Writing - some highlights

Abstracts

- Nature has the clearest guidelines & this almost works for all

One or two sentences providing a **basic introduction** to the field, comprehensible to a scientist in any discipline.

Two to three sentences of **more detailed background**, comprehensible to scientists in related disciplines

One sentence clearly stating the **general problem** being addressed by this particular study

One sentence summarising the main result (with the words "**here we show**" or their equivalent)

Two or three sentences explaining what the **main result** reveals in direct comparison to what was thought to be the case previously, or how the main result adds to previous knowledge.

One or two sentences to put the results into a more **general context**

Two or three sentences to provide a **broader perspective**, readily comprehensible to a scientist in any discipline, may be included in the first paragraph if the editor considers that the accessibility of the paper is significantly enhanced by their inclusion. Under these circumstances, the length of the paragraph can be up to 300 words. (The above example is 190 words without the final section, and 250 words with it).

basic introduction

more detailed background

general problem

here we show

main result

general context

broader perspective

During cell division, mitotic spindles are assembled by microtubule-based motor proteins[1, 2]. The bipolar organization of spindles is essential for proper segregation of chromosomes, and requires plus-end-directed homotetrameric motor proteins of the widely conserved kinesin-5 (BimC) family[3]. Hypotheses for bipolar spindle formation include the 'push–pull mitotic muscle' model, in which kinesin-5 and opposing motor proteins act between overlapping microtubules[2, 4, 5]. However, the precise roles of kinesin-5 during this process are unknown. Here we show that the vertebrate kinesin-5 Eg5 drives the sliding of microtubules depending on their relative orientation. We found in controlled *in vitro* assays that Eg5 has the remarkable capability of simultaneously moving at ~ 20 nm s^{-1} towards the plus-ends of each of the two microtubules it crosslinks. For anti-parallel microtubules, this results in relative sliding at ~ 40 nm s^{-1}, comparable to spindle pole separation rates *in vivo*[6]. Furthermore, we found that Eg5 can tether microtubule plus-ends, suggesting an additional microtubule-binding mode for Eg5. Our results demonstrate how members of the kinesin-5 family are likely to function in mitosis, pushing apart interpolar microtubules as well as recruiting microtubules into bundles that are subsequently polarized by relative sliding. We anticipate our assay to be a starting point for more sophisticated *in vitro* models of mitotic spindles. For example, the individual and combined action of multiple mitotic motors could be tested, including minus-end-directed motors opposing Eg5 motility. Furthermore, Eg5 inhibition is a major target of anti-cancer drug development, and a well-defined and quantitative assay for motor function will be relevant for such developments.

What tense where?

Abstract- refers to your results	Past tense
Introduction- discussing current background and facts	Present tense
Methods- what was done	Past tense
Results- what was found	Past tense
Discussion- what is significant	Past tense to summarise findings, with present
Conclusions-summarise the main findings and the major implications	Go wild
Figures and Tables	Present tense to refer to figures, tables and graphs

https://learn.canvas.net/courses/1505/pages/lesson-verb-tenses-in-scientific-writing?module_item_id=177875
http://services.unimelb.edu.au/__data/assets/pdf_file/0009/471294/Using_tenses_in_scientific_writing_Update_051112.pdf

Citations

Why? What? How many?

See Homo Citans article

Citations: how?

- Web of Science, Google Scholar, … etc
- Try a variety of search terms
- Look in the citing articles (forwards & backwards)
- Look at the full publication list of important authors
- Look beyond titles

When should you start thinking the paper you'd like to write?

A. When you first start work on a project

B. When you first get some results

C. When you have all the problems sorted out and have some final results

D. When your supervisor tells you to

So what is an outline?

- A skeleton of a paper
- A structure to agree on with your supervisor before you start writing
- A planning tool
- A way to organise your thoughts

Before we get started…

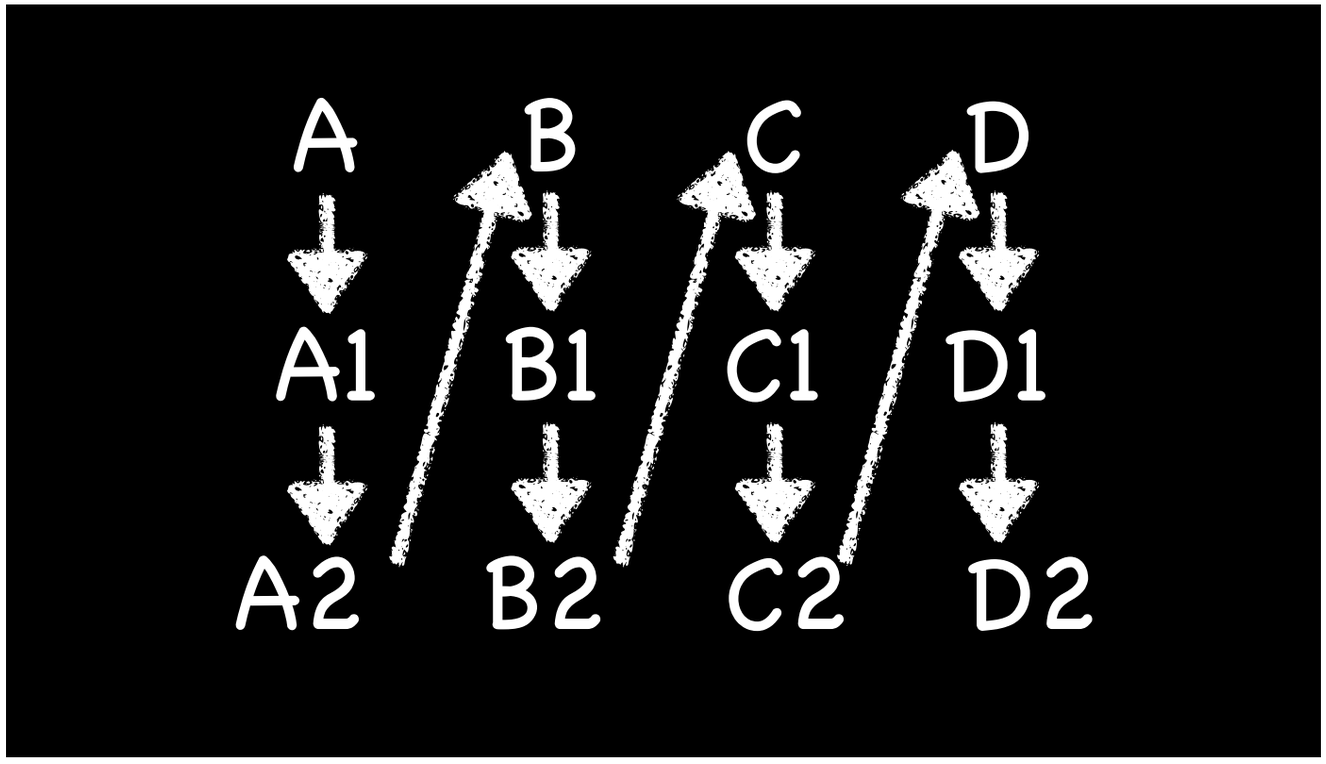
- Shouldn’t a paper be very formal?

- What about a grumpy old professor?

Why do we need scientific stories?

- You have all the pieces BUT your audience/reader comes in cold
- Research results can be extremely specialised BUT you can be speaking to a general audience
- Sometimes people need to be told WHY something is interesting
- Since we were little folks we have been listening to/reading stories and we all like a good story
- A good narrative can make it easier to hold all the important pieces together

A multi-layered story



Some Types of Scientific Stories

- Different types of stories are better suited to different types of problems

- Answer two questions:
    - What have you discovered?

    - Why is it interesting?

- Then think about what sort of narrative is effective for presenting that story.
  For example:

    - ....

Some Types of Scientific Stories

- Different types of stories are better suited to different types of problems
- Answer two questions:
    - What have you discovered?
    - Why is it interesting?
- Then think about what sort of narrative is effective for presenting that story.
  For example:
    - A historical account of discovery
    - Verification of a previous prediction
    - A surprising development going against previous intuition
    - A new class of knowledge
    - ....

