

Lecture 4

- Atomic physics e-databases
- Emission line identification
- Line identification exercise using e-databases

NIST Home > PML > Physical Reference Data > Atomic Spectra Database

<https://www.nist.gov/pml/atomic-spectra-database>

Version History & Citation Information | Disclaimer

NIST Atomic Spectra Database

Version 5

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.

GROUND STATES & IONIZATION ENERGIES

Ground states and ionization energies of atoms and atomic ions.

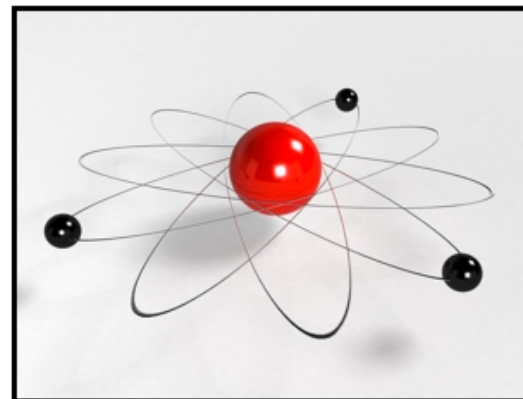
Additional information about the database may be obtained through the following links:

Atomic Spectroscopy Intro	Outlines basic atomic physics concepts, explains terminology and notation.
ASD Intro & Contents	Introduction to and contents of the Atomic Spectra Database.
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 Spectroscopy Data Center](#) has carried out these critical compilations. The Data Center is located in the Physical Measurement Laboratory at the

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NIST ASD Team

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NIST Atomic Spectra Database Lines Form

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

Spectrum Spectrum: e.g., Fe I or Na; Mg;
 Lower Wavelength: or Upper Wavenumber (in cm⁻¹):
 Upper Wavelength: or Lower Wavenumber (in cm⁻¹):
 Units: nm

Dynamic Plots Dynamic Plots
 Line Identification Plot: Line Identification Plot:
 Saha-LTE Spectrum: Saha-LTE Spectrum:
 Electron Temperature Electron Temperature T_e(eV): Doppler-broadened spectrum Doppler-broadened spectrum
 Electron Density Electron Density N_e(cm⁻³): Ion Temperature Ion Temperature T_i(eV): (if T_i ≠ T_e)

Grotrian Diagram
 Java subwindow size: Java subwindow size:
 640 x 640 800 x 640 1024 x 768
 Group by configurations Group by configura
 multiplicity Term multiplicity
 Show only radiatively linked levels Show on
 (requires Java2)
Java Security Level should be Medium. For Java 8 Update 2
 Java Control Panel exception site list.

Output Options
 Format output:
 No JavaScript
 Energy Level Units:
 Display output:
 Page size:
 Output ordering: Wavelength
 Multiplet Multiplet

Optional Search Criteria
 Maximum lower level energy: (e.g., 100000)
 Maximum upper level energy: (e.g., 400000)
 Transition strength bounds will apply to:
 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
 Only with diagnostics
 Include diagnostics data
 Bibliographic Information: TP references, Line references
 Wavelength Data: Observed
 Ritz
 Observed - Ritz (difference)
 Wavenumber (in cm⁻¹)
 Wavelengths: Vacuum (< 200 nm) Air (200 - 1,000 nm)
 Vacuum (< 1,000 nm) Wavenumber (> 1,000 cm⁻¹)
 Vacuum (< 200 nm) Air (200 - 2,000 nm)
 Vacuum (all wavelengths)
 Vacuum (< 185 nm) Air (> 185 nm)
 Wavenumber (all wavelengths)
 Transition strength: A_{ki}A_{ki} g_kA_{ki}g_k in units of 10⁸ s⁻¹
 f_{ik}f_{ik} S_{ik}S_{ik} log(gf)
 Relative Intensity Relative Intensity
 Transition Type: Allowed (E1) Forbidden (M1, E2, ...)
 Level information: Configurations Terms Energies

