RELIC 1.0

Rare Earth Level and Intensity Calculations

User Guide

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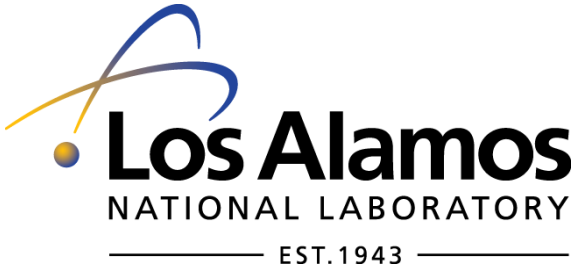

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1. Introduction

Thank you for your interest in RELIC, and welcome to the RELIC user community. RELIC was developed at Los Alamos National Laboratory (LANL) with the goal of providing a user-friendly and self-consistent tool that can be offered under a free license. RELIC stands for "Rare Earth Level and Intensity Calculations". It is a software package that performs calculations of $[Xe]4f^N$ wavefunctions and energy levels of the tripositive rare earth ions (from Pr^{3+} to Tm^{3+}) as well as electronic transition intensities between them. In addition, RELIC offers a number of basic quantum mechanical functions, and it calculates several derived quantities that are relevant for the optical spectroscopy of rare earths.

This marks the first release of the RELIC software package. It comes with an extensive set of functions, and we hope that RELIC proves to be a useful tool in your research. We are interested in your feedback. If you find any errors or deficiencies, or if you have suggestions for additional functionality please let us know so we can consider your input for incorporation in future RELIC releases. We continually strive to improve RELIC and will provide updated versions as needed.

The RELIC developers can be contacted at:

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This user guide contains important information on the terms of use of the RELIC software as well as on the details of using each of the functions. Please read the user guide carefully so that you get the most benefit from the software and are also aware of its capabilities as well as limitations.

2. License Agreement, Terms of Use, and Limitations

The use of RELIC 1.0 is governed by the Software End User Agreement (see Appendix A: Software End User License Agreement). By downloading and installing the software distributed with this agreement, you are confirming your acceptance of this software and agreeing to become bound by the terms of this license agreement.

Please note: Whenever you publish work (peer-reviewed papers, proceedings, oral and poster presentations, lectures, theses, etc.) that has used RELIC or contains any results obtained from RELIC you agree to add a reference to the following paper:

M.P. Hehlen, M.G. Brik, K.W. Krämer, "50th anniversary of the Judd-Ofelt theory: An experimentalist's view of the formalism and its application", J. Lumin., 136 (2013) pp. 221-239.

This above publication gives a detailed description of all equations used in RELIC 1.0 as well as the preferred methods of application of this quantum mechanical framework. It can be accessed at http://dx.doi.org/10.1016/j.jlumin.2012.10.035. Alternatively, an official hardcopy reprint can be requested from the first author (see 1. Introduction for contact information).

The RELIC 1.0 software is distributed through Los Alamos National Laboratory (LANL). LANL maintains a list of RELIC users so that we can communicate the release of software upgrades to the community. It is therefore important that each user register individually and obtain his/her own free copy of RELIC. Your RELIC registration information will not be used for any other purpose or shared with any third party.

We have exercised utmost care in the implementation of the formalism and have performed extensive testing and cross-referencing of RELIC 1.0 with other codes. However, there is always a small chance of errors in the code, and we cannot be responsible for any respective consequences to the end user (see Appendix A: Software End User License Agreement).

3. RELIC Software Overview

3.1. System Requirements

The RELIC 1.0 software was written in National Instruments LabView 2011 (Full Development System) in order to take advantage of the strong mathematical and graphical functions of LabView. The National Instrument Application Builder was used to create the RELIC 1.0 stand-alone executable that is distributed to users along with associated database files. It is therefore not necessary for the user to own a license of LabView in order to legally run RELIC 1.0. The software was developed and tested on a Windows 7 Professional (64-bit) machine with Intel Core i7 CPU (2.80 GHz) and 8 GB of RAM. RELIC 1.0 is distributed to run on this environment, and it has not been tested on any other configuration.

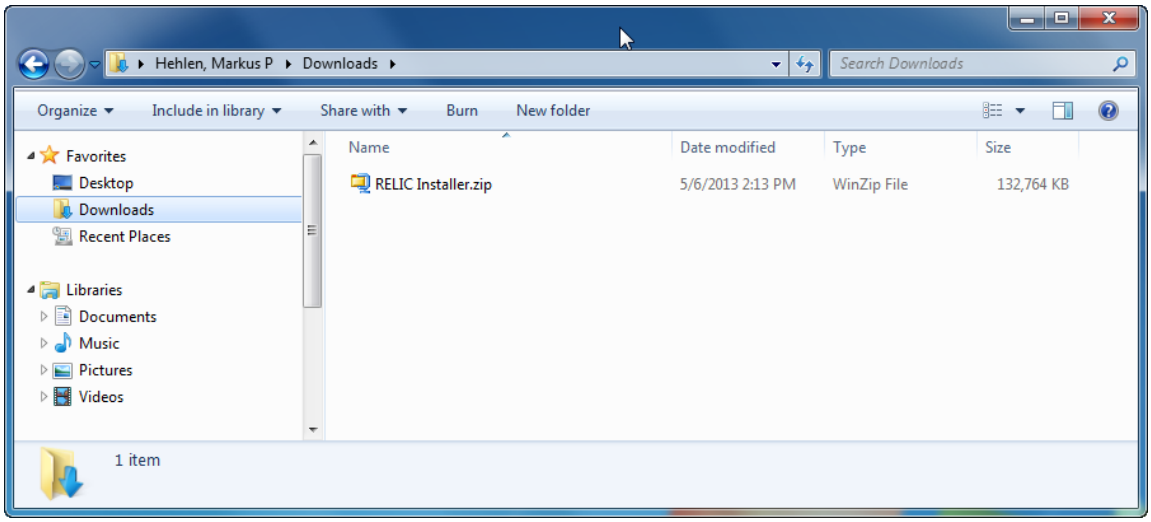
3.2. RELIC Installation

RELIC is downloaded as a zip file. Once extracted, the software can be installed on your PC through an Installer. The following steps guide you through the initial installation of the RELIC 1.0 software and its associated database files.

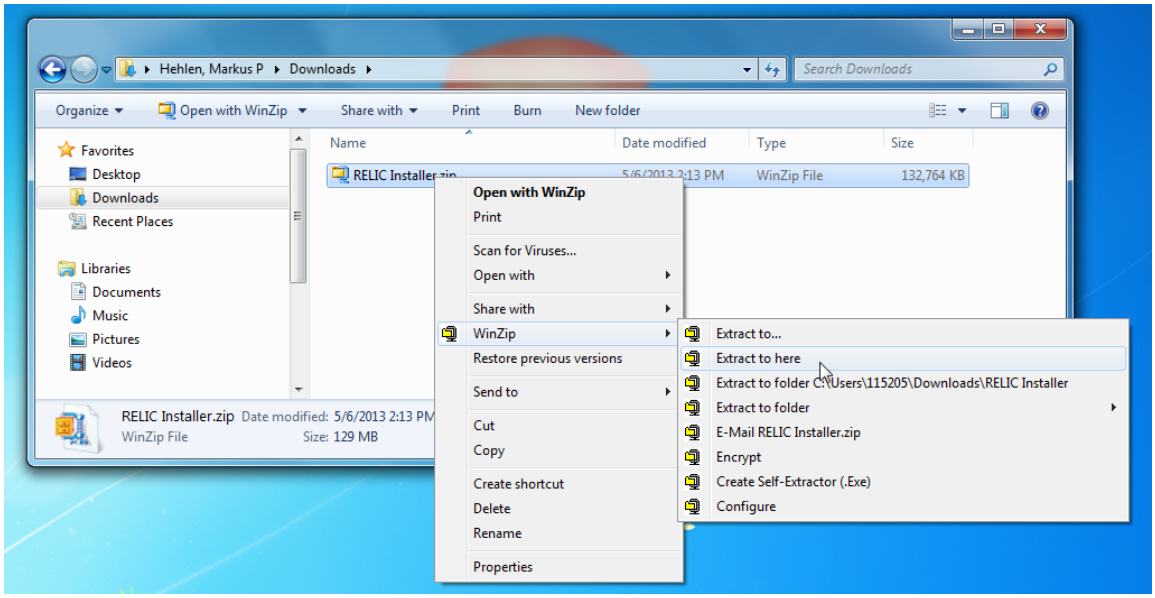
1. Register at the Los Alamos National Laboratory RELIC website to become a licensed user

2. Download the zip file containing the latest RELIC distribution into the "Downloads" folder on your computer.

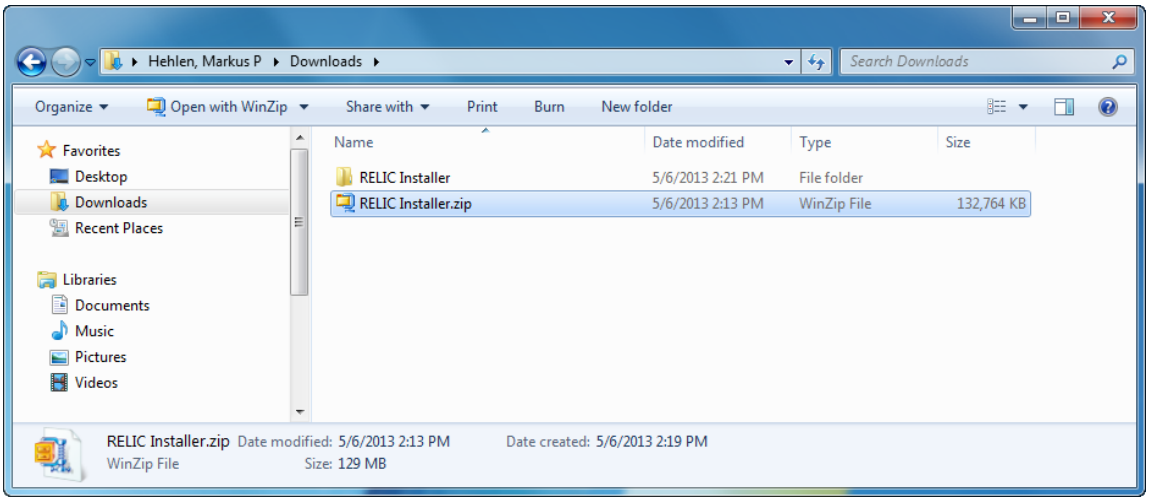
3. Open Windows Explorer and navigate to the Downloads folder to locate the RELIC Installer.zip file.



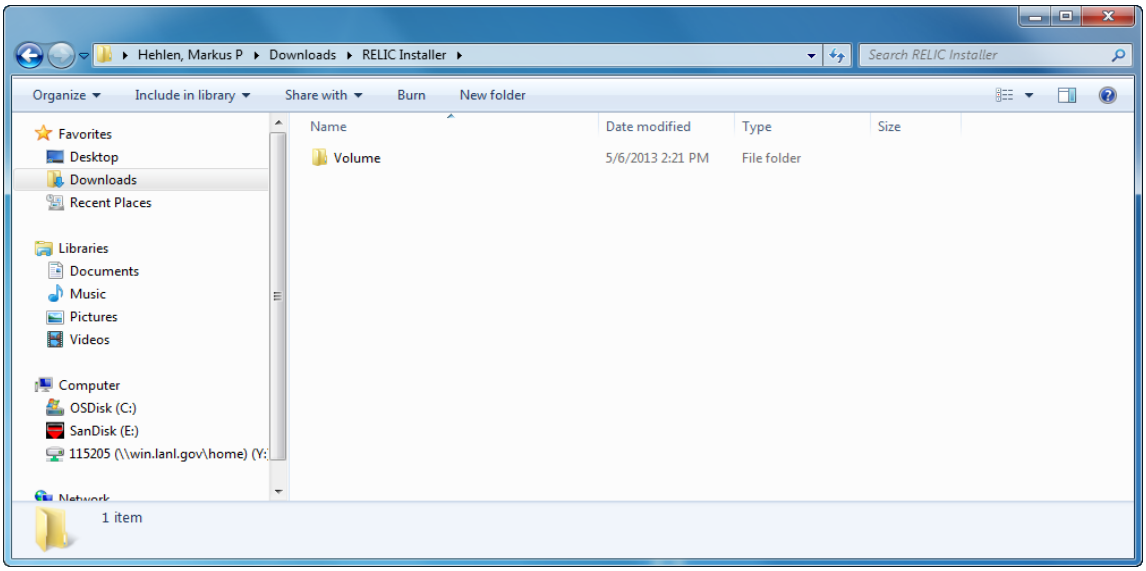
4. Right-click on the zip file and chose "Extract to here" to extract the zip file to the current folder. Note that this step requires you to have the WinZip software installed on your computer.



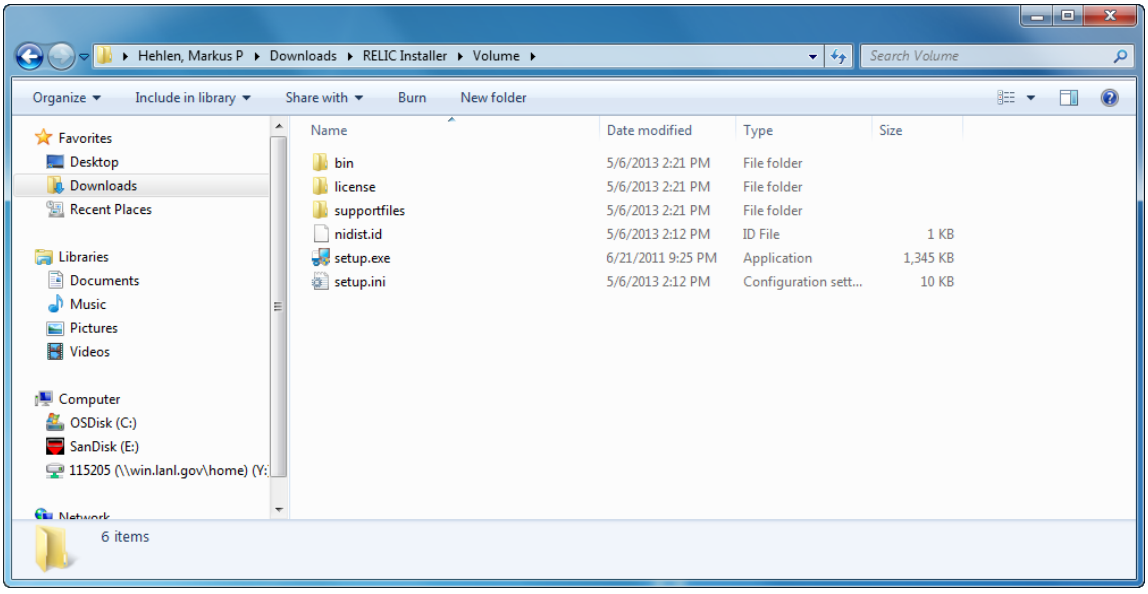
5. After the extraction has been completed, you see a new folder RELIC Installer. Double click on it to access its contents.



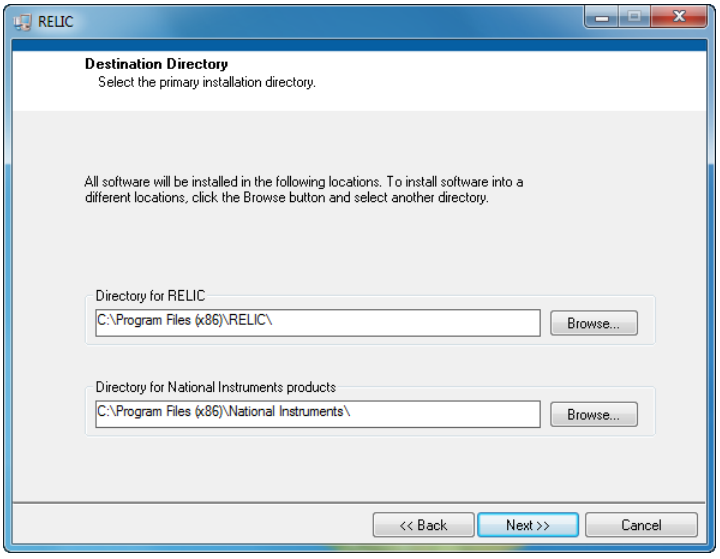
6. Double-click on the subfolder Volume to open it.



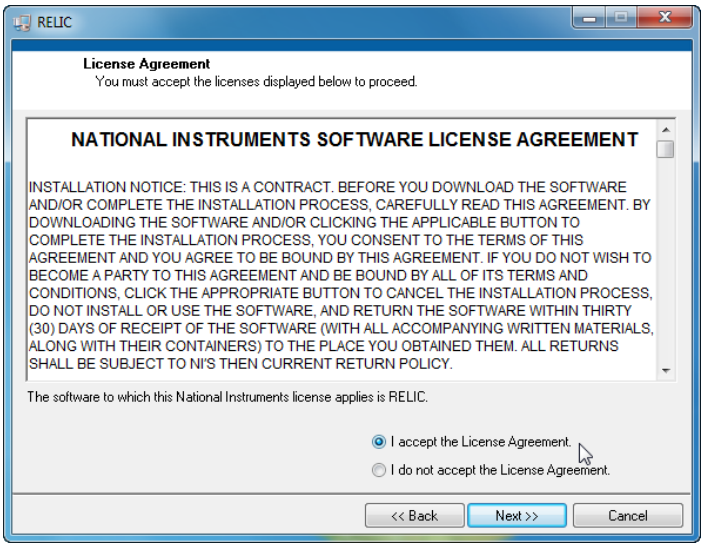
7. Double-click on Setup.exe to start the installation process.



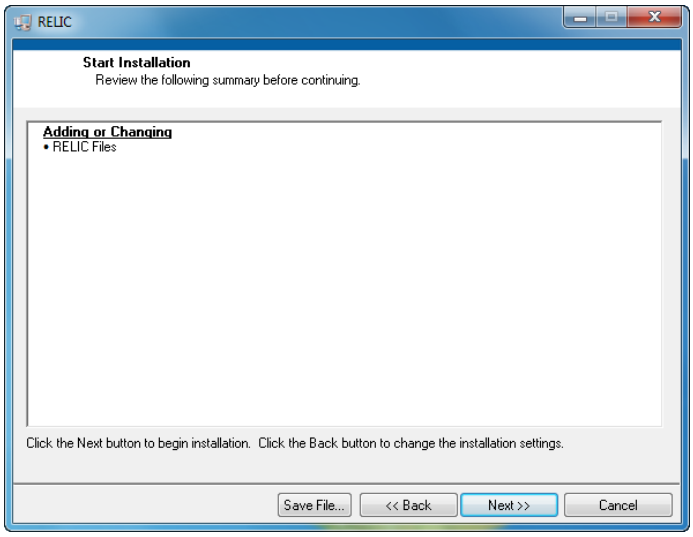
8. The RELIC Installer will start. Click Next to accept the creation of the new program folders. Do not change those.



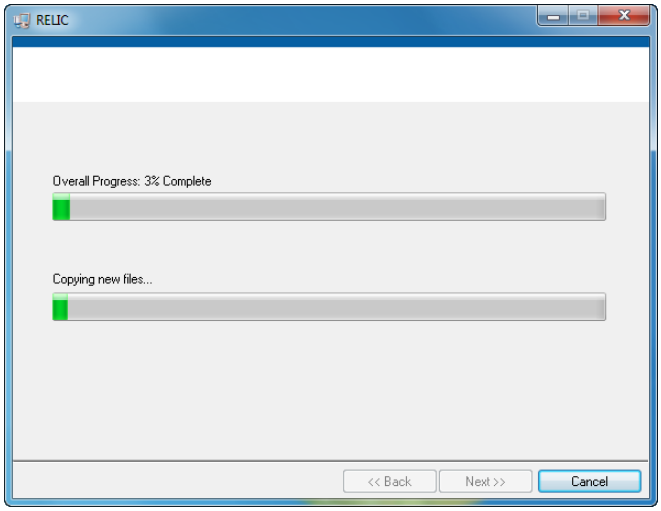
9. Accept the National Instruments License Agreement. This agreement covers the use of the LabView Run Time Engine, which executes the RELIC software. Click Next.



