Social media and science

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SOCIAL MEDIA EXPLAINED

TWITTER I'M EATING A # DONUT

FACEBOOK I LIKE PONUTS

FOURSQUEE THIS IS WHERE I EAT DONUTS

INSTAGRAM HERE'S A VINTAGE PHOTO OF MY PONUT

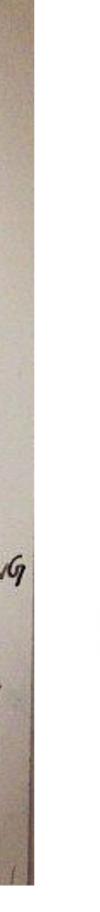
YOU TUBE HERE I AM EATING A DON'T

LINKED IN MY SKILLS INCLUDE DONUT EATING

PINTEREST HERE'S A PONUT RECIPE

LAST FM NOW LISTENING TO "DON UTS"

- I'M A GOOGLE EMPLOYER WHO EATS DONUTS.





SCIENTISTS AND THE

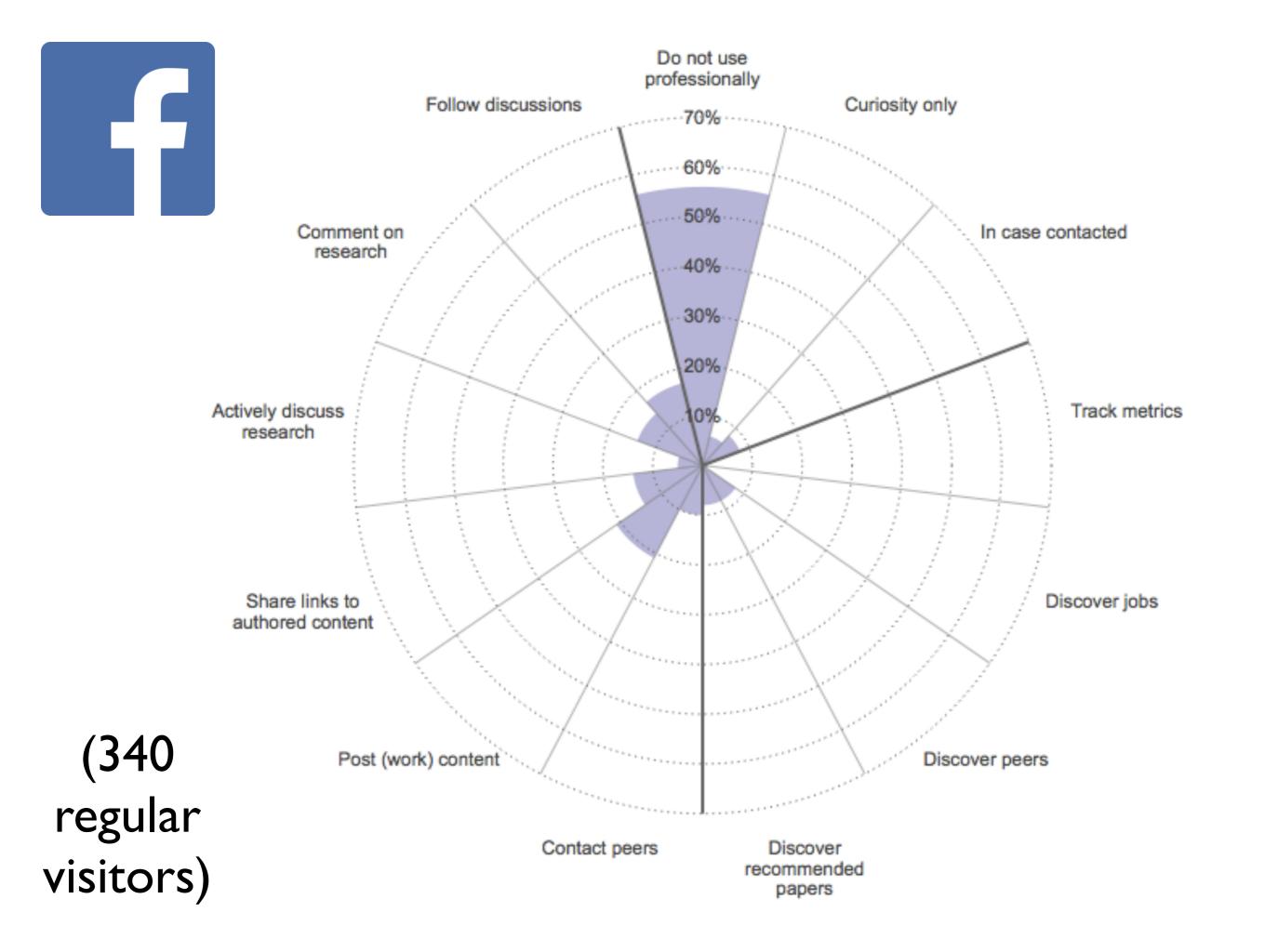
Giant academic social networks have taken off to a degree that no one expected even a few years ago.

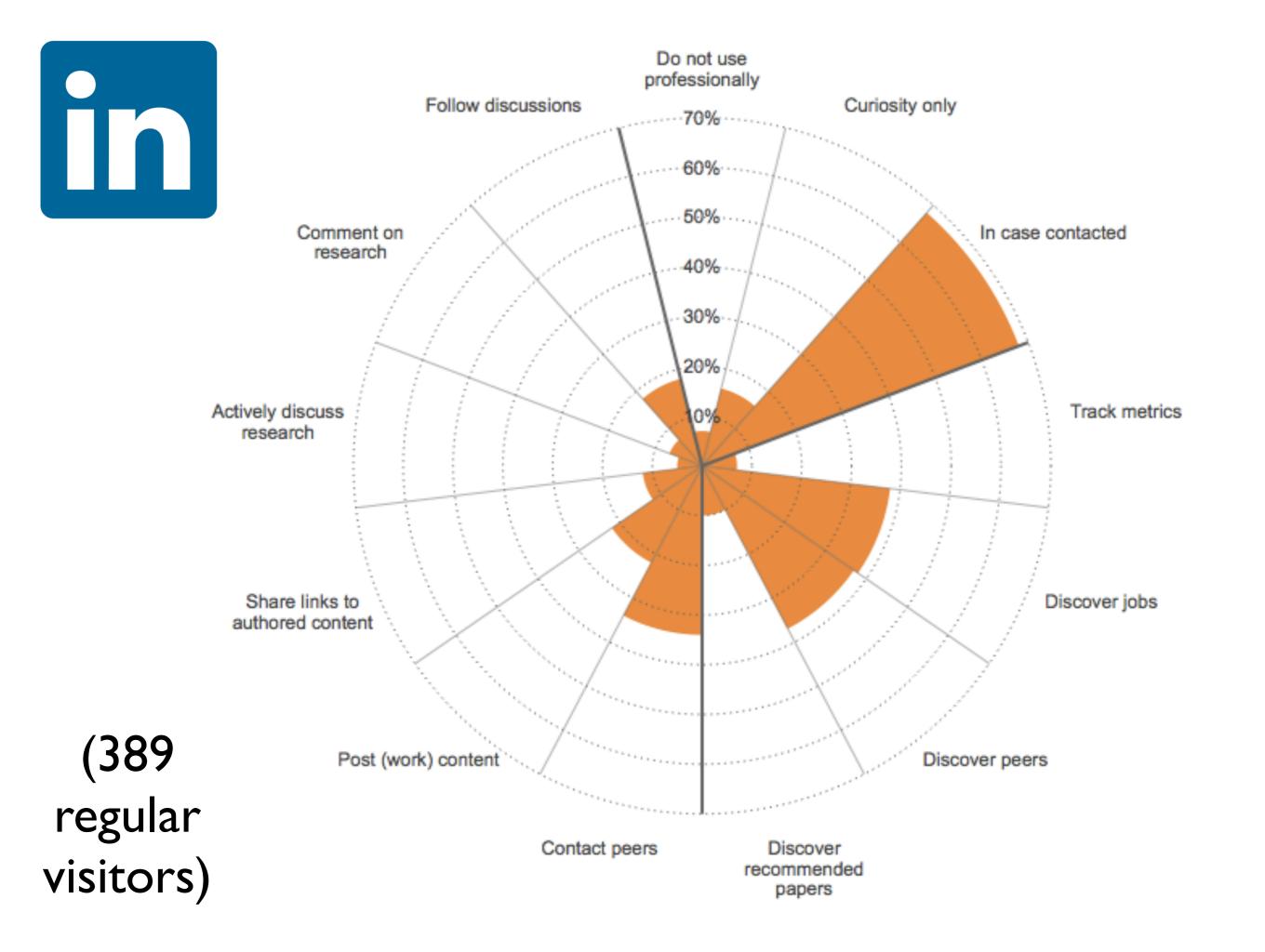
A Nature survey

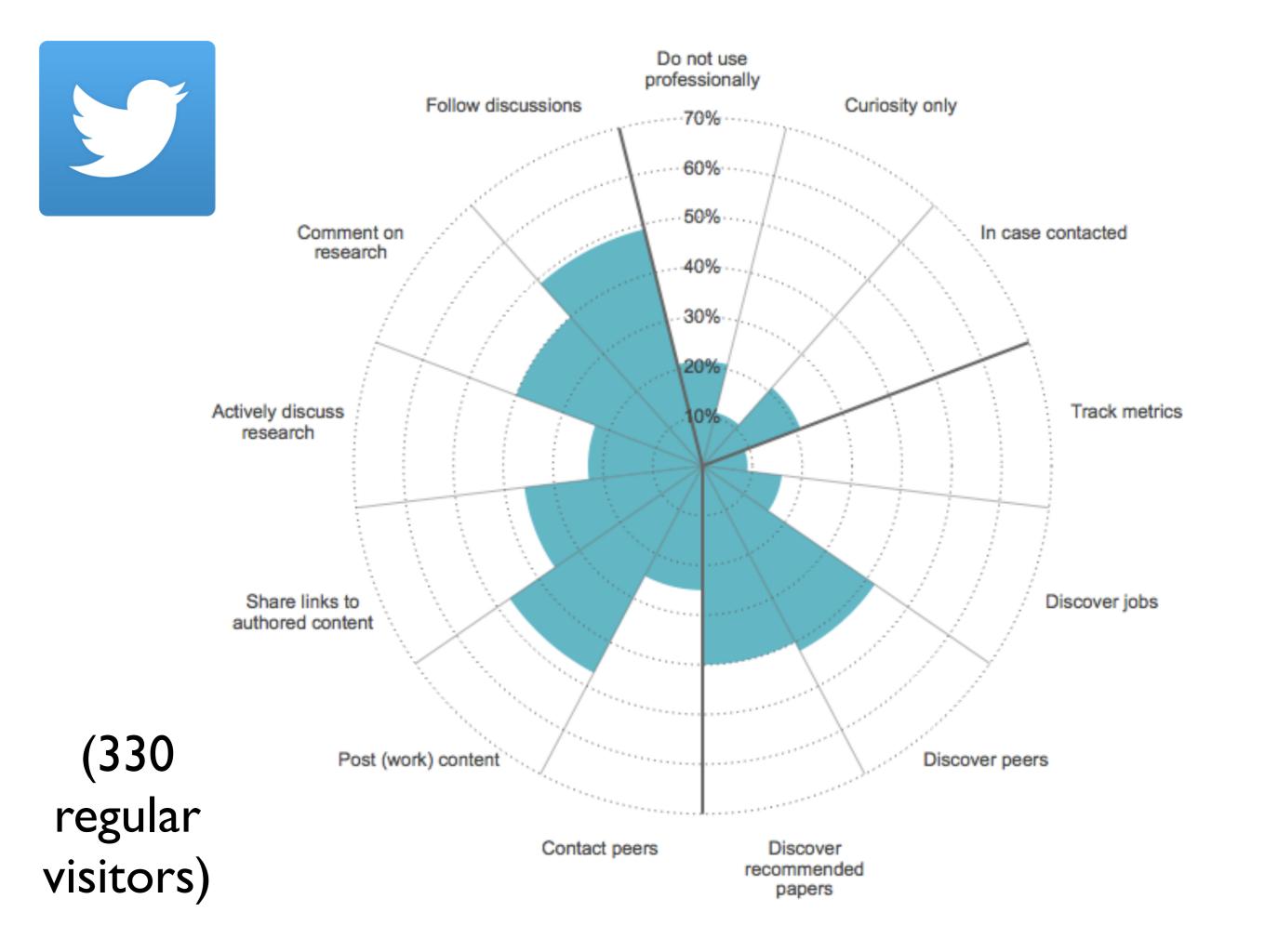
A *Nature* survey explores why.

