Chemistry in New Zealand

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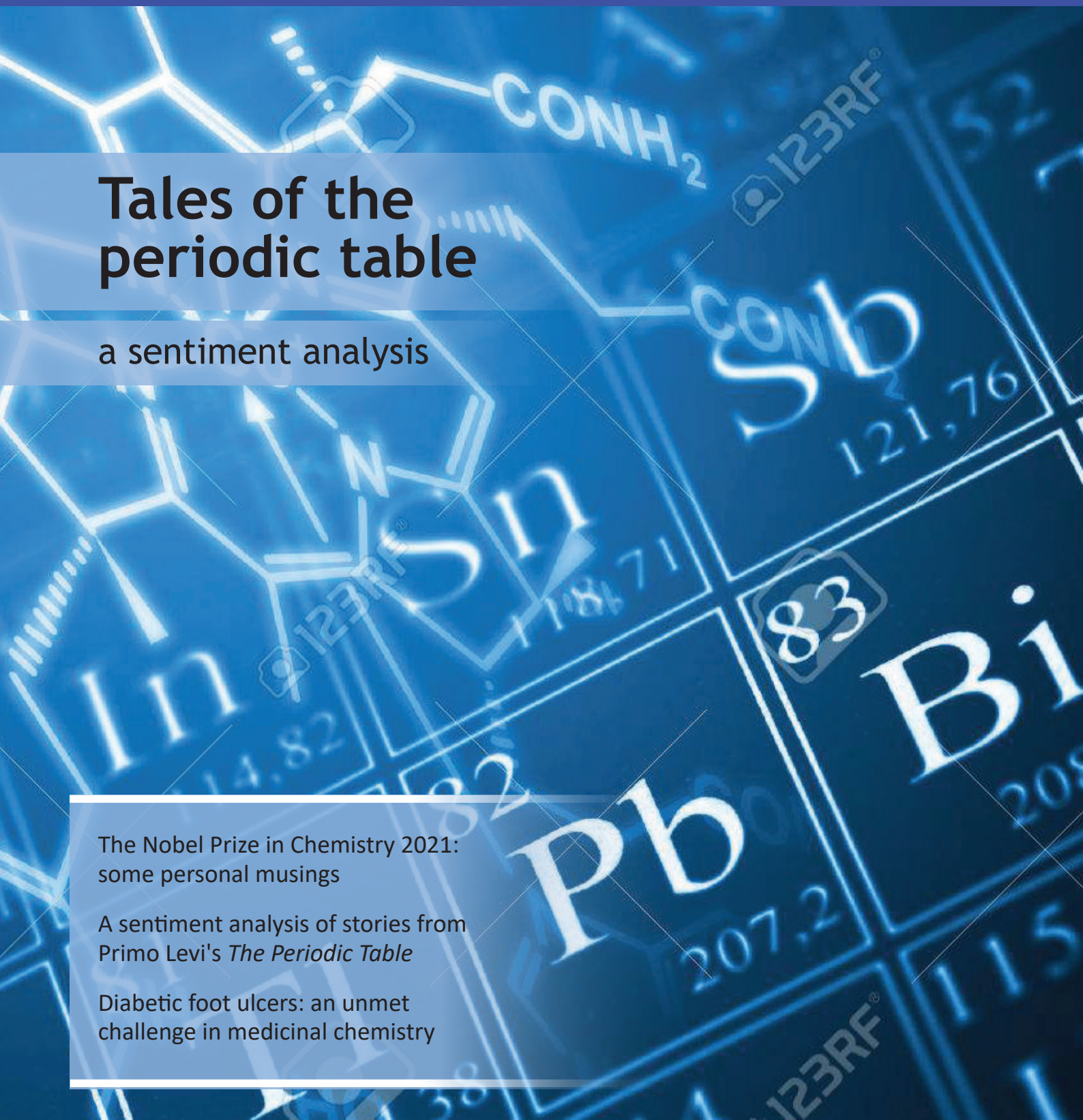

Tales of the periodic table

a sentiment analysis

The Nobel Prize in Chemistry 2021: some personal musings

A sentiment analysis of stories from Primo Levi's *The Periodic Table*

Diabetic foot ulcers: an unmet challenge in medicinal chemistry

Published on behalf of the New Zealand Institute of Chemistry in January, April, July and October.

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Chemistry in New Zealand

VOLUME 86, NO.1, JANUARY 2022

Articles and features

Other columns

Comment from the President

Kia ora koutou

Greetings to all NZIC members. With this edition, I bid you a very Happy New Year 2022 and hope that you had a safe and peaceful Christmas period with a good long break to relax. I think 2021 is a year many of us, including myself, would want to put firmly behind us, a little like 2020. By the time this edition appears, we will be working under the New Zealand government's new "traffic light system" which further advocates the importance of vaccinations against the COVID-19 virus and where we might have some more freedom to go about life and work without the disruption of frequent lockdowns.

Some of you may have noticed that our last issue was a double one. This was caused by some unavoidable delays in production which took us some time to work through. However, due to the fine efforts of Catherine Nicholson and her team, we were able to get this issue out to you which we hope you enjoyed.

Now that we are already in January 2022, it is important that I make mention of our NZIC Prizewinners of 2021. Last year, we had many high quality entries to the various prizes offered and so the awarding panels had a very difficult time deciding on the prize recipients. The details of these are already given on our website but in brief, these were Professor Martyn Coles from VUW who won the Maurice Wilkins Centre Prize for Chemical Science, Dr Anna Garden, University of Otago, who won the Easterfield Award, Dr Brendon Gill (Fonterra) who won the Douglas Pharmaceuticals Prize for Industrial and Applied Chemistry, Ms. Qing Wang who won the JEOL Brian Halton award for the best paper in the field of chemistry published by a New Zealand university student, and Jo Standley who won the sciPAD Denis Hogan award for Chemical Education.

Due to the events of 2021 with COVID lockdowns and the like, we were unfortunately not able to award these in person to the recipients at various events across the country and so had to send these via mail. I hope that you will join with me in warmly congratulating the prize winners for their excellent achievements in chemistry. We are fortunate to have had many high calibre applicants to choose from. To all applicants, we send out a vote of thanks for sharing your achievements with us.

On the NZIC front, there have been a number of changes both in terms of people and in where we host our webpages.

Firstly, I am delighted to announce the appointment of our new Publishing Designer, Natalie Bould. Natalie has wide ranging experience as a journalist, subeditor and graphic designer, and has worked across a number of sectors which include media, non-profit organisations and local government. She will bring a wide range of technical skills to the role and is particularly interested in combining good design with the written word to create publications that people want to engage with.

Natalie will be closely involved with our move into a digitised version of CiNZ. We look forward to working with her and the subcommittee headed by Associate Professor Vyacheslav Filichev from Massey University, as they implement this change.

We acknowledge the efforts of Raoul Solomon, our former publishing editor, especially in the design of the new NZIC logo that features on the cover of this issue.

Secondly, I would like to announce that we are moving our NZIC webpage off a website which had been hosted by Ackama, a web hosting company associated with the Royal Society Te Apārangi, to another provider. By the time this column appears, this change will have been cemented in place. We anticipate the web address URL will be the same as that used previously to access the NZIC webpages so you will not notice a great change. It was important that we carried out this change as we need a stable website to allow us to crack on with our plans to deliver to members a fully digitised *Chemistry in New Zealand* journal this year.

Noho ora mai

Michael Mucalo, NZIC President

NEWS

AUCKLAND

University of Auckland

STAFF SUCCESSES

Ira Mautner, who works with Michel Nieuwoudt and others in the Photon Factory won a Best Poster Presentation Award at the 12th International Conference on Skin Ageing and Challenges, 2021. This was titled, "Development of portable Raman spectroscopy as a clinic tool for assessing photodamage in skin."

Orbis Diagnostics (a spinout from UOA chemistry staff Matheus Vargas, David Williams and Cather Simpson) partnered with Air New Zealand to test staff's COVID-19 immunity levels in a trial of the rapid testing platform they developed. For more information see: https://www.orbisdiagnostics.com/announcements/orbis-conducts-trial-of-immunity-levels-with-air-new-zealand

Dr Ziyun Wang, was awarded a Fast Start Marsden Grant for his application, "Understanding selectivity determinants in CO2 electrochemical reduction reaction."

Dr Joel Rindelaub (Research Fellow in SCS) was the subject of a feature in the NZ Herald weekend magazine, Canvas, that discussed his motivation for conveying science to the public. His communication methods now extend to rapping about the coronavirus!

Geoff Waterhouse has been awarded a James Cook Research Fellowship for the project, "Catalysing the decarbonisation of New Zealand's energy sector." Geoff's two-year Fellowship will target the discovery of efficient non-precious metal electrocatalysts for the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), key processes in a number of emerging energy conversion and storage devices such as fuel cells, rechargeable metal-air batteries and water electrolysers.

Professor Jadranka Travas-Sejdic was one of the recipients of the HRC 2020 NZ-China Covid-19 Collaboration Fund. Jadranka received funding for a two-year project entitled, "Printed sensing strips for sensitive and reliable detection of SARS-CoV-2."

New Faces

Dr Christopher Larsen has accepted a position as a lecturer in inorganic chemistry commencing August 2022. Chris is a PhD graduate from the University of Otago, who has held postdoctoral positions at the University of Basel and Stanford University before becoming an independent Ambizione Fellow at the University of Geneva.

Dr Danaé Larsen joined us mid-September 2021 as a lecturer in Food Science. She graduated with a PhD from SCS and has held postdoctoral positions in chemical and materials engineering at UoA and at Heidelberg University, Germany.

Dr Marie-Anne Thelen joins us in January as a Professional Teaching Fellow with particular responsibility for our articulation agreement with Northeast Forestry University (NEFU) in China.

STUDENT SUCCESSES

PhD completions

Nabangshu Sharma successfully defended his PhD thesis entitled, "Harnessing the potential of proteins for sustainable development: from bioremedijation to drug discovery" on 13 August. During his PhD, Nabangshu explored the use of enzyme technology for environmental remediation as well as developed new methodologies to study enzymatic processes and protein-protein interactions.

PhD Student Prizes

Oscar Shepperson won the prize for the best student talk entitled, "Total synthesis of novel antimicrobial β-hairpin capitellacin via rapid flow-based SPPS assembly and regioselective on-resin disulfide cyclisation" at the Royal Australian Chemical Institute – Peptide Users Group (PUG) 2021 Symposium held in Melbourne (and by zoom).

Miriama Wilso, was awarded runner up for Best Student Poster at the Testing the Waters 5 Conference held in Brisbane.

Qing Wang, a MacDiarmid Institute-funded PhD student, was awarded the NZIC's JEOL Brian Halton Award. The Brian Halton Award is awarded for an outstanding paper in the field of chemistry published by a New Zealand University student.

Qing's paper entitled, "Molten NaCl-assisted synthesis of porous Fe-N-C electrocatalysts with a high density of catalytically accessible FeN4 ac-

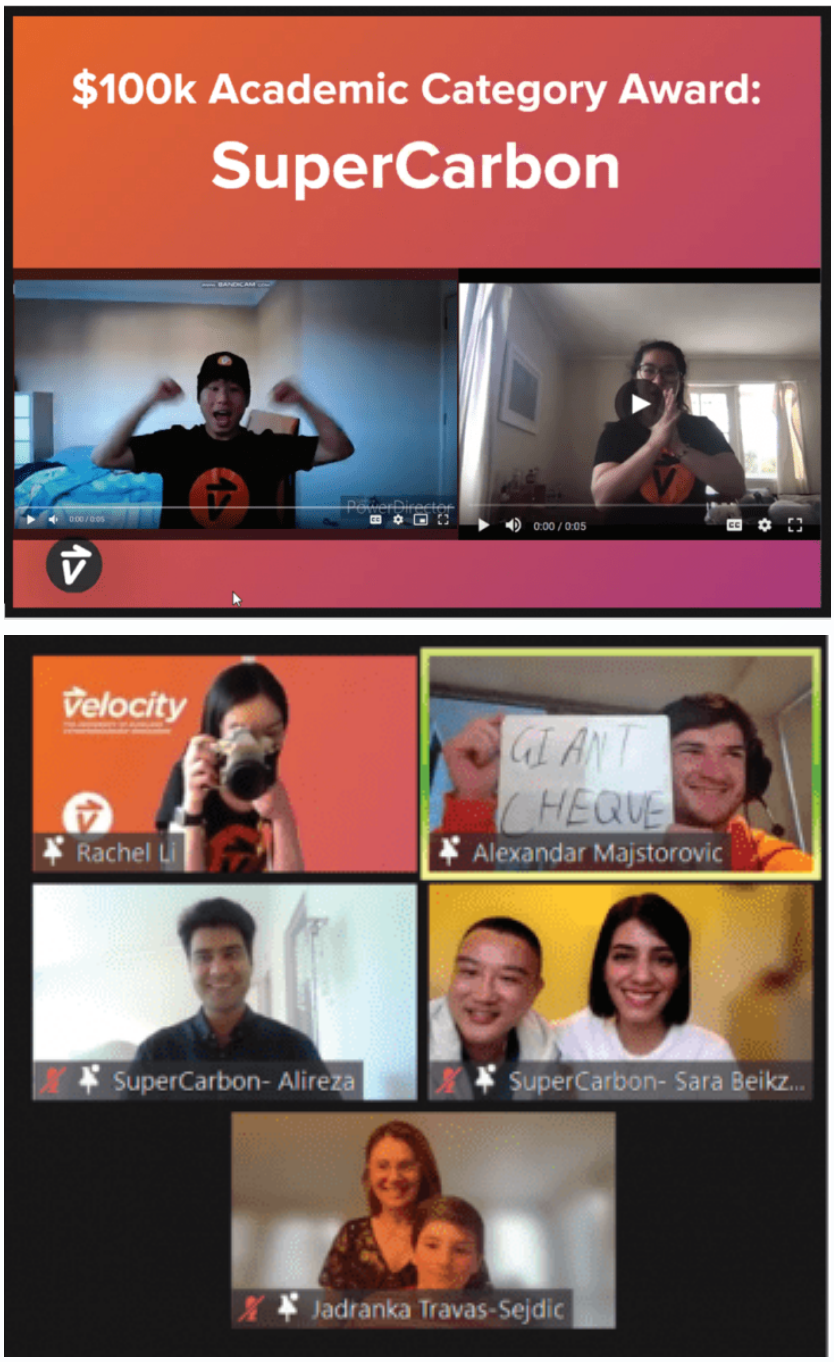
tive sites and outstanding oxygen reduction reaction performance" published in Advanced Energy Materials (impact factor 29.368), reports a novel synthetic strategy towards Fe-N-C electrocatalysts for fuel cells. This work supports the development of a carbon-neutral hydrogen economy in New Zealand (https://doi.org/10.1002/aenm.2021002).