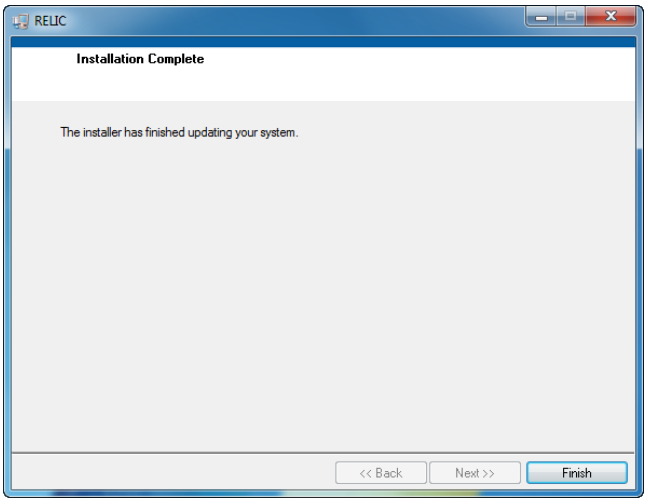
10. This page gives a summary of what will be installed. Click next to begin the installation of the RELIC files.



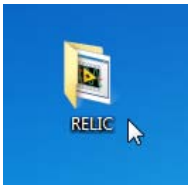
11. It may take several minutes to install all components as indicated by the progress bars.



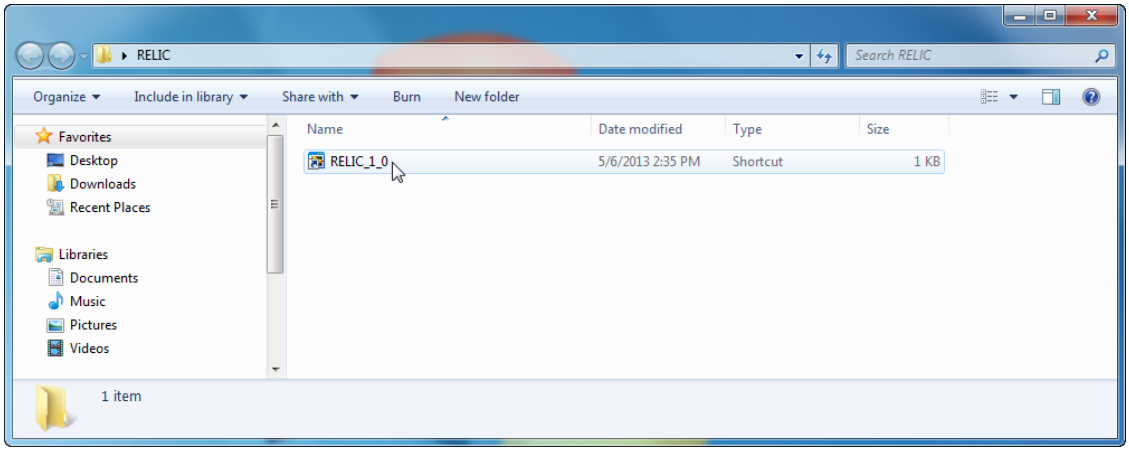
12. The installer will notify you once the installation has been completed. Click Finish to complete the process.



13. A shortcut to the RELIC software has been placed on the desktop. Double click on it.



14. Double-click on RELIC_1_0 to start the program.



15. RELIC will start up and you will see the RELIC main page. This completes the installation.

Table 1: Files contained in the RELIC 1.0 distribution.

Filename	Description
RELIC_1_0.exe	RELIC 1.0 stand-alone executable
RELIC_1_0.ini	RELIC 1.0 configuration file
RELIC_1_0.aliases	RELIC 1.0 support file
CFP.F2	Coefficients of fractional parentage for F2
CFP.F3	Coefficients of fractional parentage for F3
CFP.F4	Coefficients of fractional parentage for F4
CFP.F5	Coefficients of fractional parentage for F5
CFP.F6	Coefficients of fractional parentage for F6
CFP.F7	Coefficients of fractional parentage for F7
ELE.F1	Electrostatic matrix elements for F1
ELE.F2	Electrostatic matrix elements for F2
ELE.F3	Electrostatic matrix elements for F3
ELE.F4	Electrostatic matrix elements for F4
ELE.F5	Electrostatic matrix elements for F5
ELE.F6	Electrostatic matrix elements for F6
ELE.F7	Electrostatic matrix elements for F7
STATES.F1	$^{2S+1}L(\sigma)$ terms for F1
STATES.F2	$^{2S+1}L(\sigma)$ terms for F2
STATES.F3	$^{2S+1}L(\sigma)$ terms for F3
STATES.F4	$^{2S+1}L(\sigma)$ terms for F4
STATES.F5	$^{2S+1}L(\sigma)$ terms for F5
STATES.F6	$^{2S+1}L(\sigma)$ terms for F6
STATES.F7	$^{2S+1}L(\sigma)$ terms for F7
RELIC_1_0_UserGuide.pdf	RELIC 1.0 User Guide (this document)

3.3. Database Files

Table 1 lists all the files that have been placed in the RELIC program folder. For RELIC to work properly, it is essential to keep all distributed files in that one directory. To ensure proper operation, none of these files should be altered in any way.

RELIC calculations use three types of databases for each [Xe]$4f^n$ electron configuration. Do not change any of these files. The databases are:

- STATES.Fn: Databases containing the LS terms for the [Xe]$4f^n$ electron configurations. The first few LS(σ) terms of the [Xe]$4f^3$ electron configuration as contained in STATES.F3 are shown as an example below:

```
4S
4D
4F
4G
4I
2P
2D1
2D2
:
```

- CFP.Fn: Databases containing the coefficients of fractional parentage (CFP) [1]. The three columns are the SL final state ([Xe]$4f^n$), the SL parent state ([Xe]$4f^{n-1}$), and the corresponding CFP. The first few entries for the [Xe]$4f^3$ configuration as contained in CFP.F3 are shown as an example below:

```
4S     3F       1.00000000000
4D     3P      -0.65465367071
4D     3F      -0.47140452079
4D     3H      -0.59093684028
4F     3P       0.26726124191
4F     3F      -0.81649658093
4F     3H       0.51176631572
4G     3P       0.51176631572
4G     3F      -0.47140452079
2D1    3F      -0.62360956446
 :
```

- ELE.Fn: Databases containing the electrostatic matrix elements for the [Xe]$4f^n$ electron configurations [1]. The first two columns are the two coupling SL states followed by 4 columns containing the e_0, e_1, e_2, and e_3 coefficients of the respective Slater integrals [1, 2]. The first few entries for the [Xe]$4f^3$ configuration as contained in CFP.F3 are shown as an example below:

```
4S     4S         3.000000      0.000000      0.000000      0.000000
4D     4D         3.000000      0.000000      0.000000     33.000000
4F     4F         3.000000      0.000000      0.000000      0.000000
4G     4G         3.000000      0.000000      0.000000     12.000000
4I     4I         3.000000      0.000000      0.000000    -21.000000
2P     2P         3.000000      3.000000      0.000000    -11.000000
2D1    2D1        3.000000      3.000000   -122.571429     -4.714286
2D1    2D2        0.000000      0.000000   -384.065046     19.695643
2D2    2D2        3.000000      3.000000    161.571429      1.714286
2F1    2F1        3.000000      9.000000      0.000000      0.000000
2F1    2F2        0.000000      0.000000      0.000000    -28.142495
 :
```

4. Using RELIC

4.1. RELIC Folders

As described in the previous section, the installation creates a RELIC folder C:\Program Files. This folder contains the RELIC software executable, other support files, as well as the database files for the LS terms, coefficients of fractional parentage, and the electrostatic matrix elements (Table 1).

In addition, RELIC creates a new folder at C:\RELIC Data when RELIC runs the first time. This is the folder where all sample-specific data files created by the user during the course of the work are being stored. The folder will contain the following user-created files:

- Input files (extension INP): contain the input parameters for specific samples
- Archive files (extension ARC): contain the reduced matrix elements of the $U^{(2)}$, $U^{(4)}$, $U^{(6)}$, and L+gS tensors calculated by the user for specific samples
- Decay files (extension DEC): contain the results for a radiative decay calculation (rates, branching ratios, lifetimes) performed by the user for specific samples

As the calculation for a specific sample proceeds, the three respective files (INP, ARC, DEC) depend on each other. All three files are required to reside in the C:\RELIC Data folder for proper operation of RELIC.

4.2. Getting Started

When you first run RELIC you are asked to accept the Software End User License Agreement as shown in Figure 1. Click on the “Disclaimers and Terms of Use” button in the “Main Menu” and either accept or decline the Software End User Agreement by clicking on the respective button at the bottom of the “Workspace” field. All RELIC functions will activate after you accept the Software End User Agreement.

You will find screenshots of the RELIC user interface throughout this User Guide. We have highlighted program control functions with red boxes, data input fields with green boxes, and data output fields with blue boxes.

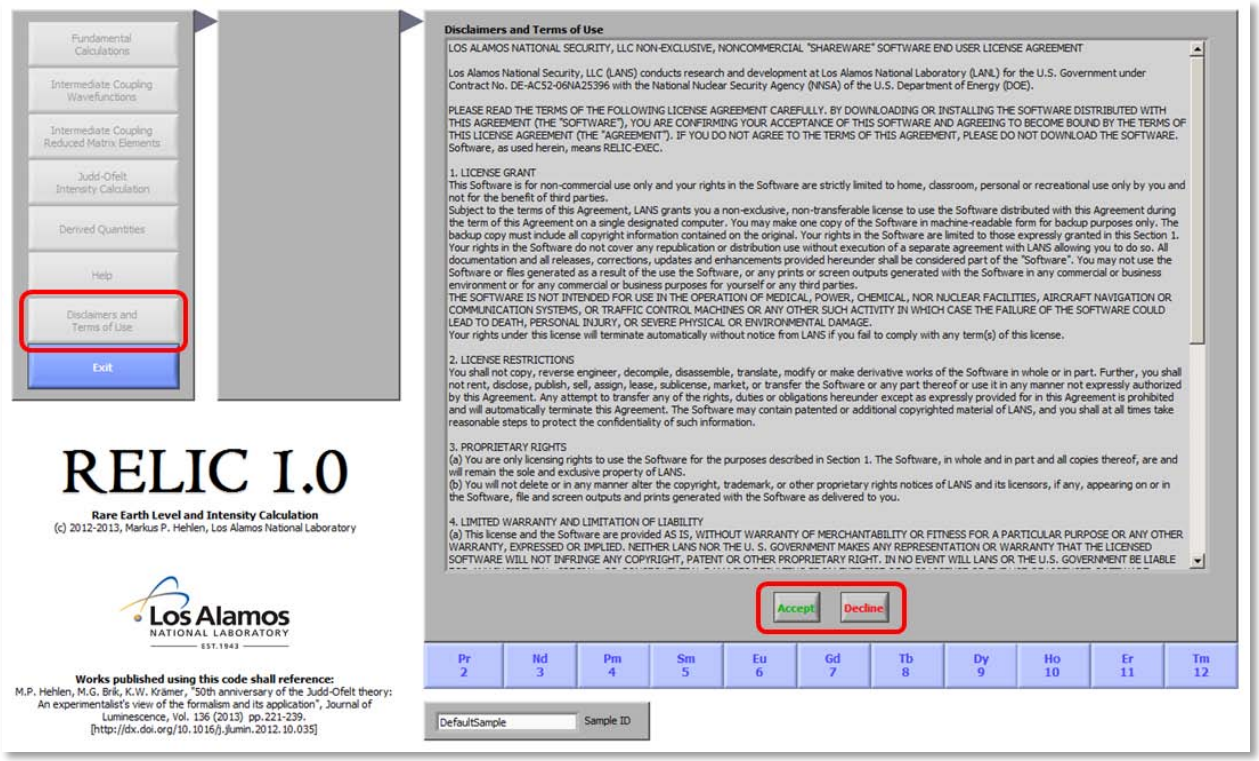


Figure 1: Accepting the Software End User Agreement.

4.3. General Considerations

RELIC is operated through a graphical user interface (GUI). A screenshot of a typical RELIC page is shown in Figure 2. All functions are accessed by clicking on the respective button in the *Main Menu*. Depending on your *Main Menu* choice, the functions in the *Sub Menu* change. At this point you can return to the *Main Menu* by clicking the Return button in the *Sub Menu*. You can exit RELIC by clicking the Exit button in the *Main Menu*.

Once you click on a function in the *Sub Menu* several input and/or output windows appear in the *Workspace* field. The number and type of windows depend on the function you have activated. Each function will be discussed in detail in the following. By clicking the OK button in the bottom right corner you can exit the *Workspace* field and return to the *Sub Menu*.

You also find the sequence and abbreviations for the rare earth ions from Pr^{3+} to Tm^{3+} along with the number of 4f electrons for the respective $[Xe]4f^{2}$ to $[Xe]4f^{12}$ configurations. This bottom bar is just for reference and has no accessible function.

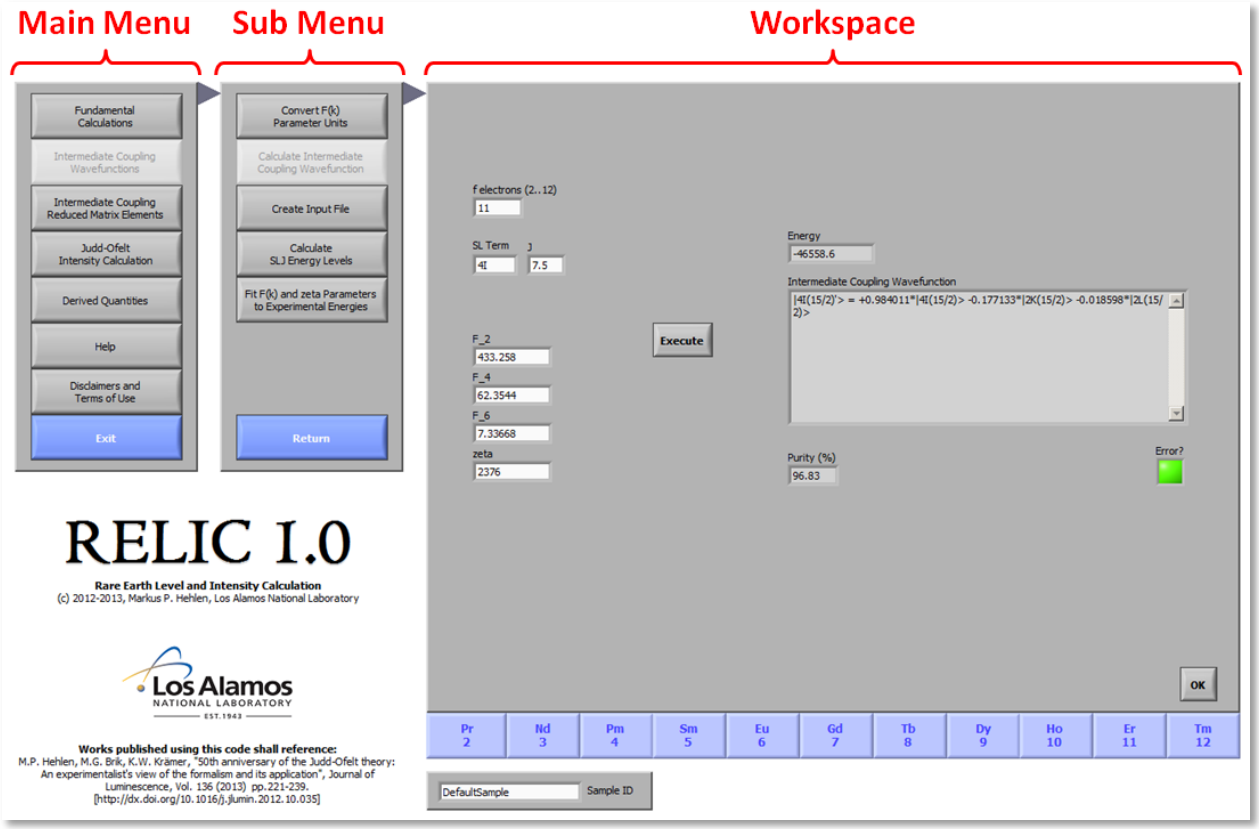


Figure 2: Example screenshot of the RELIC graphical user interface.

At the bottom of the GUI you see a box for entering the name of the sample you want to work on. All sample-specific files you create and edit (INP, ARC, DEC) will be assigned a filename that corresponds to the Sample ID entered in this box. If you do not enter a sample ID, then the name "DefaultSample" will be used. Changing the sample ID in this box allows you to work with different samples and keep the respective data organized in separate files within the C:\RELIC Data folder.

4.4. Fundamental Calculations

RELIC 1.0 makes extensive use of fundamental quantum mechanical quantities such as the coefficients of fractional parentage, electrostatic matrix elements, Wigner 3j and 6j symbols, and reduced matrix elements of the $V^{(1x)}$, $U^{(k)}$, and L+gS tensor operators. You do not have to access these low-level functions if you are only interested in calculating wavefunctions, energy levels, or oscillator strengths. However, explicit access to each of these functions is provided by clicking the "Fundamental Calculations" button in the Main Menu. As shown in Figure 3, this brings up a new Sub Menu with buttons for these 7 functions.

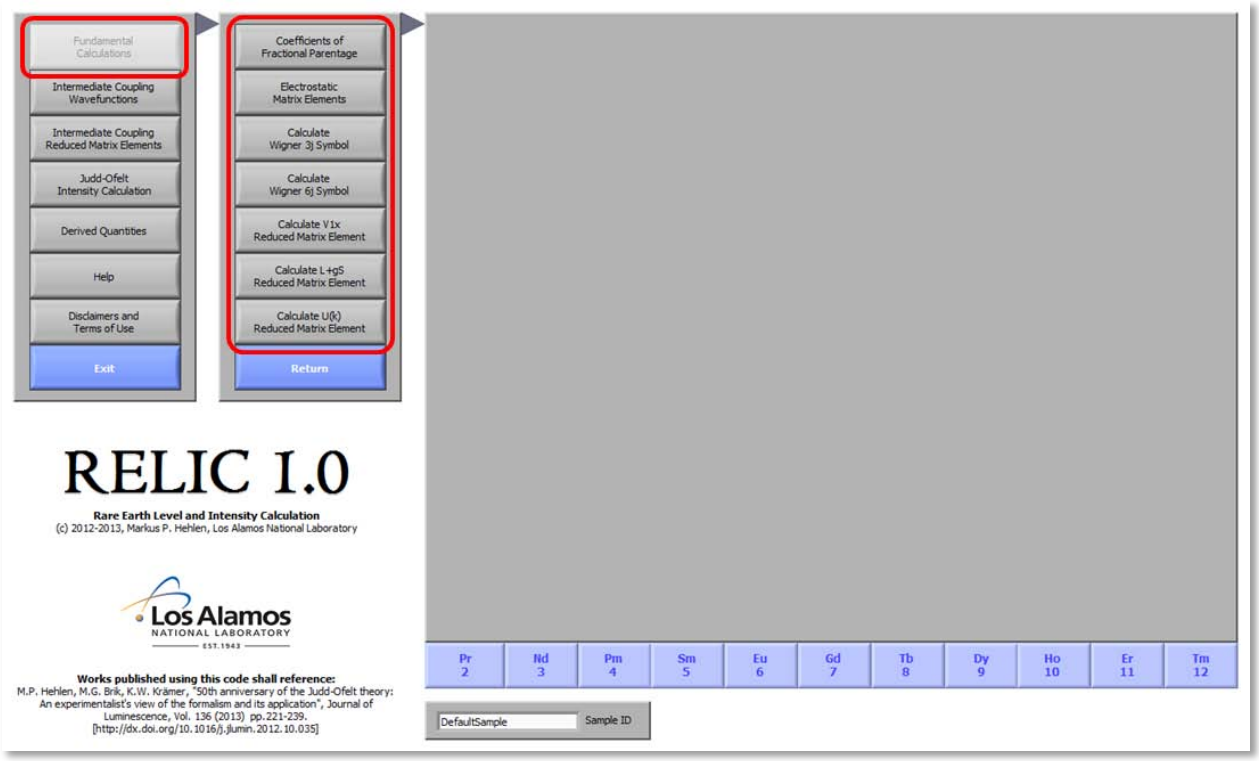


Figure 3: Sub menu activated by clicking the "Fundamental Calculations" button in the Main Menu.

