

JOES User Manual

<https://omasgroup.org/joes-software/>

Note: Chromaticity (CIE) calculations are no longer available as they will be moved to a specific colorimetric application. DOI will be available here soon.

By using this application, you are obliged to cite:

A. Ćirić, S. Stojadinović, M. Sekulić, M.D. Damićanin, JOES: An application software for Judd-Ofelt analysis from Eu^{3+} emission spectra, J. Lumin. 205 (2019) 351–356.
<https://doi.org/10.1016/j.jlumin.2018.09.048>.

The algorithm and equations the app applies are given in this research paper.

The software is published with a GPLv3 License. It is free to use and share. It can be modified, under this license's terms.

Software Requirements: Java, which can be freely downloaded here:

<https://www.java.com/en/download/>

Chances are that it is already installed on your PC/MAC.

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JOES - Judd-Ofelt from Emission Spectra

File Help

Input

Spectrum Units:
☐ W ☒ Counts (default)

Refractive Index:

Overall Quantum Yield
Observable Lifetime

☐ Remove Background (Minimum)

Input Data Preview

Nanoparticles

☐ Is particle diameter much smaller than emission wavelength?

Filling Factor
Surrounding Media Refractive Index

INPUT									
min [nm]	max [nm]	Area	Ω [cm ²] x 1E20	Tr. Prob. [1/s]	β	n	ν [1/cm]	λ [nm]	
$^5D_0 \rightarrow ^7F_1$									
$^5D_0 \rightarrow ^7F_2$									
$^5D_0 \rightarrow ^7F_4$									
$^5D_0 \rightarrow ^7F_6$									

Wavelength range $^5D_0 \rightarrow ^7F_0$: 570 – 585, 7F_1 : 585 – 600, 7F_2 : 610 – 630, 7F_3 : 640 – 660, 7F_4 : 680 – 710, 7F_5 : 740 – 770, 7F_6 : 810 – 840

Calculate

By using this software cite following article:
doi: 10.1016/j.jlumin.2018.09.048

CIE calculations are moved to a new Project, doi will be soon given here

Symmetry - Europium as a spectroscopic probe

Number of emission bands for terminal state:

7F_0 7F_1 7F_2 7F_3 7F_4 Point Group Symmetry: A_0 Asymmetric Ratio, R =

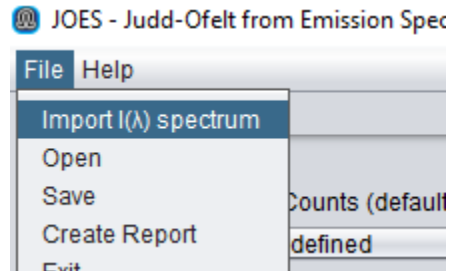
This is the JOES default screen. The application is very simple to use, just please follow this user manual.

Requirements for use are:

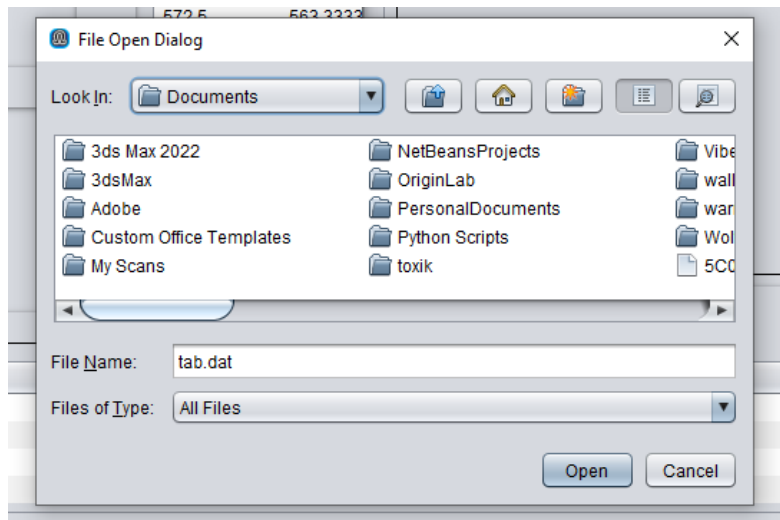
1. Emission spectrum, given with comma-separated values, or tab-separated values. Both txt and dat files work. The input file cannot have a header that contains some text, only the spectrum data is allowed.
2. Values of refractive index for $^5D_0 \rightarrow ^7F_{1,2,4}$ transitions. Alternately, the user can choose the host matrix from the drop-down list. Note that some materials, like the pure metals, in the list have $n < 1$, and they cannot be used for Judd-Ofelt analysis (they exist there as the refractive index values are obtained from the refractive index database).
3. For the small nanoparticles, the effective refractive index values should be used instead of the bulk refractive index. Then the filling factor and the surrounding media refractive index should be provided.

