Using The Cowan Code

ZJS

April 10, 2015

The Cowan code is talked about all the time in AMO circles. I wanted to learn how to use it to examine a couple issues in our experiment as well as write up the process so that it would be easier for other students in YavuzLab to learn how to use the code for their own investigations. Specifically, I am interested in predicting Eu^{3+}transition wavelengths and magnetic dipole strengths for use in our EuYSO project. As a result, this tutuorial is heavily geared toward that objective and unfortunately isn't very comprehensive, although I did includ a section on calculating Rb electric dipole transitions.

1 How does it work?

I will not go into detail here because I do not understand very well how it works. In my defense it is complicated and the fact that this is still widely used i take as evidence of both the quality of the program and the giant task replacing it would be. The short story is that the Cowan code uses a relativistic Hartree-Fock approach, a variational approach giving an approximate solution to the Schrodinger equation by numerically solving it in a self-consistent manner using a linear combination of input wavefunctions. The program (really a suite of programs) allows for the calculation of electronic wavefunctions, atomic (ionic- in our case) energy levels, as well as transition wavelengths, lifetimes, and oscillator strengths. Different programs have different tasks. Quoting directly from Cowan's documentation:[1]:

> (1) RCN calculates one-electron radial wavefunctions (bound or free) for each of any number of specified electron configurations, using the Hartree-Fock or any of several more approximate methods. The principal output, for each configuration, consists of the center- of-gravity energy (Eav) of the configuration, and those radial Coulomb (Fk and Gk) and spin-orbit (zeta) integrals required to calculate the energy levels for that configuration.
>
> (2) RCN2 is an interface program that uses the output wave- functions from RCN (on a file called tape2n) to calculate the configuration-interaction Coulomb integrals (Rk) between each pair of interacting configurations, and the electric-dipole (E1) and/or electric quadrupole (E2) radial integrals between each pair of configurations. RCN2 prepares an output file called out2ing that (after being renamed ing11) serves as input to RCG.
>
> (3) RCG sets up energy matrices for each possible value of the total angular momentum J, diagonalizes each matrix to get eigenvalues (energy levels) and eigenvectors (multi-configuration, intermediate-coupling wavefunctions in various possible angular-momentum-coupling representations), and then computes M1 (magnetic dipole), E2, and/or E1 radiation spectra, with wavelengths, oscillator strengths, radiative transition probabilities, and radiative lifetimes. Other options, when a continuum (free) electron is present, are photoionization cross- sections, autoionization transition probabilities, total lifetimes, branching ratios for autoionization, and plane-wave Born collision strengths.
>
> (4) When higher accuracy results are desired, RCE can be used to vary the various radial energy parameters Eav, Fk, Gk, zeta, and Rk to make a least-squares fit of experimental energy levels by an iterative procedure. The resulting least-squares-fit parameters can then be used to repeat the RCG calculation with the improved energy levels and (presumeably) wavefunctions.
>
> Reference: Robert D. Cowan, "The Theory of Atomic Structure and Spectra," (University of California Press, Berkeley, 1981), esp. Chapters 8 and 16.

---

[1] http://www.tcd.ie/Physics/people/Cormac.McGuinness/Cowan/Code/Lanl/readme

It's interesting and a bit challenging to use a program that's so very old. Apparently the program was originally started in 1964 but it's a testament to its staying power that people still use it. In any case, this snippet from the documentation gives a flavor:

> ...terminology will be used in places that dates from the time when computer input consisted of punched cards: The word "card" may be used to refer to a line of an input file or FORTRAN source file, and the word "deck" to refer to an input file–set of cards–or portion thereof. Characters "punched" in specific columns of these cards are, of course, to be typed into the corresponding columns of the input line.