NIST Atomic Spectra Database Lines Data

All Spectra: 24 Lines of Data Found

Example of how to reference these results:
 Kramida, A., Ralchenko, Yu., Reader, J., and NIST ASD Team (2013). NIST Atomic Spectra Database (ver. 5.1). [Online]. Available: <http://physics.nist.gov/asd> [2014, April 2]. National Institute of Standards and Technology, Gaithersburg, MD.
[BibTex Citation](#) (new window)

Wavelength range: 5321 - 5323 Å
 Wavelength in: vacuum below 2000 Å, air between 2000 and 20000 Å, vacuum above 20000 Å
 Highest relative intensity: 830

Ion	Observed Wavelength Air (Å)	Ritz Wavelength Air (Å)	Rel. Int. (?)	A _{ki} (s ⁻¹)	Acc.	E _j (cm ⁻¹)	E _k (cm ⁻¹)	Lower Level Conf., Term, J	Upper Level Conf., Term, J	Type	TP Ref.	Line Ref.
Fe I	5 321.1076	5 321.1074	355	2.13e+06	C	35 767.564	- 54 555.418	3d ⁷ (⁴ F)4p	z ³ G° 4	3d ⁷ (⁴ F)4d	e ³ H 4	T5720 L11631
Zr I	5 321.26		25									L3475
Re I	5 321.28		35									L3475
W I	5 321.282	5 321.259	3w			18 116.84	- 36 904.16	5d ⁵ (⁴ G)6s	⁵ G 2	*		L153
Ca III	5 321.288	5 321.287	90	1.56e+08	B	341 601.46	- 360 388.68	3s ² 3p ⁵ (² P° _{3/2})5p	2 [³ /2] 2	3s ² 3p ⁵ (² P° _{3/2})5d	2 [⁵ /2]° 3	u33 L1405
Gd I	5 321.50		130									L3475
Xe III	5 321.57	5 321.38+	1bl			181 684.94	- 200 471.83	5s ² 5p ³ (² D°)4f	³ H 4	5s ² 5p ³ (² D°)6d	³ G° 5	L7270
Ni IV	5 321.60			1.0e-02	E	24 651.4	- 43 437.5	3p ⁶ 3d ⁷	² P 1/2	3p ⁶ 3d ⁷	² F 5/2	E2 T4605
Co II	5 321.7033		m(Co I)	2.4e+07	C+	91 408.494	- 110 194.244	3d ⁷ (⁴ F)4d	e ³ D 3	3d ⁷ (⁴ F _{9/2})4f	2 [³ /2]° 2	T6999 L9429
Gd I	5 321.78		280									L3475
Fe I	5 321.8342	5 321.8351	347			29 313.008	- 48 098.293	3d ⁶ 4s ²	a ¹ I 6	3d ⁶ (³ H)4s4p(³ P°)	¹ I° 6	L11631
Sr III	5 321.909	5 321.933	12			290 831.39	- 309 616.33	4p ⁵ (² P° _{1/2})4f	2 [⁷ /2] 3	4p ⁵ (² P° _{1/2})6d	2 [⁵ /2]° 2	L1771
Kr I	5 322.02	5 322.01+	2			92 294.4012	- 111 079.06	4s ² 4p ⁵ (² P° _{3/2})5p	2 [⁵ /2] 3	4s ² 4p ⁵ (² P° _{3/2})9d	2 [⁵ /2]° 3	L7408
Fe I	5 322.0404	5 322.0405	830	5.29e+04	C	18 378.186	- 37 162.746	3d ⁶ 4s ²	a ³ P ₂ 2	3d ⁷ (⁴ F)4p	y ³ F° 3	T5720 L11631
S II	5 322.205	5 322.216	7			140 708.89	- 159 492.83	3s ² 3p ² (¹ D)4p	² D° 5/2	3s ² 3p ² (³ P)4d	² D 5/2	L5883
Fe II	5 322.2361	5 322.2366	400	1.67e+07	C+	84 326.967	- 103 110.835	3d ⁶ (⁵ D)4d	⁶ P 5/2	3d ⁶ (⁵ D ₄)4f	2 [¹]° 3/2	T6892c83 L18349c139
Rb I	5 322.3800	5 322.375+	3			12 578.950	- 31 362.331	4p ⁶ 5p	² P° 1/2	4p ⁶ 10s	² S 1/2	L7459
O II	5 322.525	5 322.502	2			248 515.30	- 267 298.23	2s ² 2p ² (³ P)4p	² P° 3/2	2s ² 2p ² (³ P)6s	² P 3/2	L10621
Fe III	5 322.74		10									L1171
Pr II	5 322.76		430									L3475
Kr II	5 322.77	5 322.74+	60hl			139 101.568	- 157 883.65	4s ² 4p ⁴ (³ P)5p	² P° 1/2	4s ² 4p ⁴ (³ P)6s	⁴ P 3/2	L7386
Xe III	5 322.80	5 322.88+	1			184 594.45	- 203 376.04	5s ² 5p ³ (² P°)6p	³ D 3	5s ² 5p ³ (² D°)6d	¹ D° 2	L10579
I II	5 322.80	5 322.81	400			84 222.19	- 103 004.04	5s5p ⁵	³ P° 1	5s ² 5p ³ (⁴ S°)6p	³ P 0	L7360
Tm II	5 322.99		16									L3475

