

How to Write a Good Paper

- Titles -

The following information was drawn from a group exercise that took place in May 2019. 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
- are short (~10 words)
- contain action words (e.g., predicting, tuning, etc.)

Bad Titles...

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

Examples of Good Titles...

- Influence of Counterion Structure on Conductivity of Polymerized Ionic Liquids
- Predicting Monomers for Use in Aqueous Ring-Opening Metathesis Polymerization-Induced Self-Assembly

- Abstracts/TOC Graphics -

The following information was drawn from a group exercise that took place in May 2019. We took the most read articles on 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 three sections: impact/importance, methods, key results/conclusions
- are self-contained, the conclusions address/fill in the gap mentioned earlier
- follow the 6-sentence abstract guidelines, with slight expansion if needed

Bad Abstracts...

- contain raw experimental data
- contain a lot of technical jargon and acronyms/abbreviations
- use strong words that are a matter of opinion (excellent, versatile, synergy)
- have too much of one thing (e.g., introduction)

Good TOC Graphics...

- present a single take-home message in cartoon format

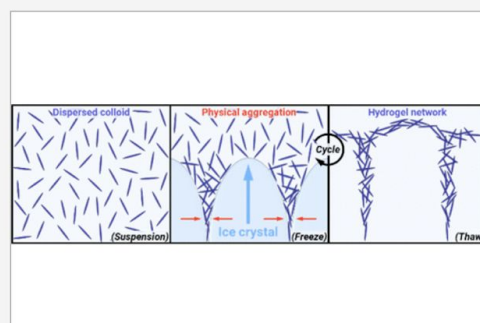
Bad TOC Graphics...

- 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... ([link](#))

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.



- Introductions -

The following information was drawn from two group exercises that took place in June 2019. We took a recent issue of *Macromolecules* (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. We also analyzed the "sections" that were common amongst most introductions and their order. Then we came to a consensus on what makes a good introduction, and what to avoid.

Good Introductions...

- have these basic sections
 - a big picture background (4-5 sentences) ending with a grand challenge (or gap) in the field
 - a narrower picture background (5-10 sentences) that focuses the reader on what work/approaches have been done by us and others to address this grand challenge
 - a clear "gap" sentence that focuses the reader on what this paper is trying to address
 - a brief description of what this paper did (e.g., what system you studied, 3-4 sentences) along with an explanation of why you chose this system (3-4 sentences)
 - then a brief summary of 1-2 main results/take-home message (keep it simple and avoid data, 2-4 sentences)
 - a one-sentence implications statement about how this work will impact others
- contain 1 simplified figure/scheme
- clearly explain all key concepts that are necessary to understand the work/context without getting into the nitty gritty details

Bad Introductions...

- have too long of any of the above sections
- are missing one or more of the above sections
- include equations and undefined concepts (e.g., epitaxy)
- have too many gap statements
- go back and forth between sections

Example of a Good Introduction (full paper)... ([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. We took five 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 your work and the field? (1-3 sentences)
- Abbreviations with meaning - for example NBE for norbornene as opposed to M1.
- 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 Introductions...

- 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.
- Talk extensively about figures located in the SI.

Example of a Good Results & Discussion... ([link](#))

- Conclusions -

The following information was drawn from a group exercise that took place in June 2019. We took a recent issue of ACS Macro Lett and individually voted on whether we liked each conclusion, commenting on what we liked or didn't like about them. We also looked for comment 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 summary of what they did (1-2 sentences)
 - a brief summary of the key results (note: for full articles, we definitely liked having this section, whereas we were more split on whether communications needed to have a results summary)
 - an explicit discussion of the implications of the work (1-3 sentences)
- shorter sentences with simple words/terms were best
- define all terms (even if defined in the paper b/c some people read the conclusion after the abstract)

Bad Conclusions...

