How to Write a Good Paper

- Titles -

The following information was drawn from group exercises that took place in May 2019 & Fall 2021. We took a recent issue of ACS Macro Lett and individually voted on whether we liked each title, commenting on what we liked or didn’t like about them. Then we came to a consensus on what makes a good paper title, and what to avoid.

Good Titles...

● we can understand exactly what was done
● contains the “what” and the “how” (in that order)
● are between 6-15 words
● contain action words (e.g., predicting, tuning, etc.)

Bad Titles...

● contain unnecessary words (e.g., synthesis, properties, design, toward, use in, etc.)
● contain redundant words
● contain complex words
● are too long (>15 words)
● are too short (<6 words)
● hard to tell what is new or interesting
● have too little information
● missing the “how”
● use unfamiliar acronyms
● force fit catchy terms (e.g., “keep xx on track”)

Examples of Good Titles...

● Rate Control of Helix Oscillation of Poly(arylacetylene)s Achieved by Design of Side-Group Structures
● Influence of Counterion Structure on Conductivity of Polymerized Ionic Liquids
● Ring Size-Dependent Solution Behavior of Macrocycles: Dipole–Dipole Attraction Counteracted by Excluded Volume Repulsion
● Predicting Monomers for Use in Aqueous Ring-Opening Metathesis Polymerization-Induced Self-Assembly
The following information was drawn from group exercises that took place in May 2019 & Fall 2021. We took a recent issue of ACS Macro Lett and individually voted on whether we liked each abstract/TOC combination, commenting on what we liked or didn’t like about them. Then we came to a consensus on what makes a good paper abstract, and what to avoid.

**Good Abstracts...**
- contain five sentences/sections in this order:
  - (1) challenge/problem statement - what are you trying to solve/address/understand
  - (2) how did you go about addressing it (not too detailed)
  - (3) what did you actually do (more detailed)
  - (4) what are the most important results (should relate to your challenge/problem statement)
  - (5) impact/importance of the results
- are self-contained

**Bad Abstracts...**
- are missing any one of the 5 sections mentioned above
- contain too much raw experimental data
- contain a lot of technical jargon and acronyms/abbreviations (think about your audience)
- use strong words that are a matter of opinion (excellent, versatile, synergy)
- contain too much of one thing (e.g., results)

**Good TOC Graphics...**
- present a single take-home message in cartoon format

**Bad TOC Graphics...**
- overly complex with multiple take-home messages
- use actual data plots that require one to take the time to interpret
- contain neon green or other offensive colors
- are too technical (e.g., photos of polymers before/after stretching with ruler)

**Example of a good Abstract & TOC Graphics...**
Abstract

Gels are attractive for applications in drug delivery, tissue engineering, and 3D printing. Here, physical colloidal gels were prepared by freeze–thaw (FT) cycling of cellulose nanocrystal (CNC) suspensions. The aggregation of CNCs was driven by the physical confinement of CNCs between growing ice crystal domains. FT cycling was employed to form larger aggregates of CNCs without changing the surface chemistry or ionic strength of the suspensions. Gelation of CNC suspensions by FT cycling was demonstrated in water and other polar solvents. The mechanical and structural properties of the gels were investigated using rheometry, electron microscopy, X-ray diffraction, and dynamic light scattering. We found that the rheology could be tuned by varying the freezing time, the number of FT cycles, and concentration of CNCs in suspension.

Like this text abstract but not the TOC...

Abstract

Currently, only 5% of thermoset carbon fiber reinforced polymer composites (CFRP) are recycled into lower-value secondary products. Highly efficient closed-loop recycling of both thermoset resin and carbon fiber is a major challenge. Here, we report a sustainable approach for the closed-loop recycling of the resin and fiber from CFRPs. Thiol-functionalized carbon fiber (TCF) obtained by functionalization with a thiol-ended hyperbranched polymer, and then an epoxy-ended degradable hyperbranched polymer (HT\textsubscript{3}) are used to prepare HT\textsubscript{3}/TCF composites, which show considerable acid resistance and mechanical performance. The cured composites are controllably depolymerized into monomers and oligomers with high recyclability (89%), which can be utilized to prepare HT\textsubscript{3} and the precursor of cross-linked HT\textsubscript{3}. A total of 100% of the carbon fibers are recovered and reused to fabricate composites without deterioration of performance. The results provide a method for designing high-performance composites and a pathway for high efficiency closed-loop recycling.