A historical account of discovery

- This should be the one you're least likely to use (but you may be tempted)
- Use it when the point of the story is the history
- Otherwise, the way you came to a discovery isn't often the most effective way to explain it after the fact - generally, you were puzzled beforehand so that's not necessarily a good place to start
- A good choice for a Nobel Prize lecture... but maybe not a Masters thesis

The Conquest of Taxol

Kyriacos C. Nicolaou* and Rodney K. Guy

Much has been written about taxol, one of the newest weapons against cancer, and its producer, the Pacific Yew tree (*Taxus brevifolia*).[1] In this article, the authors give a frank and behind-the-scenes account of their encounter with this well-known molecule, which they and their collaborators faced as a synthetic target.[2–6] Once again total synthesis is found to offer excellent opportunities for developing new synthetic strategies and novel reactions. The team of chemists who took up this challenge emerged with valuable experience and confidence in their skills.

Keywords: natural products · taxol · total syntheses

1. Introduction

Rarely has a molecule received as much media attention as taxol (**1**, Fig. 1) has in recent years. Taxol and its producer, the Pacific Yew, earned their positions of public prominence after a long association between the yew and humans. By 1991 taxol was a "celebrity molecule", hailed as a miracle drug against cancer but in desperately short supply.[7, 8a] The media frenzy surrounding taxol focused daily attention on issues of life and death for cancer patients who desperately needed the drug, on the yew tree whose exclusive taxol-producing ability meant sure death for the tree, and on a rare owl species whose natural habitat was being destroyed systematically by the logging of the same forests that harbor the yew. The ethical and pragmatical dilemma that accompanied the discovery of taxol was fiercely argued by doctors, environmentalists, and politicians. The solution, they all agreed, was to find an alternative source of taxol. Chemists and biologists were challenged to find a solution. Today taxol is obtained semisynthetically from baccatin III, which is isolated from the needles of the European Yew, *Taxus baccata*.[8b]

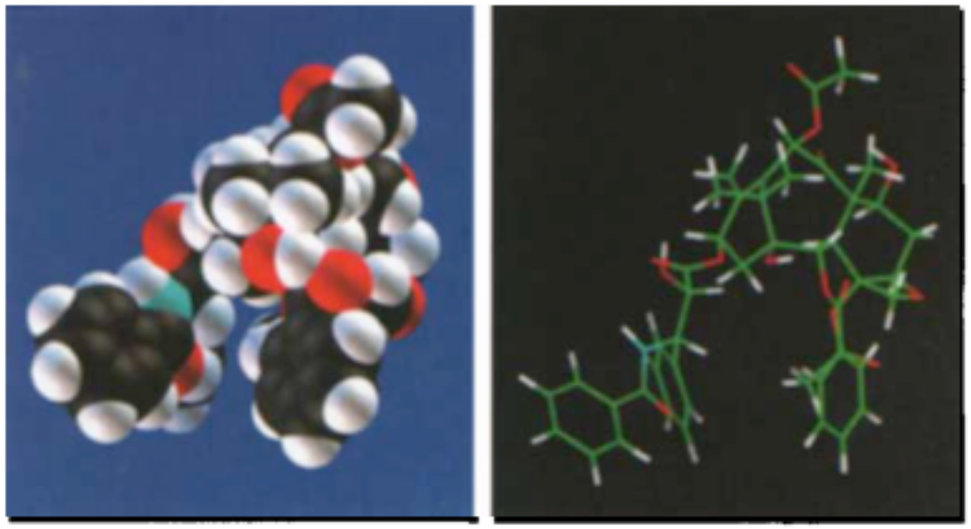
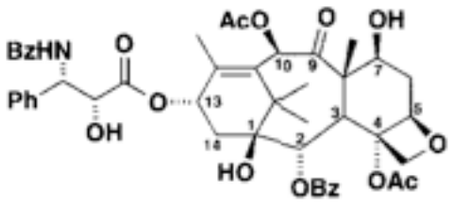


Fig. 1. Structure of taxol (**1**): top left: space-filling model, top right: stick model. The two models were generated by computer.



1

2. Embarking on the Taxol Project: The First Proposal to NIH

3. The Conquest

3.1. The Exhilarating Triumphant Moments

It was 11:00 pm on Wednesday, January 19, 1994, when the phone rang. Georgette, my wife, woke me up saying, "There's a man with an accent on the phone for you." Reluctant and very sleepy, I picked up the phone and said, "Hello?" It was Hiroaki Ueno asking me to come to the lab immediately because he wanted to talk to me. "What is it?" I said, "Can we talk tomorrow?" My thoughts started to turn to some bad accident in the lab. "No," he said, "You have to come now. It is very important, we have some news." To press me to come, Hiroaki put Jin-Jun on the line, who also insisted that I come to the lab, by saying, "We have the compound—we made taxol!" "I'll be there in five minutes," I said slamming the phone down and jumping out of bed. I put on my jogging suit and ran out the door to the car, saying to Georgette, "I have to go. They say they have some good news they finished taxol. I'll be back soon." In five minutes I was in my office looking at the spectra. The NMR spectra of synthetic and authentic intermediate **67** were identical. The synthetic and retrosynthetic sequences had been bridged! Only five already secured steps remained; our goal was only a matter of days if not hours from completion! Satisfied with what I saw, I left saying, "I'll see you tomorrow morning to discuss whatever we have to do to polish the work and write up the paper."

The next morning, I was in my office early pacing back and forth until everyone on the project arrived. Hiroaki was still in the lab when I arrived, having spent all night and morning bringing up material for a repeat of the final stages. Jin-Jun and Philippe were both away interviewing for jobs. The rest of the team, consisting of visiting professor Elias Couladouros from the University of Athens, research associates Johanne Renaud, K. Paulvannan, anad Zhen Yang, and graduate students Kip Guy, Chris Claiborne, and Erik Sorensen arrived shortly, and we decided that they would press around-the-clock until all intermediates leading to taxol were finally characterized and the final sequence was repeated; I was to immediately start working on preparing the manuscript. By the afternoon of Friday, January 21, 1994, the manuscript on the total synthesis of taxol was dispatched to *Nature*. Our paper was accepted, after peer review, on Monday, January 31, 1994, and scheduled to be published on Thursday, February 17, 1994.

Verification of a previous prediction

- In this case, the objective can be stated very simply, and is generally known at the outset of the project
- What was predicted?
- Why was it hard to verify?
- What have you done?

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Observation of Top Quark Production in $\overline{p}p$ Collisions with the Collider Detector at Fermilab

A different kind of collaboration

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(Received 24 February 1995)

A surprising development going against previous intuition

- Can be constructed to provide a nice narrative for explaining to a general audience why a result is surprising

    - What was the previous intuition?
    - Why should your system follow this?
    - What happens instead?
    - Rebuilding intuition

J|A|C|S
COMMUNICATIONS

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When Things Are Not as They Seem: Quantum Interference Turns Molecular Electron Transfer "Rules" Upside Down

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In the last half-century, understanding of molecular electron transfer[4] has advanced significantly. From this body of knowledge, three "rules of thumb" for trends in rates of electron transfer can be deduced: (1) Increasing molecular length leads to decreasing rate. (2) Transport through a fully conjugated bridge is greater than through a saturated bridge. (3) A larger energy difference between the donor and acceptor energy levels and the bridge levels leads to decreased electron transfer rates. These rules of thumb are not universal; however, significant deviations are not widespread and provide insight into novel phenomena.

Figure 2. The molecular orbital eigenenergies for the isolated molecules (left) show the large band gap typical in the saturated system and the much smaller gap in the conjugated systems. The gold Fermi energy is shown for comparison. The HOMO and LUMO of the short/long system (right) show delocalization across all three arms, giving no indication that there should be any difference between the different paths beyond their differing length.

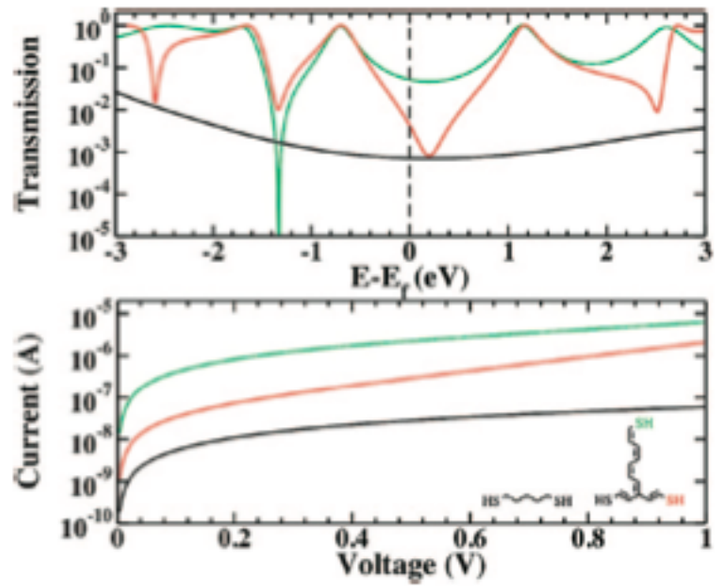

Figure 3. The transmission (above) and current (below) through the long system (green), short system (red), and dtp (black). The dramatic differences between the long system and the short system cannot be predicted from conventional understanding of molecular electron transfer.

