

expdata2tex: Experimental Data to \LaTeX

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A simple GUI that emits experimental data as LaTeX

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Introduction

This is a simple GUI which I created in order to make it easier to “texify” experimental data. Simple usage is given below. So far it has only been tested on Ubuntu 10.04 and is only expected to run on Linux without problems.

You are also able to save files. The format is plain text, with rows separated by “|” and columns by “~”.

Icons have been borrowed from the KDE Oxygen theme (GPL).

Required Packages

You need to install mhchem, it may not work with older versions. To run this, you will need Python, PyQt4 and Qt4.

New Commands

These might be useful for your preamble. Some version of these will be required.

```
\newcommand{\alphad}[0]{\left[ \alpha \right]_{\text{D}}^{\text{20}}}% The opt rot symbol
\newcommand{\HNMR}[0]{\textsuperscript{1}\text{H}}
\newcommand{\CNMR}[0]{\textsuperscript{13}\text{C}}
\newcommand{\JNMR}[1]{\textit{J}^{\sim\sim\#1}\text{ hertz}}
```

The Program

Proton Data Tab

Enter in the data, an example is shown below. To underline text, highlight it, then use Ctrl-U to underline it.

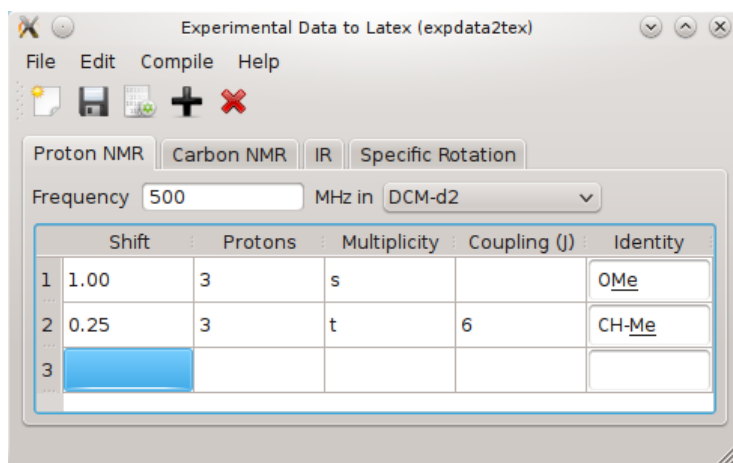


Figure 1: Screenshot of the Proton Tab

Carbon Data Tab

Enter in the data, an example is shown below. To underline text, highlight it, then use Ctrl-U to underline it.

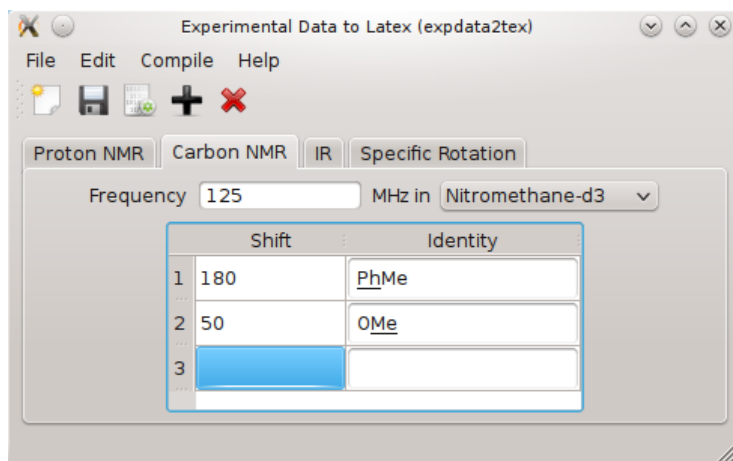


Figure 2: Screenshot of the Carbon Tab

IR Data Tab

Enter in the data, an example is shown below. Text cannot be highlighted.

