McNeil Group Handbook

Policies, Procedures, and Guidelines

Last Updated: August 2024

http://mcneilgroup.chem.lsa.umich.edu/

Core Values

Everyone – regardless of race, ethnicity, gender, sexuality, age, nationality, religion, ability, or socioeconomic status – is welcomed, valued, and respected within our group.

Each individual is valued for their different perspectives and the different paths they took to arrive here, as well as the different paths they take when they leave. Each individual's cultural norms or standards will be respected, and we will not expect anyone to assimilate to white, heteronormative standards. We believe that everyone has something unique to contribute to the group.

We will celebrate successes, and at the same time, we will recognize that we are all here to learn and part of learning involves making mistakes. We aim to separate the mistakes from the people making them and to collectively learn from them. Respectful dialogue is expected at all times. We feel empowered to speak up when a community member isn't upholding these core values. We are all here to learn, grow, thrive, and support each other.

We value teaching, mentoring, and outreach activities aimed at encouraging the next generation of scientists to be successful.

We value teamwork and collaboration. The quality of the science we produce is more important than the quantity of results. We aim to use our time, resources, and skills to perform research with integrity and to benefit society.

Additional Resources

(The following resources were assembled in Summer 2020 by the McNeil Group.)

- "White Privilege: Unpacking the Invisible Knapsack" by Peggy McIntosh
- "Walking While Black" by Garnette Cadogan
- "The White Space" by Elijah Anderson
- "The Disturbing Return of Scientific Racism" by Angela Saini
- NY Times videos: "A conversation on race."
- The Michigan League 21-day Racial Equity Challenge
- Bystander Intervention and Conflict De-escalation in the Workplace training by Hollaback!
- "Interrupt the Systems" Robin DiAngelo on "White Fragility" and Anti-racism on Life Kit
- "Unlocking Us" with Brene Brown with Ibram X. Kendi on How to be an Antiracist."
- "Unequal Opportunity Race" by Kimberle Crenshaw and Luke Harris
- "Patent Racism" on Planet Money
- "Uncovering the Greenwood Massacre, Nearly a Century Later" on 60 Minutes
- "The Danger of a Single Story" by Chimamanda Ngozi Adichie
- "This Land is Your Land" by Crooked Media
- "The Urgency of Intersectionality" by Kimberle Crenshaw
- "The Diversity–Innovation Paradox in Science" by McFarland et al.
- "The Pressure to Assimilate" by Montrai Spikes

Your Health & Well-Being

(Adapted with permission from Jen Heemstra)

Philosophy

We are all here to grow as scientists & people by pursuing ambitious research goals. However, this goal should not come at the cost of your health and well-being. Your mental and physical health are the most important consideration in all that you do while in our lab. Moreover, success should not come at the cost of maintaining your interests/hobbies or healthy relationships in your life. You are more likely to be successful if you take care of yourself and give time to the things outside of work that matter to you. Below are some general guidelines but every situation is unique, and Anne is always open to discussion, so don't hesitate to ask.

Mental and physical health concerns

If you are not feeling well, either physically or mentally, take the time off you need to seek out help. If you have an acute situation that requires help, take the day (or a few days) off with no questions asked. If you are going to be out for more than 3 days or miss a group meeting, give Anne a heads up so that she knows you are okay – no need to give details, it is sufficient to Slack and say that you have a "personal health emergency." If you need to take more substantial amounts of time off, you can work with Anne and the department to facilitate this absence. Being an undergraduate, grad student, or postdoc is stressful. We all care about you and are here to support you – just let us know how we can help.

- For help contact: Counseling and Psychological Services (CAPS) at (734)764-8312 or the University Health Service (UHS) at (734)764-8320. For confidential support related to sexaul assault call (734)936-3333.

Personal emergencies

Chances are that a life situation will arise during your time in our lab. In these situations, the top priority is taking care of yourself and dealing with the situation. Communicate with Anne to let her know that you are dealing with something and approximately how much time you will need off. You can share as much or as little detail as you feel comfortable with. These situations are inherently stressful, so also make sure you are taking care of yourself and getting help if needed.

Work-life integration

I want you to push your limits to explore what you are capable of. The key is to know when to give yourself a break or some time off. Similar to playing sports, you advance by pushing out of your comfort zone, but if you push too hard you end up injured and stuck on the sidelines. Managing your motivation and work habits while integrating interests and commitments outside of work is a key self-leadership skill that will serve you well throughout your career, and now is a great time to build that skill.

Resources on Campus

The Rackham Graduate Student Emergency Fund is intended to help meet the financial needs of Rackham graduate students who encounter an emergency situation or one-time, unusual, or unforeseen expenses during their degree program.

The Rackham Postdoctoral Fellows Emergency Fund is intended to help meet the financial needs of postdocs who encounter an emergency situation or one-time, unusual, or unforeseen expenses.

For U-M students, staff, faculty, and surrounding community, the Center for Education of Women+ offers opportunities for scholarships, emergency grants, sponsorships, fellowships, and more for a range of situations and life circumstances.

If you or someone you know is feeling overwhelmed, depressed, and/or in need of support, several services are available. The Chemistry Department has an embedded counselor (Ashley Jacobs) who is available for appointments. Email: ashjacob@umich.edu to schedule a one-on-one consultation.

For additional or outside help, contact Counseling and Psychological Services (CAPS) or email: caps-uofm@umich.edu. You may also consult University Health Service for other health needs and for alcohol or drug concerns.

Title IX prohibits discrimination on the basis of sex, which includes sexual misconduct — including harassment, domestic and dating violence, sexual assault, and stalking. I encourage anyone dealing with sexual misconduct to talk to someone about their experience, so they can get the support they need. Confidential support and academic advocacy can be found with the Sexual Assault Prevention and Awareness Center (SAPAC) on their 24-hour crisis line, (734)936-3333. Such violations can also be non-confidentially reported to the Office for Institutional Equity.

Work Expectations

Your success in graduate school is not correlated with the number of hr/wk that you work, but how well you use the time you have (approx. 5 years). Just physically being in the lab is not enough, you need to focus your time and effort when in the lab on experiments (and readings) that move the project forward and your learning.

A good general guideline to keep in mind is that your project and your learning should move forward each day. To accomplish this task, you should set daily goals for your research project and for your own intellectual growth, and check in with those goals at the end of each day. Some goals should be experiment-based, but some goals should also involve reading the literature to learn more about an important aspect of your project.

Try to avoid being in a materials- or equipment-limited world. You should get into the habit of planning far enough ahead so that you don't have to wait for a chemical or piece of equipment to arrive. Similarly, bringing up starting materials should not be a daily goal, rather it should be happening in the background. Your daily goals should always include key experiments where the results intellectually move the project forward.

Weekly goals can also be helpful, along with monthly goals, although keep in mind that these are more projections than goals, and they may change as new results are acquired. Frequent "research direction" meetings with Anne can also be helpful, especially when unexpected results throw a wrench into your weekly or monthly plan.

Other really useful tips and strategies to monitor "how well" you are doing can be found in the self-evaluation document on our group website. By the time you graduate, you should be able to answer "yes" (or equiv) to all the questions in that document. The self-eval can serve as a great "to-do" list for your own professional growth.

Vacations: Each graduate student/post-doc is allotted 21 days of vacation per calendar year (Jan-Dec). This number is inclusive of all UM-recognized holidays. Note that sick days do NOT count as a vacation day. If you join the lab mid-year, the number of vacation days will be prorated based on the start date. To keep track of everyone's dates, there is a shared Google calendar. You should write your initials on the date(s) you will be taking off AND what vacation day that is for you (e.g., 10/21 2024). Vacation days can roll over into the next calendar year.

Lab Safety

General

- Make sure you complete the UM-OSHA Comprehensive Laboratory Safety Training course and read the Chemistry Department Safety Manual before initiating research. Upload a copy of your completion certificate to the McNeil Group "Shared Drive" Safety Folder prior to starting lab work.

- Make sure you read and sign all lab-relevant SOPs (binder in kitchen).

- Make sure that you complete the safety checklist (next page) and send a signed copy (PDF) to Anne before beginning research. Upload a copy onto the McNeil Group "Shared Drive" Safety Folder as well.

- Notify the group safety officers AND Anne immediately if you have been injured or spilled a toxic, caustic, or flammable compound.

