natsci — Science notation style guide

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1 Introduction

This style guide outlines some LATEX basics and some typesetting conventions using the natsci package. It is aimed at English and Czech users, but should be easily adaptable for everyone. This document should be read side-by-side with its source code.

2 General

Normal text is written as it is and line breaks in the code are treated only as spaces. The number of spaces between words does not matter.

However, a completely empty line signifies a new paragraph. Note that it must be completely empty (may contain only spaces). Any comments or commands count as non-empty.

Alternatively, a new paragraph can be created by a command, but that is usually not necessary. Sometimes

you want a line break without a new paragraph. That is done using two backslashes.

Different styles of text are roman (upright), **bold**, *italics*, *emphasised* (usually italics, but can be globally changed), *bold italics*, sans-serif, **sans-serif bold**, *sans-serif italics* (*oblique*), mono-spaced, mono-spaced *italic*.

2.1 Escaping characters

There are some characters that have meaning in \LaTeX and have to be "escaped" when you actually want to display them. These are &, %, \$, #, _, {, }, ~, ^, \. The empty curly braces are not necessary, but prevent disappearence of spaces that follow them. (If you don't want a space after them, you can omit the braces.)

2.2 Unicode characters

The package uses X五序下X, which can directly typeset the whole of Unicode. However, the characters need to be supported by the font, and there is not a single font that would cover the whole of Unicode. This means that one would have to manually switch fonts if characters outside of the body font are needed. This can be done automatically for predefined Unicode ranges using the ucharclasses package, as demonstrated for the Han characters (漢字) in the header of this file.

2.3 Unicode abbreviations

There are some Unicode characters that have TEX shorthands consisting of ASCII characters. These are more explicit and easier to type than the actual Unicode characters, which is why we shall use them.

Space sizes. There are different sizes of spaces in typesetting which are represented by different characters in Unicode. LATEX automatically inserts a larger space following a full stop. This is appropriate following a sentence, but not for other uses of full stop, e.g. in abbreviations. There, the space should be escaped using a backslash, which achieves a normal sized space. Compare e.g. spacing to e.g. spacing. This is only in English language.

Non-breaking spaces. In some cases, spaces should not change into line breaks. This is done using the tilde symbol. Let's say that we don't want the initials to separate, like in A. Přáda. This also suppresses the large spacing after a full stop that is present in English.

Dashes and hyphens are typed by 1 to 3 ASCII hyphens. For hy-phe-na-ted words use a single one. For ranges of numbers, use two, which give you an en-dash (e.g. 1–2). For pauses — em-dashes are used, which are represented by three hyphens.

English quotation marks are created using backticks for the front and apostrophes for the back, like 'this' or "this". Make sure that you don't use the typewriter double quote ", which can cause troubles. Czech quotation marks, however, are typed using the double-quote character followed by quotations as previously, like "this". (This works only in Czech texts.)

Non-breaking hyphens Sometimes there are hyphenated words that should not be split across lines. We use the extdash package and the hyphens are done as follows: 2-propanol.

2.4 References

You can refer to other places in the document using the \ref command. This refers to a place labelled with the appropriate \label command. This refers to section 2.3 on page 2. If these labels are inside numbered environments like sections, subsections, equations, figures or tables, they carry the appropriate number in the ref command and the page number in the pageref command. It is customary to name labels with prefixes eq:, fig: and tab: for equations, figures and tables respectively.

2.5 Footnotes

Footnotes are simple done like this.* You can write the footnote text[†]outside of the paragraph, if appropriate.

^{*}My first footnote.

[†]My second footnote

3 Mathematical equations

LATEX has a special math mode that needs to be triggered by a command.

Inline mathematics is written either using dollar signs like this x = y (this is the old TEX macro) or using escaped parentheses x = y. These two are completely equivalent, even though the latter one is somewhat neater and makes it easier to search for a missing one.

Display mathematics is written either using escaped brackets.

$$x = y$$

or using the equation* environment.

$$x = y$$

These two are equivalent. The * means that the equation is not automatically numbered. Please refrain from using the old T_EX double dolar macro \$\$ x=y \$\$. This is poorly defined and breaks things. For automatically numbered equations, use the \equation environment.

$$x = y \tag{1}$$

Note that empty lines prior to \[or \begin{equation} matter. Display equations are parts of paragraphs or paragraphs themselves, and the spacing reflects this. Also, note that spaces can be used to separate individual commands, but just like in normal mode, any number of spaces counts as a single space. Other environments that you may want to use are align (aligned equations, arrays of equations), multline (not a typo) (one equation split across line) and gather (not-aligned equations, one per line). (Please don't use array, it causes problems.)