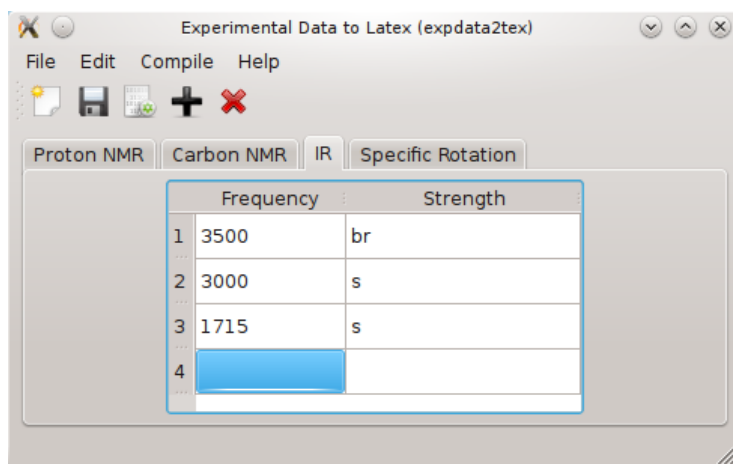


Figure 3: Screenshot of the IR Tab

AD Tab

Enter the data as shown. There is no drop down box for the solvent, specify it yourself.

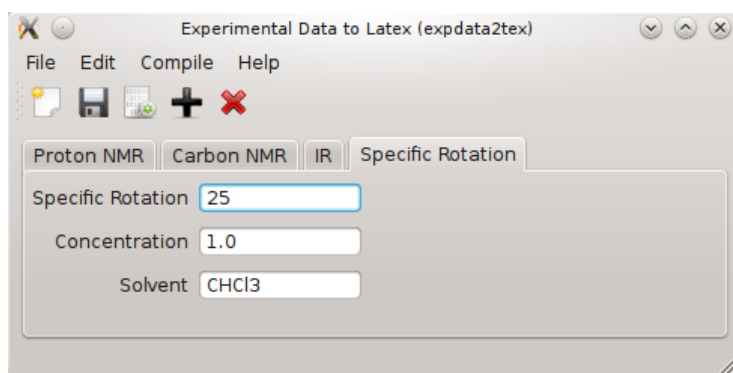


Figure 4: Screenshot of the AD Tab

Compile

Pressing the compile button will supply you with a pop up window containing the \LaTeX source. Copy and paste this into your document. You will probably need to supply the new commands given above, or specify them yourself.

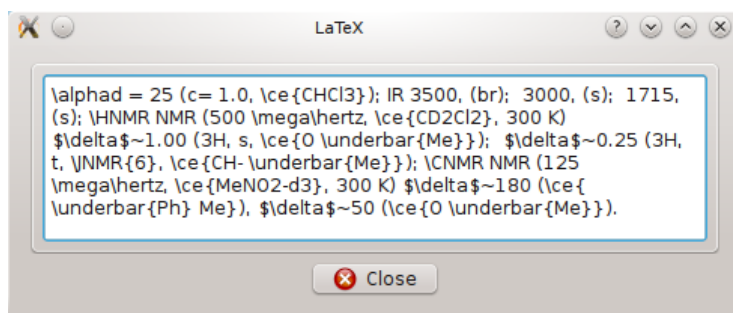


Figure 5: Screenshot of the Generated \LaTeX

```
\alphad = 25 (c= 1.0, \ce{CHCl3}); IR 3500, (br); 3000, (s); 1715, (s);%
\HNMR NMR (500 \mega\hertz, \ce{CD2Cl2}, 300 K) $\delta$~1.00 (3H, s, \ce{O \underbar{Me}});%
$\delta$~0.25 (3H, t, \JNMR{6}, \ce{CH- \underbar{Me}});%
\CNMR NMR (125 \mega\hertz, \ce{MeNO2-d3}, 300 K)%
$\delta$~180 (\ce{ \underbar{Ph} Me}), $\delta$~50 (\ce{O \underbar{Me}}).%
```

Produces: $[\alpha]_D^{20} = 25$ (c= 1.0, CHCl_3); IR 3500, (br); 3000, (s); 1715, (s); ^1H NMR (500 MHz, CD_2Cl_2 , 300 K) δ 1.00 (3H, s, OMe); δ 0.25 (3H, t, $J = 6$ Hz, CH^- Me); ^{13}C NMR (125 MHz, $\text{MeNO}_2\text{-d}_3$, 300 K) δ 180 (PhMe), δ 50 (OMe).

In cases such as

$\text{CH-} \text{Me}$

You may need to use

$\text{CH}\text{---}\text{Me}$

Other than that, it does the majority of formatting for you.

Shortcuts

Here are a list of shorcuts specified in the program.

Shortcut	Action
Tab	Go to next cell
Ctrl-U	Underline Selected
Ctrl-N	New File
Ctrl-O	Open File
Ctrl-S	Save
Ctrl-Alt-C	Compile
F1	Help
Alt-N	Add New Row