Import spectrum file

First click on **File > Import spectrum**



File open dialog will appear.



The default file extension is **.txt**. If your file is in **.dat** or some other format, choose "**All Files**".

Select the file. The file must be formatted in the form:

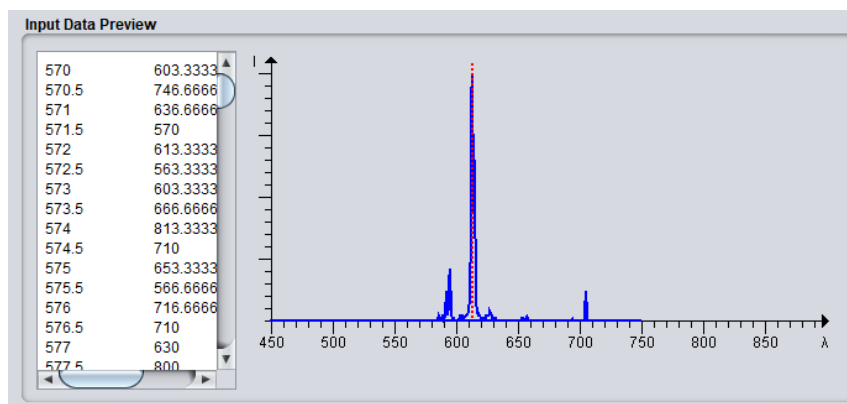
wavelength, intensity

or

wavelength intensity

i.e. comma-separated or tab-separated. Unit of intensity is not important at this step.

If the file is correct, you will see the data and the spectrum in the **Input Data Preview** panel:



If you wish for the background to be removed, JOES can automatically subtract the baseline, but only by subtracting the minimum of the spectrum. For that option, before clicking on Calculate button, select the **Remove Background** checkbox:

☐ Remove Background (Minimum)

Units

Select units in which the spectrum intensity is recorded:

Input

Spectrum Units:

☐ W ☒ Counts (default)

The default value is in counts as the most spectrofluorometers record in that manner. Some spectrometers do record irradiance, thus the spectrum is proportional to **W** – select that option in that particular case.

Refractive Index

Judd-Ofelt parameters' calculation strongly depends on the correct values of the refractive index. Firstly, the choice must be made if the user wants to provide for the values of refractive index for each of the emission peaks, or select the material from our drop-down list:

Input

Spectrum Units:
☐ W ☒ Counts (default)

Refractive Index

Overall Quantum Yield

Observable Lifetime

☐ Remove Background (Minimum)

If the “**User defined**” is selected, please provide the refractive index values in the table, for each of the emissions $^5D_0 \rightarrow ^7F_{1,2,4,6}$.

INPUT								
	min [nm]	max [nm]	Area	Ω [cm ²] x 1E20	Tr. Prob. [1/s]	β	n	v
$^5D_0 \rightarrow ^7F_1$								
$^5D_0 \rightarrow ^7F_2$								
$^5D_0 \rightarrow ^7F_4$								
$^5D_0 \rightarrow ^7F_6$								

If the user selects the host matrix from the drop-down list, the refractive index values will be automatically filled out.

input

Spectrum Units:
☐ W ☒ Counts (default)

Refractive Index

Overall Quantum Yield

☐ Remove Background (Minimum)

Nanoparticles

☐ Is particle size much smaller than emission wavelength

Ag - Silver
 AgCl - Silver Chloride
 Al - Aluminium
 Al₂O₃ - Amorphous, thin film
 AlSb - Aluminium Antimonide
 Au - Gold
 B₄C - Boron Carbide

If the particle size is much smaller than the wavelength of light, the effective refractive index should be used instead. JOES can apply this correction if that option is selected and given values provided:

Nanoparticles

☐ Is particle diameter much smaller than emission wavelength?