SOCIAL NETWORK

Nature **512**, 126–129 (2014)









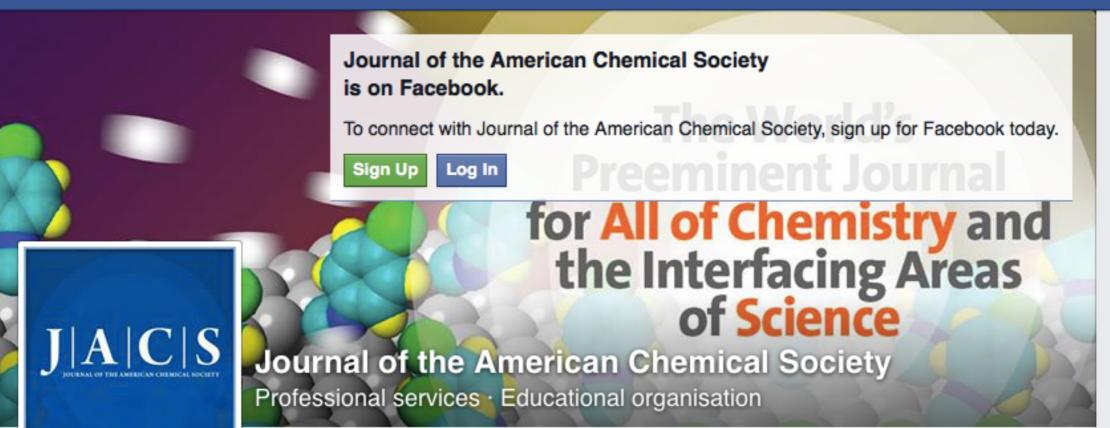
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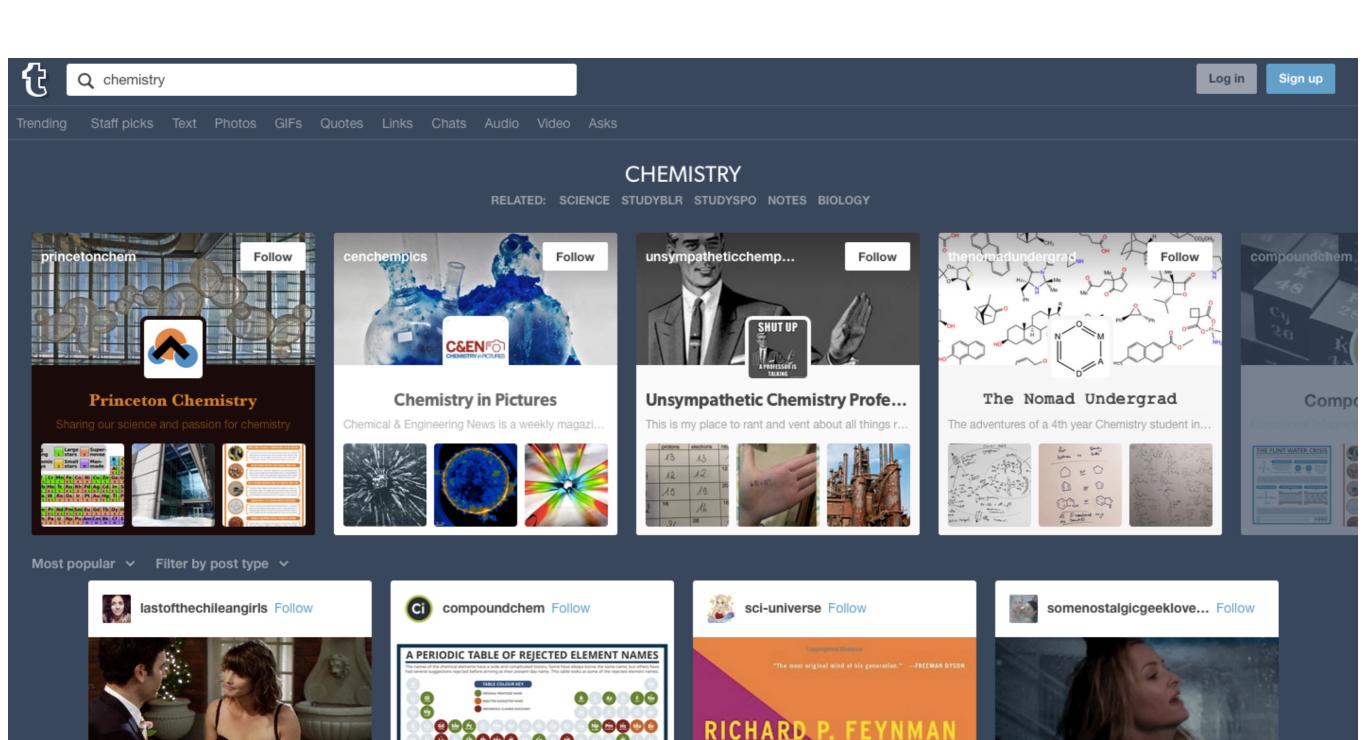


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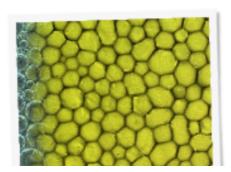












Chemistry in Pictures

C&EN's Chemistry in Pictures launched in early 2014 to showcase the beauty of chemistry, chemical engineering, and the allied sciences. Through visually compelling photos and images, Chemistry in Pictures provides a window into the fascinating world of scientific research and discovery.

We draw our content from several sources: scholarly journals, C&EN editors, and reader submissions. If you have just one cool photo, or if you have 100, we'd love to hear from you at **CENChemPics@acs.org**. It can be a photo, an SEM, a micrograph, or any other type of image as long as it is visually compelling.

Chemistry in Photography Contest

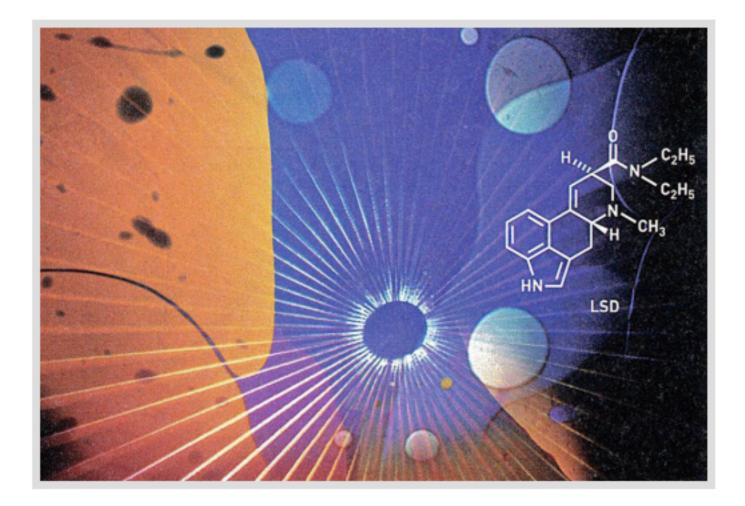
We want your photos! Give your chemistry photography exposure and share your images to participate in the **C&EN Photography Contest** launching June 1st.

the watch glass

A random walk through 90 years of C&EN

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JAN 11



Chemist Albert Hofmann, who first synthesized LSD, was born today in 1906. Here's his account of the first trip:

http://labphoto.tumblr.com/

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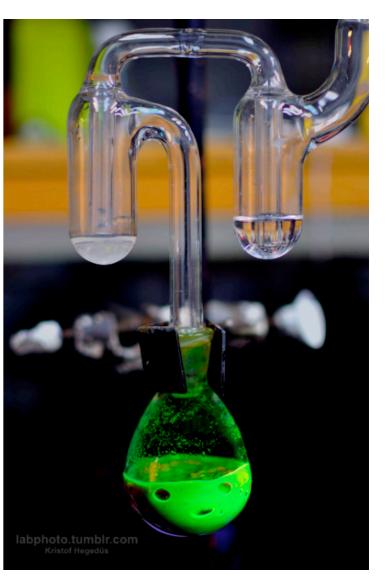




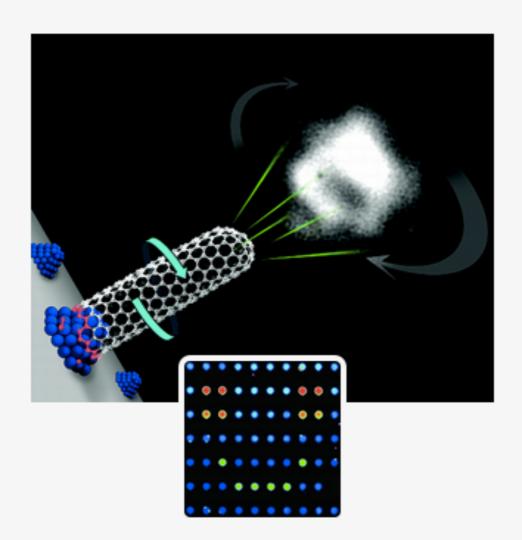








http://tocrofl.tumblr.com/



TOC ROFL

funny table-of-contents images from scientific journal articles. inspired by crazy TOC images and http://blogs.discovermagazine.com/discoblog/category/ncbi-rofl/

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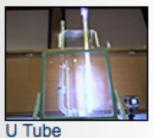
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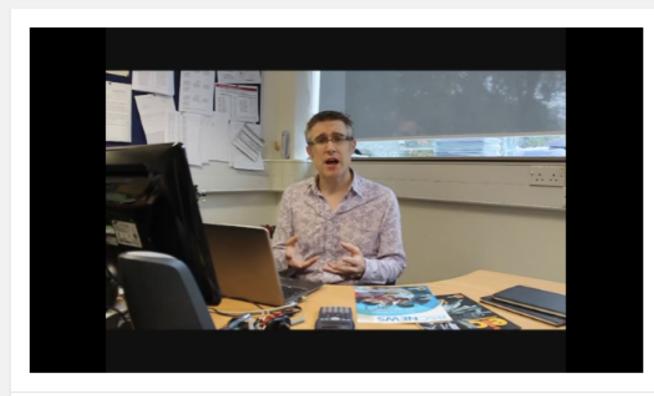
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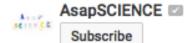




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The Speaking of Chemistry team has made some resolutions for 2016. Watch the video to find out what you can expect from us in the coming year, then share your #ChemResolution with us in the comments.

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THE CHEMISTRY OF BREAD-MAKING

Baking bread may seem like a very simple process. It's a combination of only four different ingredients: flour, water, yeast, and salt. However, there's a lot of science in how these four ingredients interact, and how varying them varies the bread's characteristics.



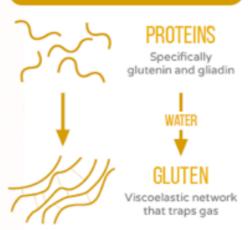


KNEAD THE DOUGH



BAKE THE BREAD

FLOUR, WATER & SALT



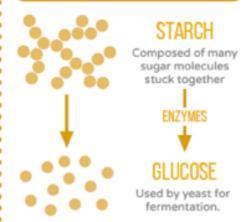
Flour contains high levels of glutenin and gliadin proteins. These classes of proteins are collectively referred to as gluten. When water is added, these proteins form a network held together by hydrogen bonds & disulfide cross-links. Kneading uncoils gluten proteins, strengthening the network and the dough.



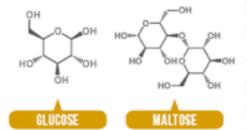
THE ROLE OF SALT

ADDS FLAVOUR TO BREAD SLOWS DOUGH FERMENTATION STRENGTHENS GLUTEN STRUCTURE MAKES DOUGH MORE ELASTIC

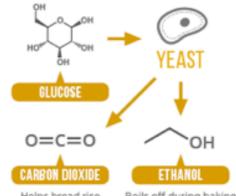
STARCH & SUGAR



Flour contains starch, long chains of connected sugar molecules. Amylase converts starch to maltose; maltase in yeast converts this to glucose. Along with other sugars, this can be used by the yeast for fermentation, and is also involved in the flavour-forming browning reactions that help to form the bread's crust.



YEAST & FERMENTATION



Boils off during baking Helps bread rise

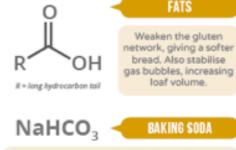
Yeast are single-celled fungi that help convert sugars in the bread mix into carbon dioxide. The bubbles of carbon dioxide formed cause the bread to rise; kneading makes their size more uniform. Sour dough breads contain both bacteria and wild yeasts. The lactic acid produced by bacteria can sometimes give a sour taste.

SOUR DOUGH 100:1

Both feed on sugars; yeasts in sour dough can't break down maltose, bacteria can

BACTERIA:YEAST

OTHER INGREDIENTS



BAKING SODA

FATS

Weaken the gluten

bread. Also stabilise

loaf volume.

Sodium bicarbonate. Combined with moisture and acidity, produces carbon dioxide, which can help bread rise. Can cause bitterness.

NaHCO₂ CREAM OF TARTAR

BAKING POWDER

Also sodium bicarbonate, but with cream of tartar (potassium bitartrate), an acid ingredient that activates the bicarbonate.

More commonly known as vitamin C, it helps to strengthen the dough's gluten network.

A POLYSACCHARIDE HAT IS PRODUCED BY THE BACTERIUM XANTHOMONAS CAMPESTRIS

XANTHAN GUM

Used in the production of gluten-free breads.





THE NEW YORKER

JANUARY 29, 2016

THE END OF TWITTER

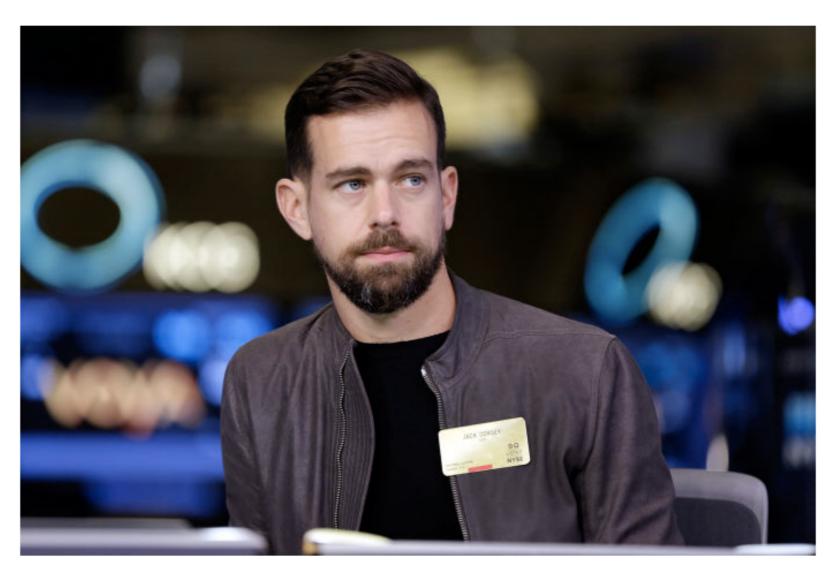
BY JOSHUA TOPOLSKY











Twitter might rebound in the wake of Jack Dorsey's reappointment as C.E.O., but the service is still in trouble. PHOTOGRAPH BY RICHARD DREW / AP

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28 day summary with change over previous period

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Tweets 50 1233.3%

nature

Nature Chemistry @ @NatureChemistry

305K ↑215.3%

Tweet impressions

Profile visits

9,688 128.2%

Mentions

388 128.2%

Followers

125K 12,417

Jan 2016 • 29 days so far...