4.4.1. Coefficients of Fractional Parentage (CFP)

Activating the "Coefficients of Fractional Parentage" function brings up the Workspace fields shown in Figure 4. Enter any number of f-electrons ranging from 2 to 7 in the respective input field and click the "Execute" button (circled by green box). RELIC will retrieve the CFPs for this configuration from the respective data file (see Table 1) and display them in the output field (circled by blue box). The output field has a scroll bar on the right hand side that allows scrolling though the entire list of CFP. The 3 columns in the table are the final (daughter) $|SL\rangle$ term of the [Xe]4f^N configuration, the parent $|SL\rangle$ term of the [Xe]4f^{N-1} configuration, and the respective CFP. You can bring up the CFPs for another configuration by updating the number in the "f-electrons" field and again clicking the "Execute" button. Return to the Sub Menu by clicking the "OK" button.

For the development of RELIC, the CFPs were taken from the original works of Nielsen and Koster [1]. This CFP database was subsequently double-checked against the CFPs published by published by Johns Hopkins University [3] to ensure correctness and consistency.

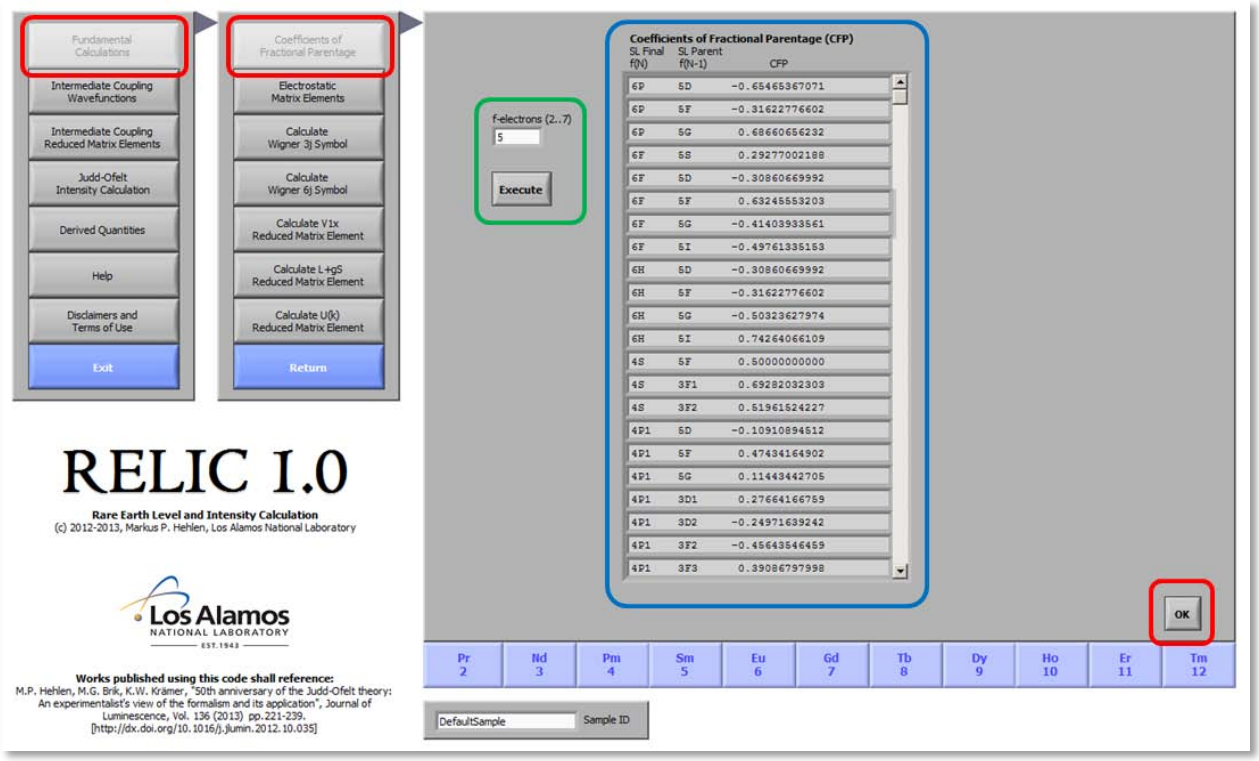


Figure 4: *Displaying the coefficients of fractional parentage.*

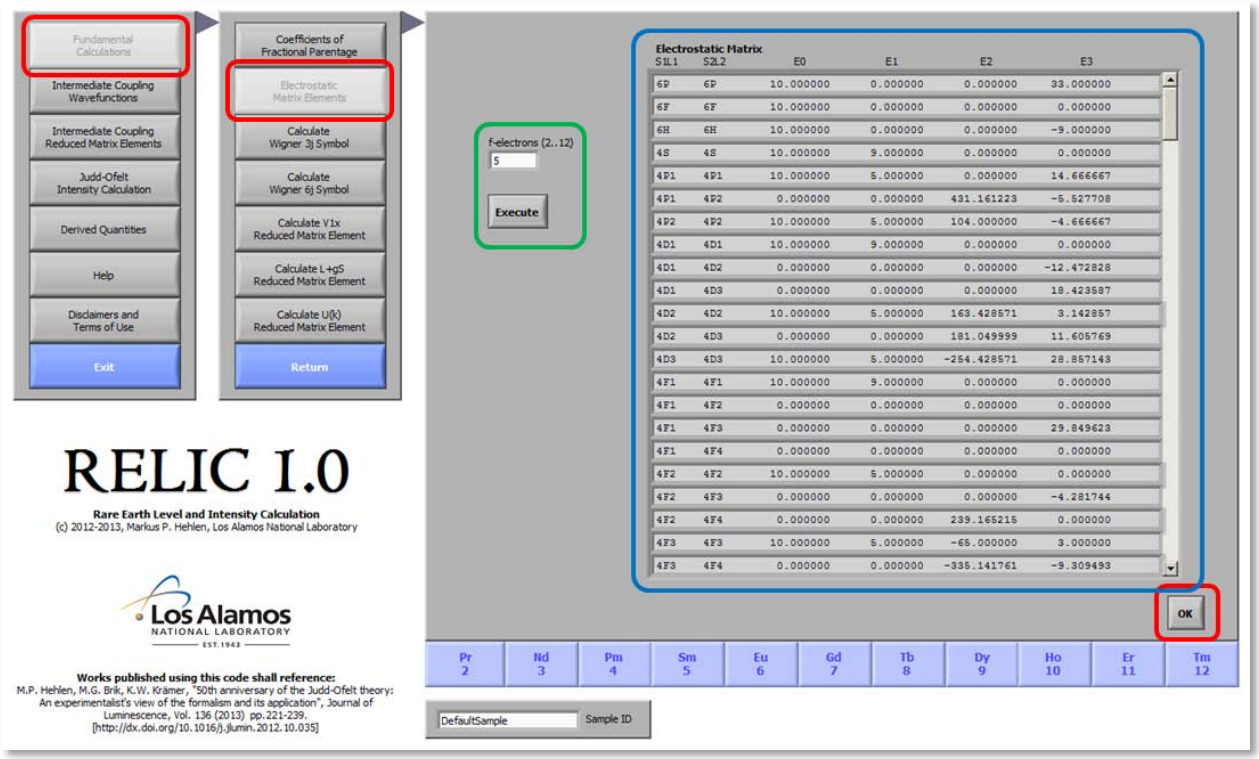


Figure 5: *Displaying the electrostatic matrix elements.*

4.4.2. Electrostatic Matrix Elements

Activating the “Electrostatic Matrix Elements” function brings up the Workspace fields shown in Figure 5. Enter any number of f-electrons ranging from 2 to 7 in the respective input field and click the “Execute” button (circled by green box). RELIC will retrieve the electrostatic matrix elements for this configuration from the respective data file (see Table 1) and display them in the output field (circled by blue box). You can bring up the electrostatic matrix elements for another configuration by updating the number in the “f-electrons” field and again clicking the “Execute” button. Return to the Sub Menu by clicking the “OK” button.

The output field has a scroll bar on the right hand side that allows scrolling though the entire list of electrostatic matrix elements. The 6 columns in the table are the first and second $|SL\rangle$ term that couple followed by the coefficients e_0, e_1, e_2, and e_3 of the sum [2]

$$\langle 4f^n SL|\hat{H}_e|4f^n S'L'\rangle = \sum_{k=0}^{3} e_k E^{(k)} \tag{1}$$

In (1), the coefficients $E^{(0)}$, $E^{(1)}$, $E^{(2)}$, and $E^{(3)}$ are given by the relations

$$\begin{aligned} E^{(0)} &= F_{(0)} - 10F_{(2)} - 33F_{(4)} - 286F_{(6)} \\ E^{(1)} &= \left(70F_{(2)} + 231F_{(4)} + 2002F_{(6)}\right)/9 \\ E^{(2)} &= \left(F_{(2)} - 3F_{(4)} + 7F_{(6)}\right)/9 \\ E^{(3)} &= \left(5F_{(2)} + 6F_{(4)} - 91F_{(6)}\right)/3 \end{aligned} \tag{2}$$

where $F_{(0)}$, $F_{(2)}$, $F_{(4)}$, and $F_{(6)}$ are the electrostatic interaction parameters [2]. The electrostatic matrix elements in RELIC 1.0 were taken from the original works of Nielsen and Koster [1] and the databases were double-checked manually.

4.4.3. Calculate Wigner 3j Symbol

Activating the “Calculate Wigner 3j Symbol” function brings up the Workspace fields shown in Figure 6. Enter the 6 numbers that make up the Wigner 3j symbol and click the “Execute” button (circled by green box). RELIC will calculate the respective Wigner 3j coefficient and display it in the output field (circled by blue box). You can calculate another Wigner 3j symbol by updating the 6 numbers and again clicking the “Execute” button. Return to the Sub Menu by clicking the “OK” button.

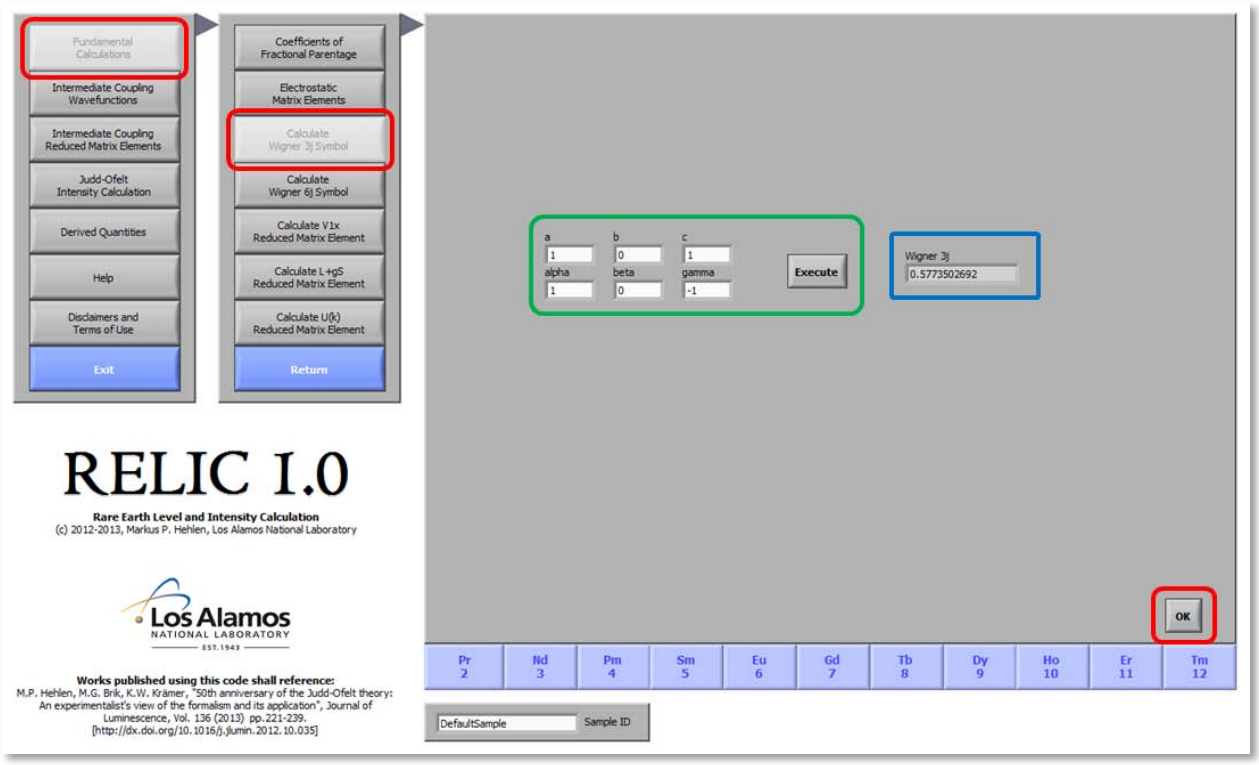


Figure 6: *Evaluating Wigner 3j symbols.*

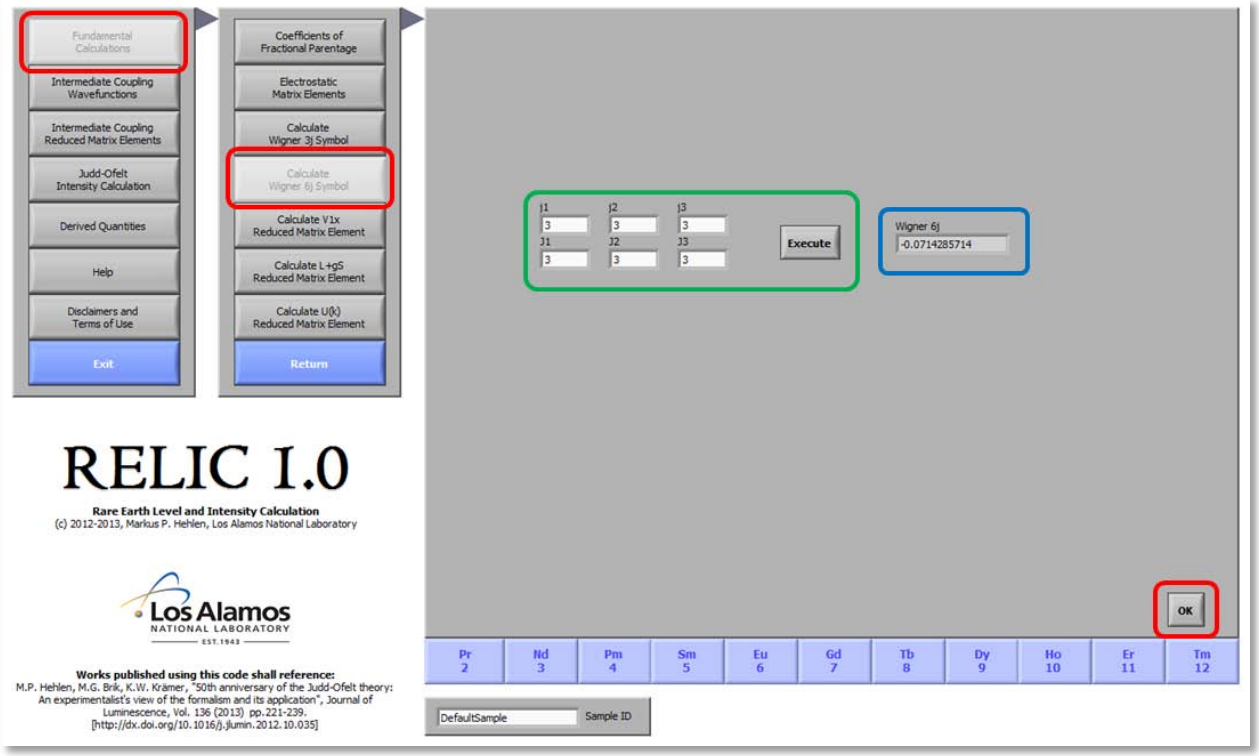


Figure 7: *Evaluating Wigner 6j symbols.*

The Wigner 3j coefficient is calculated according to

$$\begin{pmatrix} a & b & c \\ \alpha & \beta & \gamma \end{pmatrix} = (-1)^{a-b-\gamma}\sqrt{\Delta(a,b,c)}\sqrt{(a+\alpha)!\,(a-\alpha)!\,(b+\beta)!\,(b-\beta)!\,(c+\gamma)!\,(c-\gamma)!}\sum_t \frac{(-1)^t}{x(t)} \quad (3)$$

where $x(t) = t!(c-b+t+\alpha)!(c-a+t-\beta)!(a+b-c-t)!(a-t-\alpha)!(b-t+\beta)!$, the sum is taken over all t for which all factorials in $x(t)$ are ≥ 0, and the triangle coefficient is given by $\Delta(a,b,c) = (a+b-c)!(a-b+c)!(-a+b+c)!/(a+b+c+1)!$ [2].

4.4.4. Calculate Wigner 6j Symbol

Activating the "Calculate Wigner 6j Symbol" function brings up the Workspace fields shown in Figure 7. Enter the 6 numbers that make up the Wigner 6j symbol and click the "Execute" button (circled by green box). RELIC will calculate the respective Wigner 6j coefficient and display it in the output field (circled by blue box). You can calculate another Wigner 6j symbol by updating the 6 numbers and again clicking the "Execute" button. Return to the Sub Menu by clicking the "OK" button.

The Wigner 6j coefficient is calculated according to [2]

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ J_1 & J_2 & J_3 \end{Bmatrix} = \sqrt{\Delta(j_1,j_2,j_3)\Delta(j_1,J_2,J_3)\Delta(J_1,j_2,J_3)\Delta(J_1,J_2,j_3)}\sum_t \frac{(-1)^t(t+1)!}{f(t)} \quad (4)$$

where $\Delta(a,b,c)$ is the triangle coefficient (see 4.4.3. Calculate Wigner 3j Symbol), the sum is taken over all t for which all factorials in $f(t)$ are ≥ 0, and

$$f(t) = (t-j_1-j_2-j_3)!(t-j_1-J_2-J_3)!(t-J_1-j_2-J_3)! (t-J_1-J_2-j_3)!(j_1+j_2+J_1+J_2-t)!(j_2+j_3+J_2+J_3-t)!(j_3+j_1+J_3+J_1-t)! \quad (5)$$

4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element

Activating the "Calculate V(1x) Reduced Matrix Element" function brings up the Workspace fields shown in Figure 8. Enter the number of f-electrons of the configuration of interest, the $|SL\rangle$ term of the first state, the rank x of the V(1x) tensor operator, the $|SL\rangle$ term of the second state, and click the "Execute" button (circled by green box). RELIC will calculate the respective $V^{(1x)}$ reduced matrix element and display it in the output field (circled by blue box). You can calculate another $V^{(1x)}$ matrix element by updating the input fields and again clicking the "Execute" button. Return to the Sub Menu by clicking the "OK" button.

