Section 13: Layout & Language of a scientific paper

Kallia Katsampoxaki-Hodgetts
School of Sciences and Engineering
A Spectrum of Genres: From Chemistry specific to general

1. Expert
2. Scientific
3. Student
4. General

AUDIENCE
What parts does a paper consist of?
Primary research vs. Review article

- Original research
  - Method
  - Results
- Not original research
  - Summary of existing research
Primary research journal article: organization and structure

The hourglass structure of a scientific paper

- Introduction
- Methods
- Results
- Discussion

General → Specific → General
Introduction

1. Introduce the Research Area
   1.1 Identify the research area
   1.2 Establish the importance of the research area
   1.3 Provide essential background information about the research area

2. Identify a Gap (or Gaps)

3. Fill the Gap
   3.1 Introduce the current work
   3.2 Preview key findings of the current work

Figure 6.1 A visual representation of the move structure for a typical Introduction section.
Central to the entire discipline of X is the concept of ……

Xs are one of the most widely used groups of antibacterial agents and have been extensively used for decades to …

Questions have been raised about the safety of prolonged use of …

To date there has been little agreement on what...

However, there is no reliable evidence that ……

The purpose of this paper is to review recent research into the The main questions/issues addressed in this paper are: a, b, c.
Methods section

1. Describe Materials
   (e.g., materials, chemicals, samples, cultures, sampling sites, general reaction conditions)

2. Describe Experimental Methods
   - Describe procedure(s)
   - Describe instrumentation

3. Describe Numerical Methods (if applicable)
   (e.g., statistical analyses, theoretical computations)

Figure A visual representation of the move structure for a typical Methods section.
Possible Items for a Methods Section

A table of chemicals with their physical properties (e.g., mp, MW, ρ)
Amounts of reagents used in a synthesis (e.g., mg, mmol)
Directions for preparing a stock solution
The quality (grade) of chemicals used
The names and locations of chemical vendors
The brand names of commercial instrumentation used
A diagram of a distillation apparatus
An illustration of a novel or custom-built apparatus
Operating conditions for a gas chromatograph
Equations used to calculate percent yield or dilution ratios
A list of disposable equipment (e.g., rubber gloves, Bunsen burners)
Step-by-step instructions of the procedure
Warnings to other scientists about unusual hazards
Quantitative statements of reaction times and temperatures
Descriptions of the physical appearances of synthesis products
IR or NMR data confirming product purity
Statistical packages used (including the name of the software)
Reports of other software used to keep track of data (e.g., Excel)
Results Section

Ordering your information
1: a statement that locates the figures where the results can be found
2: statements that present the most important findings
3: statements that comment on the results
Discussion Section

Specific Reference to the Study: A reference to the main purpose or hypothesis of the study;

A review of the most important findings (remind readers of results), whether or not they support the original hypothesis, and whether they agree with the findings of other researchers;

Possible explanations for or speculations about the findings; Summary of the work

Limitations/implications and applications of the study that restrict the extent to which the findings can be generalized.

Recommendations for further study.
Being critical

- A serious weakness with this argument, however, is that ......
- One of the limitations with this explanation is that it does not explain why...
- Many writers have challenged Jones' claim on the grounds that ........
- However, such explanations tend to overlook the fact that......
Discussing findings

- A strong relationship between X and Y has been reported in the literature.
- Prior studies that have noted the importance of ...
- In reviewing the literature, no data was found on the association between X and Y.
- As mentioned in ......,
- In the current study, X provided the largest set of significant clusters of ......
- It is interesting to note that in all seven cases of this study......
- This inconsistency/discrepancy may be due to ...
- This rather contradictory result may be due to ..
Writing an Abstract

1. **State What Was Done**
   1.1 Identify the research area and its importance
   1.2 Mention a gap addressed by the work
   1.3 State purpose and/or accomplishment(s) of work

2. **Identify Methods Used**
   (i.e., procedures and/or instrumentation)

3. **Report Principal Findings**
   3.1 Highlight major results (quantitatively or qualitatively)
   3.2 Offer a concluding remark

Figure 1 A visual representation of the move structure for a typical journal article abstract.
Abstract: State what was done

In this study, we report the chemical synthesis and functionalization of magnetic and gold-coated magnetic nanoparticles and the immobilization of single-stranded biotinylated oligonucleotides onto these particles. (From Kouassi and Irudayaraj, 2006)
Abstract: Identify methods used