- We never set out to challenge the "rules of thumb".
- We were looking for interference effects for other reasons.
- We made this short paper when we realised that the results we were sitting on also challenged conventional wisdom in the field.

A new class of knowledge

- This could be a new experimental technique, reaction or new phenomenon.

- It is very difficult a first paper to capture what will develop as the important implications

Tunneling through a controllable vacuum gap

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(Received 30 September 1981; accepted for publication 4 November 1981)

We report on the first successful tunneling experiment with an externally and reproducibly adjustable vacuum gap. The observation of vacuum tunneling is established by the exponential dependence of the tunneling resistance on the width of the gap. The experimental setup allows for simultaneous investigation and treatment of the tunnel electrode surfaces.

PACS numbers: 73.40.Gk

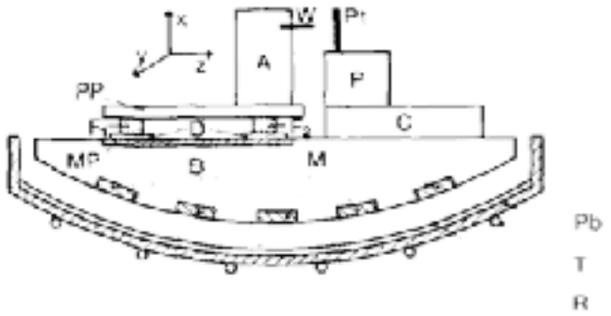


FIG. 1. Schematic of the tunneling unit and magnetic levitation system. Components and operation are described in the text. Liquid-He circulating in the tubes T cools the lead bowl Pb, which is thermally shielded by Al-coated mylar foils (not shown).

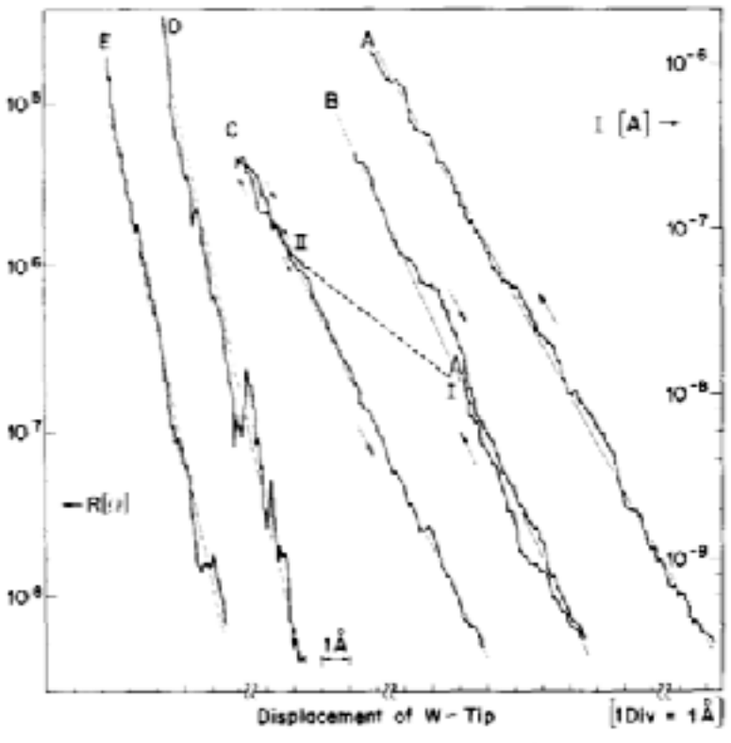
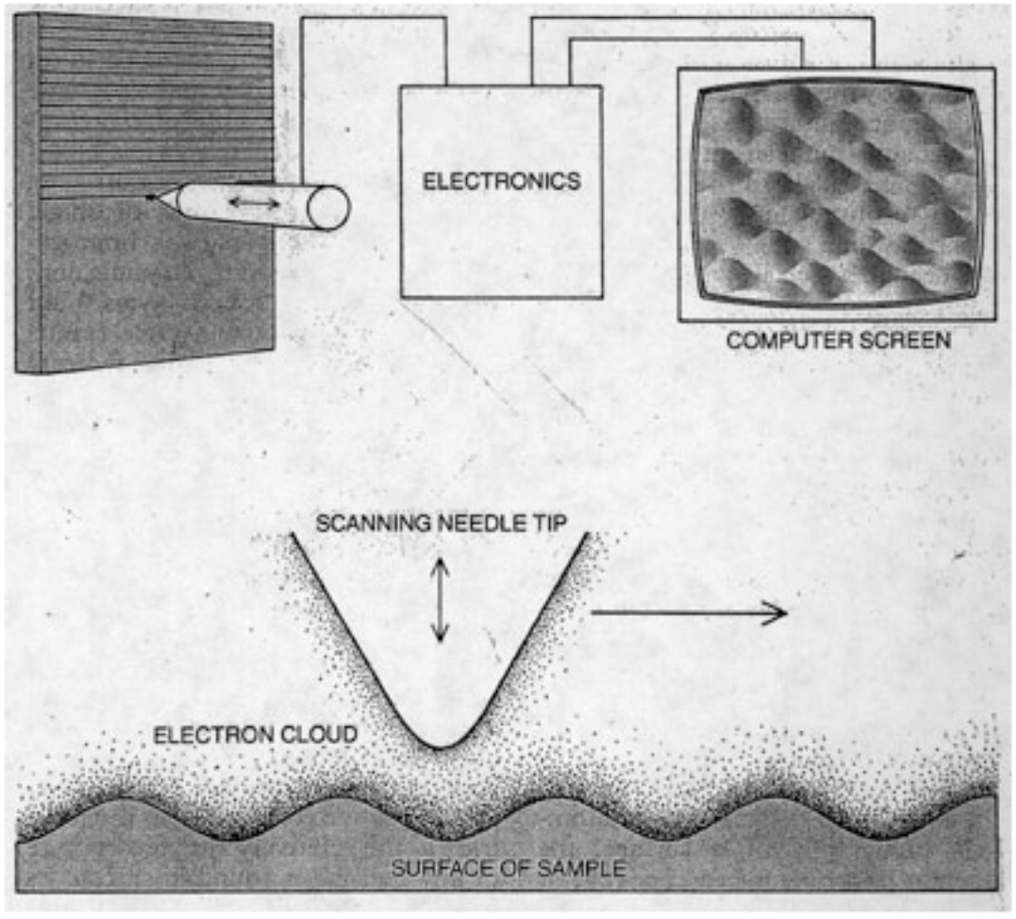


FIG. 2. Tunnel resistance and current vs displacement of Pt plate for different surface conditions as described in the text. The displacement origin is arbitrary for each curve (except for curves B and C with the same origin). The sweep rate was approximately 1 Å/s. Work functions $\phi = 0.6$ eV and 0.7 eV are derived from curves A, B, and C, respectively. The instability which occurred while scanning B and resulted in a jump from point I to II is attributed to the release of thermal stress in the unit. After this, the tunnel unit remained stable within 0.2 Å as shown by curve C. After repeated cleaning and in slightly better vacuum, the steepness of curves D and E resulted in $\phi = 3.2$ eV.



Stories Summary

- When you have pieces of your research in place, think very carefully about the most effective story to communicate them.