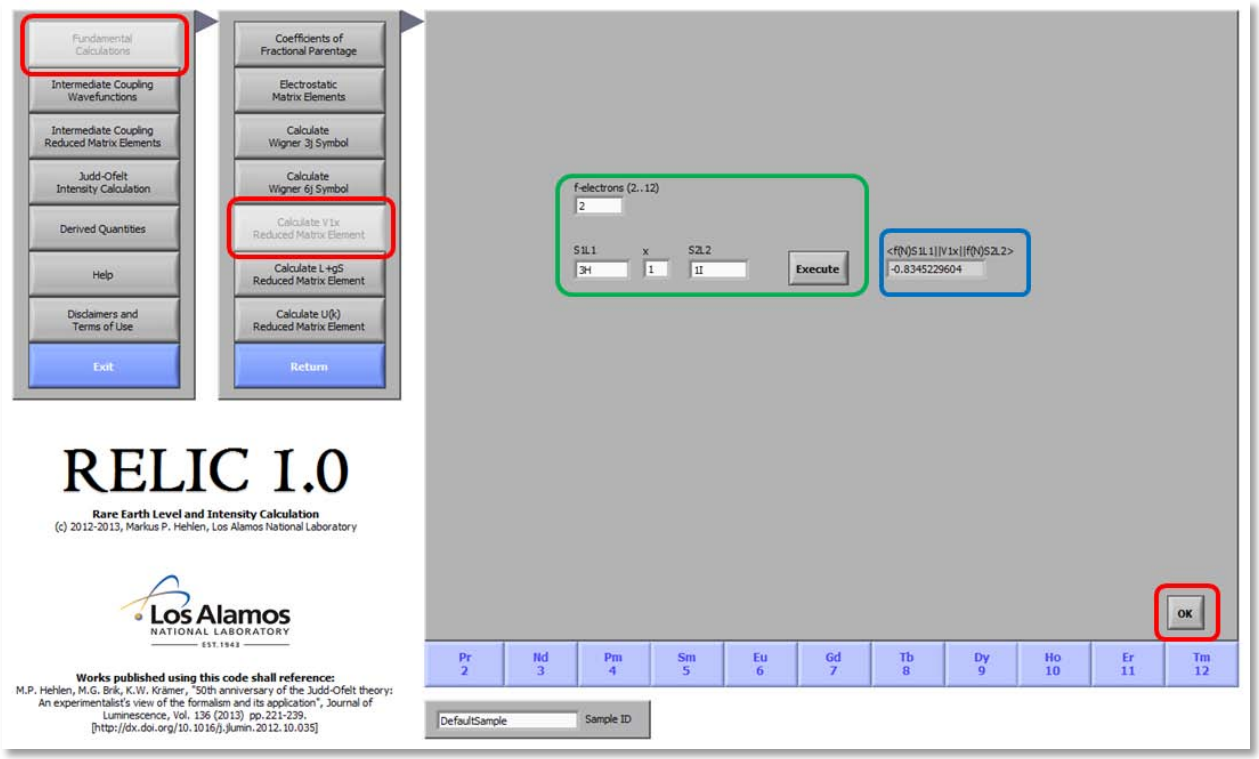


Figure 8: Calculating the matrix element of the $V^{(1x)}$ tensor operator.

In RELIC, $|SL\rangle$ terms are entered alphanumerically by first giving the number for the spin multiplicity (2S+1), followed by a character signifying the angular orbital momentum (L), and finally (if applicable) a number indicating the seniority number. The seniority number is omitted by default and is only added if there exist more than one $|SL\rangle$ state with the same S and L for the given configuration. The characters signifying the angular orbital momentum are given by the usual conventions shown in Table 2.

For example, a $|SL\rangle$ term with S=3/2 and L=4 would be entered as "4G". As another example consider the $|SL\rangle$ term with S=1/2 and L=5 of the [Xe]$4f^3$ electron configuration. There exist two such terms, and they would be entered as "2H1" and

"2H2", where the last number represents the seniority number 1 and 2, respectively, that is used to distinguish them.

Table 2: *Letter symbols for the orbital angular momentum quantum numbers.*

L=	0	1	2	3	4	5	6	7	8	9	10	11	12
	S	P	D	F	G	H	I	K	L	M	N	O	Q

The $V^{(1x)}$ reduced matrix element is calculated according to [2]

$$\left\langle l^N SL \left\| \mathrm{V}^{(1x)} \right\| l^N S'L' \right\rangle = N\sqrt{s(s+1)(2s+1)(2S+1)(2L+1)(2S'+1)(2L'+1)} \times \sum_{\psi\left(l^{N-1}\right)} \left(l^{N-1}\overline{SL} \middle| l^N SL \right) \begin{Bmatrix} S & S' & 1 \\ s & s & \bar{S} \end{Bmatrix} \begin{Bmatrix} L & L' & x \\ l & l & \bar{L} \end{Bmatrix} (-1)^{\bar{S}+\bar{L}+S+L+s+l+x+1} \tag{6}$$

where $s = ½$ and $l = 3$ (for *f*-electrons). RELIC automatically chooses the correct sign of the matrix element by using the relation $\left\langle l^{14-N} SL \left\| \mathrm{V}^{(1x)} \right\| l^{14-N} S'L' \right\rangle = (-1)^x \left\langle l^N SL \left\| \mathrm{V}^{(1x)} \right\| l^N S'L' \right\rangle$ for the conjugate $4f^{14-N}$ electron configuration [1].

4.4.6. Calculate L+gS Reduced Matrix Element

Activating the "Calculate L+gS Reduced Matrix Element" function brings up the Workspace fields shown in Figure 9. Enter the $|SL\rangle$ term and J quantum number of the first state followed by the $|SL\rangle$ term and J quantum number of the second state, and then click the "Execute" button (circled by green box). RELIC will calculate the respective L+gS reduced matrix element and display it in the output field (circled by blue box). Refer to Section *4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element* for instructions on how to enter the $|SL\rangle$ terms. The J quantum number is a multiple of (1/2). Non-integer J values are entered as decimals, and integer J values are entered as that integer number. For example, J=13/2 is entered as "6.5", and J=4 is entered as "4". You can calculate another L+gS matrix element by updating the input fields and again clicking the "Execute" button. Return to the Sub Menu by clicking the "OK" button.

The L+gS matrix element is calculated according to [2]

$$\left\langle l^N SL\, J \left\| \mathrm{L} + g\mathrm{S} \right\| l^N SLJ' \right\rangle = g\sqrt{J(J+1)(2J+1)} \tag{7}$$

for $J' = J$ and

$$\left\langle l^N SL\, J \left\| \mathrm{L} + g\mathrm{S} \right\| l^N SL\,(J-1) \right\rangle = (g-1)\sqrt{\frac{(S+L+J+1)(J+L-S)(J+S-L)(S+L-J+1)}{4J}} \tag{8}$$

for $J' = J - 1$, where $g = 2.002319304362$ is the *g*-factor of the electron.

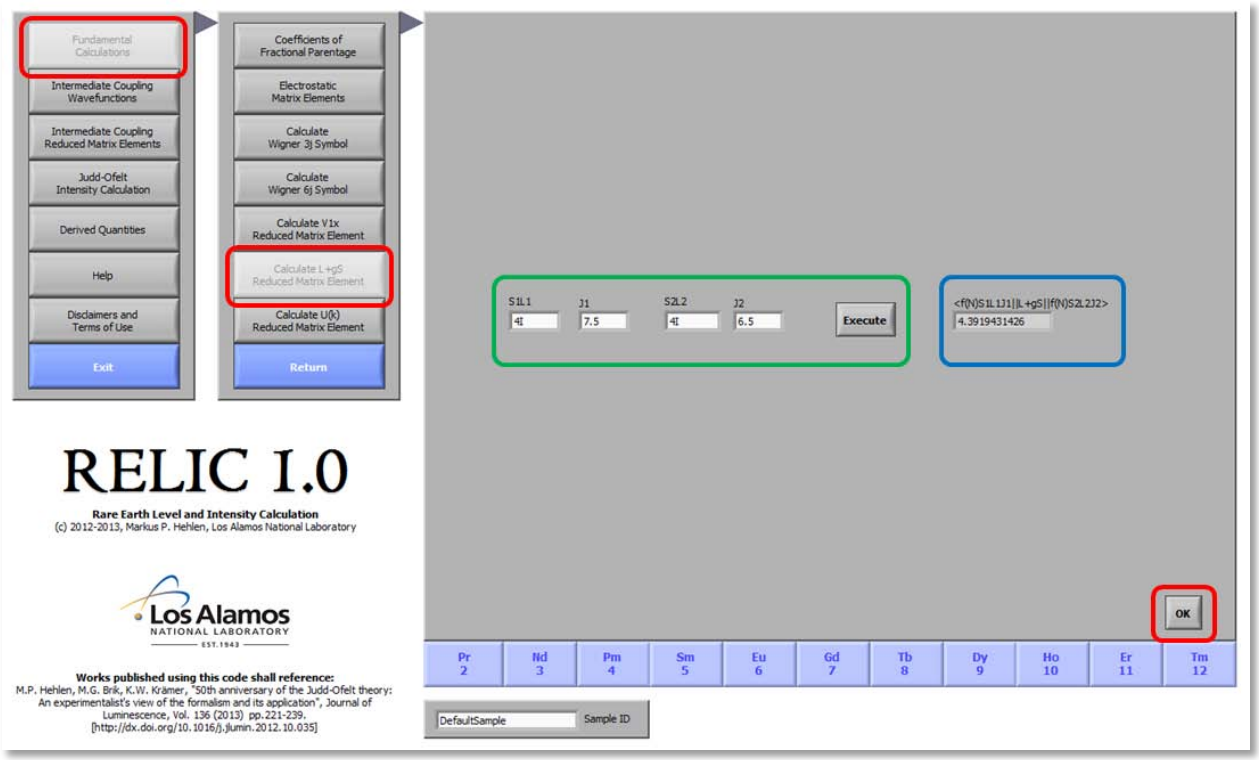


Figure 9: Calculating the matrix element of the L+gS tensor operator.

4.4.7. Calculate U(k) Reduced Matrix Element

Activating the "Calculate U(k) Reduced Matrix Element" function brings up the Workspace fields shown in Figure 10. Enter the $|SL\rangle$ term of the first state, the rank k of the $U^{(k)}$ tensor operator, followed by the $|SL\rangle$ term of the second state, and then click the "Execute" button (circled by green box). RELIC will calculate the respective $U^{(k)}$ reduced matrix element and display it in the output field (circled by blue box). Refer to Section *4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element* for instructions on how to enter the $|SL\rangle$ terms. You can calculate another $U^{(k)}$ matrix element by updating the input fields and again clicking the "Execute" button. Return to the Sub Menu by clicking the "OK" button.

The $U^{(k)}$ reduced matrix element is calculated according to [2]

$$\left\langle l^N SL \left\| \mathrm{U}^{(k)} \right\| l^N SL' \right\rangle = N\sqrt{(2L+1)(2L'+1)} \sum_{\psi\left(l^{N-1}\right)} \left(l^{N-1}\overline{SL} \middle| l^N SL \right) \begin{Bmatrix} L & l & \overline{L} \\ l & L' & k \end{Bmatrix} (-1)^{\overline{L}+L+l+k} \tag{9}$$

RELIC automatically chooses the correct sign of the matrix element by using the relation $\left\langle l^{14-N} SL \left\| \mathrm{U}^{(k)} \right\| l^{14-N} S'L' \right\rangle = -(-1)^k \left\langle l^N SL \left\| \mathrm{U}^{(k)} \right\| l^N S'L' \right\rangle$ for the conjugate $4f^{14-N}$ electron configuration [1].

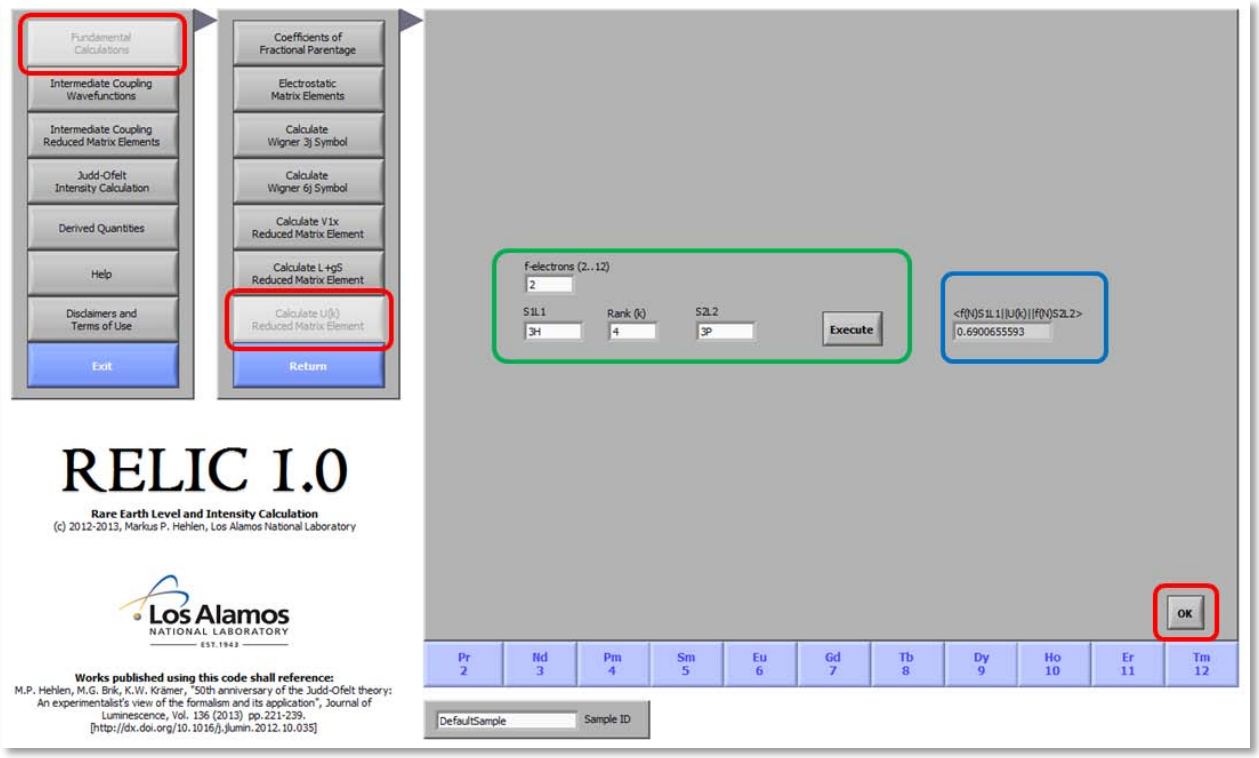


Figure 10: Calculating the matrix element of the $U^{(k)}$ tensor operator.

4.5. Intermediate Coupling Wavefunctions

Clicking on "Intermediate Coupling Wavefunctions" in the Main Menu brings up a new Sub Menu with buttons for 5 functions as shown in Figure 11. This group of functions allows for the calculation of individual $|SLJ\rangle$ wavefunctions, calculations of $|SLJ\rangle$ energy levels for a material, and the least-squares fitting of the electrostatic $F_{(k)}$ and spin-orbit ζ parameters to a set of experimental barycenter energies. This group of functions also

allows for the creation of an input file that contains experimental data obtained for a sample.

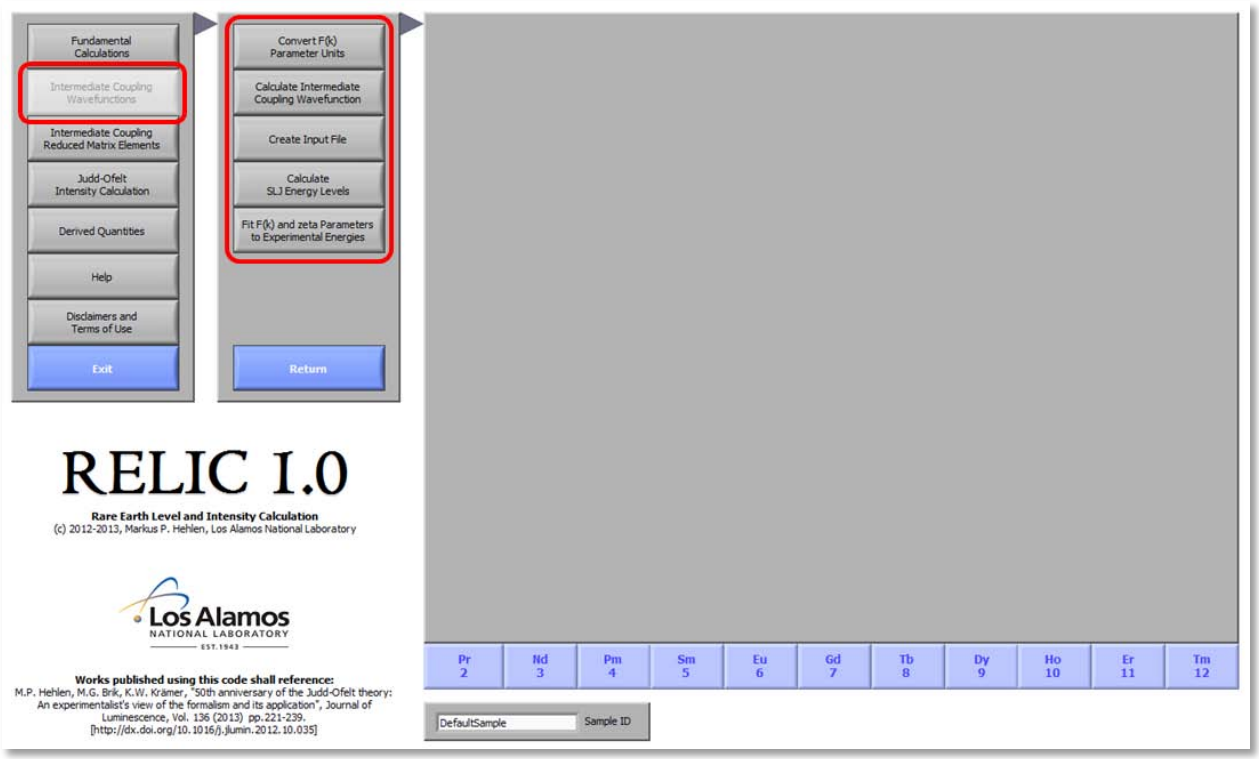


Figure 11: Sub menu activated by clicking the "Intermediate Coupling Wavefunctions" button in the Main Menu.

4.5.1. Convert $F_{(k)}$/ $F^{(k)}$ Parameter Units

There are two definitions for the electrostatic parameters common in the literature, $F_{(k)}$ and $F^{(k)}$, where k=2,4,6. Both represent an energy and are given in units of wavenumbers [cm^{-1}]. RELIC 1.0 consistently uses the $F_{(k)}$ representation. The two representations are related by [2]

$$\begin{aligned} F_{(0)} &= F^{(0)} \\ F_{(2)} &= F^{(2)}/225 \\ F_{(4)} &= F^{(4)}/1089 \\ F_{(6)} &= 25F^{(6)}/184041 \end{aligned} \tag{10}$$

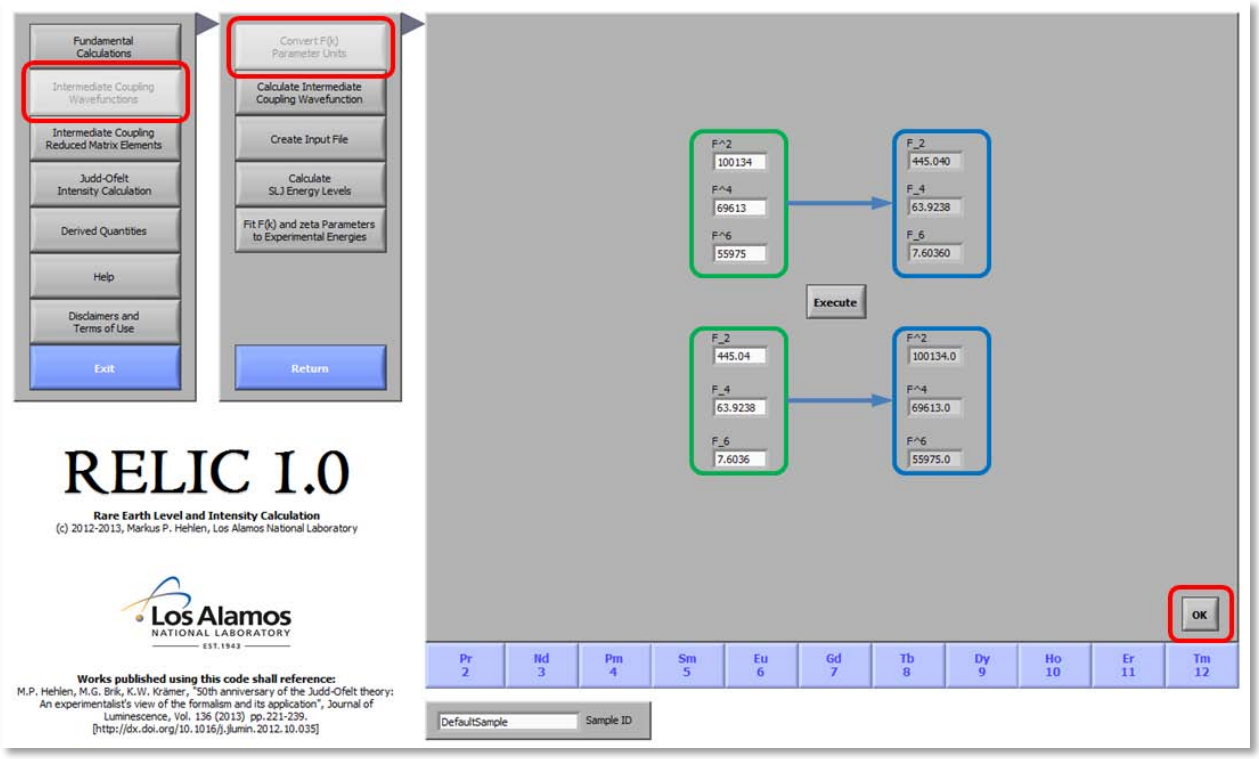


Figure 12: Performing $F^{(k)} \leftrightarrow F_{(k)}$ electrostatic parameter conversions.

