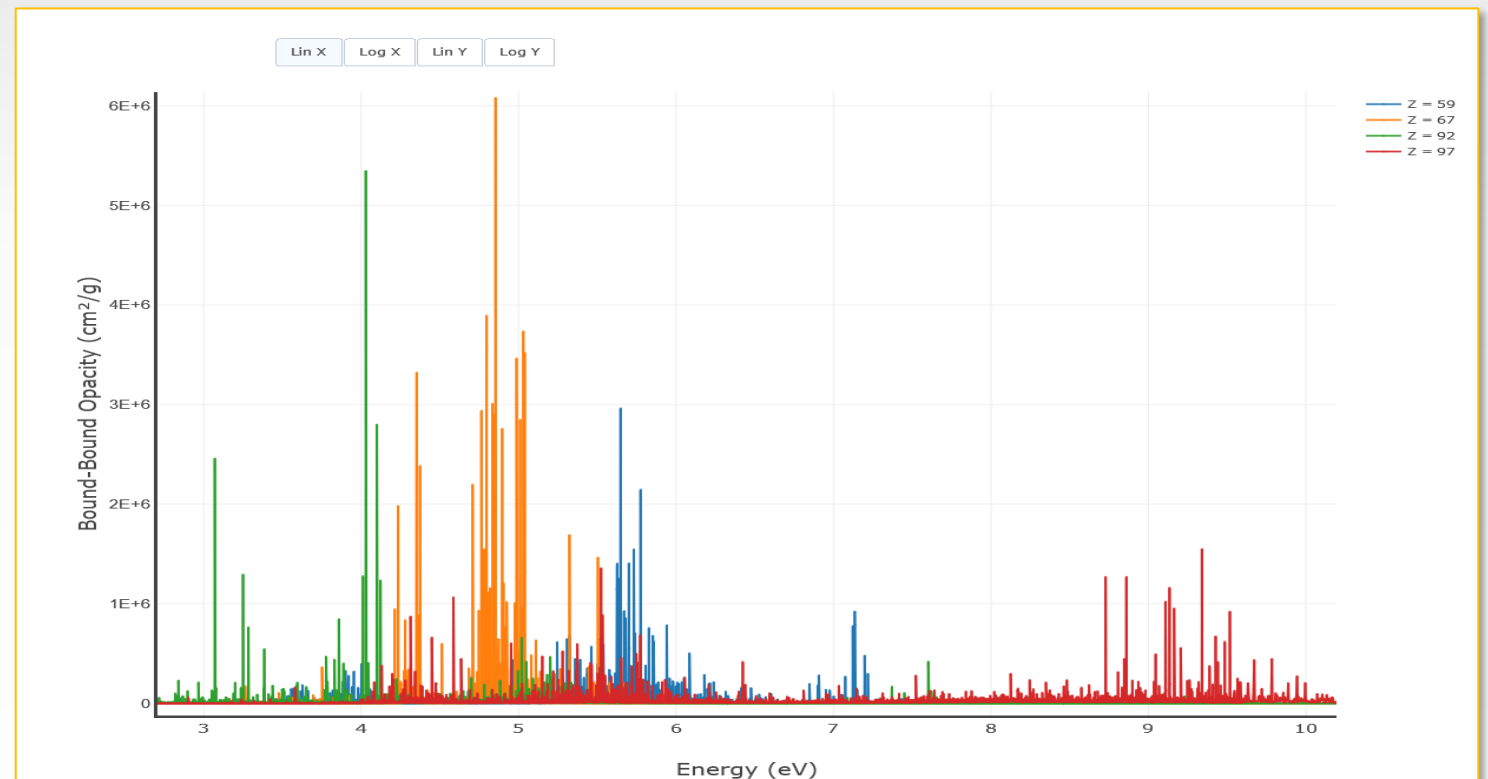
K. Olsen, C.J.Fontes, C.L.Fryer, A.L. Hungerford, R.T. Wollaeger, O. Korobkin, Yu. Ralchenko

- LANL LTE opacities for $57 \leq Z \leq 70$, $89 \leq Z \leq 102$
- Temperatures: 0.01—5 eV
- Densities: 10^{-20} — 10^{-4} g/cm³
- Photon energy grid: 14,900 points

Fontes et al, *Mon. Not. Roy. Astron. Soc.* **493**, 4143 (2020)

Fontes et al, *Mon. Not. Roy. Astron. Soc.* **519**, 2862 (2023)

- Tables and graphs:
 - Total opacities
 - Scattering
 - Absorption
 - Bound-bound
 - Bound-free
 - Free-free



NIST Atomic Bibliographic Databases: references to *the latest data*

- Updated regularly (~2 weeks)
- **Atomic Energy Levels and Spectra**
 - **23,607** references, 1802-2026
- **Atomic Transition Probabilities**
 - **10,572** references, 1914-2025
- **Atomic Lines Broadening and Shifts**
 - **7,237** references, 1889-2026
- Search options
 - Elements/ions
 - Isoelectronic sequence
 - Word/pattern
 - Publication years
 - Publication source
 - Method type
 - Keywords
 - General category
 - Specific subjects of interest