



THE OHIO STATE UNIVERSITY



Workshop on:

**”ATOMIC STRUCTURE AND TRANSITIONS:  
COMPUTATION USING SUPERSTRUCTURE PRO-  
GRAM”**

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- **Textbook: ”Atomic Astrophysics and Spectroscopy”  
A.K. Pradhan & S.N. Nahar (Cambridge U Press, 2011)**
- **Computation: Ohio Supercomputer Center (OSC)‘**

**• Notes from workshops given to universities**

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# SUPERSTRUCTURE (SS)

The program SUPERSTRUCTURE (SS) calculates number of quantities for atomic structure and atomic processes. The useful ones are the energies of atomic states and transition parameters, such as, oscillator strengths, line strengths, and radiative decay rates or Einstein's A-coefficients. There are a few references for the atomic structure program SUPERSTRUCTURE (SS). The main references are:

1. Eissner, W., Jones, M., Nussbaumer, H. *Comput. Phys. Commun.* 8, 270 (1974)
2. Eissner, W., Jones, M., Storey P., Nussbaumer, H. *Comput. Phys. Commun.* (draft 1994)
3. Nahar S.N., Eissner, W., Chen, G.X., Pradhan, A.K., *A&A* 408, 789 (2003) (transitions of types E2, M1, E3 and M2 by Werner Eissner)
4. Eissner W, in *The Effects of Relativity on Atoms, Molecules, and the Solid State* (Edited by S. Wilson et al., Plenum Press, New York), p.55 (1991)

## SUPERSTRUCTURE files:

- For your use, go to my website:

<http://www.astronomy.ohio-state.edu/~nahar/teaching.html#program>

- Download files to your laptop: "struct.f", ssinar17, ssout.bp.ar17, sspnl.ar17, runss, rss, and the document. You will upload these files to your workshop or w account (it starts with w followed by a number) that you received from the lecture class
- Check that you can login to you w-account. Follow as:
  1. Download "putty" from internet to your computer & click to open the login window - Or open a "terminal" window on your laptop
  2. Type: ssh w....@oakley.osc.edu → to login (Omit "ssh " if you are using putty) and hit return button
- Please note that after typing each command, you will hit the <return> key

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3. password: type the password given next to you w-id and hit the return key
4. You should be in your account for work. Type:  
mkdir sstutorial → to create your directory "sstutorial"
5. type: exit and hit return key → to logoff [Upload SS files to your w-account:](#)
6. On your laptop terminal, type: sftp w.....@oakley.osc.edu
  - Type password at prompt
7. Type: cd sstutorial → to go to directory "sstutorial"
8. Type: put struct.f → to upload the file to sstutorial directory
  - Keep on using put command to upload all SS-files
9. Type: quit → to get out of transfer mode

## Running SUPERSTRUCTURE:

10. Now login to your w-account in the same way explained above
11. Type: cd sstutorial → to go your directory "sstutorial"
12. type: ls (to see the files in the directory)
13. File "struct.f" → Program SUPERSTRUCTURE
14. File "runss" → script file to compile "struct.f" and create executable with name "structx" of the program:
  - Type: ./runss → to create "structx"
15. File "ssin.ar17" → an example input file for struct.f. This example is for He-lie Ar, Ar XVII
  - Type: cp ssin.ar17 ssin → to copy file "ssin.ar17" to "ssin"
16. File "rss" → contains the command to run structx for an atomic system
  - Type: "rss" → to run structx for the present case: Ar XVII
17. type: ps → to see the job status of structx & whether the run has finished
18. If the job is done, you will see in directory the two files "ssout" and fort.7

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- i) File "ssout" → output file containing energy levels, transitions, etc. This file will have the same contents as "ssout.bp.ar17"
- ii) "fort.7" → output file containing potential and wave functions of the atom. This will have the same content as in "zsspnl.ar17"

## Input file for SUPERSTRUCTURE:

- We look at the contents of file "ssin". SS reads all lines in defined format specified in program struct.f. So make sure all numbers are specified in the exact columns. You can use the example file to create your own input file.
- "ssin" contains a set of configurations encoded in numerical notation. The first few lines of ssin are:

```
-2-1 0 0  21 11512 11513 11514 11515 11516
          11517 11518 11519 1151A 22 23 24 25 26
          12513 12514 12515 12516 12517 12518 12519 1251A
          13514 13515 13516 13517 13518
```

- Ignore first two numbers "-2-1" on the first line
- The next two numbers "0 0" tell the program how many subshells starting from "1s" orbital are filled in all listed configurations. This example shows that there is no common filled subshell in the configuration list.
- Rest of the numbers are encoded configurations. Each number tells how many electrons (occupancy number) are in the specified orbitals.
  - i) The first number or configuration "21" states that there are two electrons in the first orbital which is "1s". So the spectroscopic configuration is:  $1s^2$
  - ii) The second number or configuration "11512" states that there is 1 electron in the first orbital (1s), then "5" is the separator between two orbitals, and then 1 electron in the 2nd orbital (2s). Hence the spectroscopic configuration is:  $1s2s$

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iii) The third configuration "11513" says that 1 electron in orbital (1s) and 1 electron in the 3rd orbital (2p). Again "5" is the separator between two orbital information.