Activating the "Convert F(k) Parameter Units" function brings up the Workspace fields shown in Figure 12. Enter the $F^{(k)}$ values in the top left fields (circled by green box) and then click the "Execute" button to convert them to the respective $F_{(k)}$ values (circled by blue box). In analogy, $F_{(k)}$ values can be converted to the respective $F^{(k)}$ values by using the lower fields in the same manner. You can do another conversion by updating the input fields and again clicking the "Execute" button. Return to the Sub Menu by clicking the "OK" button.

4.5.2. Calculate Intermediate Coupling Wavefunction

Activating the "Calculate Intermediate Coupling Wavefunction" function brings up the Workspace fields shown in Figure 13. Enter the number of f-electrons for the configuration at hand, enter the $|SL\rangle$ term of the desired wavefunction (Refer to Section 4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element for instructions on how to enter the $|SL\rangle$ terms), enter the J value of the desired wavefunction (Refer to Section 4.4.6. Calculate L+gS Reduced Matrix Element for instructions on how to enter J values), enter the electrostatic parameters $F_{(2)}$, $F_{(4)}$, $F_{(6)}$ (in [cm^{-1}]; note that RELIC uses $F_{(k)}$ representation; see Section 4.5.1. Convert F(k)/ $F^{(k)}$ Parameter Units), enter the spin-orbit coupling constant (in [cm^{-1}]), and then click the "Execute" button (circled by green box). The function calculates the energy (in [cm^{-1}]), the wavefunction, and the purity of the $|SLJ\rangle$ term. The purity is the contribution of the $|SLJ\rangle$ term (in %) to the overall

wavefunction, i.e. $1/c_i^2$ where c_i is the coefficient of the $|SLJ\rangle$ term in the wavefunction. Note that energies are given on an arbitrary absolute scale because the $F_{(0)}$ parameter, which produces an uniform shift of all $|SLJ\rangle$ energy levels, has been omitted. Energies should be referenced relative to the $|SLJ\rangle$ ground state of the given configuration, which can be found by using Hund's rules [2]. The output section also contains an "Error?" indicator. It is green if no error occurred in the calculation, and it is "red" if the requested $|SLJ\rangle$ term was not found for the given [Xe]$4f^N$ electron configuration. You can calculate another wavefunction by updating the input fields and again clicking the "Execute" button. Return to the Sub Menu by clicking the "OK" button.

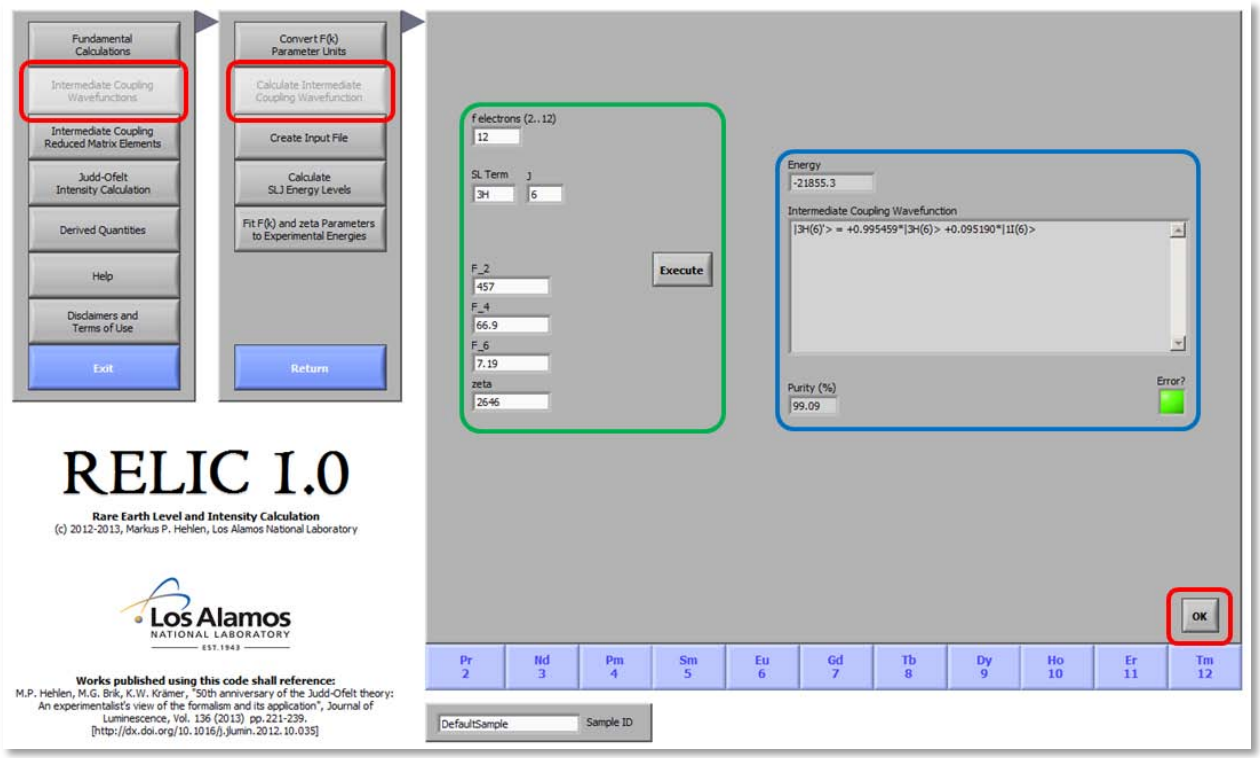


Figure 13: Calculating an intermediate coupling wavefunction (associated energy) of an $|SLJ\rangle$ term of an [Xe]$4f^N$ electron configuration given a set of electrostatic ($F_{(2)}$, $F_{(4)}$, $F_{(6)}$) and spin-orbit coupling (ζ) parameters.

4.5.3. Create Input File

The next function allows you to create an input file that contains the various parameters for a specific sample. *Before* you activate this function be sure to enter the "Sample ID" in the respective box at the bottom of the workspace. We will use an Er3+-doped glass as one of the examples in this guide, and the respective Sample ID was entered as "ErGlass". It is advisable to keep Sample IDs to a maximum length of 8 characters (no

spaces or special characters). Examples of good input filenames are “ErYLF” or “TmZBLAN”, while “Pr:YAG” or “Er YAG crystal” are not advisable.

Activating the “Create Input File” function brings up the Workspace fields shown in Figure 14. Here you can enter the experimental energies (in [cm^{-1}]) and experimental oscillator strengths for transitions from one $|SLJ\rangle$ multiplet (SL and J initial) to another $|SLJ\rangle$ multiplet (SL and J final), information on the material refractive index or dispersion (Sellmeier coefficients), electrostatic ($F_{(k)}$), spin-orbit coupling (ζ), and Judd-Ofelt intensity ($\Omega_{(k)}$) parameters, the number of 4f electrons, a one-line text description for a specific sample. The various fields are discussed in more detail below.

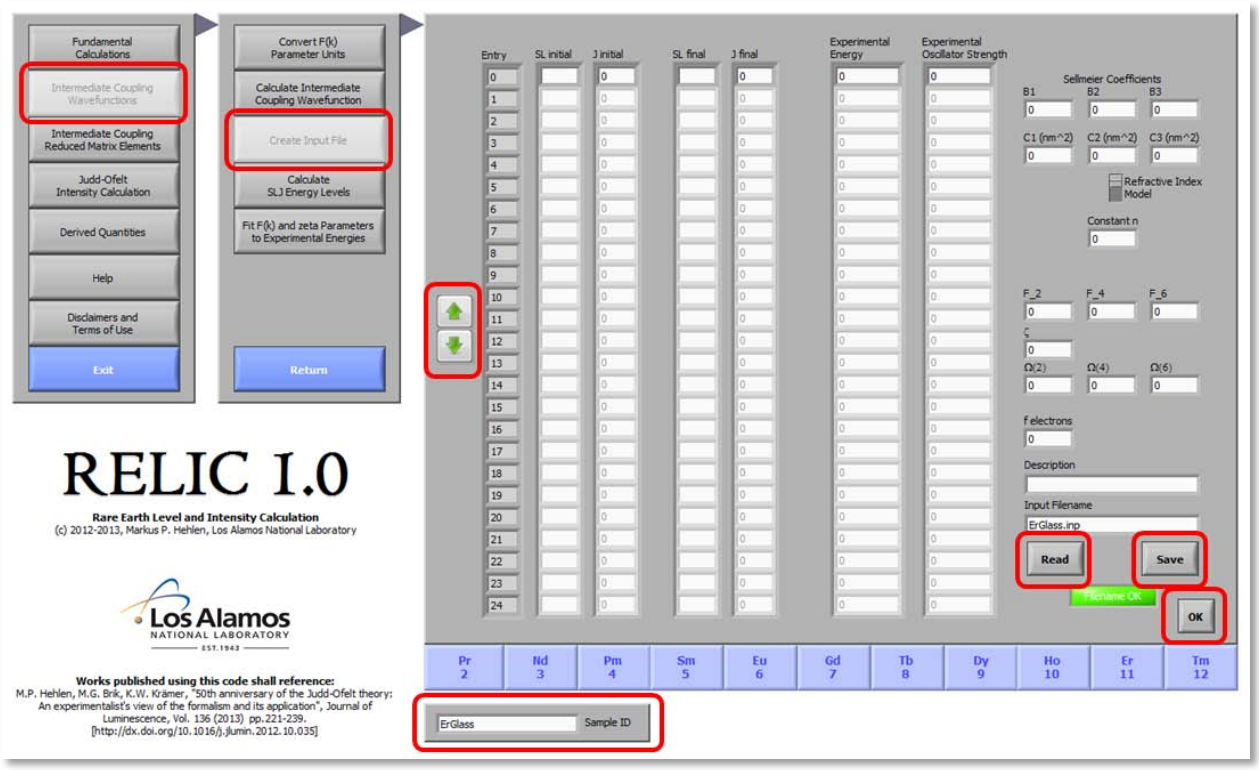


Figure 14: Workspace for creating and editing material specific input files. The buttons used to navigate the workspace are circled red (see text).

There are five navigation buttons in the workspace shown in Figure 14:

- The “Save” button saves all data currently entered in the various fields into a text file having the name specified in the “Filename” field.

- The “Read” button loads the data contained in the file specified in the “Filename” field and populates the respective fields in the workspace. This allows you to read an existing files, make changes, and then click “Save” again to store the latest version. If the specified filename was not found when clicking “Read” then

the indicator below will turn red and say “Invalid Filename”. Correct the filename and click “Read” again. If the file was found then the indicator below will say “Filename OK”.

- If you have more than 24 transitions, you can use the “up” and “down” arrow buttons on the left side of the workspace to navigate through the list.

- Click the “OK” button to return to the Sub Menu. Note that any changes will be lost unless you click “Save” before “OK”.

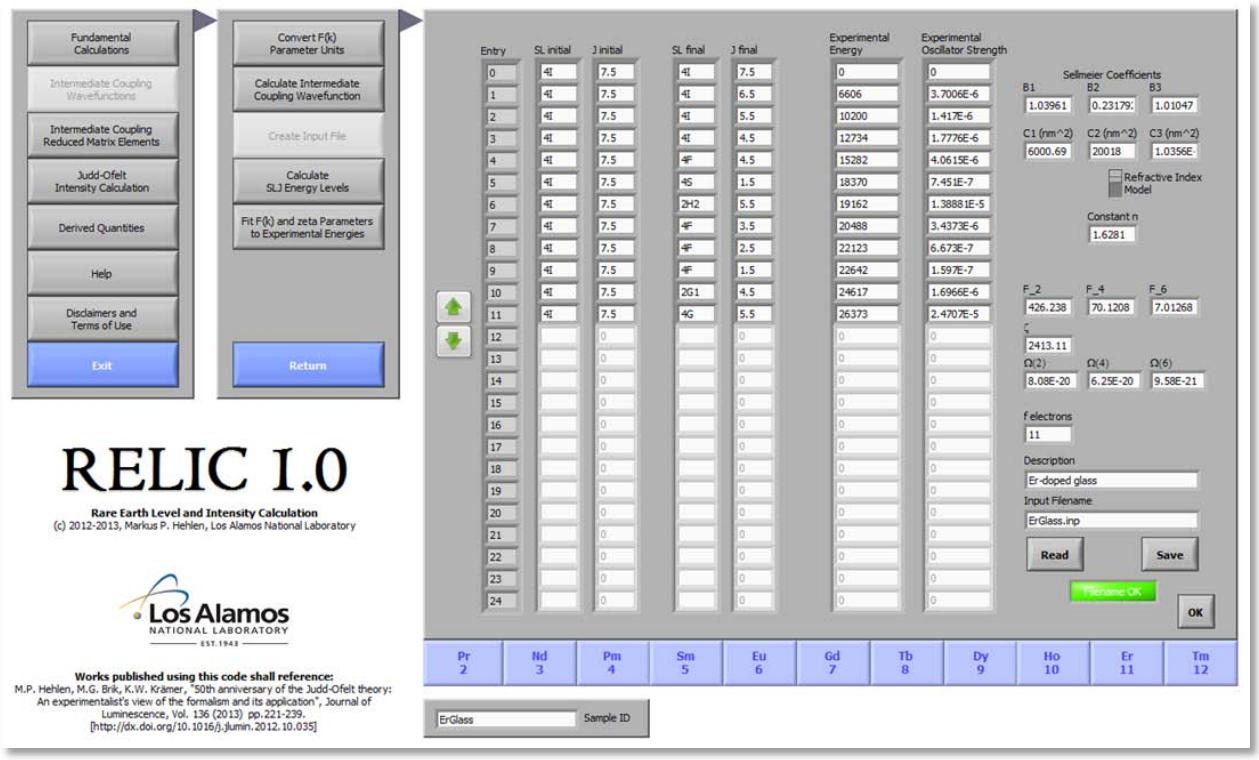


Figure 15: Example of an input file being edited.

Figure 15 shows an example of an input file being edited. The data is for an Er^{3+}-doped oxyfluoride glass. Let’s look at the various fields more closely:

- First note that the number of 4f electrons is given as 11 to indicate the $[Xe]4f^{11}$ electron configuration of Er^{3+}.

- The “Description” field contains a simple one-line text to identify the data. The filename is automatically chose as “ErGlass.INP” to conform with the file naming rules described above.

- The center portion of the workspace contains information for absorption transitions from the $^4I_{15/2}$ ground state multiplet (SL initial = "4I" and J initial = "7.5") to a total of 10 excited state multiplets***. It is mandatory to have the first entry contain the ground state multiplet for both the initial and final states along with an energy and oscillator strength of zero.*** This tells RELIC 1.0 the ground state of the system and thus the energy reference. Note that for this configuration, it is necessary to add the seniority number for some of the multiplets (such as 2H2 and 2G1) as this was described in Section 4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element.

- The fields in the top right corner of the workspace provide refractive index information. One can choose to use a wavelength-independent refractive index by entering a value in the "Constant n" field and setting the "Refractive Index Model" control switch to the *down* position. Alternatively, one can enter the B and C coefficients for up to three terms of the Sellmeier equation and setting the "Refractive Index Model" control switch to the *up* position, as shown here. In this case, the wavelength-dependent refractive index is calculated according to

$$n(\lambda)^2 = 1 + \sum_{i=1}^{3} \frac{B_i \lambda^2}{\lambda^2 - C_i} \tag{11}$$

  where B_i and C_i are phenomenological material constants that are typically obtained from a fit of Eq.(11) to a number of refractive index measurements at different wavelengths. It is important to note that the unit of wavelength is [nm], and thus the unit of the C_i paremeter is [nm^2]. If less than three terms are used in the Sellmeier equation then the other terms must be set to zero.

- The example in Figure 15 also shows that the fields for the electrostatic interaction parameters ($F_{(2)}$, $F_{(4)}$, $F_{(6)}$ in units of [cm^{-1}]), the spin-orbit coupling constant (ζ in units of [cm^{-1}]), and the Judd-Ofelt intensity parameters ($\Omega_{(2)}$, $\Omega_{(4)}$, $\Omega_{(6)}$ in units of [cm^2]) are populated. It is not necessary to populate all fields, but inputs some fields are required depending on the calculations that will be performed.

- It is a good idea to use separate Sample IDs for different samples in order to clearly manage multiple projects.

4.5.4. Calculate SLJ Energy Levels

Activating the "Calculate SLJ Energy Levels" function brings up the Workspace fields shown in Figure 16. It allows you to calculate the $|SLJ\rangle$ energy levels for the configuration as well as $F_{(k)}$ and ζ parameters specified in an input file. The input filename is automatically chosen as the one corresponding to the specified "Sample ID".

If you need to change the sample ID, click “OK” to exit this function, update the “Sample ID” field, and then reactivate the function.

Click “Execute” to start the calculation. The indicator below the “Execute” button will turn yellow during the calculation. Upon completion, the energies of all $|SLJ\rangle$ energy levels of the given [Xe]4f^n electron configuration will be given in the output fields on the right side. Use the up/down buttons to navigate through the list if needed. Return to the Sub Menu by clicking the “OK” button.

