

JUDD-OFELT FITTING Matlab PROGRAM

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Rare earth doped fiber characterization

The accurate estimation of the lanthanide photonic device numerical simulation parameters is essential for predictive modelling. The key parameters that are needed for predictive modelling of lanthanide ion-doped photonic devices are emission and absorption cross-sections and the photoluminescence life time. The values of these parameters are obtained usually indirectly from measurements. The measurements can be performed on either a section of a lanthanide-doped fire that is used for the realization of the photonic device or on a bulk glass sample. The bulk glass sample can be obtained either from the fire preform or made separately. In principle, the most useful and predictive results are obtained by measuring emission and absorption cross sections and the photon life time directly for the fire section.

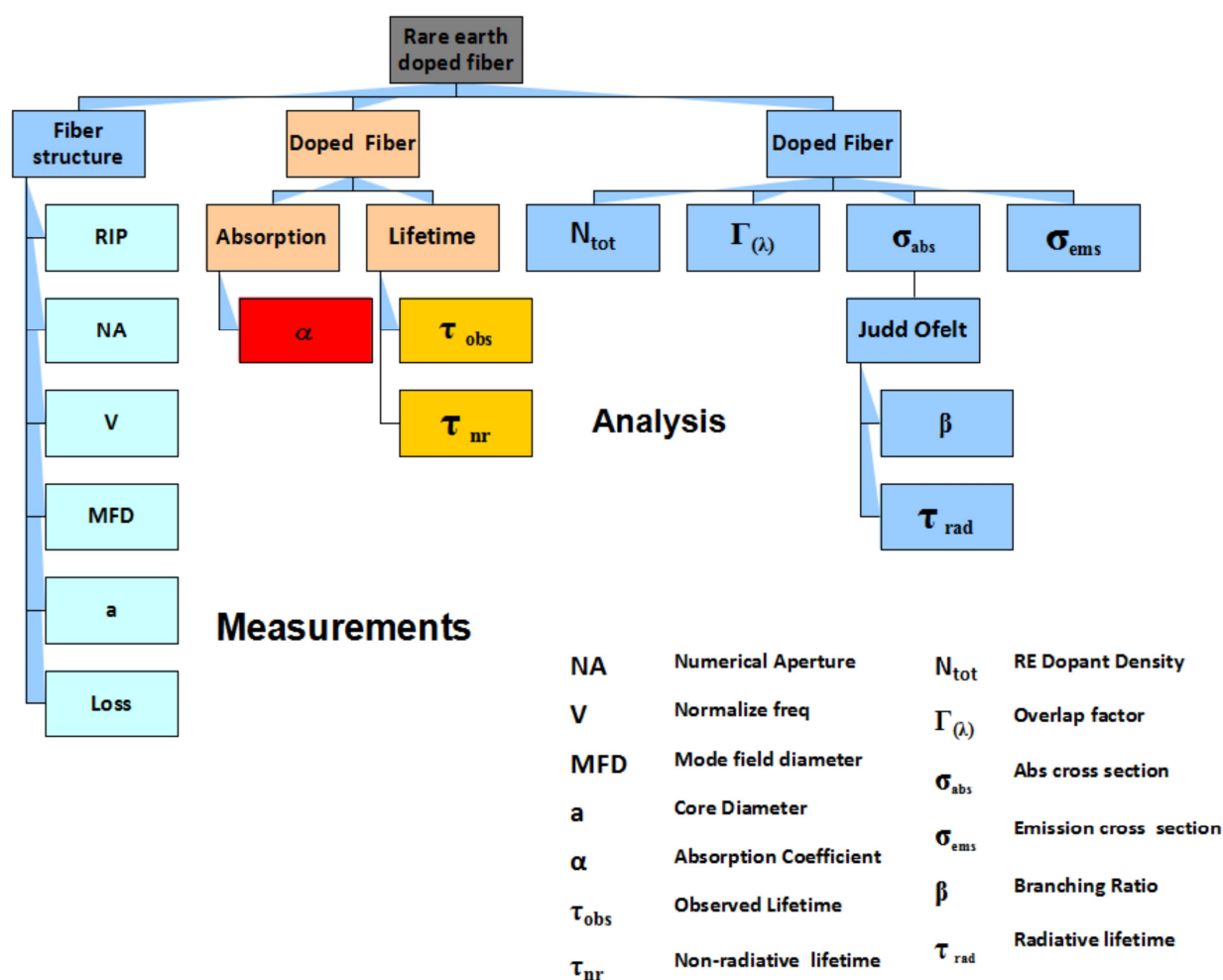
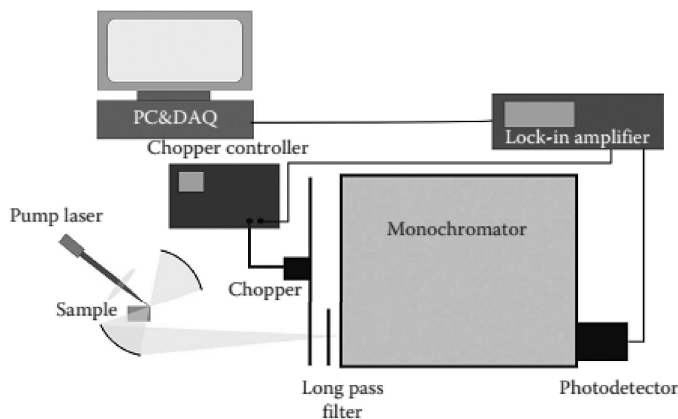