- re-hash their discussion of the key results
- contain too many useful words (e.g., versatile, excellent, etc)
- contain numerical data/results
- rely on acronyms
- 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

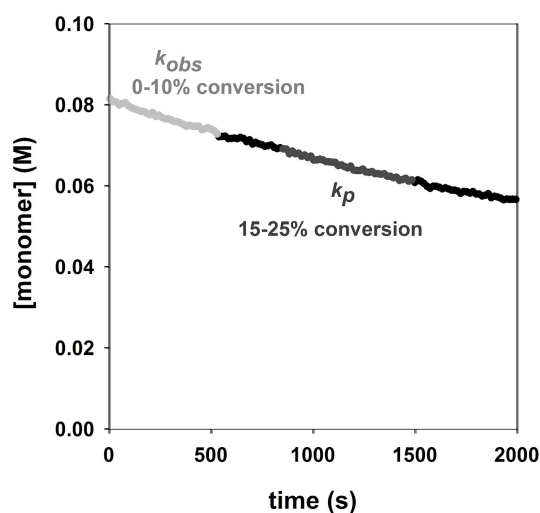
All plots should be created in SigmaPlot. The plot size should be square; I recommend setting the plot dimensions to 3.0 x 3.0 inches. Almost all plot axes should start at 0,0 unless it really doesn't make sense to do so (e.g., with retention volume in GPC). The axis labels should be simple, and contain 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 following 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!

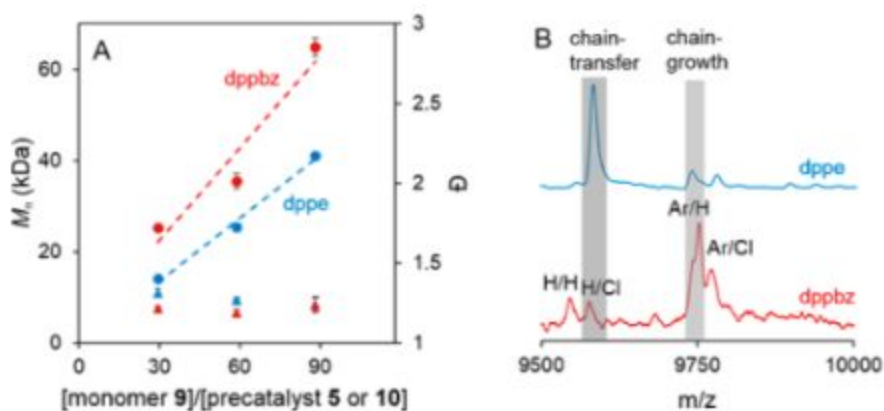
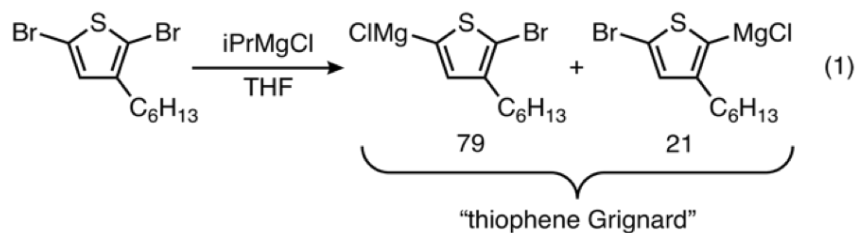


Figure 3. (A) Plot of M_n and dispersity (D) of PTz-OR versus the monomer/catalyst ratio using either precatalyst **5** (blue) or precatalyst **10** (red) and monomer **9**. (B) MALDI-TOF-MS analysis of PTz-OR obtained via either precatalyst **5** or **10** and monomer **9**.

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.