- Lab coats and safety glasses must be worn when doing work, either at your bench, hood, or sink OR if you are talking/standing next to someone who is working at the bench, hood, or sink. If you see someone working without a lab coat and/or safety glasses, please remind them of the appropriate personal protective equipment needed for working in the lab. If the problem persists, please notify Anne.

- Open-toed shoes and shorts/skirts (without leggings) cannot be worn in the lab.

- Headphones (even single-ear wearing) are not allowed in the lab.

- Notify group members when you are leaving for the night. This habit helps to ensure that nobody is working alone!

- For additional safety resources, please consult the "safety information" section of the group website.

Guidelines for a Safe Working Area

Bench and Hood Area

- Your workspace should not be cluttered. You must be able to place a new vial/flask/beaker on your bench. All reagent and solution bottles must be clearly labeled without use of chemical abbreviations.

- Nothing can be hanging off the edge of benches or shelves. Flammable solvents and reagents cannot be located within 18" of the ceiling.

- No objects can be within the back 4" of your hood unless it is on a shelf. Check that all water, air and N_2 lines are secured with copper wire. Ensure all tubing and power cords are free of defects.

- All chemical waste must be clearly labeled with no chemical abbreviations and dated. Chemical waste should be capped when not in use. Glass containers containing chemical waste within 4' of a drain must be in a secondary container.

Instrument Room and Shared Space

- If you are responsible for an instrument that generates chemical waste, ensure that the waste bottle is properly labeled, dated, placed in a secondary container and has an appropriate cap.

- Claim any chemicals left in the balance area and return them to the proper place.

Emergencies

Call the Department of Public Safety by dialing **911** from a campus phone or **734-763-1131** from a cell phone. Call **Chris Peters** (Departmental Lab Safety) at **734-763-4527** or **chrpeter@umich.edu** or **Tracy Stevenson** (Departmental Lab Safety) at **734-764-7316** or **steventi@umich.edu**.

Lab Entry – Safety Checklist

*Please complete the following checklist with your mentor and/or the group safety officer, and return an signed, scanned copy as a pdf file to Anne **before** beginning to work in the lab. Also upload a copy to the McNeil Group "Shared Drive" Safety Folder.*

Student	*Mentor*	*Task*
		I have completed the online OSHA safety training and uploaded my certificate on Drive.
		I have read the University of Michigan chemical hygiene plan and the group-specific hygiene plan, and have read and signed all SOPs (blue binders) and become familiarized with their contents.
		I have received safety glasses and a lab coat and agree to wear them at all times when in lab. I am aware of acceptable clothing to wear in lab.
		I have completed a safety walk-through of the lab with the group safety officer. I am aware of the location and operation of the safety shower, eye wash, fire extinguisher, blast shield, and fire alarm in ALL of the group laboratory rooms.
		I know how to access MSDS (material safety data sheets), and I will refer to these if I have any questions about the safe handling of any reagent.
		I am aware of emergency phone numbers and department contact numbers in the event of an accident, chemical spill, or other emergency.
		I will be properly trained (i.e., read the SOP and talk to an experienced user) before handling any new (to you) compounds.
		I will maintain a safe and clean work environment, will properly label and dispose of hazardous materials, and will safely store and handle all chemical reagents.
		I understand that no food or drink is allowed in the labs (except the kitchen areas).
		I have discussed with my mentor how to properly handle and label chemical waste (solid & liquid) related to my research.
		I will conduct my research with honesty and integrity and will not intentionally fabricate or misrepresent any scientific data.

		I will consult with Anne on any issue that poses a safety concern. If I see an unsafe operation being conducted, I will ask the coworker to correct the problem, and I will consult with Anne if the problem persists or is repeated.
		I will seek advice from experienced group members about all new procedures, and I will consult with Anne if any procedure poses a potential safety concern.
		I have viewed the group job list and will consult the appropriate person before using any equipment for which I have not yet received proper training.
		I have access to the McNeil Group OneNote lab notebook and I am aware of the lab protocols for keeping complete and accurate records of my research.
		I have read the entire group manual and understand what is expected of me.
		I agree with all of the above items and will upload this signed document to drive.

Group Policies

Group Collaborations

Collaborations are a vital part of the scientific enterprise. In the McNeil Group, members are encouraged to participate in both external collaborations (within and/or outside of the Michigan department) as well as internal collaborations (group members working together on related projects). There are many benefits to these collaborations. Oftentimes, the project's timeline can be expedited when multiple people are working together. In addition, your collaborators can give research projects added areas of expertise and new directions.

When you agree to engage in a collaborative project, you are committing to providing the collaborator with the highest possible quality of materials. The group policy is that with each sample you must provide (as a PDF file) the notebook page that corresponds to the exact procedure used to make the sample, a copy of the ^{1}H NMR spectrum of that sample, the yield and estimated purity, and any other relevant characterization data (e.g., the GPC for polymers or elemental analysis). It is imperative that all lab members conform to the above criteria to ensure a productive collaboration. Also, you should cc Anne on ALL communications with collaborators, no matter how small the detail or communication.

Research Group Meetings

Research group meetings occur every week. (See the McNeil Group "Shared Drive" Group Meeting Schedule folder for the schedule.)

Each member of the presenting subgroup has 10–15 min to present something that they want to discuss. Students should think carefully about how to use this time. Do you want us to help you troubleshoot an experiment? Do you need help with planning what experiments to do next? Do you want a second opinion on your data analysis and interpretation? Do you think your project should switch directions? Or do you just want to update us on your latest findings? Then the student should craft a short (but polished) slide presentation with all necessary information to accomplish their goal. A few general guidelines: All experiments should be accompanied by the notebook page and with a chemdraw scheme and literature references. All data should be processed as if publishing it (do not post raw data) and the analysis should be clearly depicted using ChemDraw and Illustrator/Photoshop.

In addition, each week 2-3 students will have an individual meeting with Anne. Once or twice a year, the group will go off-site for a retreat where everyone will give a formal research presentation.

Literature Group Meetings

Your first goal is to pick a paper that you think will be of interest to other group members. You can browse recent issues of polymer/materials journals or pull from articles highlighted by C&E News or other organizations, or from an upcoming seminar speaker. Next, read the paper carefully and then share with the group at least one week prior to the meeting.

When preparing your talk, you should first identify at least three main take-home messages that you want to share with the group. Then structure your talk around those messages. One take-home message should convey the impact of this work in the context of what was already known in the literature. To do this, you will need to read several papers that preceded this work and share what was found/known in enough detail for us to understand it. Another take-home message should be related to the new insights gained through the work in the paper you are highlighting. Don't simply rely on their figures/tables, etc. You should present it in the way that makes the most sense as a whole. You should analyze their data and conclusions and create slides that have, in some cases, original graphics from you on them. You do not need to highlight everything! Pick out the most interesting results. A third take-home message should be a "teaching moment" for the group. Dig into a complex concept in the paper, learn more about it, and share/teach it to the group.

You should end your presentation with a brief discussion of an idea that this work sparked in you. Examples include: What would you do next if this was your project? How does this connect with your work or other work in the field?

Public Presentations of Research

All forms of public research presentations, whether conference talks, posters, or published papers are a reflection of the entire research group and *therefore must be approved by Anne 2 days in advance of their presentation*.

Rotation Students

Rotation students should plan to work *at least* 20 hrs per week in the lab. At the end of the semester, rotation students will present a 30 min formal presentation on their work to the group.

Undergraduate Researchers

All undergraduates are expected to work 3 h/credit-hour and can only perform research if a graduate student or post-doc is also in the lab. The undergraduates are expected to attend and participate in all group meetings.

Data Storage: McNeil Group Shared Drive

After joining the group you should set up some space on the McNeil Group "Shared Drive" to store all data, publications, presentations, and candidacy- and thesis-related documents. Please create separate sub-folders for "processed data", "presentations", "publications", "candidacy", and "thesis".

Slack

Slack is a cloud-based app that we use for all group communication. All students should join our Slack team "McNeil Group" when you start. Channels should be used to send messages to large groups of people. For example, the "conjugated polymers" channel sends a message to everyone in that subgroup, whereas messages posted to the "random" channel go to everyone. Slack can also be used to send direct (private) messages to anyone in the group, including Anne. You can also start "conversations" with several people at any time by creating a direct message to more than one person. Slack should be used for all file sharing as well, you can upload/download, share via Google drive, etc. One really nice feature of Slack is that both the files and messages are text searchable.

