Tutorial number 1 : Using GASP

1. Download and install gasp (Graphical AutoStructure Package)

    weblink: http://connorb.freeshell.org/gasp/

    download the gasp.tar file into your home directory

    You will need java and fortran compiler.

2. Learn how to use an atomic structure package called 'GASP' to calculate energy levels and A-values.

    First of all log into adas.physics.auburn.edu, then from the shell prompt

    ssh -X username@adas.physics.auburn.edu

Once you are logged in, do the following:

Install and run the atomic structure package called GASP

    (1) mkdir gasp
    (2) cd gasp
    (3) cp ../gasp.tar .
    (4) tar -xvf gasp.tar
    (5) make
    (6) java -jar gaspstart.jar &

Hopefully at this point, the GASP gui should appear on your desktop.

[Overview of the package : 5 mins]

Let us try He-like Ne, as our first test case.

Nuclear charge

Number of electrons

LS or LSJ resolution

Choose up to the 3d to be valence subshells.

$1s^2$ configuration with one electron promoted

Note that you should type the following into the Advanced options tab

under the SALGEB append box type : RAD='ALL'

When the code runs it will give you a list of energies. It also writes a file called adf04ic. In the terminal window type

nedit adf04ic &

You will then have a file that you can use to compare the energies and A-values with NIST.

Tutorial number 2 :
Optimizing atomic structure using GASP

The aim in this tutorial is to allow you explore some of the issues required in calculating accurate energy levels and A-values. We are assuming that our wavefunctions are constructed from a set of basis functions. Until now we have considered the basis functions from single configurations only. e.g. the $1s^2\,2s^2\,{}^1S$ is considered to be purely made up from basis functions from the $1s^2\,2s^2$ configuration. In reality states can be made up of basis functions from more than a single configurations. i.e. the term that we call $1s^2\,2s^2\,{}^1S$ is mostly $1s^2\,2s^2$ but is also partly $1s^2\,2p^2$.
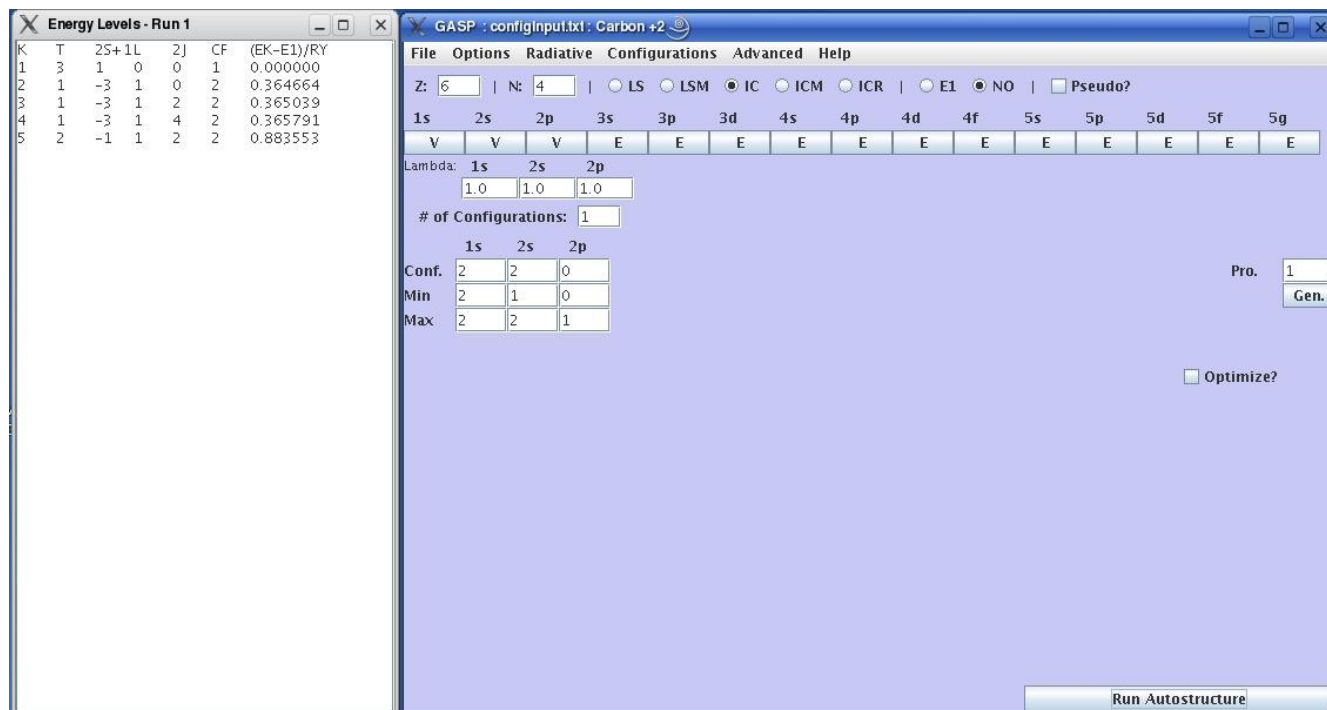
A more detailed explanation is given in the attachment from Cowan's atomic structure book. The main idea is that the more configurations you include in your atomic structure calculation, the more accurate your energy levels and wavefunctions (hence A-values) will be. So the question is what configurations should be included. Here is a summary of the rules that Cowan gives:

(1) Configurations within the same complex (i.e. n-shell) will dominate the configuration interaction.
(2) Configurations of the same parity will mix.
(3) Configurations with either one or two electron differences will mix.
(4) Configurations that contain the same LS term will mix.

Consider the case of Be-like systems as a worked example. Say we wish to calculate energies and A-values for Be-like carbon (C^{2+}). We wish energies for the $1s^2\,2s^2$ and $1s^2\,2s2p$ configurations. The NIST energies are:

So our first attempt using GASP would be to calculate the atomic structure for the $1s^2\ 2s^2$ and $1s^2\ 2s2p$ configurations. This would look like:

Energy Levels - Run 1

K	T	2S+1L	2J	CF	(EK–E1)/RY
1	3	1	0	0	1	0.000000
2	1	-3	1	0	2	0.364664
3	1	-3	1	2	2	0.365039
4	1	-3	1	4	2	0.365791
5	2	-1	1	2	2	0.883553

GASP : configinput.txt : Carbon +2

File   Options   Radiative   Configurations   Advanced   Help

Z: 6 | N: 4 | ○ LS ○ LSM ◉ IC ○ ICM ○ ICR | ○ E1 ◉ NO | ☐ Pseudo?

1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f	5g
V	V	V	E	E	E	E	E	E	E	E	E	E	E	E

Lambda:
1s	2s	2p
1.0	1.0	1.0

# of Configurations: 1

	1s	2s	2p		
Conf.	2	2	0	Pro.	1
Min	2	1	0		Gen.
Max	2	2	1		

☐ Optimize?

Run Autostructure

Notice that the energies are terrible!

Consider the configurations that would mix strongly with the $1s^2\ 2s^2$ configuration. The strongest contribution is for n-shell jumps within the same complex (i.e. n=2) that have the same parity (even) and that contain the same term as the $1s^2\ 2s^2$ configuration. The $1s^2\ 2p^2$ configuration is within the same complex, has even parity and has allowed terms **^{1}S**, ^{1}D and ^{3}P. So it should mix with the $1s^2\ 2s^2$ configuration. So if we now do a structure calculations for

$1s^2\ 2s^2$
$1s^2\ 2s\ 2p$
$1s^2\ 2p^2$

We should get an improvement in our structure. We would include this in our GASP calculation by:

Notice that the energies are much improved.

TO DO:

Calculate energy levels for Ar^{5+} (Al-like argon), which has a ground configuration of $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p$. Calculate energies using only this configuration and the $1s^2\ 2s^2\ 2p^6\ 3s\ 3p^2$ configuration. Then try to improve your atomic structure by including configurations that should mix strongly with the ground configuration.