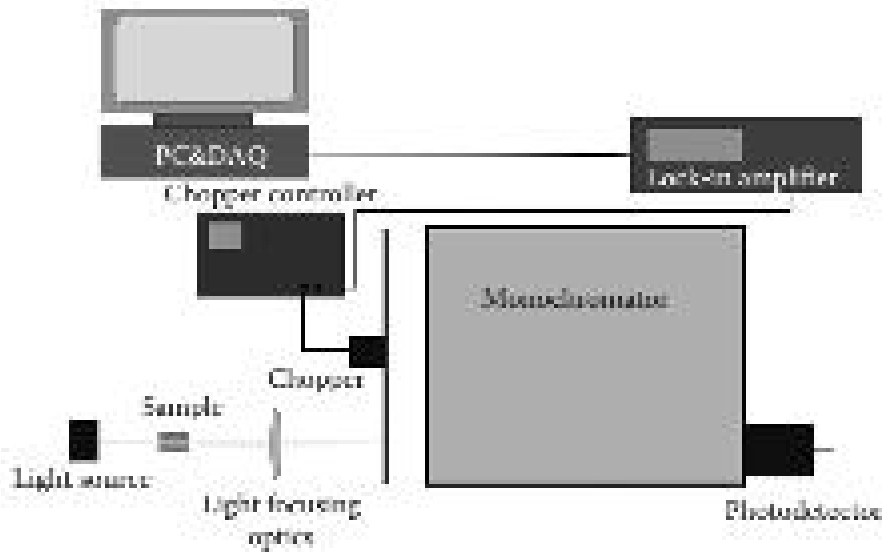
Figure 1: Dope Fiber characterization and analysis

This, however, is usually not straightforward and requires a development of a dedicated measurement setup. Measuring the parameters using a bulk glass sample on the other hand, involves performing standard measurements that can be carried out in most optical laboratories, using standard measuring equipment. We outline the measurement procedures for the bulk glass sample first.

The basis for the extraction of the emission and absorption spectra and of the photoluminescence lifetime of lanthanide ion doped bulk glass samples are two standard measurements, that is, the photoluminescence measurement and the optical absorption measurement. To measure the absorption cross-section spectrum, a doped glass sample with two parallel flat surfaces needs to be prepared. The measurement itself is carried out typically using a Fourier transform infrared spectrophotometer (FTIR). The values of absorption cross-section can be calculated directly from the absorption measured by FTIR, if the sample thickness is known. A typical experimental setup for photoluminescence spectrum measurement consists of a pump laser, chopper, photoluminescence collection optics, a long pass filter that prevents the scattered pump radiation from entering the monochromator, a monochromator, a photodetector, a lock-in amplifier, and a computer that controls all devices and collects the data samples through a data acquisition (DAQ) board (Figure 7.13).