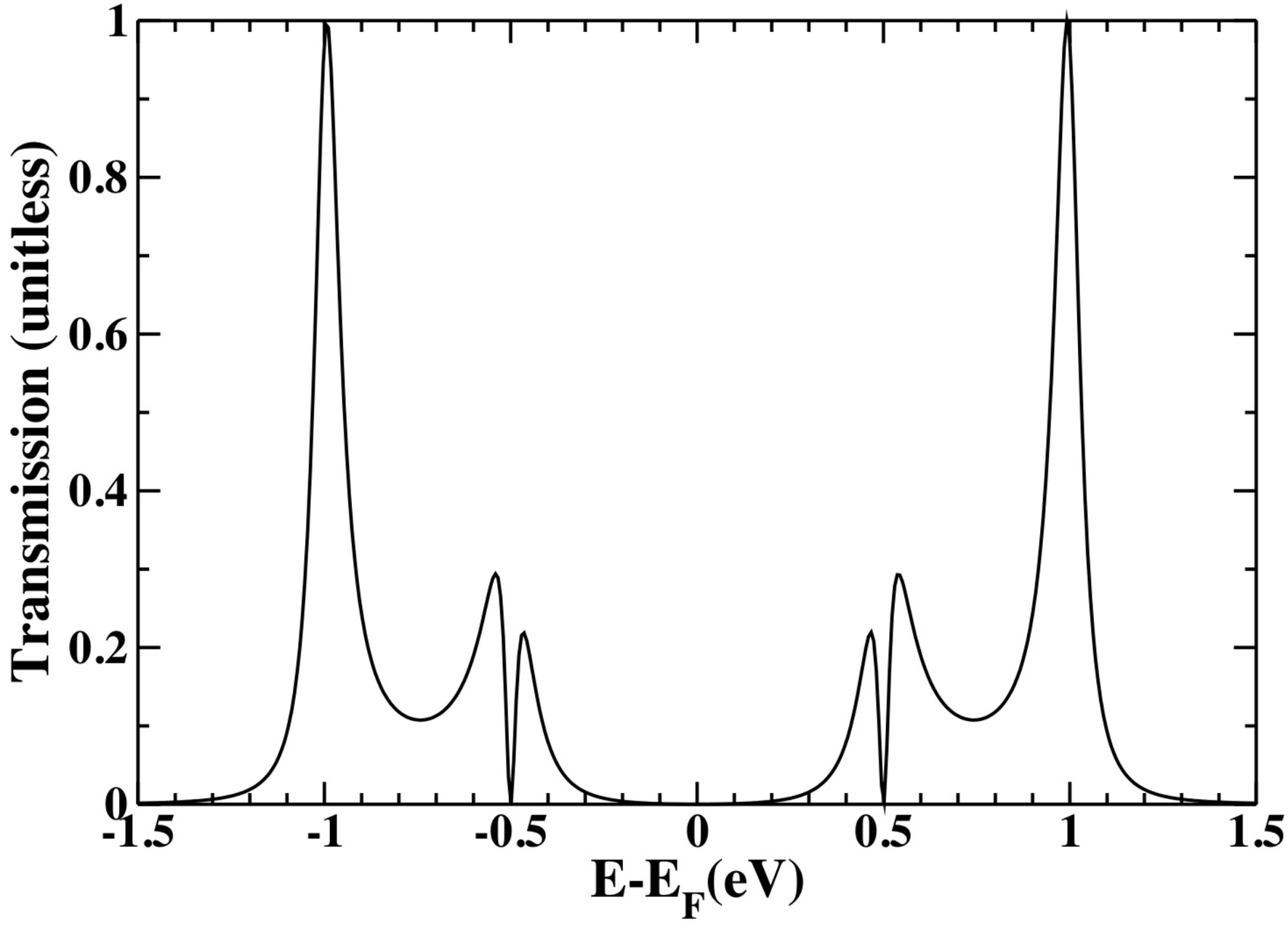
- The story may be the same one you would have imagined at the start of the project, but it also may be completely different.

- The right story will make it easier for both you and your reader/audience.

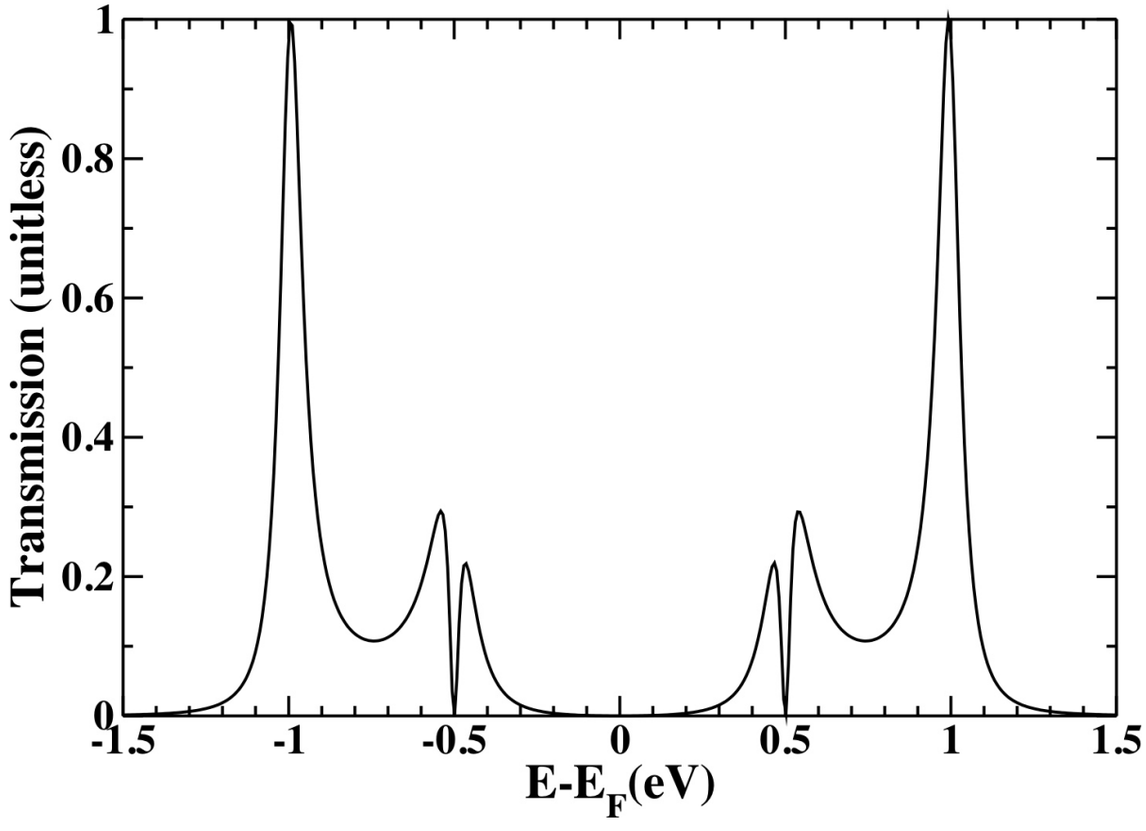
- Enjoy telling your stories!

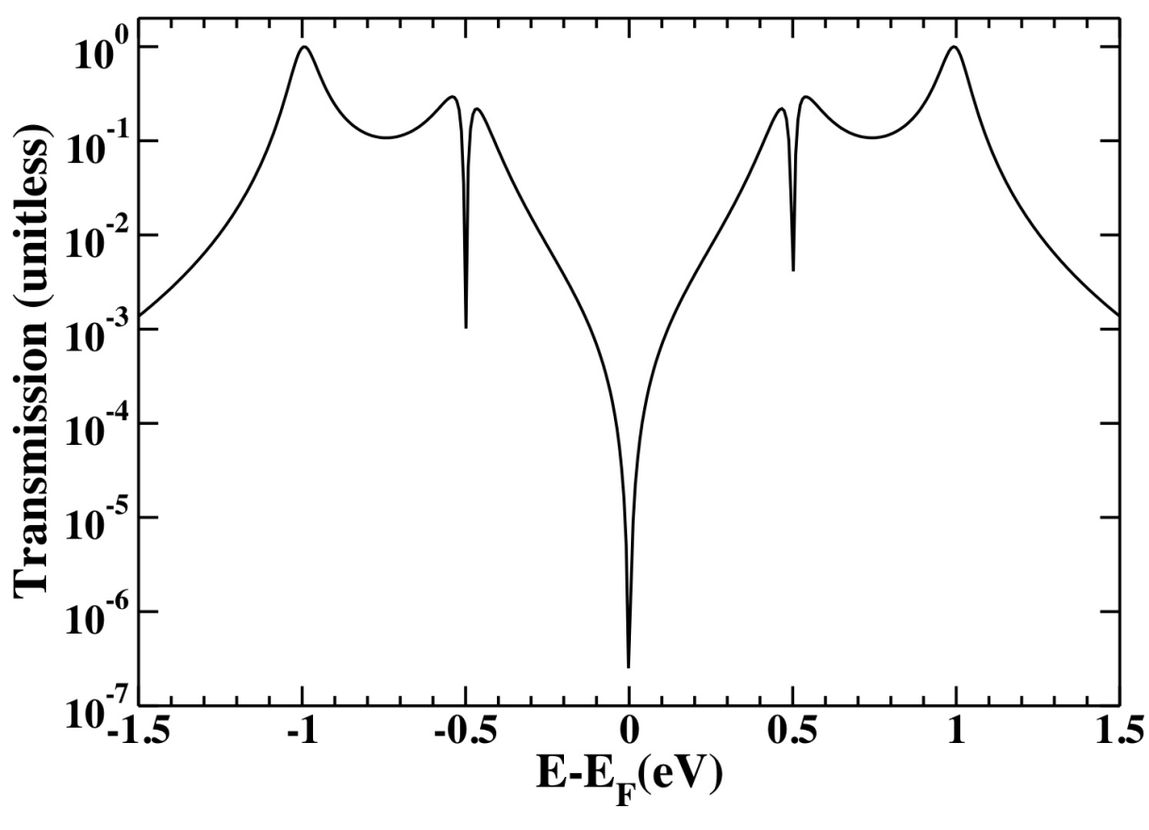
Graphs

I want to make a graph....