PhD student Sara Beikzadeh, research fellow Alireza Akbarinejad and Professor Jadranka Travas-Sejdic were the core of the winning team in the academic category at the 2021 Velocity 100k Challenge Grand Finals for their entry, SuperCarbon. They were one of five winning teams. The SuperCarbon public disclosure statement is:

"SuperCarbon is a ground-breaking technology with sustained antimicrobial and antiviral properties and multiple applications, including electroceutical wound dressings, antivirus and antibacterial face masks, anti-pathogen air filters, and antiaging beauty facial devices. Our lead product, the HealectricCarbon wound dressing uses microcurrents to accelerate healing in chronic and acute wounds and to prevent infection. It can significantly improve patient outcomes whilst markedly decreasing healthcare costs."

Alex Risos was one of five winners in the Velocity 100k Challenge with his company RisosEnterprises. His publicity for the company states, "Waterborne E. coli testing is a monumental effort, prohibitively expensive and takes days to yield results. Eighty percent of New Zealanders are not only unhappy with environmental water but especially with their drinking water.

"RisosEnterprises is working on technology that is much faster and more accurate than any existing water testing instrumentation to date. This cuts down testing costs and reaction times to critically enable widespread testing for effective countermeasures. RisosEnterprises are creating the Waicorder (TM), a star-trek inspired water tricorder that everyone can use to sense water quality anywhere, anytime. Communities will benefit from a healthier environment and drinkable water, while private industry cuts down on production losses, especially beverage manufacturers."



The SuperCarbon team were winners in the 2021 Velocity 100k Challenge

Forensic Science PhD student Courtney Lynch was awarded first place in the SGS Research Showcase for her poster titled, "Pick and mix-tures: decoding forensic stains with RNA". Courtney is based at ESR Ltd, where she is supervised by Douglas Elliot and Rachel Fleming.

Thuy Trang Pham was named on the Dean's List. This is an excellent achievement, with fewer than 30 PhD graduates from throughout the university making it to the Dean's List last year. Trang was supervised by Jon Sperry on the project, "Synthetic applications of the chitin-derived platform 3-acetamido-5-acetylfuran (3A5AF)."

AUT

NEW FACES

Welcome back Anau Lautaha. Anau has taken up a Dodd-Walls Centre funded research position with Professor Nicola Brasch and will be carrying out studies on photoactive molecules which release nitroxyl (HNO).

Marina Kisa was awarded a summer studentship under the supervision of Dr Taniela Lolohea. Marina will be working on the project, "Atmospheric plasma 'plants' – exploring plasma deposition onto seedlings towards improved growth of radish plants."

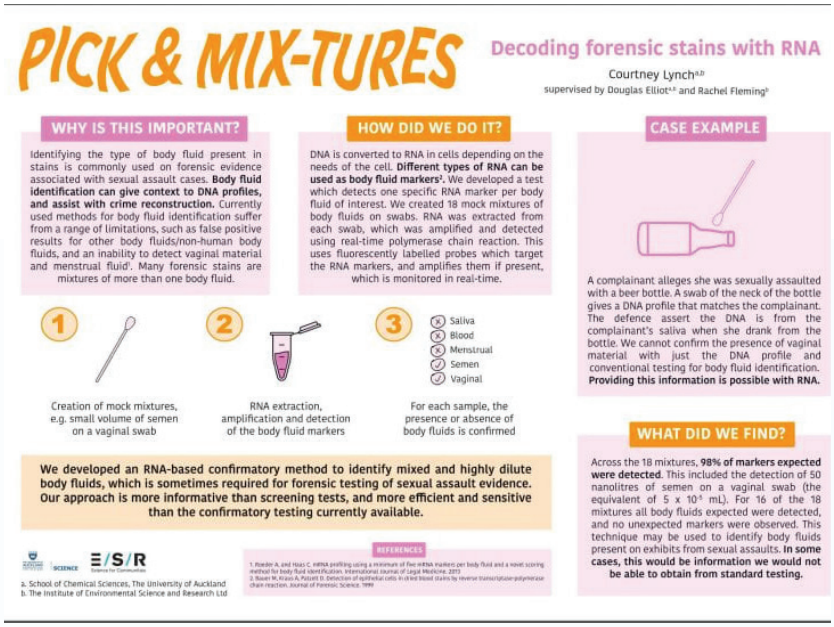
Jade Williamson will be doing a summer studentship under the supervision of Dr Cassandra Fleming. Jade will be working on, "The design and synthesis of two-photon excitable fluorescent histone deacetylase inhibitors."

Shaun D'zousa was also awarded a summer studentship and will be working with Dr Jack Chen on a project entitled, "Stimuli-responsive nanocontainers for targeted drug delivery."

CONGRATULATIONS

Dr Jack Chen was awarded KiwiNet Tier 1 funding for the project, "Cellulose-based surfactants." Jack's team will be developing sustainably-produced surfactants for applications in industry as emulsifiers, wetting agents and solubilisers.

Dr Jack Chen was nominated to be a member of the Science of Synthesis Early Career Advisory Board, with the two-year term beginning 1 January 2022.



Vinay Bharadwaj has successfully defended his PhD thesis entitled, "Mechanistic studies on the photodecomposition of caged N-hydroxysulfonamides incorporating the 2-nitrobenzyl, (2-nitrophenyl)ethyl and (6-bromo-7-hydroxycoumarin-4-yl) methyl chromophores." Vinay was supervised by Professor Nicola Brasch.

MANAWATU

CONGRATULATIONS

Congratulations to the following staff for their recently announced promotions:

- **Dr Helen Fitzsimons** to Senior Lecturer Range 2.
- **Dr Tammy Lynch** to Associate Professor.
- **Dr Jonathan Marshall** to Associate Professor.
- **Associate Professor Patrick Biggs** to Professor.
- **Associate Professor Mark Waterland** to Professor.
- **Professor Paul Plieger and Associate Professor Gareth Rowlands** were both made Fellow of the Royal Society of Chemistry.

On 21 September 2021 at the 72nd meeting of the Division of Colloid and Surface Chemistry held by the Chemical Society of Japan, Associate Professor Catherine Whitby gave an invited seminar titled, "Yielding to stress: the effect of interparticle interactions on how Pickering emulsions flow."

Courtney Lynch (below) and her winning poster (above).

3rd year undergraduate student Braydon Nikolaison won the SFS Summer Vacation Scholarship for chemistry majors. He will be working with Associate Professor Catherine Whitby on a project titled, "Investigating the interfacial rheology of protein nanoparticles at oil-water interfaces."

WAIKATO

UNIVERSITY OF WAIKATO

CONGRATULATIONS

Congratulations to Lewis Dean and Sravan Bandaru, who both successfully completed their PhDs (Lewis with Michèle Prinsep and Sravan with Graham Saunders).

Congratulations also to two former PhD students. Brendan Gill (supervised by Merilyn Manley-Harris) won the Douglas Pharmaceuticals Prize for Industrial and Applied Chemistry and is a senior research scientist at Fonterra. Hayden Thomas (supervised by Graham Saunders) has been appointed as a research officer in the School of Science and is predominantly in charge of the NMR spectrometer and other instrumentation such as the ICPMS.

The School of Science held their Postgraduate conference online in October 2021. There were 37 oral presentations and 20 posters. The day was well attended, with 147 participants.

Sebastian Hopker (supervised by Adam Hartland and Megan Grainger) won the best geoscience-related oral presentation, sponsored by the Geoscience Society of New Zealand.

Shaun McNeil (supervised by Merilyn Manley-Harris) won the prize for best chemistry-related oral presentation, sponsored by the NZIC Waikato Branch.

Edie Thomas (supervised by Megan Grainger) won the prize for best poster, sponsored by the Waikato Science Club.

Hill Laboratories

Hill Laboratories have been conducting saliva testing for COVID-19 since late 2020, with services focused into the aged care sector. They have now been awarded accreditation for their COVID testing services.

Hill Labs utilises the "SalivaDirect" methodology in their Hamilton-based laboratory, a non-invasive method which was developed by New Zealander Anne Wyllie's group at the Yale School of Public Health in the USA.

This non-proprietary method has been made publically available and has been implemented in many laboratories globally, with millions of tests successfully conducted. It has been fully validated, and is now referenced in many publications in peer-reviewed journals.

Initially, Hill Laboratories will be delivering saliva testing services for COVID to businesses, preferably working through existing partners who specialise in the collection of human biological samples.

CANTERBURY

UNIVERSITY OF CANTERBURY

AWARDS

Laura Revell

Dr Laura Revell has won the prestigious Royal Society Te Apārangi Cooper Award - Early Career Research Excellence Award - Technology, Applied Science and Engineering for her research into climate change and atmospheric science.

"I am honoured to receive the 2021 Cooper award, and the acknowledgement it brings for my field of atmospheric chemistry and climate research," says Dr Revell.

GRANTS

Congratulations for success in the latest Marsden round.

Professor Antony Fairbanks, School of Physical and Chemical Sciences at UC, is PI on a $921,000 grant for his research, "Radically different; new reactions of unprotected sugars in aqueous solution."

Dr Laura Revell, School of Physical and Chemical Sciences, is AI on a $921,000 grant for "Electromagnetic scattering by particles of arbitrary size and shape with application to microplastics."

Daniel Foley

Congratulations for grants from the Canterbury Medical Research Foundation (CMRF)

Dr Daniel Foley in the School of Physical and Chemical Sciences, has received $109,946, for a project that aims to develop safe and effective treatments based on a better understanding of key molecular mechanisms underlying breast cancer.

Dr Foley said the Canterbury region has a notably higher number of cancer registrations than the national

average. Every day, breast cancer claims the lives of two New Zealand women. Māori women have one of the highest incidences of breast cancer worldwide – 60% higher than Pākehā. https://buff.ly/3oLEK43

Tim Allison

Dr Tim Allison in the School of Physical and Chemical Sciences, has received $110,00 to study "How a crucial toxin is secreted from Mycobacterium tuberculosis to kill immune cells." In this project, Tim and postdoctoral researcher Dr Thu Ho will work toward understanding the structure and assembly of specific proteins within the exotoxin secretion system of M. tuberculosis, the pathogenic bacterium responsible for greater 1 million deaths per year.

PhD Completions

Congratulations to Andrea Mascherpa who successfully defended his PhD thesis. Andrea's thesis was titled, "The production of phosphorylated glycoconjugates" and he was supervised by Antony Fairbanks. The viva voce exam took place over Zoom and Andrea was examined by Dr Philip Rendle (Ferrier Research Institute).

Congratulations to Xin Qiu who successfully defended his PhD thesis titled, "New protecting group free transformations of carbohydrates" and supervised by Professor Antony Fairbanks. The viva voce exam took place over Zoom and Xin was examined by Professor David Larsen (Otago).

RNZ Interview: Supplements

Do natural health supplements work? University of Canterbury toxicology Professor Ian Shaw says the evidence is low. He criticises statements by supplement businesses that sound like medicinal claims and mislead consumers. For more see the link to his interview on 1 November 2021:

https://www.rnz.co.nz/national/programmes/checkpoint/audio/2018818702/supplements-natural-does-not-always-mean-safe-professor

Retirement: Alison Downard

Professor Alison Downard gave her final lecture in October and we all popped in to surprise her. After 33 years at UC she is retiring at the end of the year. We will miss her!

Alison completed her PhD on "Electron transfer reactions of organometallic clusters" at the University of Otago in 1979. After a postdoctoral position overseas, she returned to New Zealand and began lecturing at the University of Canterbury in 1988. She gained her Professorship in 2009 and is an Emeritus Investigator with the MacDiarmid Institute.

In 2014 Alison was awarded the RH Stokes medal from the Royal Australian Chemical Institute. The medal is awarded in recognition of distinguished research in the field of electrochemistry carried out mainly in Australasia.

That same year she was elected as a Fellow of the Royal Society of New Zealand.

In 2017, Alison was featured as one of the Royal Society Te Apārangi's 150 women in 150 words. https://buff.ly/3vntRH7

Alison has published more than 100 refereed papers on various aspects of electrochemistry.

She has undertaken various leadership roles including Associate Dean

Alison Downard

of Science (1999-2004) and Head of Department of Chemistry (2009-2010). Alison's research has made pioneering discoveries involving the chemical modification of surfaces at the nanoscale, leading to new electrodes with applications in energy storage and conversion.

Alison is looking forward to spending more time in the great outdoors.

Microplastics publication in *Nature*

Aotearoa New Zealand scientists recently found that microplastics – which are in our rivers, oceans and land – are also in the air we breathe. Now local scientists have discovered airborne microplastic pollution is likely to directly affect climate change.

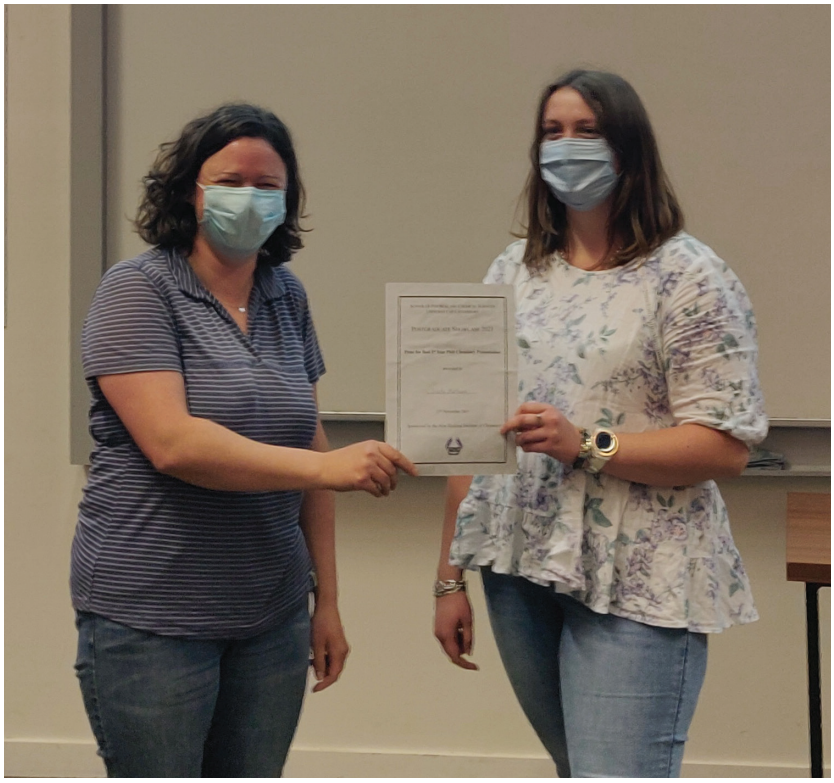
Dr Laura Revell, along with University of Canterbury colleagues Dr Peter Kuma and Professor Sally Gaw and MacDiarmid Institute researchers Professor Eric Le Ru and Dr Walter Somerville at Te Herenga Waka, reviewed concentrations of airborne microplastics reported by previous studies. The findings in the paper entitled, 'Direct radiative effects of airborne microplastics' were published in *Nature* (https://buff.ly/3E0YLrL). Some of the findings included:

"Airborne microplastic pollution will become more severe in future—not only are microplastics durable but, based on current production and waste management trends, the abundance of plastic accumulated in

landfills and the environment is projected to double over the next three decades.