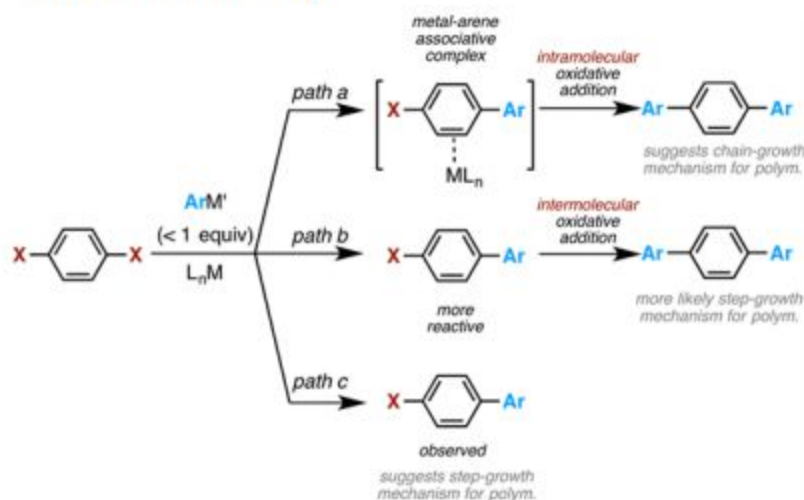


Schemes

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.

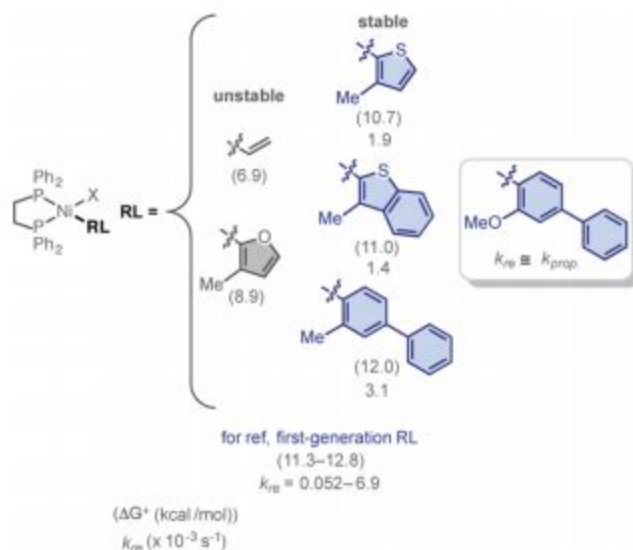
Scheme 1. Difunctionalized Products Can Be Obtained via Two Different Pathways



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 Ligands⁷³



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.

Table 1 Results of the competition experiments^a

Equiv. of 3 ^b	P _{intra} : P _{inter}			
	1a	1b	1c	1d
1	95 : 5	65 : 35	97 : 3	98 : 2
2	91 : 9	55 : 45	94 : 6	96 : 4
10	69 : 31	28 : 72	78 : 22	87 : 13
50	40 : 60	13 : 87	49 : 51	71 : 29
100	32 : 68	11 : 89	40 : 60	64 : 36

^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.

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 ¹H and ¹³C NMR spectra, as well as the HRMS results, elemental results, rate profiles, GPC data, etc should be uploaded to

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 ($\text{Ni}(\text{cod})_2$) 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 P_2O_5 . 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 **S2**,¹ and **2b–2f**² 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 N_2 overnight. All other compounds were used without further purification unless otherwise noted. Compounds **S1–S3**,¹ **1a–h**,^{2,3} **2a–b**,⁴ and **3**⁵ were prepared from modified literature procedures. Throughout this document H_2O refers to deionized H_2O , 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

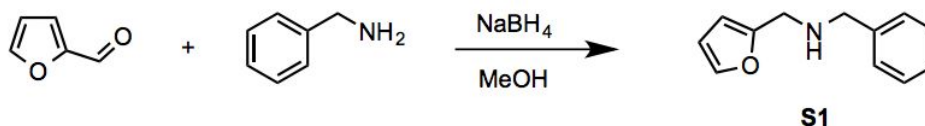
NMR Spectroscopy – ^1H and ^{13}C NMR spectra for all compounds were acquired in d_6 -DMSO or D_2O on a Varian vnmr 700 operating at 700 and 176 MHz, or a Varian Inova 500 operating at 500 and 126 MHz. The chemical shift data are reported in units of δ (ppm) relative to tetramethylsilane and referenced by residual protic solvent. An asterisk was used to indicate residual H_2O 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 λ_{max} for each compound. All experiments were run in triplicate at rt.

