

# Proteínas capaces de cristalizar en un intervalo de pH amplio

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```
# knitr::opts_chunk$set(eval = FALSE)
# switch global para evaluar funciones o no.
```



# Chapter 1

## Dependencias

La reproducción correcta de esta bitácora depende de varios programas instalados en un sistema operativo linux.

### 1.1 Sistema operativo

El sistema operativo usado es Fedora 36 (<https://getfedora.org/>) en su versión *workstation*.

```
uname -r # Imprime la versión del núcleo de linux.
```

```
## 5.17.8-300.fc36.x86_64
```

### 1.2 Minería de datos

La extracción de datos se realiza con **gemmi** (<https://github.com/project-gemmi/gemmi>), que ya viene dentro de la colección de programas de **ccp4** (<https://www.ccp4.ac.uk/>).

Para la limpieza y transformación de datos se usa:

- **awk** (<https://www.gnu.org/software/gawk/>)
- **bash** (<https://www.gnu.org/software/bash/>)
- **grep** (<https://www.gnu.org/software/grep/>)
- **R** (<https://www.r-project.org/>)
- **sed** (<https://www.gnu.org/software/gawk/>)
- **tidyverse** (<https://www.tidyverse.org/>)

La instalación de R conviene hacerla como la describo en el siguiente enlace <https://murpholinox.github.io/2021/05/01/installRsansTexLivedeps.html>. La instalación del **tidyverse** depende a su vez de la instalación de las siguientes librerías en el sistema operativo:

```
sudo dnf install openssl-devel libcurl-devel
```

Advertencia: Si se tiene instalado chimera-daily se tendrá un conflicto con openssl-devel. En ese caso se tiene que instalar openssl1.1-devel y tanto chimera-daily como rstudio corren sin problemas.

Los programas restantes (awk, bash, grep y sed) vienen instalados por defecto en el sistema operativo usado.

## 1.3 Configuración

Además de la instalación correcta de los programas anteriores, se tienen que cargar las siguientes librerías de R.

```
library(dplyr)
library(ggplot2)
library(readr)
library(knitr)
library(kableExtra)
library(stringdist)
library(svglite)
library(bookdown)
library(rmarkdown)
library(renv)
```

### 1.3.1 Manejo de dependencias

El manejo de dependencias, de manera interna, se da automáticamente gracias a renv.

```
renv::consent() # Da permiso a renv.4
```

```
## * Consent to use renv has already been provided -- nothing to do.
```

```
renv::init() # Inicia renv.
```

```
# Para ver las dependencias.
cat renv.lock
```

## 1.4 Sesión

Imprime información de la sesión activa de R.

```
sessionInfo()
```

```
## R version 4.1.3 (2022-03-10)
## Platform: x86_64-redhat-linux-gnu (64-bit)
```