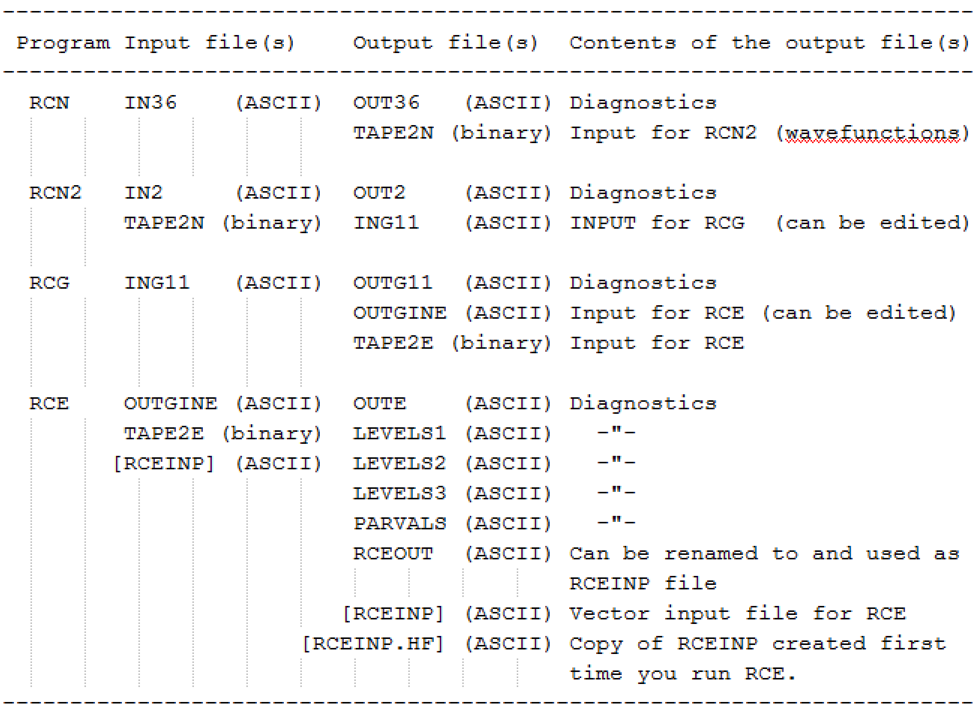
2 How do you work it?

2.1 Installation/Distribution to Use:

I would recommend the Alexander Kremida distribution[2] and refer to his readme for installation information. This distribution has the distinct advantage of being already compiled to run on Windows. There are other versions that include utilities and such but they are not compiled and so would require getting compilation to work. Thus far i haven't been successful at that, but potentially that would be a better route as they have potentially very useful utilities. There are also utilities in PERL that come with Kramida version but i haven't tried to get those to work; that could also be fruitful. There are a variety of distributions and versions. Cormac McGuiness's website is a the place to look: https://www.tcd.ie/Physics/people/Cormac.McGuinness/Cowan/

2.2 Programs and File Dependencies

So as i mentioned above, the program is actually a suite of programs. There are four: RCN, RCN2, RCG, and RCE. Upon correctly installing the programs, go to the cmd window and navigate to the "work" directory he has in place. You can run the programs in sequence there: RCN RCN2 RCG RCE. The output of each program supplies the inputs for the next: A table of the different files from Kramida's documentation gives you a better picture of the flow.



```
------------------------------------------------------------------------
 Program Input file(s)    Output file(s)  Contents of the output file(s)
------------------------------------------------------------------------
  RCN    IN36     (ASCII)  OUT36    (ASCII) Diagnostics
                           TAPE2N (binary) Input for RCN2 (wavefunctions)

  RCN2   IN2      (ASCII)  OUT2     (ASCII) Diagnostics
         TAPE2N (binary)   ING11    (ASCII) INPUT for RCG  (can be edited)

  RCG    ING11    (ASCII)  OUTG11   (ASCII) Diagnostics
                           OUTGINE  (ASCII) Input for RCE (can be edited)
                           TAPE2E (binary) Input for RCE

  RCE    OUTGINE (ASCII)   OUTE     (ASCII) Diagnostics
         TAPE2E (binary)   LEVELS1  (ASCII)   -"-
        [RCEINP]  (ASCII)  LEVELS2  (ASCII)   -"-
                           LEVELS3  (ASCII)   -"-
                           PARVALS  (ASCII)   -"-
                           RCEOUT   (ASCII) Can be renamed to and used as
                                            RCEINP file
                          [RCEINP]  (ASCII) Vector input file for RCE
                       [RCEINP.HF]  (ASCII) Copy of RCEINP created first
                                            time you run RCE.
------------------------------------------------------------------------
```