Linear or Log.





Errors & Lines of best fit

- Experimental data has error/uncertainty
- Part of accurate reporting of results is accurate reporting of uncertainty
- There are different kinds of error bars (see error bars article)

An Example

JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

ARTICLE

pubs.acs.org/JACS

Evidence for Quantum Interference in SAMs of Arylethynylene Thiolates in Tunneling Junctions with Eutectic Ga—In (EGaIn) Top-Contacts

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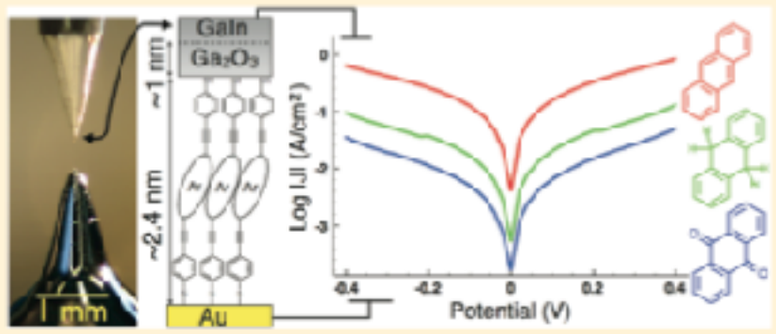
Supporting Information

ABSTRACT: This paper compares the current density (J) versus applied bias (V) of self-assembled monolayers (SAMs) of three different ethynyl-thiophenol-functionalized anthracene derivatives of approximately the same thickness with linear conjugation (AC), cross-conjugation (AQ), and broken-conjugation (AH) using liquid eutectic Ga—In (EGaIn) supporting a native skin (~1 nm thick) of Ga_2O_3 as a nondamaging, conformal top-contact. This skin imparts non-Newtonian rheological properties that distinguish EGaIn from other top-contacts; however, it may also have limited the maximum values of J observed for AC. The measured values of J for AH and AQ are not significantly different ($J \approx 10^{-1}$ A/cm^2 at $V = 0.4$ V). For AC, however, J is 1 (using log averages) or 2 (using Gaussian fits) orders of magnitude higher than for AH and AQ. These values are in good qualitative agreement with gDFTB calculations on single AC, AQ, and AH molecules chemisorbed between Au contacts that predict currents, I, that are 2 orders of magnitude higher for AC than for AH at $0 < |V| < 0.4$ V. The calculations predict a higher value of I for AQ than for AH; however, the magnitude is highly dependent on the position of the Fermi energy, which cannot be calculated precisely. In this sense, the theoretical predictions and experimental conclusions agree that linearly conjugated AC is significantly more conductive than either cross-conjugated AQ or broken conjugate AH and that AQ and AH cannot necessarily be easily differentiated from each other. These observations are ascribed to quantum interference effects. The agreement between the theoretical predictions on single molecules and the measurements on SAMs suggest that molecule—molecule interactions do not play a significant role in the transport properties of AC, AQ, and AH.



Distinguishing data

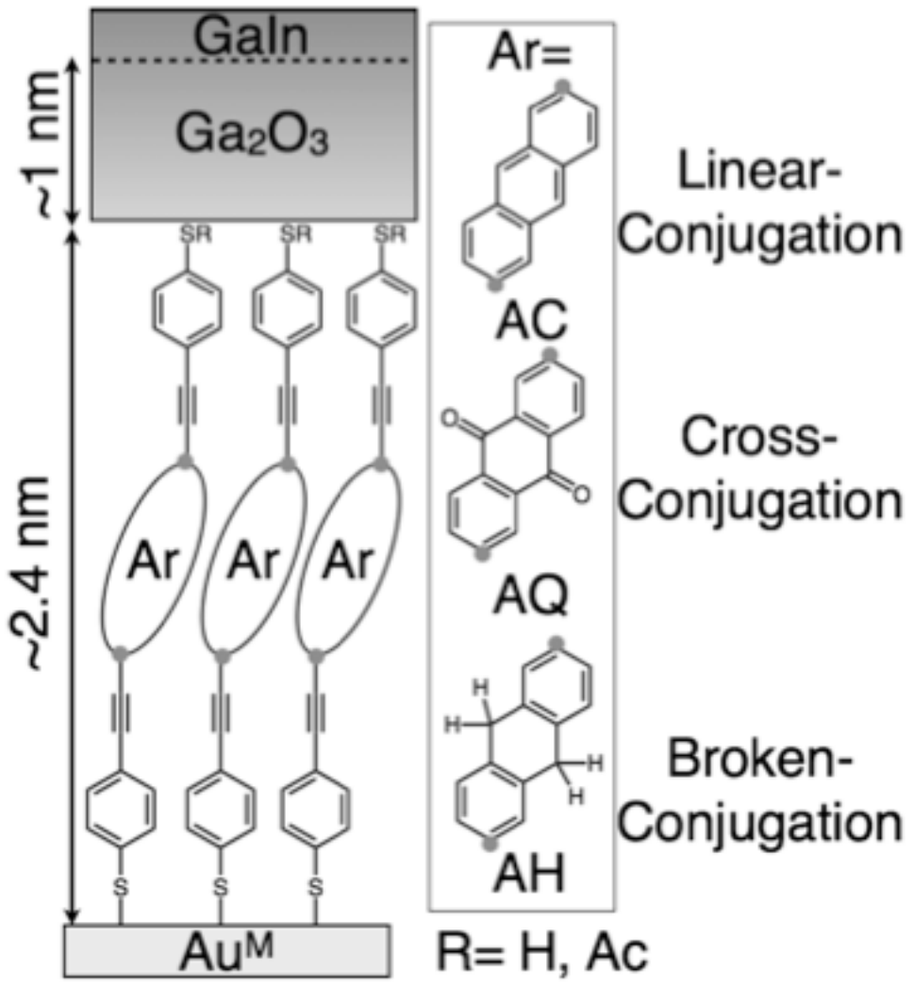


Figure 1. Schematic of the tunneling junctions (not to scale) of gold-on-mica supporting SAMs of thiolated arylethynylenes with cores of anthracene (AC; linear-conjugation), 9,10-anthraquinone (AQ; cross-conjugation), or 9,10-dihydroanthracene (AH; broken-conjugation) connected at the 2,6 positions (indicated with gray circles). The thiolate groups at the GaIn|Ga_2O_3 interface comprise a random mixture of free thiols and thioacetates.

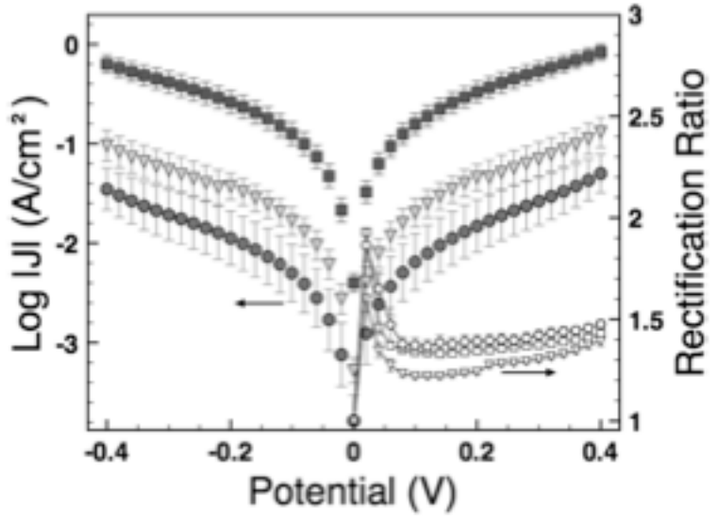


Figure 2. Left axis: plots of the geometric mean of $\log|J|$ versus V for AC (■), AQ (●), AH (▼). Error bars represent the standard error. Right axis: plots of the rectification ratios for AC (□), AQ (○), and AH (▽) versus $|V|$ computed from the arithmetic mean of $J(+V)/J(-V)$ for each trace. Error bars are computed from the standard error, SEM. These data show that AC (linear-conjugation) is at least 1 order of magnitude more conductive than AH (broken-conjugation) and AQ (cross-conjugation) while AH is slightly more conductive than AQ, though in some places the error bars overlap and thus we cannot conclude that they differ significantly from each other.