TWEET HIGHLIGHTS

Top Tweet earned 34.2K impressions

Odds on names of those 4 new elements? @philipcball, @scburdet, @chronicleflask, @ericscerri & @geochembrett discuss bit.ly/1QyNkM1

♠2 **t**₹20 ♥23

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Top Follower followed by 121K people



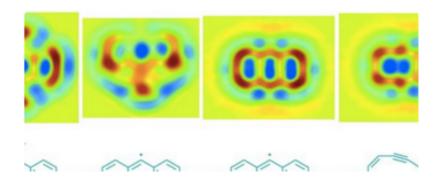
Top mention earned 601 engagements



C&EN

@cenmag · Jan 27

Poke! Chemists nudge molecule to react, then watch bonds break and form ow.ly/Xzouw New @naturechemistry pic.twitter.com/gGtLGkxe1A



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Get your Tweets in front of more people



Promoted Tweets and content open up your reach on Twitter to more people.

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JAN 2016 SUMMARY

Tweets

50

Profile visits

9,859

Tweet impressions

306K

Mentions

394

How we've used Twitter

Commissioned News & Views articles Commissioned In Your Element articles Found papers to cover in Research Highlights Ideas for Editorials Highlight our journal content Highlight content in other journals Highlight interesting chemistry news stories Interact with our community Answer questions Pose questions Report from conferences Retweets of job/postdoc opportunities

A great question

Who is the greatest chemist of all time?

These eight simple words pose a question that is far from simple to answer. The first obvious problem is with the concept of 'greatness' — how should this be defined and measured? After all, greatness doesn't come with a handy SI unit. Continuing to analyse the question further, would everyone agree with exactly what is meant by the term 'chemist'? There are some prominent historical figures that both chemists and physicists would claim as their own — and the boundaries between disciplines are perhaps more blurred today than they have been since the days when scientists of any stripe were called 'natural philosophers'.

Another complication is a fundamental (and unavoidable) one associated with all questions and polls of this type — the influence of time. Consider the world of sport for example — when a team or an individual becomes very successful, comparisons are often made with so-called 'greats' of a bygone era. But in the same way as it would be impossible for the Manchester United teams of 1968 and 1999 to play one another to inform a fair comparison¹, how do we judge the relative merits of the contributions that Wöhler and Woodward made to chemistry?

The technical challenges involved in

or ranking. We asked the greatest-chemist question on our journal's Twitter feed² back in early January and gave a comprehensive round-up of the responses we received on the Sceptical Chymist blog³. We received a total of 86 votes, with 36 different names put forward as the greatest — Linus Pauling came out on top with 16 votes.

To our surprise, there were some truly great chemists missing from the list. No Gibbs, no Dalton and no Priestley. One omission in particular, that of the only person to be awarded two Nobel Prizes in Chemistry, sparked some debate in the blogosphere at the Curious Wavefunction⁴ and Second Messenger⁵. Was Sanger's

name missing because chemists tend to focus on

fundamental topics such as structure and bonding rather than more applied aspects? And, as discussed at There (& Hopefully) Back Again⁶, should our evaluations of the 'greatness' of a scientist change when we consider

not just their

contributions to physics?' Einstein received the most votes, with Newton and Maxwell trailing in second and third places, respectively, and a total of 61 others were nominated.

One would somewhat confidently predict Einstein to top the physics survey, but would any of us have picked Pauling to lead the chemistry one with the same certainty? The cat is out of the bag now,

but it's also worth bearing in mind the subtle difference between asking 'Who is the greatest chemist?' and asking 'Who do you think would top a poll of greatest chemists?' Another difference is that Einstein and the photos of him with stereotypical 'mad-genius' hair have crossed into popular culture — and this is certainly not the case with Pauling.

Is the lack of a recognisable figurehead in chemistry a problem? If there was an Einstein-like figure we could point to, would this help to brighten up chemistry's somewhat tarnished public image? It might also serve our community better than generic images of men and women in

lab coats and googles standing in front of

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All you can tweet

Nature Chemistry signed up for a Twitter account in March 2009. More than 5,000 tweets later, what have we learned and how do we use it?

When cramming an informative and selfcontained message into only 140 characters (including spaces!), clarity is a virtue.

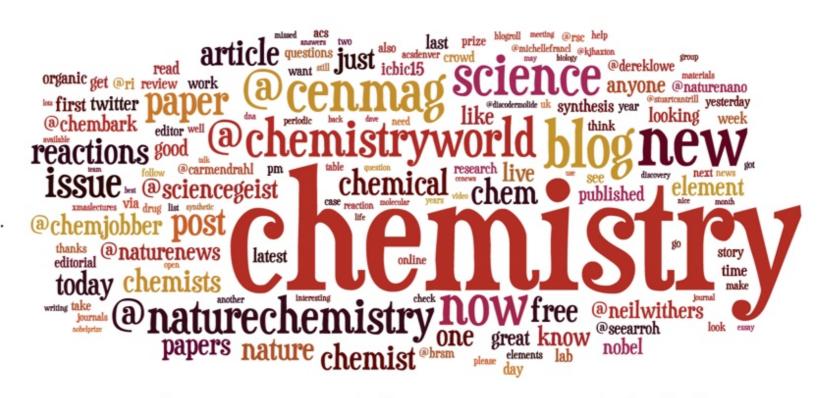
With subjects that sometimes rely on specialist language, such as chemistry, composing tweets can be quite challenging.

We use Twitter to point out any interesting chemistry-related content, including papers, news stories and blog posts.

We retweet chemistry-related job opportunities and internships that we think might be of interest to our followers.

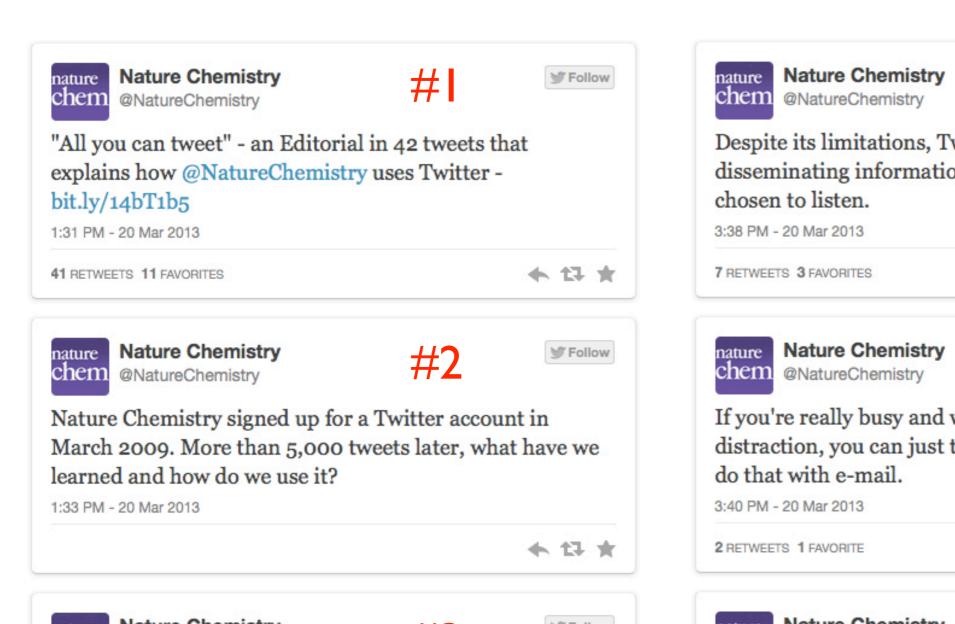
Our tweets range from serious topics (chemical safety) to the light-hearted (such as chemistry-themed music parodies: http://bit.ly/cmmbk).

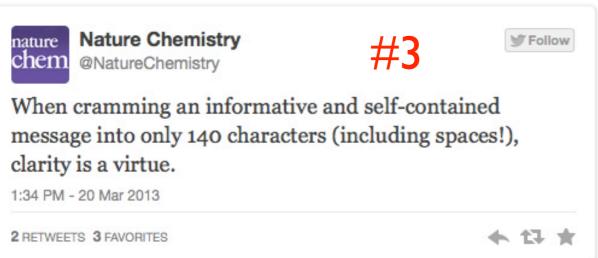
We share our Articles and other content from *Nature Chemistry* on Twitter, but that's only a small fraction of what we tweet about.

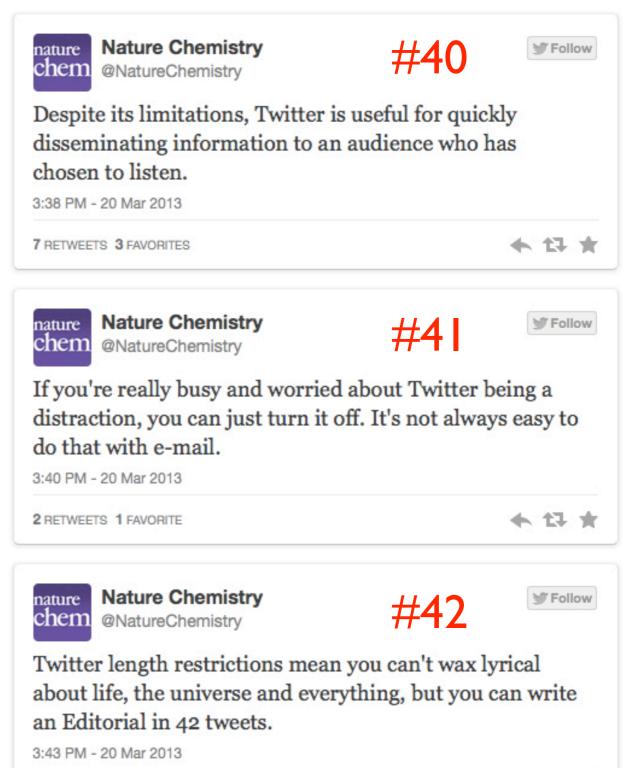


Our tweet referencing a tongue-in-cheek blog post by @DrRubidium about misuse of the term 'organic' is our most retweeted. We commissioned @davidkroll to review @bstockwell's book, 'The quest for the cure', after he tweeted about it (http://bit.ly/qftcure).

http://bit.ly/twittertorial







小 口 ★

5 RETWEETS 2 FAVORITES

All you can tweet

Nature Chemistry signed up for a Twitter account in March 2009. Nearly 5,000 tweets later, what have we learned and how do we use it?

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We share our fescarch Articles and other content from Nature Chemistry on Twitter, but that's only a small fraction of what we tweet

Journal Twitter streams - especially automated ones - full of just their own content can resemble RSS feeds and are a missed opportunity.

There are quite a few chemistry journals with an active presence on Twitter and we maintain a list of them (http://bit.ly/chemjnls).

Only a tiny proportion of visitors to our website come through Twitter, but it's not just about that; we use it to engage with our

instant - two-way connection between the journal's editors and its followers.

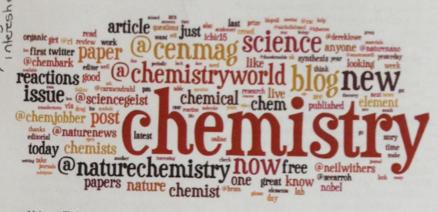
All of the Nature Chemistry editors (past and present) have contributed to the journal's Twitter feed, albeit some more than others.

Ideas for research highlights come from many different sources, including tweets by chemists about papers that catch their eye.

Twitter can be a great way to crowd-source answers to a question — there are lots of experts (and others.) just waiting to chime in.

Have a problem with a reaction or want to know what the odd piece of glassware might know.

As of mid-February 2013 we had Jecrued more than 70,000 followers, aided by a short spell on Twitter's who-to-follow list for 'science'.



Using @TwitonomyApp (http://bit.ly/ twitonomy) we have analysed just under 3,200 tweets that we sent between April 2011 and

Of 3,197 tweets scrutinized by Twitonomy, 1,492 (47%) of them have, so far, been retweeted a total of 5,865 times fan average of

Our tweet referencing a tongue-in-cheek blog post by @DrRubidium about misuse of 7 the term 'organic' is our most retweeted 166

From April 2011 to February 2013, we posted an average of 4.79 tweets per day, with an average of 0.39 links in each one.

A Wordle (http://www.wordle.net/) made from more than 3,000 of our tweets shows that the word 'chemistry' dominates (pictured).

Apart from 'chemistry' and its derivatives. Twitter provides a direct — and effectively \(\square \text{other words that often appear in our tweets} \) include, 'science', 'blog', 'paper' and 'new'.

Unsurprisingly, the vast majority of our tweets are about chemistry — whether in the context of concepts, publishing or people.

The accounts of other chemistry publications frequently get mentioned in our tweets, most notably those of @ChemistryWorld and @cenmag.

The Twitter handles of chemistry bloggers feature prominently in our tweets, including @ChemBark, @Chemjobber, @SeeArrOh and @sciencegeist.