Grad School Skills Development

Here we suggest some year-specific goals for graduate students because it is oftentimes difficult to assess your progress because there are few concrete milestones in graduate school. It's easy to feel like an imposter when you don't know how to assess yourself. (Special thanks to Jessica Tami for leading this group discussion in Feb 2022.)

Year 1

- Learn to effectively search through the literature to answer specific questions and keep up-to-date with the latest science in your field. Some resources to use are: Reaxys, SciFinder, Web of Science, Google Scholar, and checking ASAPs of the journals you read. Read as much as you can. This guideline is true for every year of graduate school and beyond.

- Learn to extract the important information from papers efficiently. Start by reading introductions to situate yourself in your field and understand what has been done previously. Then read the abstracts and conclusions. Then incorporate results and discussion. Eventually, with a lot of practice, you will look at figures and understand the novelty or improvement of methods without having to read the entire paper. Try paraphrasing published work to improve on your scientific writing. How would you phrase the introduction? How would you conclude the paper?

- Build self confidence and comfort with relevant lab techniques, lab equipment, and instruments. This comes with practice! We also have manuals by all of our instruments in case you forget something.

- Attend seminars (aim for 1 per week) and be engaged. Read a paper by the speaker before attending. In addition, pay attention to the speaker's presentation skills and aesthetics so you can learn how to present *your* research most effectively. If you learn one thing (even if it isn't science) at a seminar, it was worth your time.

- Apply to fellowships! There are a lot of fellowships for 1st and 2nd year graduate students (NSF, NDSEG). You will understand your project in a deeper way and get practice with scientific writing.

- THIS IS YOUR TIME TO MAKE MISTAKES! If you make a mistake, it is not the end of the world. You will learn and probably never make the mistake again. Remember that the health and safety of our lab members is paramount. Please do not be afraid to ask questions. It's better to ask and do something correctly than say nothing and potentially hurt yourself. Your first year is all about learning, learning, learning. Not producing, producing, producing.

Year 2

- Practice public speaking. Explain your project to a variety of people. How would you tell your parents about your science? Your younger sibling? A tenured professor in your field? An assistant professor in another department? Internal symposia (Karle, Macro, etc.) are good opportunities to practice your speaking skills. Participate in all relevant ones.

- Ask yourself about the *what*, *how*, and *why*'s. What do reagents do in your reaction flask? What is the mechanism? Why are you using this number of equivalents? How will I purify the crude reaction mixture? Thinking ahead will help you answer questions during group meetings, subgroups, and candidacy.

- Know your basics from classwork and how they apply to your project. Know your basics on chemistry terminology, like: "alkylation reaction" or "de-chlorination." Learn how to answer questions eloquently and make educated guesses and hypotheses on the spot. This is a follow-up to point #2. You will not always know every answer to every question but when you know the basics of your project, you can generally guide yourself to the answer. And if all else fails…do what everyone does and say: "That's an interesting question!"

- Continue attending seminars. Start building the confidence to ask the speaker any questions you might have.

- This needs to be reiterated: read, read, read!

- Continue applying to fellowships as you are still eligible!

- Draw writing inspiration from papers that do similar science to your project. Start writing an intro to your first paper. This exercise will help you see gaps in your own project and knowledge. Don't be afraid to put words on paper, your first draft will never be your final product. Just get started!

Year 3

- Start thinking about your future career and explore different career paths. Attend career workshops and give informational interviews. Start networking with people who have this career, as their advice and support will be really helpful. McNeil Group alumni, Twitter, LinkedIn, and DiversifyChemistry are good sources for finding people to interview.

- Attend different professional development activities. The university and department put on a lot of events for resume building, public speaking, scientific writing, etc.

- Continue attending seminars and reading the literature!

- Attend an external conference (ACS) and present your work.
- Get involved with grant-writing, paper-writing, and/or helping write a Perspective or Review article.
- Mentor an undergraduate or a rotation student.

Year 4

- Go to job recruitment sessions to start preparing for future job searches. Network with professionals who work in industry, government, academia, etc.
- Mentor an undergraduate or a junior graduate student.
- Continue attending seminars and reading the literature!
- Attend a more specialized external conference (Gordon, etc.) and present your work.
- Get involved with grant-writing, paper-writing, and/or helping write a Perspective or Review article.
- Start planning your thesis chapters and consider adding a new project and/or starting a collaboration.

Year 5

- Start applying for jobs and/or postdoc positions in early Fall.
- Start writing your thesis. Whenever you think you should start writing, start a month earlier! It takes longer than you think AND it is due to your committee 14 days before your defense.
- Mentor an undergraduate or a junior graduate student.
- Continue attending seminars, conferences, and reading the literature!
- Get involved with grant-writing, paper-writing, and/or helping write a Perspective or Review article.

Post-docs

- Don't be afraid to try *new* things! You are supposed to *grow* a ton during your postdoc time so look for opportunities to develop new skills and research directions.

- Consider applying to different jobs (industry, academia, government, non-profits, etc) to see which feels right. Reassessing your goals is OKAY! Do what is best for you.

- Practice for the job that you want. If you want to be a professor, apply to teach a class. Ask to meet with seminar speakers when they come through Michigan. If you want to go to industry, try to get involved with collaborations with other groups and manage those collaborations so that productive scholarship results.

- Be efficient with experimental designs and your time.

- Mentor an undergraduate or a junior graduate student.

- Continue attending seminars, conferences, and reading the literature!

- Get involved with grant-writing, paper-writing, and/or helping write a Perspective or Review article.

Mentoring Checklist

Please complete the following checklist with your mentor, and return a signed, scanned copy as a pdf file to Anne and upload a copy to the McNeil Group "Shared Drive" mentoring folder.

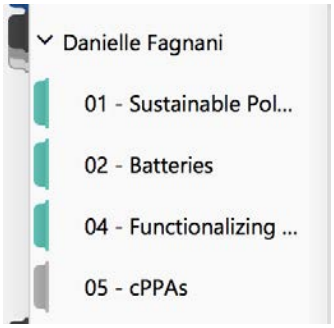
Trained	*Proficient*	*Task / Skill*
		Safety
		I have completed the "lab entry - safety checklist" and sent a PDF copy to Anne and uploaded it onto Drive.
		I understand how to be a safe worker in the lab on my specific research project and have demonstrated it.
		I understand what "good chemical hygiene" refers to (clean workspaces, clean shared spaces, returning chemicals to their original location, etc.) and demonstrated it.
		Navigating the lab
		I understand what is expected of me from subgroup presentations.
		I understand what is expected of me for the online laboratory notebook pages and how to store/backup my data.
		I am properly storing and labeling my samples.
		I can navigate to shared online resources like training manuals, Drive, and library/web resources.
		I know how to search the department's chemical inventory and how to order supplies and reagents.
		I understand the group guidelines on how to make figures.
		I have watched tutorials for ChemDraw and Adobe Illustrator and can use those for my presentations.
		Searching the literature
		I have demonstrated effective searching using Reaxys, SciFinder, and Web of Science.
		I have set up alerts for research papers related to my project.
		I have crafted a preferred method to save and annotate papers related to my project (e.g., Zotero, Notability, etc).