Query time: 0.9 sec

If you did not find the data you need, please [inform the ASD Team](#).



THE ATOMIC LINE LIST V2.05B1G

<http://www.pa.uky.edu/~peter/newpage/>

Welcome to the atomic line list !

This is a beta version of the next release of the Atomic Line List. It has not been fully tested and is likely to change without prior notice. It is being offered for testing purposes only. If you notice any problems with the content or the interface, please report these to the maintainer at the email listed at the bottom of this page.

This is a compilation of approximately 1.55 million allowed, intercombination and forbidden atomic transitions with wavelengths in the range from 0.6 Å to 1000 μm. Its primary intention is to allow the identification of observed atomic absorption or emission features. The wavelengths in this list are all calculated from the difference between the energy of the upper and lower level of the transition (except for hydrogenic lines, which are a weighted average of all the fine structure components). Only a very limited attempt has been made to include observed wavelengths.

When attempting to identify an observed line, usually many possible candidates can be found in this list. In order to facilitate narrowing down the number of possible identifications a selection tool is presented which allows imposing, apart from the wavelength, several additional criteria.

The following documentation is available:

- [Instructions](#) for querying the line list.
- [Documentation](#) on how this line list was compiled.
- [Contents](#) of this line list.
- [Copyright Notice/Disclaimer](#).

Please note that publication of the entire line list, or any large part of it, is only allowed with permission of the author.

Please acknowledge use of the Atomic Line List (including the URL) in each paper that contains data from this list.

The author kindly thanks the following people (in alphabetical order) who contributed to this list by providing data and/or helpful insights:

K.M. Aggarwal, M.A. Bautista, C.F. Fischer, R. Kisielius, S.N. Nahar, M.J. Seaton, T. Sochi, D.A. Verner.

Constructing this web page would be impossible without the continued efforts of many people generating the energy level and transition probability data, and making them publicly available. Please acknowledge this effort by citing the original source(s) of the data you include in your paper!