The sample should be prepared in such a way that the effect of reabsorption is minimized as much as possible. The lanthanide ion doping concentration should not be too high to avoid the upconversion effects. However, it should be also noted that a low dopant concentration results in a weak photoluminescence signal. The pump laser should operate at the wavelength that corresponds to one of the absorption bands of the given lanthanide ion. The optical signal is chopped after passing the chopper at the frequency that should be adjusted, taking into account the photoluminescence lifetime of the observed transition. Nearly the same setup can be used for the measurement of the photoluminescence lifetime. The output signal from the photo-detector should be in this case, however, connected to a scope via a trans-impedance amplifier instead of using a lock-in amplifier. The value of the photoluminescence lifetime is extracted from the exponentially decaying part of the waveform observed on the scope. Finally, we note that if FTIR is not available, the absorption cross section can be also measured using a modified setup of that used for the photoluminescence analysis. In this modified setup, the pump laser needs to be replaced with a white light source (Figure 7.14).



The cutback method is the other method often used for measuring the total absorption of an Doped fiber. The cutback method involves comparing the optical power transmitted through a long piece of doped fiber to the power transmitted through a very short piece of the fiber. The cutback method requires that a test fiber of known length L be cut back to a length of approximate 2 m. It requires access to both ends of the fiber. The cutback method begins by measuring the output power P_y of the test fiber of known length L . Without disturbing the input conditions, the test fiber is cut back to a length of approximate 2 m. The output power P_x of the short test fiber is then measured and the fiber attenuation A and the attenuation coefficient a are calculated.

Once the absorption spectrum, photoluminescence spectrum, and photoluminescence lifetime are measured, the emission and absorption cross-sections and the photoluminescence lifetime corresponding to the radiative part of the transition can be obtained in a number of ways. As mentioned, the absorption cross-section can be directly obtained from the FTIR absorption measurement if the sample thickness is known, which is the case if the bulk glass sample is correctly prepared. The photoluminescence spectrum measurement on the other hand provides only the shape of the photoluminescence cross-section spectrum. It has to be therefore scaled to obtain the absolute values of the emission cross-section. For this purpose, either the Fuchbauer-Ladenburg theory or McCumber theory is applied. Additionally, the data provided by the absorption measurement can be applied to investigate the efficiency of the radiative transitions in lanthanide ions using the Judd-Ofelt theory.

Furthermore, very often, only a limited range of measurements can be carried out in the laboratory using the available equipment. In such situations, FuchtbauerLadenburg theory, McCumber theory, and Judd-Ofelt theory can be used to obtain all the required information. We list in the following the main useful formulae that stem from these three theories.

Judd-Ofelt Theory

We outline first the application of the Judd-Ofelt theory to a measured absorption cross-section spectrum. This technique allows the transition strength to be extracted from the absorption cross-section spectrum. Simply stated, the Judd-Ofelt theory describes the intensities of lanthanide and actinide transitions in solids and solutions. The utility of the Judd-Ofelt theory is that it provides a theoretical expression for the line strength [1, 2]

$$S_{ED} = \sum_{t=2,4,6} \Omega_t \left| \left\langle f^n [SL]J \parallel U^{(t)} \parallel f^n [S'L']J' \right\rangle \right|^2$$

Through this expression, the Judd-Ofelt theory allows for the calculation of manifold-to-manifold transition probabilities, from which the radiative lifetimes and branching ratios of emission can be determined. A Judd-Ofelt analysis relies on accurate absorption measurements, specifically the integrated absorption cross section over the wavelength range of a number of manifolds. From the integrated absorption cross-section, the so-called line strength, S_m , can be found,

$$S_m = \frac{3ch(2J+1)}{8\pi^3 e^2 \bar{\lambda}} n \left(\frac{3}{n^2 + 2} \right)^2 \int_{\text{manifold}} \sigma(\lambda) d\lambda$$

where J is the total angular momentum of the initial ground manifold, found from the $2S+1L_J$ designation. $\sigma(\lambda)$ is the absorption cross section as a function of wavelength. The integral of absorption cross section over wavelength is termed the *bandsum*. The mean wavelength, $\bar{\lambda}$, can be found from the first moment of the absorption cross section data,