Like this TOC graphic but the abstract is missing the problem statement...

Abstract

In this Letter, we report that two amines can be coupled together rapidly and quantitatively through amine–thiol scrambling using a bisvinyllogous thioester conjugate acceptor under mild conditions. The resulting bisvinyllogous amide conjugate acceptors can be decoupled via an ethylene diamine-induced cyclization. Four representative conjugate acceptors have been utilized in the couple–decouple reactions, which were monitored and characterized by nuclear magnetic resonance, high-resolution mass spectrometry, and UV–vis spectroscopy. Further, we applied these small-molecule-based "click–declick" reactions to polymer synthesis and degradation. Highly cross-linked polymers, i.e., plastics, were quantitatively synthesized by simple reactions between commercial tris(2-aminoethyl)amine and the conjugate acceptors without solvent and any initiator or catalyst through ball milling within 60 min. Significantly, these thermosetting plastics can be degraded within 3–24 h via addition of ethylene diamine. The multiple architectures, application to plastics synthesis, and chemically triggered clean degradation to the thermosets at mild conditions with little input of energy herald a new generation of “intelligent” materials.
- Introductions -

The following information was drawn from multiple group exercises that took place in Summer 2019 and Fall 2021. We took a recent issue of Macromolecules and JACS (full papers) and ACS Macro Letters (communications) and individually voted on whether we liked each introduction, commenting on what we liked or didn’t like about them. Then we came to a consensus on what makes a good introduction, and what to avoid.

**Good Introductions...**

- address these questions
  - what is the problem/challenge that you are trying to solve?
  - why does it matter? why do we need to solve it?
  - what is your approach/hypothesis about tackling this problem? what is the rationale?
  - what are your most significant findings? provide context to understand them
  - how do your findings impact the field?

- general guidelines
  - open with the need and then follow with your approach
  - consider using shorter, digestible paragraphs
  - each paragraph should have a smooth transition from the previous one
  - clearly explain all key concepts that are necessary to understand the work/context without getting into the nitty gritty details
  - contain 0-1 simplified scheme

**Bad Introductions...**

- are too long (we found ~600-1000 words was appropriate for full papers)
- are disorganized, jumping around from concept to concept without a clear understanding of where its going
- no clear gap or challenge stated
- have too many gap statements and its not clear which one(s) are being addressed
- not clear why the work is needed or what was learned
- no hypothesis stated
- includes equations and undefined complex concepts that are specific to a subfield
- include specific results (e.g., #) without context to understand them

**Example of a Good Introduction (full papers)...** ([link](#))

**Example of a Good Introduction (communication)...** ([link](#))
- Results & Discussions -

The following information was drawn from a group exercise that took place in July 2019 and December 2021. We took 5-6 recent papers (both communications & full articles) from different journals and individually voted on whether we liked each “results & discussion” section, commenting on what we liked or didn’t like about them. We also analyzed the language/phrases that were common among most “results & discussions.” Then we came to a consensus on what makes a good “results & discussion” and what to avoid.

**Good Results & Discussions...**

- Tell a story from start to finish, bringing the reader through the project with multiple guideposts that recap what was learned and inform on what is coming next.
- Consistent paragraph structures:
  - Rationale for why the upcoming experiments were done (1-3 sentences).
  - Description of key results (3-5 sentences).
  - Rationalization of the results (1-3 sentences).
  - Implications of the results. What does this mean for the story and/or the field? (1-3 sentences)
- Each paragraph should have a single goal or take-home message.
- Abbreviations with meaning - for example NBE for norbornene as opposed to M1.
- Use descriptive text that will be understandable to a non-expert.
- Figures should tell the story without text. Use of color, cartoons, and schemes to help guide data interpretation were all highly valued. See [here](#) for a really good example.
- Transitional phrases were really helpful. “We hypothesized” “We anticipated” “To understand” “When then rationalized that”
- Used sub-section headings to help guide the reader on how the parts connect together.