Recent Developments

The atomic line list has undergone extensive development in the past few years. Much of the software generating the line list, as well as the program doing the line selection for the web page have been replaced with 11,000 lines of new C++ code. All this work was necessary to restructure the internal data files and facilitate future upgrades of the line list. The primary goal will be to make the list complete for all elements, as far as data are available. This release starts this process by making the list complete for all 4th row elements. Future releases will start adding 5th, 6th, and 7th row elements. The second goal is to add more transition probability data from additional sources. Finally, an effort will be made to include observed wavelengths, especially for forbidden transitions. These are the most important user-visible changes that are implemented in this version:

- NEW** The request form has been improved. An option for specifying the radial velocity of the emitting source has been added, thus making Doppler-shift corrections by hand unnecessary. Multiplet searches can now be done by simply clicking on the term field in the output. The maximum number of lines in the output has been increased to 5000. Multiple wavelength ranges can now be supplied at once. Plain and LaTeX mode now produce truly HTML-free output when saved to disk.
- NEW** The search tool has been improved. The output will now always be correctly sorted, the search criteria are repeated in the output for later reference, and a few minor bugs have been solved.
- NEW** Selection rules for intercombination, magnetic dipole (M1) and electric quadrupole (E2) transitions have been improved. Magnetic quadrupole (M2) and electric octupole (E3) transitions have been added to the list. This makes the list more accurate and complete.
- NEW** The theory for calculating level energies of hydrogenic ions has been fully updated following Section IV of Mohr, Taylor, & Newell, 2008, Rev. Mod. Phys. 80, 633. Furthermore, data for the following ions have been updated/amended: He I, Be II, Be III, C IV, Ca III, Mn VII, Fe V, Ni X. Data for the elements Gallium through Krypton have been added. Transition probability data have been added from the NIST ASD v3.0 database and the MCHF/MCDHF collection (C.F. Fischer et al.).

Selection Criteria

Selection Criteria

All fields in the request form have default values and may be left unspecified

Wavelength range:

(e.g. 6500-6600, or 6545+/-1, the "-" or "+/-" symbols are optional)
(multiple queries, each on a separate line, are allowed)

Wavelength Unit: Type:

Radial velocity: vrad (in km/s) cosmological redshift z

A positive value means that the observed wavelength typed above is redshifted w.r.t. the laboratory wavelengths in the output.

Min. relative wavl. accuracy:

Upper limit in percent.

Element/spectrum:

h..fe

(e.g. C II, or C II-IV, or C, or C-O; query is not case sensitive; multiple lines of input are allowed)

Minimum abundance: Depl. factor:

Logarithmic number density, relative to log(H) = 12.

Lower level energy range: Unit:

Upper level energy range:

Maximum for principal quantum number n:

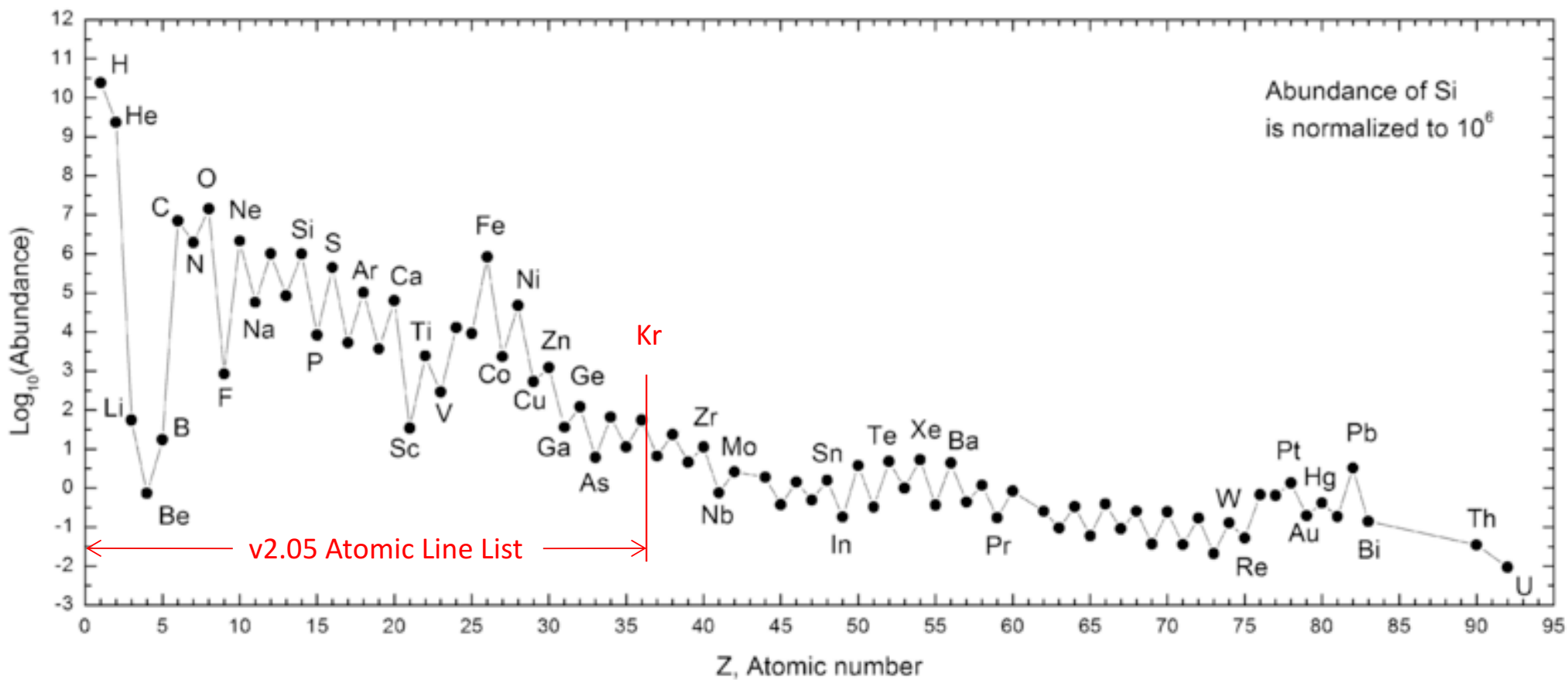
Transition types: All Types Nebular Select: E1 IC M1 E2 M2 E3

Transitions from auto-ionizing levels: Suppress Show

Customize Output

Output format (Check each item you want included in the output):

- Wavelength accuracy
- Spectrum
- Transition type
- Configuration
- Term
- Angular momentum: as J as g combine with term
- Transition probability: as A_{ki} as g_kA_{ki} as f_{jk} as S as log(gf)
- Level energies



Selection Criteria

All fields in the request form have default values and may be left unspecified

Wavelength range:

(e.g. 6500-6600, or 6545+/-1, the "-" or "+/-" symbols are optional)
(multiple queries, each on a separate line, are allowed)

Wavelength Unit: Type:

Radial velocity: vrad (in km/s) cosmological redshift z

A positive value means that the observed wavelength typed above is redshifted w.r.t. the laboratory wavelengths in the output.

Min. relative wavl. accuracy:

Upper limit in percent.

Element/spectrum:

h..fe

(e.g. C II, or C II-IV, or C, or C-O; query is not case sensitive;
multiple lines of input are allowed)

Minimum abundance: Depl. factor:

Logarithmic number density, relative to log(H) = 12.

Lower level energy range: Unit:

Upper level energy range:

Maximum for principal quantum number n:

Transition types: All Types Nebular Select: E1 IC M1 E2 M2 E3

Transitions from auto-ionizing levels: Suppress Show

Customize Output

Output format (Check each item you want included in the output):

- Wavelength accuracy
- Spectrum
- Transition type
- Configuration
- Term
- Angular momentum: as J as g combine with term
- Transition probability: as A_{ki} as $g_k A_{ki}$ as f_{jk} as S as log(gf)
- Level energies