$$\bar{\lambda} = \frac{\sum \lambda \sigma(\lambda)}{\sum \sigma(\lambda)}$$

where Ω_t are the Judd-Ofelt parameters and the term in brackets are doubly reduced matrix elements in intermediate coupling. A Judd-Ofelt analysis minimizes the square of the difference between S_m and S_{ED} , with Ω_t as adjustable parameters. In practice, the Judd-Ofelt theory is used to determine a set of phenomenological parameters, Ω_λ ($\lambda = 2, 4, 6$), by fitting the experimental absorption, Eq. (2), or emission measurements, in a least squares difference sum, with the Judd-Ofelt expression, Eq. (1). This is most efficiently done in the following way. First, the line strength in Eq. (2) is written as a $1 \times N$ column matrix, S_j^m , and Eq. (1) is also written in matrix form as,

$$S_j^m = \sum_{i=1}^3 M_{ij} \Omega_i$$

where M_{ij} are components of a $N \times 3$ matrix for the square matrix elements of $U^{(2)}$, $U^{(4)}$ and $U^{(6)}$. The Ω_k are components of a 1×3 matrix for the Judd-Ofelt parameters Ω_2 , Ω_4 and Ω_6 . Note that N represents the number of transitions to fit, which depends on the number of absorption manifolds actually measured. Since there are only three Judd-Ofelt parameters, then N must be greater than 3. For example, since Ytterbium (Yb) has only has one absorption manifold, the Judd-Ofelt theory cannot be applied to Yb. Next, the sum of the squared difference is formed,

$$\sigma^2 = \sum_{j=1}^N \left(S_j^m - \sum_{i=1}^3 M_{ij} \Omega_i \right)^2$$

and minimized by taking the derivative $d(\sigma^2)/d\Omega$ and setting the result equal to zero,

$$\frac{\partial(\sigma^2)}{\partial \Omega_k} = -2 \sum_{j=1}^N M_{jk} \left(S_j^m - \sum_{i=1}^3 M_{ij} \Omega_i \right) = 0$$

The set of Judd-Ofelt parameters that minimizes the sum of the squared difference of measured and theoretical linestrength is written in matrix form, $\mathbf{\Omega}^{(0)} = (\mathbf{M}^\dagger \mathbf{M})^{-1} \mathbf{M}^\dagger$, where \mathbf{M}^\dagger is the adjoint of \mathbf{M} . Due to the large number of calculations to be made, matrices are suitable for computer based calculations. Once the Judd-Ofelt parameters are determined, they can be used to calculate transition probabilities, $A(J;J')$, of all excited states from the equation,

$$A(J';J) = \frac{64\pi^4 e^2}{3h(2J'+1)\lambda^3} \left[n \left(\frac{n^2+2}{3} \right)^2 S_{ED} + n^2 S_{MD} \right]$$

where n is the refractive index of the solid, S_{ED} and S_{MD} are the electric and magnetic dipole line strengths, respectively. In this equation J' is the total angular momentum of the upper excited state. Electric dipole linestrengths, S_{ED} , are calculated from each excited manifold to all lower lying manifolds using the matrix elements, $U^{(\lambda)}$, and Judd-Ofelt parameters.

EXAMPLE:

Usually the $\text{Tm } ^3\text{H}_5$ manifold is excluded from the Judd-Ofelt fitting due to the fact that it has a strong magnetic dipole component. The transition probabilities given in Eq. 7 include both electric and magnetic dipole contributions. The calculation of magnetic dipole transition probabilities is more straightforward than the calculation of electric dipole transitions. The transition probability for MD transitions can be written as

$$A_{\text{MD}} = \frac{64\pi^4 e^2}{3h(2J+1)\bar{\lambda}^3} n^3 \left(\frac{h}{2mc} \right)^2 \left| \langle f^n [SL]J \| \mathbf{L} + 2\mathbf{S} \| f^n [S'L']J' \rangle \right|^2$$

The matrix elements of the MD operator, $\mathbf{L} + 2\mathbf{S}$, as well as the 4 f^n intermediate coupled wavefunctions, are required to make this calculation. The matrix elements can be calculated from Eqs. 11-13.

