

# Quarto Template for PNAS Submissions

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Please provide an abstract of no more than 250 words in a single paragraph. Abstracts should explain to the general reader the major contributions of the article. References in the abstract must be cited in full within the abstract itself and cited in the text.

template | demo

A word of warning: This template will fail with a “Not in outer par mode” warning if you try to compile it with less than one page of text. The template relies on having a full first page which is styled separately. If you see a warning to the tune of “LaTeX Error: Not in outer par mode.” or referencing `\end{document}`, try writing more or adding filler text and recompiling.

## Using this template

If your first paragraph (i.e. with the `\dropcap`) contains a list environment (quote, quotation, theorem, definition, enumerate, itemize...), the line after the list may have some extra indentation. If this is the case, add `\parshape=0` to the end of the list environment. This PNAS journal template is provided to help you write your work in the correct journal format. Instructions for use are provided below.

Note: please start your introduction without including the word **Introduction** as a section heading (except for math articles in the Physical Sciences section); this heading is implied in the first paragraphs.

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**Format.** Many authors find it useful to organize their manuscripts with the following order of sections: title, author line and affiliations, keywords, abstract, significance statement, introduction, results, discussion, materials and methods, acknowledgments, and references. Other orders and headings are permitted.

**Manuscript Length.** A standard 6-page article is approximately 4,000 words, 50 references, and 4 medium-size graphical elements (i.e., figures and tables). The preferred length of articles remains at 6 pages, but PNAS will allow articles up to a maximum of 12 pages.

**References.** References should be cited in numerical order as they appear in text; this will be done automatically via bibtex, e.g. (1) and (1 2 3 4). All references cited in the main text should be included in the main manuscript file.

**Data Archival.** PNAS must be able to archive the data essential to a published article. Where such archiving is not possible, deposition of data in public databases, such as GenBank, ArrayExpress, Protein Data Bank, Unidata, and others outlined in the [Information for Authors](#), is acceptable.

## Significance Statement

Authors must submit a 120-word maximum statement about the significance of their research paper written at a level understandable to an undergraduate educated scientist outside their field of speciality. The primary goal of the significance statement is to explain the relevance of the work in broad context to a broad readership. The significance statement appears in the paper itself and is required for all research papers.

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Please provide details of author contributions here.  
Please declare any competing interests here.

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**Table 1. Comparison of the fitted potential energy surfaces and ab initio benchmark electronic energy calculations**

Species	CBS	CV	G3
1. Acetaldehyde	0.0	0.0	0.0
2. Vinyl alcohol	9.1	9.6	13.5
3. Hydroxyethylidene	50.8	51.2	54.0

nomenclature for the TSs refers to the numbered species in the table.

**Language-Editing Services.** Prior to submission, authors who believe their manuscripts would benefit from professional editing are encouraged to use a language-editing service (see list at <https://www.pnas.org/author-center/language-editing>). PNAS does not take responsibility for or endorse these services, and their use has no bearing on acceptance of a manuscript for publication.

**Figures and Tables.** Figures can be included using Quarto's syntax, code chunks, or with LaTeX. For simple figures, Quarto syntax is typically easiest. Full details are available in [the Quarto documentation](#).



**Figure 1.** Placeholder image of a frog with a long example legend to show justification setting.

Tables can similarly be included using Quarto's syntax, code chunks, or with LaTeX. I tend to use code chunks, but LaTeX works very well for classic tables, like regression tables or summary statistics.

**Digital Figures.** EPS, high-resolution PDF, and PowerPoint are preferred formats for figures that will be used in the main manuscript. Authors may submit PRC or U3D files for 3D images; these must be accompanied by 2D representations in TIFF, EPS, or high-resolution PDF format. Color images must be in RGB (red, green, blue) mode. Include the font files for any text.

Images must be provided at final size, preferably 1 column width (8.7cm). Figures wider than 1 column should be sized

to 11.4cm or 17.8cm wide. Numbers, letters, and symbols should be no smaller than 6 points (2mm) and no larger than 12 points (6mm) after reduction and must be consistent. Figures and tables should be labelled and referenced in the standard way using the `\label{}` and `\ref{}` commands. Figure Figure 1 shows an example of how to insert a column-wide figure. To insert a figure wider than one column, please use the `figure*` environment. Figures wider than one column should be sized to 11.4 cm or 17.8 cm wide. Use `SCfigure*` environment for a wide figure with side legends, such as Figure 2.

In Quarto, we can do these by setting the `fig-env` command to `figure*` or `SCfigure*`

**Tables.** Tables should be included in the main manuscript file and should not be uploaded separately.

**Single column equations.** Authors may use 1- or 2-column equations in their article, according to their preference. To allow an equation to span both columns, use the `\begin{figure*}...\end{figure*}` environment mentioned above for figures. Note that the use of the `widetext` environment for equations is not recommended, and should not be used.

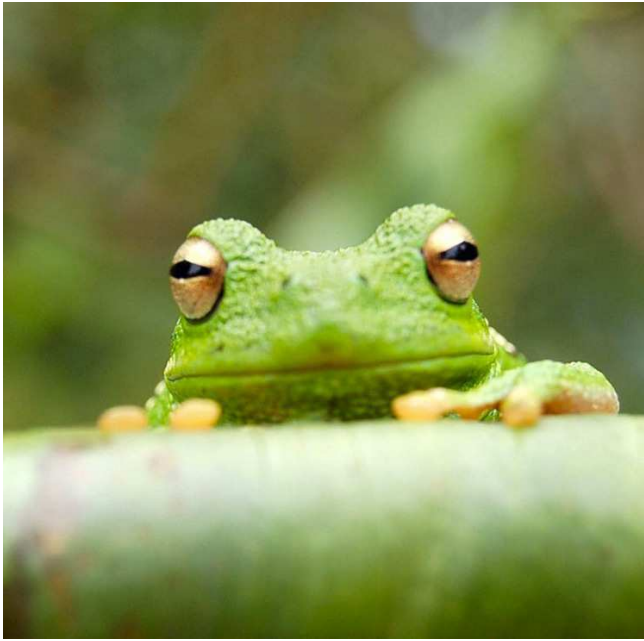
## Material and Methods

**Supporting Information Appendix (SI).** Authors should submit SI as a single separate SI Appendix PDF file, combining all text, figures, tables, movie legends, and SI references. SI will be published as provided by the authors; it will not be edited or composed. Additional details can be found in the [PNAS Author Center](#). The PNAS Overleaf SI template can be found [here](#). Refer to the SI Appendix in the manuscript at an appropriate point in the text. Number supporting figures and tables starting with S1, S2, etc. Authors who place detailed materials and methods in an SI Appendix must provide sufficient detail in the main text methods to enable a reader to follow the logic of the procedures and results and also must reference the SI methods. If a paper is fundamentally a study of a new method or technique, then the methods must be described completely in the main text.

**SI Datasets.** Supply .xlsx, .csv, .txt, .rtf, or .pdf files. This file type will be published in raw format and will not be edited or composed.

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## References



**Figure 2.** This legend would be placed at the side of the figure, rather than below it.

$$\begin{aligned}(x + y)^3 &= (x + y)(x + y)^2 \\ &= (x + y)(x^2 + 2xy + y^2) \\ &= x^3 + 3x^2y + 3xy^2 + y^3.\end{aligned}$$

[1]

**ACKNOWLEDGMENTS.** Please include your acknowledgments here, set in a single paragraph. Please do not include any acknowledgments in the Supporting Information, or anywhere else in the manuscript.