Wavelength range: 5322 +/- 2 Unit: Angstrom Type: Air

Radial velocity: 0 km/s

Wavelength accuracy upper limit: 5%

Element/Spectrum: H -Zn I-IV

Minimum line strength: no restrictions

Include lines without atomic data: true

Minimum abundance: no minimum

Lower level energy range: no restrictions Unit: eV

Upper level energy range: no restrictions

Maximum for principal quantum number n: no restrictions

Transition types included: all

Transitions from auto-ionizing levels: included

-LAB-WAVL-ANG-AIR-[SPECTRUM][TT]-----TERM-----[J_i-J_k]-[A_ki]-[f_ik]-[TPF]-[LEVEL-ENERGY-EV]-[REF]-

5270.	Be II	E1	2D-2Do	5/2 - 5/2	133.100000 - 135.448000	050
5270.	Be II	E1	2D-2Do	5/2 - 3/2	133.100000 - 135.448000	050
5270.	Be II	E1	2D-2Do	3/2 - 5/2	133.100000 - 135.448000	050
5270.	Be II	E1	2D-2Do	3/2 - 3/2	133.100000 - 135.448000	050
5319.7	Zn III	E1	5Go-3/2[7/2]	3 - 4	30.499000 - 32.829020	ASD
5319.8	Cl I]	E1	4So-2P	3/2 - 1/2	11.854420 - 14.184400	ASD
5319.8	Cl I]	E1	4So-2P	3/2 - 3/2	11.854420 - 14.184400	ASD
5319.8	Cl I]	E1	4So-2D	3/2 - 3/2	11.854420 - 14.184400	ASD
5319.8	Cl I]	E1	4So-2D	3/2 - 5/2	11.854420 - 14.184400	ASD
5320.00	O II]	E1	2Do-4P	3/2 - 3/2	30.749346 - 33.079230	ASD
5320.0373	Fe I]	E1	b3D-v5Po	3 - 2	3.641640 - 5.971505	061
5320.041	[V II]	E2	a3P-c3F	1 - 3	1.427648 - 3.757512	ASD
5320.1	Zn III	E1	5/2[3/2]-3Fo	2 - 2	32.474140 - 34.804000	ASD
5320.123	Ni II]	E1	4P-2Po	1/2 - 1/2	14.414626 - 16.744454	ASD
5320.134	Mn II	E1	x3Go-e3G	5 - 4	10.403808 - 12.733631	ASD
5320.183	V I]	E1	z6Do-e4F	5/2 - 5/2	2.256274 - 4.586076	ASD
5320.202	N II	E1	5Po-5P	2 - 1	4.20E+07 1.07E-01 3 27.974052 - 30.303845	03
5320.231	Cl II]	E1	3Po-3F	1 - 2	18.029934 - 20.359715	ASD
5320.324	V III]	E1	e4D-y4Go	3/2 - 5/2	17.547722 - 19.877462	ASD
5320.3502	Fe II	E1	y4Ho-e4G	7/2 - 7/2	8.266315 - 10.596043	ASD
5320.367	Cu I	E1	2Po-2D	1/2 - 3/2	7.645595 - 9.975327	ASD
5320.367	Cu I	E1	2Po-2D	3/2 - 3/2	7.645595 - 9.975327	ASD
5320.364	Cr II]	E1	e6F-r4Go	11/2 - 9/2	10.910777 - 13.240499	ASD
5320.406	Cr II]	E1	d2F-4Fo	5/2 - 5/2	6.284463 - 8.614167	ASD
5320.429	Ca III	E1	3Fo-1/2[1/2]	2 - 1	40.352844 - 42.682538	087
5320.430	Fe II	E1	4F-v4Fo	7/2 - 7/2	9.111872 - 11.441566	ASD
5320.435	Cr I]	E1	b3P-y3Fo	1 - 2	3.369422 - 5.699113	ASD
5320.44	O II	E1	F[3]o-2D	5/2 - 3/2	31.755547 - 34.085240	ASD
5320.440	F II	E1	3P-3Do	2 - 3	1.58E+07 9.37E-02 3 30.584679 - 32.914368	01
5320.4453	Ni I	E1	5Fo-5/2[1/2]	2 - 1	3.739750 - 6.069437	ASD
5320.466	Ne III]	E1	5Go-3G	4 - 3	58.520838 - 60.850516	008
5320.466	Ne III]	E1	5Go-3G	2 - 3	58.520838 - 60.850516	008
5320.466	Ne III]	E1	5Go-3G	3 - 3	58.520838 - 60.850516	008
5320.467	Fe II	E1	f4D-2[2]o	5/2 - 5/2	10.522645 - 12.852322	ASD
5320.49	Sc I]	E1	4P-2Po	5/2 - 3/2	4.534445 - 6.864110	ASD
5320.55	Ar III]	E1	1F-5Do	3 - 2	28.174670 - 30.504316	069,068
5320.5526	Ne II	E1	3/2[1/2]-3/2[5/2]o	1 - 2	5.28E+03 3.73E-05 6 18.381621 - 20.711261	023