Getting to know people (and their 7 four found is? Ask Twitter, someone on there of opinions) through Twitter has been useful and had led to the commissioning of content for

> A Commentary article (http://bit.ly/ chempublic) co-authored by @sciencegeist came about following numerous interactions

with him on Twitter.

After spotting a tweet by @kevinbookermilb lauding a paper in @angew_chem we asked him to write about it for us (http://bit.ly/flowchem).

Twitter exchanges about our 'In Your Element' series of essays resulted in @DavidMLindsay, @SimonHiggins_60 and @ kjhaxton each writing one.

We commissioned @davidkroll to review @bstockwell's book, 'The quest for the cure', after he tweeted about it (http://bit.ly/qftcure).

Bloggers we have got to know on Twitter (@JessTheChemist, @Synthetic Remark, @azmanam and @karlDcollins) have penned our Blogroll column.

In 2011 we used Twitter to ask who the greatest chemist of all time was - the responses inspired an Editorial (http://bit.ly/ gr8chem).

A handful of chemistry editors and journalists are on Twitter and following them gives you a behind-the-scenes look at the publishing world.

Twitter is particularly useful for highlighting new chemistry blogs and was how we learned of those written by @BRSM_blog and @vinylogous.

Filtering tweets is relatively easy; you can control the signal-to-noise ratio by choosing who to follow and by creating themed lists.

Hashtags - Abich ark included in tweets in the form of '#hashtag' — are handy for tracking or finding tweets on a particular topic.

A very active chemistry-related hashtag popularized by @Doctor_Galactic — is #realtimechem, where chemists tweet about their daily lives.

K # 18 19 26

New and old media collide...

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Volume 92 Issue 39 | Web Exclusive

Issue Date: September 29, 2014 | Web Date: September 24, 2014

20 Chemists Worth Following On Twitter

A panelist-selected primer for newcomers to the social network

By Lauren K. Wolf

Department: Science & Technology

Keywords: twitter

Everybody loves a good "Top 10" list, right?

Turns out that's not always true. Last week, Science magazine published "The Top 50 Science Stars of Twitter," a list attempting to collect the most-followed, most-cited scientists regularly putting their thoughts into 140-character snippets. The list was assembled in response to comments made by genomics researcher Neil Hall, who suggested that scientists should stop wasting time on Twitter and publish more papers.

The list that Science produced was just as heavily criticized as Hall's comments. The chemistry community was particularly irked over the fact that neuroscientists, biologists—even physicists—made the list





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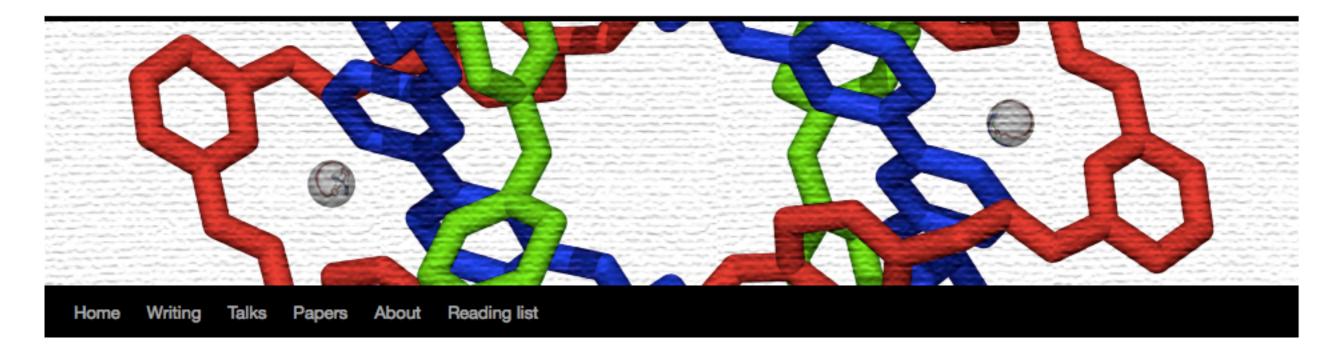
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← Animal authors I did a Nobel thing... →

100 chemists on Twitter

Posted on September 22, 2014

This is not a list of the top 100 chemists on Twitter. For a start, I'm not really comfortable defining 'top'. Most followers? Most tweets? Shiniest avatar? Funniest bio? Most well-known in the real world? (Define 'well-known' and 'real world', go on, I dare you). Secondly, not everyone on this list is necessarily a card-carrying chemist, but they are all people who, more often than not, have something to say on Twitter about chemistry in all its many guises.

This is essentially a starter pack for those interested in hearing about some chemistry on Twitter (and was, perhaps obviously, inspired by the list that Science put out last week that

Find me

E-mail: stuart at stuartcantrill.com Twitter: @stuartcantrill

Recent posts

- Imperfect impact
- Chemistry journal citation distributions
- Back to the future (of chemistry publishing)
- All your base are belong to JACS
- 115 years of JACS titles

Top posts & pages

- The heaviest naturally occurring element on Earth?
- The smallest chiral hydrocarbon?
- 100 chemists on Twitter



http://bit.ly/chemjnls

Should researchers tweet?

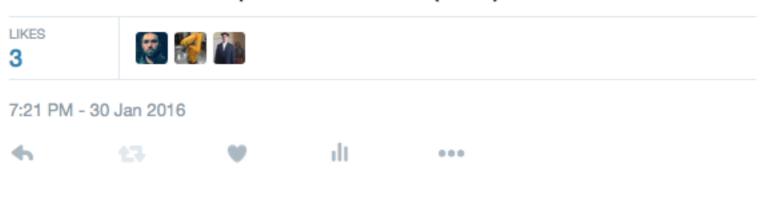


Highly tweeted articles were 11 times more likely to be highly cited than less-tweeted articles

(A total of 4208 tweets cited 286 distinct JMIR articles)



Chemtweeps! I'm giving a talk on Monday & a large part of it will be about social media and Twitter in particular... (1/2)





So, tell me in a tweet why you use Twitter. Would like to put some direct quotes/tweets in talk (credited of course)

Stuart Cantrill @stuartcantrill

LIKES

Chemtweeps! I'm giving a talk on Monday & a large part of it will be about social media and Twitter in particular... (1/2)

RETWEETS

11

📸 🚳 🕼 🞯 🗟 🦝 oe 🌠 🔯











7:22 PM - 30 Jan 2016



17









Well, it's useful for crowdsourcing talks...

Networking





@stuartcantrill It's done more networking for me than LinkedIn has.



Networking





@stuartcantrill Started as a way to keep track of friends, now I talk to tons of great scientists I'd otherwise never get to. Amazing.



Networking (in real life too)





.@stuartcantrill Because I have met more interesting chemists in person (thanks to Twitter) than through any other medium.

TRETWEET LIKES

1 7

1:54 AM - 31 Jan 2016









Different perspectives (and not all work)



Broaden your horizons



@stuartcantrill twitter = worldwide random coffee machine chats. Very ≠ perspectives, broaden your horizon.



Broaden your horizons



@stuartcantrill Helps give perspective on chemistry beyond your own work - very easy to get lost down a rabbit hole if you're not careful.



Different perspectives (and good for connections)





@stuartcantrill instantly connects me across multiple fields w folk junior to senior—so many perspectives I'd never otherwise get so easily!



...and this





@stuartcantrill also, snark.

RETWEET

LIKES







7:39 PM - 30 Jan 2016



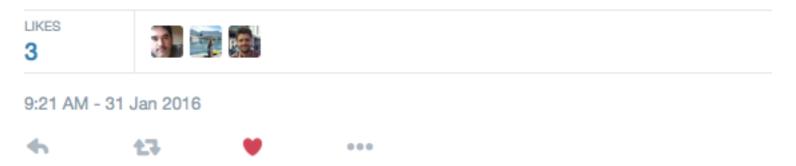








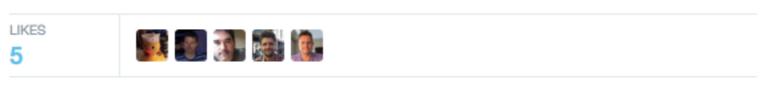
@stuartcantrill Twitter connects me to interesting chemists doing fantastic work, folk that I otherwise won't have a chance to meet.







@stuartcantrill Keeps me connected to an international array of chemists that I am otherwise rather isolated from



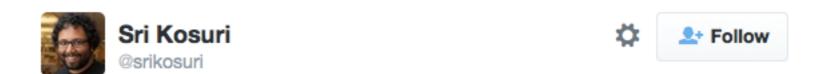
4:50 AM - 31 Jan 2016



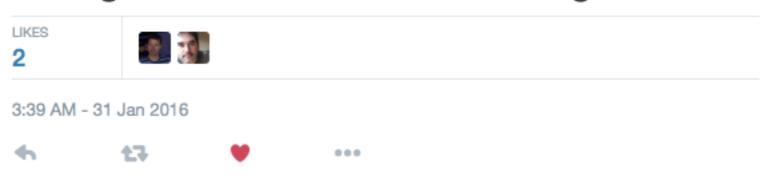








@stuartcantrill Hard to travel with young fam. Easiest way to keep abreast of banter and finding out what's new and exciting.



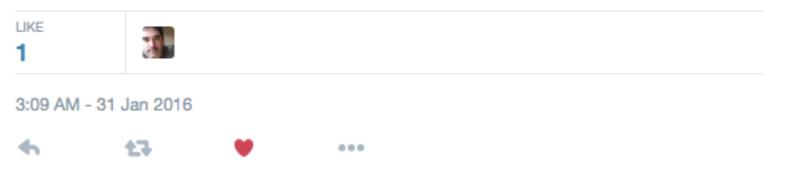


@stuartcantrill it helps to connect with others in field. We can see each other once a year at meetings but tweet every day





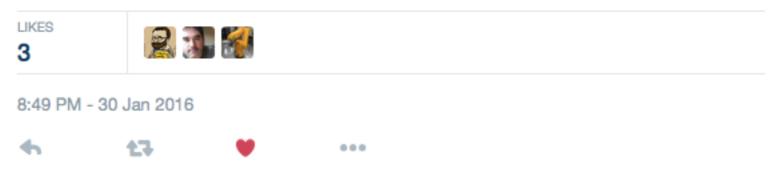
@stuartcantrill Twitter helps connect chemists, increasing the impact of our research and keeps me up-to-date with the latest research.



Connections to collaborations to co-authors!



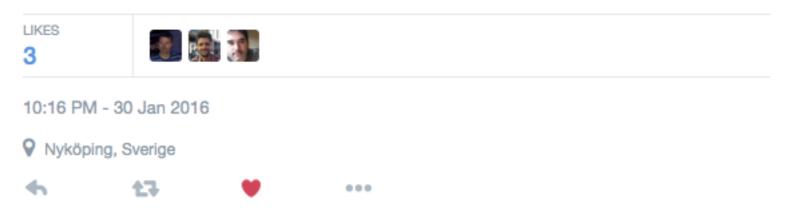
@stuartcantrill discover people who eventually become friends who eventually become collaborator, and co-author. happened to a few of us.



Lots of different people on Twitter



@stuartcantrill cause its just as easy to talk to editors and top professors as with grad students



It's like a conference!





@stuartcantrill Twitter is the biggest international scientific conference in the world 24/7 where everyone is an invited speaker.

T:39 PM - 30 Jan 2016







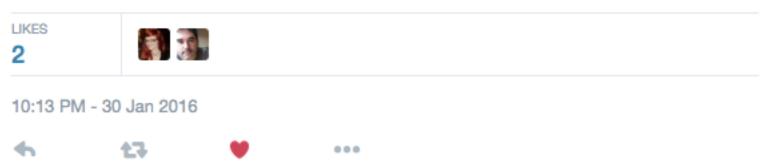


It's like a conference!





@stuartcantrill it's a 24/7, free chemistry conference. What more could you want?



It has other benefits too...



It's like a conference bar!



@stuartcantrill It's the bar at a conference I've not been to before with people I've mostly never met, where science and Lego are both cool



Community





@stuartcantrill It's all about community for me.



Community





@stuartcantrill Chem Twitter is a great mini community of mind.

11:56 PM - 30 Jan 2016







000

Community





Following

To witness dialog within communities I might not connect with otherwise (and hopefully vice versa!)

Stuart Cantrill @stuartcantrill

Chemtweeps! I'm giving a talk on Monday & a large part of it will be about social media and Twitter in particular... (1/2)

LIKES











6:37 AM - 31 Jan 2016







•••

Community and support



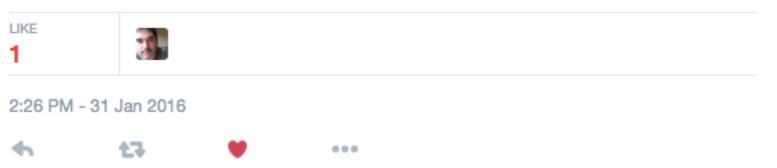
@stuartcantrill sense of a larger community is nice, grad school can be pretty isolating. Nice to hear from others with similar experiences



Community and support



.@stuartcantrill Able to engage wideer network of peers. Comforting to know others facing similar challenges. Also, the laughs...



Community and support

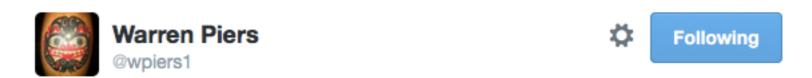




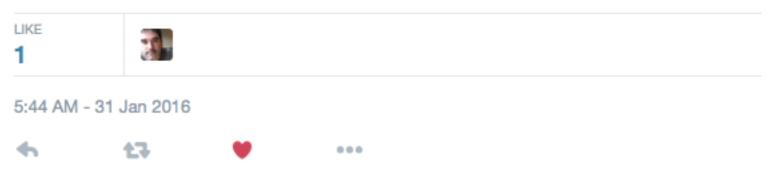
@stuartcantrill a great way 2 see commonality of challenges in all areas of science; 2 give/receive support. We're humans, after all. Mostly.