Since plastic degrades through age and exposure to UV light to produce secondary microplastics, we expect microplastics to be present in Earth's atmosphere for many years to come. In the absence of serious efforts to address microplastic pollution, mismanaged plastic waste could exert an influence on climate in the future.

Future research should assess whether microplastics influence climate regionally; anthropogenic aerosols have been linked to changes in heat extremes, and microplastics may similarly influence local and regional climate. This is especially true of urban environments, where airborne microplastics are already present on the order of hundreds to thousands of microplastic particles per cubic metre and may already contribute locally to atmospheric heating and/or cooling".



Associate Professor Sarah Masters (left) presents postgraduate student Brooke Matthews with the prize for best first year PhD presentation.

Techweek Talk

Dr Anna Farquhar completed her PhD at the University of Canterbury School of Physical and Chemical Sciences in 2017. For her PhD, Anna studied graphene and designed electrode materials based on graphene to be used in supercapacitor electrodes. After finishing her PhD she completed a postdoc at the University of Alberta, Canada, before starting work as a senior scientist at Aeroqual in Auckland.

Aeroqual is a company that specialises in air quality monitoring. As a member of the R&D team at Aeroqual, Anna's work involves studying various types of sensor technology including electrochemical gas sensors, metal oxide semiconducting sensors and optical particle sensors. This work includes developing new sensor materials for different gases, as well as improving and understanding the behaviour of commercially available gas sensors.

Check out this video where she discusses her work https://buff.ly/3pgazCi

Recently Anna gave an invited talk at the "Deep tech creating an economic boost for NZ" Techweek event in Christchurch organised by the MacDiarmid Institute and attended by Hon Dr Megan Woods, Minister of Research, Science and Innovation.

Postgraduate Student Research Showcase 2021

The School of Physical and Chemical Sciences held its 2021 Postgraduate Showcase afternoon on 25 November 2021. This was an all-day event that celebrated the research endeavours of our MSc and PhD postgraduate students. There were 20 presentations over three sessions, followed by a fantastic plenary seminar by Dr Anna Garden (University of Otago). At the conclusion of the Showcase, the judges (Associate Professor Deb Crittenden, Associate Professor Chris Fitchett and Associate Professor Sarah Masters) had the tough decision of determining our prize winners. These were:

- The prize for best Master's presentation went to Hayden Masterton (Gaw research group), for his presentation entitled, "Plastics as vectors for metals in the marine environment" sponsored by RSC-NZ.

- The prize for best first year PhD presentation went to Brooke Matthews (Kruger research group), for her presentation entitled, "Hoffman-like hybrid ultramicroporous materials for selective gas adsorption" sponsored by NZIC.

- The prize for best second year PhD presentation (Ralph H. Earle Jr Seminar Prize) went to Joel Schuurman (Brooksby research group) for his presentation entitled, "Modifying perovskite electrodes for solar cells." This prize was bequeathed to the School by the late Ralph H. Earle Jr., who strongly believed that chemists

should appreciate the importance of being able to verbally communicate their subject.

■ Finally, our prize for best third year PhD presentation went to Max Caplin (Foley research group), for his presentation entitled, "Synthesis of topologically complex fragments for drug discovery" sponsored by RSC-NZ.

OTAGO

The Otago branch of the NZIC is pleased to continue to sponsor prizes at the Aurora Energy Otago Science and Technology Fair. This year we awarded 11 prizes to the following young chemists - congratulations to all! Aaron Hill, "Elephant toothpaste"; Callum Attwell, "Removing oil experiments"; Cerys Thomas, "pHaecal matters!"; Dan Kelleher, "Don't overreact"; Harriet Rowe, "Save our waterways"; Jomana Moharram, "Poison in your backyard: fractionation of leaf extracts"; Liv Buckby, "Are shellfish strong or not?"; Niamh Clark, "Squashed tomatoes"; Odin Hyink, "A beginners guide to not killing your fish"; Rata Jameson, "Finding a light source in the produce section"; Viktor Mann, "Removing oil experiments."

UNIVERSITY OF OTAGO, DEPARTMENT OF CHEMISTRY

AWARDS

There have been a number of prizes and fellowships awarded recently. Keith Gordon received the University of Otago Distinguished Research medal, giving his medal lecture on 18 November 18 entitled, "Using light to unpick complex materials; from solar cells to krill oil." Anna Garden was awarded the 2021 Easterfield Medal from the NZIC. Charlie Ruffman was award a Rutherford Postdoctoral Fellowship to be taken up at the University of Auckland.

Five years of funding has been secured (on both the NZ and German sides) by co-leaders Sally Brooker (Otago) and Paul Jerabek (Helmholz Zentrum Hereon, Hamburg) of the German-NZ Green Hydrogen alliance. In partnership with Ngāi Tahu, they will foster green hydrogen relationships between the two countries, and provide opportunities for investment and collaboration with high-value industrial and research partners.

Courtney Ennis was awarded a Marsden grant for his project, "Laboratory exploration of co-crystal minerals for planetary chemistry: assisting NASA Dragonfly's search for the origins-of-life on Titan."

The group of Keith Gordon has been busy with PhD submissions and defences. Joseph Mapley and Piumika Samanali Garagoda Arachchige (Samanali) submitted their PhD theses titled "Spectroscopic and computational investigations of charge transfer excited states" and "Using vibrational spectroscopy and chemometrics to understand structure and properties in biological systems" respectively. Kārlis Bērziņš ("Low-frequency Raman spectroscopy in pharmaceutical applications"), Jeremy Rooney ("Analyses on low temperature curing waterborne coil coatings") and Chima Robert ("Vibrational spectroscopic analysis of complex systems") successfully defended their theses, with Karlis being placed on the sciences divisional list of exceptional doctoral theses. Jeremy and Karlis have started working as postdoctoral fellows in the Gordon group.

Peter Remoto and Sam Harris recently completed their honours course with the group. Peter investigated dehydration processes in pharmaceuticals using low frequency Raman spectroscopy, while Sam studied an interesting series of cationic donor-acceptor dyes. Lea Muetzel has also completed an undergraduate research project correlating the spectroscopic properties of a range of laundry detergents to their end user performance.

Lea, Peter, Joshua Kirkham and Lia Heremia joined the group over the summer. Lea is working with Joseph to study a series of organic dyes. Peter is working on using low frequency Raman spectroscopy to evaluate softening transitions in glassy materials. Lia and Joshua are working with Sara on creating model GI tissue phantoms and testing the newly developed multi-spectroscopic probes for disease diagnosis respectively.

Keith Gordon gave a virtual invited talk at the Asian Photochemistry Conference (APC2021) in November. The meeting was hosted from Yonsei University in Korea. His talk entitled, "Excited state complexity in metal complexes with ILCT and MLC states" was in the Spectroscopy and Dynamics section of the meeting.

Article

The Nobel Prize in Chemistry 2021 - some personal musings

ANTONY J. FAIRBANKS

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Keywords: *Nobel Prize, organocatalysis, synthesis, enamine, iminium*

One Wednesday morning in Stockholm; one Wednesday night in New Zealand

On the night of Wednesday 6th October our household stayed up a little later than usual to watch the live YouTube feed from the Royal Swedish Academy of Sciences for the 2021 Nobel Prize in Chemistry announcement. I have to confess that this year was the first time I have ever done this.

Why this year, and not previous years you may ask? Well, this year I was really gunning for Katalin Karikó to win the Prize, perhaps along with her long-term collaborator Drew Weissman. Who is Katalin Karikó you may perhaps ask, as she's not a chemist that many of us will have heard of – well at least not until last year!

As many now know, she is the inventor of the RNA vaccines that we have all been taking; the genius behind both the Pfizer/BioNTech and the Moderna jabs. Having looked into the RNA vaccine development a little deeper, I was delighted to discover that a key aspect of those RNA vaccines was the incorporation of a C-glycoside analogue of uridine into the sequence;[1] of course this struck a chord with a carbohydrate chemist. Moreover, Karikó's personal story is one that resonates with those who have faced grant rejection, and suffered at the hands of anonymous peer-review, and it should be told in full in these pages at some point in time. However, now is not that time.

Back to the hall in Stockholm, full of gilded portraits. After a short hiatus, the Secretary General of the Royal Swedish Academy of Sciences, Göran K. Hansson, was seated, and then followed the announcement[2], at about 10.45pm NZ time, that this year the prize was to be shared by Benjamin List and David MacMillan for their work on organocatalysis. Honestly, I felt a bit flat; I thought Karikó would be a shoo-in.

Antony Fairbanks undertook both his first degree and DPhil in chemistry at Oxford, the latter with Professor George Fleet. After two postdocs (Professor Pierre Sinaÿ, École Normale Supérieure, Paris and Professor Steve Ley, Cambridge) he became an independent academic at Oxford in 1996. In 2009 he moved to UC and was Head of the Department of Chemistry from 2010-2014 during the Christchurch earthquakes. He is an organic chemist with research interests focussed on carbohydrate chemistry and biology. Antony has authored/co-authored >160 scientific publications. In 2018 he was awarded the NZIC Maurice Wilkins Centre Award for Chemical Science.

"Surely this is the mark of true genius; to see something so beautiful and simple that everyone else has missed?"

I texted a colleague who was also watching – similar feelings. Surely Karikó should have won? But then I thought a bit more deeply, "Isn't organocatalysis just fantastic?" And wasn't it top of my personal list for the best development in organic chemistry in the last 20 years? Maybe I needed to think about this a bit more? I switched off the YouTube feed, and headed off to bed.

Mulling things over

The next day the prize was of course a topic of conversation at work, and I began to think about the 2021 award again. Catalysis is undoubtedly exceptionally useful, and asymmetric catalysis the most useful method for the creation of chirality. However, enzymes aside, catalysis in synthetic organic chemistry has long been the preserve of the transition metals. For example, the 2001 Nobel Prize was shared by Sharpless (1/2), and Noyori and Knowles (1/4 each), for their seminal work on asymmetric transition metal-catalysed oxidation and reduction reactions respectively.

More recently, transition metals triumphed again in 2010, when Heck, Negishi, and Suzuki shared (1/3 each) the prize for palladium-catalysed cross-coupling reactions. And of course, one cannot forget the 2005 triumph of our good friend Bob Grubbs (an Erskine fellow at UC when the prize was announced), when he shared the prize (1/3 each) with Chauvin and Schrock

for transition-metal catalysed olefin metathesis. So, in the world of catalysis, transition metals rule supreme and you can't really do anything that useful without them, particularly in attempts to control stereochemistry. That is unless you can do molecular biology and clone and express an enzyme, which may be able to help you out as long as your substrate scope isn't too broad.

Then, along come List and MacMillan, and all of this prevailing thought goes out of the window right at the start of the new millennium.

Organocatalysis is such a wonderfully simple concept – that you can control the stereochemical outcome of a reaction by simply adding a catalytic amount of a small organic molecule to your reaction process; the key point being that if the catalyst is chiral, and you add only one enantiomer of it, then you can control the enantioselectivity of the overall bond forming process.

It was a brilliant development for the 'simple' organic chemist like myself; one who loves curly arrows and solid lines to represent bonds. Gone are electron counting problems, confusing catalytic cycles, and 'magic' bond rearrangements steps; everything can once again be rationalised simply pushing the good old curly arrow.

The advent of organocatalysis was something like an 'emperor's new clothes' moment for organic chemistry. Sitting in the Ilam Homestead at the University of Canterbury Club (formerly the University of Canterbury Staff club) mulling the Nobel announcement over a beer a few days later, one thought that resonated with Jim Coxon and myself was that, back in the early 2000s when we had just read the papers of List and MacMillan, we had both thought to ourselves, "Why didn't I think of that? It's so obvious!"

So, surely this is the mark of true genius; to see something so beautiful and simple that everyone else has missed?

Benjamin List, Director of the Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany. Photo courtesy of David Ausserhofer / MPG.

The first discoveries: Benjamin List

List's first seminal contribution to the field concerned enamine catalysis of the aldol reaction. At UC I teach the aldol reaction and its applications in synthesis in the second half of the second year of undergraduate study (200-L). As you all know, the aldol is a simple and highly useful C-C bond forming reaction involving attack of one carbonyl compound (either as the enolate formed by deprotonation by a base, or in the enol tautomeric form) onto the carbonyl of another (Scheme 1A).

Students learn about the inherent problems of controlling crossed aldol reactions, such as how to control which component is the electrophile and which is the nucleophile, and also about the use of enamines. Enamines are readily formed by reaction of carbonyls with secondary amines (Scheme 1B) and are reactive, yet neutral 'enolate equivalents'. They are very useful for making C-C bonds; chemistry that was pioneered by Gilbert Stork back in the 1950s.[3] So, surely chiral enamines have been extensively used to control the stereochemical outcome of these types of reactions for almost as long as enamines have been around?

Well, actually no.