Many 4 f^n intermediate coupled wavefunctions can be found in the literature. The wavefunctions for Tm^{3+} ions in this example are taken from Krupke [7]. Generally speaking, the wavefunctions, like the matrix elements, are independent of the host material since the energy levels of a given lanthanide ion vary only by relatively small amounts (\sim several hundred cm^{-1}) from host to host. This is due to the weak perturbation that the crystal field of the host has on the optically active site of the lanthanide ion embedded in the host material. The intermediate coupled wavefunctions are shown here for Tm^{3+} ions in table E1, taken from the article by Krupke.

If we wish to find the magnetic dipole line strength for the $^3\text{H}_5 \rightarrow ^3\text{H}_6$ transition, for instance, then the matrix element is calculated using the wavefunctions in table E1 and then utilizing Eq. A5. This is shown below.

$$\langle [^3\text{H}_5] \| \mathbf{L} + 2\mathbf{S} \| [^3\text{H}_6] \rangle = 0.9953 \langle ^3\text{H}_5 \| \mathbf{L} + 2\mathbf{S} \| ^3\text{H}_6 \rangle + 0.0973 \langle ^3\text{H}_5 \| \mathbf{L} + 2\mathbf{S} \| ^1\text{I}_6 \rangle = 3.2393$$

$$\text{So, } \left| \langle [^3\text{H}_5] \| \mathbf{L} + 2\mathbf{S} \| [^3\text{H}_6] \rangle \right|^2 = 10.4931$$

Table E1. Intermediate coupled wavefunctions for Tm^{3+} ions.

$$\begin{aligned} [^3\text{H}_6] &= 0.9953|^3\text{H}_6\rangle + 0.0973|^1\text{I}_6\rangle \\ [^3\text{F}_4] &= 0.7817|^3\text{F}_4\rangle - 0.2804|^3\text{H}_4\rangle + 0.5567|^1\text{G}_4\rangle \\ [^3\text{H}_5] &= 1.0000|^3\text{H}_5\rangle \\ [^3\text{H}_4] &= 0.7522|^3\text{H}_4\rangle + 0.5395|^3\text{F}_4\rangle - 0.3785|^1\text{G}_4\rangle \\ [^3\text{F}_3] &= 1.0000|^3\text{F}_3\rangle \\ [^3\text{F}_2] &= -0.8738|^3\text{F}_2\rangle + 0.4654|^1\text{D}_2\rangle + 0.1408|^3\text{P}_2\rangle \\ [^1\text{G}_4] &= 0.7393|^1\text{G}_4\rangle + 0.5963|^3\text{H}_4\rangle - 0.3128|^3\text{F}_4\rangle \\ [^1\text{D}_2] &= 0.6400|^1\text{D}_2\rangle + 0.6284|^3\text{P}_2\rangle + 0.4422|^3\text{F}_2\rangle \\ [^1\text{I}_6] &= 0.9953|^1\text{I}_6\rangle - 0.0973|^3\text{H}_6\rangle \\ [^3\text{P}_0] &= 0.9719|^3\text{P}_0\rangle - 0.2353|^1\text{S}_0\rangle \\ [^3\text{P}_1] &= 1.0000|^3\text{P}_1\rangle \\ [^3\text{P}_2] &= -0.7650|^3\text{P}_2\rangle + 0.2023|^3\text{F}_2\rangle + 0.6114|^1\text{D}_2\rangle \\ [^1\text{S}_0] &= 0.9719|^1\text{S}_0\rangle + 0.2353|^3\text{P}_0\rangle \end{aligned}$$

Rearranging Eq. E1 and using $\hbar = 6.5826 \times 10^{-16}$ eV-s, $c = 2.998 \times 10^{17}$ nm/s, $e^2 / \hbar c = 1/137$, the fine structure constant, and $mc^2 = 0.511$ MeV, the constant factor is determined to be

$$\frac{64\pi^4 e^2}{3h} \left(\frac{\hbar}{2mc} \right)^2 = 2.698 \times 10^{10} \text{ nm}^3 / \text{s}$$