The human side of science



@stuartcantrill I like to get (and provide) a glimpse of the human beings behind the science.



The human side of science





@stuartcantrill ...because you see the characters behind the names and interact. Characters who wouldn't want any more e-mails.

10:55 PM - 30 Jan 2016







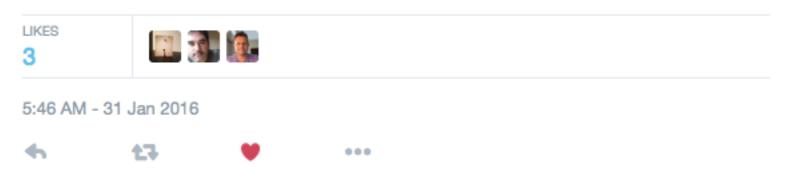


The human side of science





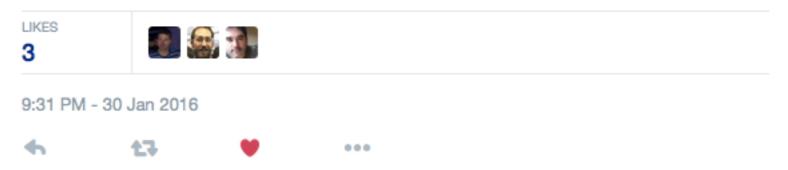
@stuartcantrill it is, in effect, the human side of professional interaction lacking in some other mediums



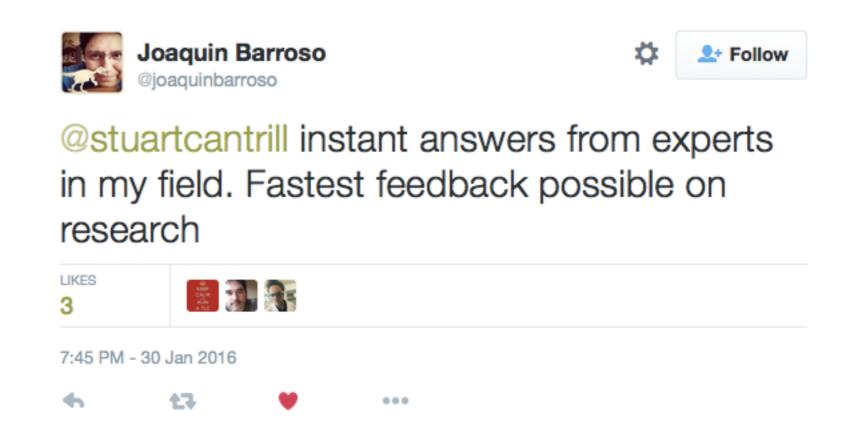
News, connections, community, humanity...!



@stuartcantrill awesome news aggregator, good to see what's happening in other fields, making contacts in other communities, be human



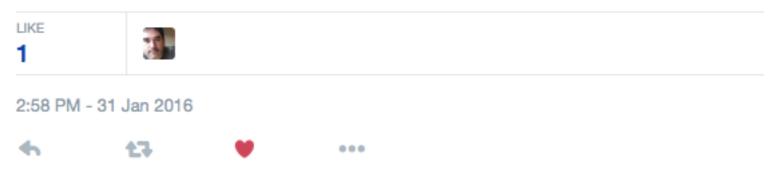
Answers to questions and feedback



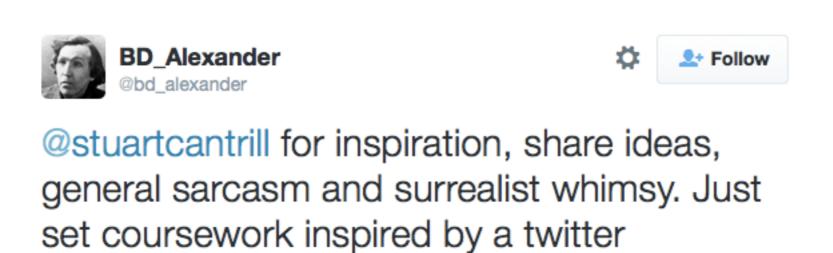
Great resource for chemical education



@stuartcantrill as a schoolteacher I get great access to academics and frontier chemistryideas, links, blogs and help w stuff too



Great resource for chemical education



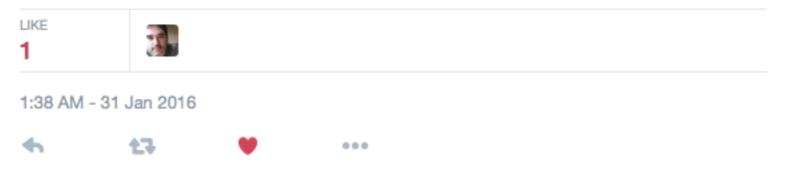
1 10:05 AM - 31 Jan 2016

discussion.

Straight to the source of science



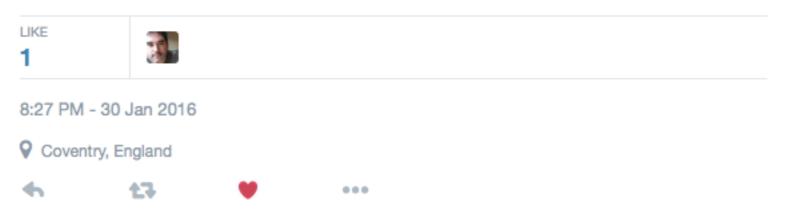
@stuartcantrill I can have a direct conversation with people involved with scientific work rather than gatekeepers of information.



Straight to the source of science



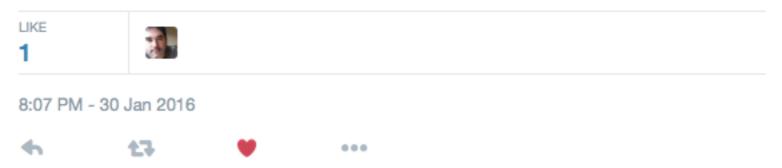
To talk directly with those most engaged in #science and #healthcare @stuartcantrill. It's brilliant. #thanks



Keeping up-to-date with chemistry



@stuartcantrill to keep up to date about science/chemistry, by being informed instantly about the latest news, through experts



Keeping up-to-date with chemistry



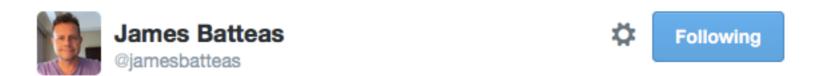
@stuartcantrill to keep up with news, find advice, make friends, reading tweets from conferences I can't attend, to find papers



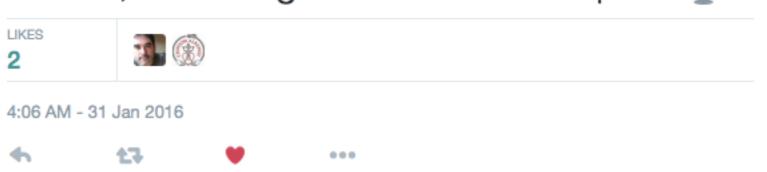
Keeping up-to-date and promoting interesting stuff



And don't forget the cocktails...!



@stuartcantrill Worldwide scientific and social engagement, and cocktail recipes of course, can't forget the cocktail recipes.



I think this sums it up nicely...



@stuartcantrill twitter is the people I WISH I knew. It's for finding the needles in the vast haystack.



This too...





.@stuartcantrill Great to find so many things I otherwise wouldn't - kind of like random adjacent interesting papers in printed journals



And maybe this...





@stuartcantrill Twitter is the only place where evidence and opinion are instantly aggregated and filtered through trusted friends.



Also: good for yelling; possibly addictive...



For measuring self-worth... and complaining?



entirely on RTs & mentions. Also, I like to complain. Gives me a captive audience



and...





@stuartcantrill and it beats working

LIKE 1



12:43 AM - 31 Jan 2016





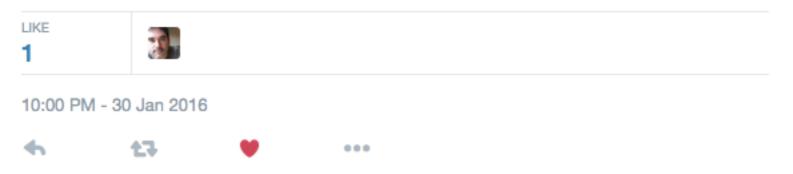


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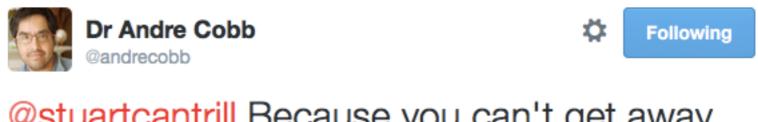
Because you have to?



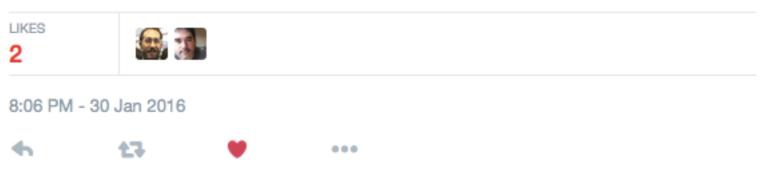
@stuartcantrill Because I see a future in which academic work performance is partly linked to number of followers.



A place to be a little bit more yourself



@stuartcantrill Because you can't get away with flippant, pithy aphorisms in publications.



A place for deep (or sarcastic) answers



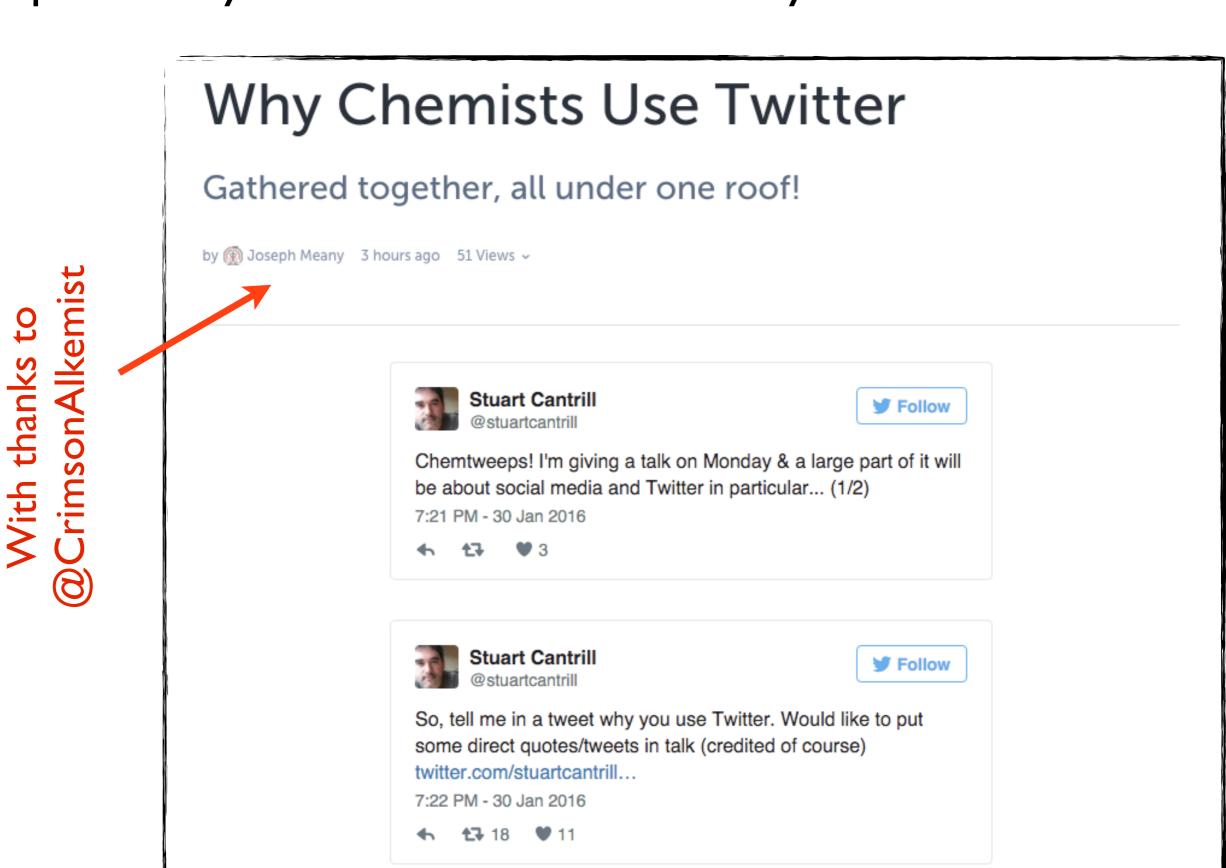
@stuartcantrill Trying to fit deep (or sarcastic) answers into 140 characters is a fun challenge. Also, new interesting friends



To sum up again: a bit of everything, including humour



https://storify.com/CrimsonAlkemist/why-chemists-use-twitter



What others say...

An infinity of hypotheses

The Biologue Chronicles

FRANÇAIS

ENGLISH

WELCOME MESSAGE

A SCIENTIST'S ACCOUNT TO TWITTER

FEBRUARY 24, 2015 BY AVERGER

Some of my colleagues often asked me what I am doing on Twitter. Below are some of my answers.

Twitter, the micro-blogging platform may be viewed as fascinating for some people but also frightening and boring for others. It is certainly a controversial subject. But Twitter is a diamond in the rough for the scientific community: keeping up with current research in real time, follow conferences, improve your professional network, bibliography search,...