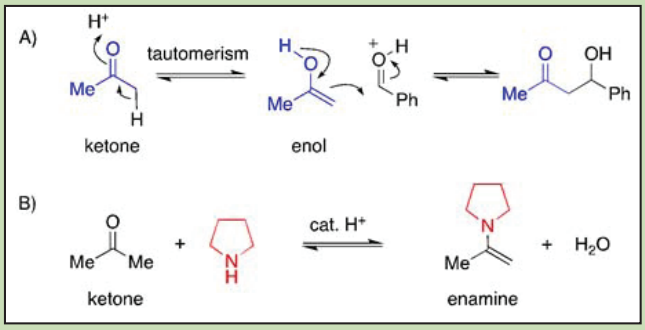
Hindsight is a wonderful thing. Looking back, what is remarkable is that two versions of an asymmetric intramolecular aldol reaction catalysed by the chiral secondary amine proline had been reported as far back as 1971; the Hajos–Parrish–Eder–Sauer–Wiechert reaction.[4,5] Although appreciated at the time as the first asymmetric aldol reaction, applications were limited and only ever intramolecular.

Only some 30 years later did List have the insight to examine and develop the use of proline as an asymmetric catalyst for intermolecular aldol processes. The first seminal work by List was submitted for publication on Dec 7th 1999[6], and detailed the proline-catalysed crossed aldol reaction of acetone with a series of benzaldehydes. The products of these reactions were preferentially formed as the (R)-enantiomers, with enantiomeric excess (ee) of ~75% (Scheme 2A).

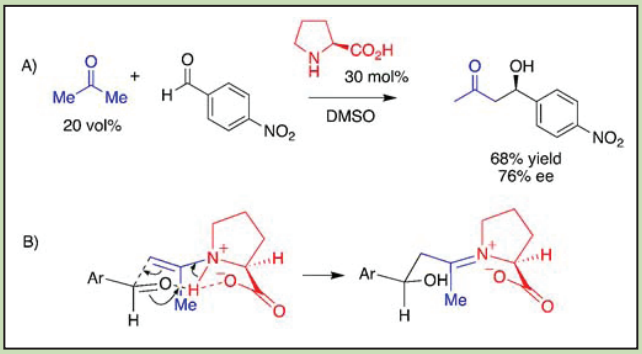
Varying the catalyst structure revealed that both the pyrrolidine and the carboxylic acid of proline were essential for effective catalysis. The mechanism

was assumed to proceed via an enamine intermediate, formed in situ by reaction of the proline and the ketone. The carboxylic acid of the enamine protonated the aldehyde carbonyl activating it to attack; all of this occurring via a cyclic Zimmerman–Traxler chair-like transition state in which the aldehyde substituent occupies an equatorial position (Scheme 2A).

So, this was an example of a bifunctional catalyst: the amine of the proline activated the enol form of the ketone to generate a better nucleophile, by forming an enamine, and the carboxylic acid also assisted by activating the aldehyde carbonyl to attack. The observed enantioselectivity of the reaction was a result of the cyclic transition state and the proline stereochemistry. Once the new C-C bond was formed, the enamine reverted to the ketone, and regenerated proline, which then catalysed further reactions. All beautifully simple, and easily rationalised.



Scheme 1. A) an acid-catalysed crossed aldol reaction; B) enamine formation by reaction of a carbonyl with a secondary amine



Scheme 2. List's proline-catalysed asymmetric crossed aldol reaction

David W. C. MacMillan

The Diels-Alder reaction, first reported almost a century ago[7], and for which Otto Diels and Kurt Alder won the 1950 Nobel Prize in Chemistry, is probably the best method of making 6-membered rings, particularly as 4 new stereogenic centres are made in a single step and the relative configuration of these can be controlled.

We all learn the basic reaction mechanism (Scheme 3A) at an early stage as chemistry undergraduates, it being the best-known example of a cycloaddition, and probably the first pericyclic reaction that many students encounter.

Making the Diels–Alder reaction enantioselective makes this reaction even more powerful, and probably elevates it to the lofty status of 'the most useful reaction for the creation of complex stereochemistry in a single step'. Up until 1999, enantioselective Diels–Alder reactions[8] had almost exclusively[9] relied on the use of asymmetric Lewis acid catalysts – species which could coordinate to the dienophile and activate it to reaction by lowering the energy of the lowest unoccupied molecular orbital (LUMO) (Scheme 3B). In fact, most of the time a stoichiometric amount of the Lewis acid was required, so the term catalyst is often rather inappropriate!

Princeton chemistry professor and 2021 Nobel laureate in chemistry, David MacMillan. Photo courtesy of Denise Applewhite, Princeton University, Office of Communications.

At the end of the 1990s, MacMillan had for some time been examining the use of secondary amines to activate carbonyl compounds by making iminium ions in situ. With hindsight it is so obvious that positively charged iminium ions are much better electrophiles than neutral aldehydes/ketones but making and reacting such species catalytically had been overlooked; people had been focusing almost entirely on carbonyl activation using Lewis acids.

MacMillan had the insight to put two things together – and the result was

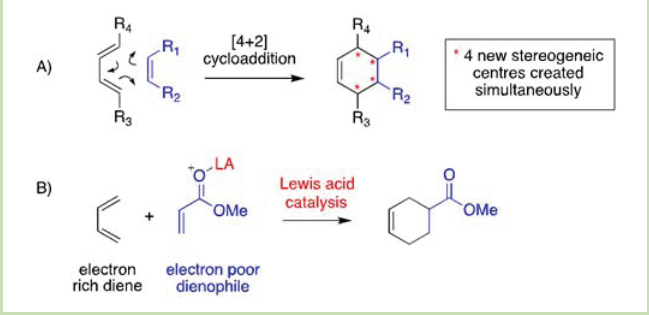
the first asymmetric organocatalysed Diels–Alder reaction. His seminal publication was submitted to JACS on Jan 7th 2000, a month after List had submitted the proline-catalysed aldol reaction to the same journal. The concept, again based on the use of a chiral secondary amine, was beautifully simple.

An α,β-unsaturated aldehyde would condense with the catalytic amount of a chiral secondary amine, to make an iminium ion in situ. This iminium ion would be considerably more electrophilic than the corresponding α,β-unsaturated aldehyde, and consequentially the energy of the LUMO of the alkene would be lowered.

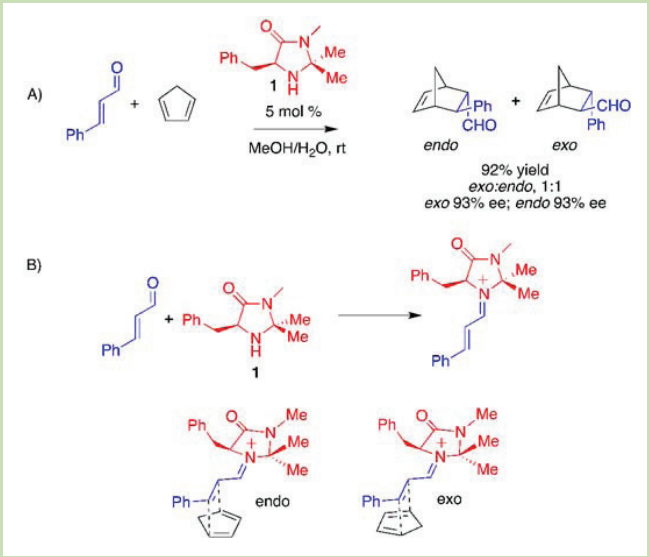
Its reaction with a diene in a standard electron demand Diels–Alder reaction (which relies on the HOMO-diene-LUMO-dienophile interaction) would therefore be significantly accelerated, and would out compete any reaction of the diene with the α,β-unsaturated aldehyde itself. The asymmetry of the amine would then control the facial selectivity of the Diels–Alder reaction. After the cycloaddition, hydrolysis of the iminium ion would re-form the amine catalyst, and give the aldehyde product enantioselectively.

MacMillan's first paper investigated reaction between cyclopentadiene and cinnamaldehyde (Scheme 4A) and examined the effect of several different chiral secondary amines as catalysts. All of the chiral amines tested, including the methyl ester of proline, led to the selective formation of one enantiomer of the products, but amine 1 proved to be the most effective.

Rather perversely, the diastereoselectivity of the reaction tuned out to be harder to control than the enantioselectivity, and both the endo and exo diastereomers were formed in approximately equal amounts (Scheme 4A). However, with catalyst 1 each diastereomer was formed almost exclusively as a single enantiomer (99% ee in both cases) demonstrating the power of the



Scheme 3. The Diels-Alder reaction



Scheme 4. MacMillan's asymmetric Diels-Alder reaction via iminium catalysis

"Suddenly everything seemed possible using a small (or sometimes not so small) chiral organic molecule – the sky was the limit."

chiral catalyst to completely control the iminium ion geometry and the facial selectivity of the reaction of the dienophile (Scheme 4B). This was the first enantioselective amine-catalysed Diels–Alder reaction.

The goldrush

Organic chemists are not sheep, even less so lemmings, but literally hundreds of us read these initial papers in the 2000s and thought something like: "there be gold in them there hills." The goldrush[11] that followed was extensive, well-documented, and far too large to summarise in this short article. However, it had one real difference to 'normal' goldrushes; in this case the seam didn't give out, but it kept giving, and giving, and giving.

In 2005, approximately ~250 research papers were published on organocatalysis; by 2007 this had risen to ~580 papers per year. Following on from the first discoveries published in early 2000, List and MacMillan rapidly pushed the boundaries and opened up new vistas for both enamine and iminium ion catalysis and improved upon their early results. Many others joined in these studies. Suddenly everything seemed possible using a small (or sometimes not so small) chiral organic molecule – the sky was the limit.

Numerous fantastic discoveries and applications were made along the way,

and it would be wrong not to mention a few. For me some of the highlights have been: asymmetric Brønsted acid catalysis, for example by chiral phosphoric acids[11]; asymmetric H-bonding catalysis, for example by chiral thioureas[12] and asymmetric counterion catalysis[13] (a broader term which incorporates some examples of the above).

Our research group also caught the gold fever and even though application in carbohydrate chemistry was less obvious, we applied chiral Brønsted acid catalysis to glycosylation reactions in an attempt to exert reagent control on the stereochemical outcome of glycosylation. Although our results were very modest at best[14], they were the first in this aspect of the field, and many others have subsequently gone on to improve upon them or develop alternative applications of organocatalysis in sugar chemistry.

After the goldrush

Unlike the Neil Young song, there was no 'burned-out basement'. In contrast to many real-world gold rushes, there was no desolate aftermath, no despair, nor the dashing of false hopes. In fact, more than 20 years after those first two seminal papers appeared, organocatalysis is still going strong, finding new exciting, innovative, and useful applications.

A Scopus search for the year 2020 pulls up 474 publications which list the term in title, keywords or abstract, as hits. The legacy of the early discoveries of List and Macmillan is therefore considerable, and without them this field would probably still not exist (yet). Moreover, in the intervening years the two new Nobel laureates have done anything but rest on their laurels; they have both continued to lead and inspire the field. Furthermore, MacMillan is almost singlehandedly responsible for starting another 'organic chemistry goldrush' – this time in photoredox catalysis[15]. So, if you watch this space, in ~20 years' time they may well have just given him a second Nobel.

Conclusions

If you watch the whole of the Nobel Prize YouTube video,2 you will see that, when the floor is opened to questions, one of the journalists attending asks about "the inventors of the mRNA vaccines, which are the only reason we're all standing in the room today." The Nobel Committee of course "declines to comment on other nominations." So, clearly, I was not alone in my initial feelings. Yes, Karikó must surely win a Nobel for her enormous contribution to the fight against Covid, and for the multitude of other applications of her RNA-vaccine technology that are yet to come. Weissman should share in that prize too.

However, my initial feelings watching the Nobel announcement were misguided. I was wrong; List and MacMillan are truly worthy winners. Organocatalysis is a beautiful concept that had been passed over by several generations of organic chemists. The genius of List and MacMillan is that they saw opportunity based on elementary mechanism and reactivity, and used rational design to creative amazingly simple new asymmetric synthetic methods. Their vision, and the beauty, simplicity and huge potential of organocatalysis were all so compelling that their pioneering work immediately inspired multitudes of organic chemists to hugely expand the field. Given the ongoing work in the field, and the exciting discoveries that continue to appear, their legacy is enduring. I conclude by sending my sincere congratulations to them both, and also to their co-workers and research groups who have worked so hard and should of course also share in this moment of glory.

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Article

Tales of the periodic table: a sentiment analysis

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Keywords: *fiction, periodic table, quest, sentiment, mood*

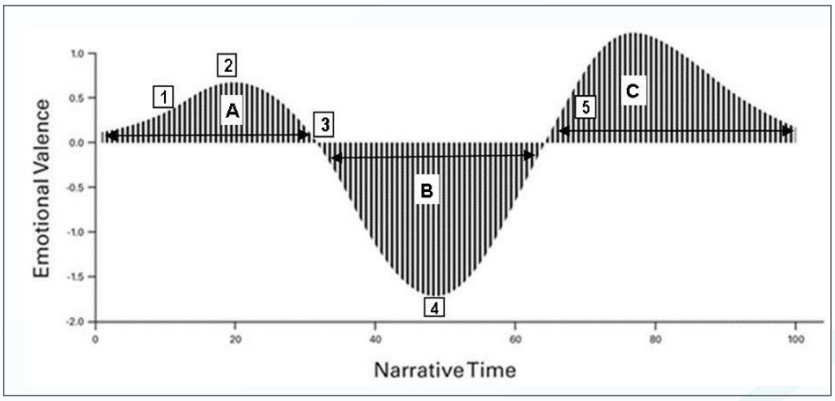
Introduction

Sentiment analysis – often undertaken in a marketing context – can be also applied to scientific writing, as in a previous article in this journal[1]. This article extends that analysis further to books written for the public by scientists involved in the discovery of the double helix as the structure of DNA, which confirms a previous inference that scientific discoveries are analogous to fictional quests.

This idea is then applied to writings about research into the periodic table.

Compilations of essays or papers that reflect the chronology of the table's development are found to show a trend in sentiment or mood – determined from their abstracts or summaries – which resembles that of a fictional quest. Quests are characterised by initial enthusiasm (more positive sentiment); being followed by a time of disappointments (more negative sentiment), which may be mediated by 'helpers' (co-workers, in this context) and frustrated by 'monsters' (e.g. negative reviewers, in this context).

Although success follows, there are inevitably final ordeals to be overcome before the goal is achieved. Analysis of papers related to the development of a periodic table specifically for earth scientists shows similar trends. The paper also shows how the order of papers in a compilation could be varied by the editor in order to mimic a quest – or, indeed, another form of fictional plot – either to foster reader interest or to enhance the ease of perusal of the compilation.