```
## Running under: Fedora Linux 36 (Workstation Edition)
##
## Matrix products: default
## BLAS/LAPACK: /usr/lib64/libflexiblas.so.3.1
##
## locale:
## [1] LC_CTYPE=en_US.UTF-8      LC_NUMERIC=C
## [3] LC_TIME=en_US.UTF-8      LC_COLLATE=en_US.UTF-8
## [5] LC_MONETARY=en_US.UTF-8  LC_MESSAGES=en_US.UTF-8
## [7] LC_PAPER=en_US.UTF-8     LC_NAME=C
## [9] LC_ADDRESS=C             LC_TELEPHONE=C
## [11] LC_MEASUREMENT=en_US.UTF-8 LC_IDENTIFICATION=C
##
## attached base packages:
## [1] stats      graphics  grDevices datasets  utils      methods    base
##
## other attached packages:
## [1] renv_0.15.4      rmarkdown_2.14   bookdown_0.26    svglite_2.1.0
## [5] stringdist_0.9.8 kableExtra_1.3.4 knitr_1.39       readr_2.1.2
## [9] ggplot2_3.3.6    dplyr_1.0.9
##
## loaded via a namespace (and not attached):
## [1] pillar_1.7.0      compiler_4.1.3    tools_4.1.3      digest_0.6.29
## [5] viridisLite_0.4.0 evaluate_0.15      lifecycle_1.0.1  tibble_3.1.7
## [9] gtable_0.3.0      pkgconfig_2.0.3   rlang_1.0.2      cli_3.3.0
## [13] rstudioapi_0.13   parallel_4.1.3    yaml_2.3.5       xfun_0.30
## [17] fastmap_1.1.0     xml2_1.3.3        httr_1.4.3       withr_2.5.0
## [21] stringr_1.4.0     systemfonts_1.0.4 hms_1.1.1        generics_0.1.2
## [25] vctr_0.4.1        webshot_0.5.3     grid_4.1.3       tidyselect_1.1.2
## [29] glue_1.6.2        R6_2.5.1          fansi_1.0.3      tzdb_0.3.0
## [33] purrr_0.3.4       magrittr_2.0.3    scales_1.2.0     ellipsis_0.3.2
## [37] htmltools_0.5.2   rvest_1.0.2       colorspace_2.0-3 utf8_1.2.2
## [41] stringi_1.7.6     munsell_0.5.0     crayon_1.5.1
```

## 1.5 Contacto

Me puedes contactar por correo electrónico en gmail o ibt.





## Chapter 2

# Hello bookdown

All chapters start with a first-level heading followed by your chapter title, like the line above. There should be only one first-level heading (#) per .Rmd file.

### 2.1 A section

All chapter sections start with a second-level (##) or higher heading followed by your section title, like the sections above and below here. You can have as many as you want within a chapter.

#### An unnumbered section

Chapters and sections are numbered by default. To un-number a heading, add a {.unnumbered} or the shorter {-} at the end of the heading, like in this section.



## Chapter 3

# Cross-references

Cross-references make it easier for your readers to find and link to elements in your book.

### 3.1 Chapters and sub-chapters

There are two steps to cross-reference any heading:

1. Label the heading: `# Hello world {#nice-label}`.
  - Leave the label off if you like the automated heading generated based on your heading title: for example, `# Hello world = # Hello world {#hello-world}`.
  - To label an un-numbered heading, use: `# Hello world {-#nice-label}` or `{# Hello world .unnumbered}`.
2. Next, reference the labeled heading anywhere in the text using `\@ref(nice-label)`; for example, please see Chapter 3.
  - If you prefer text as the link instead of a numbered reference use: any text you want can go here.

### 3.2 Captioned figures and tables

Figures and tables *with captions* can also be cross-referenced from elsewhere in your book using `\@ref(fig:chunk-label)` and `\@ref(tab:chunk-label)`, respectively.

See Figure 3.1.

```
par(mar = c(4, 4, .1, .1))
plot(pressure, type = 'b', pch = 19)
```

Don't miss Table 3.1.

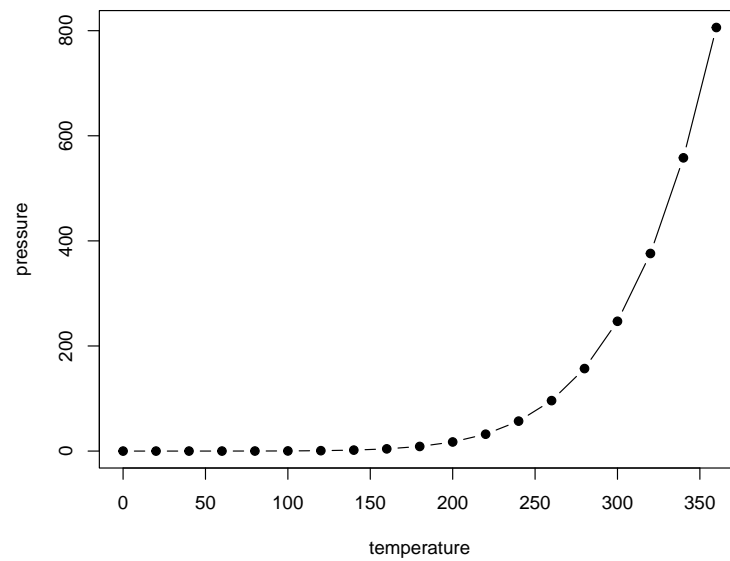


Figure 3.1: Here is a nice figure!

