

NIST2Stout

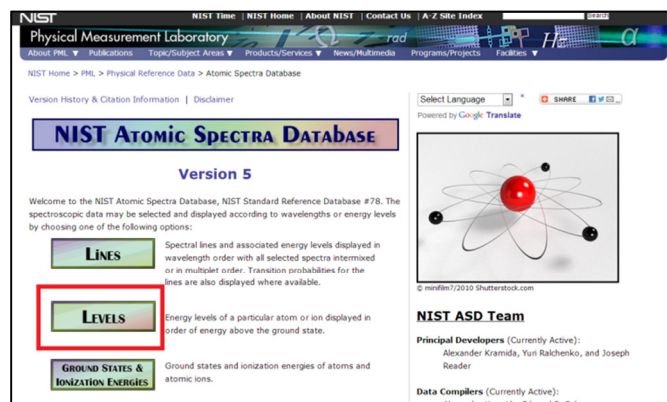
1. Setting up files:

1.1. NIST Levels File:

Go to the [NIST Atomic Spectral Database](https://physics.nist.gov/ASD/).

Click “Levels”

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



NIST Atomic Spectra Database Levels Form

Best viewed with the latest version

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

Spectrum: Co XI e.g., Fe I or Mg Li-like or Z=59 II

Level Units:

Format output:

Display output:

Page size:

Term ordered: ☐ term energy ☐

Energy ordered: ☒

Level information: ☒ Principal configuration ☒ Principal term ☒ Level ☒ J ☐ Landé-g ☐ Leading percentages

Bibliographic references: ☐

Level splitting: ☐

T_e (eV)

for partition function:

The results columns should look like this:

Co XI 18 Levels Found
Z = 27, CI 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

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

Co XI 18 Levels Found
Z = 27, CI 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.

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

The screenshot shows the NIST Atomic Spectra Database interface. The 'Spectrum' section at the top has a dropdown for 'Spectrum' (set to 'Co XI'), and input fields for 'Lower Wavelength', 'Upper Wavelength', and 'Units' (set to 'Å'). Below this are sections for 'Dynamic Plots' (with options for 'Line Identification Plot' and 'Saha-LTE Spectrum'), 'Grotian Diagram' (with options for 'Java subwindow size', 'Group by configurations', and 'Show only relatively linked levels'), 'Output Options' (with options for 'Format output', 'Energy Level Units', 'Display output', and 'Page size'), and 'Additional Criteria' (with options for 'Lines', 'Bibliographic information', and 'Wavelength data').

Continue to edit parameters on the Line form

The screenshot shows the 'Line form' section of the NIST Atomic Spectra Database interface. It includes input fields for 'Format output' (set to 'ASCII (text)'), 'Energy Level Units' (set to 'cm-1'), 'Display output' (set to 'in its entirety'), 'Page size' (set to '15'), 'Output ordering' (set to 'Wavelength'), and 'Optional Search Criteria' (with fields for 'Maximum lower level energy', 'Maximum upper level energy', 'Transition strength bounds will apply to', 'Minimum transition strength', 'Maximum transition strength', 'Accuracy minimum', and 'Relative intensity minimum'). The 'Additional Criteria' section on the right includes options for 'Lines', 'Bibliographic information', 'Wavelength data', 'Wavelengths is', 'Transition strength', 'Transition Type', and 'Level information'.

Select the lines and copy them to the clipboard.

CO XI. 9 LINES OF DATA FOUND
Z = 27, CI isoelectronic sequence

Wavelength in: vacuum below 2000 Å, air between 2000 and 20000 Å, vacuum above 20000 Å

Primary data sources					
Energy Levels:		Sugar and Corfas 1985; Shirai et al. 2000.			
Lines:		Shirai et al. 2000.			
Transition Probabilities:		Fuhr et al. 1988.			

Ak1 s ⁿ⁻¹	Acc.	E1 (cm ⁻¹)	E2 (cm ⁻¹)	Type
4.7e+09	D	0	631680	
1.94e+11	C	0	6315140	
1.86e+11	C	19345	631680	
1.3e+11	C	0	582510	
4.38e+10	C	19345	582510	
4.50e+09	C	0	313630	
1.9e+09	C	19345	313630	

Ak1 s ⁿ⁻¹	Acc.	E1 (cm ⁻¹)	E2 (cm ⁻¹)	Type
1.3e+02	B	0	19345	M1
3.6e-02	D	0	19345	E2

Query time: 0.2 sec

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

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.