Clear conclusions can be difficult

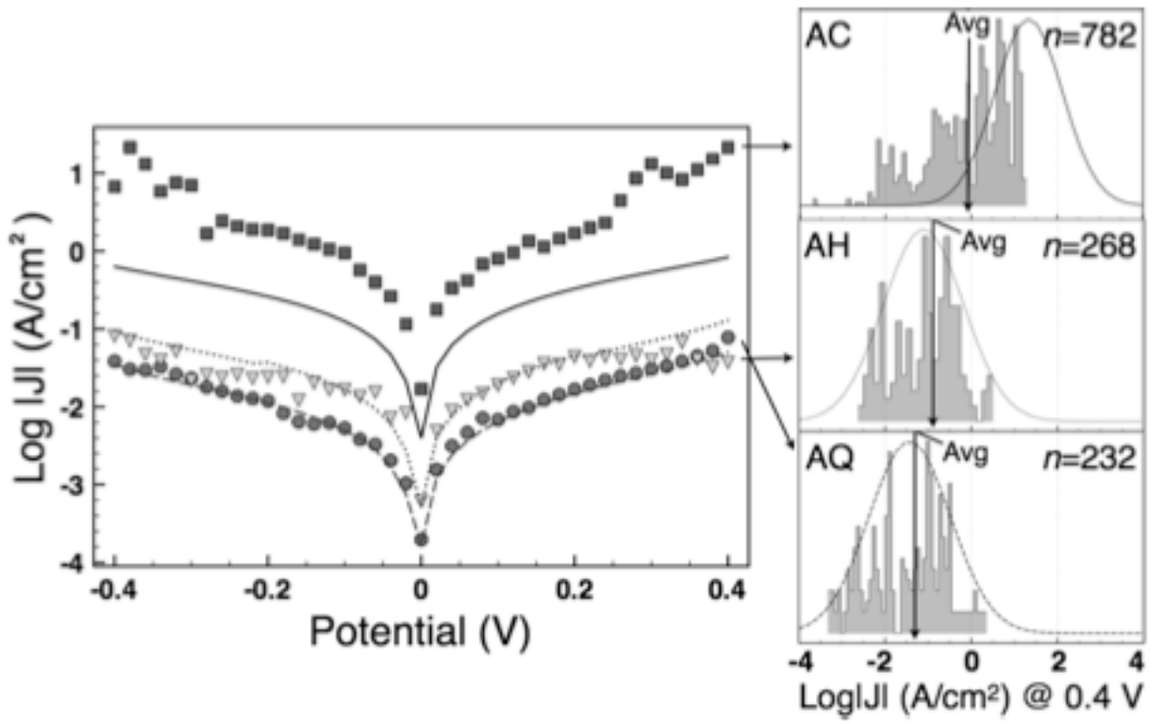


Figure 3. Left: plots of the geometric mean (lines) and Gaussian ($\mu_{\log}$) mean (symbols) of $\log|J|$ versus V for AC (solid line; ■), AH (dotted line; ▼), and AQ (dashed line; ●). Right: plots of the normalized histograms of $\log|J|$ at 0.4 V and the Gaussian fits for AC (top; solid line), AH (center; dotted line), and AQ (bottom; dashed line). The value of the geometric mean of $\log|J|$ is indicated with a solid arrow, and n is the total number of traces. These data reveal no appreciable difference between the geometric and Gaussian means for AH and AQ and clearly show that we cannot make a meaningful distinction between AH and AQ. The data for AC, however, form a truncated Gaussian distribution such that the Gaussian mean is more than an order or magnitude higher than the geometric mean. In either case, AC is clearly more conductive than either AH or AQ.

Summary: Making Graphs

- ALWAYS label axis - NO EXCEPTIONS
- Scale or cut axis to provide the clearest presentation of the important aspects of the data
- Use legends AND describe in figure captions
- Use error bars AND say what kind of error it is
- Don’t “connect the dots” - use a line of best fit
- Make sure fonts are readable
- Consider using insets for chemical structures or a different perspective

Graphs Exercise

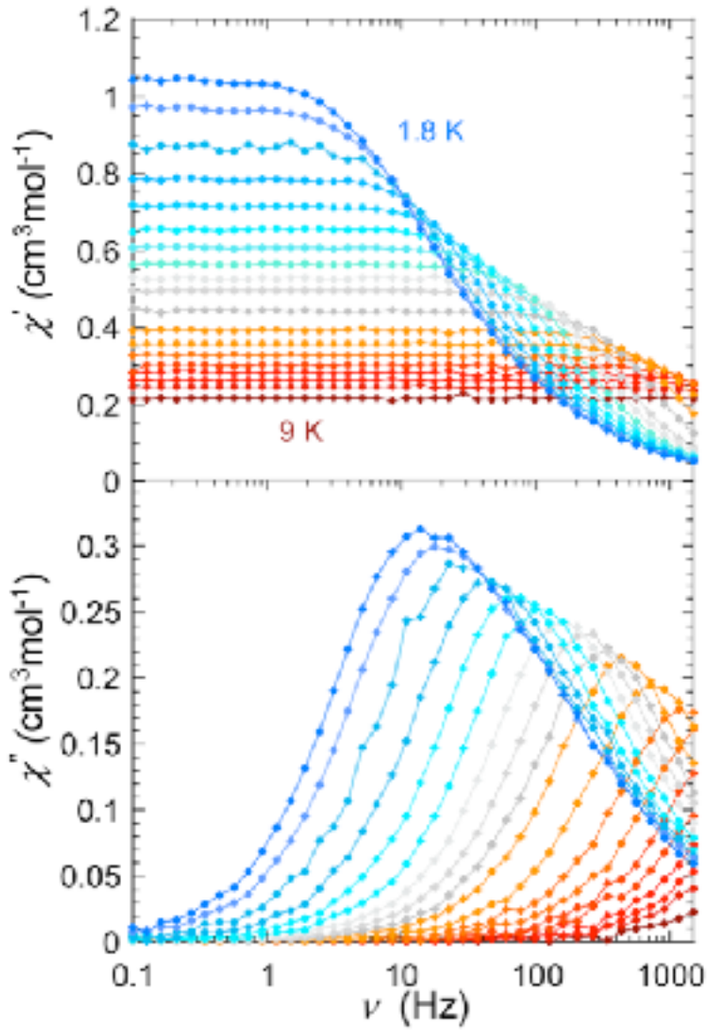


Figure 5. Frequency dependence of the in-phase (top) and out-of-phase (bottom) susceptibility between 1.8 and 9 K under a 600 Oe applied dc field.

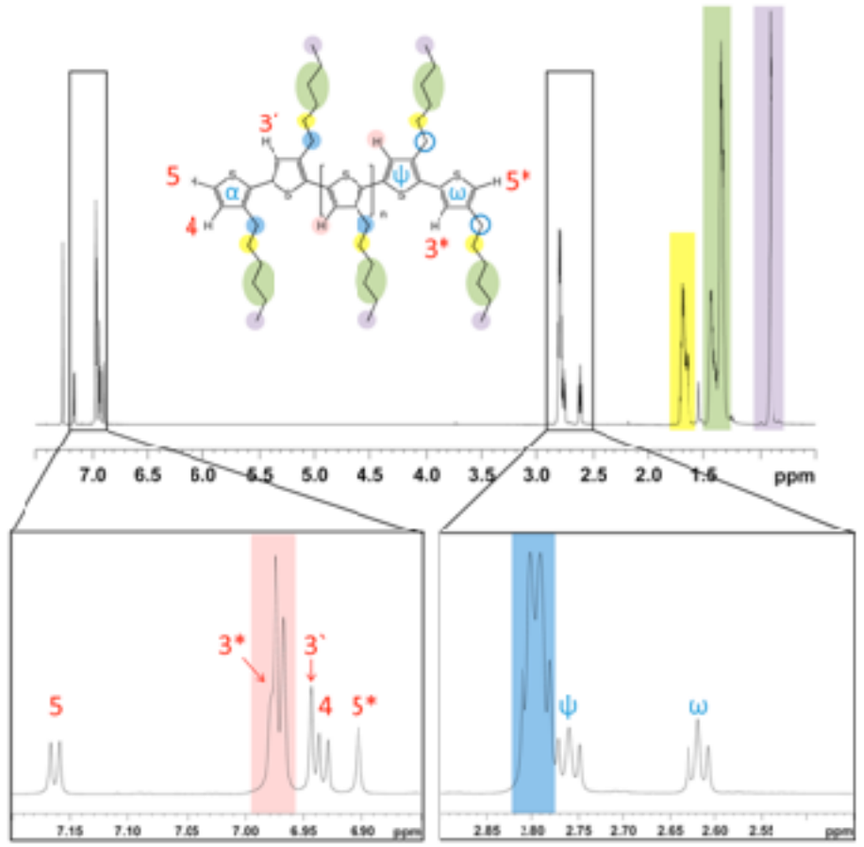


Figure 3. Assignment of the signals in the ^{1}H NMR spectrum (700 MHz, $CDCl_3$) of $(3HT')_8$, indicating high isomeric purity.