Figure 1: Cowan code programs and file dependencies

---

[2] http://das101.isan.troitsk.ru/cowan.htm

As you can see, in many cases one or more of the output files of one program are used as inputs for the subsequent program. The suite of programs requires you create/modify two files in order to run: IN36 and IN2. Technically, you can/have to also edit ING11, but in my experience, the settings you might want to change are carried through from the file IN2. It's better to set them in IN2 because otherwise you have to manually modify ING11 for each time you run RCN2, because executing RCN2 creates/rewrites the ING11 file on you.

As far as output is concerned, for our purposes the output information: levels, lifetimes, and line strengths was contained in OUTG11. The LEVELS files generated by RCE are also interesting/easier to read but contain less information.

To find more information about the programs, refer to the documentations files. Included in the Kramida distribution are a readme he has prepared (README_Kramida) as well as 3 documents from Cowan titled: RCN_DOC, RCG_DOC, and RCE_DOC. These documents contain information on what the individual programs do was well as details on the input and output. Most of this tutorial info came from RCN_DOC and RCG_DOC.

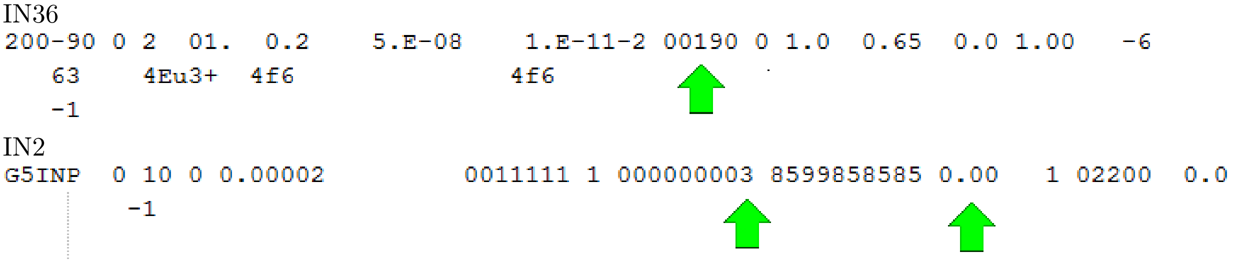
3 Examples

3.1 $Eu^{3+}4F$ Magnetic Dipole Spectrum

For our negative index experiment, i'm very interested in the magnetic dipole spectrum. In addition to information about the green line that we work with at 527nm, i'd like to know about other optical decay routes as well as the relative strengths of the lines. It would be great to understand the spectral composition of fluorescence we observe from the crystal as well as understand the relative rates of different optical (and non-radiative, though Cowan can't help us with that) decay mechanisms. Let's see how the Cowan code can help us.

3.2 Control and Configuration Cards for Eu^{3+}

One of the main things to figure out, and sort of your first step, when trying to use the Cowan code is how to set the "control cards." It's kind of interesting because this language is alluding to actual punch cards. That way of describing things was still in the computing vernacular at the time the programs were originally written. In practice, it's kind of annoying because rather than say, a text file with a list of parameters you can edit, you need to edit the first line of files IN36 and IN2. Also, you have to pay attention to the location of characters, i.e. the character column numbers. It goes without saying a text editor that notes the column is handy in this task. I'll also note here that the top line constitutes the "control card" whereas the next line in the following is the "configuration card". You can have multiple such entries, "cards" in the IN36 file. Let me just point out a few columns of note for our purposes in fig 2:



IN36

```
200-90 0 2  01.  0.2    5.E-08    1.E-11-2 00190 0 1.0  0.65  0.0 1.00   -6
   63    4Eu3+  4f6              4f6
   -1
```

IN2

```
G5INP  0 10 0 0.00002         0011111 1 000000003 8599858585 0.00   1 02200  0.0
        -1
```

Figure 2: Control and Configuration Cards in IN36 and IN2

As far as IN36 is concerned, as you can see there are many parameters, see Cowan's documentation for more information. Most don't need to be changed, but there is one that we should change, indicated by the green arrow. Column 46 should be changed from 0 to 1, as indicated. Evidently, this means we're working with relativistic corrections which is especially important for us as we're working with a heavy element.

