

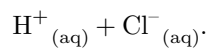
The quichem package

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1 Introduction

quichem (pronounced */kwi-keh-m/*) is a utility written in pure Python designed to take the pain out of typing chemical equations into the computer. For example, typing in `h=aq=cl-aq` will create an output of:



This L^AT_EX package facilitates the use of quichem markup in L^AT_EX documents. The quichem Python package must already be installed and on the PYTHONPATH in order for this package to operate. In addition, the mhchem package must be installed, as quichem uses it for typesetting.

2 Usage

This document describes how to use the quichem package in L^AT_EX documents. For other information about quichem such as its syntax, please see the documentation files at the quichem GitHub page. This package makes use of `\write18`, which therefore must be enabled in the L^AT_EX compiler being used (e.g. with `-shell-escape`).

2.1 Python-side Setup

Before using this package in L^AT_EX, quichem must be installed with the Python executable to be used by this package. Installation of the Python package is performed with `<python> setup.py install`. The installation can be checked by ensuring that `<python> -m quichem.tools.latex` outputs “Congratulations! Your quichem installation is set up with LaTeX support.”

2.2 Including the Package

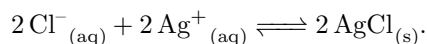
To include the quichem package, add `\includepackage [<python>] {quichem}` to the document header. `<python>` is an optional keyword argument specifying the path to the Python executable. By default, quichem tries to run “python”.

E.g., `\includepackage[python=/usr/bin/python3]{quichem}`.

2.3 Macros

`\qc` Typesets the provided quichem markup, e.g., `\qc{2cl-aq=2ag=aq=/2agcl;s}` renders as $2 \text{Cl}^-_{(\text{aq})} + 2 \text{Ag}^+_{(\text{aq})} \rightleftharpoons 2 \text{AgCl}_{(\text{s})}$. This macro creates a temporary file in the document directory named `_quichem_temp.dat`, which can be safely deleted after document compilation.

`\dqc` Has the same function as `\qc`, but centers the output on its own line, e.g., `\dqc[.]{2cl-aq=2ag=aq=/2agcl;s}` renders as:



Takes an optional parameter containing L^AT_EX code to place after the quichem output. Useful for grammatical elements such as periods or commas.

3 Implementation

```
1 \NeedsTeXFormat{LaTeX2e}[1994/06/01]
2 \ProvidesPackage{quichem}[2014/03/27 quichem]
3
4 \RequirePackage{kvoptions}
5 \RequirePackage[version=3]{mhchem}
```

```

6
7 \DeclareStringOption[python]{python}[python]
8 \ProcessKeyvalOptions*
9
10 \newcommand{\@qc}[1]{\immediate\write18{
11   \quichem@python\space -m quichem.tools.latex "#1" > _quichem_temp.dat}
12   \leavevmode\unskip\input{_quichem_temp.dat}\unskip}

\qc

13 \newcommand{\qc}[1]{\@qc{#1}}

\dqc

14 \newcommand{\dqc}[2][\begin{center}]{\@qc{#2}#1\end{center}}

15 \endinput

```

Change History

2014-03-27
 General: Initial version 1

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Numbers written in *italic* refer to the page where the corresponding entry is described; numbers underlined refer to the code line of the definition; numbers in roman refer to the code lines where the entry is used.

Symbols	\input 12	R
\@qc 10, 13, 14		\RequirePackage . . . 4, 5
B	L	
\begin 14	\leavevmode 12	
D	N	S
\DeclareStringOption . 7	\NeedsTeXFormat 1	\space 11
\dqc <u>14</u>	P	U
E	\ProcessKeyvalOptions 8	
\end 14	\ProvidesPackage 2	\unskip 12
\endinput 15	Q	
I	\qc <u>13</u>	W
\immediate 10	\quichem@python 11	\write 10