A number of cigarettes were tested including three pure-tobacco-type cigarettes, an experimental reference cigarette, and 11 commercial cigarettes. Due to the complexity of the smoke particulate matter, the pesticides were identified only after each sample was subjected to a multistep cleanup process that included phenyl solid-phase extraction, an acid wash, aminopropyl solid-phase extraction, and normal phase liquid chromatography fractionation. (Adapted from Dane et al., 2006)
Abstract: report principal findings

Variations in the temperature between 10 and 30 °C did not affect the H₂ concentration in a fashion that suggested thermodynamic control through a constant energy gain. In another set of experiments, H₂ levels at constant ionic strength were independent of the chloride concentration between 10 and 110 mmol chloride per liter. These findings demonstrate that the partial equilibrium approach is not directly applicable to the interpretation of reductive degradation of chlorinated ethenes. We also present recalculated thermodynamic properties of aqueous chlorinated ethene species that allow for calculation of in situ Gibbs free energy of dechlorination reactions at different temperatures. (From Heimann and Jakobsen, 2006)
Components of Writing conventions

- Abbreviations/Acronyms
- Level of Detail
- Conciseness
- Level of Formality
- Word Choice
- Structure
- Formatting
- Verb
  - Tense/Voice/Parallelism/Punctuation/Subject-verb Agreement/Word Usage
- Graphics: Tables and Figures
Abbreviations

- Are abbreviations used in this paper?
- Can you work out whether or not we need to use the full term?
What do these stand for?

- *et al.*
- *i.e.*
- *e.g.*
- *sp.*
- *spp.*
Common abbreviations

- **et al.** and others. Referring to studies by more authors
- **e.g.** For example
- **i.e.** that is, in other words, namely
- **sp.** Species (singular)
- **spp.** species. (plural)
Abbreviations that do not need to be defined for a chemistry audience

- at. wt
- NMR
- bp
- RNA
- DNA
- U.S.
- equiv
- fp
- mp
- UV
- IR
- v/v
- w/v
- w/w
- wt
Answers

- Atomic weight
- Nuclear magnetic resonance
- Boiling point
- Ribonucleic acid
  Deoxyribonucleic acid
- United States
- Equivalent (s)

- Freezing point
- Melting point
- Infrared
- Ultraviolet
- Volume per volume
- Weight per volume
- Weight per weight
- weight
Nominalizations allow several words to be summarized in a single word

Without a nominalization
○ After we distilled the product, it was a colorless liquid. (10 words)

With a nominalization
○ After distillation, the product was a colorless liquid. (8 words)

Nominalizations can also minimize awkwardness, adding to the fluidity and clarity of your writing.

Awkward
○ The ability to deprotect the carboxylic acid and to simultaneously cleave from the resin will provide compounds with the desired side chain.

Less awkward
○ The deprotection of the carboxylic acid and the simultaneous cleavage from the resin will provide compounds with the desired side chain. (Adapted from Hergenrother, 2002)
### Table 2.2 Common nominalizations used in chemistry writing.

<table>
<thead>
<tr>
<th>Absorption</th>
<th>analysis</th>
</tr>
</thead>
<tbody>
<tr>
<td>activation</td>
<td>luminescence</td>
</tr>
<tr>
<td>concentration</td>
<td>measurement</td>
</tr>
<tr>
<td>conductivity</td>
<td>oxidation</td>
</tr>
<tr>
<td>conversion</td>
<td>preparation</td>
</tr>
<tr>
<td>Dependence</td>
<td>presence</td>
</tr>
<tr>
<td>diffusion</td>
<td>calculation</td>
</tr>
<tr>
<td>addition</td>
<td>comparison</td>
</tr>
<tr>
<td>aggregation</td>
<td>reaction</td>
</tr>
<tr>
<td>emission</td>
<td>reactivity</td>
</tr>
<tr>
<td>excitation</td>
<td>reduction</td>
</tr>
<tr>
<td>extraction</td>
<td>synthesis</td>
</tr>
<tr>
<td>formation</td>
<td>treatment</td>
</tr>
<tr>
<td>intensity</td>
<td>efficiency</td>
</tr>
<tr>
<td>agreement</td>
<td>purification</td>
</tr>
</tbody>
</table>
Graphics: Tables and Figures (1)

- All tables and figures should be put into a contextual framework in the corresponding text.
- Should present information in a format that is easily evaluated by the reader, stands alone, summarises data and is sequentially numbered.
Tables and figures (2)

- Where do captions/legends go?
Tables and Figures (3)
Number tables and figures (Arabic numerals)

- Title TABLES fully in a legend placed ABOVE the table.