This post does not aim to be a scientist's guide to social media in general and to Twitter in particular. The objective is simply to share my experiences as a scientist in social media. As Zen Faulkes (@DoctorZen) quite rightly stated here: 'Everything that happens on social media has been happening at conference for as long as there have been conference (informal conversations). Social media is just the biggest research conference in the world'.

(click to enlarge the images)

1- A bibliography search tool

1a- Scientific journals twitter accounts. Forget Pubmed, RSS feed or eTOCs. Just follow your favorite journal on Twitter. So far, I have a list of 291 journals.

RECENT POSTS

Eventually they
will understand November 9,
2015

Ils finiront par comprendre
November 8, 2015

A scientist's account to Twitter February 24, 2015

Mon petit twitter scientifique illustré February 20, 2015

#jesuisCharlie #CharlieHebdo January 8, 2015

TWITTER

After the Q by @stuartcantrill 'tell me in a tweet why you use

What others say...



The amazing power of the hashtag

After I joined as an Assistant Professor, I have been using twitter a lot more. The reach and what happens subsequent to a tweet still surprises me. I will narrate a story, one that is definitely worth a read if you are an academic and still are skeptical of the twitterverse.

Commonwealth of Pennsylvania runs a program called Pennsylvania Infrastructure Technology Alliance, abbreviated as PITA (interesting abbreviation) where they encourage researchers to involve Pennsylvania companies. The rules of the program are that PA pays 1\$ for every 2\$ you can get a Pennsylvania company to commit.

I have always been quite interested in having a close connection with industry but given I was new to the Pennsylvania area, I did not have any strong connections with local companies. All of my company connections were still back in California. Now, this posed a challenge. I decided to turn

A (shouty) case study...



Excuse me, but I need to shout: A ROTAXANE OR CATENANE IS A MOLECULE, IT IS NOT SUPRAMOLECULAR! (limited audience for that tweet, I know).

RETWEETS

36

























SHOP FIND A JOB

BLOG REGISTER

HOME

NEWS

OPINIONS

FEATURES

REGULARS

JOBS

PODCASTS

WEBINARS

JM 🛠

Johnson Matthey

VISIT US AT INFORMEX. **HALL H, BOOTH 533.**

Fine Chen

What is a molecule?

28 January 2016

Philip Ball





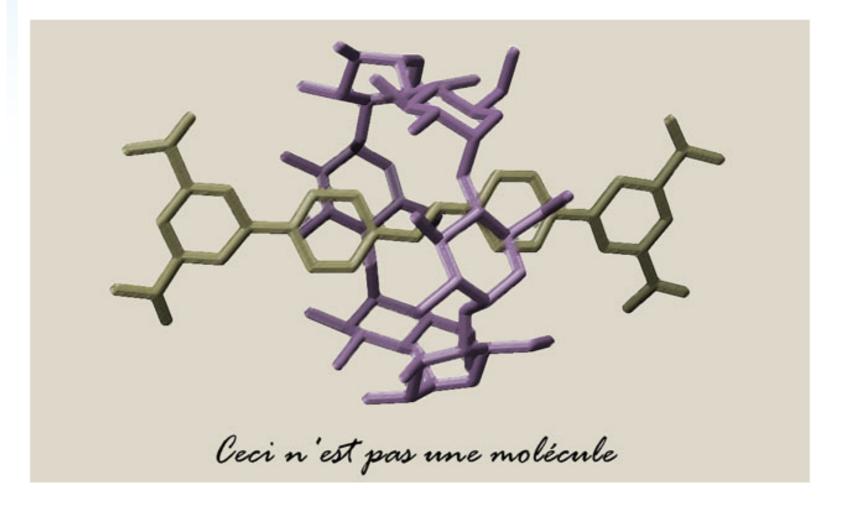




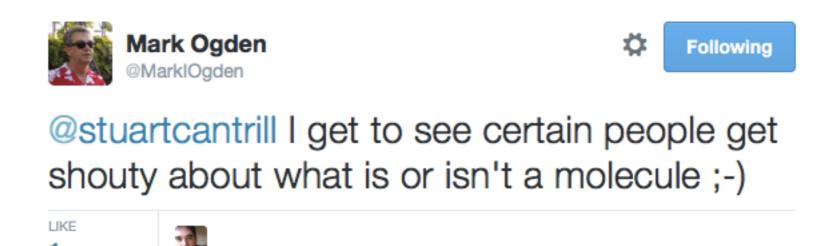




In science, as in life, words often acquire meaning through usage rather than through definition. We use 'species' and 'force' without being troubled by their imprecision. The same can be said about 'molecule'.



Some more of that Twitter hunour...



4:05 AM - 31 Jan 2016

Outreach...?



Ramo Khalifa @EndPali

1d

@ChemistryWorld @NatureChemistry @AmChemistry
@ChemistryNews I hate all of you and chemistry











@EndPali @NatureChemistry @AmChemistry
@ChemistryNews Sorry to hear that Ramo. Is it just chemistry? How do you feel about @PhysicsWorld?

06/12/2015, 22:03











Ramo Khalifa @EndPali

2m

@ChemistryWorld @NatureChemistry @AmChemistry @ChemistryNews @PhysicsWorld just chemistry









#realtimechem

(Story by @carmendrahl)

SCIENCE & TECHNOLOGY

REAL-TIME COMMUNITY

With the Twitter hashtag #REALTIMECHEM, chemists worldwide incubate ideas, share snaps

CARMEN DRAHL, C&EN WASHINGTON

All tweets with

#RealTimeChem

(as of press time):

Tweets on Nov. 7.

Average tweets

(as of press time):

SOURCE: Inpay.com

per day since

Nov. 7, 2012

2012, alone:

"WHAT ARE YOU working on?" It's a question every chemist has addressed, typically in the corridor or at a conference. With the advent of smartphones and the social network Twitter, a growing band of chemists is addressing it in a different way-publicly, online, and in real time.

The phenomenon is called #RealTimeChem, after the label, or hashtag, that participants use. To join in, chemists need only sign up for Twitter, then use the service to share or "tweet" what they're up to-whether meeting a client or setting up a distillation. Researchers on every continent except Antarctica have taken part.

"This is a low-cost, low-barrier way to network," says Adam Azman, a chemistry lecturer at Butler University. For a chemist who can't travel or is learning how to build professional relationships, #RealTimeChem is a virtual watercooler. Mixed in with a typical day's real-time tweets are messages about journal articles

or reaction troubleshooting. And of course, oohing and aahing over pretty pictures of crystals or lasers, a smattering of which are shown here. Azman, who tweets under the name @azmanam, inspired the movement. His livetweeted attempts to determine the proprietary composition of a cleanser attracted advice from chemists in multiple countries.

Many chemists tweet about what they do, says Jason Woolford (@doctor_galac tic), who launched the community by holding an official "#RealTimeChem Day" on Marie Curie's birthday, last Nov. 7. The label is an umbrella to bring those individuals or small communities together, he says.

"It has really taken off, more than I thought it would," says University of Leeds postdoc Jessica Breen (@JessTheChemist), who coined the #RealTimeChem name. Daily tweets don't match the all-time high from Nov. 7, but



conversation levels among a smaller group have stayed consistent since then. Woolford, who just joined the Royal Society of Chemistry as a publishing editor, is planning a #RealTimeChem week for April.

Real-time tweeting isn't for everyone. "I was slightly concerned with intellectual property issues," wrote Marvinthefish, a chemist based in Cambridge, England, on his blog. He ended up participating but tweeted only "fairly generic" images. Some workplaces, including his, block Twitter

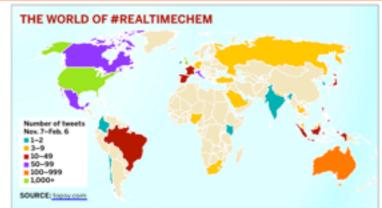
for productivity reasons. But chemists who can participate relish the camaraderie they find online. One group's #RealTimeChem chatter has led to an independent project, a website called Blog Syn. The project aims to complement established journals and websites that verify published synthetic procedures. Blog Syn team

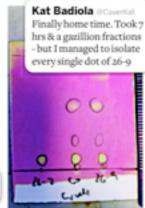
member Matthew Katcher (@katmatcher), a Princeton University chemistry graduate student, says he's glad he's taking part in #RealTimeChem. "It makes you feel like part of a community."■

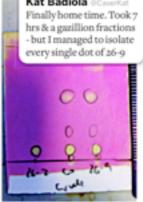
















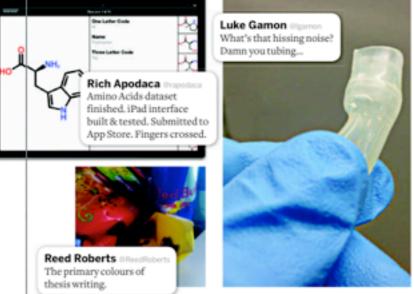
Matthew Katcher Ok, here we go! Forgot how colorful nitroarenes can be







& VIDEO ONLINE



Why did Blog Syn launch? What reactions are

being evaluated? Find out at http://cenm.ag/rtc.

WWW.CEN-ONLINE.ORG 31 FEBRUARY 25, 2013 WWW.CEN-ONLINE.ORG 3O FEBRUARY 25, 2013

most pragmatic approach is to introduce simulation constraints. By fixing the chemical composition, novel polytypes can be explored through crystal structure prediction, with many successes for microporous materials⁴. Alternatively, by fixing the crystal structure, the screening of different combinations of elements can be used to identify previously overlooked stable compositions^{5,6}. As search algorithms are improving, such constraints are gradually being overcome^{7,8}.

In the work of Poeppelmeier, Zunger and co-workers¹, a valiant route was taken. They chose to fix the valence state of their target compounds to satisfy the 18-electron rule, and screen both the chemical composition and crystal structure. From 483 chemically plausible ternary compounds with 18 valence electrons, 83 have been previously reported, leaving 400 'missing' compounds. A rigorous multi-step selection process was implemented (Fig. 1 shows one such process), and validated by 'searching' known compounds — the method did correctly predict their stability and structures. A crystal structure search was carried out to ensure a global minimum configuration was identified, and the vibrational spectrum of each candidate material was investigated to confirm its dynamic stability. Finally, thermodynamic calculations were performed to ensure stability with respect to each competing phase. This screening procedure ensures that fanciful predictions of hypothetical compounds with exotic properties are avoided. In the end only 54 candidates

survived — that is, were predicted to be stable — and of these, 15 new materials were successfully synthesized.

One of the roles of materials prediction in this study is to reduce the possible phase space and direct synthetic efforts to the most realistic and important targets. The simulations also provide valuable information to expedite the characterization of the novel compounds, ranging from predicted crystal structure parameters to vibrational and electronic spectral signatures. For all 15 materials predicted then synthesized in the study, the simulated and measured X-ray and electron diffraction patterns are in very good agreement. Although in the past materials modelling has been largely responsive to experiment, the predictive power of modern simulation techniques is becoming increasingly apparent.

The 18-electron compounds predicted to be stable are distributed amongst eight structure types. Phenomenologically, compounds with one transition metal (such as MgPdTe) are found to be metallic; those with two transition metals (such as TaIrSn) have a gap between their valence and conduction bands. The potential applications of these new materials with unconventional chemical bonding are wide ranging. For example, HfIrAs is a topological semimetal of interest in quantum electronics, ZrNiPb is a small-gap semiconductor with a large Seebeck coefficient suitable for thermoelectric applications, and ZrIrSb is a rare example of a transparent p-type conductor with high conductivity of holes.

It is an exciting time for materials chemistry. The ability to synthesize materials of increasing complexity continues to astound. Even fundamental thermodynamic limits can be overcome, as metastable structures and kinetically stable compositions are accessible through non-equilibrium growth techniques. The challenge now is not simply to make new compounds, but to enable new functionality. The combination of theory and simulation has adopted a new role in the field, as a quantitative tool that can direct and inform experimental synthesis and characterization. When used appropriately, it can help to navigate the immense structural and compositional landscape at a fraction of the time and cost of an empirical search. The googol of possible materials may contain a room-temperature superconductor, the next high-voltage battery, or indeed, a viable photocatalyst for splitting H₂O or converting CO₂ into a chemical feedstock. The quest is to find them.

Aron Walsh is in the Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, UK.

e-mail: a.walsh@bath.ac.uk; Twitter: @lonepair

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- 2. Curtarolo, S. et al. Nature Mater. 12, 191-201 (2013).
- 3. Jain, A. et al. APL Mater. 1, 011002 (2013).
- 4. Woodley, S. M. & Catlow, R. Nature Mater. 7, 937–946 (2008).
- 5. Castelli, I. E. et al. Energy Environ. Sci. 5, 9034 (2012).
- Chen, S., Gong, X. G., Walsh, A. & Wei, S.-H. *Phys. Rev. B* 79, 165211 (2009).
- 7. Meredig, B. et al. Phys. Rev. B 89, 094104 (2014).
- 8. Zhang, W. et al. Science 342, 1502–1505 (2013).

Blogging...



BLOGGING

WE'RE GOING TO NEED MORE MONKEYS.

WE'RE GOING TO NEED MORE MONKEYS.

ВгоесіиС

The infinite monkey theorem states that a monkey hitting keys at random on a typewriter keyboard for an infinite amount of time will almost surely type a given text, such as the complete works of William Shakespeare.

Blogging on the sidelines

Bloggers shouldn't be relegated to the sidelines of the scientific literature, argues Michelle Francl.