Voyage and Return	**1|** Anticipation and 'fall' into another world	**2|** Initial fascination, whose unfamiliarity may exhilarate	**3|** Frustration stage, with intruding shadow	**4|** Nightmare: a shadow dominates and threatens survival	**5|** Thrilling escape and return
Comedy	**A|** A 'little world' in which people are confused, frustrated and shut off from each other		**B|** Worsening confusion and darkness; a 'nightmarish tangle'		**C|** Previously unrecognised things come to light, changing perceptions and dispersing shadows: the 'little world' becomes happy

Fig. 1. Stages in 'voyage and return' and 'comedy' fictional plots - two of Christopher Bookers 'seven basic plots' - overlain on a plot of aggregated compilation of 'emotional valence' (i.e. mood or sentiment) as a function of 'narrative time'

Types of story

The identification of several 'types' of fiction and the computerised evaluation of mood or sentiment of text has enabled the characterisation of works of fiction in terms of their mood or sentiment. As shown by the two examples in Fig. 1, most of these types of fictional story show a phase of initial optimism (i.e. positive sentiment), followed by at least one 'reversal of fortune' (i.e. negative sentiment) before matters are successfully resolved at the story's end.

Quests have a rather more complicated variation of mood, the stages of which are identified in Fig. 2[4]. Because quests seem akin to scientific discoveries, it is tempting to explore similarities between the stages of quests and the development of scientific knowledge and ideas.

Sentiment analysis

The trend of sentiment in successive chapters of a 'classic' scientific tale – The Double Helix[6] – shows a succession of personal highlights and disappointments and research successes and failures culminating in the final discovery of the structure of DNA. One demonstration of a quantitative approach to determining success or failure is to make judgements on whether words evoked positive feelings (e.g. "successful", "excited",

etc.) or negative feelings (e.g. "embarrassed", "angry", "disappointed", etc.) and then count the frequency of such words in chapters of The Double Helix, which results in a pattern of 'highs' and 'lows', trending to a positive end, but showing clear setbacks along the way[7]. Perhaps inevitably, it has been recognised that the process of allocating words to emotions and then counting them for chapters or other defined stages in a manuscript can be computerised[8], and the 'highs' and 'lows' can then be manipulated to generate a simplified graph of sentiment versus the timeline of a story[9].

A version of this process is shown for The Double Helix in Fig. 3A. For this diagram the sentiment analysis was undertaken using a package developed for analyzing consumers' comments. Although various versions of sentiment analysis have been developed for use with social media as well as for evaluating products and services[10].

For this particular study the website's generic version was used on each complete chapter. The sentiment is expressed in terms of 'polarity' (negative, neutral or positive), with the confidence shown as a percentage. From this polarity and percentage, a sentiment score can be defined in which negative sentiment can have scores ranging from 0 to 0.99, neutral sentiment can have scores ranging from 1.0 to 1.99, and positive sentiment can have scores ranging from 2.00 to 3.00.

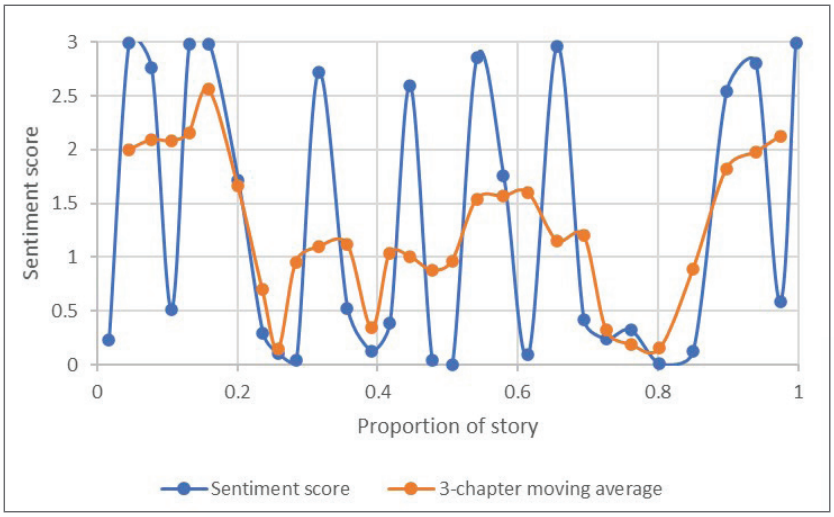


Fig. 3A. Variation of sentiment score with proportion of story for *The Double Helix*. Sentiment analysis was undertaken on each of the 30 chapters (including the Epilogue) that comprise the story. The three-chapter moving average sentiment scores in this version of the story are rather lower than the three-section moving average sentiment scores in *The Third Man of the Double Helix* (see Fig. 3B).

The diagram shows wide variation in sentiment scores as the story proceeds, but the extremes of the curve can be ameliorated by taking a 3-chapter moving average of the sentiment scores. This process yields a pattern of sentiment with the progress of the plot that is reminiscent of the quest (compare Fig. 3A with Fig. 2).

James Watson's candid admission, "I am aware that other participants in this story would tell parts of it in other ways, sometimes because their memory of what happened differs from mine and, perhaps in even more cases, because no two people ever see the same events in exactly the same light. In this sense, no-one will ever be able to write a definitive history…"[11] His view is supported by the result of the same kind of analysis undertaken on the chapters in Maurice Wilkins's reminiscences, shown in Fig. 3B[12], which although it shows a variation in sentiment scores for the sections of its chapters, that variation is not the same as determined for the chapters in Watson's book.

Type of plot			Stages of the plot		
The Quest	**1|** The Call: recognition of need for journey	**2|** Journey across hostile terrain with companions and helpers, albeit with monsters and temptations to covercome	**3|** Success by 'arrival', but frustrations remain	**4|** The final ordeals - a last series of tests	**5|** After a last thrilling escape from death the kingdom or life-transforming treasure is won
Sentiment	Typical trend of sentiment through the story ➲				
Positive					
Neutral					
Negative					

Fig. 2. Typical variation of mood with stages of a fictional quest. An example of a fictional quest is "The Lord of the Rings", although it has been argued that in that particular book sub-plots of other types can be inferred in addition to its being a quest.[5]

This diagram shows three strong excursions into negative sentiment between the grey ('Crick') and brown ('Nobel') markers; they are similar – but they are not the same as – those in the middle section of Fig. 3A.

The negative sentiment is also not as strongly expressed in The Third Man of the Double Helix as it is in The Double Helix. This is consistent with Wilkins' contention that Watson's then-controversial book was written for "an era when popular science tended to present a rather noble and heroic picture of the scientific endeavor". In fact, Wilkins' writing style harks back to that 'heroic' style.

In his foreword to Watson's book, the noted crystallographer of the time, Sir Lawrence Bragg, commented that Watson's book was "not a history, but an autobiographical contribution to *a history which will some day be written"* (italics added)[14]. He would doubtless have made the same comment in respect of Wilkins's book. Bragg implied that there can be a definitive history, a stance few would subscribe to today, and which this paper indicates is certainly not the case for the periodic table.

This initial example reminds us that different people will interpret the same 'facts' differently, and the same person will look at those facts differently on different occasions: there is no single true story of any scientific endeavour. Such differences can also arise because the preferred way of telling stories changes over time: an example of which is the recent move away from interpretations of science history as hero-led scientific revolutions[15] to interpretations inferring slower 'ecological' change.[16]

The Periodic Table as a quest

The possibility of the development of the periodic table being interpreted as a quest has been suggested previously[17], because its overall 'story' includes sections that match Booker's stages of a quest – 'the call', 'the journey', 'arrival and frustration',

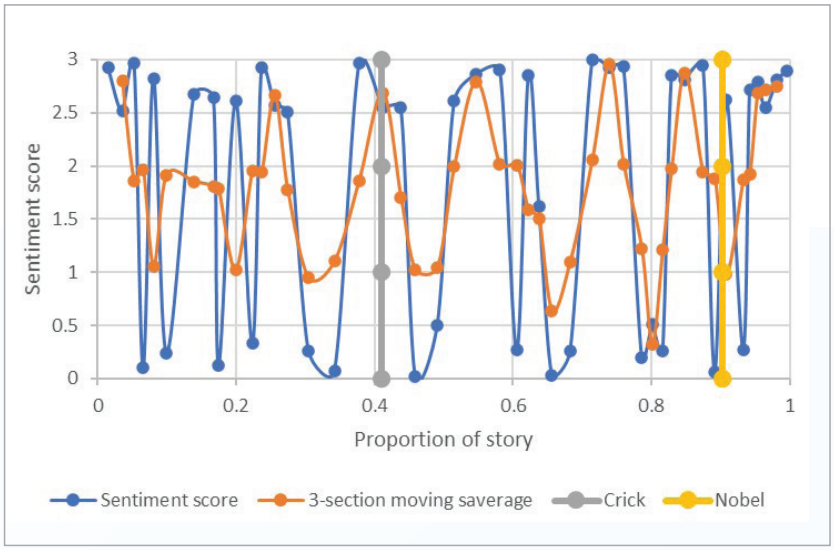


Fig. 3B. Variation of sentiment score with proportion of story for *The Third Man of the Double Helix*. Each of the ten chapters is divided into several clearly demarcated sections; sentiment analysis was undertaken on each of these 46 sections. The heavy grey line and the heavy brown line are the places in the book where Francis Crick ('Crick' in the legend) and the real prospect of winning a Nobel Prize ('Nobel' in the legend) are first mentioned; these correspond to the first page and the last page of *The Double Helix* (see Fig. 3A), respectively.

'the final ordeal' and the equivalent of 'the life-renewing goal' (see Fig. 2), as well as requiring 'companions and helpers' to achieve the quest.

This interpretation is not compromised by most modern scholars' contention that there is no single definitive version of the 'story' of the periodic table, nor of the quest itself. Consistent with that stance, a reviewer of Eric Scerri's book *The Periodic Table: Its Story and Its Significance*[18] observed what it was not:

"It is not simply a plodding, step by step history nor a collection of all known tabular arrangements of the elements. The author describes developments, explains what led to them, comments on them and discusses their implications", noting too that "it reflects the personal interests of the author"[19].

In brief, it is Scerri's book – his 'take' on the facts of the development of the Periodic Table, and, thereby, his interpretation of the quest (or other form of story) referred to in the previous section. However, the chronology is more-or-less tied to historical dates for the research described, although Scerri warns the reader that, on occasion, he "will not avoid looking ahead…."[20]

The simple form of sentiment analysis described earlier for The Double Helix and The Third Man of the Double Helix is applied here to the conclusions (either actual or inferred) for each of the ten chapters in The Periodic Table: Its story and its significance (Table 1). The variation of sentiment with chapter number, effectively with time – as Scerri makes clear[21] – is shown in Fig. 4.

The plot of sentiment score versus chapter number shows it as positive at the start and end of the book – consistent with all of Booker's types of plot, including the quest. The highly negative sentiment of some of the early chapters might seem surprising until it is realised that these correspond to the time at which Mendeleev's Periodic Table was being 'tested' and its predictions evaluated.

The two later excursions into negative sentiment (i.e., sentiment scores

Table 1. Sentiment of chapters in Scerri (2007)

Chapter	Title of chapter	Sentiment polarity and %[1]	Sentiment score[2]
1	The periodic system: An overview	+69.5%	2.695
2	Quantitative relationships among the elements and the origins of the Periodic Table	-82.4%	0.176
3	Discoverers of the periodic system	-65.9%	0.341
4	Mendeleev	-95.9%	0.041
5	Prediction and accommodation: The acceptance of Mendeleev's periodic system	-95.2%	0.048
6	The nucleus and the Periodic Table: Radioactivity, atomic number and isotopy	+66.0%	2.660
7	The electron and chemical periodicity	N55%	1.550
8	Electronic explanations of the periodic system developed by chemists	+74.2%	2.742
9	Quantum mechanics and the periodic table	-85.4%	0.146
10	Astrophysics, nucleosynthesis and more chemistry	+93.3%	2.933

[1] Sentiment polarity (negative [-], neutral [N], or positive [+]) and percentage determined from: https://monkeylearn.com/sentiment-analysis/

[2] Sentiment score (S) is: 1-(negative %/100), giving a range of scores from 0-0.99; or 1+(neutral %/100), giving a range of scores from 1.00-1.99; or 2+(positive %/100), giving a range of scores from 2.00-3.00. On this basis sentiment scores will be between 0 and 3.

of less than 1.0) are typical of the later 'trials' in many quests (see Fig. 2), and in this instance are inferred to correspond to the Periodic Table being challenged by the developing discipline of quantum mechanics. The similarity with the quest of Fig. 2 is more obvious if a plot of the 3-year moving average of sentiment score is considered.

On a rather shorter time-scale within the overall story of the periodic table, another book by Scerri (A Tale of Seven Scientists) profiles seven scientists who are less well-known for their contributions to the development of the table than, for example, Mendeleev or Mayer[22]. In Table 2 the result of sentiment analysis of Scerri's conclusion for the chapter about each scientist are given, with a view to determining the sentiment trend throughout the book.

Although the chapters of the book are in roughly chronological order, in terms of the range of dates of publication of the scientists' research (corresponding to about the time of Chapter 8 of Scerri 2007), the rationale for the book is also clearly defined by the role of those who he refers to as "little people" in the development of the Periodic Table:

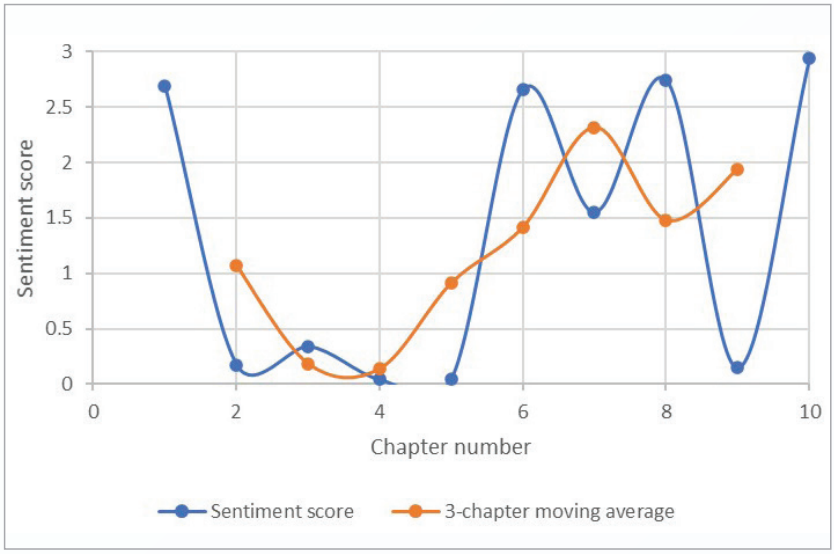


Fig. 4. Variation of sentiment score with chapter number in Scerri (2007)

"Although I believe that social context makes an important contribution to the development of science I am more interested in a radical or literal form of sociology, which regards science as a group activity rather than the work of particular individuals. Or if one must speak of individuals, as I suppose one must, I prefer to include the lesser-known individuals who provided the missing links for the heroic personalities. It is they who provide the glue and continuity …"[23]

In the chapters describing "little people" whose contribution is more directly association with 'heroes' of the time (e.g. Nicholson's association with Bohr, and Bury's association with Lewis and Langmuir) the sentiments are more positive than the chapters for van den Broek, Abegg, and particularly, Main Smith and Stoner.

