Guide to Formal Reports

In science, communication of important findings between peers often takes the form of a written publication. The report format presented here is well-established in chemistry journals and is similar to that used by journals of the American Chemical Society. Feel free to consult the literature (particularly full articles in J. Am. Chem. Soc.) for ideas about construction.

General guidelines

Writing style: You write as a researcher reporting your new results to your peers. Therefore, you maintain a professional style and terminology. Instead of referring to the “lab,” write about your “study” or “experiment.” It should go without saying that you are writing in the third person, passive voice, using perfect spelling and grammar.

Audience: Assume that your reader is acquainted with the field. S/he understands specialized terminology; for example, ‘spectrometer’ or ‘cuvette’ for a spectroscopy experiment. (An exception to this rule is the use of acronyms: as a safe rule of thumb, define an acronym the first time it is used; i.e. “light-emitting diode (LED).”) However, although your reader is familiar with the field and general terminology, s/he is not familiar with this particular experiment, so relevant background and experimental details are necessary.

Numbers and units: Nearly every number (including constants) needs units. Numbers smaller than 1 either require a zero in the ones place or should be written in scientific notation. For example, one can write 0.50 or 5.0x10^{-1}, but not .50. All measurements are reported as a mean, standard deviation, and units (i.e. $\bar{x} \pm s$ units), where $s$ has two significant figures and $\bar{x}$ matches $s$ in precision. For example, an acceptable way to report a set of length measurements would be 8.50 ± 0.13 cm, not 8.5 ± 0.13 cm.

Required Elements

Title: Do NOT use “Experiment” or “Lab” in your title. Pick something that concisely describes the important aspects of your study.

Abstract: Short (< 100 words) summary of the experiment, the interesting findings, and their implications.

2 - Purpose is clearly described; experimental techniques are mentioned; significant findings and implications are briefly described.
1 - Purpose is described; experimental techniques or the significant findings/implications are inadequately described or are missing.
0 - Purpose is inadequately described or missing. Introduction does not address any level 2 requirements.
Introduction: ≥ 3 pages. In your own words, briefly summarize the theory behind the experiment (no mathematical derivations necessary). Briefly describe your experimental system and explain why it is a good choice for testing the theoretical principles. Explicitly state the experimental outcomes and objectives, as well as the parameters that you have measured and calculated. End with a brief statement assessing the significance and implications of your results.

3 – Theory and experimental system are briefly described and referenced; experimental outcomes and objectives are explicitly stated; measured and calculated parameters are stated; significance and implications of the results are briefly stated.
2 – Two items from level 3 are missing or inadequately described.
1 – Three items from level 3 are missing or inadequately described, or no references are cited for theoretical material.
0 - Introduction does not address any of the requirements listed in level 3.

Experimental: ≥ 1 page. Summarize the experimental procedure as recorded in your lab notebook. Include enough information for the reader to reproduce the experiment using his/her own equipment.

Detailed information about sample preparation (i.e. amounts, mixing procedures) and instruments (i.e. brand, model number) is important and should be included. On the other hand, detailed operating instructions are not the focus of this section, as shown here:

The wrong way (emphasizes trivia about your specific lab conditions) –
The Ocean Optics power was turned on and the software program initialized. The sample was placed into the cuvette using a pipette. 200 nm was entered into the “Start Wavelength” dialogue box, and 500 nm was entered into the “End Wavelength dialogue box, with the resolution being 1 nm. The spectrometer was engaged by pressing “Start,” and the resulting spectrum was printed. The peak positions were entered into an Excel sheet to find the expected conjugation length, \( L \).

The right way (general method, but enough particulars) –
An Ocean Optics USB 2000 UV-Vis Spectrometer was used to collect the absorption spectra of all the molecules under study. Sample solutions were placed into a quartz cuvette, and absorption spectra were collected from 200 to 500 nm. Peak positions were determined using the Ocean Optics software package. They were converted to peak energies in eV and were then used to calculate the expected conjugation length, \( L \), of the molecule according to Equation 1:

\[
E_{\text{transition}} = \frac{(n_f^2 - n_i^2)\hbar^2}{8meL^2} + E_{\text{lim}} \tag{1}
\]

Where [define all equation terms here].

When relevant, include original (computer-generated preferred, but handwritten permitted) figures of the equipment (spectrometer, circuit, etc.) with all parts labeled.
Results and Discussion: ≥ 5 pages of text (do not count figures and tables toward this total). This narrative section is the heart of any journal article. It always moves from the specific (your experiment, your data/analysis) to the general (interpret how the experiment fits into the greater theoretical context).