- For each graph comment on:
  - What is good?
  - What is bad?
  - Anything missing?
  - Anything you'd change?

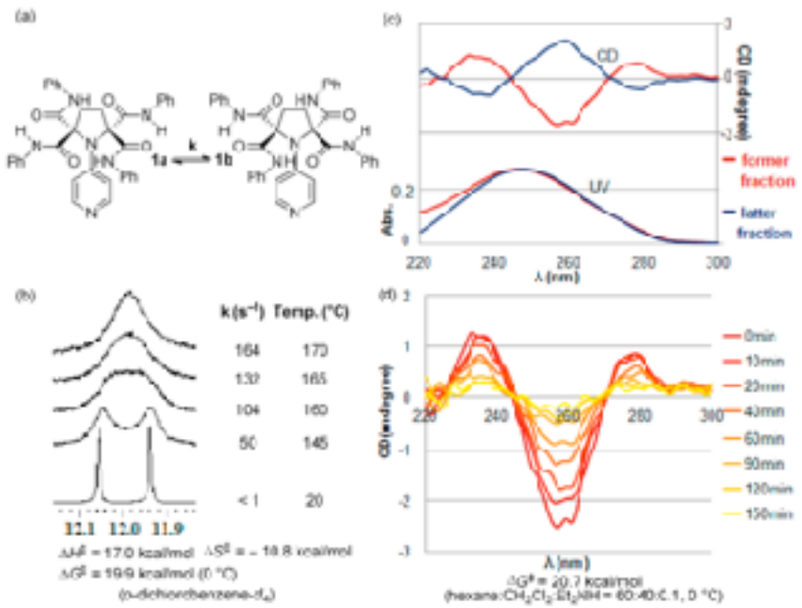
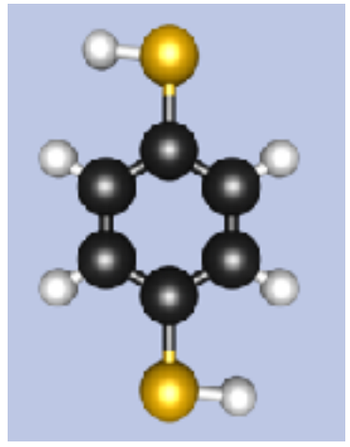


Figure 3. Analysis of the racemization barrier of **1**. (a) Interconversion of the enantiomers of **1** through rotation of the amide moieties. (b) Coalescence of the amide protons observed in a VT NMR study in *o*-dichlorobenzene-d_4. (c) CD spectra of both enantiomers in hexane:CH_2Cl_2:Et_2NH (60:40:0.1). (d) A trace of racemization was observed based on the CD spectra.

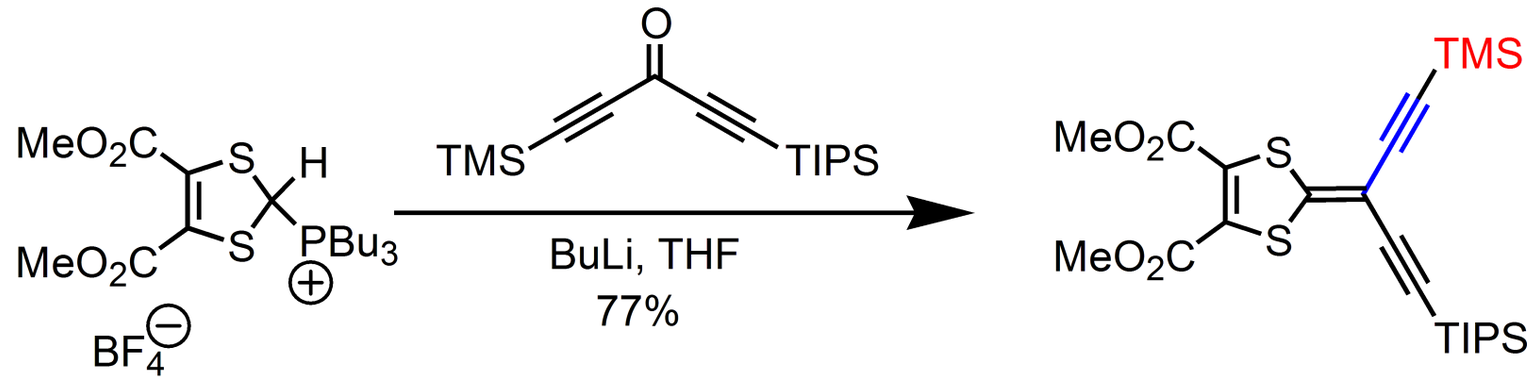
Molecules

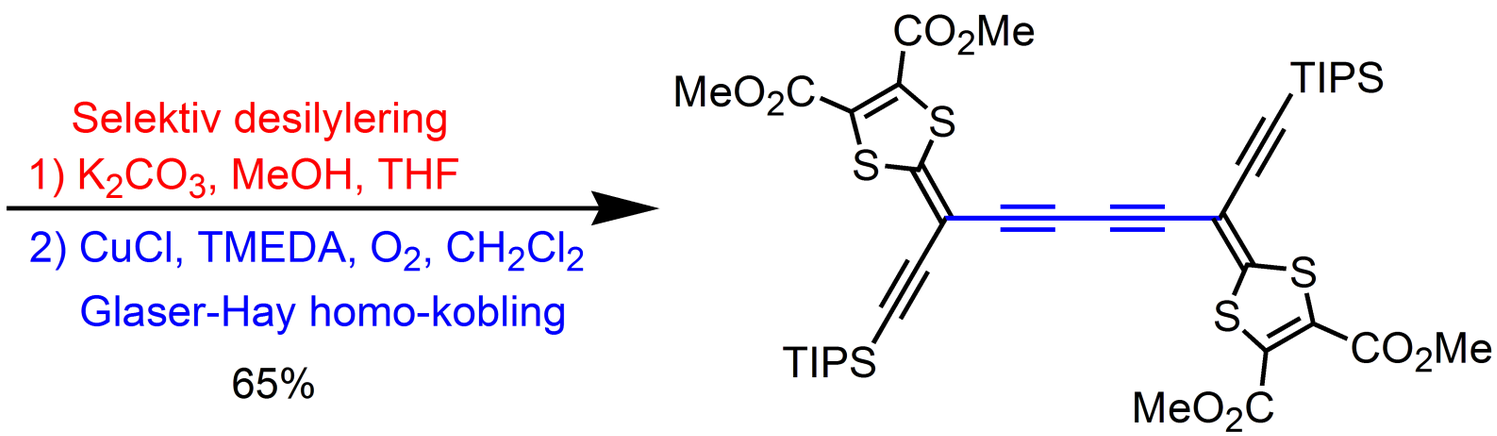
ChemDraw vs. Space Filling



- Think about what aspects you need to emphasise
- Consider your audience - a chemist can be frustrated by space filling alone, a physicist might not understand chemdraw
- Consider using both!