		I have used some online library resources like e-EROS.
		I have used an online chemistry resource including Not Voodoo, SafetyNet, etc.
Reading a paper effectively		
		I have demonstrated that I can read a paper effectively and write short summaries of the key points.
		I understand how to read papers for specific information versus general background.
		I am an active participant at the professional development meetings.
		I read papers before seminar by the speaker.
Basic synthetic lab techniques		
		I can safely operate the Schlenk line and vacuum pumps (and gauges).
		I can safely syringe and pipette solutions.
		I can safely dispose of solid, liquid, and sharps waste.
		I have demonstrated that I can run and analyze TLC plates.
		I have demonstrated that I can successfully run a column by hand.
		I have demonstrated proper use of a rotovap and can disassemble it for cleaning or repair.
		I have demonstrated proper cleaning and drying of glassware.
		I can take an ^{1}H NMR on my own (not on “Carbon”) and interpret it.
Project-specific training		

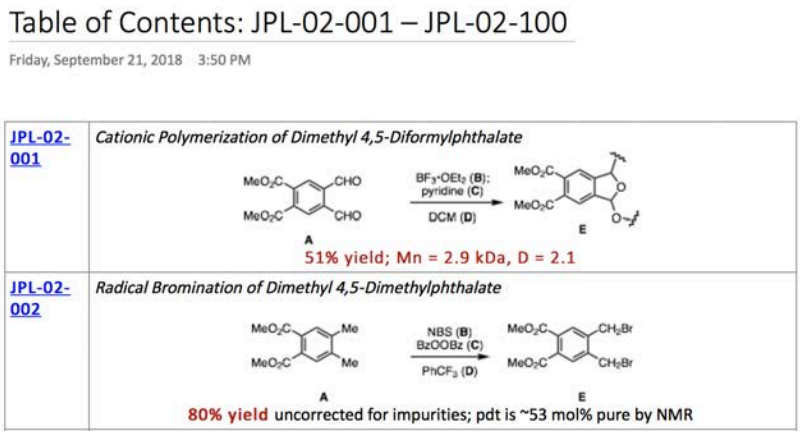
Lab Notebook (OneNote) Guidelines

General

- The McNeil Group shares a single OneNote Notebook called “McNeil Lab - General”.
- Ask Anne to initiate your notebook. Create a new “notebook” section for yourself and then create sub-sections for each project you have. Assign each notebook a different number.



- Each notebook should have as its first page a graphical TOC with hyperlinks to the experiment pages.



- Label each experiment with your initials, notebook #, and page #.

- Every experiment you do MUST be accompanied by an entry in your lab notebook.

- Keep your electronic notebook up to date! At the end of day, your notebook should be updated and make sure all data files have been uploaded. Consistent notebook-keeping is an essential part of being a scientist!

- We should be able to find this data after you have graduated. OneNote keeps a copy, but you should backup all your data files onto the Turbo volume before you leave/graduate.

Experiment Pages - for syntheses

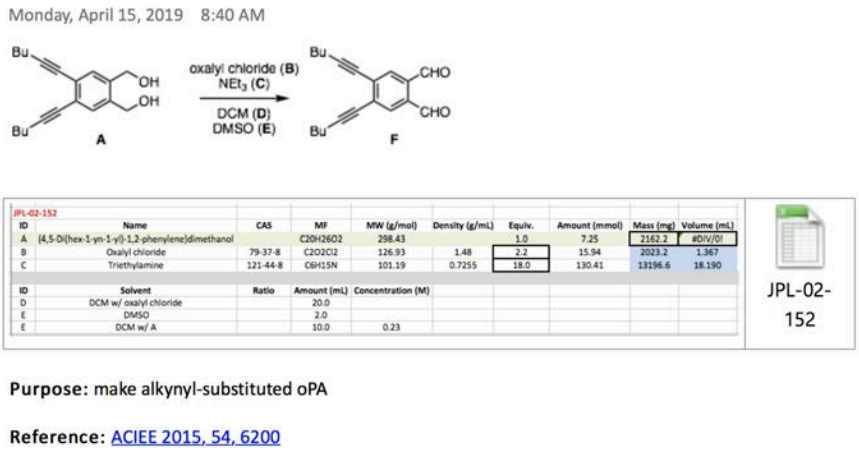
First Section

- Start the page with a date, title and reaction scheme (as appropriate).

- State the purpose of this experiment. What are you trying to do and why? How does it relate to previous experiments you've done?

- Include any references to the literature or previous notebook pages relevant to the experiment.

- Note that if you are repeating a procedure, you must record it as a new experiment. You can copy/paste from the previous experiment, but be sure to update it with any changes that you make, including quantities of starting materials used, workup conditions, chromatography conditions, etc.



Monday, April 15, 2019 8:40 AM

JPL-02-152

ID	Name	CAS	MF	MW (g/mol)	Density (g/mL)	Equiv.	Amount (mmol)	Mass (mg)	Volume (mL)
A	(4,5-Di(hex-1-yn-1-yl)-1,2-phenylene)dimethanol		C20H26O2	298.43		1.0	7.25	2162.2	#DIV/0!
B	Oxalyl chloride	79-37-8	C2O2Cl2	126.93	1.48	2.2	15.94	2023.2	1.367
C	Triethylamine	121-44-8	C6H15N	101.19	0.7255	18.0	130.41	13196.6	18.190

ID	Solvent	Ratio	Amount (mL)	Concentration (M)
D	DCM w/ oxalyl chloride		20.0	
E	DMSO		2.0	
E	DCM w/ A		10.0	0.23

JPL-02-152

Purpose: make alkynyl-substituted oPA

Reference: ACIEE 2015, 54, 6200

- For syntheses, add a reagent table that includes molecular weights, mols/equiv, masses or volumes. Record masses based on the accuracy of the balance, and volumes based on the accuracy of the syringes. Record the source of each reagent (lab notebook page or commercial supplier), the date opened and the batch number (if purchased).

- Record the actual quantities added to the accuracy of the instrument you used to measure it. For example, if you intended to add 10 g and you weighed out 10.230 g –

record the 10.230 g. Be sure to re-calculate the mols/equiv based on what you actually measured, not what you intended.

- Make sure to include the time at which you start the experiment as well as when you finish it. If you work on the experiment over multiple days, record a new date and time for each part of the experiment on the same notebook page.

Procedure Notes

- Record every action and observation. The more detail you provide, the easier it will be for you (or someone else) to learn from and reproduce your work. Use past tense to describe the experiments. Use full sentences, in paragraph form.

- Be sure to indicate the time involved for all steps (e.g., stirred for 3 h) and the temperature (e.g., at rt). Always indicate whether the reaction was performed under inert atmosphere (e.g., under N_2 or in the glovebox) or ambient conditions (e.g., open to air).

- If you are doing an action, like a freeze-pump-thaw cycle or bubbling H_2 through your solution, be sure to indicate the times (e.g., for 10 min) for each step.

- Estimate approximate volumes for workup conditions (e.g., approx. 10 mL of water was added to quench the reaction), including LLE (e.g., ~50 mL of DCM was added and the organic layer was separated).

- Provide explicit details about what you see: Is the reaction homogeneous or heterogeneous? Does that change over the course of the reaction? Is there a color observed? Is your product colored?

- If you used a reagent that required some purification, be sure to state that here, ideally referencing another notebook page where that purification was recorded. Similarly, if you are using an anhydrous solvent, state whether that's from a commercial source (e.g., Sure-Seal bottle) or our solvent system or dried by you with activated sieves (state the sieve size and activation method too!).

Procedure:
To an oven dried 100 mL RBF was added a solution of **ran20Br** (46 mL, 60 mg, 35.0 µmol, 1.0 equiv Br) in dry THF (added by rinsing the vial containing polymer sequentially with aliquots of THF). To this flask was added DMF (25 mL). The reaction was stirred for 5 min at 60 °C then and NaN_3 (25 mg, 0.385 mmol, 11 equiv) was added in one portion with stirring. The flask was equipped with a reflux condenser and the reaction was stirred under N_2 for 2 h at 100 °C before cooling to r.t.* The THF was removed *in vacuo*, and the remaining polymer was precipitated into cold MeOH (50 mL), filtered, and the solids were rinsed with cold MeOH (30 mL). The remaining solid was dissolved in $CHCl_3$ and precipitated into cold MeOH (30 mL) and centrifuged, and the supernatant was removed. The pellet was resuspended in cold MeOH, placed in the freezer for 10 min, centrifuged, supernatant decanted. The pellet was dried *in vacuo* to yield a purple powder (49 mg, 79% for the 2 steps). avg RU mass = 174.485, #RU's = 68.37.

- If you prepare a sample for analysis, state how that sample was prepared (e.g., 0.05 mL of the crude reaction mixture was diluted with 2 mL Et_2O, then filtered through a small plug of silica and analyzed using the “lower-high” method on the GC–MS).

