

EXPDATA2TEX: EXPERIMENTAL DATA TO  $\text{\LaTeX}$

AUTHOR: RUSSELL CURRIE

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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 extensively 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 “~”. An example file “example.db” has been included for you to play around with.

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 ]_{D}^{\{20\}} } % The opt rot symbol
\newcommand{\HNMR}[0]{\textsuperscript{1}H }
\newcommand{\CNMR}[0]{\textsuperscript{13}C }
\newcommand{\JNMR}[1]{\textit{J}~\sim\#1 \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.

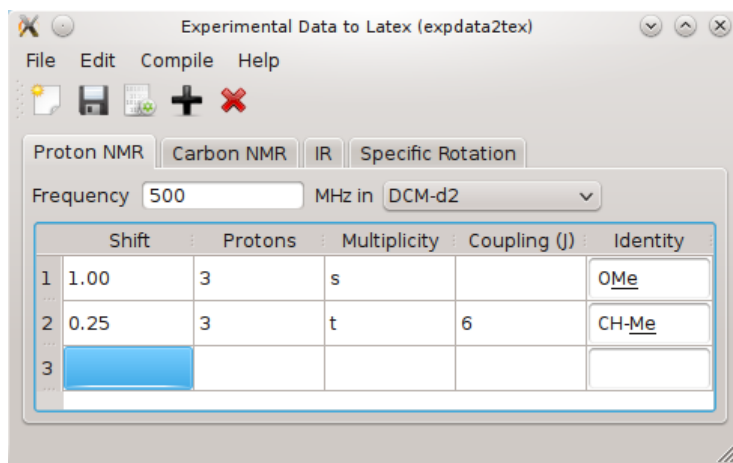


Figure 1: Screenshot of the Proton Tab

### Carbon Data Tab

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

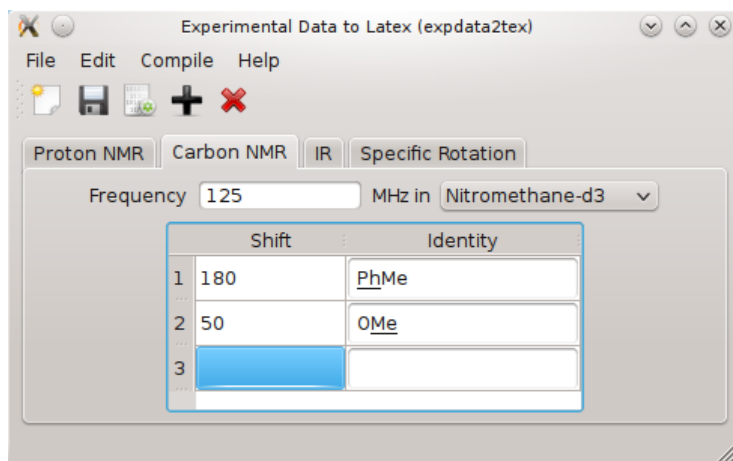


Figure 2: Screenshot of the Carbon Tab

## IR Data Tab

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