Regarding IN2 there are two entries i'd like to point out, indicated by the arrows. The first, column 49, needs to be set to 1, 2 or 3 if you want the code to output magnetic dipole transitions. If it's set to zero you won't get any M1 output. The second, columns 61-65, needs to be made small if you want to see weak transitions. Since the magnetic dipole transitions we're looking at are weak, if this remains set to 5 as it was in the IN2 file i modified, you won't get any magnetic dipole transition output. Setting it to zero seemed to work for me. Note: you won't find information about these in Cowan's RCN (and RCN2) documentation, because the values are directly carried through to the ING11 file. If you edit them here you won't have to mess with the ING11 file. Information about these entries can be found in Cowan's RCG documentation.

The "configuration card" for our system is quite simple as we're examining magnetic transitions inside an f orbital rather than electric dipole transitions between different orbitals. Our "configuration card" is the second line of IN36. The first entry (col 2-5) is the atomic number: 63. The next entry, (col 10) is 1+ degree of ionization, i.e. 4. Following that (col 11-28) is a label: Eu3+ 4f6; this isn't actually used in the calculation. Next (col 33-35) is the orbital specification: 4f. Last (col 36-37) is the occupation number, for us we have 6 electrons in the 4f. Note: in principle you can have more entries, the -1 on the next line indicates it's the end of the group.

3.3 Eu output

Two pages in this document following this discussion are output selected from the OUTG11 file produced by the code for Eu3+. It's the magnetic dipole spectrum of the couple dozen or so lowest lying lines. Let's see if we can locate some information of interest. Let's examine the first entry to pin down what all the columns are. Going across the first row with numbers, the first is the energy of the level, the next is J, following that is the configuration. This is the decaying level.

Where it decays to is given on the subsequent line(s). In this case, there is only one level, but for others there can be more/many levels, e.g. for the 5D1. The line starts with just a number for the transition. Notice on this second line, J=0, as the only transition from 7F1 is to 7F0. After the configuration, next is the change in energy, for this transition it's 430 wavenumbers, followed by the corresponding transition wavelength in angstroms. Following that is a logarithm of the oscillator strength. Note: this is log base 10. We can exponentiate this to find the oscillator strength; doing so we find that the oscillator strength for this transition is quite small, approx 2E-7. Now we can also relate the oscillator strength to the item in the next column, the decay rate. They're different ways of expressing the strength of the transition. They are related through some factors, see Cowan's book[3] eq 14.38:

$$gA = \frac{8\pi^2 e^2 \sigma^2}{mc} gf$$

e and m are the charge and mass of the electron respectively. Sigma is the wavenumber (need to convert to /m to be dimensionally consistent). One note with respect to this expression, there's an implicit factor of $1/4\pi\epsilon_0$. If we evaluate this expression, we find: 0.02479Hz, consistent with the Cowan code output for the optical decay rate of the transition given in the next column: 0.0248Hz, this 7F1-7F0 transition is extremely weak. Note: the last item in the line CF/BR is some kind of cancellation factor involved in the calculation; i don't understand its meaning.

The last line for a group (starting with SUM...) contains a couple items of interest. It starts with 3 zeros, at least for the magnetic dipole transitions, but stronger transitions give numbers. I don't know what these are supposed to be, as it doesn't appear to be the total oscillator strength, although its possible that it is supposed to be but that there is a glitch so that it's giving the wrong value. I haven't been able to straighten this out by looking at the documentation, it remains a hole in this tutorial.