If you want to number equations manually, you use the tag command

$$x = y \tag{4}$$

4 Mathematical typesetting conventions

The document uses unicode-math, which means that you can type mathematical symbols directly using their Unicode characters. However, since there are no Unicode keyboards, it is usually more convenient to use the related ASCII macros.

Variables All variables are typeset in *italics/slanted/oblique*. This includes fundamental constants that do not vary. (We can imagine a hypothetical situation when they do.)

$$x,y,i,j,e$$
 (elementary charge), c (the speed of light)

Vector variables are typeset in **bold italics**. (They are still variables.) For this, use the vc command.

$$F = ma$$

Matrix/tensor variables are typeset in bold sans-serif font. For these the command mat was defined. (In addition, a command transp was defined for transpose T)

$$c^{\mathsf{T}}Hc = E$$

Mathmatical alphabets If you want a more direct control, below is the list of all the mathematical alphabets that exist in Unicode. (These commands can also be used without the curly braces, in which case they apply to the next symbol, like this \mathcal{L} . However, with curly braces it is more explicit what you mean.)

$aA\xi\Xi$	$aA\xi\Xi$	$aA\xi\Xi$	$aA\xi\Xi$	$aA\xi\Xi$	$aA\xi\Xi$	a $A\xi\Xi$	aA $\xi \Xi$
aΑξΞ	$aA\xi\Xi$	$aA\xi\Xi$	oA $\xi\Xi$	$aA\xi\Xi$	$a\mathcal{A}\xi\Xi$	$a\mathcal{A}\xi\Xi$	$a\mathcal{A}\xi\Xi$
$a\mathcal{A}\xi\Xi$	$\mathfrak{a}\mathfrak{A}\xi\Xi$	$\mathfrak{a}\mathfrak{A}\xi\Xi$	aA $\xi\Xi$	aΑξΞ	$aA\xi\Xi$	aAξΞ	

Non-variables All other objects, like operators, labels, abbreviations, function names or units, must be typed upright. This also applies to mathematical constants that are usually denoted by letters, like e (Euler's number), i (imaginary unit), π (circumference of a circle of a unit diameter). Basic functions, like trigs and logs have their own commands. For differentials d, e, i and π , new commands were defined for their upright versions ue, ud, ui, upi. Similarly, the difference, the upright capital delta is used Δ , which has been assigned the macro uDelta. For derivatives, the package diffcoeff provides a simpler notation than explicitly writing fractions.

If you want to specify that something should be upright in the math mode, you have a few options.

```
symup effigy Symbols from the mathematical upright alphabet. No spaces, no ligatures
             and specific spacing. Use for mathematical symbols that are upright letters
             (differentials, mathematical constants)
```

math* Uses math font and its variations without ligatures and spaces. Ideal for multiletter operators.

```
mathrm effigy
    mathup effigy Equivalent to mathrm
    mathit effigy
    mathbf effigy
mathbfit effigy
    mathsf effigy
  mathtt effigy
                  Use only for compatibility purposes.
```

mathtext* "Old" definitions of the math* commands that are not updated throughout

```
mathtextrm effigy
mathtextit effigy
mathtextbf effigy
```

text effigy Gives the same result as text outside of the math mode (including the font, spaces and ligatures). Can also use textrm, textbf, textit, textsf, texttt just like outside of math mode.

See examples below.

$$\sin x, \ln \Delta H_{\text{fus}}^{\Theta}, \int \mathrm{d}x, \mathrm{e}^{\mathrm{i}\pi}, \mathbf{A}^{\mathsf{T}}, \frac{\mathrm{d}f(x)}{\mathrm{d}x}, \left. \frac{\mathrm{d}^3 f}{\mathrm{d}x^3} \right|_{x=0}, \left(\frac{\partial^3 f(x,y)}{\partial x^3} \right)_{y=0}$$

Also note the standard state symbol Θ , which has been assigned the std macro.