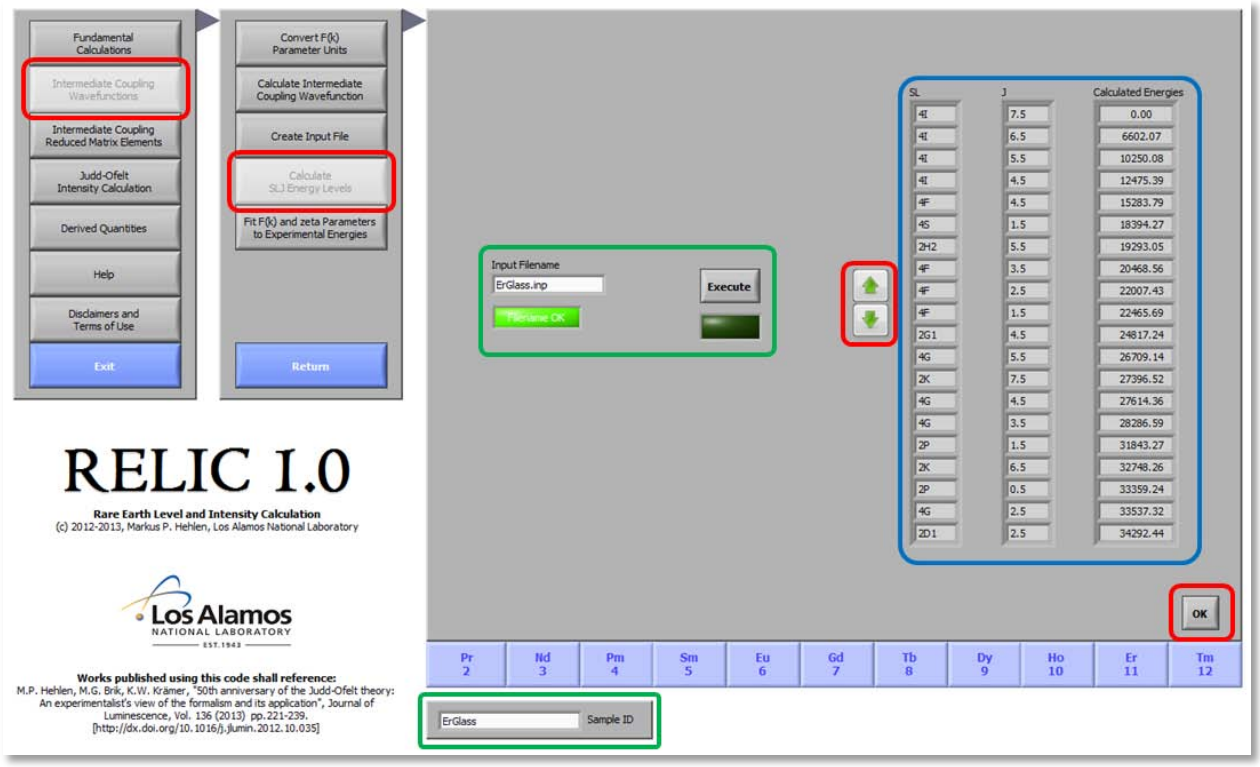


Figure 16: Calculating the intermediate coupling $|SLJ\rangle$ energy levels using the information provided in an input file.

4.5.5. Fit $F_{(k)}$ and ζ Parameters to Experimental Energies

Activating the “Fit F(k) and Zeta Parameters to Experimental Energies” function brings up the Workspace fields shown in Figure 17. The function performs a least-squares fit of calculated $|SLJ\rangle$ energy levels to a set of experimental $|SLJ\rangle$ energy levels by adjusting the $F_{(k)}$ and ζ intermediate coupling parameters. The function that is being minimized is the sum of the squares of the *relative* errors of the energies [2].

The input filename is automatically chosen as the one corresponding to the specified “Sample ID”. You can also specify the function and parameters tolerances that

determine the endpoint of the least squares fit. A value of 0.001 for both these tolerances is recommended. The fit function will use the $F_{(k)}$ and ζ parameters currently stored in the input file as starting values for the optimization. Absent any other information, use the $F_{(k)}$ and ζ parameters shown in Table 3 as starting values. These values are averages derived from a compilation of many published studies [2] and should provide a useful starting point.

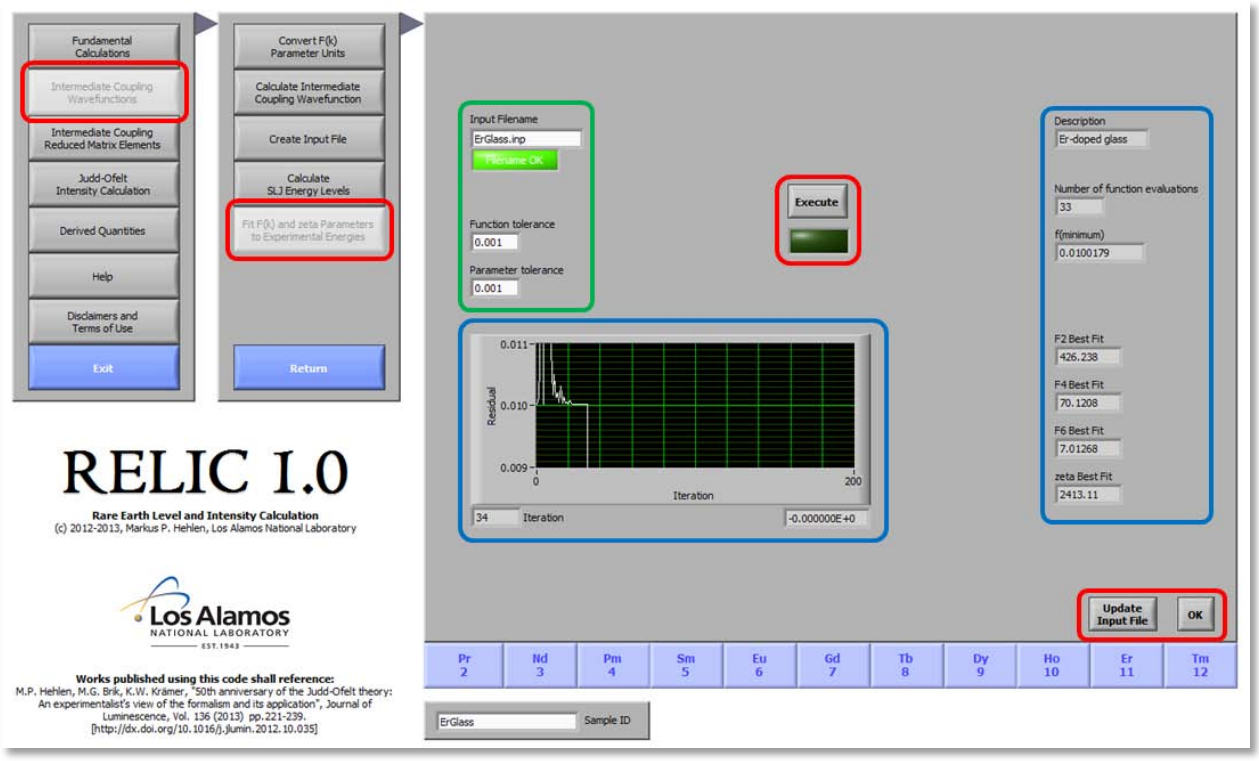


Figure 17: Fitting $F_{(k)}$ and ζ intermediate coupling parameters to a set of experimental $|SLJ\rangle$ energy levels.

Click "Execute" to start the calculation. The indicator below the "Execute" button will turn yellow during the calculation. The graph shows the evolution of the function residual as the calculation proceeds through the iterations. The current iteration and function residual are also shown numerically below the graph. Note that a full matrix diagonalization is being performed for *each* iteration. Therefore, the calculation can be time consuming for configurations with many 4f electrons/holes. Upon completion, the result of the fitting is shown on the right side of the workspace. This includes the total number of iterations performed, the minimum function residual, and the best $F_{(k)}$ and ζ parameters found by the fit. If you wish, click on the "Update Input File" button to overwrite the current $F_{(k)}$ and ζ parameters in the input file by these new best fit parameters. The best fit parameters will not be saved if you do not click on the "Update Input File" button. Return to the Sub Menu by clicking the "OK" button.

Table 3 lists values for the $F_{(k)}$ and ζ parameters that can be used as reasonable starting values. They were derived from a survey of a large number of RE-doped compounds [2]. If you have no specific set of $F_{(k)}$ and ζ parameters to begin with, it is recommended that you use these respective values as starting point for fitting intermediate coupling wavefunctions.

Table 3: Recommended $F_{(k)}$ and ζ starting parameters in [cm^{-1}].

RE^{3+}	$F_{(2)}$	$F_{(4)}$	$F_{(6)}$	ζ
Pr	306	46.8	4.57	746
Nd	322	47.5	4.87	876
Pm	339	50.1	4.83	1013
Sm	353	53.0	5.49	1166
Eu	371	54.8	5.75	1334
Gd	382	56.7	5.93	1477
Tb	399	59.0	6.01	1704
Dy	409	61.8	6.53	1922
Ho	421	63.2	6.80	2138
Er	436	66.1	6.92	2379
Tm	457	66.9	7.19	2646

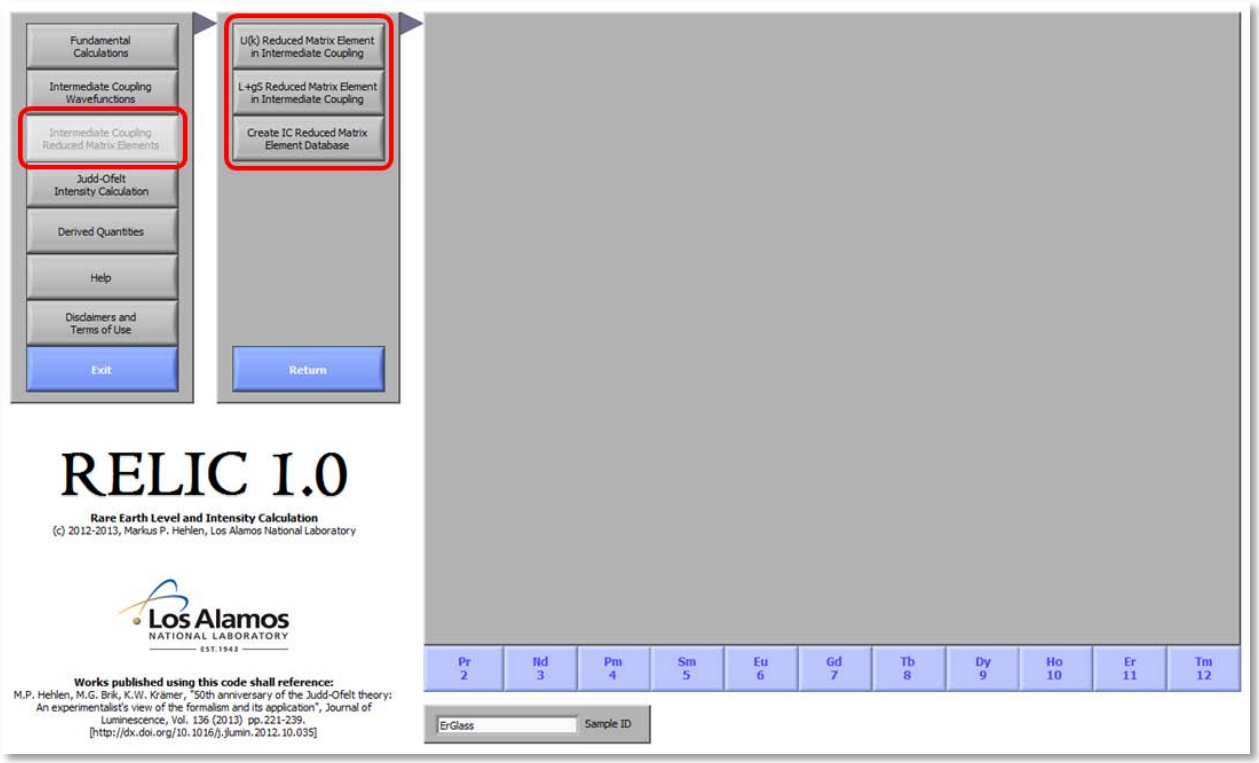


Figure 18: Sub menu activated by clicking the "Intermediate Coupling Reduced Matrix Elements" button in the Main Menu.

4.6. Intermediate Coupling Reduced Matrix Elements

Clicking on “Intermediate Coupling Reduced Matrix Elements” in the Main Menu brings up a new Sub Menu with buttons for 3 functions as shown in Figure 18. This group of functions allows for the calculation of individual reduced matrix elements of the $U^{(k)}$ and L+gS tensor operators. It also allows for the creation of a database of reduced matrix elements for a specific compound that is specified by a set of $F_{(k)}$ and ζ parameters.

4.6.1. $U^{(k)}$ Reduced Matrix Element in Intermediate Coupling

Activating the “U(k) Reduced Matrix Element in Intermediate Coupling” function brings up the Workspace fields shown in Figure 19. This function calculates the reduced matrix element of the $U^{(k)}$ tensor operator between two $|SLJ\rangle$ multiplets in intermediate coupling. The function first calculates the intermediate coupling wavefunctions of the two the wavefunction of the two $|SLJ\rangle$ multiplets and then calculates the reduced matrix element by performing the summation in Eq. (12) over the respective wavefunction coefficients c_i.

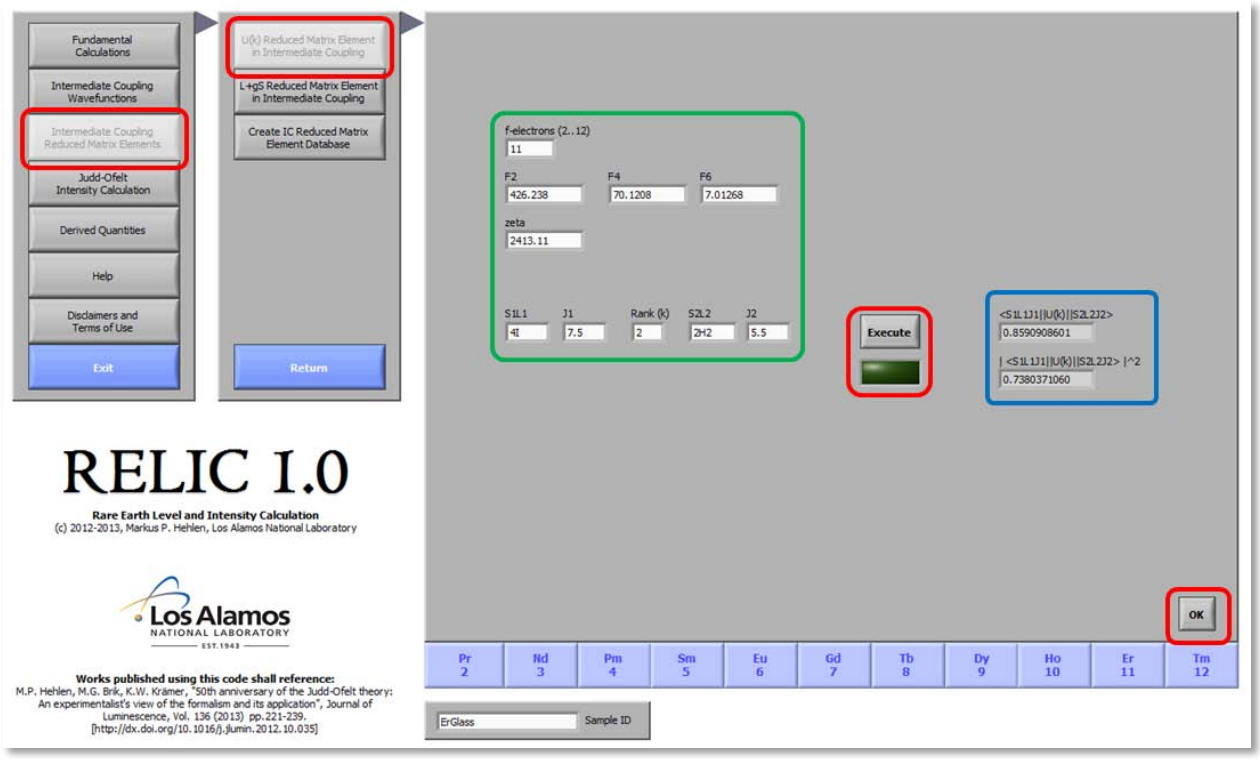


Figure 19: Calculating a reduced matrix element of the $U^{(k)}$ tensor operator in intermediate coupling approximation.

$$\langle l^n SLJ \| U^{(k)} \| l^n S'L'J' \rangle' = \sum_i \sum_j c_i c_j \langle l^n SLJ \| U^{(k)} \| l^n S'L'J' \rangle \tag{12}$$

To perform the calculation, enter the number of f-electrons for the configuration at hand, the $F_{(k)}$ and ζ parameters values, the $|SL\rangle$ term (Refer to Section 4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element for instructions on how to enter the $|SL\rangle$) and J of the two coupling states, and the rank k of the $U^{(k)}$ operator. Click "Execute" to start the calculation. The indicator below the "Execute" button will turn yellow during the calculation. As a result, the reduced matrix element $\langle l^n SLJ \| X \| l^n S'L'J' \rangle'$ and its square will be displayed. Return to the Sub Menu by clicking the "OK" button.

4.6.2. L+gS Reduced Matrix Element in Intermediate Coupling

Activating the "L+gS Reduced Matrix Element in Intermediate Coupling" function brings up the Workspace fields shown in Figure 20. This function calculates the reduced matrix element of the L+gS tensor operator between two $|SLJ\rangle$ multiplets in intermediate coupling. The function first calculates the intermediate coupling wavefunctions of the two the wavefunction of the two $|SLJ\rangle$ multiplets and then calculates the reduced matrix element by performing the summation in Eq. (13) over the respective wavefunction coefficients c_i.

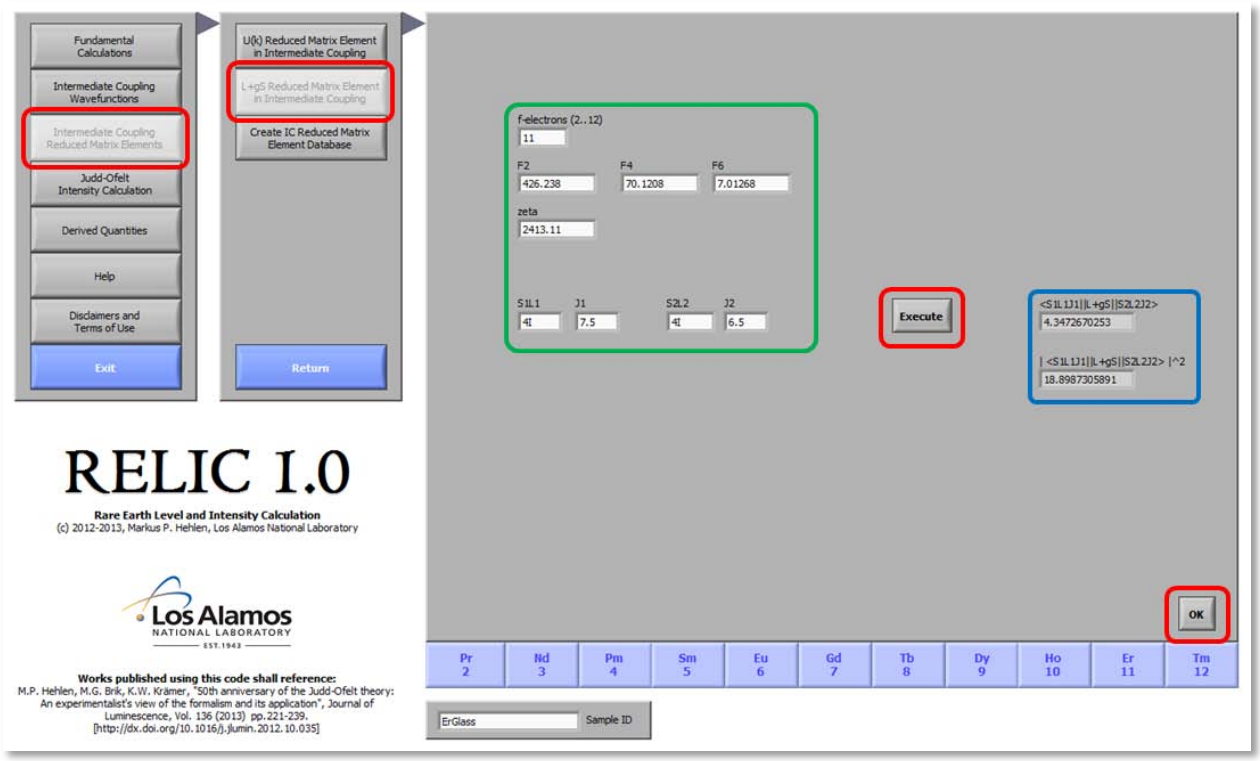


Figure 20: Calculating a reduced matrix element of the L+gS tensor operator in intermediate coupling approximation.

$$\langle l^n SLJ \| L + gS \| l^n S'L'J' \rangle' = \sum_i \sum_j c_i c_j \langle l^n SLJ \| L + gS \| l^n S'L'J' \rangle \tag{13}$$

To perform the calculation, enter the number of f-electrons for the configuration at hand, the $F_{(k)}$ and ζ parameters values, and the $|SL\rangle$ term (Refer to Section 4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element for instructions on how to enter the $|SL\rangle$) and J of the two coupling states. Click "Execute" to start the calculation. As a result, the reduced matrix element $\langle l^n SLJ \| L+gS \| l^n S'L'J' \rangle'$ and its square will be displayed. Return to the Sub Menu by clicking the "OK" button.