Filling Factor

Surrounding Media Refractive Index

This checkbox must be selected before clicking on the Calculate button. The filling factor is the fraction of the space occupied by the particle, for example, if particles contain 70% of space, and 30% is air, the filling factor is 0.7. The surrounding media is most commonly air, and in that case, the surrounding media refractive index is equal to 1. Make sure to click only once on Calculate button after selecting the “**Is particle diameter much smaller**” checkbox, as the correction is applied each time the Calculate button is clicked.

Wavelength ranges

A necessary input is the wavelength range for each of the transitions:

	INPUT	
	min [nm]	max [nm]
$^5D_0 \rightarrow ^7F_1$	585	600
$^5D_0 \rightarrow ^7F_2$	610	630
$^5D_0 \rightarrow ^7F_4$	680	710
$^5D_0 \rightarrow ^7F_6$		

If the user does not enter the values manually, the default values will be provided. After the default values are entered, the user must check them and click on Calculate button again.

Optional inputs

Optionally, the observable lifetime or quantum yield values can be input, which allows for the calculation of the PL quantum efficiency and the Sensitization efficiency.

Overall Quantum Yield Observable Lifetime

Calculation

After clicking on **Calculate** button, the Judd-Ofelt parameters, Transition probabilities, branching ratios, barycenter energies, centroids, and areas appear in the table. Note that the values for Judd-Ofelt parameters should be multiplied by 10^{-20} for the correct value.

In the bottom right corner is displayed the **Asymmetric Ratio**.

Input

Spectrum Units: ☐ W ☒ Counts (default)

Refractive Index: Nb2O5 - Niobium pentoxi...

Overall Quantum Yield Observable Lifetime

☐ Remove Background (Minimum)

Nanoparticles

☐ Is particle diameter much smaller than emission wavelength?

Filling Factor

Surrounding Media Refractive Index

Input Data Preview

570,603.33333
570,5746.66667
571,636.66667
571,5,570
572,613.33333
572,5,663.33333
573,603.33333
573,5,666.66667
574,813.33333
574,5,710
575,653.33333
575,5,666.66667
576,716.66667
576,5,710
577,630
577,5,800

INPUT

	min [nm]	max [nm]	Area	Ω [cm ²] x 1E20	Tr. Prob. [1/s]	β	n	ν [1/cm]	λ [nm]
$^5D_0 \rightarrow ^7F_1$	585	600	371,580.933		181.909	0.154	2.33	16,861.633	593.062
$^5D_0 \rightarrow ^7F_2$	600	640	1,885,623.117	6.48	923.116	0.784	2.329	16,280.885	614.217
$^5D_0 \rightarrow ^7F_4$	680	715	148,757.483	1.117	72.825	0.062	2.301	14,229.648	702.758
$^5D_0 \rightarrow ^7F_6$			0	0.0	0	0			

Wavelength range $^5D_0 \rightarrow ^7F_0: 570 - 585$, $^7F_1: 585 - 600$, $^7F_2: 610 - 630$, $^7F_3: 640 - 660$, $^7F_4: 680 - 710$, $^7F_5: 740 - 770$, $^7F_6: 810 - 840$

Calculate

By using this software cite following article:
doi: 10.1016/j.jlumin.2018.09.048

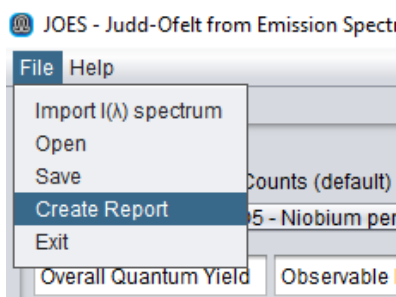
CIE calculations are moved to a new Project, doi will be soon given here

Symmetry - Europium as a spectroscopic probe

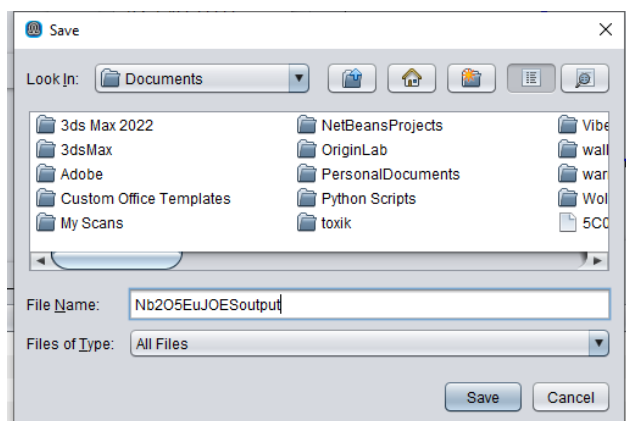
Number of emission bands for terminal state:

7F_0 7F_1 7F_2 7F_3 7F_4 Point Group Symmetry: A_0 Asymmetric Ratio, R = 5.103

These are not all of the calculations the program performs. For that, the report must be generated. Click on **File > Create Report**:



Choose the location and name for your report file:



And it will be saved as an **HTML** file, which the user can open with an internet browser:



A part of the report is displayed in the image below:

Judd-Ofelt from Emission Spectra of Eu^{3+} incorporated in Nb_2O_5 - Niobium pentoxide

Peaks:

- $^5\text{D}_0 \rightarrow ^7\text{F}_1$: Integrated from 585.0 nm to 600.0 nm, Area [arb. units] = 371580.9333499995
- $^5\text{D}_0 \rightarrow ^7\text{F}_2$: Integrated from 600.0 nm to 640.0 nm, Area [arb. units] = 1885623.1166750006
- $^5\text{D}_0 \rightarrow ^7\text{F}_4$: Integrated from 680.0 nm to 715.0 nm, Area [arb. units] = 148757.48334499993
- $^5\text{D}_0 \rightarrow ^7\text{F}_6$: Integrated from null nm to null nm, Area [arb. units] = 0.0

Refractive indexes

- $n(^5\text{D}_0 \rightarrow ^7\text{F}_1) = 2.3304$
- $n(^5\text{D}_0 \rightarrow ^7\text{F}_2) = 2.3287763623981874$
- $n(^5\text{D}_0 \rightarrow ^7\text{F}_4) = 2.3006828949507043$
- $n(^5\text{D}_0 \rightarrow ^7\text{F}_6) = \text{NaN}$

Judd-Ofelt Parameters:

- $\Omega_2 = 6.48 \times 10^{-20} \text{ cm}^2$
- $\Omega_4 = 1.117 \times 10^{-20} \text{ cm}^2$
- $\Omega_6 = 0.0 \times 10^{-20} \text{ cm}^2$

== Derived Quantities ==

Radiative Transition Probabilities

- $A(^5\text{D}_0 \rightarrow ^7\text{F}_1) = 181.909 \text{ s}^{-1}$
- $A(^5\text{D}_0 \rightarrow ^7\text{F}_2) = 923.116 \text{ s}^{-1}$
- $A(^5\text{D}_0 \rightarrow ^7\text{F}_4) = 72.825 \text{ s}^{-1}$
- $A(^5\text{D}_0 \rightarrow ^7\text{F}_6) = 0.0 \text{ s}^{-1}$

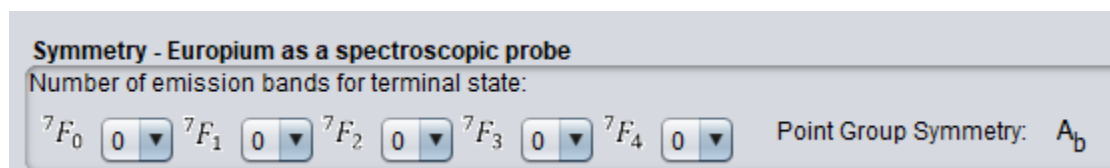
Experimental Branching Ratios and Theoretical Branching Ratios

- $\beta(^5\text{D}_0 \rightarrow ^7\text{F}_1) = 0.1544417598467785; 0.1544418432264851$
- $\beta(^5\text{D}_0 \rightarrow ^7\text{F}_2) = 0.7837295362098278; 0.7837294589269919$
- $\beta(^5\text{D}_0 \rightarrow ^7\text{F}_4) = 0.06182870394339372; 0.061828697846523174$

The report displays the Judd-Ofelt parameters, relevant data, and the derived quantities, as explained in the above-mentioned research article.

Symmetry

This part has nothing to do with the Judd-Ofelt analysis. The program can be additionally used to calculate the symmetry around the Eu^{3+} ion, given that the spectrum is well resolved and that the Stark peaks are observable for each relevant transition. The user needs to enter the number of Stark peaks for each transition $^5\text{D}_0 \rightarrow ^7\text{F}_J$:



Symmetry - Europium as a spectroscopic probe

Number of emission bands for terminal state:

$^7\text{F}_0$ $^7\text{F}_1$ $^7\text{F}_2$ $^7\text{F}_3$ $^7\text{F}_4$ Point Group Symmetry: A_0