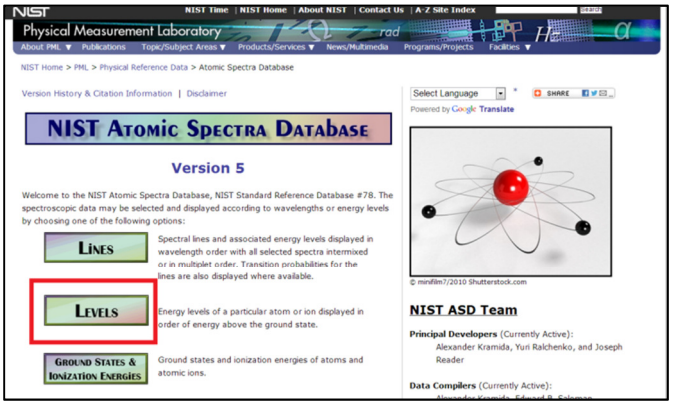
NIST2Stout

1. Setting up files:

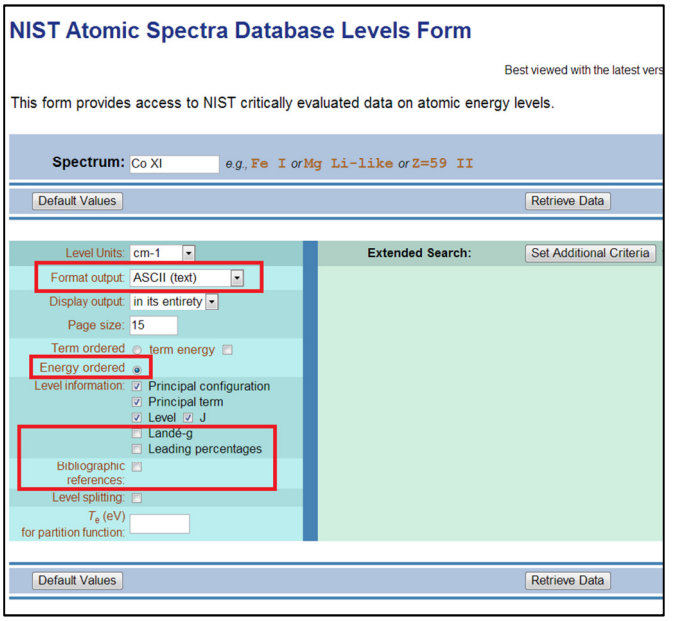
1.1. NIST Levels File:

Go to the [NIST Atomic Spectral Database](#).

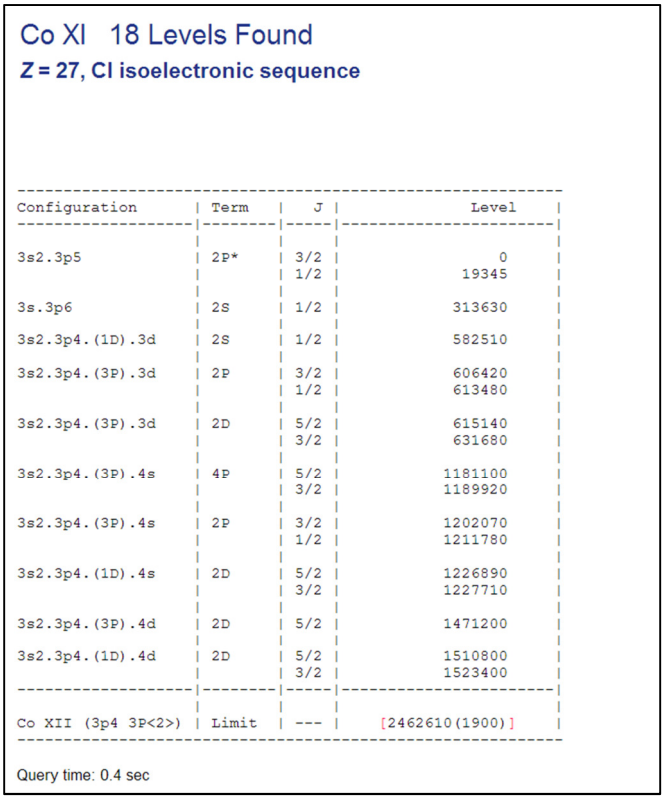
Click “Levels”



Input the spectrum you are looking for and set the parameters as shown to the right.