4.6.2. Create IC Reduced Matrix Element Database

Activating the "L+gS Reduced Matrix Element in Intermediate Coupling" function brings up the Workspace fields shown in Figure 21.

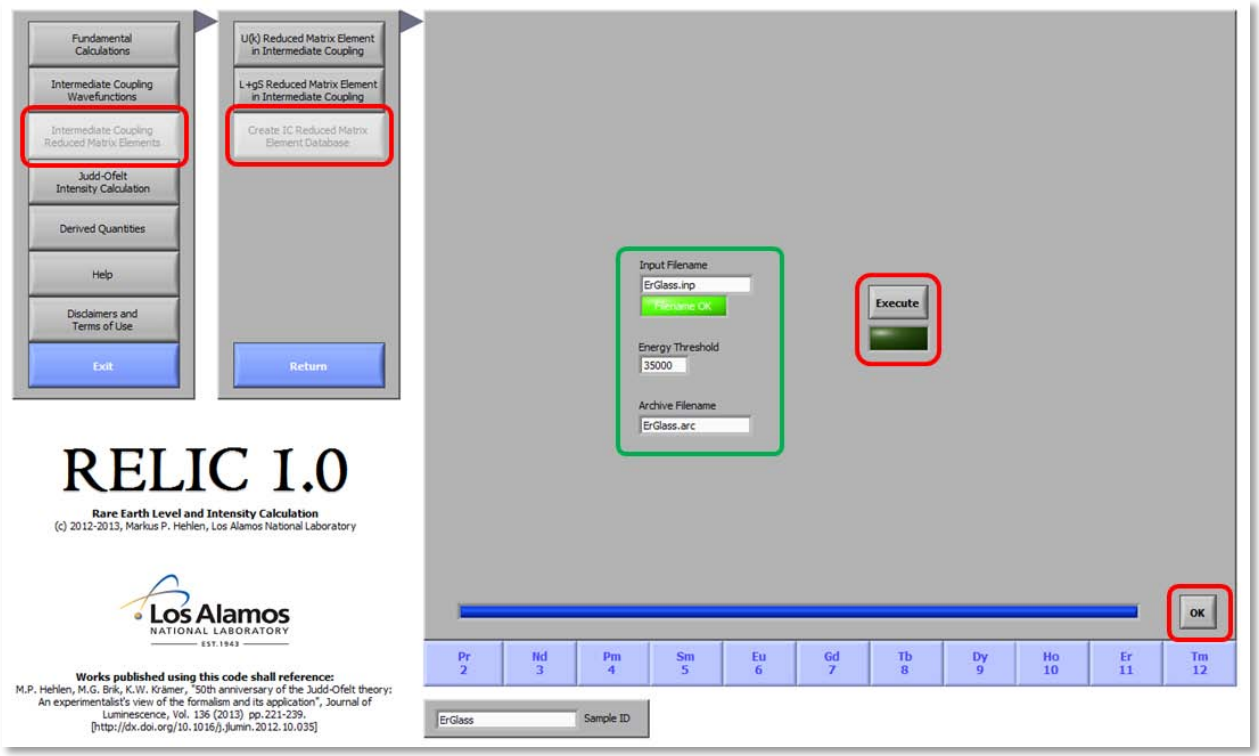


Figure 21: Creating a database of $U^{(k)}$ and L+gS reduced matrix elements in intermediate coupling approximation.

This function calculates the reduced matrix elements of the $U^{(k)}$ and L+gS tensor operators in the intermediate coupling approximation for a specific sample that is characterized by a set of $F_{(k)}$ and ζ parameters. The matrix elements are calculated between all $|SLJ\rangle$ multiplets for which the energy difference is less or equal to a user-defined threshold energy. This speeds up the calculation by only calculating matrix elements for transitions of interest. The $U^{(k)}$ and L+gS reduced matrix elements are stored in an archive file. The archive filename is the Sample ID followed by the extension ".arc", and it is located in the C:\RELIC Data folder. ***Creation of such an archive file is required for all subsequent Judd-Ofelt intensity calculations and the respective derived quantities.***

To create the reduced matrix element database, enter the energy threshold and click "Execute" to start the calculation. The calculation progress is indicated by the blue progress bar at the bottom of the workspace. Note that the calculation can be rather time-consuming for systems with many f-electrons. When the calculation is finished, click "OK" to return to the sub-menu.

4.7. Judd-Ofelt Intensity Calculation

Clicking on "Judd-Ofelt Intensity Calculation" in the Main Menu brings up a new Sub Menu with buttons for 3 functions as shown in Figure 22.

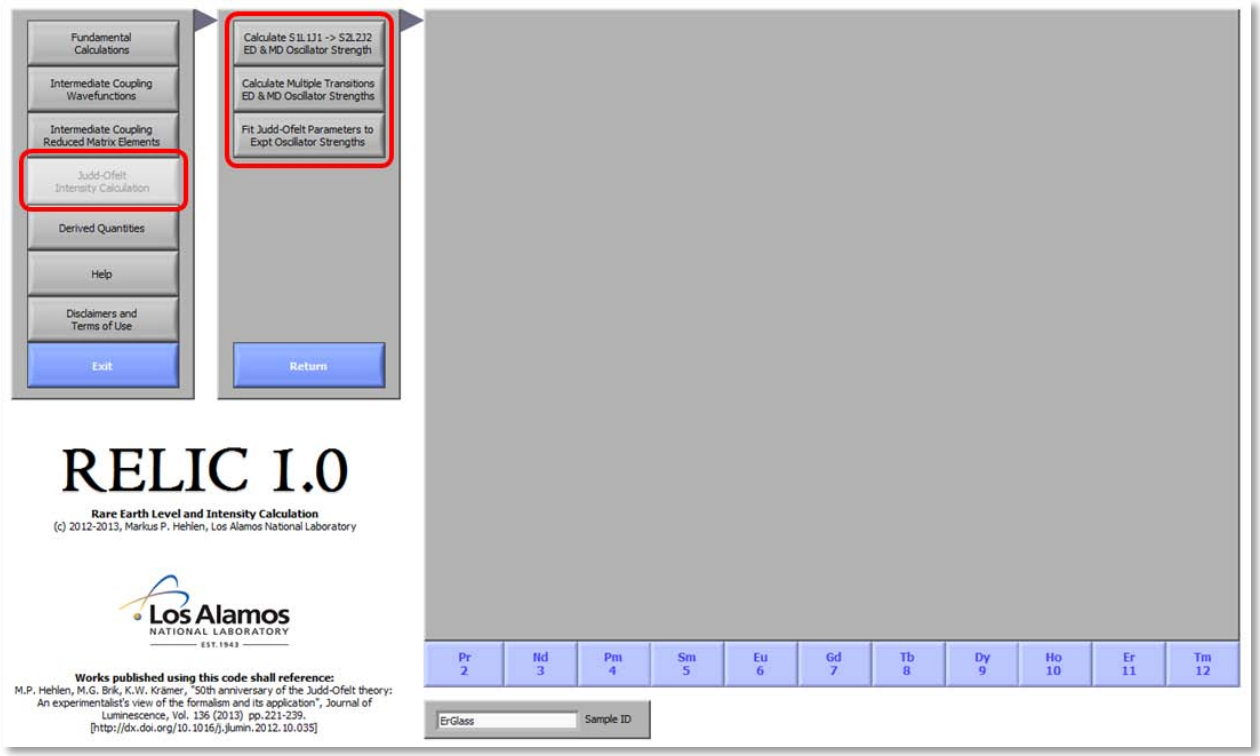


Figure 22: Sub menu activated by clicking the "Judd-Ofelt Intensity Calculation" button in the Main Menu.

This group of functions allows for the calculation of electric-dipole (ED) and magnetic-dipole (MD) oscillator strengths as well as the fitting of Judd-Ofelt intensity parameters $\Omega_{(\lambda)}$ to a set of experimental oscillator strengths. Note that you must have created a reduced matrix element database before using any of these functions (see 4.6.2. Create IC Reduced Matrix Element Database).

4.7.1. Calculate S1L1J1→S2L2J2 ED & MD Oscillator Strength

Activating the "Calculate S1L1J1->S2L2J2 ED & MD Oscillator Strength" function brings up the Workspace fields shown in Figure 23.

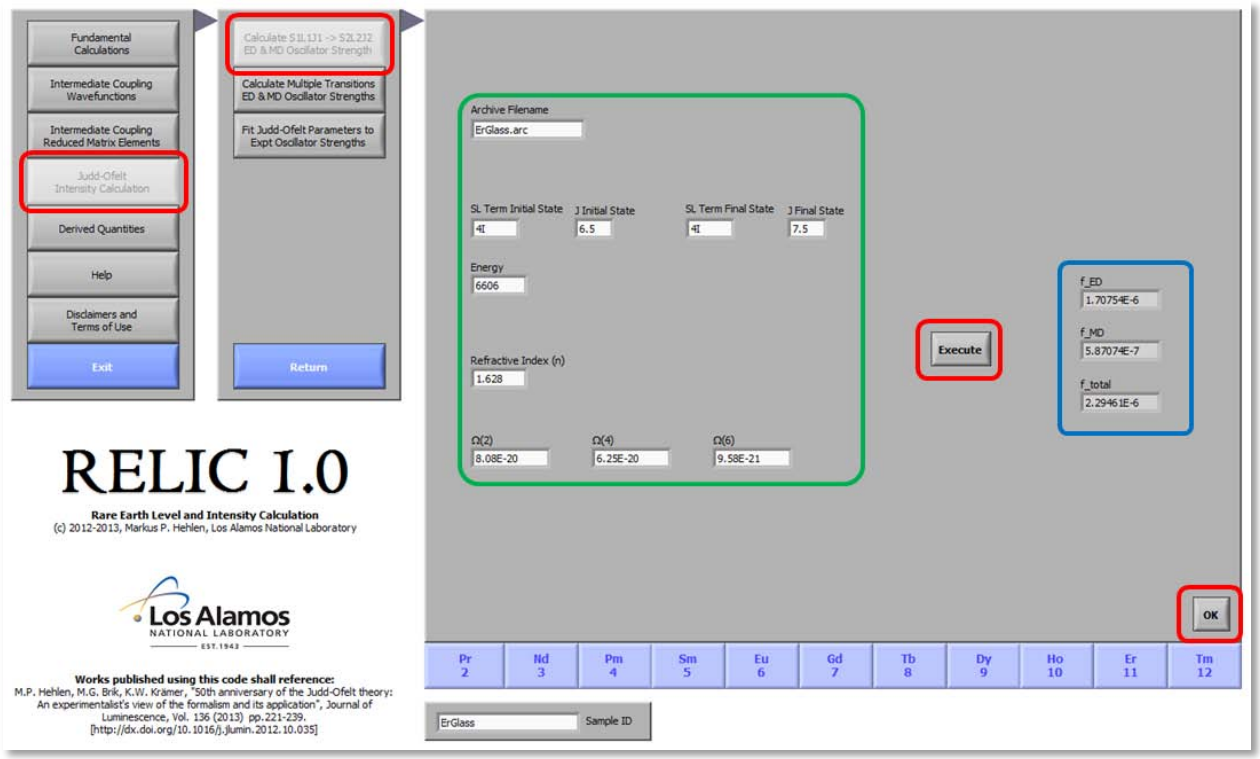


Figure 23: Calculation of ED and MD oscillator strength of a $|SLJ\rangle \rightarrow |S'L'J'\rangle$ transition in the framework of the Judd-Ofelt model.

This function calculates the electric-dipole (ED) and magnetic-dipole (MD) oscillator strength of an $|SLJ\rangle \rightarrow |S'L'J'\rangle$ <u>*absorption*</u> transition in the framework of the Judd-Ofelt model. The respective formulae are shown below [2], and the reduced matrix elements are taken from the respective database file (.arc file).

$$f_{ED}^{abs} = \frac{8\pi^2 m_e}{3h} \frac{\nu}{(2J+1)} \frac{\chi_{ED}^{abs}}{n} \sum_{\lambda=2,4,6} \Omega_{(\lambda)} \left| \langle l^n SLJ \| \mathrm{U}^{(\lambda)} \| l^n SL'J' \rangle \right|^2 \quad (14)$$

$$f_{MD}^{abs} = \frac{h\nu}{6m_e c^2} \frac{n}{(2J+1)} |\langle l^n SLJ \| \mathrm{L} + g\mathrm{S} \| l^n SLJ' \rangle|^2 \tag{15}$$

To perform the calculation, enter the $|SL\rangle$ term (Refer to Section 4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element for instructions on how to enter the $|SL\rangle$) and *J* of both initial and final state of the transition, the energy of the transition, the refractive index at the transition energy, and the three Judd-Ofelt intensity parameters $\Omega_{(2)}$, $\Omega_{(4)}$, and $\Omega_{(6)}$ in units of [cm^2]. Click "Execute" to start the calculation. The ED, MD, and total (ED+MD) oscillator strengths are shown as a result. Return to the Sub Menu by clicking the "OK" button.

4.7.2. Calculate Multiple Transition ED & MD Oscillator Strengths

Activating the "Calculate Multiple Transitions ED & MD Oscillator Strengths" function brings up the Workspace fields shown in Figure 24.

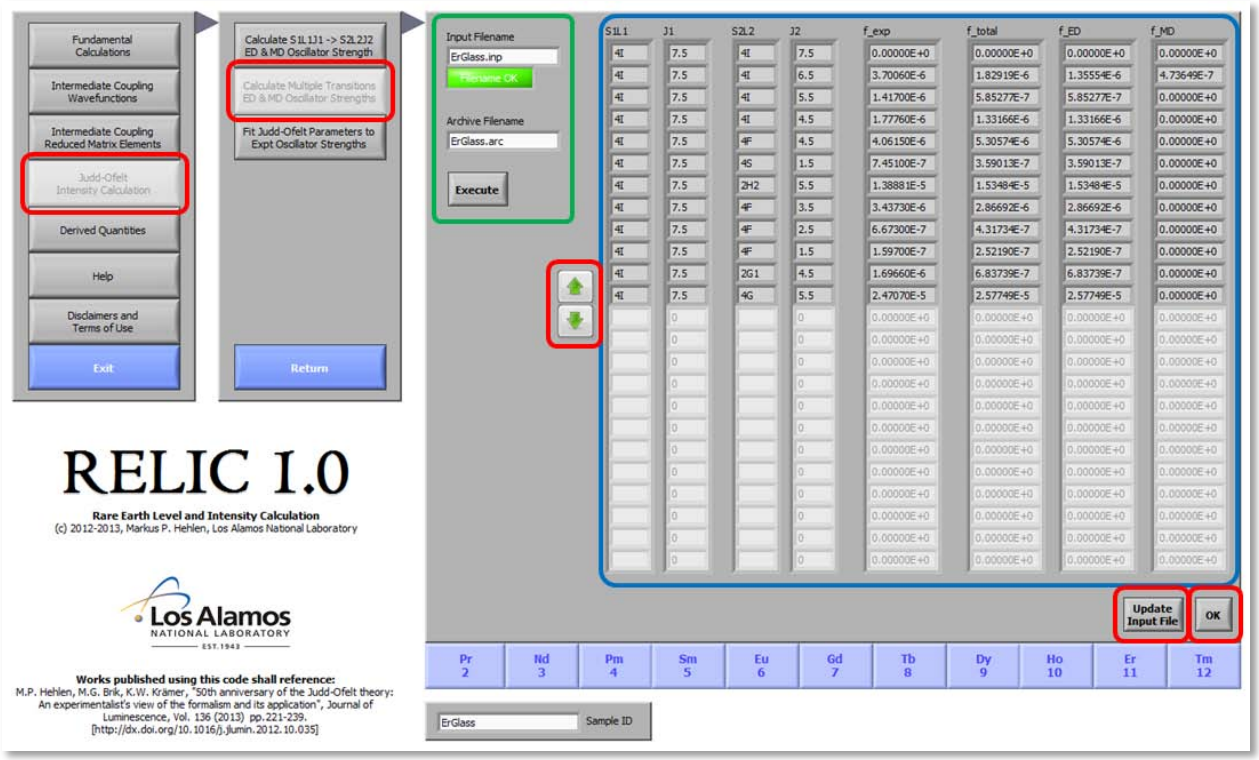


Figure 24: Calculation of the ED and MD oscillator strengths of all transitions defined in the input file.

This function calculates the electric-dipole (ED) and magnetic-dipole (MD) oscillator strength of all transition defined in the input file. They are calculated according to Eqs.

(14) and (15), and the Judd-Ofelt intensity parameters $\Omega_{(\lambda)}$ given in the input file. The reduced matrix elements are taken from the respective database file (.arc file). Click the "Execute" button to perform the calculation. The output table shows the $|SLJ\rangle \rightarrow |S'L'J'\rangle$ transition, the experimental oscillator strength, and the calculated total (ED+MD), ED, and MD oscillator strength. If you have more than 24 transitions, you can use the "up" and "down" arrow buttons on the left side of the workspace to navigate through the list. If desired you can click the "Update Input File" button to write the calculated oscillator strengths to the input file for future reference. Return to the Sub Menu by clicking the "OK" button.

4.7.3. Fit Judd-Ofelt Parameters to Experimental Oscillator Strengths

Activating the "Fit Judd-Ofelt Parameters to Expt Oscillator Strength" function brings up the Workspace fields shown in Figure 25. The function performs a least-squares fit of calculated total (ED+MD) oscillator strengths to a set of experimental oscillator strengths by adjusting the $\Omega_{(2)}$, $\Omega_{(4)}$, and $\Omega_{(6)}$ Judd-Ofelt intensity parameters. The function that is being minimized is the sum of the squares of the *relative* errors of the oscillator strengths [2].