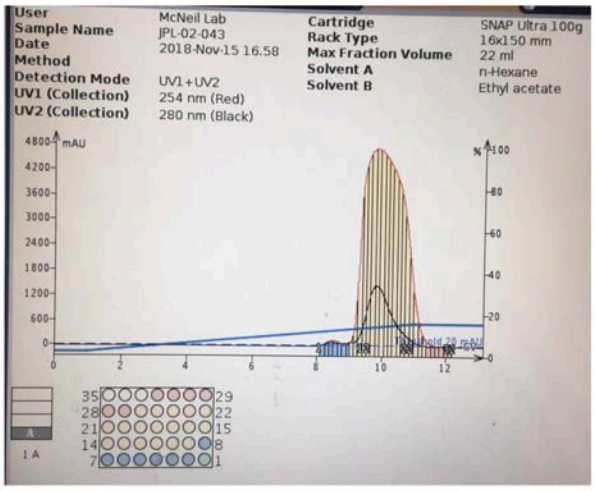
Characterization Data

- At a minimum, you should include: (i) some visual representation of your data (screenshot, photo, or PNG file), (ii) some words that summarize what the data means, and (iii) a link to the actual raw data file.

- Indicate in your notebook the file name and date acquired for all data relating to that experiment. You should also include pertinent information about the instrument the data was acquired on.

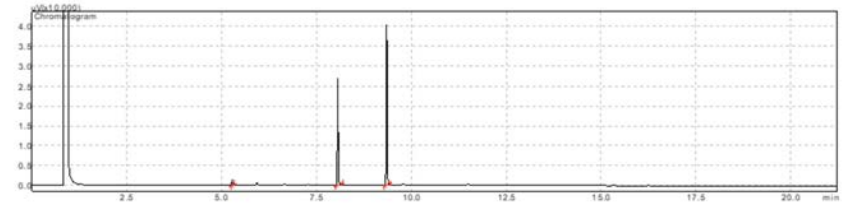
- Copy/paste or insert as an image a screenshot of the raw data (e.g., for GPC, GC, NMR, Biotage, etc).

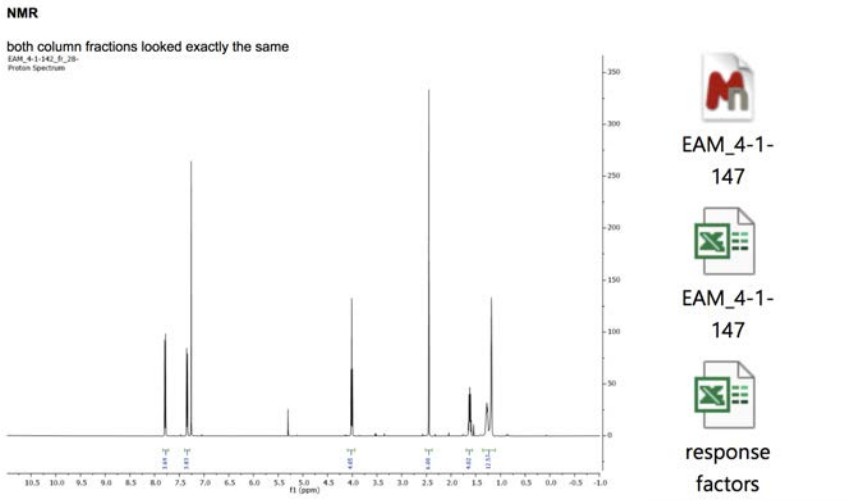
Purified on Biotage (100 g column, 1 –> 15% EtOAc in hex, fracs 9–32) and put on high vac to give a pale yellow solid (1.17 g, 79% yield)



GC

prod plus C22





- If you decide that for one reason or another you don't think the data obtained is valid, note this in your notebook and state your reasoning. Otherwise, interpret your data and indicate what the next steps should be based on your data.

Conclusion:

First issue: added 10x the amt of catalyst I wanted to. Next time will be careful to add less! Next, the product co-elutes with C22 (DUH), so will need to change GC standards before running this experiment again. I'm guessing low conversion is because the catalyst died (turned black). Will try again but leave the reaction at 0 the whole time. JACS paper cited above seems to indicate that changing the eq of grignard won't have a large effect on yield (even tho I'm seeing some mono-funct).

Experiment Pages - for microplastics research

Sample identity and preparation

- Indicate the amount of sample used by mass or volume.
- *For generated solutions*: indicate the solvent, concentration, volume, and how the solution was mixed.
- *For generated particles*: cite the notebook page for samples that were created in-lab along with any characterization data of the generated samples.
- *For commercial standards*: detail the supplier, batch number, size, shape, identity, density, and color.
- *For environmental samples*: indicate the origin and any previous isolation attempts (i.e., sample history).

Experimental details

- List the protocol for preparing all solutions including filtering conditions (type of filter), solvent, type of filtration, and components.

- Include glassware cleaning conditions and substrate preparation protocol, if any.

- Note experimental observations and time conditions of all reactions (e.g., digestion).

- *For environmental sampling*: include information on location, date, weather conditions, description of instrumentation or tools used, time of collection, images of collection, and note plastic use.

- *For microplastic capture*: include information on pump model and rate, details on flow conditions, capture medium, material for capture (pore size, mass, layers), tubing identity, and include an image of the setup.

- *For microplastic extraction and isolation:* include information on chemical supplier information and concentration, digestion protocol, density separation protocol, staining protocol, and resting time (if applicable).

- *For probe tack:* include information on method parameters, probe material, any sanding completed for polymer probes, the number of samples, probe pokes per sample, film thickness, sample preparation procedure, observed thickness via microscopy, and link the adhesive synthesis notebook page.

Analysis information

- Include the name of any assistants and their contribution to your results.

- List the location, name, and parameters of any instrumentation used.

- Include information on the number of samples or particles analyzed as well as a description of subsampling protocol, if any.

- Export and link raw files or indicate the file location if they are too large to attach in OneNote.

- Include searched libraries, software, and conditions of spectral identification.

- *For SEM*: include information on citation/acknowledgement criteria, sputtering time and coating type, detector used, high voltage, beam intensity, magnification, and view field.

- *For optical image collection*: include information on the magnification, number of tiles in mosaic, and indicate whether a mosaic or single image was collected.

- *For flow cytometry*: include information on acquisition volume, flow rate, stop option and value, and voltage setup.

Experiment Pages - for e-chem/battery research

Stock solutions

- Oftentimes we use stock solutions (e.g., 0.5 M KPF_6 in MeCN) so it is helpful to either make a notebook page which details how you make your stock solutions or include those details in each experiment.

- Important details to include are: solvent supplier and grade, electrolyte supplier, if electrolyte was recrystallized, how it was recrystallized (solvent(s) volume, solid volume, temperature, time), how electrolyte was dried (vacuum oven, temperature, time).

- Were the stock solutions dried over sieves in the glovebox (size, brand, pretreatment)?

Electrodes

- How were the electrodes made? What materials were used? Where were they purchased? How are they cleaned or polished? What solution is contained in your reference electrode? When was the reference electrode prepared / how long has it been used?

Material synthesis

- Hyperlink synthesis notebook page and include how the material was dried before bringing it into the glovebox.

Procedure notes

- How was the experiment set up? What electrodes were used? Solvents? What settings were used on the potentiostat?

- CV: reference electrode, counter electrode, working electrode; vessel (e.g., 20 mL vial); concentration of material and supporting electrolyte, scan rate

- BE: galvanostatic? CCCV? Electrodes?, capacity cut off, voltage cutoff, charging rate, number of cycles

- Electrasyn: anode, cathode, volume, current/voltage, time, reference electrode (if used), stirring rate, alternating current (if used)

- Battery: Electrodes (any pretreatment?), gaskets, O-rings, membrane/separator, flow field, volume, concentration, flow rate, tubing (on the cell and the pump), EIS conditions, GCPL conditions (or other technique)

Characterization data

- Include all raw data on an excel sheet and make sure the file name corresponds to the notebook page. If data needs to be further worked up, include those excel sheets too.

- Include a few sentences to explain results (what were you looking for and what did the experiment tell you?)

- It is also helpful to include all raw data files in your notebook. This can be done by saving the folder containing the raw data as a .zip file and uploading it to the notebook page.