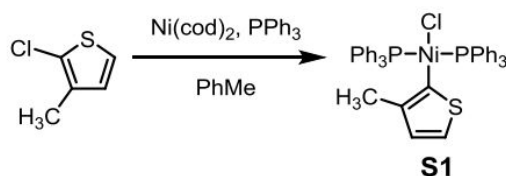
- The third section is dedicated to “syntheses” of all materials generated during the course of the work. It should be self-contained, meaning that if you had to make it for this paper because it was not commercially available, then its synthesis should appear here...even if we (or someone else) previously 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:



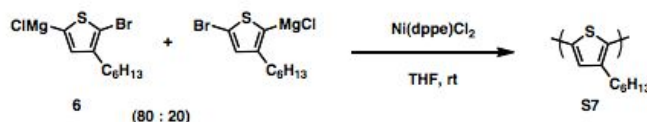
N-Benzyl-1-(furan-2-yl)methanamine (S1). 2-Furaldehyde (300 μL , 3.63 mmol) and benzylamine (360 μL , 3.30 mmol) were combined in dry MeOH (9 mL) and stirred under N_2 for 18 h. The solution was then treated with NaBH_4 (279 mg, 7.38 mmol) in small portions, and stirred under N_2 . After ~ 1 h, no starting material was visible by TLC. The reaction was carefully quenched with H_2O (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 $\text{C}_{12}\text{H}_{14}\text{NO}^+$, 188.1070. Found, 188.1066.

Sample Organometallics Experimental Procedure:



[Bis(triphenylphosphine)](3-methylthiophene)nickel(II) chloride (S1). A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, $\text{Ni}(\text{cod})_2$ (139 mg, 0.506 mmol, 1.00 equiv), PPh_3 (262 mg, 1.00 mmol, 1.98 equiv), toluene (4 mL), and 2-chloro-3-methylthiophene (82 μL , 0.75 mmol, 1.5 equiv) were added. The solution was stirred at rt for 30 min and turned from dark red homogeneous solution to orange heterogeneous mixture. The reaction was removed from the glovebox. Addition of hexanes (30 mL) led to an orange precipitate. The solid was filtered and washed with hexanes (20 mL) and cold MeOH (5 mL). The resulting solid was recrystallized from 1/3 (v/v) THF/hexanes (approx. 20 mL), to give 299 mg of **S1** as an orange solid (84% yield). Elemental analysis: Calcd for $\text{C}_{41}\text{H}_{35}\text{ClNiP}_2\text{S}$, C, 68.79; H, 4.93; Found C, 68.49; H, 4.88.

Sample Polymerization Experimental Procedure:



S7. In the glovebox an oven-dried 20 mL vial was equipped with a stir bar and charged with **6** (1.0 mL, 0.20 mmol, 1.0 equiv) and THF (3.5 mL). The pre-initiated catalyst solution (0.50 mL, 0.0013 mmol, 0.0063 equiv) was added. After 1 h the reaction was quenched with HCl (5 mL, 5 M) then extracted with CHCl_3 (3 x 5 mL). The combined organic layers were washed with water (2 x 5 mL) and brine (1 x 5 mL) and concentrated in vacuo. The resulting solid was washed with methanol to give 30 mg of **S7** as a dark purple solid (quant.).

- The fourth section is dedicated to the “characterization” (e.g., ^1H , ^{13}C , ^{19}F NMR spectra) of the compounds found in the synthesis section. The figures should all have the same x-axis scaling (e.g., 0–8 ppm for all ^1H NMR spectra). Be sure to check the journal if any particular guidelines are required for submission. I recommend making a template of just the axes and then pasting the spectra (without axes) into the template for consistency. Each figure should also have chemical structure and structure number. If the peak splitting is hard to see, then insets should be created as well. The figure caption should list the peak positions to 2 decimals (both ^1H and ^{13}C), coupling constants (italicize the J), and the number of protons (based on the integration).