Atomic Line List version: 2.05b18 Constructed: 2014-05-13 13:23 GMT

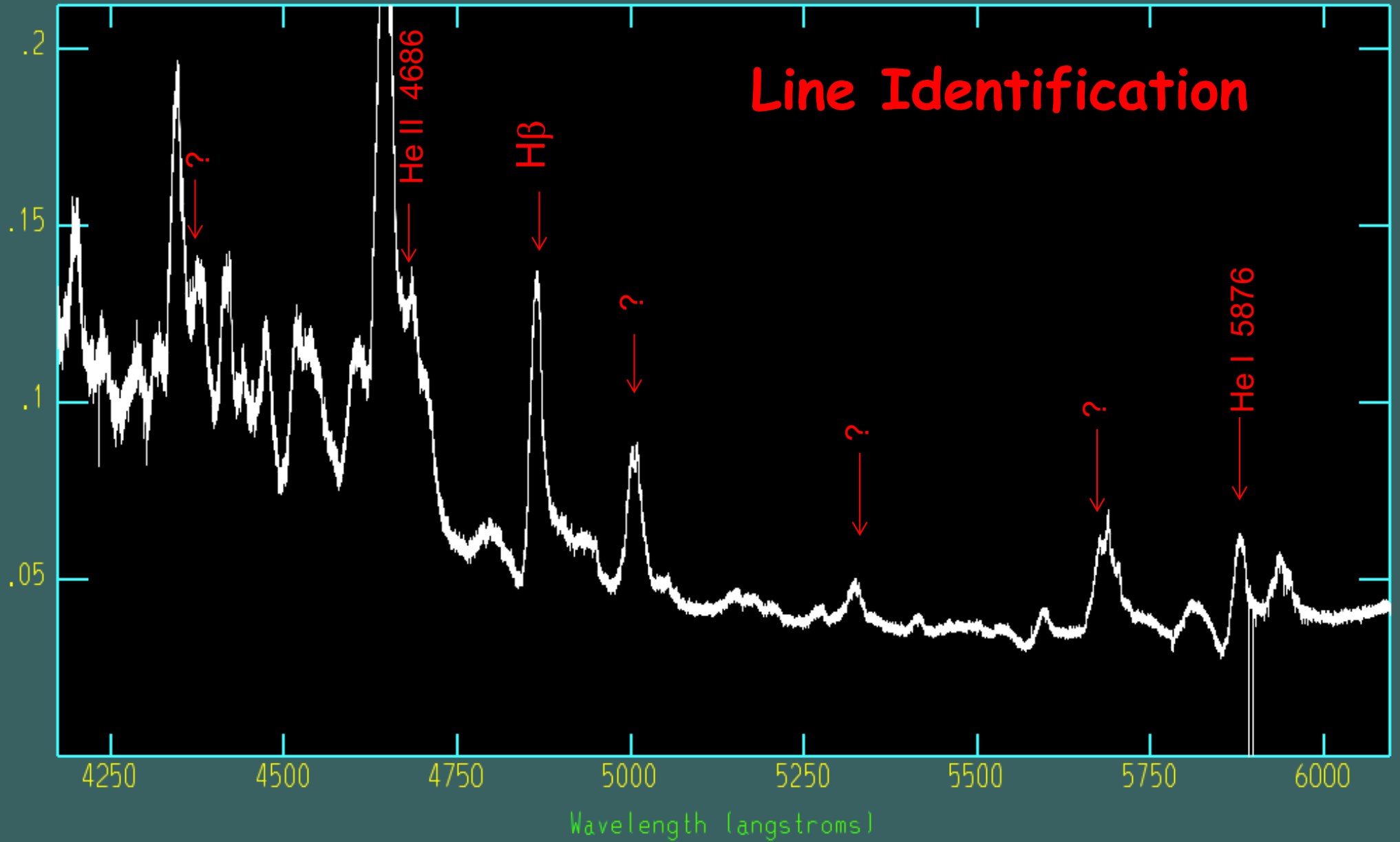
Wavelength range: 0 - inf Unit: Angstrom Type: Air