Summary

Ultimately, your electronic lab notebook, collections of spectra and other data, and the supporting information documents are the ***most important*** things you will prepare as a scientist during your PhD. You should take pride in these items and spend the time to prepare a solid foundation to support your claims. This documentation can and will be used to verify that indeed these experiments were run and that the results are as you claim. If there are errors in these records, then it can call into question deeper issues ranging from carelessness, negligence, to scientific fraud. These can result in serious consequences, including getting expelled from the PhD program. **Do not take these issues lightly!**

Collecting and Archiving Scientific Data

Uncertainty in Measurements – Significant Figures

All measurements have some level of uncertainty. Significant figures include all the digits you are certain about PLUS one additional uncertain digit. See attached discussion. Note that our balances are uncertain in the *last* digit you can read.

Counting Significant Figures

Leading zeros are not significant. 0.008 has one significant figure
Captive zeros are significant. 1.02 has three significant figures
Trailing zeros are significant. 40.00 has four significant figures

Rules for Rounding

In a series of calculations, carry the extra digits through to the final result and then round. If the digit to be removed is less than 5, the preceding digit does not change. (1.33 = 1.3) If the digit to be removed is greater than 5, the preceding digit goes up by one. (1.36 = 1.4) Only look at the first number to the right of the significant figure. (4.348 = 4.3) If the digit is 5, then round to the closest even number. (1.35 = 1.4 and 1.65 = 1.6)

Calculations and Significant Figures

For multiplication and division, the answer should have the same number of significant figures as the least precise measurement. (4.56 x 1.4 = 6.4) For addition or subtraction, the answer should have the same number of decimal places as the least precise measurement. (12.1 + 1.103 = 13.2)

Advice for Running Reactions

- For a great reference on synthesis and lab techniques, check out the "Not Voodoo" website by Alison Frontier (University of Rochester) at http://chem.chem.rochester.edu/~nvd/. See also, "The Laboratory Companion" by Gary S. Coyne and John S. Wiley and "Advanced Practical Organic Chemistry" by J. Leonard, B. Lygo, and G. Procter. See also, senior members of our research group.

- Start with pure reagents and chemicals. See "Purification of Laboratory Chemicals" by Armarego and Chai for detailed information on how to purify common reagents and solvents. Garbage In = Garbage Out!

- Run reactions on a small scale the first time (~100 mg or less!). After you have worked out the reaction conditions and purification procedure you can scale up. Do not scale up a reaction more than 3-fold of your previous successful attempt.

- Monitor your reactions by TLC. You can supplement TLC with GC analysis, crude NMR spectra, and IR. None of these techniques are a substitute for TLC.

- Always work up reactions immediately upon completion.

- Take the time to identify by-products the first time through a synthesis.

Labeling and Storing Compounds

- Label all vials with a structure AND the notebook page number. Use a small white label and attach to the vial with reinforced clear tape. Sharpie's do not last the test of time!

- Store all synthesized materials in small disposable vials with screwcaps. Please do not store any compound in an expensive flask with ground glass joints.

- Indicate the amount of material inside the vial on the screwcap (e.g., 52 mg).

- Store all synthesized compounds either near your bench or in your assigned shared refrigerator. Do not store your compounds on the group chemical cabinets or in the group refrigerator.

Searching and Reading the Literature

Searching the past literature

Reaxys & SciFinder Scholar

Excellent resources when searching for specific chemical reactions & conditions.

ISI Web of Science

There are several very useful functions of this website.

A. Cited References Search

Use this search to find all articles that cite a key paper. This search is especially useful because you can also find articles that cite the paper that cited your key paper!

B. General Topic Search

Use the "and" command to link two concepts and use "*" to expand. For example, if you want to search for fluorescent polymers, but also want to include any search where "fluorescence" is also used. Your search command would read "fluor* and polymer."

C. Author Search

Use this search to find all articles published by an author. You can then refine this search using keywords, dates, or document type, etc.

Note that both search engines allow you to refine your results by narrowing the list and by analyzing the list. For example, if you are searching for a starting material, you can refine your SciFinder result list by "commercial availability." Or if you are searching for articles with a name like John Smith, you can refine by first analyzing the "institution type" and then only select those articles by John Smith at University of Michigan. Other useful tools include Wikipedia, Google, Google Scholar, "Comprehensive Organic Transformations" by Larock, and eROS (encyclopedia of reagents for organic synthesis.)

Google

This search engine can provide a useful starting point for any literature search.

Reading the Current Literature

You should aim to read one new paper each day of the week. Keeping up with the current literature is essential to becoming a creative, independent, and successful scientist. You should aim to gain breadth (by reading newly published papers *outside your project area*) and depth (by reading newly published papers *in your project area*). Balance your reading

between breadth and depth. To set yourself up for success, here are some strategies and tips from group members on how to identify papers to read.

Research App

Most folks in the group (included Anne) have gravitated to the Researcher App. Receive content from specific journals, or create keyword (or author or topic) searches and have papers delivered in a newsfeed type style to your device (similar to RSS feeders). Read, bookmark, or save for later.

Publication Alerts

- ***Google Scholar*** You can set alerts for specific authors or keywords.
- ***ACS Journals*** You can sign up to receive alerts for new papers published in specific journals, or set alerts for specific keywords in newly published papers in ACS journals, or set an alert for when specific publications have been cited.
- ***SciFinder Scholar (or Web of Science)*** You can set alerts for papers published with specific keywords and set a frequency of emails.

Other Tips

As you identify papers to read, assign them to a specific day so that you always have a paper on deck and are not spending time looking for something to read each day. Then prioritize reading that designated paper for that day first thing in the morning, when you arrive at work.

When deciding whether you want to add a paper to your “deck”, read the title, then abstract, then scan the figures. If you are still interested to know more, add it to your reading list.

How to Write a Conference Abstract

The following advice was excerpted (and edited) from "How to write a scientific abstract in six easy steps."

1. **Introduction. In one sentence, what's the topic?** Phrase it in a way that your reader will understand. The readers are others in your field, so they know the background work, but want to know specifically what topic your paper covers.

2. **State the problem you tackle**. What's the key research question? Again, in one sentence. Remember, your first sentence introduced the overall topic, so now you can build on that, and focus on one key question within that topic. If you can't summarize your presentation in one key question, then you don't yet understand what you're trying to present. Keep working at this step until you have a single, concise (and understandable) question.

3. **Summarize (in one sentence) why nobody else has adequately answered the research question yet**. The trick is *not* to try and cover all the various ways in which people have tried and failed; the trick is to explain that there's this one particular approach that nobody else tried yet (hint: it's the thing that your research does). But here you're phrasing it in such a way that it's clear it's a gap in the literature. So use a phrase such as "previous work has failed to address…".

4. **Explain, in one sentence, how you tackled the research question.** What's your big new idea?

5. **In one sentence, how did you go about doing the research that follows from your big idea**. Did you run experiments? This is likely to be the longest sentence, but don't overdo it – we're still looking for a sentence that you could read aloud without having to stop for breath. Remember, the word 'abstract' means a summary of the main ideas with most of the detail left out.

6. **As a single sentence, what's the key impact of your research?** Here we're not looking for the outcome of an experiment. We're looking for a summary of the implications. What's it all mean? Why should other people care? What can they do with your research?

Sample Abstract

(Note: Anne submitted this actual abstract in 2009 for a CERMACS invited talk. It follows quite closely to the format described on the previous page. Use this sample as a guide. Numbers were added to indicate which "how to" is relevant.)

(1) Conjugated polymers are the principal components in emerging technologies due to their beneficial properties, including the ability to synthetically tune the optical and electronic character, their low materials cost, and their facile deposition using solution processing. (2) Recent studies have shown that the nanoscale organization in polymer films may be as important as the π-conjugation in terms of device performance. (3) Surprisingly, there have been few studies aimed at controlling these phase separation processes, in part due to the limited number of polymer architectures available. (4) Recent reports of controlled chain-growth synthesis of π-conjugated polymers using nickel and palladium catalysts have revitalized the search for new materials with specific thermodynamic and optoelectronic properties. (5) This talk will highlight our efforts towards a mechanistic understanding of these chain-growth polymerizations, their utilization in the syntheses of new π-conjugated copolymers with unique microstructures, and (6, sort of) the implications for their use in emerging technologies.

The Paper Writing Process

Stage 1

Before drafting any manuscript, you should compose an outline. I recommend going through all your old subgroup files to remind yourself of all the experiments you did. Schedule a meeting with Anne to outline the tentative paper. Come prepared with a comprehensive outline.