**Bad Results & Discussions...**

- Make the reader work hard to understand the results.
- Have disparate sections that seem unrelated without transitional phrases or sub-section headings between them.
- Descriptions of results without a clear understanding of why the experiments were done.
- Descriptions of results without their implications.
- Contain too many abbreviations and acronyms. It breaks up the flow of sentences and makes the reader work harder to understand/comprehend the experiments.
- Contains too much numerical data rather than describing trends in the data or the implications of the data.
- Talk extensively about figures located in the SI.

**Example of a Good Results & Discussion...** ([link](#)) and ([link](#))
The following information was drawn from a group exercise that took place in January 2022. We took a recent issue of Angew. Chem. and individually voted on whether we liked each paper’s collection of figures/charts/schemes, commenting on what we liked or didn’t like about them. We also looked for common features among the ones we liked. Then we came to a consensus on what makes a good figure/chart/scheme, and what to avoid.

Good Figures/Charts/Schemes...
- The reader looking at the figure/chart/scheme can immediately understand what the “take-away” message is without having to read the caption or main text.
- Have one key take-away message per figure/chart/scheme. Do not try to convey too much information in one.
- Use complementary colors (and not too many of them) to highlight important features or structural changes. Shading in parts of structures can also be useful rather than using bold or a lot of colors.
- Use consistent capitalization, fonts, and font sizes throughout.
- Use consistent structure sizes and specs throughout.
- Are symmetrical and minimize white space.
- Often include a cartoon depiction of the experiment alongside the data for easier interpretation.
- For complex or large structures, include both cartoon and chemdraw versions in the same figure and use the same cartoon throughout the paper.
- For multiple spectra, consider using dotted lines to label peaks from one to another rather than individually labeling or coloring peaks.

Bad Figures/Charts/Schemes...
- The reader must also read the caption and main text to understand the “take-aways” from the figure/chart/scheme.
- Are too busy with too much information trying to be conveyed.
- Contain too much text or a lot of duplicated text.
- Contain a lot of different data types without a clear understanding of what is being done in each experiment, and how they relate to each other (if at all).
- Make the reader work too hard.
- Use things like i, ii, iii and then never define them in the figure or caption.

Examples of good figures/charts/schemes... (link and link)
- Conclusions -

The following information was drawn from group exercises that took place in June 2019 and Winter 2022. We took a recent issue of ACS Macro Lett and Polymer Chemistry and individually voted on whether we liked each conclusion, commenting on what we liked or didn’t like about them. We also looked for common sections/structures among the ones we liked. Then we came to a consensus on what makes a good conclusion, and what to avoid.

**Good Conclusions...**

- have these basic sections
  - a brief statement about why the work is important/necessary/significant
  - a brief summary of their approach (1-2 sentences)
  - a brief summary of the key results and context for those results (how does this compare to other materials/work in the field?)
  - an explicit discussion of the implications of the work (1-3 sentences)
- shorter sentences with simple words/terms were best
- 1-2 paragraphs preferred
- define all terms (even if defined in the paper b/c some people read the conclusion after the abstract)
- ok and maybe even helpful to include cross-references, and/or new references to support the impact statements

**Bad Conclusions...**

- re-hash their discussion of the key results (e.g., “using MALDI to determine end-groups, we...”)
- contain too many value judgement words (e.g., versatile, excellent, etc)
- contain too much numerical data/results
- rely on acronyms introduced in the paper but not in the conclusions
- reference figures or SI
ChemDraw Guidelines

After opening ChemDraw, go to File and then Apply Document Settings from and choose ACS Document 1996. Proceed to draw your structures and reaction schemes. (There are a lot of great tutorials here and here on the web for learning and mastering ChemDraw. There is also a comprehensive 300+ page user guide and list of shortcuts)

Pay attention to the little details, like centering text over arrows, aligning and distributing the structures in a reaction, using the same sized arrows in a single scheme and paper. Use a circle as a scaffold to create a mechanistic cycle and guide arrow placement, etc. Color can be a really useful tool. Iron is a good color for the main structures, then use midnight and cayenne to highlight parts of structures. (Note: These colors refer to choices on Macs, which you should be using for all paper figures.) Avoid greens and yellows. Do not switch between CH3 and Me in a figure or set of figures. Make sure square planar complexes are actually square planar and that the substituents are aligned (vertically/horizontally) on any metal catalyst.