The results columns should look like this:



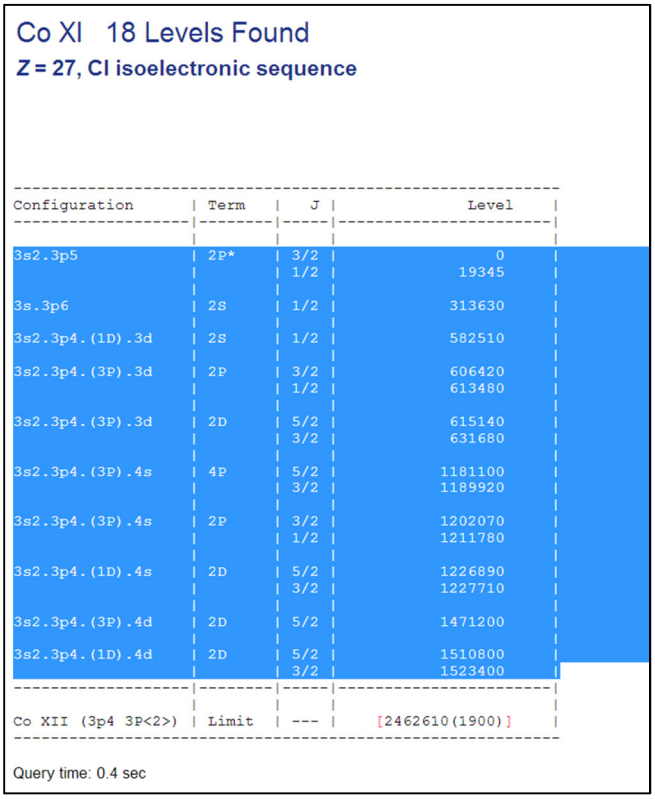
Co XI 18 Levels Found

Z = 27, Cl isoelectronic sequence

Configuration	Term	J	Level
3s2.3p5	2P*	3/2	0
		1/2	19345
3s.3p6	2S	1/2	313630
3s2.3p4.(1D).3d	2S	1/2	582510
3s2.3p4.(3P).3d	2P	3/2	606420
		1/2	613480
3s2.3p4.(3P).3d	2D	5/2	615140
		3/2	631680
3s2.3p4.(3P).4s	4P	5/2	1181100
		3/2	1189920
3s2.3p4.(3P).4s	2P	3/2	1202070
		1/2	1211780
3s2.3p4.(1D).4s	2D	5/2	1226890
		3/2	1227710
3s2.3p4.(3P).4d	2D	5/2	1471200
3s2.3p4.(1D).4d	2D	5/2	1510800
		3/2	1523400
Co XII (3p4 3P<2>)	Limit	---	[2462610(1900)]

Query time: 0.4 sec

Higlight the levels you want to include and copy them to the clipboard.



