

Template for preparing your Brief Report submission to PNAS using Overleaf

Author One^{a,c,1}, Author Two^{b,1,2}, and Author Three^a

^aAffiliation One; ^bAffiliation Two; ^cAffiliation Three

This manuscript was compiled on October 17, 2019

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

Keyword 1 | Keyword 2 | Keyword 3 | ...

1 This PNAS journal template is provided to help you write
2 your work in the correct journal format. Instructions for
3 use are provided below.

4 Note: please start your introduction without including the
5 word “Introduction” as a section heading (except for math arti-
6 cles in the Physical Sciences section); this heading is implied
7 in the first paragraphs.

8 Guide to using this template on Overleaf

9 Please note that whilst this template provides a preview of the
10 typeset manuscript for submission, to help in this preparation,
11 it will not necessarily be the final publication layout. For
12 more detailed information please see the [PNAS Information
13 for Authors](#).

14 If you have a question while using this template on Overleaf,
15 please use the help menu (“?”) on the top bar to search for [help
16 and tutorials](#). You can also [contact the Overleaf support team](#)
17 at any time with specific questions about your manuscript or
18 feedback on the template.

19 **Author Affiliations.** Include department, institution, and com-
20 plete address, with the ZIP/postal code, for each author. Use
21 lower case letters to match authors with institutions, as shown
22 in the example. Authors with an ORCID ID may supply this
23 information at submission.

24 **Submitting Manuscripts.** All authors must submit their arti-
25 cles at [PNAScentral](#). If you are using Overleaf to write your
26 article, you can use the “Submit to PNAS” option in the top
27 bar of the editor window.

28 **Format.** Many authors find it useful to organize their
29 manuscripts with the following order of sections; title, au-
30 thor line and affiliations, keywords, abstract, introduction,
31 results, discussion, materials and methods, acknowledgments,
32 and references. Other orders and headings are permitted.

33 **Manuscript Length.** The maximum length of a Brief Report
34 article is 20,000 characters, including all text, spaces, and
35 the number of characters displaced by equations and graphical
36 elements. Brief Reports typically include no more than 2
37 graphical elements (e.g., figures and tables) and Supporting
38 Information is limited to essential supporting datasets and
39 videos; additional methods, tables, or figures are not permit-
40 ted.

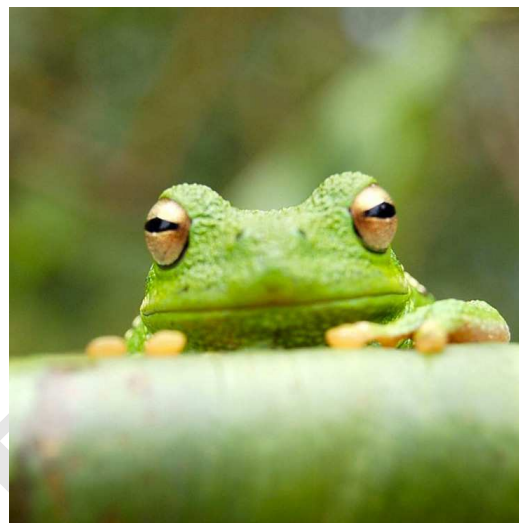


Fig. 1. Placeholder image of a frog with a long example legend to show justification setting.

References. References should be cited in numerical order as
they appear in text; this will be done automatically via bibtex,
e.g. (1) and (2, 3). 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, Ar-
rayExpress, Protein Data Bank, Unidata, and others outlined
in the [Information for Authors](#), is acceptable.

Language-Editing Services. Prior to submission, authors who
believe their manuscripts would benefit from professional edit-
ing are encouraged to use a language-editing service (see list at
[www.pnas.org/page/authors/language-editing](#)). PNAS does
not take responsibility for or endorse these services, and their
use has no bearing on acceptance of a manuscript for publica-
tion.

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

Please provide details of author contributions here.

Please declare any competing interests here.

¹A.O.(Author One) contributed equally to this work with A.T. (Author Two) (remove if not applicable).

