# PlotCAS
# A CASSCF/CASPT2 spectrum plotting program

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# 1 Quick guide

## 1.1 The main window

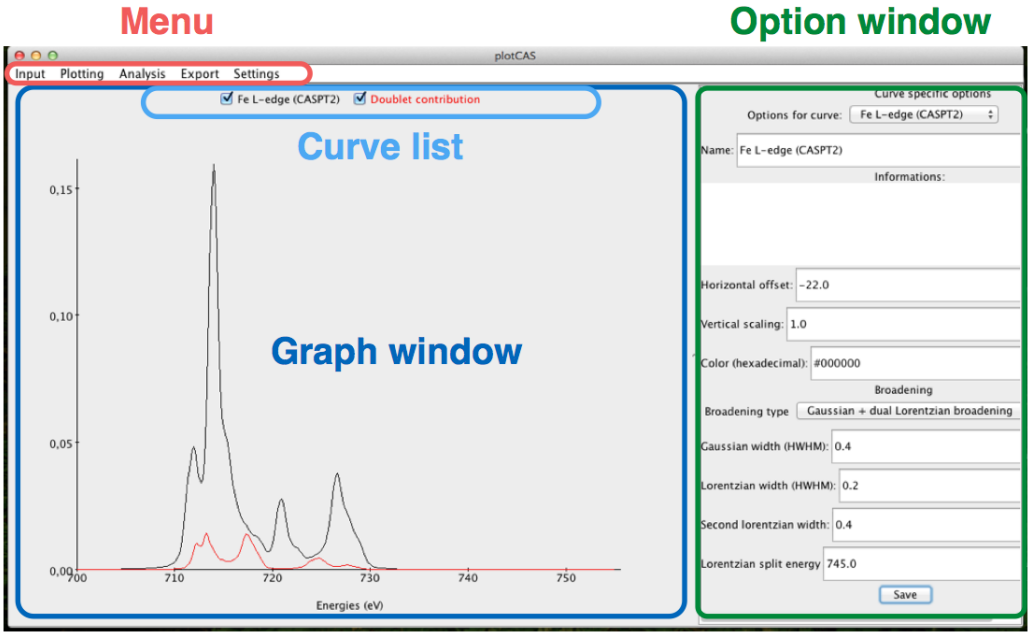


Figure 1: A window of PlotCAS

## 1.2 Creating a graph

You can choose 3 different types of input data to create a graph. The first one is an already existing XY file, which is a list of lines with format:

```
#comments
energy1 intensity1
energy2 intensity2
...
```

This is particularly useful if you have an experimental spectrum which you want to superpose your result to. For this, you simply click on "XY curve" in the "input" menu, as seen in image 2. Then write the XY file in the upper box of the option window. Select the native unit of the spectrum (the unit of the energies). Then give a name to the curve and click "Create curve".

You can also create a spectrum from a list of transition energies and oscillator strength. Click on "List of transitions" in the "input" menu and

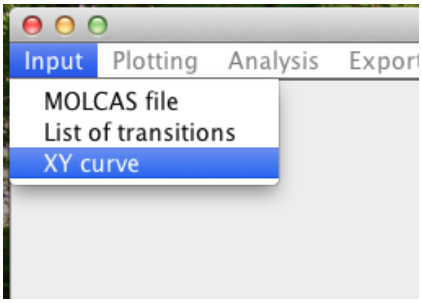


Figure 2: The XY curve menu

follow the same step as for the XY curve. The format of the list of transitions is about the same as the one of XY curve, but you must also indicate the total number of transitions in the first line.

```
#comments
ntransitions
energy1 intensity1
energy2 intensity2
...
```

Finally, you can plot a spectrum directly from a Molcas output which contains a RASSI section. For this, click on "MOLCAS file" in the "input" menu. Click on "Select File" to find the file on your computer and then click on "Load". The program will analyse your log file and especially the RASSI section to find the relevant informations (see fig. 3). You can then choose (if available) to plot the spectrum using the spin-free of spin-orbit data, the dipole and/or quadrupole moment intensities. If you have more than 1 ground state, for example in case of (quasi)-degenerate ground states, you can select the range of them as ordered in the RASSI output, and weight them with a Boltzman factor (default temperature 298K). Finally, write a name for the curve and click on "Create curve".

The curve will then appear in the Graph window, using default parameters. By repeating the above operations, you can superpose as many curves as you want. You can selectively hide some of the curves by clicking on the check boxes in the curve list section on top of the graph window.

## 1.3 Plotting options

When you create a curve for the first time, the programs tries to use the optimal horizontal and vertical scale. Those can be changed at any moment by clicking on "General settings" in the "Plotting" menu. You can manually

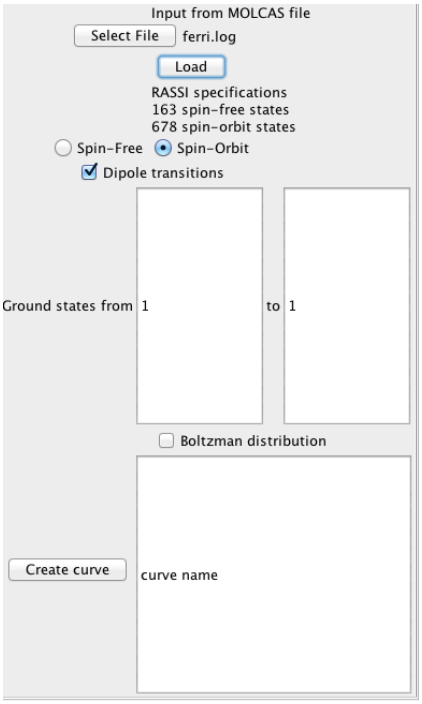


Figure 3: The Molcas input option window

edit those values, and in case of the absorption range, you can also click on "Adjust to graph" to select the optimal value. There you can also select the number of curve points (hence the resolution). Finally, you can select the final unit of the graph (all curves will be converted to this unit). Once you have changed the setting, click on "Redraw" to save them and redraw all the curves.

There are also curve-specific settings that you can change by clicking on "Curve options" in the "Plotting" menu. First select the curve you want to edit. You can then change its name or add some comments for you to remember later. You can also shift the curve horizontally or scale it vertically. You can change its color, using hexadecimal code. If the curve was drawn from a list of transition or a Molcas file, you can also change the default broadening. Select the broadening type and then enters the different parameters. Currently, you can use a gaussian (which typically models thermal effects), a gaussian convoluted with a Lorentzian (which typically models the natural width due to the lifetime of the excited state) and a gaussian convoluted with 2 Lorentzian, in case your spectrum has to parts with distinct lifetime (for example in core-hole spectroscopy).

Once selected, those parameters will be the default parameters for the

next curves. You can also save them by clicking on "Save settings" in the "Plotting" menu. The option window shows all the settings. At the bottom of the option window, you can choose to overwrite an already existing setting or "create new", in which case you should give a name to the setting. Then click on "Save setting". To retrieve those settings at any moment (including an other session of the program), just click on "Load settings" in the "Plotting" menu, select the name of the setting and click on "Load".

## 1.4 Exporting data

You can export a png file of the graph by clicking on "Picture" in the "Export" menu. Select the desired dimensions (in pixel) of the picture and "save as". Note that small dimensions may give overlapping image and text.

You can also save each curve as a XY file for plotting in alternative programs (MS excel, Open-Office calc or gnuplot for example). Just click on "Curve XY" in the "Export menu", then choose the curve and click on "Export". A pop-up window will appear with the xy values.