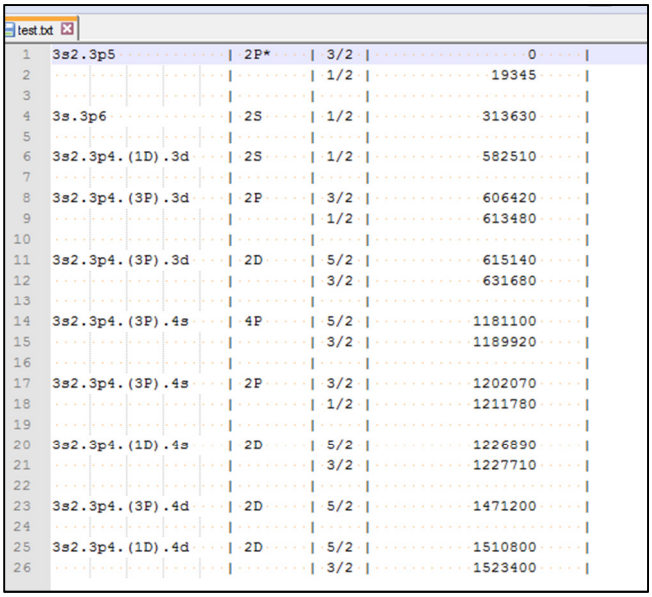
Co XI 18 Levels Found

Z = 27, Cl isoelectronic sequence

Configuration	Term	J	Level
3s2.3p5	2P*	3/2	0
		1/2	19345
3s.3p6	2S	1/2	313630
3s2.3p4.(1D).3d	2S	1/2	582510
3s2.3p4.(3P).3d	2P	3/2	606420
		1/2	613480
3s2.3p4.(3P).3d	2D	5/2	615140
		3/2	631680
3s2.3p4.(3P).4s	4P	5/2	1181100
		3/2	1189920
3s2.3p4.(3P).4s	2P	3/2	1202070
		1/2	1211780
3s2.3p4.(1D).4s	2D	5/2	1226890
		3/2	1227710
3s2.3p4.(3P).4d	2D	5/2	1471200
3s2.3p4.(1D).4d	2D	5/2	1510800
		3/2	1523400
Co XII (3p4 3P<2>)	Limit	---	[2462610(1900)]

Query time: 0.4 sec

Paste the contents into an empty text file. The name of the file should be X.NIST.txt, where X is whatever you want the base output name to be.

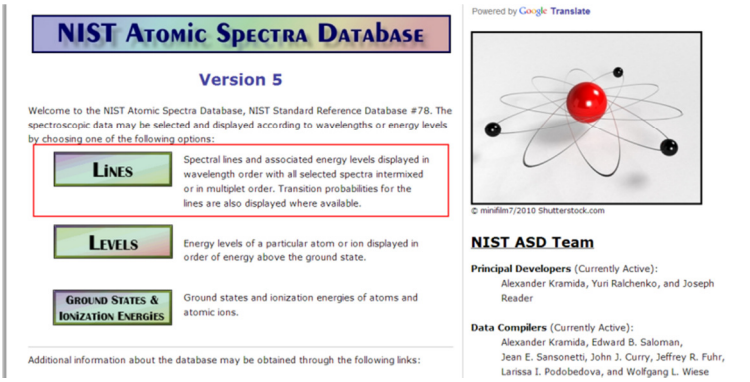


test.txt

1	3s2.3p5	2P*	3/2	0
2			1/2	19345
3				
4	3s.3p6	2S	1/2	313630
5				
6	3s2.3p4.(1D).3d	2S	1/2	582510
7				
8	3s2.3p4.(3P).3d	2P	3/2	606420
9			1/2	613480
10				
11	3s2.3p4.(3P).3d	2D	5/2	615140
12			3/2	631680
13				
14	3s2.3p4.(3P).4s	4P	5/2	1181100
15			3/2	1189920
16				
17	3s2.3p4.(3P).4s	2P	3/2	1202070
18			1/2	1211780
19				
20	3s2.3p4.(1D).4s	2D	5/2	1226890
21			3/2	1227710
22				
23	3s2.3p4.(3P).4d	2D	5/2	1471200
24				
25	3s2.3p4.(1D).4d	2D	5/2	1510800
26			3/2	1523400

1.2 NIST Lines File:

Go to the Lines section of the NIST Atomic Spectral Database



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:

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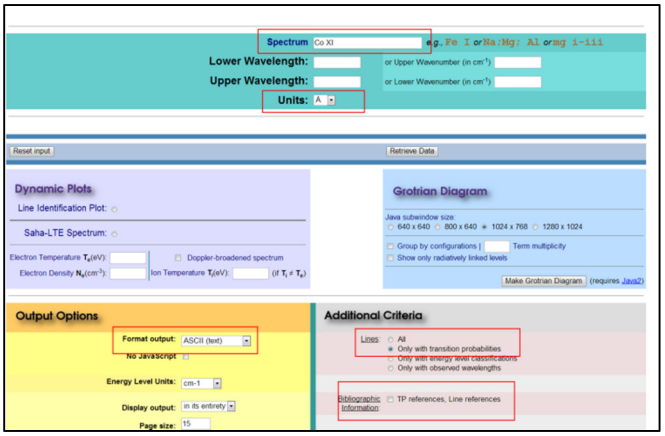
NIST ASD Team