The spectroscopic configuration is: 1s2p

- The orbitals are encoded in the following convention:

1	2	3	4	5	6	7	8	9	A	B	C	D	E	F	G	H	I	J	K	L
1s	2s	2p	3s	3p	3d	4s	4p	4d	4f	5s	5p	5d	5f	5g	6s	6p	6d	6f	6g	6h

- Please decode all the configurations just to verify them.
- These configurations are also specified in the beginning of the output file "ssout".
- At the end of configuration list, there is a line with numbers as:

```
0      0      -1Xfe21kshl
```

keep the line as it is

- The next line is:

```
18  00 1010  0  0 -1  0  0  0  0  7 -0  0  0 Y
```

Only the first 3 numbers of this line are changed as needed, but keep the rest numbers as they are.

1st number = 18 = Z (nuclear charge of the atom)

2nd number = 00 (optimization set, ignore it at this time)

3rd number = 1010 - the first 10 = total number of orbitals included in the configuration set and hence is equal to number of  $\lambda$  parameters) The next 10 = how many should be optimized). Keep these two numbers same for the time being

- Values of the 10  $\lambda$  parameters. (Try to keep them close to 1 except for the first 1s, 2s orbitals)

- The next lines are (leave them as they are):

```
0
```

```
0 0 0 0
```

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## Output files of SUPERSTRUCTURE:

We will first check the energy values of the atomic states from our run of SS. Open up the file "ssout" by typing

vi ssout

- SS prints out energies for LS terms in table with column heads:

Table "I T K\*CM ..." (line 242 of ssout)

and for fine structure levels in table with column heads

Table "K LV K\*CM 2\*S+1 L 2J CF (EK-E1)/RY " (line 1239 in ssout).

- We check fine structure levels for direct comparison with NIST
- Go down to the table of energies (line number 1239).

Some of the columns are: K=energy index

2\*S+1 = Spin multiplicity (e.g. for first energy in the table it is 1)

L = total orbital angular momentum (for the first energy it is 0, that, is L = S)

2J = 2 times the total angular momentum (for the first state 1S, J=0 and hence, 2J=0)

CF = configuration numbers of the configurations given in input file "ssin"

(EK-E1)/RY = Relative energy of the state in Rydberg (Ry) (for example, the ground state is at 0 Ry)

- For the run you had, the table energy states should read as 1S0, 3S1, 3P0 etc.
- First check how good the energies are in comparison to experimental values. The experimental values are available at the NIST website which is at

[http : //physics.nist.gov/PhysRefData/ASD/index.html](http://physics.nist.gov/PhysRefData/ASD/index.html)

This website is accessible to everyone. So go to this website.

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At the NIST website:

Click on box "LEVELS" -> this will open up the option page

2) At the "Spectrum" box, type in "Ar XVII", and at the "Level Units:" box, scroll down to choose "Rydberg" unit.

3) click on the "Retrieve Data"

- You will come to a page where it will say "NIST Atomic Spectra Database Levels Data" and little bit below it will say "Ar XVII 45 Levels Found"

- Below it is the table of experimental energies. See that for the second level, SS gives an energy of 3S0 as 228.364952 Ry and NIST table gives 228.15015 Ry. So the energy compares well. Check rest of the energies to see how good calculated energies in comparison to experimental energies.

LS state and J-level:

- An energy state (correctly a LS "state" or "term") can be written as  $(2S+1)L^{\pi}$

where  $2S+1$  = spin multiplicity

$L$  = Total orbital angular momentum,  $\pi$  = parity

- For a LS state, we do not specify the total angular momentum  $J$ . For a fine structure level, we do and write the level as

$(2S+1)L_J^{\pi}$

where  $J$  = J-value from angular momentum sum of  $L+S$ .  $L+S$  is a vector addition, that is, the values are from  $L+S, \dots, -L-S$  giving a total of  $2J+1$  values. Example: 3P state has  $S=1$  and  $L=1$ . So  $L+S$  gives  $J=0,1,2$ . These 3 levels 3P0, 3P1, 3P2 are called the fine structure components of 3P.

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- LS term energy can be calculated from its fine structure components using

$$E(\text{LS}) = \frac{\sum_{\text{J}}(2\text{J} + 1)E(\text{J})}{\sum_{\text{J}}(2\text{J} + 1)}$$

## Some comments on comparison:

- SS predicts complete set of energies from the given list of configurations. But observed energies may not be complete. NIST usually lists the identified energies. An energy level can be seen, but it needs to be identified spectroscopically.