ChemDraw tips



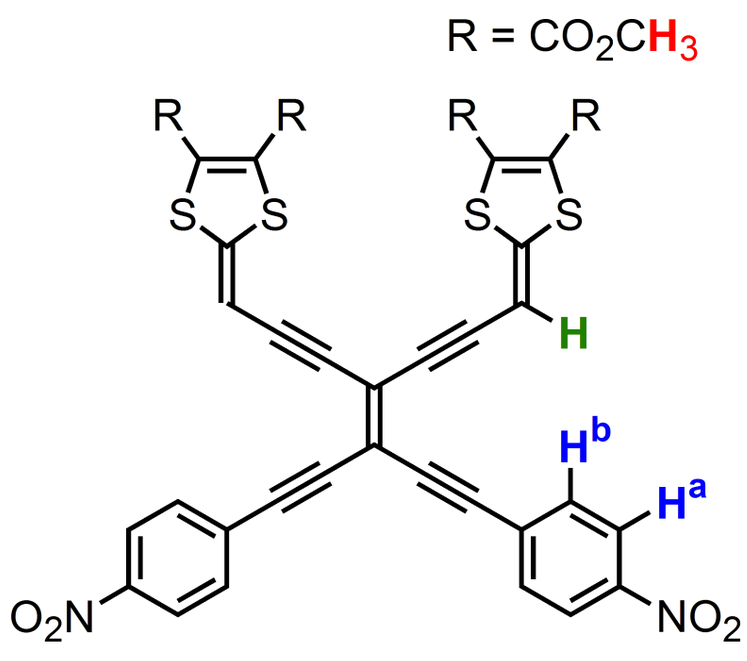


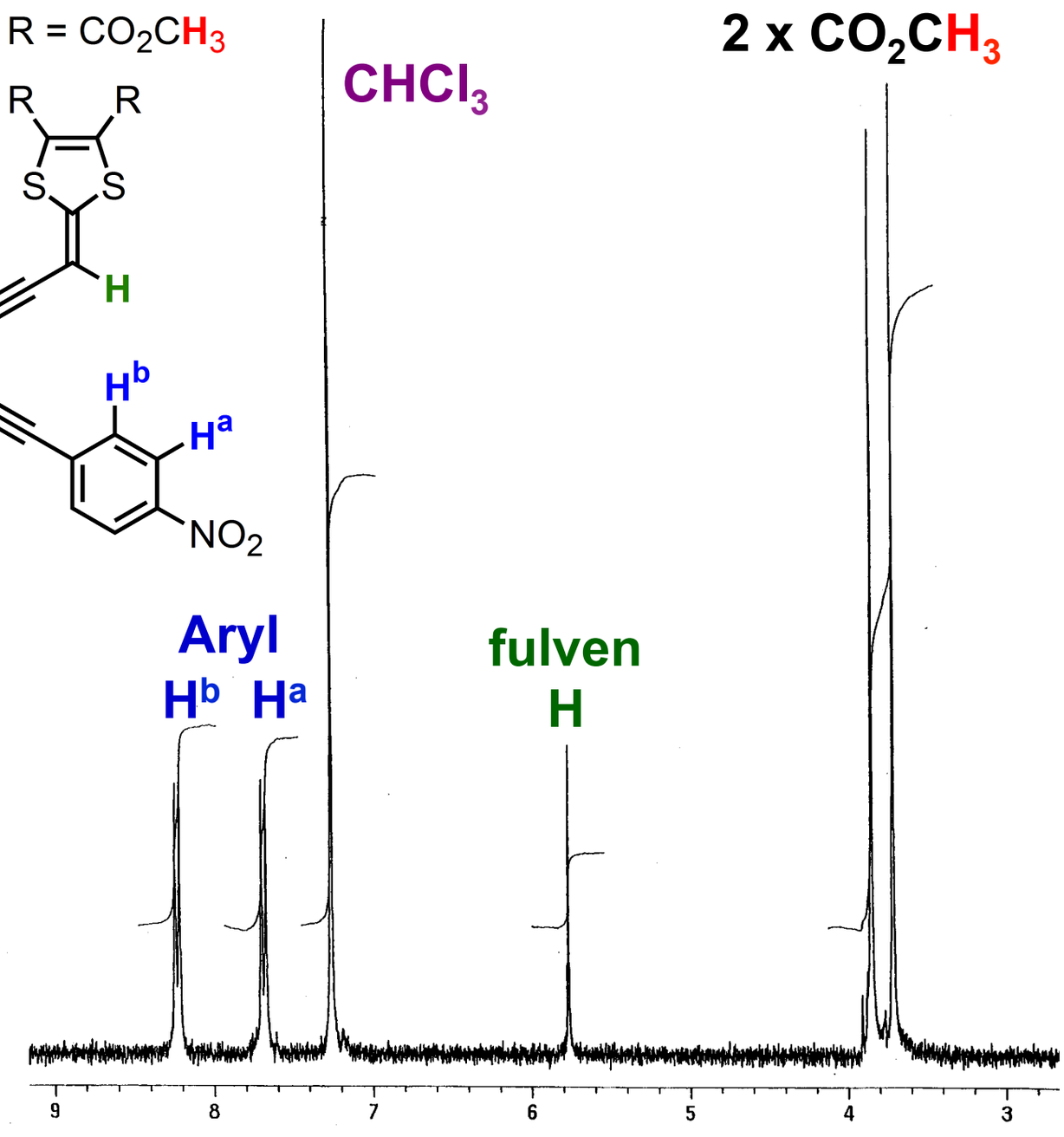
TMS = $SiMe_3$

TIPS = $Si(i\text{-}Pr)_3$

TMEDA = $Me_2NCH_2CH_2NMe_2$

Spectra (NMR, MS, etc)





Powerpoint science

J|A|C|S
ARTICLES
Published on Web 03/15/2007

Influence of Defects on the Electrical Characteristics of Mercury-Drop Junctions: Self-Assembled Monolayers of *n*-Alkanethiolates on Rough and Smooth Silver

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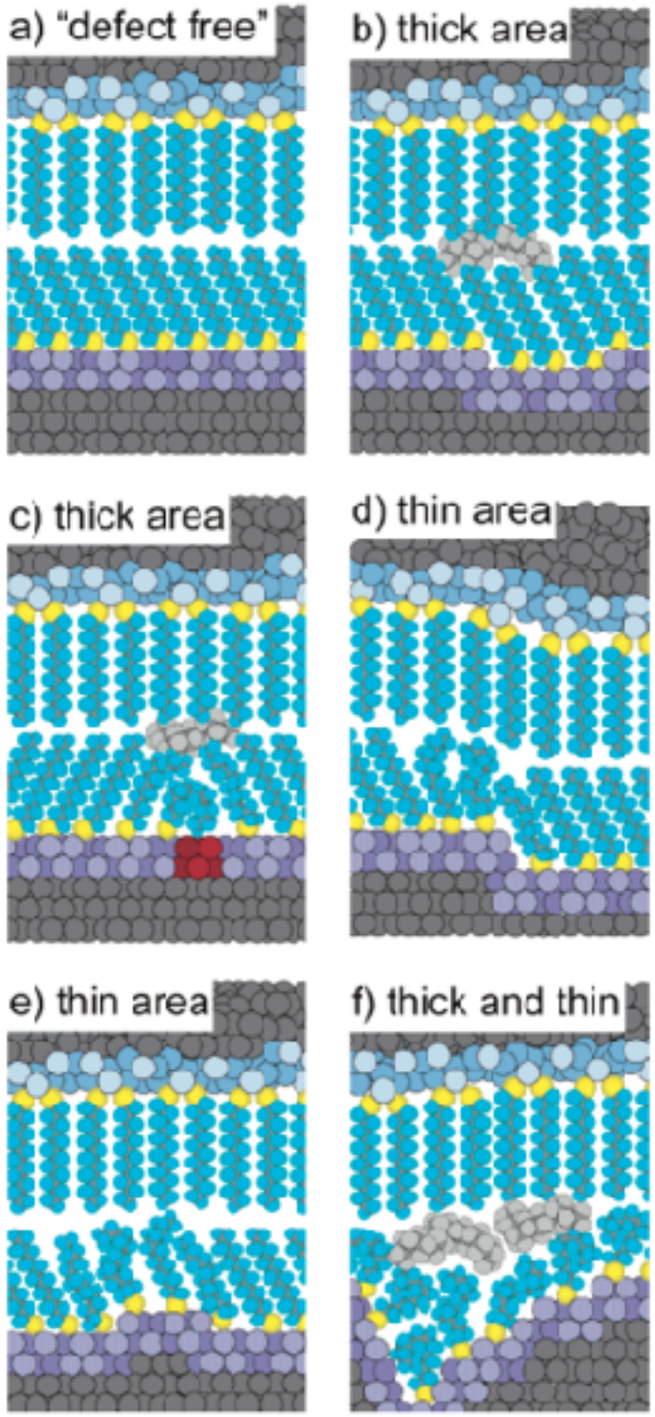
Two sandwiched monolayers



- We generally think in “defect-free” terms
- If defects dominate the properties, defect-free thinking can lead you astray
- Try not to let that influence your hypotheses
- Try not to let this thinking pollute your explanations, unless it is provable.