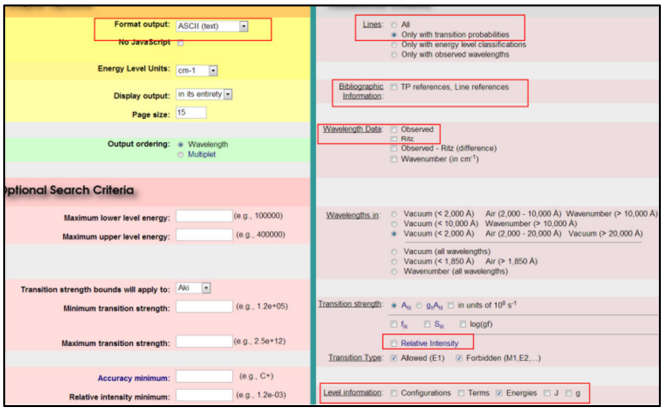
Principal Developers (Currently Active):
Alexander Kramida, Yuri Ralchenko, and Joseph Reader

Data Compilers (Currently Active):
Alexander Kramida, Edward B. Saloman, Jean E. Sansonetti, John J. Curry, Jeffrey R. Fuhr, Larissa I. Podobedova, and Wolfgang L. Wiese

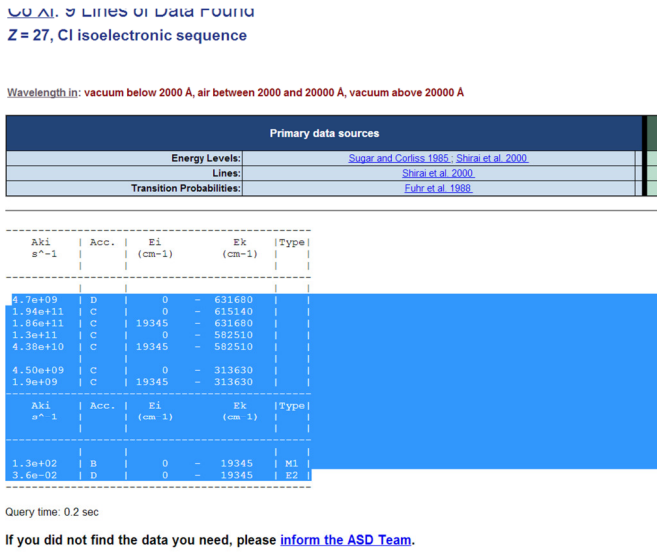
Enter the spectrum to match the levels file and edit the following parameters



Continue to edit parameters on the Line form



Select the lines and copy them to the clipboard.



Paste the line data to a blank text file. Name the text file X.tp.NIST.txt where X is the same base name used for the level file.

2. Running the script:

The program has 2 parts, nist2stout.py and n2sWrapper.py. The program can be run for one species with nist2stout.py or in a batch mode with n2sWrapper.py.

2.1 Running for a Single Species:

Running the program for a single species has a simple syntax. From the command line enter nist2stout.py <name of level file> <name of line file>. The code will run and you will end up with X.nrg.txt and X.tp.txt.

2.2 Running as a Batch:

Consider this directory structure:

<Base>

    <Ar>

        ar_2.nist.txt

        ar_2.tp.nist.txt

    <Be>

        be_3.nist.txt

        be_3.tp.nist.txt

        be_4.nist.txt

        bet_4.tp.nist.txt

You can automatically run NIST2Stout on all of these species by copying nist2stout.py and n2sWrapper.py to the Base directory. Then execute n2sWrapper.py with no other parameters. The code will go through all subdirectories looking for matching pairs of level files (X.nist.txt) and line files (X.tp.nist.txt). For each pair it finds, it will execute nist2stout.py as in

described in Section 2.1. The Stout formatted files should end up in the same directories as the NIST source files for that species.

3. Gotchas and Troubleshooting:

- Make sure that all of the levels necessary to reference the transitions in the lines file (X.tp.nist.txt) are included in the levels file (X.nist.txt).

- Make sure that you have all of the necessary columns (and no others) included in the levels and lines files.