Begin with several narrative paragraphs presenting your data. Intersperse tables, graphs, and figures that summarize the raw data and calculated results contained in these paragraphs. Report all calculated values with their uncertainty (ex. Planck’s constant was calculated to be 6.673 ± 1.248 × 10⁻³⁴ J⋅s)

Next, reflect on your data and assess its quality and reliability. Identify overarching trends; for example, how did a molecule’s UV-Vis absorption depend on the length of its conjugated portion? Address (in narrative form) the following questions: Is the data precise (self-consistent) and/or accurate (consistent with others’ measurements of the same or similar quantities)? What are the main sources of uncertainty? Might any systematic error be present? How might you improve your precision or accuracy? A few prodding questions will be given in each lab handout in order to get you started.

Finally, interpret and assess your results in the general context of others’ work and the big picture. How do your results compare to results obtained by other researchers (i.e., your classmates or reported literature values)? Do they corroborate or contest the hypotheses being tested (and can you tell that based on your uncertainty)? Again, pay attention to specific prodding questions in your handouts.

Results and Discussion – overall structure and style
2 – Results and discussion are presented in narrative format supported by tables and figures; narrative moves from the specific to general.
1 – Results and discussion are presented in narrative format without tables and figures; OR narrative does not move from the specific to the general.
0 – Results are reported only in isolated tables and figures and not described in narrative form.

Interpretation of Results – context of study:
3 – Important features of the experimental data are identified and interpreted; overarching trends are identified and interpreted; uncertainty of calculated
quantities is stated and examined; uncertainty is used to identify sources of error and suggest methods for improving experimental precision. 0.5 pt deductions are made for insufficient interpretation in any of these categories (experimental data, uncertainty, or error identification/methods for improvement). 0 – none of the level 3 elements have been included, or maximum deductions met.

**Interpretation of Results – general context**

3 – Results are compared to other reported literature values (with citations); results are interpreted as supporting or refuting the relevant theory; the significance and physical meaning of the results is assessed; prodding questions from the lab handout are sufficiently addressed.
2 – One item from level 3 is missing or inadequate.
1 – Two items from level 3 are missing or inadequate.
0 – Three or more of the items in level 3 are present or inadequate.

**Conclusions**: In a short paragraph (>5 sentences), summarize the results. Show how your results, analysis, and interpretation meet the objectives of your study as stated in the Introduction.

3 – Results are summarized; success of experiment is identified; theoretical principles supported (or refuted) by the results are identified; significance of experimental results is restated.
2 – One item from level 3 is missing or inadequate.
1 – Two items from level 3 are missing or inadequate.
0 – Conclusion inadequate or missing.

**References**: Consult and cite ≥ 3 references. The lab handout does not count towards this total. At least one must be a print source. Acceptable references include books, academic-affiliated or science-dedicated chemistry and physics websites, journal articles, and reference books. Wikipedia is NOT an acceptable reference, although it can be a useful starting point. Cite a source when directly quoting its text or numbers or if it forms the main basis for a point you make in your text.

Citations will follow the ACS format. A good guide can be found through the University of Wisconsin-Madison.1 In-text citations are indicated by superscripted, consecutive numbers that correlate to the Reference list, as seen in the previous sentence.

Cite the CRC as follows: *CRC Handbook of Chemistry and Physics*, [X] ed. Lide, D.R., ed. CRC Press: Boca Raton, FL, [year]; Chapter [Y], p [Z].

Cite handouts as follows: Davis, K.L. and Bryant, M.A. “Title of Experiment,” September 2010.

2 – ≥ 3 properly-cited, acceptable reference sources (≥ 1 is a print source).
1 – ≤ 1 print source, OR improper citation format.
0 – 2+ level 3 items are missing. Alternatively, citing a general website or not consulting at least three references results in an immediate zero.
Appendix: Include one computer-generated sample calculation for each calculated value, as well as a propagation of the uncertainty when applicable. Attach instrumental output data (spectra, etc.), as well as carbon copy pages of your lab notebook, to the end of the report.

Appendix – Original Data
2 – Original instrumental outputs are attached; carbon copies of notebook pages are attached and adequately describe the experimental procedure.
1 – One data output or notebook page is missing.
0 – 2+ data outputs or notebook pages are missing, or the notebook pages inadequately describe procedure.