Although Janet's position remains unresolved[24], sentiment analysis suggests that perhaps – akin to the pigs in the allegorical novel Animal Farm [25]– perhaps not all "little people" are equal, despite Scerri's claim to the contrary[26].

Table 2. Sentiment of chapters in Scerri (2016) - A Tale of Seven Scientists

Chapter	Title of chapter	Life span of 'little' person	Time range of publications	Sentiment polarity and % †	Sentiment score ‡
[E]	Foreword			+87.0%	2.870
[B]	Biographical background			N66.3%	1.663
1	Introduction			+56.1%	2.561
2	John Nicholson	1881 _ 1955	1911 _ 1912	+62.5%	2.625
3	Anton van den Broek	1870 – 1926	1907 – 1913	-96.2%	0.038
4	Richard Abegg	1869 – 1910	1904	-68.1%	0.319
5	Charles Bury	1890 – 1968	1921 – 1922	+60.2%	2.602
6	John D. Main Smith		1923 – 1927	-99.1%	0.009
7	Edmund Stoner	1899 – 1968	1924 – 1925	-91.0%	0.090
8	Charles Janet	1849 – 1932	1927 – 1930	+64.8%	2.648
9	Bringing things together			N67.2%	1.672

† Sentiment polarity (negative [-], neutral [N], or positive [+]) and percentage determined from: https://monkeylearn.com/sentiment-analysis/

‡ Sentiment score is: 1-(negative %/100), giving a range of scores from 0-0.99; or 1+(neutral %/100), giving a range of scores from 1.00-1.99; or 2+(positive %/100), giving a range of scores from 2.00-3.00. On this basis sentiment scores will be between 0 and 3.

The variations of sentiment score in the chapters of A Tale of Seven Scientists are shown in Fig. 5. The variation is rather different from those derived for fictional stories. Perhaps this is not surprising when it is recalled that the simpler plots determined from fiction are essentially 'heroic' tales, whereas this tale is – by Scerri's own admission – about "little people" and for a limited time.

Although the title of another of Scerri's books *A Tale of Seven Elements*[27] might imply an emphasis on chemistry of these particular elements, in fact the focus of the book is as much if not more about the people involved in the discovery of seven elements during the first half of the twentieth century.

This book is another small-scale analysis of a component of the longer story of the periodic table. The nationalities of the scientists involved, the politics of their respective countries, and the influence of the 1914-1918 and 1939-1945 global wars makes this 'tale' rather more complex than that described for A Tale of Seven Scientists, and, accordingly, has made the selection of appropriate passages from each chapter for sentiment analysis perhaps less rep-

Fig. 5. Variation of sentiment score by chapter in Scerri (2016) - *A Tale of Seven Scientists*

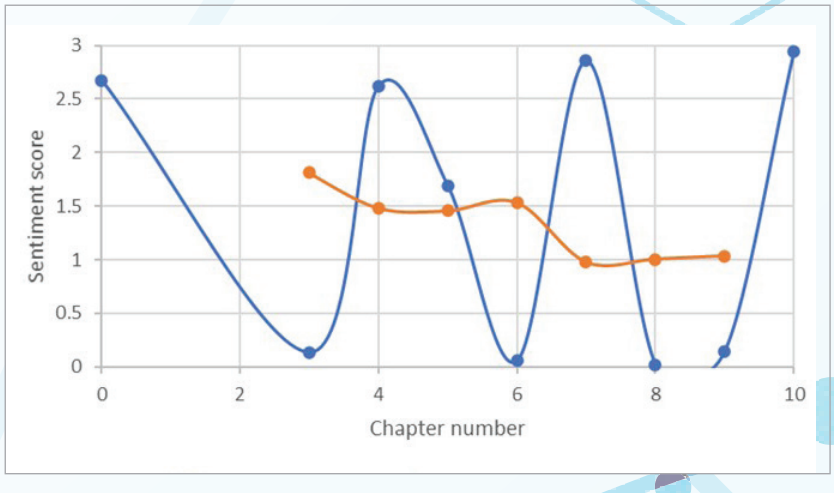


Fig. 6. Variation of sentiment score by chapter in Scerri (2013) - *A Tale of Seven Elements*

Table 3. Sentiment of chapters in Scerri (2013) – *A Tale of Seven Elements*

Chapter	Title of chapter	Senior discoverer*	Date of element's discovery	Sentiment polarity and %†	Sentiment score‡
0	Introduction			+67.5%	2.675
1	From Dalton to the discovery of the periodic system ¶			N66.3%	1.663
2	The invasion of the Periodic Table by physics ¶			+56.1%	2.561
3	Proactinium (atomic no. 91)	Lisa Meitner (Otto Hahn)	1917	-63.3%	0.367
4	Hafnium (atomic no. 72)	George Hevesy (Dirk Coster)	1923	+62.4%	2.624
5	Rhenium (atomic no. 75)	Walter & Ida Noddacks (Otto Berg)	1925	N68.5%	1.685
6	Technetium (atomic no. 43)	Emilio Segrè	1937	-94.6%	0.054
7	Francium (atomic no. 87)	Marguerite Perey	1939	+85.6%	2.856
8	Astatine (atomic no. 85)	Emilio Segrè (Dale Corson & Alexander MacKenzie)	1940	-98.6%	0.014
9	Promethium (atomic no. 61)	J.A. Marinsky (L.E. Glendenin)	1945	-85.7%	0.143
10	From missing elements to synthetic elements			+94.7%	2.947

*'Senior discoverer', is as shown in Scerri (2013, p. xvi, fig. 0.1); other contributors to the discovery are in parentheses

†Sentiment polarity (negative [-], neutral [N], or positive [+]) and percentage determined from: https://monkeylearn.com/sentiment-analysis/

‡Sentiment score is: 1-(negative %/100), giving a range of scores from 0-0.99; or 1+(neutral %/100), giving a range of scores from 1.00-1.99; or 2+(positive %/100), giving a range of scores from 2.00-3.00. On this basis sentiment scores will be between 0 and 3.

¶ Scerri (2013, p. xxxiii) informs the reader that Chapters 1 and 2 "are condensed versions of most of the chapters of my 2007 book on the periodic table [viz., Scerri, E.R. 2007]. You may, therefore wish to skip to Chapter 3, which begins relating the discovery of the seven elements." Accordingly, these chapters are not included in this analysis.

resentative and certainly more difficult. Table 3 shows the sentiment polarity and percentages as well as the sentiment score calculated for extracts from each chapter's conclusion; the graph of variation of sentiment with time (Fig. 6) broadly resembles that of Fig. 5.

Non-chronological stories

In the three previous examples, the order of chapters is essentially that of history. In a thematic compilation of scientists' work this need not be the case – and certainly is not in Mendeleev to Oganesson: A Multidisciplinary Perspective on the Periodic Table, for which the contributions were obtained in response to invitations to current experts/specialists in disciplines associated with the Periodic Table, following a global meeting held in Cuzco, Peru.

Table 4 shows the chapters in their order in the book; also included are the sentiment polarity and % as well as the sentiment scores, determined from the editors' short summaries of the chapters which are provided in the Introduction to the book.

The variation of sentiment polarity and the variation of sentiment scores inferred for the chapters of Scerri and Restrepo (2018) is shown in Fig. 7. Most chapters are of positive sentiment; with the overall trend with chapter number being positive (shown as the dotted line in Fig. 7). However, the variation of sentiment does not correspond obviously with any of the fictional plots described earlier.

Of course, the variation of sentiment throughout the book could be very different if the order of the essays was changed. As an example, consider if the book was arranged with papers relating to the origins of the periodic table came first, followed by the general papers relating to electron configurations and quantum mechanics, followed by papers relating to the placement of elements in the table, and ending with papers discussing the form of the table.

Within these four groups, the essays might have been arranged with an essay with positive (or at least neutral) sentiment to start and end, bookending those essays with less positive sentiment, leading to the variation of sentiment with the amended order of essays shown in Fig. 8.

It would also be possible to rearrange the order of papers in such a compilation to either cluster or separate papers with very different sentiment scores so as to achieve an 'improved' storyline. As an example, the essays in Mendeleev to Oganesson: A Multidisciplinary Perspective on the Periodic Table could have been arranged in an adjusted order that was deliberately designed so that the trend in sentiment resembled that of a fictional plot, i.e., an artificial time-line could have been constructed.

If a quest was the preferred type, and the desired outcome was a particular form of the periodic table, say, the Periodic Table for earth scientists, essays that refer to 'valence' (currently Chapter 13), 'cations' (also Chapter 13), 'chemical properties' (currently Chapter 4) – all of which bear on 'ionic potential', should be in close proximity to the essay by Railsback (currently Chapter 11).

Table 4. Sentiment of chapters in Scerri and Restrepo (2018)

Chapter	Title of chapter / essay	Author(s) of essay	Theme or discipline†	Sentiment polarity and %†	Sentiment score‡
1	Heavy, superheavy….Quo vadis	Paul J. Karol	Nuclear chemistry	+79.4%	2.794
2	Nuclear lattice model and the electronic configuration of the chemical elements	Jozsef Garai	Structural chemistry	-48.7%	0.513
3	Amateurs and professionals in chemistry: The case of the periodic system	Philip J. Stewart	Forms of the periodic table	N56.3%	1.563
4	The periodic system: A mathematical approach	Guillermo Restrepo	Mathematics	N67.4%	1.674
5	The "chemical mechanics" of the Periodic Table	Arnout Ceulemans & Pieter Thyssen	Mathematical physics	+55.8%	2.558
6	The grand periodic function	Jan C.A. Boeyens	Mathematical chemistry	+52.8%	2.528
7	What elements belong in Group 3 of the Periodic Table?	Eric Scerri & William Parsons	Chemistry / placement of elements in table	+77.7%	2.777
8	The Periodic Table retrieved from density functional theory based concepts: The electron density, the shape function and the linear response function	Paul Geerlings	Theoretical chemistry	+61.1%	2.611
9	Resemoticization of periodicity: A social semiotic perspective	Yu Liu	Semiotics/ forms of table	+76.7%	2.767
10	Organizing the transition metals	Geoff Rayner-Canham	Forms of table	+95.4%	2.954
11	The earth scientist's periodic table of the elements and their ions: A new periodic table founded on non-traditional concepts	L. Bruce Railsback	Placement of elements in table / forms of table	N64.6%	1.646
12	The origins of Mendeleev's discovery of the periodic table	Masanori Kaji	Social history	+99.8%	2.998
13	Richard Abegg and the Periodic Table	William B. Jensen	Placement of elements in table	N60.9%	1.609
14	The chemist as philosopher: D.I. Mendeleev's 'The Unit' and 'Worldview'	Michael D. Gordin	History / Philosophy	+57.2%	2.572
15	The philosophical importance of the Periodic Table	Mark Weinstein	Philosophy	+67.4%	2.674

† Sentiment polarity (negative [-], neutral [N], or positive [+]) and percentage determined by https://monkeylearn.com/sentiment-analysis/ from editors' summaries (Scerri and Restrepo 2018, pp. 4-6)

‡ Sentiment score is: 1-(negative %/100), giving a range of scores from 0-0.99; or 1+(neutral %/100), giving a range of scores from 1.00-1.99; or 2+(positive %/100), giving a range of scores from 2.00-3.00. On this basis sentiment scores will be between 0 and 3.

The sentiment scores of these three chapters could then be arranged in a sequence that could define "the final ordeals" of a quest referred to in Fig. 2, viz., Chapter 4, (sentiment score 1.674), followed by Chapter 13 (sentiment score 1.609), followed by Chapter 11 (sentiment score 1.646). Leaving the order of the remaining two chapters as they are shown in Fig. 8, the variation of sentiment becomes as shown in Fig 9.

Particularly noticeable is the shape of the 3-chapter moving average sentiment score, which now resembles that of a quest. Although such a re-arrangement of the text might seem strange to those who write about science, it can serve either as a means of improving the storytell-

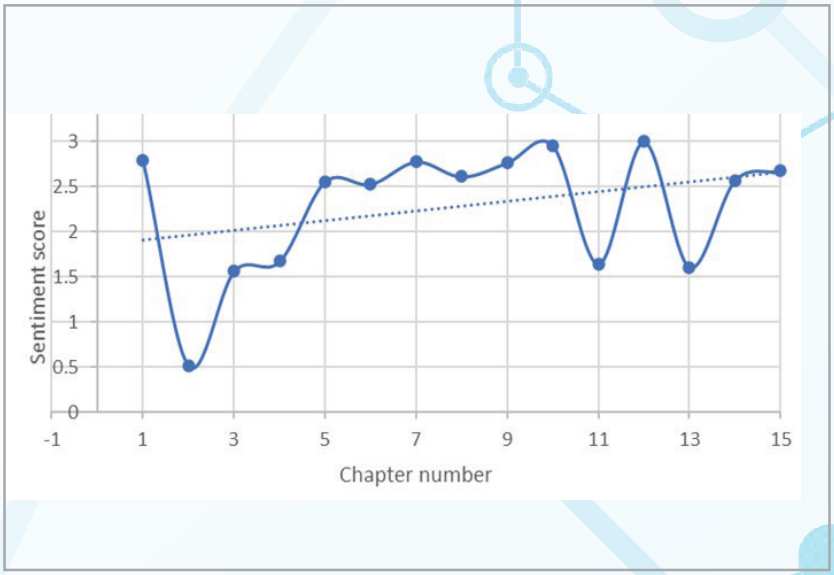


Fig. 7. Variation of sentiment score in Scerri and Restrepo (2018) - ***Mendeleev to Oganesson: A Multidisciplinary Perspective on the Periodic Table***

ing or making a particular outcome of the story more prominent, and can be used in a story where a strict chronological sequence of events is not required.