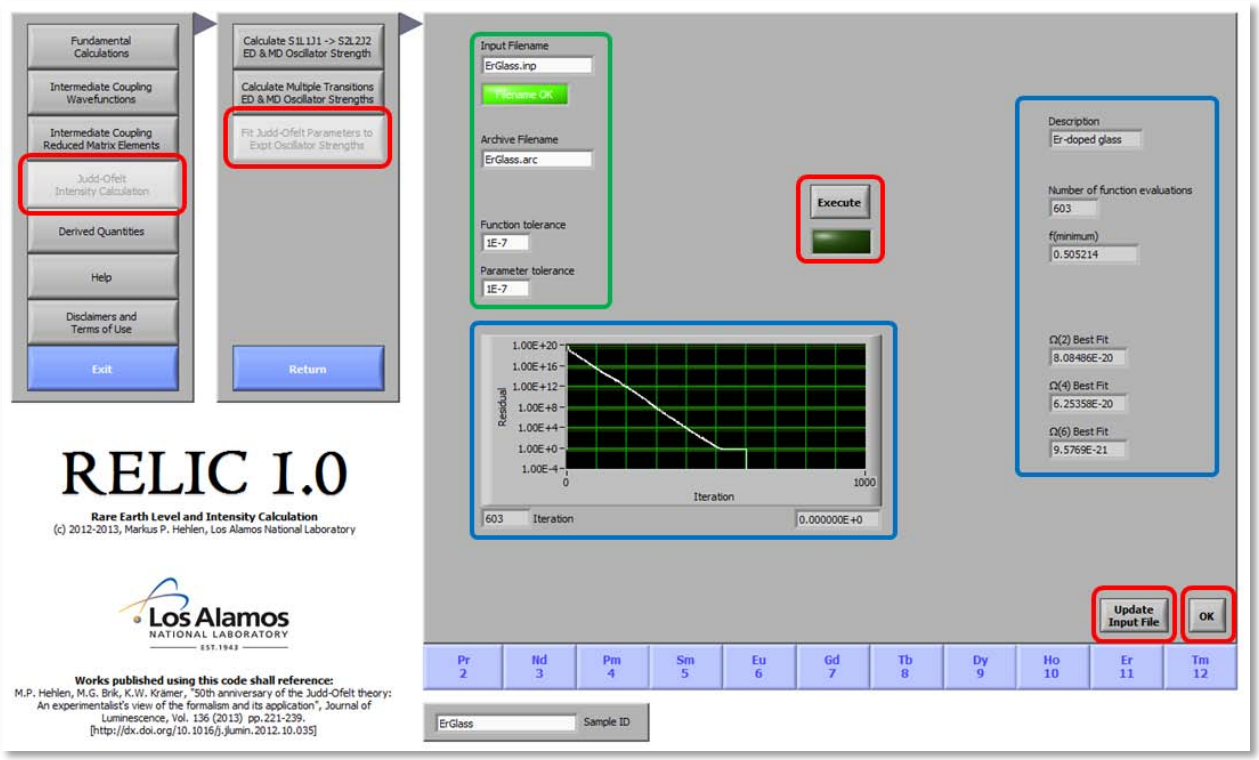


Figure 25: Fitting of the $\Omega_{(2)}$, $\Omega_{(4)}$, and $\Omega_{(6)}$ Judd-Ofelt intensity parameters to a set of experimental oscillator strengths.

You can specify the function and parameters tolerances that determine the endpoint of the least squares fit. A value of 1E-07 for both these tolerances is recommended. The fit function will use the $\Omega_{(2)}$, $\Omega_{(4)}$, and $\Omega_{(6)}$ Judd-Ofelt intensity parameters currently stored in the input file as starting values for the optimization. The oscillator strengths evaluated during the fit are calculated according to Eqs. (14) and (15), and the reduced matrix elements are taken from the respective database file (.arc file). Click "Execute" to start the calculation.

The indicator below the "Execute" button will turn yellow during the calculation. The graph shows the evolution of the function residual as the calculation proceeds through the iterations. The current iteration and function residual are also shown numerically below the graph. Upon completion, the result of the fitting is shown on the right side of the workspace. This includes the total number of iterations performed, the minimum function residual, and the best $\Omega_{(2)}$, $\Omega_{(4)}$, and $\Omega_{(6)}$ Judd-Ofelt intensity parameters found by the fit. If you wish, click on the "Update Input File" button to overwrite the current $\Omega_{(2)}$, $\Omega_{(4)}$, and $\Omega_{(6)}$ Judd-Ofelt intensity parameters in the input file with these new best fit parameters. The best fit parameters will not be saved if you do not click on the "Update Input File" button. Return to the Sub Menu by clicking the "OK" button.

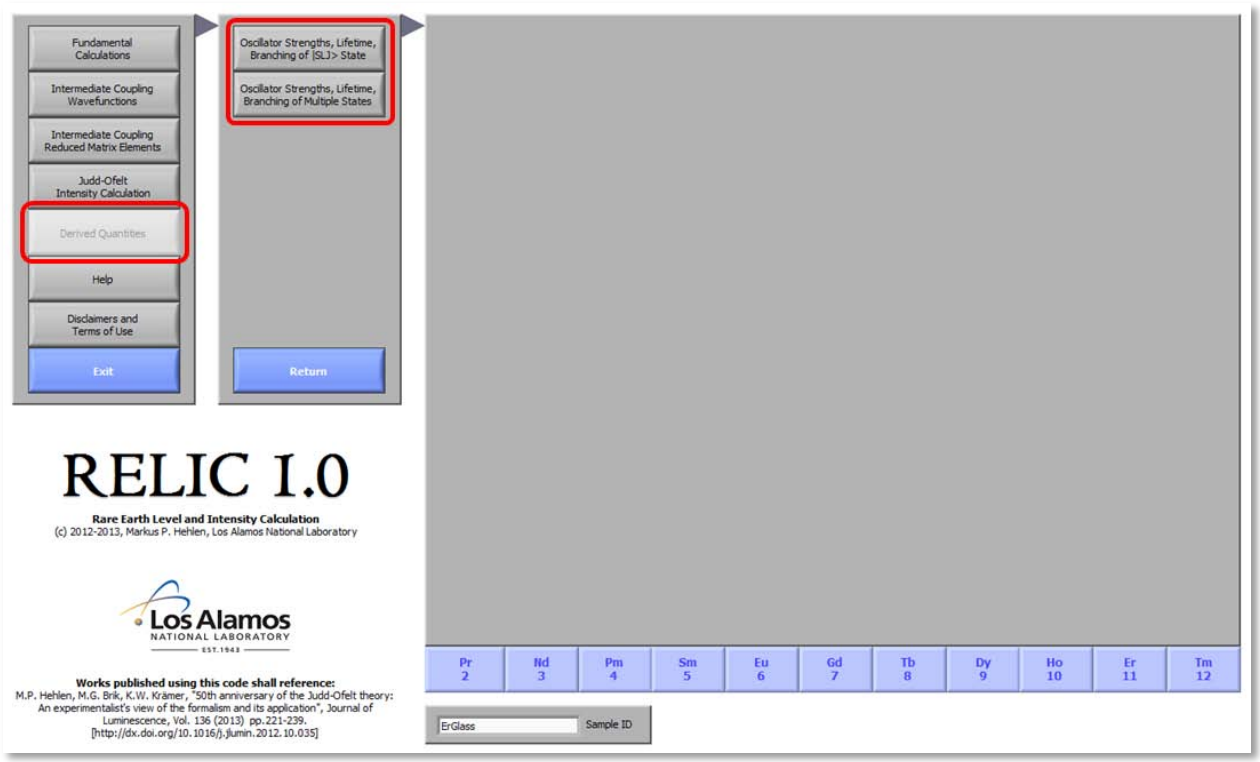


Figure 26: Sub menu activated by clicking the "Derived Quantities" button in the Main Menu.

4.8. Derived Quantities

Clicking on “Derived Quantities” in the Main Menu brings up a new Sub Menu with buttons for 2 functions as shown in Figure 26. This group of functions allows for the calculation of electric-dipole (ED) and magnetic-dipole (MD) oscillator strengths and radiative rates as well as respective radiative lifetimes and branching ratios of excited $|SLJ\rangle$ states. Note that you must have created a reduced matrix element database before using the second function (see 4.6.2. Create IC Reduced Matrix Element Database).

4.8.1. Oscillator Strengths, Lifetime, and Branching Ratio of |SLJ> State

Activating the “Oscillator Strength, Lifetime, Branching of |SLJ> State” function brings up the Workspace fields shown in Figure 27. The function calculates the ED and MD oscillator strengths for transitions from one particular excited $|SLJ\rangle$ state to all lower energy $|SLJ\rangle$ states. This calculation does not use the reduced matrix element database but rather performs a full matrix diagonalization using the parameters provided.

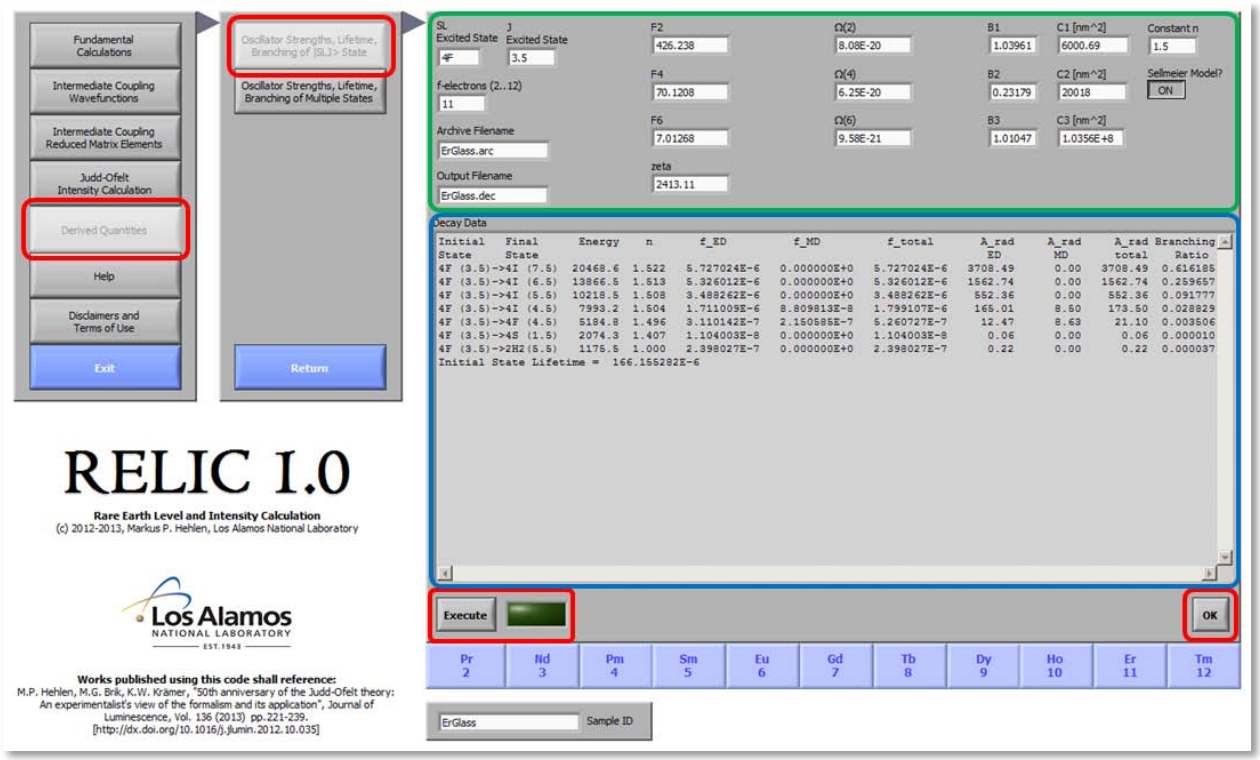


Figure 27: Calculation of all ED and MD oscillator strengths and associated radiative rates and branching ratio for a $|SLJ\rangle$ excited state.

To perform the calculation, the $|SL\rangle$ term (Refer to Section 4.4.5. Calculate $V^{(1x)}$ Reduced Matrix Element for instructions on how to enter the $|SL\rangle$) and J of the excited state of interest. Also enter the number of f-electrons for the configuration at hand, the $F_{(k)}$ and ζ parameters values, and the Ω_λ Judd-Ofelt intensity parameters. You must also provide a refractive index either by entering a constant refractive index (and turning the "Sellmeier Model?" button OFF) or by entering the coefficients of the Sellmeier equation (and turning the "Sellmeier Model?" button ON). Click "Execute" to start the calculation. The indicator next to the "Execute" button will turn yellow during the calculation. The final result is displayed in the "Decay Data" field as well as stored in C:\RELIC Data under a filename consisting of the Sample ID and the extension ".dec". The output consists of the various $|SLJ\rangle \rightarrow |S'L'J'\rangle$ transitions, their respective energies, refractive indices, the ED, MD, and total (ED+MD) oscillator strengths, the ED, MD, and total (ED+MD) radiative rates (in [s^{-1}]), and the radiative branching ratio. The overall radiative lifetime (in [s]) is also given. Return to the Sub Menu by clicking the "OK" button.

4.8.2. Oscillator Strengths, Lifetimes, and Branching Ratios of Multiple States

Activating the "Oscillator Strengths, Lifetime, Branching Multiple States" function brings up the Workspace fields shown in Figure 28.

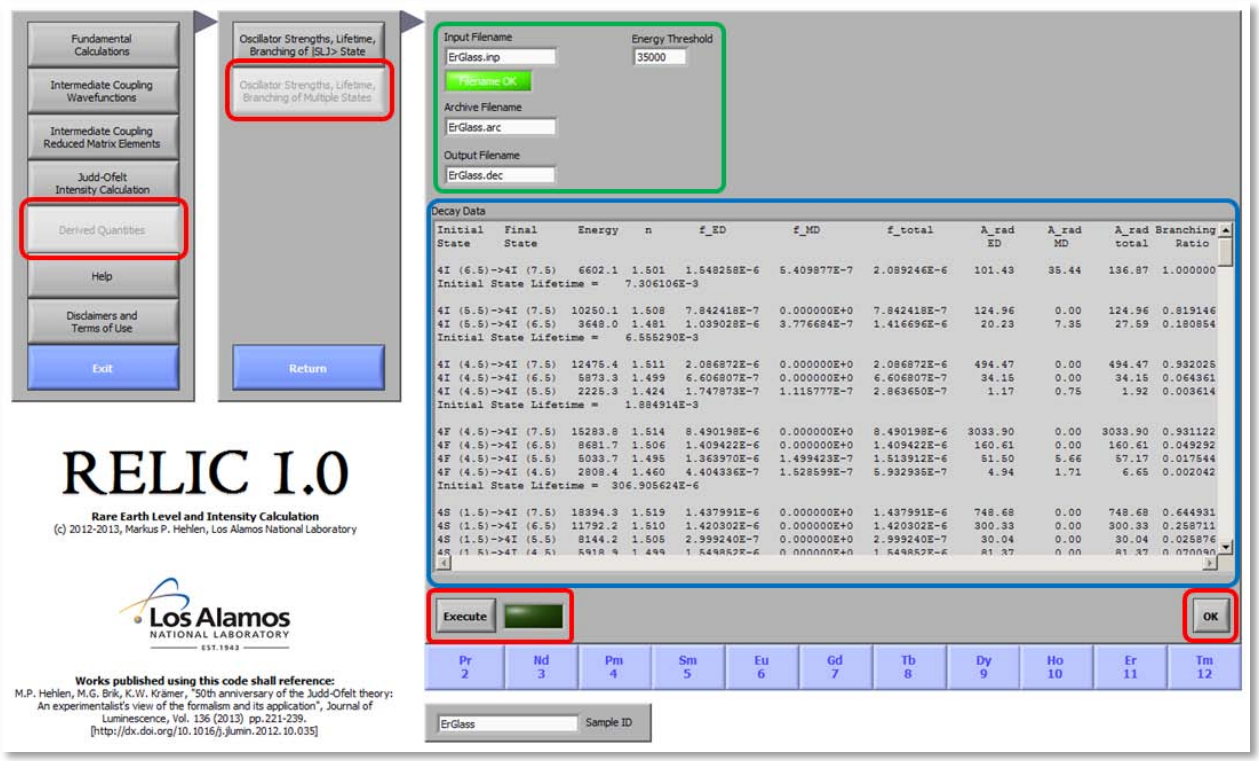


Figure 28: Calculation of all ED and MD oscillator strengths and associated radiative rates and branching ratio for a all $|SLJ\rangle$ excited states with energies less than a user-specified threshold energy.

The function calculates the ED and MD oscillator strengths and associated rates and branching ratios for each excited $|SLJ\rangle$ state up to a user-specified threshold energy. This function uses the reduced matrix elements in the respective database file (.arc file).

To perform the calculation, enter the energy threshold up to which you want to consider excited states. Click “Execute” to start the calculation. The indicator next to the “Execute” button will turn yellow during the calculation. The final result is displayed in the “Decay Data” field as well as stored in C:\RELIC Data under a filename consisting of the Sample ID and the extension “.dec”. The output consists of detailed decay information for each excited state up to the specified threshold energy. For each excited state this includes the various $|SLJ\rangle \rightarrow |S'L'J'\rangle$ transitions, their respective energies, refractive indices, the ED, MD, and total (ED+MD) oscillator strengths, the ED, MD, and total (ED+MD) radiative rates (in [s^{-1}]), and the radiative branching ratio. The overall radiative lifetime (in [s]) is also given. Return to the Sub Menu by clicking the “OK” button.

4.9. Help

Clicking on “Help” in the Main Menu brings up the workspace shown in Figure 29. Click “OK” to open the RELIC 1.0 User Guide (the present document) or click “Cancel” to return to the Main Menu.

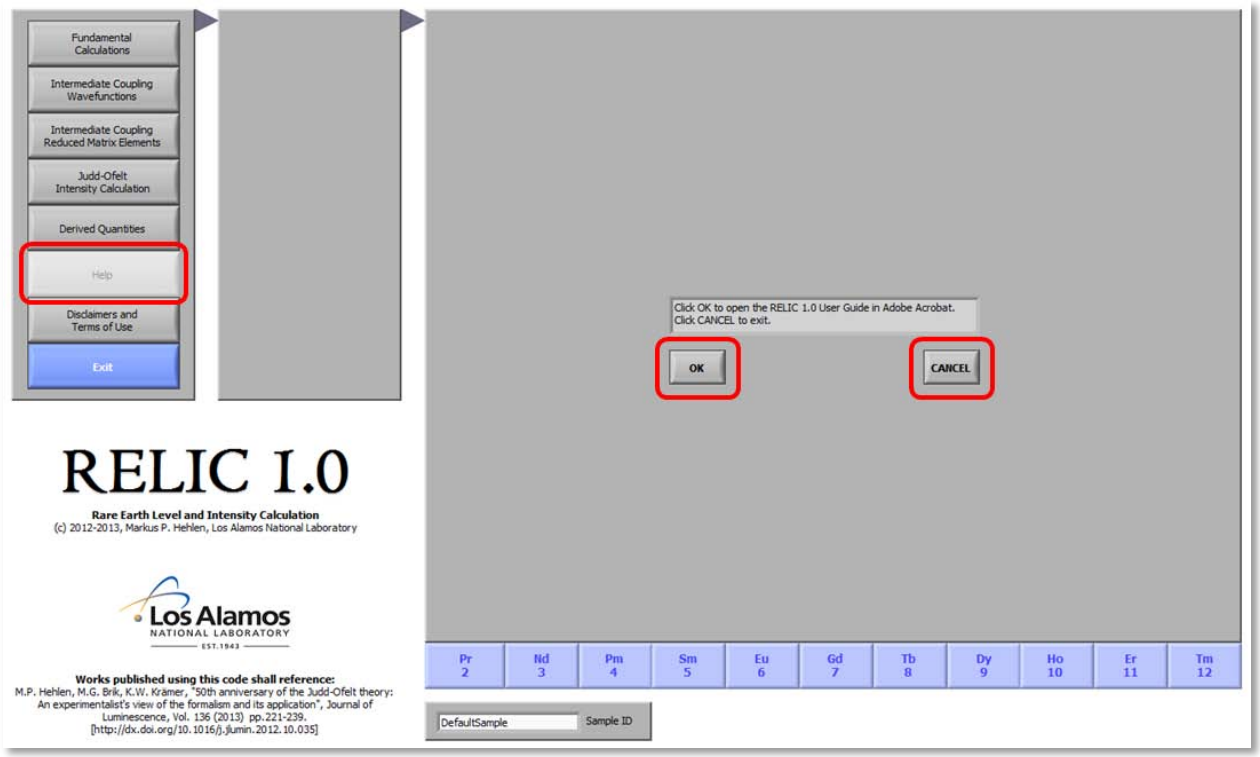


Figure 29: Workspace activated by clicking the “Help” button in the Main Menu.

Bibliography

[1] C. W. Nielsen and G. F. Koster, Spectroscopic Coefficiencts for the p, d, and f Configurations, Cambridge: The MIT Press, 1963.

[2] M. P. Hehlen, M. G. Brik and K. W. Krämer, "50th anniversary of the Judd-Ofelt theory: An experimentalist's view of the formalism and its application," *J. Lumin.,* vol. 136, pp. 221-239, 2013.

[3] "Multi-Electron Coefficients of Fractional Parentage for p, d, and f Electrons; File "b1f_all.txt" for the "1-body CFPs for f electrons"," Johns Hopkins University, [Online]. Available: http://www.pha.jhu.edu/groups/cfp/.

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