Following that, the next entry is the overall radiative lifetime for the level. It appears this is given by the inverse of the sum of the decay rates times the J-multiplicity of the originating level. I don't understand why it is specified this way.

The last item on the line is the sum of all the decay rates, i.e. the total decay rate.

---

[3] The Theory of Atomic Spectra and Structure by Robert D. Cowan

```
1          MAG DIP SPECTRUM     (ENERGIES IN UNITS OF  1000.0 CM-1 =    0.12 EV)

    1      Eu3+  4f6           ---      Eu3+  4f6

           E      J     LEVEL        DELTA E  LAMBDA(A)  LOG GF GA(SEC-1) CF/BR

     * * *     -67.071  1.0   1 (7F) 7F      Eu3+  4f6          * * *

    1    -67.502  0.0  1 (7F) 7F        0.430 232361.387  -6.697 2.480E-02  1.00

 SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 1.210E+02 SEC  SUMGA= 2.480E-02

     * * *     -66.329  2.0   1 (7F) 7F      Eu3+  4f6          * * *

    2    -67.071  1.0  1 (7F) 7F        0.742 134768.992  -6.184 2.402E-01  1.00

 SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 2.082E+01 SEC  SUMGA= 2.402E-01

     * * *     -65.389  3.0   1 (7F) 7F      Eu3+  4f6          * * *

    3    -66.329  2.0  1 (7F) 7F        0.941 106299.583  -5.953 6.580E-01  1.00

 SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 1.064E+01 SEC  SUMGA= 6.580E-01

     * * *     -64.329  4.0   1 (7F) 7F      Eu3+  4f6          * * *

    4    -65.389  3.0  1 (7F) 7F        1.059  94387.870  -5.857 1.041E+00  1.00

 SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 8.646E+00 SEC  SUMGA= 1.041E+00

     * * *     -63.205  5.0   1 (7F) 7F      Eu3+  4f6          * * *

    5    -64.329  4.0  1 (7F) 7F        1.124  88936.516  -5.870 1.136E+00  1.00

 SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 9.681E+00 SEC  SUMGA= 1.136E+00

     * * *     -62.054  6.0   1 (7F) 7F      Eu3+  4f6          * * *

    6    -63.205  5.0  1 (7F) 7F        1.151  86877.146  -6.047 7.937E-01  1.00

 SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 1.638E+01 SEC  SUMGA= 7.937E-01

     * * *     -50.658  0.0   1 (5D) 5D3     Eu3+  4f6          * * *

    7    -67.071  1.0  1 (7F) 7F       16.413   6092.631  -7.056 1.581E+01 -0.07

 SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 6.326E-02 SEC  SUMGA= 1.581E+01

     * * *     -48.811  1.0   1 (5D) 5D3     Eu3+  4f6          * * *

    8    -67.502  0.0  1 (7F) 7F       18.691   5350.285  -7.751 4.134E+00 -0.01
    9    -67.071  1.0  1 (7F) 7F       18.260   5476.382 -10.353 9.871E-03  0.00
   10    -66.329  2.0  1 (7F) 7F       17.518   5708.343  -6.708 4.013E+01 -0.10
```

```
  11    -50.658  0.0  1 (5D) 5D3        1.847  54143.040  -6.376 9.581E-01  1.00

SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 6.633E-02 SEC  SUMGA= 4.523E+01

    * * *     -46.187  2.0   1 (5D) 5D3     Eu3+  4f6          * * *

  12    -67.071  1.0  1 (7F) 7F        20.884   4788.332  -8.066 2.498E+00  0.00
  13    -66.329  2.0  1 (7F) 7F        20.142   4964.729  -9.813 4.167E-02  0.00
  14    -65.389  3.0  1 (7F) 7F        19.201   5207.967  -6.595 6.244E+01 -0.15
  15    -48.811  1.0  1 (5D) 5D3        2.624  38111.690  -5.964 4.987E+00  1.00

SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 7.146E-02 SEC  SUMGA= 6.997E+01

    * * *     -43.109  6.0   1 (5L) 5L      Eu3+  4f6          * * *

  16    -63.205  5.0  1 (7F) 7F        20.096   4976.112  -9.201 1.694E-01  0.06
  17    -62.054  6.0  1 (7F) 7F        18.945   5278.448  -8.325 1.132E+00  0.01

SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 9.988E+00 SEC  SUMGA= 1.302E+00

    * * *     -43.105  3.0   1 (5D) 5D3     Eu3+  4f6          * * *

  18    -66.329  2.0  1 (7F) 7F        23.224   4305.842  -8.670 7.698E-01  0.00
  19    -65.389  3.0  1 (7F) 7F        22.284   4487.620 -10.210 2.044E-02  0.00
  20    -64.329  4.0  1 (7F) 7F        21.224   4711.632  -6.651 6.713E+01 -0.26
  21    -46.187  2.0  1 (5D) 5D3        3.082  32444.617  -5.827 9.441E+00  1.00

SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 9.048E-02 SEC  SUMGA= 7.737E+01

    * * *     -41.933  7.0   1 (5L) 5L      Eu3+  4f6          * * *

  22    -62.054  6.0  1 (7F) 7F        20.121   4969.968 -10.491 8.724E-03 -1.00
  23    -43.109  6.0  1 (5L) 5L         1.176  85041.741  -5.822 1.391E+00  1.00

SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 1.072E+01 SEC  SUMGA= 1.399E+00

    * * *     -40.903  2.0   1 (5G) 5G3     Eu3+  4f6          * * *

  24    -67.071  1.0  1 (7F) 7F        26.168   3821.474  -7.803 7.187E+00  0.81
  25    -66.329  2.0  1 (7F) 7F        25.426   3932.997  -7.580 1.133E+01  0.28
  26    -65.389  3.0  1 (7F) 7F        24.485   4084.106  -8.119 3.041E+00 -0.06
  27    -48.811  1.0  1 (5D) 5D3        7.908  12645.932  -8.914 5.081E-02  0.28
  28    -46.187  2.0  1 (5D) 5D3        5.284  18925.722  -8.522 5.595E-02  0.11
  29    -43.105  3.0  1 (5D) 5D3        2.202  45420.709  -8.531 9.525E-03 -0.19

SUMFI= 0.0000  0.0000 =  0.0000  RAD.LIFE= 2.306E-01 SEC  SUMGA= 2.168E+01
```