When you are ready to “move” your structures into another document, first select all. Then go to Object and choose Object Settings. Change the “bold width” to 0.03 and the “line width” to 0.015. Then save your file as both a .cdx and .png. Do not do any re-scaling or sizing in ChemDraw.

Open the png file in Adobe Photoshop. Then go to Image and choose Image Size. Use a calculator to determine the new width and height (in inches or cm) by multiplying the original values by some %. The smallest you should re-size a ChemDraw image is 65% (usually what I prefer for papers and grants). Most importantly, once you pick a re-size value, stick with it for all images within a single paper. Note that for single column figures, the max size is 3.3 cm and for double-column figures, the max size is 6.5 cm.

In some cases, you may want to enhance your image in Adobe Illustrator. Open and modify the original png file (before re-sizing). Illustrator enables you to add more diverse shapes (1D, 2D, 3D)/colors and you can even map your chemical structures onto 3D images.
Plot/Figure/Equation/Scheme/Chart/Table Guidelines

Plots
All plots should be created in SigmaPlot. The plot size should be square; I recommend setting the plot dimensions to 3.0 x 3.0 inches. Almost all plot axes should start at 0,0 unless it really doesn’t make sense to do so (e.g., with retention volume in GPC). The axis labels should be simple, and contain the units in parentheses. Also, do not capitalize the axis labels. The data on the plot should be clear/readable and labeled so that the take-home message is easily interpreted. Please do not use “legends” or figure captions. Do not give the plot a title either. The plot itself should be self-explanatory. Use color sparingly; use grayscale and dashed lines as a starting point.

Please follow the follow guidelines for plot formatting:
Plot dimensions: 3.0 x 3.0
Axis and Tick Sizes: 3 pt (only use major ticks)
Axis Font: 16 Arial Bold

Figures
First and foremost, figures have processed data (plots, spectra, etc). Sometimes chemical structures and/or reactions can be added to supplement the data, but a figure must have some data! In general, stick to one column figures (width 3.3 cm) unless there is a really strong justification for using the two column width (6.5 cm). Note that two plots can fit side-by-side into a single column figure without appearing too small. Figure captions should be concise and contain essential experimental information!
**Equations**

Equations usually contain either mathematical relationships or a single chemical transformation. Number them sequentially in the manuscript (hint: place the # in the chemdraw version to keep the sizing the same). Equations do not contain titles or captions.

\[ \text{Equation 1} \]

**Schemes**

A scheme is a series of equations that make more sense when grouped together. A good rule of thumb is that if it has more than one reaction arrow, it is likely better represented as a scheme. Schemes require titles.
which are generally placed above the chem draw (though be sure to check the journal requirements). The title should briefly describe the main conclusions of the scheme.

**Scheme 1. Difunctionalized Products Can Be Obtained via Two Different Pathways**

![Scheme 1 Diagram]

**Charts**

A chart is a collection of structures, sometimes with data associated with them. Chart titles are generally placed above the data and briefly describe the major findings.

**Chart 2. Second-Generation Reactive Ligands**

![Chart 2 Diagram]

**Tables**

I generally avoid tables unless absolutely necessary. Tables are most useful when you run a series of reactions with varying conditions or substrates. Before making a table, consider whether a chart might be a better method of presenting the data.
Supporting Information Guidelines

Philosophy

This document is an incredibly important document and one that should replicate the results you obtained as depicted exactly in your lab notebook. Every section of SI should be associated with a searchable experiment number from your notebook and data files. Original electronic copies of the $^1$H and $^{13}$C NMR spectra, as well as the HRMS results, elemental results, rate profiles, GPC data, etc should be uploaded to