I have to admit that my first reaction to Royce Murray's recent editorial in *Analytical Chemistry*¹, warning scientists about science 'bloggers', was irritation. Judging by the reaction of some of my colleagues — bloggers and otherwise — I was not alone. Still, as much as my blogger's fingers itched to post about the irony of someone lionizing scholarly publication, while simultaneously disregarding the published work of the lexicologists at the OED (who have considered 'blogger' to be an English word

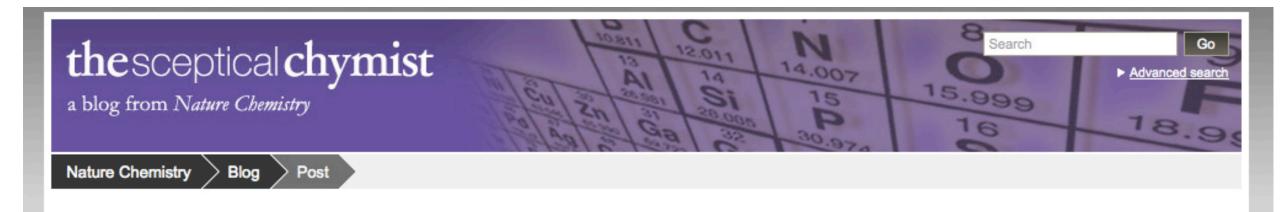
science currently trades, or at least academic science. But I wonder if we conflate the easily countable product (number of publications in peer-reviewed journals and the number of citations they receive) with the product we really care about (furthering interesting developments in the field).

Biologist and blogger Bora Zivkovic argues³ that the communication of results is "the essential last step of the scientific process." Many of us see the journal article as that last step — the moment when a plethora

evolutionary pressures on the field. These conversations act as filters for research, from the conversation at group meetings, which leads you to discard a line of work, to the peer-review process a submitted manuscript undergoes. Post-publication commentary such as citation, media coverage, blog reactions or (perish the thought) a retraction would seem to carry no positive evolutionary weight — the chick has been successfully hatched. Still, such processes can and do feed back into decisions about future choices. How



The Sceptical Chymist...



Previous post

Blogroll: Chemistry in crowds

Next post

Reactions: Felice Grandinetti

NATURE CHEMISTRY | THE SCEPTICAL CHYMIST

50 things you might not know about Nature Chemistry

25 Apr 2013 | 00:59 BST | Posted by Stuart Cantrill | Category: Journal journeys |

Edit

On Monday I realized that our May 2013 issue is our 50th issue. To celebrate, we have compiled 50 (hopefully) interesting tidbits of information about the journal that you might not have been aware of. Apologies for the length of this post, but it seemed like cheating to do fewer than 50...

- The first formal manuscript submission (i.e., made through our online submission system rather than being e-mailed to us before that went live) arrived on the 25th July 2008. It was sent out to three referees and was then, alas, declined for publication on the 5th September 2008.
- 2. The first Nature Chemistry research Article was <u>published</u> on February 22nd 2009. The corresponding author was <u>Makoto Fujita</u> and the paper was entitled: *Minimal nucleotide duplex formation in water through enclathration in self-assembled hosts*. According to Web of Science, as of today it has been cited 62 times.
- 3. We published 471 research Articles (not including review-type articles) in the first 50 issues of *Nature Chemistry*. On average, that's just under 9-and-a-half papers per issue.
- 4. As of today, according to Web of Science our most cited research Article (in fact, our most-cited piece of

Current issue

July 2013, Vol 5 No 7 pp 547-636

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E-alert



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nature.com blogs home

Recent comments on this blog

A sharply intellectual man. I appreciate the desire to learn Latin; pulling the veil of English dominance from the works ... Read more

- Daniel Efford

Reactions: Felice Grandinetti

I'm a little confused. How could you reorganize the table as to make Neon the first noble gas while maintaining ...

Read more >

- Daniel Efford

Neon behind the signs





A comprehensive overview of chemical-free consumer products

Alexander F. G. Goldberg¹ and CJ Chemjobber^{2*}

Manufacturers of consumer products, in particular edibles and cosmetics, have broadly employed the term 'Chemical free' in marketing campaigns and on product labels. Such characterization is often incorrectly used to imply — and interpreted to mean — that the product in question is healthy, derived from natural sources, or otherwise free from synthetic components. We have examined and subjected to rudimentary analysis an exhaustive number of such products, including but not limited to lotions and cosmetics, herbal supplements, household cleaners, food items, and beverages. Herein are described all those consumer products, to our knowledge, that are appropriately labelled as 'Chemical free'.

ARTICLES NATURE CHEMISTRY

References

- 1. 'Chemical-free' sunscreen: http://campl.us/bmnl
- 2. 'Chemical-free' chemistry set: http://sciencegeist.net/my-chemically-fueled-life/
- 4. 'Chemical-free' eggs: http://justlikecooking.blogspot.com/2012/07/chemophobia-vacation-style.html

Acknowledgments

CJC thanks Carmen Drahl for pioneering this important topic in the modern chemistry blogosphere. A.F.G.G. thanks the Azrieli Foundation for an Azrieli Postdoctoral Fellowship.

Author contributions

Both authors contributed equally to the main text.

Additional information

Correspondence should be addressed to ${\it chemjobber@gmail.com}, including \ requests \ for \ reprints \ and \ permission \ information.$

Competing financial interests

The authors declare no competing financial interests, though would have short-sold 'Rubber Ducky Sunscreen' on principle if it was publicly traded.

IN THE PIPELINE

Derek Lowe's commentary on drug discovery and the pharma industry. An editorially independent blog from the publishers of *Science Translational Medicine*.



JANUARY 29, 2016

Alkermes Hits a Wall in Depression

8:16 AM

In case you hadn't seen it, CNS drug development recently did what it's really good at doing: disappointing people late in the clinic. Alkermes had their candidate for depression, ALKS-5461, fail not one, but two Phase III trials. That's especially, well, depressing because the therapy had been thought to have real potential in a ... Read More

Comments: (17) | No Trackbacks | No Pings

Category: Clinical Trials, The Central Nervous System

JANUARY 28, 2016

The Management Hat

12:49 PM

On this anniversary, I wanted to point back to an older post here: Roger Boisjoly and the

The Baran Laboratory

Search Baran Lab Blog

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Recent Comments

Duc Tien commented on J Org Chem Is New Zh Org Khim: "Trên thị trường hiện nay, có rất nhiều loại máy phun sơn phục vụ cho các công trình dân dụng và..."

Duc Tien commented on Baran Lab Does Steroids: "Trên thị trường hiện nay, có rất nhiều loại máy phun sơn phục vụ cho các công trình dân dụng và..."

Duc Tien commented on Antroquinonol Blog Post Hello I Worked: "Trên thị trường hiện nay, có rất nhiều loại máy phun sơn phục vụ cho các công trình dân dụng và..."

Duc Tien commented on Strain Release Amination Your Guide To_14: "Trên thị trường hiện nay, có rất nhiều loại máy phun sơn phục vụ cho các công trình dân dụng và..."

Ryan G. commented on Strain

Thursday, January 14, 2016

Strain-Release Amination – Your Guide to Make Super-Paxil!

HELLO AND WELCOME TO MARSII: This post chronicles the path that we took to solve a 45 YEAR OLD PROBLEM and how this led to our exploration of privileged strained ring systems that look like they come from another planet.

It all started in late 2014 when we were approached by Pfizer to provide a kilo-scale synthesis of [1.1.1]Bicyclopentylamine - that's right.....1KG!!

Large scale synthesis is unprecedented and expensive (3 kg ~\$150 k)

PF-4735165-01

PF-1060219

	current*
Wuxi	3kg @ \$48,148/kg, LT=15 wks
	5kg @ \$35,736/kg, LT=15 wks
	10kg @ \$27,811/kg, LT=16 wks
Inogent	3kg @ \$46,754/kg, LT=14 wks
	5kg @ \$35,876.20/kg, LT=14 wks
	10kg @ \$31,627.70/kg, LT=15 wks
Asymchem	3kg @ \$77,741/kg, LT=13 wks
	5kg @ \$66,088/kg, LT=14 wks
	10kg @ \$54,979/kg, LT=15 wks

NOTE: Pfizer would be providing PF-01060219 (this material typically accounted for <5% of overall cost)

- Only a short term solution MAY exist that gets us through R1.
- · The scale-up is not a solved problem.
- · There is a risk that the chemistry may not be solved in time to address post R1 needs.

CHEMJOBBER

1. HELPING CHEMISTS FIND JOBS IN A TOUGH MARKET. 2. TOWARDS A QUANTITATIVE UNDERSTANDING OF THE QUALITY OF THE CHEMISTRY JOB MARKET.

e for chemists? Dude -- it's always bad.*

eck should I know? Quantifying the hat this blog is about. That, and helping

nelpful tips, career questions or angry
-at- gmail dotcom. All correspondence is
get an e-mail back? It's okay to try again.)

gets hungry sometimes, and likes to eat il me, and sometimes I can get it to cough tways happy to try.)

this is a joke. Mostly.)

3-6257

unday Conversation Sts Winner Does ow, CG. Put up or shut up."

ented on C Readers Respond To ised exactly this question with the ask force."

ented on C Readers Respond To ised exactly this question with the SUNDAY, JANUARY 31, 2016

Sunday conversation: STS winner != Nobel Prize winner

From the New York Times and its book advertisements thinkpieces, a really dumb conclusion from Wharton professor Adam Evans:

THEY learn to read at age 2, play Bach at 4, breeze through calculus at 6, and speak foreign languages fluently by 8. Their classmates shudd parents rejoice at winning the lottery. But to paraphrase T. S. Eliot, their careers tend to end not with a bang, but with a whimper.

Consider the nation's most prestigious award for scientifically gifted high school students, the Westinghouse Science Talent Search, called to science by one American president. From its inception in 1942 until 1994, the search recognized more than 2000 precocious teenagers as fit percent ended up making the National Academy of Sciences, and just eight have won Nobel Prizes. For every Lisa Randall who revolutionize physics, there are many dozens who fall far short of their potential...

Wait a minute, is this guy actually arguing that all STS winners have the potential to be Nobel Prize winners? That is a wildly wrong statement; chooses to be an undergraduate biology professor? No chance of a Nobel there - are they falling short of their potential? This is also evidence to Evans has no idea about what it takes to win a Nobel Prize in the sciences.

Here's his concluding paragraphs:

Evidence shows that creative contributions depend on the breadth, not just depth, of our knowledge and experience. In fashion, the most of come from directors who spend the most time working abroad. In science, winning a Nobel Prize is less about being a single-minded genius being interested in many things. Relative to typical scientists, Nobel Prize winners are 22 times more likely to perform as actors, dancers or times more likely to write poetry, plays or novels; seven times more likely to dabble in arts and crafts; and twice as likely to play an instrummusic.

No one is forcing these luminary scientists to get involved in artistic hobbies. It's a reflection of their curiosity. And sometimes, that curiosi flashes of insight. "The theory of relativity occurred to me by intuition, and music is the driving force behind this intuition," Albert Einstein mother enrolled him in violin lessons starting at age 5, but he wasn't intrigued. His love of music only blossomed as a teenager, after he storand stumbled upon Mozart's sonatas. "Love is a better teacher than a sense of duty," he said.

Hear that, Tiger Moms and Lombardi Dads? You can't program a child to become creative. Try to engineer a certain kind of success, and th an ambitious robot. If you want your children to bring original ideas into the world, you need to let them pursue their passions, not yours.

G+1 Recommend this on Google

I'm sympathetic to the idea that art helps people become creative or think differently, but I think this is a lot of post hoc reasoning meant to sel

POSTED BY CHEMJOBBER AT 11:52 AM 6 COMMENTS: LINKS TO THIS POST

Just Like Cooking

Molecular Rapscallion since Twenty Eleven

Tuesday, January 26, 2016

Tough-to-Swallow Propargylation

As I thumbed through the recent *Tet Lett* abstracts, I encountered this title:

"Regioselective propargylation of aldehydes using potassium allenyltrifluoroborate promoted by **tonsil**"

Turns out, the authors were referring to Tonsil (R), an acid-treated calcium bentonite clay, not the fleshy pockets in the back of the throat associated with immune response. I guess BRSM doesn't have to update his "Desperate Conditions" list quite yet...

See Arr Oh



Who is this masked chemist?





Accountability in Research

Policies and Quality Assurance

ISSN: 0898-9621 (Print) 1545-5815 (Online) Journal homepage: http://www.tandfonline.com/loi/gacr20

Social Media, Peer Review, and Responsible Conduct of Research (RCR) in Chemistry: Trends, Pitfalls, and Promises

Ashutosh S. Jogalekar Ph.D.

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To link to this article: http://dx.doi.org/10.1080/08989621.2015.1047705



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NaH as an Oxidant - Liveblogging!

22 JULY 2009

16.293 VIEWS



As many of you will have noticed in the comments to the previous post (which was thoroughly hi-jacked), an intriguing paper has been published in JACS by Xinbo Wang, Bo Zhang and David Zhigang Wang. In this, they suggest it is possible to oxidise benzylic alcohols to the corresponding ketones using sodium hydride (amongst other chemistry). Given that sodium hydride is, well, a hydride - this is quite something. Does it work? Hard to say without giving it a go, so I am.

What I'm Doing...

- Is there anything more colourful in the lab than sodium? I'm making some NaNp just now, and it's gorgeous! Blue/Green/Yellow/shiny... 3 weeks ago
- ... Vannusual B 2009-07-02
- Back2back papers from KCN in ACIEE; I'm on the case, but I've still got brain-hurt from the Himandrine post yesterday. Damn 3D... 2009-06-29
- It's Baran time again JACS ASAP... Post coming in a day or two, as I'm going out for dinner. Tapas, I believe... 2009-06-16
- ... How weird is following Process chemistry routes? This is the largest scale I've every worked on, and it's 1/10th of the published scale! 2009-06-13
- More updates...