Stage 2

Download the appropriate journal template and begin writing. You have (at most) four rounds of revisions, where Anne provides hand-written comments on your writing. Use your judgement, then, about when the first draft is polished enough to send along. (I recommend having a senior/experienced student read your first draft and provide comments before sending to Anne.) After four rounds of revision, Anne will "take over" and finish it up. The goal is for you to improve your writing each time so that your next manuscript's first draft starts at the level where you left off. During this time, you should also be compiling the necessary supporting information file. Please see the guidelines in this manual and use the SI template and other SI files from the group as reference. Again, use your peers for feedback before sending the first drafts to Anne. **Please DO NOT use any reference manager to insert your references. Instead, use MS Word "insert" "endnote" or "insert" "cross-reference."

Stage 3

At this point, Anne is polishing the text and figures, and may request additional figures or data (i.e., experiments). The most useful thing you as an author can do at this point is help with identifying appropriate references by performing exhaustive and comprehensive searches. In addition, it is at this point that the SI file should be edited and approved by Anne and then sent out for group edit. You are responsible for incorporating the group edit changes to the SI.

Stage 4

The manuscript will go through a group edit, usually with Anne incorporating the final changes and getting ready for submission. The SI file should be finalized and ready for submission. Anne will draft the cover letter and ask you for suggested reviewers.

Stage 5

Most papers these days go through at least 1 round of revision. For your first paper, Anne will handle the revisions while sharing the information and process with you. If this is not your first paper, you will have a chance to draft the response to reviewers and revision cover letter.

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

– Abstracts/TOC Graphics –

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

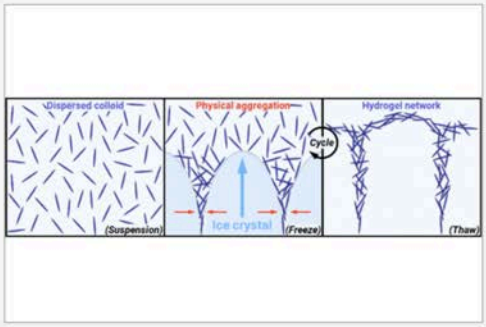
Bad TOC Graphics…

- 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

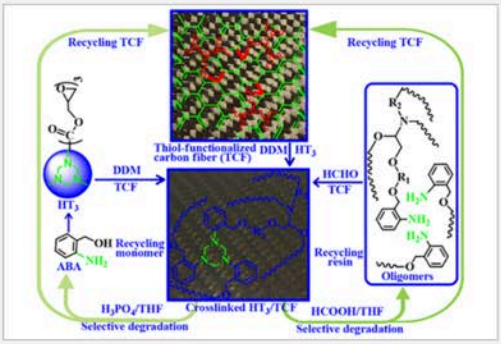
Gels are attractive for applications in drug delivery, tissue engineering, and 3D printing. Here, physical colloidal gels were prepared by freeze–thaw (FT) cycling of cellulose nanocrystal (CNC) suspensions. The aggregation of CNCs was driven by the physical confinement of CNCs between growing ice crystal 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

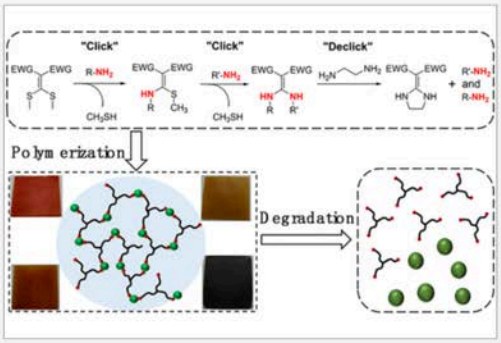
Currently, only 5% of thermoset carbon fiber reinforced polymer composites (CFRPs) are recycled into lower-value secondary products. Highly efficient closed-loop recycling of both thermoset resin and carbon fiber is a major challenge. Here, we report a sustainable approach for the closed-loop recycling 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_3) are used to prepare HT_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_3 and the precursor of cross-linked HT_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 bisvinylogous thioester conjugate acceptor under mild conditions. The resulting bisvinylogous 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 and link)

Example of a Good Introduction (communication)… (link)

- Results & Discussions -

The following information was drawn from group exercises that took place in July 2019 and December 2021. We took 5-6 recent papers 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.

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)

– Figures/Charts/Schemes –

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 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.

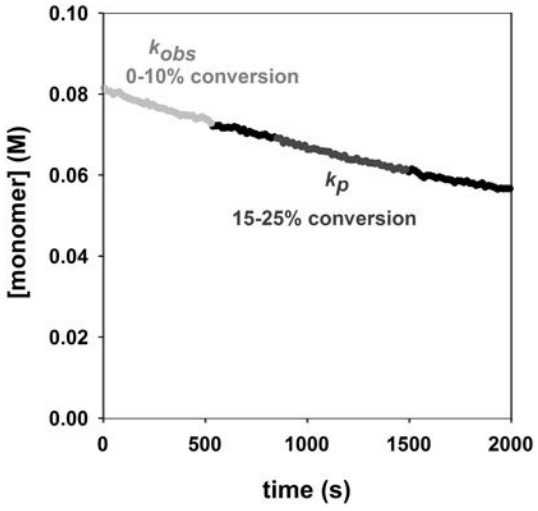
In some cases, you may want to enhance your image in Adobe Illustrator. Open and modify the original png file (before re-sizing). Illustrator enables you to add more diverse shapes (1D, 2D, 3D)/colors and you can even map your chemical structures onto 3D images.

Plot/Figure/Equation/Scheme/Chart Table Guidelines

Plots

All plots should be created in Prism or 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!

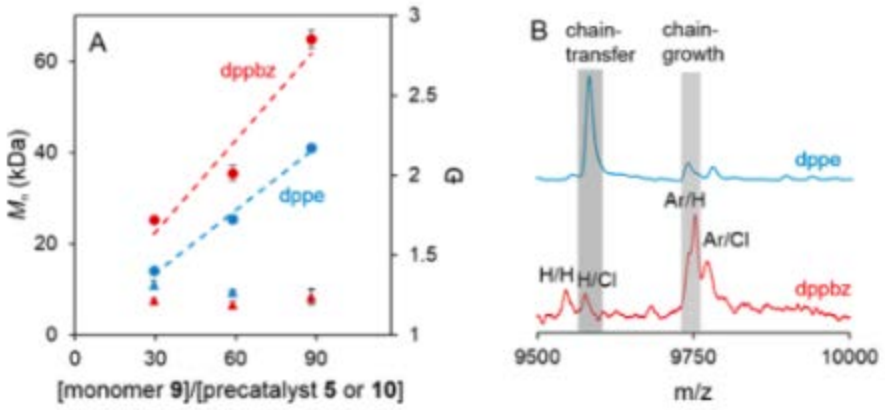
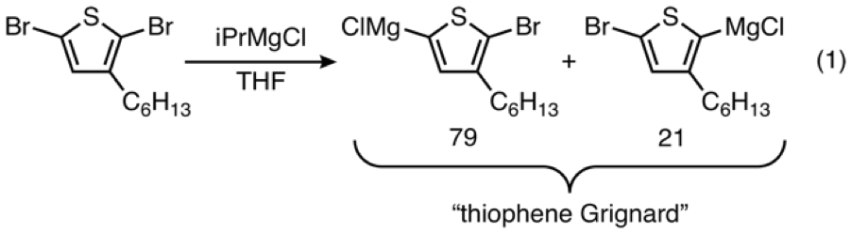


Figure 3. (A) Plot of M_n and dispersity ($Đ$) of PTz-OR versus the monomer/catalyst ratio using either precatalyst **5** (blue) or precatalyst **10** (red) and monomer **9**. (B) MALDI-TOF-MS analysis of PTz-OR obtained via either precatalyst **5** or **10** and monomer **9**.