<table>
<thead>
<tr>
<th>Equiv. of $3^b$</th>
<th>$1a$</th>
<th>$1b$</th>
<th>$1c$</th>
<th>$1d$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>95 : 5</td>
<td>65 : 35</td>
<td>97 : 3</td>
<td>98 : 2</td>
</tr>
<tr>
<td>2</td>
<td>91 : 9</td>
<td>55 : 45</td>
<td>94 : 6</td>
<td>96 : 4</td>
</tr>
<tr>
<td>10</td>
<td>69 : 31</td>
<td>28 : 72</td>
<td>78 : 22</td>
<td>87 : 13</td>
</tr>
<tr>
<td>50</td>
<td>40 : 60</td>
<td>13 : 87</td>
<td>49 : 51</td>
<td>71 : 29</td>
</tr>
<tr>
<td>100</td>
<td>32 : 68</td>
<td>11 : 89</td>
<td>40 : 60</td>
<td>64 : 36</td>
</tr>
</tbody>
</table>

$^a$ The reactions were run in THF at rt for 2 h ([Ni] = 0.02 M; [2] = 0.016 M). The reported ratios reflect the averages of three runs, with standard deviations ranging from 0.06–2%. $^b$ Relative to 2.
the group server. Your SI must conform to the above criteria or you will be asked to re-run the experiment again prior to submission.

**General Guidelines**

Open the SI group template and follow the instructions/guidelines.

- For the table of contents: You should list both the section titles as well as their starting page #. The section titles should be informative but not too lengthy. The order of sections should follow the order in which the data appears in the paper.

- The first section is “materials and supplies” and should list the source of reagents and compounds, whether and how they were purified before use.

*Sample Materials Section 1:*

I. Materials

iPrMgCl (2M in THF) was purchased in 100 mL quantities from Aldrich. Bis(cyclooctadiene)nickel (Ni(cod)) and 1,2-bis(diphenylphosphino)ethane (dppe) were purchased from Strem. All other reagent grade materials and solvents were purchased from Aldrich, Acros, EMD, or Fisher and used without further purification unless otherwise noted. THF was dried and deoxygenated using an Innovative Technology (IT) solvent purification system composed of activated alumina, copper catalyst, and molecular sieves. N-Bromosuccinimide (NBS) was recrystallized from hot water and dried over P₂O₅. Flash chromatography was performed on SiliCycle silica gel (40–63 μm) and thin layer chromatography was performed on Merck TLC plates pre-coated with silica gel 60 F254. Compounds S₂¹ and 2b–2f² were prepared from modified literature procedures.

*Sample Materials Section 2:*

I. Materials

All reagent grade materials and solvents were purchased from Sigma Aldrich, Acros Organics, or TCI. The paint thinner used was Klean-Strip paint thinner made with mineral spirits. Paints used were as follows: black oil-based paint: Rust-Oleum Professional, V7579 Gloss Black, High performance enamel; pink latex-based paint: Valspar Satin Berry Twist 530832, Spring 2014; white oil-based paint: Rust-Oleum, 7792 Gloss White, Protective Enamel. All alkyl amines and carbon disulfide were distilled prior to use. Methanol was dried over activated molecular sieves under N₂ overnight. All other compounds were used without further purification unless otherwise noted. Compounds S₁–S₃¹, 1a–h², 2a–b², and 3³ were prepared from modified literature procedures. Throughout this document H₂O refers to deionized H₂O, unless otherwise noted.

- The second section is the “general experimental” and should give specific information about the types of equipment used, and if appropriate, how the data was analyzed.

*Sample General Experimental Section:*
II. General Experimental

**NMR Spectroscopy** – $^1$H and $^{13}$C NMR spectra for all compounds were acquired in d$_6$-DMSO or D$_2$O on a Varian vnmr 700 operating at 700 and 176 MHz, or a Varian Inova 500 operating at 500 and 126 MHz. The chemical shift data are reported in units of $\delta$ (ppm) relative to tetramethylsilane and referenced by residual protic solvent. An asterisk was used to indicate residual H$_2$O in all spectra while double bars are used to indicate peaks that have been truncated. The abbreviations s, d, t, at, dd, q, and m were used to signify singlet, doublet, triplet, apparent triplet, doublet of doublets, quartet, and multiplet, respectively.