Sample ^1H and ^{13}C NMR spectra:

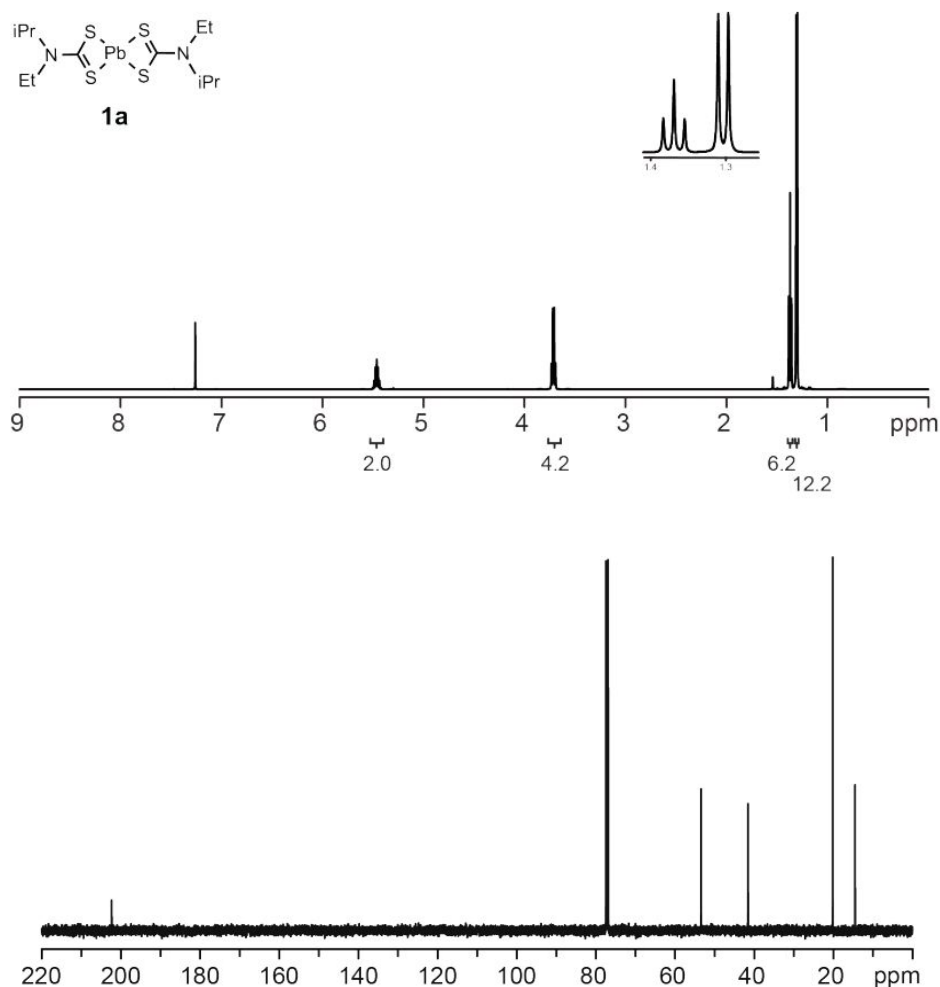


Figure S4. ¹H and ¹³C NMR spectra of **1a**. ¹H NMR (500 MHz, CDCl₃) δ 5.46 (sept, *J* = 7 Hz, 2H), 3.71 (q, *J* = 7 Hz, 4H), 1.37 (t, *J* = 7 Hz, 6H), 1.30 (d, *J* = 7 Hz, 12H). ¹³C NMR (126 MHz, CDCl₃): δ 202.32, 53.41, 41.56, 20.13, 14.50.

- From here, the list of sections should follow the order in which the data appears in the manuscript.

Common General Formatting Mistakes/Reminders

- Margins need to be justified.
- A regular hyphen (-) is used to separate elements of a compound word (i.e. “water-soluble”).
- 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).
- Degree signs (°) should be written using [option 8 on a Mac] not using a superscript o.
- There should be a space between the numbers of a temperature and the degree sign (i.e. “55 °C”, not “55° C”).
- Abbreviations: h not hours; min not minutes; d not days; s not seconds.
- Check all elemental formulas and mass spec formulas for errors/typos.
- Using fewer words is preferred (e.g. “synthesizing not the synthesis of”).
- 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.
14. "*Et al.*" and "*and coworkers*" are not interchangeable. Smith, Leone, and McNeil* would be "*Smith et al.*" or "*McNeil and coworkers.*"