

# Writing Journal Articles

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## 1 Introduction

These notes include some advice on how to write a paper for publication in a peer-reviewed journal. Considerably more extensive advice on this subject is available in other sources such as the *ACS Style Guide*.

## 2 Goals for a Paper

As Fritz Schaefer used to say, “if it isn’t published, it doesn’t exist.” Although you might present unpublished work as a poster or a talk, only a publication will elevate it to the status of a legitimate, completed project worthy of discussion. One of the most important items on your resume is how many publications you have and what journals they appear in. The first goal for a paper, then, is to conclude a project and earn credit for the work.

To achieve the first goal, it is necessary to write a paper that will pass peer review. A paper that is clear and well-organized is more likely to be accepted. Journals also only want to publish original research that will have a significant impact. Therefore it is necessary to explain how your paper differs from previous work, why your paper is important, and what new insights it presents.

The second goal for a paper is to inform the community about what you have done and why it is important. The most successful publications are those that teach others about a new discovery or a new way of looking at things. This enhances the ability of other researchers to make progress in their own projects. In more applied areas of research, published research may ultimately result in new products, devices, diagnostic procedures, etc., that can benefit society.

To achieve the second goal, you need to decide what audience you wish to reach, and write the paper appropriately. This also affects the choice of the journal to which the paper should be submitted.

Finally, a paper should have one major point, or one main thing that it is about. Trying to accomplish too much in one paper can dilute your message and make it harder for readers to understand what the paper was about.

## 3 Parts of the Paper

### 3.1 Abstract

This should be an extremely concise summary of the major findings of the article. It should not be more than 150 words, and *JACS* has been known to send back papers with abstracts longer than 100 words. The abstract is not merely an advertisement for the article — the main results should be presented directly in the abstract to the extent possible within the space allowed.

### 3.2 Introduction

This is the part where you explain why your paper is interesting. It should set up the problem, including a thorough discussion of the literature. The last part of the introduction should give a *very* brief idea (no more than a paragraph) about what is discovered in the paper. When the referee is deciding what to tell the editor about the impact of the paper, the introduction and conclusions are the sections to which he will refer.

### 3.3 Methods

For theorists, this section may also be called “Theoretical Methods.” In this section, explain *how* you did what you did. You should give sufficient detail that anyone else who is properly trained in your subfield should be able to reproduce your results. For routine applications of standard methods, this part should be as clear and concise as possible, usually 2-4 paragraphs. For papers describing the development of new theoretical approaches, this is usually the bulk of the paper, and typically there are multiple sections describing each part of the theory, with no section called “Methods.”

### 3.4 Results and Discussion

It is possible to split this into two sections, but more frequently they are combined in theory papers. This section should introduce the results and then discuss what they mean, why they are what they are, and what consequences they have. This section contains the meat of the paper and should cover any details not already explained in the methods section.

### 3.5 Conclusions

This section, of perhaps 1-3 paragraphs, should briefly summarize what the paper has discovered and go on to state the broader significance of these findings. The main point of the paper should be stated or re-stated here.

## 4 Figures

Creating figures for publication is a nontrivial task. For black and white figures, avoid bit-mapped figures (e.g., GIF, JPEG, BMP) and use Postscript, PDF, or vector graphics formats instead. For color figures, some journals prefer high-resolution bitmapped files (e.g., TIFF files). Make sure you have a resolution of at least 300 dpi. Submit figures in their intended publication size (do not make page-filling figures and assume they can be scaled down without any problem). Avoid shading in black and white figures. Avoid very tiny symbols or fonts, or tiny dashes in lines. To summarize: *the figure must be easy on the reader, not hard to see or read or understand.*

Please refer to <http://vergil.chemistry.gatech.edu/resources/figures.html> for more information.

## 5 General Suggestions

Throughout the paper, the following general rules should be helpful:

- Be concise. Don't say more than you need, except as required by the other rules.
- Be correct. If you say your data agree with experiment within 10%, then that really ought to be the case. Try to avoid making statements that are generally but not always true.
- Be clear. Don't write something that the average reader won't understand.
- Be relevant. Try to avoid lengthy discussions about issues that aren't related to the point of the paper.

## 6 Technical Points

- *Important!* For journals that use citation numbers as superscripts, the superscript comes *after* the punctuation. For example: We follow the notation of Handy *et al.*<sup>4</sup>
- Avoid superscripts on numbers, because they'll look like exponents. For example, "the mean absolute error for this method is 0.28<sup>13</sup> kcal mol<sup>-1</sup>."
- *Introduce all acronyms the first time they are used. Copy editors will insist on this very strictly, so this is something you will not be able to avoid — just go ahead and get it right in the first draft.*
- Avoid use of acronyms in titles. Possible rare exceptions might include the introduction of a new method/acronym, or cases where the acronym is much more recognizable than the full name. Any acronyms used in titles should be spelled out.

- The Latin phrase “*et al.*” is short for “*et alia*,” which means “and the others.” The *et* does not have a period because it is not abbreviated.
- If you wish to refer to a paper with only two authors, do not use *et al.* Instead, list both authors (e.g., “Sinnokrot and Sherrill”).
- For papers with more than two authors, you may refer to the paper using the last name of the first author plus “*et al.*” (for example, “Sinnokrot *et al.*”), OR using the last name of the corresponding author plus “and co-workers” (for example, “Head-Gordon and co-workers”).
- Use kcal mol<sup>-1</sup>, not kcal/mol.
- Try to use “computations,” instead of “calculations.” Especially avoid the phrase “ran calculations.”
- Try to avoid repeating a word or phrase within a sentence or pair of sentences.
- Don’t use the same sentence more than once in your paper.
- Don’t use the word “numbers” in a context where you mean “values,” e.g., don’t say “Our results are more reliable than the previously reported numbers.”
- A “level of theory” refers to a combination of a basis set and a correlation method. You might say “computed at the MP2/6-31G\* level of theory,” but avoid saying “computed at the MP2 level of theory.”
- Avoid the phrase “we looked at.” Try “we considered.”
- Try to give an appropriate number of digits in tables, etc. Don’t give more digits than are significant. For example, if you converged the Hartree–Fock computation to 6 digits in the energy after the decimal, don’t give 8. 6 digits is usually a good number for total energies, even if there are more significant digits than this. For relative energies in kcal mol<sup>-1</sup>, often 1-3 digits after the decimal is appropriate. If the theoretical methods used are not particularly accurate for the quantity being computed (e.g., DFT barrier heights), then you might want to report relative energies only to 0.1 kcal mol<sup>-1</sup>.
- *Which vs. That:* Use “that” to define a subset, and “which” to clarify all items of a set. For example, “We toured castles that had moats,” uses *that* because not all castles have moats. On the other hand, “We used NMR, which is a spectroscopic technique.”
- *Punctuation:* Use commas when a pause in the sentence is called for. Use a semicolon (;) before introducing a new independent clause in a sentence. Use a colon (:) before introducing a clarifying comment or a list (e.g., “there are three main approaches: x, y, and z.”) A semicolon can be used to separate items in a list if the items themselves contain commas

(e.g., “three approaches: density functional theory, with whatever functionals are deemed sufficiently accurate; second-order perturbation theory; and coupled-cluster theory.”)

- Use square brackets instead of parentheses if you would otherwise have parentheses within parentheses: e.g., “coupled-cluster theory with perturbative triple substitutions [CCSD(T)].”
- When using the LaTeX text formatting language, avoid defining new commands for convenience (e.g., with `newcommand`). This causes problems with the type conversion software used by the Journals.