Of course, a story might contain more than one type of plot. An example is The Lord of The Rings, in which "elements of all seven [types of plot] are woven together". Within the overall story of the periodic table reference is often made to periodic tables that are either intended or designed to meet the needs or interests of other users, either generally or specifically, (e.g., economists, inorganic chemists, metallurgists, biologists, and geoscientists). The attempt to develop each of these discipline-specific tables could be considered as quests within the overall quest of the periodic table.

A quest within a quest? A periodic table for earth scientists

Any story of the development of a periodic table for earth sciences requires the acknowledgement of an increased understanding of how ions behave in various geological environments. Crystal lattices accommodate cations largely on the basis of the size of the lattice 'hole' and the radius and charge of the ion.

The identification of ionic potential (the ratio of ionic charge to ionic radius) in the 1920s was important for this understanding. The process of uptake of ions from melts to form minerals in igneous rocks as well as the processes of sedimentation and soil formation (both low temperature environments) became better understood from the 1950s.

Much later, geochemists became aware of the characteristics of multivalent cations that were stable in hydrous high temperature and high pressure environments, such as geothermal systems. Moreover, considerable improvements were needed – and, indeed, were forthcoming – in techniques for the determination of elemental concentrations in this ever increasing range of environments.

Theme	Origins			→	Electron configuration/quantum mechanics				→	'transition'		→	Placement of elements in Periodic Table			→	Forms of the Periodic Table		
Chapter	12	14	15		6	2	5	8		4	1		13	7	10		11	3	9

Fig. 8. Upper: Allocation to themes of essays/chapters in Scerri and Restrepo (2018) - *Mendeleev to Oganesson: A Multidisciplinary Perspective on the Periodic Table*. Lower: Variation of sentiment score in a re-arranged sequence of essays/chapters.

Fig. 9. The result of further re-ordering essays / chapters in Scerri and Restrepo (2018) - ***Mendeleev to Oganesson: A Multidisciplinary Perspective on the Periodic Table*** - so that the periodic table for earth scientists is the outcome of the quest. Note that it is not necessary that the closing chapter is the subject of the quest. In this scenario, a more general paper (Essay/Chapter 9) closes the book.

In effect, Bruce Railsback's construction of his 'Earth Scientist's Periodic Table of Elements and their Ions' had to await many of these developments. Although he describes the format of his table similarly in two papers, which are separated by some fifteen years, inevitably the references reflect historic developments in understanding of geochemical environments and in analytical techniques (summarised in Table 5). Because Railsback selected rather than wrote the papers he refers to, the sentiment scores plotted in Fig. 10 are those determined from

Table 5. Distribution of references by topic and date of references in Railsback (2003) and Railsback (2018)

Main topic of reference		% of the 23 references in Railback 2003				% of the 37 references in Railsback (2018)			
		1920s-1950s	1960s-1990s	Post-2000	All dates	1920s-1950s	1960s-1990s	Post-2000	All dates
Periodic table (generic) and generic chemistry			9%		9%		3%	36%	39%
Geochemical environments	Theoretical lattices	13%	4%		17%	11%	3%	6%	20%
	Crystallization of magmas	4%	8%		12%	6%	11%		17%
	Sediments and soils		26%	4%	30%	3%	6%	3%	12%
	Geothermal		9%	4%	13%			3%	3%
Analytical techniques developed for geochemists			4%		4%		3%	3%	6%
Other			9%	4%	13%	3%		3%	3%
All categories		17%	69%	12%	100%	23%	26%	54%	100%

the authors' abstracts of the papers.

Fig. 10 shows the variation of the sentiment scores of the abstract or summary of the papers Railsback refers to in the order of date of publication: for Railsback's 2003 paper, the 23 references span the period 1928 – 2001, while for Railsback's 2018 contribution to the From Mendeleev to Oganesson … book, the 37 references span the period 1922 – 2013. Both plots show initial trends that can be interpreted as the early recognition of the importance of ionic potential in understanding geochemical processes, then some doubts, which were followed by greater optimism as theoretical understandings and analytical techniques improved.

The lower values of sentiment towards the right-hand end of Fig. 10A, which predates Railsback (2003), could be inferred to be the start of the 'final trials' of the quest and – unsurprisingly – occur in 2003, when Railsback's ideas were being articulated. This feature is more clearly shown in Fig. 10B.

In other words, while both of the sentiment plots of references in Railsback's papers show the characteristics of quest, the more recent paper's plot of sentiment score versus time has more of the shape of a quest than does the earlier one. Even

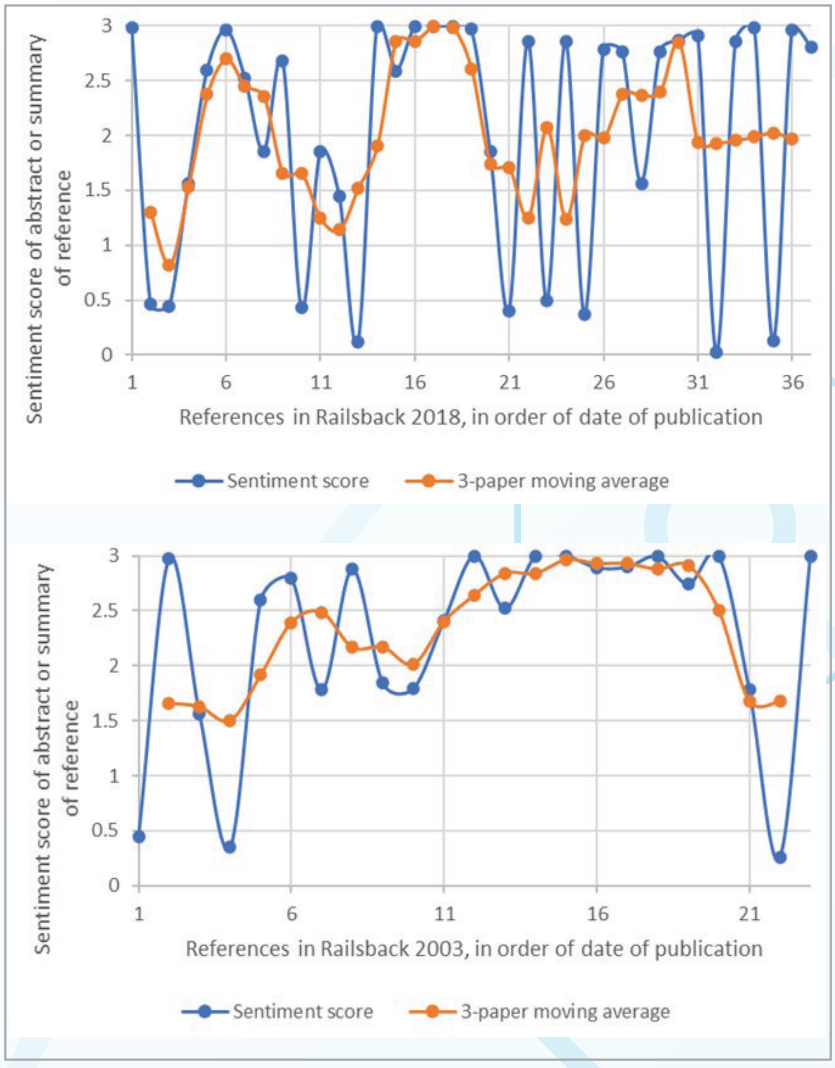


Fig. 10. Variation of sentiment score of references in Railsback (2003, 2018), in order of the date of publication of references. Sentiment scores for the abstracts or summaries of the referenced papers are determined as described earlier in this paper. Upper (A): References in Railsback (2003); and Lower (B): References in Railsback (2018).

Table 6. Sentiment of papers in proceedings of 4th International Conference on the Periodic Table

Paper no.*	Author and title of paper	Abstracts		Conclusions		Average date of references cited
		Sentiment polarity and %†	Sentiment score‡	Sentiment polarity and %†	Sentiment score‡	
F	Zhou, Q-F. Foreword for Pure and Applied Chemistry special issue 4th International Conference on the Periodic Table (Mendeleev 150), pp. 1893-1895	+87.0%		2.870		
1-5	Papers on history of the periodic table and its contributors					
1	Stewart, P. The limits of Mendeleev's insight, pp. 1915-1920	+94.5%	2.956			1942
2	Kurushkin, M. Viatscheslaw Romanoff: Unknown genius of the periodic system, pp. 1921-1928	+96.6%	2.966	+90.9% ¶	2.909	1982
3	Seaborg, D. The life and contributions to the periodic table of Glenn T. Seaborg, the first person to have an element named after him while he was still alive, pp. 1929-1939	+44.7%	2.447	+71.7%	2.717	1975
4	Ghibaudi, E. Levi's Periodic System vs. Mendeleev's Periodic System: two engaged views of chemistry between science and literature, pp. 1941-1947	+73.3%	2.773	+98.6%	2.986	1968
5	En'yo, H. History of nihonium, pp. 1949-1958	+67.0%	2.670	-84.4%	0.156	1976
6-10	***Papers on periodicity and periodic law***					
6	Pyykkö, P. An essay on periodic tables. pp. 1959-1967	-49.0%	0.510	+99.0%	2.990	1985
7	Cao, C-S.; Hu, H-S; Li, J.; Schwarz, W.H.E. Physical origin of chemical periodicities in the system of elements. pp. 1969-1999	+90.7%	2.907	+99.4%	2.994	1979
8	Atkins, P. Symmetry beneath the table, pp. 2001-2005	+76.6%	2.766			1989
9	Imyanitov, N.S. Periodic law: new formulation and equation description , pp. 2007-2021	+61.3%	2.613	+75.1%	2.751	1970
10	Babaev, E. Periodic law in chemistry and other sciences, pp. 2023-2035	-59.5%	0.405			1978
11	***Special topic paper***					
11	Balarew, C. The periodic table of chemical elements – history, nature, meaning, pp. 2037-2045	+76.6%	2.766			1884

*Paper numbers are assigned to assist in identification on Fig. 11A

† Sentiment polarity (negative [-], neutral [N], or positive [+]) and percentage determined from: https://monkeylearn.com/sentiment-analysis/

‡ Sentiment score is: 1-(negative %/100), giving a range of scores from 0-0.99; or 1+(neutral %/100), giving a range of scores from 1.00-1.99; or 2+(positive %/100), giving a range of scores from 2.00-3.00. On this basis sentiment scores will be between 0 and 3.

¶ Somewhat unusually, the conclusions to these papers are frequently personal reminiscences or reflections. Generally, they show a positive sentiment

so, the low sentiment values at the extreme right of the diagram may signify consistency with Railsback's assertion,

"The success of the new Earth Scientist's Periodic Table of the Elements and Their Ions across the past decade is that the periodic tale, as a general concept, is not a static document but instead is still subject to evolution, especially as scientific field beyond traditional chemistry increasingly use chemical perspectives. It further suggests that volumes like this one [i.e., Scerri and Restrepo 2018] are not simply ruminations on a nineteenth century invention, but instead they can be part of an ongoing process to find new meaning in the periodic concept and to make it more applicable in broader contexts in the twenty-first century."

In other words, the quest is not yet complete.

Science narratives in a journal

Rather than being compiled into a book, as was done for the Third International Conference on the Periodic Table several years after the event in 2012, selected papers from the Fourth International Conference on the Periodic Table held in 2019 were published together in an issue of the journal Pure and Applied Chemistry. The papers were gathered into three themes, as shown in Table 6, which

also shows the sentiment scores of the abstracts and conclusions (where provided) of the papers, as well as the average date of the references for each paper.

Fig. 11A shows that the sentiments of most of the papers are highly positive, although there is greater variation of the sentiment scores of papers within the second theme (i.e. papers 6-10) than for those within the first theme (i.e., papers 1-5). Typically, the references include original research papers and more recent commentary, so the average date gives an indication of the time-period covered by the paper, and facilitates a time-axis for Fig. 11B, a plot which serves no other purpose but to highlight the variability of sentiment scores for the papers on periodicity.

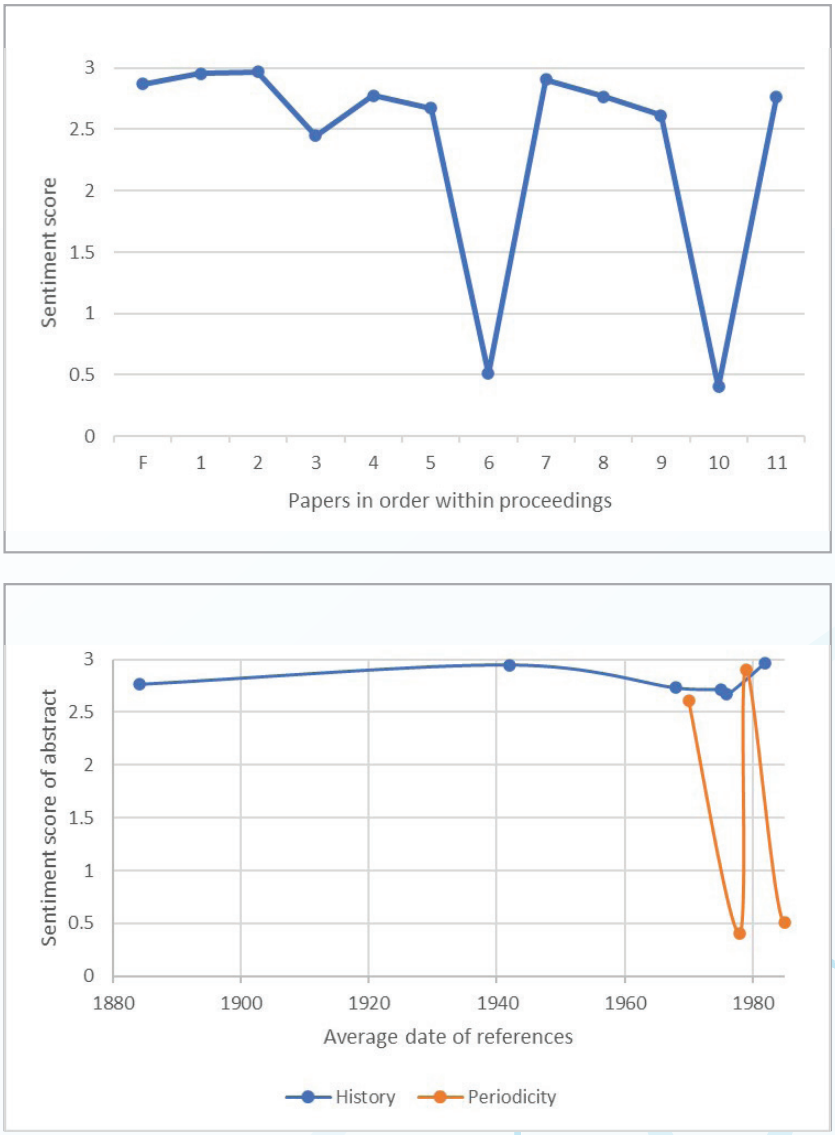


Fig. 11. Variation of sentiment score for abstracts of papers in Proceedings of 4th International Conference on the Periodic Table, published in Pure and Applied Chemistry.
Upper: Papers in order in the Proceedings.
Lower: Papers in order of average date of references for each of the sections on 'history of the periodic table and its contributor', shown as 'History' in legend of the diagram; and on 'periodicity and periodic law', shown as Periodicity' in legend of the diagram.