**High Resolution Mass Spectrometry (HRMS)** – HRMS data were obtained on a Micromass AutoSpec Ultima Magnetic Sector mass spectrometer via electrospray ionization in negative ion mode.

**UV-vis Spectroscopy** – UV-vis spectra were taken on a Perkin-Elmer Lambda 850 UV-visible spectrometer. Calibration curves were measured at the $\lambda_{max}$ for each compound. All experiments were run in triplicate at rt.

The third section is dedicated to “syntheses” of all materials generated during the course of the work. It should be self-contained, meaning that if you had to make it for this paper because it was not commercially available, then its synthesis should appear here...even if we (or someone else) previously published a synthetic procedure for it. Undoubtedly, you did it a little differently, and the SI should represent your individual work and should match the referenced notebook page exactly! In addition, you should list either the elemental analysis results OR high res mass spec results which support the identity of the compound.

**Sample Organic Experimental Procedure:**

\[
\begin{align*}
\text{Furan} & \quad + \quad \text{Benzylamine} \\
\text{MeOH} & \quad \xrightarrow{\text{NaBH}_4} \\
\text{S1} & 
\end{align*}
\]

*N-Benzyl-1-(furan-2-yl)methanamine (S1)*. 2-Furaldehyde (300 µL, 3.63 mmol) and benzylamine (360 µL, 3.30 mmol) were combined in dry MeOH (9 mL) and stirred under N$_2$ for 18 h. The solution was then treated with NaBH$_4$ (279 mg, 7.38 mmol) in small portions, and stirred under N$_2$. After ~1 h, no starting material was visible by TLC. The reaction was carefully quenched with H$_2$O (10 mL). MeOH was removed via rotary evaporation, and the aqueous residue extracted with EtOAc (3 x 10 mL). The combined organic layers were dried over MgSO$_4$, filtered, and the solvent removed via rotary evaporation. The resulting oil was purified by flash column chromatography, eluting with 14% to 20% EtOAc in hexanes to give a clear oil (518 mg, 84%). HRMS (ESI): Calcd for C$_{12}$H$_{14}$NO, 188.1070. Found, 188.1066.

**Sample Organometallics Experimental Procedure:**
Sample Polymerization Experimental Procedure:

**Sample ^1H and ^13C NMR spectra:**
Common General Formatting Mistakes/Reminders

1. Margins need to be justified.
2. A regular hyphen (-) is used to separate elements of a compound word (i.e. “water-soluble”).
3. The en-dash (–) ([option][–] on a Mac) is used for things like named reactions (“Diels–Alder”), number ranges (“1–13”), bonds (“C–O bond formation”), or negative temperatures (i.e. −35 °C, not -35 °C)
4. Degree signs (°) should be written using [option 8 on a Mac] not using a superscript o.
5. There should be a space between the numbers of a temperature and the degree sign (i.e. “55 °C”, not “55° C”).
6. Abbreviations: h not hours; min not minutes; d not days; s not seconds.
7. Check all elemental formulas and mass spec formulas for errors/typos.
8. Using fewer words is preferred (e.g. “synthesizing not the synthesis of”).
9. Use proper and consistent nomenclature for compounds.
10. HRMS \([M + H]\) versus \([M + H^+]\). Make sure that your molecular formula corresponds to the peak that you’re reporting. For example, if a proton \((H^+))\), sodium cation \((Na^+)\), etc. is present in your peak, it should also be in your molecular formula.

11. Compounds, schemes, and tables should be numbered sequentially.

12. Amounts of reagents, solvents, etc. are set aside parenthetically. For example, “The solution was washed with brine (3 x 50 mL),” not “The solution was washed three times with 50 mL of brine.”

13. “That” and “which” are not interchangeable! If removing the words that follow would change the meaning of the sentence, use “that”. Otherwise, “which” is fine.