Units and decimal numbers For the formating of numerical values and units, the package siunitx is used. The main advantage is the ability to globally change the decimal separator between dot and comma, or the way units are typeset. This can be used e.g. in making of different language versions. Therefore, all decimal numbers and numbers with units should be typeset as follows:

12345.67890	$12345,\!67890$	$1 \pm 2i$
0.3×10^{45}	$0.3 \cdot 10^{45}$	${ m kJmol^{-1}}$
$1525.3{\rm kJ}{\rm mol}^{-1}$	$10\mu\mathrm{m}$	$10\mu\mathrm{m}$
10 µl	$10^{\circ}\mathrm{C}$	$1525.3{\rm kJmol^{-1}}$
$15.3\mathrm{J}\mathrm{mol}^{-1}\mathrm{K}^{-1}$	$15.3{ m Jmol^{-1}K^{-1}}$	$1525.3{\rm kJmol^{-1}}$
4.5°	1°2′3″	

Note that the units are correctly typeset in upright font with a non-breaking space between the number and the unit. It does not matter whether decimal comma or dot is used in the source code, the output will follow the package setting. Units can be either selected by typing their abbreviations separated by dots with explicit powers, or by specific commands as demonstrate above.

5 Chemistry typesetting

The package used is chemmacros. Chemical formulas are then enclosed in the ch command, like this H_2O . This works also in the math mode like in

$$\Delta G_{\text{fus}}^{\Theta}(\text{H}_2\text{O}).$$

Alternatively, for full reactions, one can use the reaction and reaction* environments. (* again to avoid numbering)

$$\begin{split} \mathrm{H_{2}SO_{4}} + 2\,\mathrm{H_{2}O} & \Longrightarrow \mathrm{HSO_{4}^{-}} + \mathrm{H_{3}O^{+}} + \mathrm{H_{2}O} & \Longrightarrow 2\,\mathrm{H_{3}O^{+}} + \mathrm{SO_{4}^{2-}} \\ & \quad \quad ^{1}_{0}\mathrm{n} + ^{235}_{92}\mathrm{U} \longrightarrow 3\,^{1}_{0}\mathrm{n} + ^{93}_{36}\mathrm{Kr} + ^{140}_{56}\mathrm{Ba} \\ & \quad 2\,\mathrm{R-CHO} \longrightarrow \mathrm{R-COO^{-}} + \mathrm{R-CH_{2}-OH} \\ & \quad \quad \mathrm{F_{2}} + \mathrm{H_{2}O\left(s\right)} \xrightarrow{-40\,^{\circ}\mathrm{C}} \mathrm{HF(A)} + \mathrm{HOF(B)} \end{split}$$

However, the package can do much more, so feel free to explore

$$Ag^{\oplus} \stackrel{\ominus}{\cdot} \stackrel{\bigcirc}{O} - C \equiv N$$
: $Ag^{\oplus} \stackrel{\ominus}{\cdot} \stackrel{\bigcirc}{O} - N^{\oplus} \equiv C$:

SI (BIPM) **IUPAP** ISO **IUPAC NIST** letter nothing, nothing, nothing, nothing, nothing, symbols space, \cdot , \times , space, \cdot , \times , space, \cdot , \times , \cdot , \times , space, \cdot , \times , numbers ? (uses \times) X X with decimal

 \times

space, \cdot , /

Table 1: Multiplication symbols recommended by different authorities

 $\overline{?}$ (uses \times)

space, \cdot , /

 \times , \cdot

space, ·, /

6 Literature citations

 \times , \cdot

space, \cdot , /,

nothing
(when unambiguous)
cannot do

 $a \times b^{-1}$ for any of above

For citations, the package recommended today, is biblatex with biber backend. The citations are then imported from a separate .bib file, which can be automatically generated from a citation manager, like Zotero, Mendeley or EndNote.

space, \cdot , /

AS citation commands, one can use either superscripts, which is mainly when the reference is not explicitly a part of the sentence. Alternatively, you can mention them in sentence, like ref [2]. You can also reference in full like D. I. Mendeleyev, $Zeitschrift \ f\"ur \ Chemie$, 1869, 12, 405–406 or in a footnote like this. ‡

References

dots

with decimal comas

units

notes

numbers

- H. Potter and A. Dumbledore, Journal of Magical Chemistry, 2007, 58, 101–114, DOI: 10. 1143/JPSJ.58.101.
- (2) G. Gandalf and W. Saruman, *Journal of Middle-earth*, 2012, **3567**, 5568–9999, DOI: 10.1143/JPSJ.58.101.
- (3) D. I. Mendeleyev, Zeitschrift für Chemie, 1869, 12, 405–406.
- (4) L. Öhrström and J. Reedijk, $Pure\ and\ Applied\ Chemistry,\ 2016,\ 88,\ 1225–1229,\ DOI:\ 10.\ 1515/pac-2016-0501.$

[‡]L. Öhrström and J. Reedijk, Pure and Applied Chemistry, 2016, 88, 1225–1229, DOI: 10.1515/pac-2016-0501.