²To whom correspondence should be addressed. E-mail: author.twoemail.com

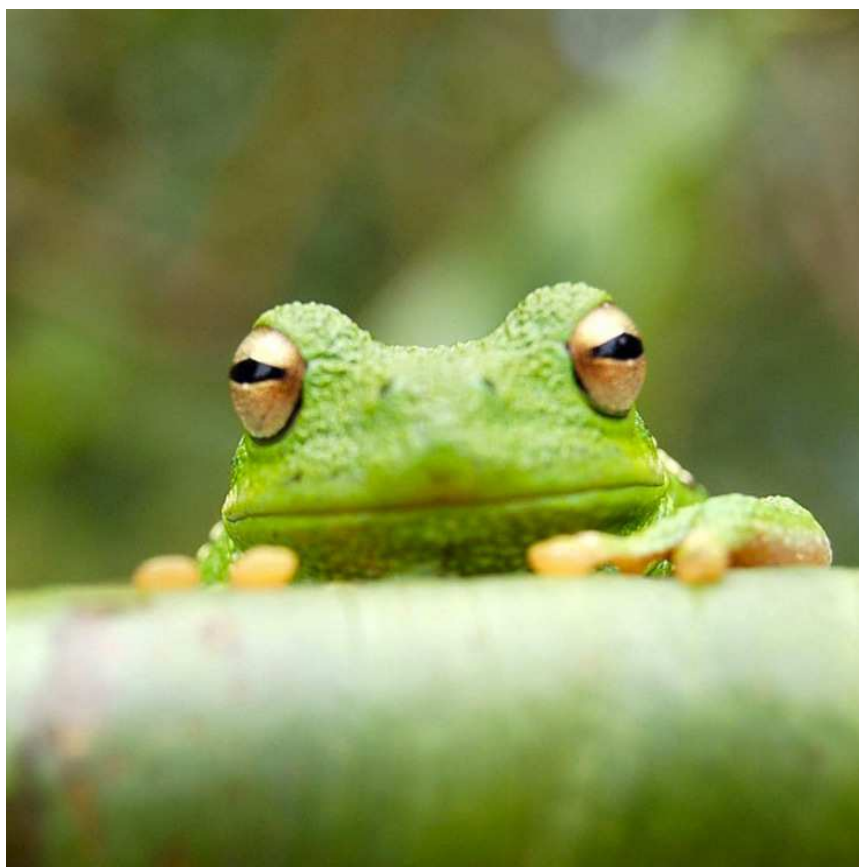


Fig. 2. This legend would be placed at the side of the figure, rather than below it.

62 must be in RGB (red, green, blue) mode. Include the font
63 files for any text.

64 Images must be provided at final size, preferably 1 column
65 width (8.7cm). Figures wider than 1 column should be sized
66 to 11.4cm or 17.8cm wide. Numbers, letters, and symbols
67 should be no smaller than 6 points (2mm) and no larger than
68 12 points (6mm) after reduction and must be consistent.

69 Figures and tables should be labelled and referenced in the
70 standard way using the `\label{}` and `\ref{}` commands.

71 Figure 1 shows an example of how to insert a column-wide
72 figure. To insert a figure wider than one column, please use
73 the `\begin{figure*}...\end{figure*}` environment. Fig-
74 ures wider than one column should be sized to 11.4 cm or 17.8
75 cm wide. Use `\begin{SCfigure*}...\end{SCfigure*}` for a
76 wide figure with side legends.

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

79 **Single column equations.** Authors may use 1- or 2-column
80 equations in their article, according to their preference.

81 To allow an equation to span both columns, use the
82 `\begin{figure*}...\end{figure*}` environment mentioned
83 above for figures.

84 Note that the use of the `widetext` environment for equa-
85 tions is not recommended, and should not be used.

86 **Supporting Information (SI).** Authors are limited to the follow-
87 ing types of SI: datasets, videos, and 3D figures. Extended
88 methods or discussion are not permitted.

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.

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.

SI Movies. Supply Audio Video Interleave (avi), Quicktime
(mov), Windows Media (wmv), animated GIF (gif), or MPEG
files and include a brief legend for each movie in the main
manuscript file. All movies should be submitted at the desired
reproduction size and length. Movies should be no more than
10 MB in size.

3D Figures. Supply a composable U3D or PRC file so that it
may be edited and composed. Authors may submit a PDF file
but please note it will be published in raw format and will not
be edited or composed.

Materials and Methods

Please describe your materials and methods here. This can be more
than one paragraph, and may contain subsections and equations
as required. Authors should include a statement in the methods

$$\begin{aligned}(x + y)^3 &= (x + y)(x + y)^2 \\ &= (x + y)(x^2 + 2xy + y^2) \\ &= x^3 + 3x^2y + 3xy^2 + y^3.\end{aligned}\tag{1}$$

106 section describing how readers will be able to access the data in the
107 paper.

108 **Subsection for Method.** Example text for subsection.

109 **ACKNOWLEDGMENTS.** Please include your acknowledgments
110 here, set in a single paragraph. Please do not include any acknowl-
111 edgments in the Supporting Information, or anywhere else in the
112 manuscript.

- 113 1. M Belkin, P Niyogi, Using manifold stucture for partially labeled classification in *Advances in*
114 *neural information processing systems*. pp. 929–936 (2002).
- 115 2. P Bérard, G Besson, S Gallot, Embedding riemannian manifolds by their heat kernel. *Geom.*
116 *& Funct. Analysis GAFA* 4, 373–398 (1994).
- 117 3. RR Coifman, et al., Geometric diffusions as a tool for harmonic analysis and structure definition
118 of data: Diffusion maps. *Proc. Natl. Acad. Sci. United States Am.* **102**, 7426–7431 (2005).

DRAFT