Equations

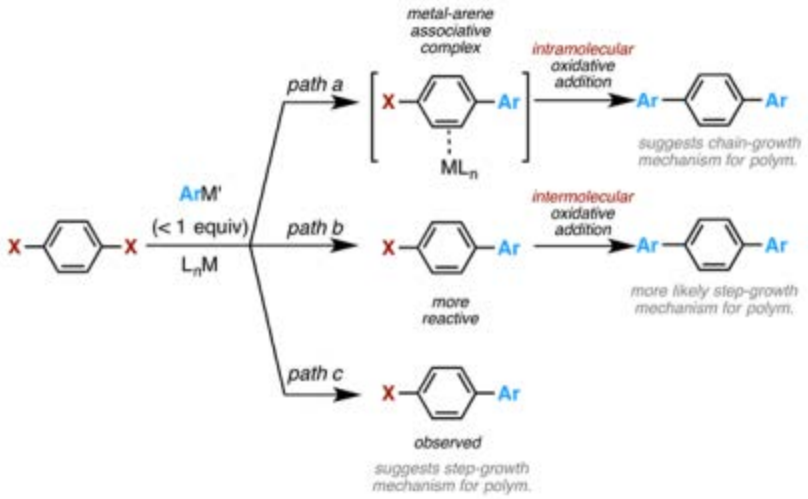
Equations usually contain either mathematical relationships or a single chemical transformation. Number them sequentially in the manuscript (hint: place the # in the chemdraw version to keep the sizing the same). Equations do not contain titles or captions.



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.

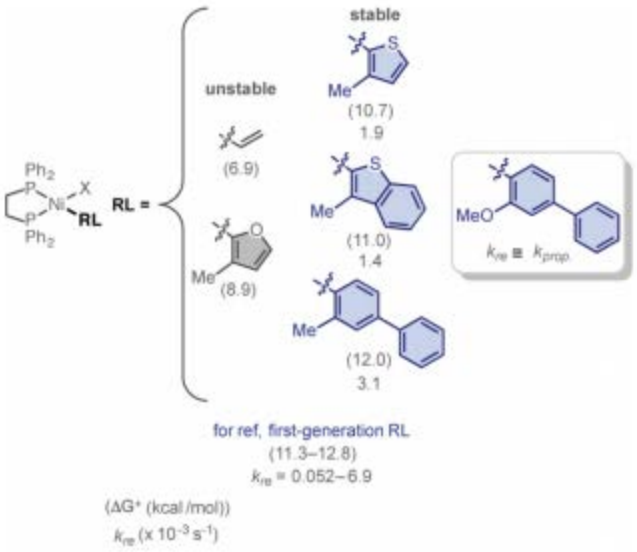
Scheme 1. Difunctionalized Products Can Be Obtained via Two Different Pathways



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 Ligands[73]



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]

	$P_{intra} : P_{inter}$			
Equiv. of **3**[b]	**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 incredibly important and one that should replicate the results you obtained as depicted exactly in your lab notebook. Every section of SI should be associated with an 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 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 ($Ni(cod)_2$) 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

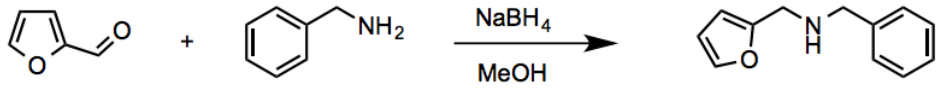
NMR Spectroscopy – ^1H and ^{13}C NMR spectra for all compounds were acquired in d_6-DMSO or D_2O on a Varian vnmr 700 operating at 700 and 176 MHz, or a Varian Inova 500 operating at 500 and 126 MHz. The chemical shift data are reported in units of δ (ppm) relative to tetramethylsilane and referenced 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.

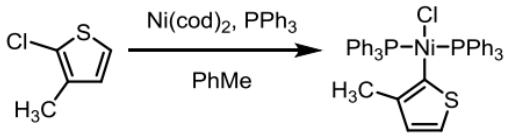
Sample Organic Experimental Procedure:



S1

***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 $C_{12}H_{14}NO^+$, 188.1070. Found, 188.1066.

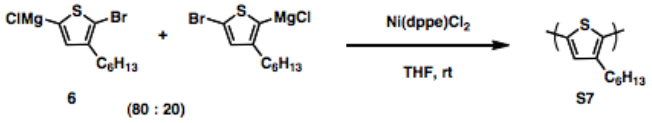
Sample Organometallics Experimental Procedure:



S1

[Bis(triphenylphosphine)](3-methylthiophene)nickel(II) chloride (S1). A 20 mL vial was equipped with a stir bar in the glovebox. Sequentially, $Ni(cod)_2$ (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 $C_{41}H_{35}ClNiP_2S$, C, 68.79; H, 4.93; Found C, 68.49; H, 4.88.

Sample Polymerization Experimental Procedure:



6 (80 : 20)

S7

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., ^{1}H, ^{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 ^{1}H 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 ^{1}H and ^{13}C), coupling constants (italicize the J), and the number of protons (based on the integration).

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

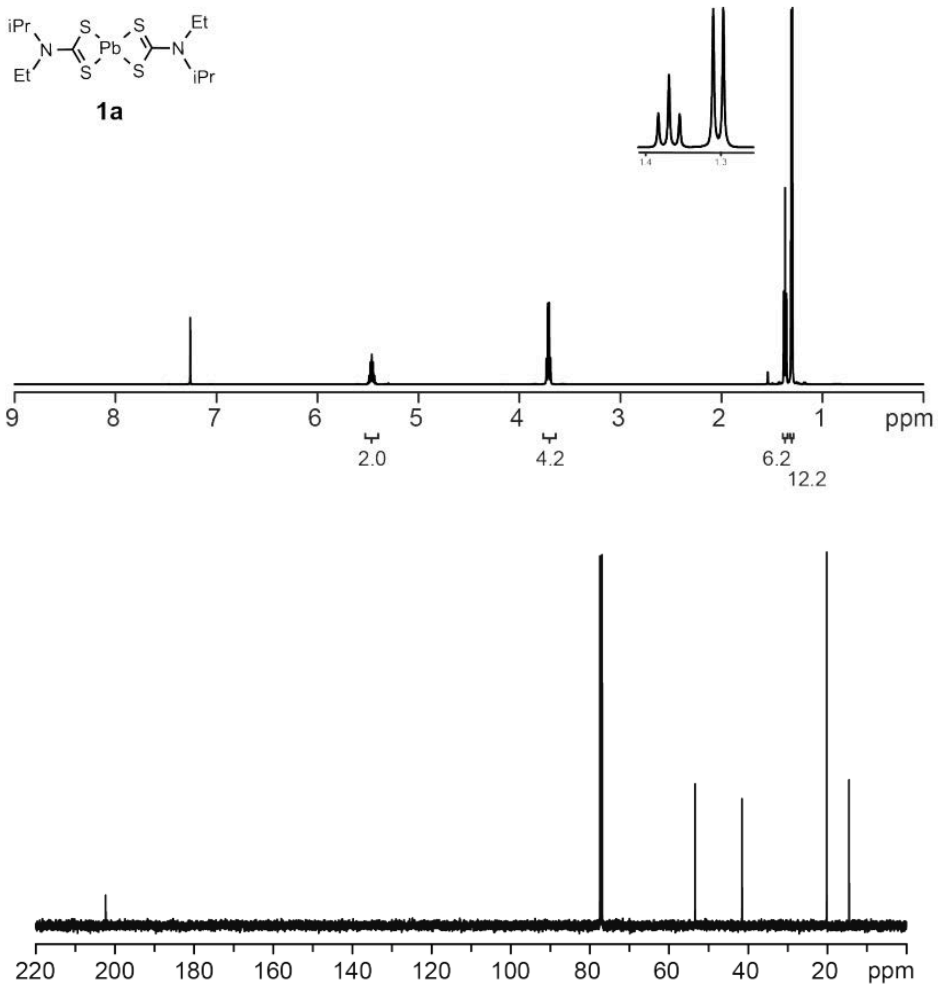


Figure S4. ^{1}H and ^{13}C NMR spectra of **1a**. ^{1}H NMR (500 MHz, $CDCl_3$) δ 5.46 (sept, *J* = 7 Hz, 2H), 3.71 (q, *J* = 7 Hz, 4H), 1.37 (t, *J* = 7 Hz, 6H), 1.30 (d, *J* = 7 Hz, 12H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 202.32, 53.41, 41.56, 20.13, 14.50.

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

Common General Formatting Mistakes/Reminders

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. Compounds that do not appear in the MS should be given an S number (e.g., Compound S1).
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.*” I prefer the “and coworkers” approach for easier attribution and retrieval of the literature.