- Experiment shows existence of energy state of 1s5s, 1s5p and 1s5d configurations, SS does not predict these because SS did not include these

- In NIST table, near the line with word "limit" means ionization energy (I). Ex, "limit-302.8628" means  $I = 302.8628$  Ry. Any level with lower energy is bound (electrons are still attached to the atomic species), and higher energy is either quasi-bound (short lived state) or continuum (electron is free).

- Now we will find out the LS states or terms resulted from these configurations.

- In "ssout" go to the LS energy table which has column heads (line number 242):

" I T K\*CM S L CF WEIGHTS (EI-E1)/RY .."

I = the running index for the LS term energies

T = is a number from a term table (ignore it)

K\*CM = energy in terms of cm-1 (ignore it)

S = the spin multiplicity,  $2S+1$

L = total orbital angular momentum

CF = configuration number according to the set in "ssin"

Weights = weight factor for mixing coefficients (ignore it)

(EI-E) = relative energy of the state in Rydberg unit

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- The first line of the table has the following numbers:

1 58 0. 1 0 1 0.000 0.000000

- So the first line of the energy table gives the first or the lowest energy, that is, 0.=ground state energy

$$2S+1 = 1$$

$$L = 0$$

$$CF = 1$$

- It means that the state is  $^1S$  and it has formed from the first configuration "1s2" we specified in "ssin".
- Note: if there is negative sign in front of  $(2S+1)$ , it means that the state is of odd parity.
- Please write in complete spectroscopic notation the first 10 energies in this table.

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## Transition parameters:

- An atomic electron can move to an upper level by absorbing a photon or to a lower level by giving out a photon
- The 3 transition parameters of interest are:
  - a) oscillator strength (f-value) (usually for moving up)
  - b) Einstein's A-value (or the radiative decay rate) for moving down,
  - c) line strength (expressed as S and is related to both A and f)
- SS output for transitions among LS states and fine structure levels:
  - The oscillator strengths (f-values), Einstein's A-value (or the radiative decay rates) for LS states are given in table "E1-DATA I P .." (line 315 in ssout.bp.ar17).
- E1 means electric dipole transition
  - The first column is the running index for the transition number
  - I and IP columns = give indices for the transitional states. They match the numbers of LS energy table
  - $A(EK)*SEC = A\text{-value in unit of } 1/\text{sec}$
  - $iI\text{---}PK\text{---}IP_i$  BSSUM - ignore these
  - $G*F = g \times f$ , where the oscillator strength (f) is multiplied by the statistical factor which is  $(2S+1)(2L+1)$
  - $F(ABS) = \text{absolute value of } f$ . Note f can be positive or negative depending on the transition to a lower or an upper level.
  - $-F(EMI)$  - ignore
  - $WAVEL/AE = \text{wavelength of the transition photon energy}$
  - $GF(VEL) = g \times f$  in velocity form
  - $SQRT(L*V)$  - ignore
- f-value is computed in two forms, "length" and "velocity" forms, to have an idea of accuracy check. Ideally these two should be the same if the wavefunction is exact.

# SUPERSTRUCTURE (SS)

- SS gives similar values for fine structure energy levels. They are in Table with headline "1. DATA FOR ELECTRIC DIPOLE ..." (line 1437 of ssout.bp.ar17)
- The transition parameters for fine structure transitions for most of the atoms and ions are available at NIST website. So we can make comparison of accuracy
- I ask you to prepare a table listing first 10 transitions given in the fine structure table (line 1437). You will write down the the energies in spectroscopic notation and put down the values of f in length and velocity forms and the percent difference between the two f-values. A-values for the E1 transitions are very important for astrophysical modeling work and lifetime calculations.
- In the same table " 1. DATA FOR ELECTRIC DIPOLE ..." (line 1437 of ssout.bp.ar17), you will find radiative decay rates (A-values) for E3 and M2 transitions. Examples:
  - Line 1447 has 5 values and they are for the forbidden M2 transition. In this line:
    - The first two numbers are the energy level indices given in the fine structure table.
    - 3rd and 4th numbers: AM2 is the radiative decay rate and S is the line strength for the forbidden M2 transition.
    - 5th number is the transition wavelength.
  - Line 1574 gives parameters for an E3 transition. It has 6 numbers: The first two numbers are the energy level indices given in the fine structure table.
    - 3rd, 4th and 5th numbers: the radiative decay rate (AE3), oscillator strength and line strength S - 6th number is the transition wavelength.
- To find A- and S-values for E2 (AQUAD), M1 (AMAG) transitions go to table with headline "2. DATA FOR ELECTRIC QUADRUPOLE AND MAGNETIC DIPOLE TRANSITIONS" (line 4742 in ssout.bp.ar17).
- Please make a short table of E2, E3, M1, M2 transitions with spectroscopic notation for the transitions.