For $J = 5$, $\bar{\lambda} = 1250$ nm, and $n = 1.65$,

$$\frac{n^3}{(2J+1)\bar{\lambda}^3} = 2.0909 \times 10^{-10} \text{ nm}^{-3}$$

Putting these factors together, the result is

$$A_{\text{MD}} = (2.698 \times 10^{10} \text{ nm}^3 / \text{s}) \times (2.0909 \times 10^{-10} \text{ nm}^{-3}) \times 10.4931 = 59.194 \text{ s}^{-1}$$

This MD value is a substantial contribution to the total transition probability when compared to the ED value from a Judd-Ofelt analysis [8]. This demonstrates clearly why the $^3\text{H}_5$ manifold was excluded from the Judd-Ofelt fit. Other manifolds can have their radiative lifetimes corrected as well by adding MD contributions. Selection rules are $\Delta S = 0$, $\Delta L = 0$ and $\Delta J = \pm 1$, which narrows the number of calculations that must be performed.

The Computer Program

All the tools have been developed up to this point, and it is now a simple matter to find the radiative lifetimes, τ_r , and the branching ratio,

$$\frac{1}{\tau_r} = \sum_J A(J'; J) \quad (16)$$

$$\beta_{J'J} = \frac{A(J'; J)}{\sum_J A(J'; J)} \quad (17)$$

This is the objective of the computer program. The procedure of a Judd-Ofelt analysis is represented in a simple flow chart shown in figure 1 below. This figure shows the major steps in the process, culminating in calculation of the radiative lifetimes, τ_r , and branching ratios, $\beta_{J'J}$. The details of all these steps have been covered and form, a hopefully clear and coherent, recipe for what is called a Judd-Ofelt analysis.

Program work in 3 different modes

Mode 0: when the mean wavelength and bandsum is available, we have to use this mode
In this case we have to provide provide bandsum (bandsum), bandsum energy levels(BEL) and mean wavelength (meanv)

%mode 0 example

NBS2=6; %number of bandsum

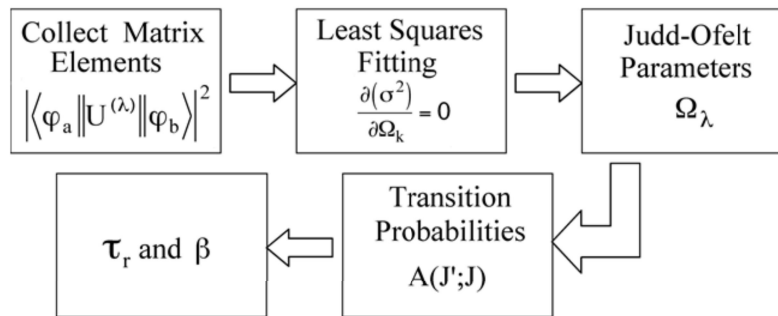
BEL2=[6 7 9 10 11 12]

bandsum2=[2.865,2.815,10.707 ,19.692,34.82 ,86.911];

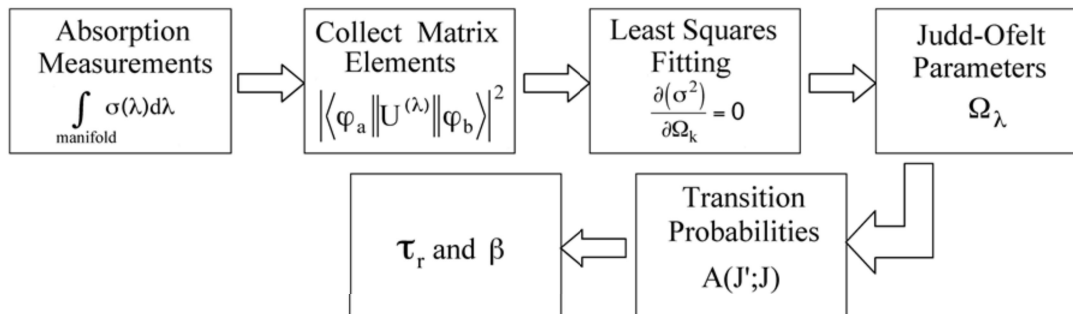
% bandsum matrix

meanv2=[3590,470,682,789,1192,1708];