Next let's look at our green line and see what we can learn from the Cowan code output. Scrolling down to transition 8, we see this is the one we want:

5D1 to 7F0. We can see the transition energy is 18691/cm, and the wavelength is computed as 535nm. The decay rate is 4.134Hz and log(gf) is -7.751, giving gf of 1.77E-8.

We would like to extract from this information a matrix element that we could use in our simulations. We can calculate this from the decay rate or oscillator strength, Cowan eq 14.33 or 14.37 respectively. (as an aside, we should see if there are any required modifications to this for magnetic dipole transitions, as these expressions were developed toward electric transitions) A couple of notes about these expressions in Cowan's book: I found them confusing because they're written as if S is dimensionless: i.e. a factor of $e^2 a_0^2$ is in the prefactor but S were to have no units. The wavenumber appears to be treated differently though, i.e. σ does have units of 1/length. Also, you have to be careful and incorporate a conversion of the wavenumber from cm^{-1} to a_o^{-1}. Let's evaluate it:

$$S = gf \frac{3h}{8\pi^2 mca_0^2\sigma} = 3.1 \times 10^{-7} e^2 a_0^2 \rightarrow \mu = 5.6 \times 10^{-4} ea_0$$

Let's organize some of this information, including calculating matrix elements for all our Eu lines of interest:

Transition		Energy (cm^{-1})	λ(nm)	$log_{10}(gf)$	gf	gA (Hz)	$\mu(ea_0)$	Notes	f $EuCl_3$[4]
$5D_0$	$7F_1$	16413	609	-7.056	8.79E-8	15.8	1.328E-3	red in fluorescence?	8.85E-8
$5D_1$	$7F_0$	18691	535	-7.751	1.77E-8	4.134	5.59E-4	our green transition	1.48E-8
	$7F_1$	18260	548	-10.353	4.44E-11	9.87E-3	2.83E-5		
	$7F_2$	17518	571	-6.708	1.96E-7	40.1	1.919E-3	yellow in fluorescence?	
	$5D_0$	1847	5414	-6.376	4.21E-7	0.958	8.66E-3		
$7F_2$	$7F_1$	742	13477	-6.184	6.55E-7	0.240	1.7042E-2		
$7F_1$	$7F_0$	430	23236	-6.697	2.01E-7	0.0248	1.2402E-2		

Table 1: Eu transitions of interest from Cowan code

A few comments on the allowed transitions: Interestingly, our transition is not particularly strong, although stronger than the 5D0-7F0 which is not computed by the Cowan code as it is doubly forbidden. It appears that there are slightly stronger red (from 5D0) and yellow (~3x stronger) transitions which I suspect are responsible for the majority of the fluorescence that we see when we put green light into the crystal. Note: i found a reference where Ofelt had calculated some of these oscillator strengths for $EuCl_3$; the numbers seem to good to be true but the seem to agree quite well with the red and green lines.

Something else that is interesting is that inter-manifold transitions are also magnetic dipole allowed, and in fact are predicted to be stronger than our transition of interst. i.e. the 5D1-5D0 is 15x stronger than the 5D1-7F0. Combined with information about non-radiative decay, we should be able to model incoherent processes pretty easily and see for example if population is accumulating somewhere it shouldn't be. Were we to look at the spectral content of the fluorescence, we would get addition information to help us understand this aspect of our system. This can only help us understand obstacles to EIT for example. I hope and expect to explore more of these issues in my thesis.

Another intersting thing to note is the difference in strength between the magnetic and electric transitions (see the next section). As you can see, our green magnetic dipole transition is about 10,000 times weaker than the electric dipole transition in Rb, as we expect for the much weaker magnetic transitions.

Another tangent that i should mention, if you look at the terms that are specified in the transitions, for example for all the transitions from the 5D1, you'll notice its specified as "1 (5D) 5D3" for the configuration, but what's the 3? it's not J; that has its own column. I think the 3 is a "seniority number;" It's another quantum number gets at the fact that the combination that gives rise to a particular L and S is not unique in a complex level like the 4f6. Different combinations can give rise to the same total L and S, i.e. term. This additional number, the seniority number, allows for distinguishing between these different combinations. I'm not sure this way of looking at this issue is valid, but the following may give us a feel as it shows how different combinations can have the same L and S (L listed at the top, S given by arrow up/down):

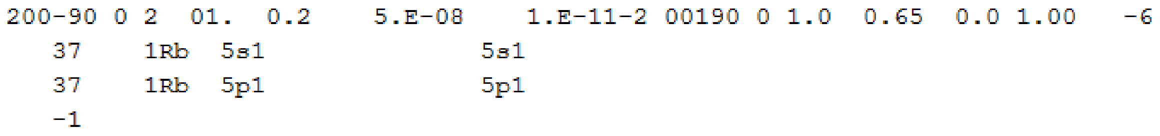
$$
\begin{array}{ccccccc}
-3 & -2 & -1 & 0 & +1 & +2 & +3 \\
\downarrow & & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow \\
 & \uparrow & \uparrow\downarrow & & \uparrow & \uparrow & \uparrow \\
 & \uparrow\downarrow & & \uparrow & \uparrow & \uparrow & \uparrow
\end{array}
$$

I don't understand how these seniority numbers are designated, but if you look through magnetic dipole spectrum output, you can spot the 5D2 and 5D1 versions of the 5D J=1 term and they have much different energies. This seems to make sense from a Hund's rules type argument that different electron arrangements are going to have different energies but the combinatorics of the complicated 4f6 level allow for some of them to have the same L and S.