```
knitr::kable(  
  head(pressure, 10), caption = 'Here is a nice table!',  
  booktabs = TRUE  
)
```

Table 3.1: Here is a nice table!

temperature	pressure
0	0.0002
20	0.0012
40	0.0060
60	0.0300
80	0.0900
100	0.2700
120	0.7500
140	1.8500
160	4.2000
180	8.8000



## Chapter 4

# Parts

You can add parts to organize one or more book chapters together. Parts can be inserted at the top of an .Rmd file, before the first-level chapter heading in that same file.

Add a numbered part: `# (PART) Act one {-}` (followed by `# A chapter`)

Add an unnumbered part: `# (PART\*) Act one {-}` (followed by `# A chapter`)

Add an appendix as a special kind of un-numbered part: `# (APPENDIX) Other stuff {-}` (followed by `# A chapter`). Chapters in an appendix are prepended with letters instead of numbers.





## Chapter 5

# Footnotes and citations

### 5.1 Footnotes

Footnotes are put inside the square brackets after a caret `^[]`. Like this one <sup>1</sup>.

### 5.2 Citations

Reference items in your bibliography file(s) using `@key`.

For example, we are using the **bookdown** package [Xie, 2022] (check out the last code chunk in `index.Rmd` to see how this citation key was added) in this sample book, which was built on top of R Markdown and **knitr** [Xie, 2015] (this citation was added manually in an external file `book.bib`). Note that the `.bib` files need to be listed in the `index.Rmd` with the YAML `bibliography` key.

The RStudio Visual Markdown Editor can also make it easier to insert citations: <https://rstudio.github.io/visual-markdown-editing/#/citations>

---

<sup>1</sup>This is a footnote.



## Chapter 6

# Blocks

### 6.1 Equations

Here is an equation.

$$f(k) = \binom{n}{k} p^k (1-p)^{n-k} \quad (6.1)$$

You may refer to using `\@ref{eq:binom}`, like see Equation (6.1).

### 6.2 Theorems and proofs

Labeled theorems can be referenced in text using `\@ref{thm:tri}`, for example, check out this smart theorem 6.1.

**Theorem 6.1.** *For a right triangle, if  $c$  denotes the length of the hypotenuse and  $a$  and  $b$  denote the lengths of the **other** two sides, we have*

$$a^2 + b^2 = c^2$$

Read more here <https://bookdown.org/yihui/bookdown/markdown-extensions-by-bookdown.html>.

### 6.3 Callout blocks

The R Markdown Cookbook provides more help on how to use custom blocks to design your own callouts: <https://bookdown.org/yihui/rmarkdown-cookbook/custom-blocks.html>



## Chapter 7

# Sharing your book

### 7.1 Publishing

HTML books can be published online, see: <https://bookdown.org/yihui/bookdown/publishing.html>

### 7.2 404 pages

By default, users will be directed to a 404 page if they try to access a webpage that cannot be found. If you'd like to customize your 404 page instead of using the default, you may add either a `_404.Rmd` or `_404.md` file to your project root and use code and/or Markdown syntax.

### 7.3 Metadata for sharing

Bookdown HTML books will provide HTML metadata for social sharing on platforms like Twitter, Facebook, and LinkedIn, using information you provide in the `index.Rmd` YAML. To setup, set the `url` for your book and the path to your `cover-image` file. Your book's `title` and `description` are also used.

This `gitbook` uses the same social sharing data across all chapters in your book—all links shared will look the same.

Specify your book's source repository on GitHub using the `edit` key under the configuration options in the `_output.yml` file, which allows users to suggest an edit by linking to a chapter's source file.

Read more about the features of this output format here:

<https://pkgs.rstudio.com/bookdown/reference/gitbook.html>

Or use:

```
?bookdown::gitbook
```

# Bibliography

Yihui Xie. *Dynamic Documents with R and knitr*. Chapman and Hall/CRC, Boca Raton, Florida, 2nd edition, 2015. URL <http://yihui.org/knitr/>. ISBN 978-1498716963.

Yihui Xie. *bookdown: Authoring Books and Technical Documents with R Markdown*, 2022. URL <https://CRAN.R-project.org/package=bookdown>. R package version 0.26.