% mean value matrix



Mode 1: When pure absorption cross section is available the code can compute and analyses the data. In this case. We have to provide absorption cross section boundaries(BSB) and bandsum energy levels(BEL), select from excel files



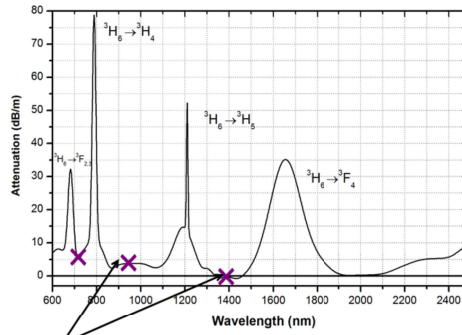
%mode 1 example

NBS=4; %number of bandsum

BSB=[0,507,1846,3866] ; % Boundaries of bandsum

BEL=[8, 10, 11, 12] ; %bandsum energy levels, select from excel files

For example for thulium doped fiber we have the following spectrum



Boundaries of bandsom (BSB)

tm-par - Notepad				
File	Edit	Format	View	Help
1S0-3H6,	0.000000,	0.000000,	0.0001553,	79592
3P2-3H6,	0.000000,	0.2645148,	0.0223155,	38193
3P1-3H6,	0.000000,	0.000000,	0.1239106,	36298
3P0-3H6,	0.000000,	0.000000,	0.0756208,	35637
1I6-3H6,	0.0106068,	0.0388558,	0.0134168,	34886
1D2-3H6,	0.000000,	0.3156233,	0.0927906,	28032
1G4-3H6,	0.0482625,	0.0748364,	0.0124885,	21374
3F2-3H6,	0.000000,	0.0000327,	0.2580804,	15116
3F3-3H6,	0.000000,	0.3163907,	0.8410927,	14510
3H4-3H6,	0.2372840,	0.1090403,	0.5947180,	12720
3H5-3H6,	0.1073904,	0.2314197,	0.6383669,	8390
3F4-3H6,	0.5374299,	0.7261070,	0.2382114,	5811

8

10

11

12

Bandsom and mean value are calculated by :

```
bandsom(i)=trapz(lamdap,sigma_sap)*1e24;
meanv(i)=(sum(lamdap.*sigma_sap)./sum(sigma_sap))./1000;
```

Mode 2: when the Judd-Ofelt Parameters are available, we can analysis the life time , branching ratio and so on. We should provide Judd-Ofelt Parameters(omega)

%mode2 example

```
omega=[7.7479 2.5110 0.7599]
```



One additional input file is provided, sellmeier.mat, which contains Sellmeier coefficients for the index of refraction calculation according to:

$$n^2 = A + \frac{B\lambda^2}{\lambda^2 - C} + \frac{D\lambda^2}{\lambda^2 - E}$$

The records are read by the program and used in the Sellmeier equation to calculate n, the index of refraction, for a given wavelength. This file can be easily edited to include any material by following the recipe outlined here and format of the file. See the Sellmeier folder in the documentation for reference information.

The computer program runs in a self-explanatory way for input and the output files should be easily readable. The files are saved in the same folder as the program. They are given names (Output.txt), containing the fit results and (transition.txt) containing the branching ratio and transition probabilities (AED & AMD), as well as the radiative lifetimes for a given manifold as a running sum for each each lower manifold. The last lifetime for a given excited manifold, therefore, represents the total sum of all inverse transition probabilities. Branching ratios are calculated by individual transition probabilities divided by the sum of all transition probabilities for a given manifold. Output is always in units of 10^{-20} cm^2 for Judd-Ofelt parameters. Then, the output files will contain information:

Wavelength is in units (nm).

Linestrengths (S) in units ($\times 10^{-20} \text{ cm}^2$).

Transition probabilities (AED & AMD) in units (s^{-1})

Lifetime in units (ms)