

## Journal Articles Essential Pieces

Journal articles generally contain the following parts:

1. Title
2. Abstract
3. Introduction
4. Methods or Experimental
5. Results
6. Discussion
7. Summary
8. Cited Literature

These sections are described below, however, much of the following has been quoted almost verbatim from the *ACS Style Guide: A Manual for Authors and Editors*, p. 17-22 (page numbers refer to 1997 edition).<sup>1</sup>

### Title

The title serves two main purposes: (1) to attract the potential audience and (2) to aid retrieval and indexing.

The title must be brief and grammatically correct but accurate and complete enough to stand alone. A two- or three-word title may be too vague, but a 14- or 15-word title is unnecessarily long. Avoid phrases such as "on the", "a study of", "research on", "report on", "regarding", and "use of". In most cases, omit "the" at the beginning of the title.

Spell out all terms in the title, and avoid jargon, symbols, formulas, and abbreviations. Whenever possible, use words rather than expressions containing superscripts, subscript, or other special notations. Do not site company names, specific trademarks, where brand names of chemicals, drugs, materials, or instruments.

### Abstract

The abstract allows the reader to determine the nature and scope of the paper and helps editors identify key features for indexing and retrieval.

The abstract should briefly state the problem or the purpose of the research, indicate the theoretical or experimental plan used, summarize the principal findings, and point out major conclusions. Do not supplement or evaluate the conclusions in the text. Although an abstract is not a substitute for the article

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<sup>1</sup> The Reed library contains two copies of the *ACS Style Guide, 3e* (QD8.5 .A25 2006). Another useful book is the American Chemical Society's *Handbook for Authors*. The Reed library contains three copies (T11 .A4 1978).

itself, it must be concise, self-contained, and complete enough to appear separately in abstract publications.

The optimal length is one paragraph, but it could be as short as two sentences. The length of the abstract depends on the subject matter and length of the paper. Between 80 and 200 words is usually adequate.

Do not cite references, tables, figures, or sections of the paper in the abstract. Do not include equations, schemes, or structures that require display on a line separate from the text. Use abbreviations and acronyms only when it is necessary to prevent awkward construction or needless repetition. Define abbreviations at first use in the abstract (and again at first use in the text).

## Introduction

A good introduction is a clear statement of the problem or project and the reasons that you are studying it. This information should be contained in the first few sentences. Give a concise and appropriate background discussion of the problem and significance, scope, and limits of your work. Outline what has been done before by citing truly pertinent literature (in most cases, this will be a single article), but do not include a general survey of semi-relevant literature. State how your work differs from or is related to work previously published. Demonstrate the continuity from the previous work to yours. The introduction can be one or two paragraphs long.

## Methods (Experimental)

Give sufficient detail about your materials and methods so that other *experienced* workers can repeat your work and obtain comparable results.

Give the names of all computer programs that you have used. If it is convenient, identify the computational method (geometry optimization, transition state search, conformer search, use of symmetry and/or constraints) and energy algorithm (force field, quantum mechanical method) used to generate each model. Alternatively, if it is more convenient, you may describe procedures generically, e.g., "Reactant and product models were produced using HF/3-21G equilibrium geometry calculations. Transition state models were produced using HF/3-21G transition state searches and were shown to have one imaginary vibration frequency."

If you calculated vibration frequencies in order to verify the nature of energy minima and/or saddle points (transition states), then say so.

When in doubt, refer back to the basic definition of "Computational Methods" given above.

## Results

Summarize the data collected and their mathematical/statistical treatment. Included only relevant data, but give sufficient detail to justify your conclusions. Use equations, figures, and tables only where necessary for clarity and brevity (computer models can be printed easily, but if you print a black and white image, some information may be lost).

When you present data, you should include the procedure that generated the data. If you present data using a figure or table, you should describe in the accompanying text how to read the figure or table.

It is important to distinguish between data and conclusions drawn from the data. The calculated energy of a model is an example of the former. The statement that one model is more stable than another is an example of the latter. Raw data is rarely interesting, so it is customary to interpret the data at the same time that it is described.

A good pattern for reporting results is to give the procedure that generated the data, and the data itself, and finally, any conclusion or interpretation that is immediately suggested by the data.

## Discussion

The purpose of the discussion is to interpret and compare the results to other work. Be objective; point out the features and limitations of your work. Relate your results to current knowledge in the field into your original purpose and undertaking the project: Have you solved the problem? What exactly have you contributed? Briefly state the logical implications of your results. Suggest further study or applications if warranted.

Present your results and discussion either as two separate sections or as one combined section if it is more logical to do so. Do not repeat information given elsewhere in the manuscript.

## Conclusions

The purpose of this section is to put your interpretation of your results in the context of the original problem. Do not repeat discussion points or include irrelevant material. Your conclusions should be based on the evidence presented, but do not present new evidence in this section.

## Cited Literature

Include specific references for all of the literature that you cite. Number your references. Alternatively, cite references using author name and year of

publication. Do not include a bibliography. Do not include references to literature that is not cited in the paper.

You can collect all of your references at the end of your paper, or you may place them at the bottom of each page.

### Figures and Tables

All figures and tables must be numbered. All figures and tables must have a descriptive title. The basic rule is that a figure or table should be understandable without reference to the text. If a figure or table contains numerical data, the units of measurement or calculation for these data must be provided.