A lingering question crops up regarding our magnetic dipole transitions. If these magnetic transition are so weak, do we need to worry about electric quadrupole transitions as well, are they of comparable strength? One would think this could be particularly important in the crystal system that is going to mix different kinds of interactions. I tried to see if the Cowan code could help me address this question by looking for D2 transitions, but didn't find anything. I changed what i thought was the correct bit of IN2 to turn on electric dipole transitions, but didn't get any electric quadrupole spectrum output. Perhaps I missed something about that option in the Cowan code documentation. Update: upon further investigation, it appears E2 transitions should be something like 1000x weaker than the M1 transitions, and so shouldn't be an issue for us.

3.4 Rubidium

We work with Rubidium a lot in YavuzLab, so let's see if we can get the Cowan code to spit out the Rb electric dipole spectrum. First, let's modify the "configuration card" in IN36. Also turn off magnetic dipole transition output in IN2, column 49, see fig 3:



```
200-90 0 2  01.  0.2    5.E-08    1.E-11-2 00190 0 1.0  0.65  0.0 1.00   -6
   37    1Rb  5s1              5s1
   37    1Rb  5p1              5p1
   -1
```

Figure 3: configuration card for Rb

Plugging in the correct terms in the "configuration card" and running the code, it spits out the dipole transitions (extracted from file OUTG11) see below. As we expect, the code calculates two electric dipole transitions between the configurations: $5S_{1/2} - 5P_{1/2}$ and the $5S_{1/2} - 5P_{3/2}$. Let's compare the transition parameters from the Cowan code to a reference(Steck line data for Rb[5]) and see how well the code does. The extracted output is a page at the end of the document and summarized below, see fig 2:

Transition	Quantity	Cowan Code	Steck Ref Paper	% difference
$5S_{1/2} - 5P_{1/2}$	λ(nm)	815	795	2.5
	gF	.764	0.342	123
	gA(MHz)	76.7	36	113
	$\mu(ea_0)$	4.53	2.99	52
$5S_{1/2} - 5P_{3/2}$	λ(nm)	803	780	3
	gF	1.55	0.7	121
	gA(MHz)	160	38	321
	$\mu(ea_0)$	6.4	4.23	51

Table 2: Comparing Cowan code to experimental data

---

[5] http://steck.us/alkalidata/

A few intersting things stand out. For one, the code seems to predict the wavelengths of the Rb E1 transitions quite well, within a few percent. The oscillator strength predictions are worse, off by a factor of 2 or so. The Decay rates are similar off by factors of 2-4. The derived matrix elements are a little better, off by about 50%. This doesn't give us any especially quantitative way to evaluate the Cowan code, but it does give us a feel for its strengths and weaknesses when applying it to Eu. Then again, maybe manifestations and sizes of error are a lot different for magnetic dipole vs electric dipole transitions. Note: i tried adjusting the empirical scaling parameters (the 8595858585 number) to see if that would result in better predictions for gf and gA but it didn't seem to make a big difference.

```
1         ELEC DIP SPECTRUM     (ENERGIES IN UNITS OF  1000.0 CM-1 =    0.12 EV)

    1      Rb  5s1              ---      Rb  5p1

            E      J     LEVEL        DELTA E  LAMBDA(A)  LOG GF GA(SEC-1) CF/BR

     * * *      12.269  0.5   1 (2P)  2P      Rb  5p1            * * *

    1      0.000  0.5  1 (2S) 2S       12.269   8150.624  -0.117 7.672E+07  1.00

 SUMFI= 0.0000 -0.3821 = -0.3821  RAD.LIFE= 2.607E-08 SEC  SUMGA= 7.672E+07

     * * *      12.448  1.5   1 (2P)  2P      Rb  5p1            * * *

    2      0.000  0.5  1 (2S) 2S       12.448   8033.257   0.190 1.603E+08  1.00

 SUMFI= 0.0000 -0.3876 = -0.3876  RAD.LIFE= 2.496E-08 SEC  SUMGA= 1.603E+08
```