Appendix – Calculations, Error, and Accuracy
2 – One sample calculation (with units) is given for each calculated result, along with propagation of uncertainty (where applicable); experimentally-determined results are within an acceptable range of accuracy (defined in the experiment).
1 – One sample calculation or uncertainty propagation is incorrect, missing or lacking units.
0 – 2+ sample calculations or uncertainty propagation are incorrect, missing, or lacking units.

Formatting
• Length: Approximately 1500-3000 words, (~10 double-spaced pages). Figures, tables, and attachments do not count towards this limit.

• Margins: 1 inch

• Spacing: 1.5 lines or double for ease in commenting. Do not turn in single-spaced pages.

• Pages must be numbered.

• Headings (Introduction, etc.) for each section are given in boldface type, separated from preceding and following text

• Table captions are placed above the table.

• Figure captions (including graphs) are placed below the figure.

• Equations and calculations must be presented in computerized format. Handwritten equations or calculations are unacceptable. Equations should be identified by consecutive numbers and referred to by those numbers in the text.

• Chemical structures must also be in computerized format (i.e., ChemSketch).
• **Tables** must be edited from the default Word format.

<table>
<thead>
<tr>
<th><strong>Word 2007 default</strong></th>
<th><strong>The right way</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Table 1. $V_0$ and $\lambda$ values</strong></td>
<td><strong>Table 1. Turn-on voltages and wavelengths for several LED lights.</strong></td>
</tr>
<tr>
<td>$V_0$</td>
<td>$\lambda$</td>
</tr>
<tr>
<td>2</td>
<td>633</td>
</tr>
<tr>
<td>2.03</td>
<td>605</td>
</tr>
<tr>
<td>2.1</td>
<td>585</td>
</tr>
<tr>
<td>2.25</td>
<td>555</td>
</tr>
<tr>
<td>2.6</td>
<td>470</td>
</tr>
</tbody>
</table>

- Table caption uses variables instead of specific terms
- Headings are unitless and in plain text
- Too many borders
- Left-justified text
- Values reported to differing numbers of significant figures

- Table caption uses terms instead of variables
- Bold headings with specific units
- Borders adjusted
- Centered text
- Values reported with uniform sig figs reflecting the experimental precision

• **Graphs** must also be edited from the default Excel format.

<table>
<thead>
<tr>
<th><strong>Excel 2007 default</strong></th>
<th><strong>The right way</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Figure 1.</strong> Plot of $V_0$ vs. $\lambda^{-1}$.</td>
<td><strong>Figure 1.</strong> Plot of the LED turn-on voltage ($V_0$) versus the inverse wavelength of the LED ($1/\lambda$).</td>
</tr>
<tr>
<td>- Legend is present</td>
<td>- Legend is removed</td>
</tr>
<tr>
<td>- Outside borders present; inner border absent</td>
<td>- Outside borders absent; inner border present</td>
</tr>
<tr>
<td>- Axes are untitled</td>
<td>- Properly titled axes, with units</td>
</tr>
<tr>
<td>- Gridlines are present</td>
<td>- Gridlines removed</td>
</tr>
<tr>
<td>- Too much white space</td>
<td>- Data fills the graph space</td>
</tr>
<tr>
<td>- Fonts too small; lines too thin</td>
<td>- Fonts enlarged; lines thickened</td>
</tr>
<tr>
<td>- Figure caption uses variables instead of specific terms</td>
<td>- Figure caption uses specific terms and defines each axis.</td>
</tr>
</tbody>
</table>
Formatting and Style – basic elements:
3 – Proper title; proper heading formatting; length, margin and spacing
requirements are fulfilled; pages numbered; computerized equations, calculations,
and chemical structures; appropriate tense and writing level for audience.
0.5 pt deductions are made for each formatting error described above.
0 – no formatting requirements from level 3 are met or maximum deductions.

Formatting and Style – Presentation of Results
2 – Raw and calculated data is summarized in one or more properly-formatted
tables; tables and figures are properly formatted and captioned.
1 – One table or figure is improperly formatted/captioned; OR insufficient number
of tables/figures are present.
0 – 2+ tables or figures are improperly formatted/captioned; OR no tables/figures
are shown.

References
(accessed July 9, 2010), part of the University of Wisconsin-Madison Chemistry Library’s
Writing Tools.