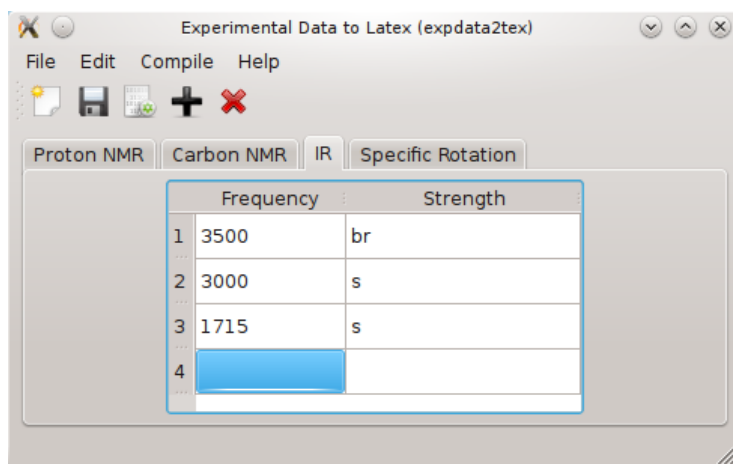


Figure 3: Screenshot of the IR Tab

## AD Tab

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

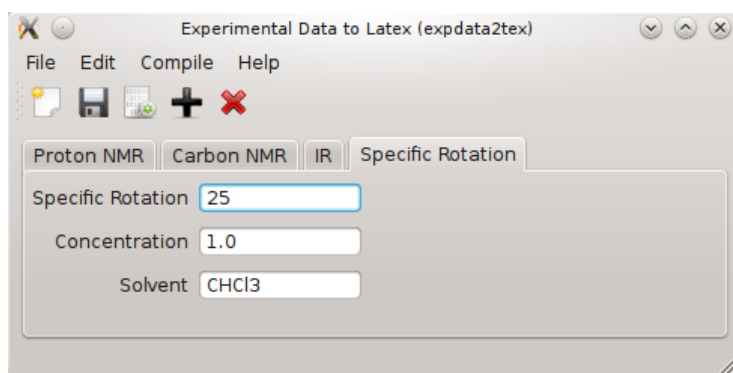


Figure 4: Screenshot of the AD Tab

## 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.

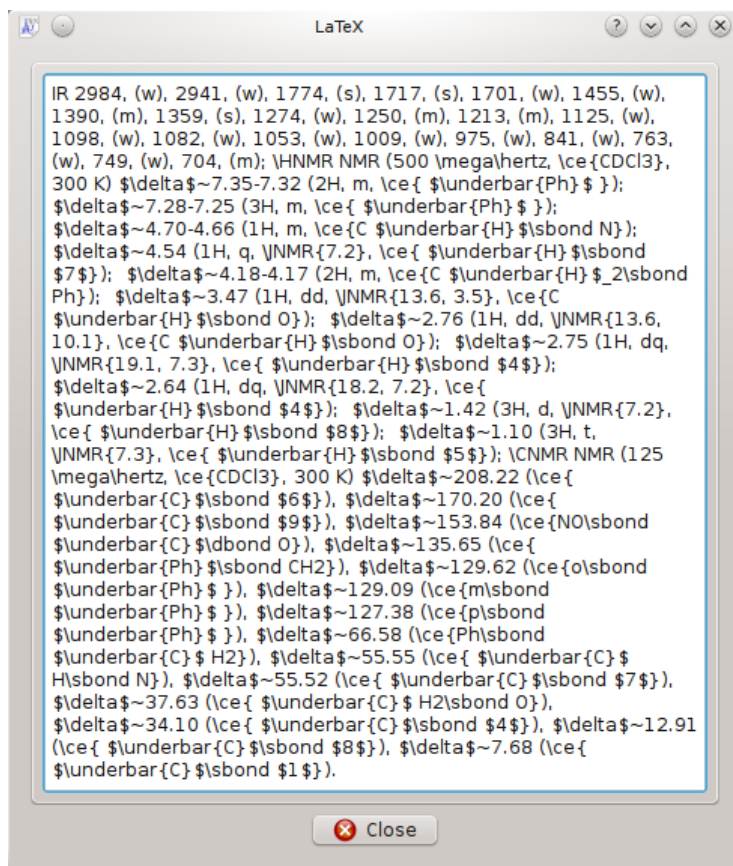


Figure 5: Screenshot of the Generated  $\LaTeX$

```
\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, \NMR{6}, \ce{CH\sbond $\underbar{Me}$});%
\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,  $\text{CHCl}_3$ ); IR 3500, (br); 3000, (s); 1715, (s);  $^1\text{H}$  NMR (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 300 K)  $\delta$  1.00 (3H, s, OMe);  $\delta$  0.25 (3H, t,  $J = 6$  Hz,  $\text{CH-Me}$ );  $^{13}\text{C}$  NMR (125 MHz,  $\text{MeNO}_2\text{-d}_3$ , 300 K)  $\delta$  180 (PhMe),  $\delta$  50 (OMe).

## 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