About Tot. Syn.

It's all about stirring pots and hoping for shiny white crystals. Read-on to see some of the best modern organic chemistry, and comments from the folks at the bench.

What I'm Reading

- Catalytic [3+2] Annulation of Aminocyclopropanes for... from Angewandte Chemie International Edition
- The Taxadiene-Forming Carbocation Cascade from Journal of the American Chemical Society: Latest

Altmetric Explorer Reports dashboard Explore the data Help -Articles from Organometallics mentioned at least once in the past 1m Articles 106 Journals [] Activity 386 × Altmetric score of 195 Tweeted by 176 On 23 Facebook Pages Mentioned in 2 Google+ posts Synthesis, Structure, and Phosphorescent Emitters from Catalytic Studies of Palladium and Reddited by 2 Natural Products: Cinchonine-Platinum Bis-Sulfoxide Derived Iridium(III) Complexes Blogged by 5 Complexes Organometallics 1 readers on Mendeley **Organometallics** 0 readers on Connotea 1 readers on CiteULike Click for more details Diazadiene Complexes of the An Early-Late Transition Metal Heavy Alkaline-Earth Metals Hybrid Analogue of Hexaborane(12) Strontium and Barium: Structures > From publisher and Reactivity Organometallics Organometallics > With handle prefix > With Medline subjects NHC-Gold-Alkyne Complexes: Activation of M-Cl Bonds with Influence of the Carbene Phosphine-Alanes: Preparation > With subjects and Characterization of Backbone on the Ion Pair Zwitterionic Gold and Copper Structure Complexes Organometallics Matching PubMed query Organometallics > Funded by Bis(pyrazol-1-yl)acetic Acid Amidophosphine-Borane > Mentioned at any time on Bearing Ferrocenyl Substituents Complexes of Alkali Metals and [Pt₂(II)((M_rS_s , S_s)-p-tolyl-binaso)₂(μ -Cl)₂][BF₄]₂ (14): A vial was charged with 100mg (0.126 mmol) 5a and 24mg (0.126 mmol) AgBF₄. 2ml CH₂Cl₂ was added, the vial was covered and the reaction was left stirring in the dark for 2 hours. After this time, the reaction was filtered over celite to remove AgCl. Solvent was then removed to leave a yellow residue in the vial, the remaining clear, yellow solution was concentrated to a volume of about 1ml, and diethyl ether was added in a dropwise manner to the stirred solution to precipitate a yellow solid. The vial was centrifuged so the supernatant solvent could be decanted off by Pasteur pipette. The yellow solid was washed twice more with ether and the dried completely under high vacuum to give 99mg (93% yield) of product.

Emma, please insert NMR data here! where are they? and for this compound, just make up an elemental analysis...

 $Pt(II)((M_sS_s,S_s)-p-tolyl-binaso)(acac)(BF_4)_2$ (154): A vial was charged with 100 mg (0.126 mmol) 5a and 24 mg (0.126 mmol) AgBF₄. 2 mL CH₂Cl₂ was added, the vial was covered and the reaction was left stirring in the dark for 2 hours. After this time, the

ChemBark

News, Analysis, and Commentary for the World of Chemistry & Chemical Research

« Hacks for Septa

Organometallics Responds to the Dorta Situation »

A Disturbing Note in a Recent SI File

August 6th, 2013

A recently published ASAP <u>article</u> in the journal *Organometallics* is sure to raise some eyebrows in the chemical community. While the paper itself is a straightforward study of palladium and platinum bis-sulfoxide complexes, page 12 of the corresponding Supporting Information file contains what appears to be an editorial note that was inadvertently left in the published document:

Emma, please insert NMR data here! where are they? and for this compound, just make up an elemental analysis...

This statement goes beyond a simple embarrassing failure to properly edit the manuscript, as it appears the first author is being instructed to fabricate data. Elemental analyses would be very easy to fabricate, and

long-time readers of this blog will recall how fake elemental analyses were pivotal to Bengu Sezen's campaign of fraud in the work she published from 2002 to 2005 out of Dalibor Sames' lab at Columbia.

The compound labeled 14 (an acac complex) in the main paper does not appear to correspond to compound 14 in the SI. In fact, the bridged-dichloride compound appears to be listed an as unlabeled intermediate in Scheme 5, which should raise more eyebrows. Did the authors unlist the compound in order to avoid having to provide robust characterization for it?



Information

- » About ChemBark
- » Ground Rules
- » Mission & Editorial Compass











Recent Comments

- » TsOH on Some VERY Suspicious TEM Images in Nano Letters
- » Organometallic chemist on Organic Achievement of 2006: Pd(IV) Intermediates Might Not Be That Rare
- » Paul Bracher on Dorta Paper Link Roundup
- » DrWater on Dorta Paper Link Roundup
- » Lila Guterman on Dorta Paper Link Poundup





John A. Gladysz Says:

August 9th, 2013 at 5:52 PM

I have been meaning to contribute a post to this blog, where there has been so much good dialog involving the Reta Dorta manuscript on the ASAP site of Organometallics (om-2013-00067 or DOI: 10.1021/om4000067). There have been hits and misses, but I'd like to thank everyone for all input and commentary. Although I write this sentence with a wink to all my friends on my masthead page (http://pubs.acs.org/userimages/ContentEditor/1219929142245/orgnd7-masthead.pdf), this has made me muse whether an Editor-in-Chief could dispense with a high-maintenance Editorial Advisory Board and simply throw the various thorny issues that arise out for adjudication on a quality blog like Chembark.

I'll attempt to address some of the many good points raised in a series of posts. I can't promise I can reply to any counterpoints (e mail traffic has been heavy and will likely remain so), but I'll be sure to read them.

A lot of comments have been made about the breakdown of the peer review process in this particular instance, and if you read to the end of this post you will get some specifics, within the confidentiality bounds that I am obliged to maintain as an Editor. However, you are going to have to bear through a general analysis of the many things that can go wrong with SI first.

The first vulnerability is in the initial submission. I don't want to put down coauthor written manuscripts, but there are some corresponding authors who have clearly never laid an eye on their SI. Without this check, and I'm talking about a word-by-word read with attention given to every reagent quantity, spectroscopic data point, significant digit cutoff, etc., major errors are much more likely to slip through. My research group uses a proofing checklist, with every author fully participating, crystallographers excepted (except for their sections).

The second vulnerability is with the referees. I want to comment that I consider the pool of reviewers used by Organometallics as extremely conscientious. But obviously there will be cases, with any journal, where the SI is neglected.

A relevant digression involves JACS manuscripts. A reviewer may decide that the manuscript does not meet certain breadth/urgency criteria, and therefore not critique the SI. When such manuscripts are resubmitted to Organometallics (often with copies of the JACS reports), we do not render an Editorial decision until we are confident that the entire manuscript has been thoroughly peer reviewed.

The third vulnerability is with the Editors. I do not expect my Editors to carry out a word-by-word examination of the SI. However, we do follow an internal check list that I could in principle share, but all of the points therein can be found in our "Author Guidelines" (http://pubs.acs.org/paragonplus/submission/orgnd7/orgnd7_authquide.pdf)

An attendant vulnerability, pointed out by several on this string, involves the submission of the revised manuscript and accompanying SI. Suppose a reviewer or Editor requests that a melting point be added. At this stage, the Editor is unlikely to check anything other than the relevant paragraph. If an author has introduced other errors by some means (many comment about fixing minor typos), these will be overlooked.

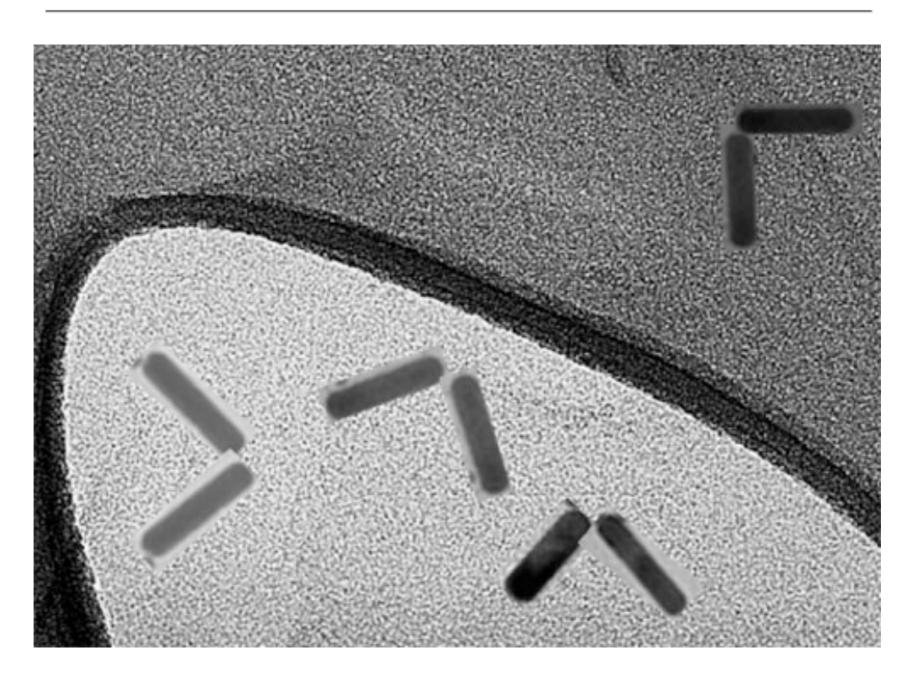
In summary, it is necessary to look at error introduction from a number of perspectives, and it may be difficult for "younger" authors with less publishing experience to view things from the inside. I'll eagerly "steal" any substantive additions that anyone offers if I ever have to present this analysis again, or incorporate it into a future Editor's Page of

Some really bad Photoshop





by mitch | science news | (463936 Views)









.@simonhiggins_60 @stuartcantrill @scburdet @fxcoudert We saw your tweets

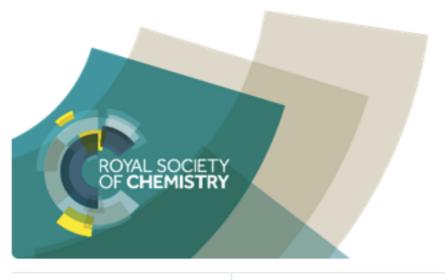
- here's some info about this retraction

We talked to the authors and decided there were grounds to retract, as per the notice.

During investigations we discovered the author list was incorrect.

We followed the recommended process to correct this, which resulted in the removal of several authors on the paper, including the corresponding author.

However we can understand how this now looks to readers, and so will now review what we can learn from this case.



RETWEETS

VLLIO

LIKES 4













A good example of listening, engaging and learning





"um, Dr Schrodinger? I opened the box and, well... we may have a problem"



It's not all just cat pictures, but even when it is, they can be quite funny...

RETWEETS 10,430

LIKES 8,693















5:35 AM - 9 Nov 2014





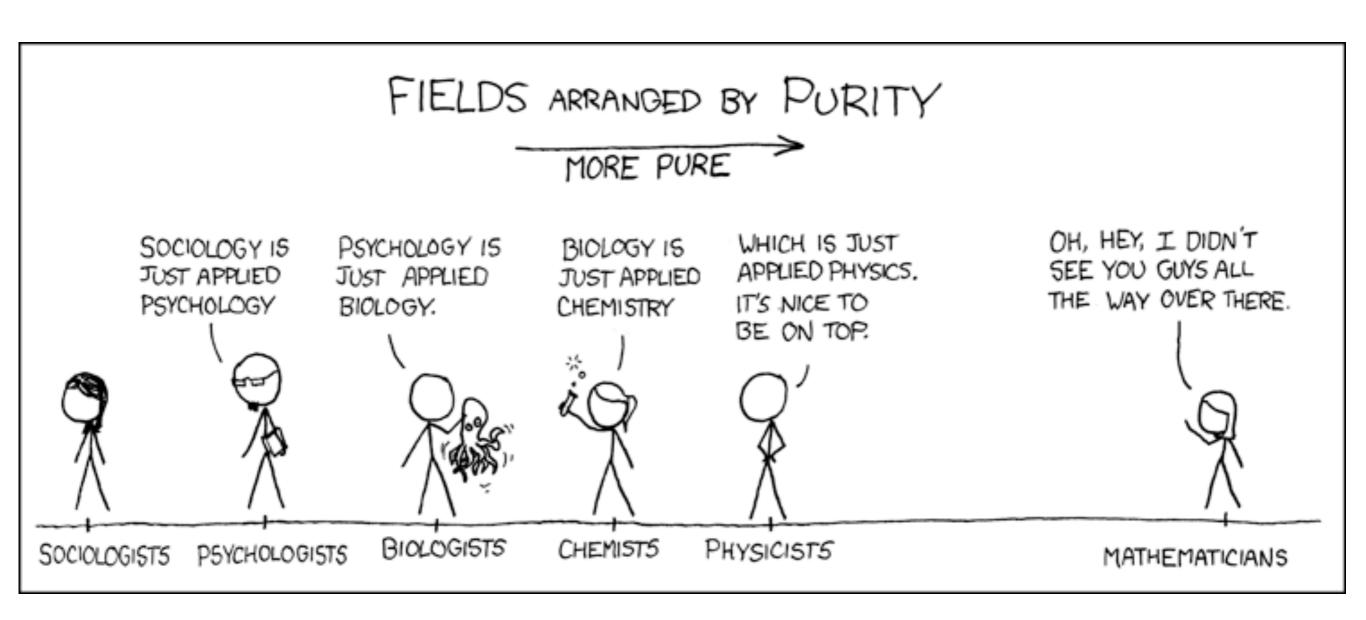






Thank you!

s.cantrill@nature.com Twitter: @stuartcantrill (and @NatureChemistry)



http://xkcd.com/435/