- Within the table, use headings to identify the nature and units of the data given. Keep vertical lines to a minimum in tables.

- Provide a full legend placed BELOW the FIGURE.

- The axes of the figure (or graph) should be specified clearly and the units identified and scaled appropriately.
<table>
<thead>
<tr>
<th>Composition</th>
<th>Nominal</th>
<th>Accurate</th>
<th>ΔM&lt;sup&gt;a&lt;/sup&gt; ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{C}<em>9\text{H}</em>{14}\text{O}_2$, $\text{M}^+$</td>
<td>154</td>
<td>154.0994</td>
<td>0.0</td>
</tr>
<tr>
<td><strong>Fragment Ions</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\text{C}<em>9\text{H}</em>{12}\text{O}$</td>
<td>136</td>
<td>136.0936</td>
<td>5.8</td>
</tr>
<tr>
<td>$\text{C}<em>9\text{H}</em>{13}$&lt;sup&gt;b&lt;/sup&gt;</td>
<td>109</td>
<td>109.1010</td>
<td>0.7</td>
</tr>
<tr>
<td>$\text{C}_7\text{H}_9\text{O}$</td>
<td></td>
<td>109.0653</td>
<td>0.2</td>
</tr>
<tr>
<td>$\text{C}_6\text{H}_9$</td>
<td>81</td>
<td>81.0704</td>
<td>0.0</td>
</tr>
<tr>
<td>$\text{C}_5\text{H}_7$</td>
<td>67</td>
<td>67.0547</td>
<td>0.1</td>
</tr>
</tbody>
</table>

<sup>a</sup> ΔM is the deviation from the nearest perfluorokerosene exact mass.

<sup>b</sup> $\text{C}_9\text{H}_{13}$ peak represents the high-abundance ion of the doublet at $m/z$ 109.
Figure 1.23  A mass spectrometer. Cl atoms are introduced on the left side of the spectrometer and are ionised to form Cl$^+$ ions, which are then directed through a magnetic field. The paths of the ions of the two isotopes of Cl diverge as they pass through the magnetic field. As drawn, the spectrometer is tuned to detect $^{35}$Cl$^+$ ions. The heavier $^{37}$Cl$^+$ ions are not deflected enough for them to reach the detector.
Most common problems

Novice writers tend not to:

- Hedge
- Paraphrase legitimately
- Write concisely (being wordy!)
- Write appropriate references
References

- Robinson et al. (2008) Write Like a Chemist, Oxford University Press; Oxford
- [http://ic.ucsc.edu/~ggilbert/envs122/ConventionsScienceWriting.html](http://ic.ucsc.edu/~ggilbert/envs122/ConventionsScienceWriting.html)
- [https://writingcenter.unc.edu/handouts/sciences](https://writingcenter.unc.edu/handouts/sciences)
- [http://www.lib.berkeley.edu/CHEM/acsstyle.html](http://www.lib.berkeley.edu/CHEM/acsstyle.html)
- [http://resources.library.lemoyne.edu/content.php?pid=104248&sid=784351](http://resources.library.lemoyne.edu/content.php?pid=104248&sid=784351)
- [http://www.phrasebank.manchester.ac.uk/introducing-work](http://www.phrasebank.manchester.ac.uk/introducing-work)
End of Section
Financing

• The present educational material has been developed as part of the educational work of the instructor.

• The project “Open Academic Courses of the University of Crete” has only financed the reform of the educational material.

• The project is implemented under the operational program “Education and Lifelong Learning” and funded by the European Union (European Social Fund) and National Resources.
Licensing Note

- The current material is available under the Creative Commons Attribution-NonCommerical-NoDerivs 4.0[1] International license or later International Edition. The individual works of third parties are excluded, e.g. photographs, diagrams etc. They are contained therein and covered under their conditions of use in the section «Use of Third Parties Work Note».

[1] http://creativecommons.org/licenses/by-nc-nd/4.0/

- As Non-Commercial is defined the use that:
  - Does not involve direct or indirect financial benefits from the use of the work for the distributor of the work and the license holder
  - Does not include financial transaction as a condition for the use or access to the work
  - Does not confer to the distributor and license holder of the work indirect financial benefit (e.g. advertisements) from the viewing of the work on website

- The copyright holder may give to the license holder a separate license to use the work for commercial use, if requested.
Reference Note

Preservation Notices

Any reproduction or adaptation of the material should include:

- the Reference Note
- the Licensing Note
- the declaration of Notices Preservation
- the Use of Third Parties Work Note (if is available)

together with the accompanied URLs.