Radial velocity: 0 km/s

Element/Spectrum: Fe II

-LAB-WAVL-ANG-AIR-[SPC]-[TT]-TERM-[J_i-J_k]-[A_ki]-[f_ik]-[TPF]-[LEVEL-ENERGY-EV]-[REF]-						
5252.506	Fe II	E1	4F-v4Fo	9/2 - 9/2	9.099664 - 11.459484	ASD
5272.049	Fe II	E1	4F-v4Fo	5/2 - 3/2	9.099935 - 11.451007	ASD
5279.822	Fe II	E1	4F-v4Fo	7/2 - 9/2	9.111872 - 11.459484	ASD
5280.046	Fe II	E1	4F-v4Fo	5/2 - 5/2	9.099935 - 11.447446	ASD
5292.694	Fe II	E1	4F-v4Fo	9/2 - 7/2	9.099664 - 11.441566	ASD
5293.306	Fe II	E1	4F-v4Fo	5/2 - 7/2	9.099935 - 11.441566	ASD
5307.034	Fe II	E1	4F-v4Fo	7/2 - 5/2	9.111872 - 11.447446	ASD
5320.430	Fe II	E1	4F-v4Fo	7/2 - 7/2	9.111872 - 11.441566	ASD
5340.033	Fe II	E1	4F-v4Fo	3/2 - 3/2	9.129866 - 11.451007	ASD
5348.237	Fe II	E1	4F-v4Fo	3/2 - 5/2	9.129866 - 11.447446	ASD

Nova T Pyxidis (14 April 2011)



Summary Procedure for Line Identification

- Measure line wavelength (from flux median & profile fit)
- Correct λ_{obs} for radial velocity shift obtained from other known lines, e.g., H β , or forbidden lines (best, because optically thin)
- Note types of lines present in spectrum, e.g., forbidden lines, heavy element lines, fluorescence excited, coronal, etc.
- Use v2.05 Line List and/or NIST line tables to list all lines within measured uncertainty of the observed wavelength, preferably with transition probabilities, A_{21} , and multiplet members listed
- Consider as potential IDs all lines of 'reasonable' abundance, level of ionization, excitation, & A_{21}
- For each candidate ID check for
 1. Other multiplet members expected to be observed
 2. Presence of lines originating from same levels of candidate line
 3. Other lines from the same (or similar) ion and excitation level, making use of Bashkin & Stoner.
- If all above criteria are met, candidate transition is reasonable ID
- The final ID assignment for any line should be consistent with the assemblage of all known lines that are present

<http://www.pa.uky.edu/~peter/newpage/> <http://www.nist.gov/pml/data/asd.cfm>