Conclusions

Sentiment analysis of fiction readily identifies a range of story types, at least one of which – the quest – is probably applicable to many of the stories of science. As an example, the story of the development of the periodic table and at least one subordinate story within it (the development of the Earth Scientist's Periodic Table of the Elements and Their Ions) show characteristic features of the quest in their plot of sentiment versus time.

In compilations of scientific essays, the order of the essays (which is not necessarily on a date/time basis) can be manipulated by the editor so that the book either resembles a fictional type or to maintain reader interest throughout the book. At the very least, choosing essays with highly positive sentiment scores as the first and last contributions to the volume is probably a good practice and might gain the approval of potential publishers.

Cautiously, it could also be suggested that authors of scientific papers and books might apply sentiment analysis to their writing prior to submission. Sentiment polarity is a measure of the emotional response of the reader, and conceivably might influence referees' and publishers' perceptions of the value of the work. Sentiment polarity might also influence scholars' perceptions of the scientific worth of a piece of work and result in their citing it.

As an example, Fig. 12 shows that for 124 of the publications authored by Eric Scerri (a particularly prolific writer of papers and books related to the Periodic Table), for which abstracts and appropriate publication details are available, there is no obvious correlation between sentiment score and the annual or total citations of his papers, but there is a weak correlation between sentiment score

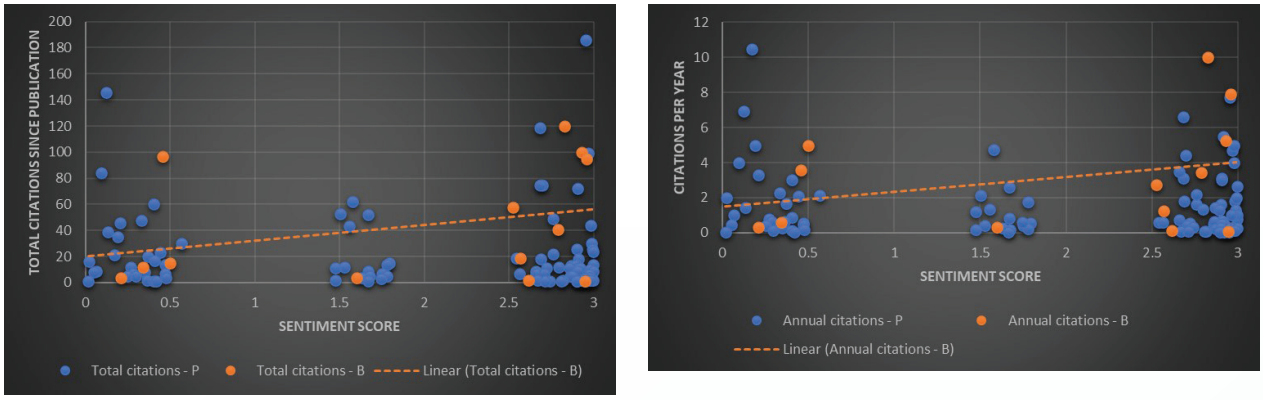


Fig. 12. Variation of citations with sentiment. Right: Sentiment score versus annual citations of Eric Scerri's papers published in journals (P) and his contributions to books (B). Left: Sentiment score versus total citations of Eric Scerri's papers published in journals (P) and his contributions to books (B).

and the annual or total citations of his contributions to books and conference proceedings. That said, any predictive relationship between sentiment score and either the number of times a paper has been cited since publication or the number of citations the paper has been cited annually since publication is likely to be problematic. This is because a reader-researcher's decision to cite an article is based on how well – or not – the content and conclusions of the potentially cited article supports – or not – the content and conclusions of the citing paper, possibly the publishing history of the author, as well as an emotional response.

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Article

A sentiment analysis of stories from Primo Levi's *The Periodic Table*

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Introduction

This article extends the application of sentiment analysis of the development of the chemists' periodic table to its application to narratives related to education and employment in laboratory practice and consulting activities, using the stories of Primo Levi as a case study.

"Born on July 31, 1919, in Turin, Italian-Jewish scientist Primo Levi graduated with honours in chemistry amid the rise of Fascism in his home country.

He later survived a year at Auschwitz during World War II against all odds. Upon his liberation in 1945, Levi began writing about his experiences and has authored the acclaimed works *If This Is a Man, The Truce* and *The Periodic Table*. The cause of his death in 1987, which was officially ruled a suicide, is the subject of some debate."

Sometimes referred to as the 'other' periodic table, Primo Levis's collection of stories bearing the title *The Periodic Table*, originally published in Italian as Il Sistema Periodico in 1975, was ranked by the Royal Institution of Great Britain in 2006 as the best science book ever published. In an article written in 2019, acknowledging the 100th anniversary of Levi's birth on 31 July 1919, London-based science writer Philip Ball noted:

"He [Levi] opened up science, and chemistry in particular, to an audience that would have never otherwise given it a thought. He celebrated the culture that was shared, he said, by 'Empedocles, Dante, Leon-

Table 1. Summary of types of content of chapters in Primo Levi's *The Periodic Table*, and inferred analogy to fictional plot [7]

Chapter (story)	Element	Provenance: biography and political context	Education (and related experience and employment)	Professional laboratory practice
1	Argon	An analogy is drawn between his family history and the inertness of argon		
2	Hydrogen	Friendship with Enrico, a later work colleague	An unauthorised childhood laboratory experience	Two activities: glassblowing; electrolysis of water
3	Zinc	First love, without desired outcome	General and inorganic chemistry at the Chemical Institute	Preparation of zinc sulfate, by reacting zinc metal with sulfuric acid
4	Iron	Iron as an analogue for strength of author's teenage friendship with an adolescent climber	Mention of Chemical Institute	
5	Potassium	Being a Jewish youth as Nazi and fascist influences in Italy increase	Appointment as a 'disciple' to the assistant at Institute of Experimental Physics	Distillation of benzene; explosive consequences of using potassium rather than sodium
6	Nickel			Employment in mine; dissolution of nickel ore in HF and its analysis
7	Lead	Follow-up of 'Nickel': two fictional (i.e. not personal) stories related to mining		
8	Mercury			
9	Phosphorus	Frustrations of early employment in factory		Failed work on anthocyanins and use of phosphoric acid in carbohydrate metabolism not realised
10	Gold	Life and capture under fascist rule; capture; alluvial gold		Describes alluvial gold occurrence
11	Cerium	Laboratory work in Auschwitz		Modifying cerium for use in cigarette lighters
12	Chromium	The varnish factory: first work after Auschwitz		Faulty transcription of recipe using chromate in paint
13	Sulfur	Managing a production system		Managing a furnace boiler related to sulfodiene
14	Titanium	A story about painting		Use of titanium as whitening agent in paint
15	Arsenic	A customer enquiry		Identification of purity of sugar – arsenic contamination; synthesis of pyruvic acid

Table continues on the following page.

ardo, Galileo, Descartes, Goethe and Einstein', as well as by 'the good craftsmen of today, or the physicists hesitating on the brink of the unknowable'."

The twenty-one stories in Primo Levi's The Periodic Table comprise a mixture of biography – which includes reference to the politics of the time at which they were written, particularly experiences related to Levi's early life (his 'provenance', if you will) – his education, particularly that related to chemistry; and his subsequent engagement in laboratory practice, including in the Auschwitz concentration camp.

Each story carries as its title the name of a chemical element: some of the names relate to an attribute of the element relevant to the story, e.g. the chemical inertness of argon has a parallel in the characteristics of his family, viz., "they were inert in their inner spirits, inclined to disinterested speculation, witty discourses, elegant, sophisticated and gratuitous discussion … an attitude of dignified abstention".

Similarly, the story entitled 'iron' relates to the strength of a childhood friendship rather than to any chemistry, i.e. iron is a metaphor for strength. The stories are generally personal narratives: this means that the chemistry in them is generally intertwined with an aspect of Levi's life experience, i.e. they are not confined to being descriptions of activities and experiences of chemistry.

Table 1 shows the distribution of Levi's stories across biography, education and the professional practice of chemistry. Highlighted in the table are those stories in which either or both of the latter two categories are dominant and to which the detailed sentiment analysis, which is central to this article, is applied.

The chemistry involved in the stories is mainly inorganic and aqueous, and, accordingly, the elements chosen by Levi for his stories are also shown in a version of the periodic table that emphasises such chemistry (see Appendix 1).

Table 1 (continued). Summary of content of chapters in Primo Levi's *The Periodic Table*, and inferred analogy to fictional plot

Chapter (story)	Element	Provenance: biography and political context	Education (and related experience and employment)	Professional laboratory practice
16	Nitrogen	A first attempt at consultancy		An unsuccessful synthesis of alloxan from bird excrement
10	Gold	Life and capture under fascist rule; capture; alluvial gold		Describes alluvial gold occurrence
11	Cerium	Laboratory work in Auschwitz		Modifying cerium for use in cigarette lighters
12	Chromium	The varnish factory: first work after Auschwitz		Faulty transcription of recipe using chromate in paint
13	Sulfur	Managing a production system		Managing a furnace boiler related to sulfodiene
14	Titanium	A story about painting		Use of titanium as whitening agent in paint
15	Arsenic	A customer enquiry		Identification of purity of sugar – arsenic contamination; synthesis of pyruvic acid
16	Nitrogen	A first attempt at consultancy		An unsuccessful synthesis of alloxan from bird excrement
17	Tin	A second and final attempt at consultancy		The trials of making stannous chloride; a ventilation hood and its demise
18	Uranium	Customer services in a factory (a retold story)		Cadmium being passed off as uranium
19	Silver	Story at a dinner party (a retold story)	^{25}th anniversary of graduation	Contamination of X-ray paper by polyphenols in water
20	Vanadium	Re-emergence of Auschwitz experiences		Contaminant affecting hardening of varnish
21	Carbon	Not a personal story, rather it is 'in some fashion, a history'		'Recycling' of carbon in organic compounds related to life, minerals, and the atmosphere

Sentiment analysis

Various versions of sentiment analysis have been developed for use with fiction, as well as for evaluating products and services; for this particular study a website's generic version was used on each chapter selected for analysis. For each paragraph in a story, the sentiment is expressed in terms of 'polarity' (negative, neutral or positive), with the confidence shown as a percentage.

From this polarity and percentage, a sentiment score can be calculated in which negative sentiment can have scores ranging from 0.0 to 0.99, neutral sentiment can have scores ranging from 1.0 to 1.99, and positive sentiment can have scores ranging from 2.00 to 3.00. In a previous analysis of narratives relating to the periodic table, the variation in sentiment score between paragraphs was often found to be large, and so the largest variations were suppressed by taking a three-paragraph moving average, which makes the major trends in sentiment score easier to visualise. The same technique has been used to assist in the visualisation of trends in this article.

Types of fictional plot

Although there are several schemes by which fictional plots have been classified, that proposed by Christopher Booker is used in this study. His

scheme provides a generic simple three-stage progression of a plot: from initial frustration to the protagonist "falling under the shadow of the dark power, which constitutes the story's main action", and eventually leading to resolution (Fig. 1). In terms of the mood or sentiment associated with the story, the initial phase is likely to be somewhat negative, becoming more negative in the middle, and positive at the end.

As variants on this generic plot, Booker identified a further five types of plot: (I) comedy; (II) rags to riches; (III) tragedy; (IV) voyage and return; (V) quest and (VI) rebirth. This paper is concerned with the 'fit' to these types of story of the overall shape of plots of sentiment score versus proportion of the story for Primo Levi's stories that focus in a particular chemical process or investigation.

Type of plot	Beginning ❶	Middle ❷	Ending ❸			
Sentiment‡						Positive
					Somewhat positive	
	Somewhat negative	Somewhat negative		Somewhat negative		
			Negative			
	0	Proportion of story ?				1.0

Fig. 1. Stages in Booker's generic plot,* and inferred sentiment

*Reference 11: Booker (2004, p. 218)

† Description of stages:

❶ "The 'beginning' of almost any story shows us the hero or heroine who is in some way undeveloped, frustrated or incomplete. This establishing of their unhappy, immature ort unfulfilled state sets up the tension needing to be resolved which provides the essence of the story."

❷ "The 'middle' of the story shows them sooner or later falling under the shadow of the dark power, the conflict with which constitutes the story's main action. In the types of story we come to early in life this threatening presence is invariably personified as outside the central figure, although later on we come to the type of story in which those same dark qualities are shown as lying in the hero or heroine themselves. Through most of the story we see its little world divided into an 'upper' realm, where the dark power holds sway, and an 'inferior' realm, where the forces of light remain in the shadows."

❸ "The 'end' of the story provides its resolution. The action eventually builds to a climax, when the forces making for threat and confusion rise to their highest point of pressure on everyone involved, and this paves the way for the 'reversal' or 'unknotting', the moment when the dark power is overthrown."

‡ In Figs. 2-7, 'sentiment score' varies between 0 (most negative sentiment) and 3.0 (most positive sentiment); the trend of sentiment as the story progresses in this generic plot is broadly similar to that seen in comedy plots.

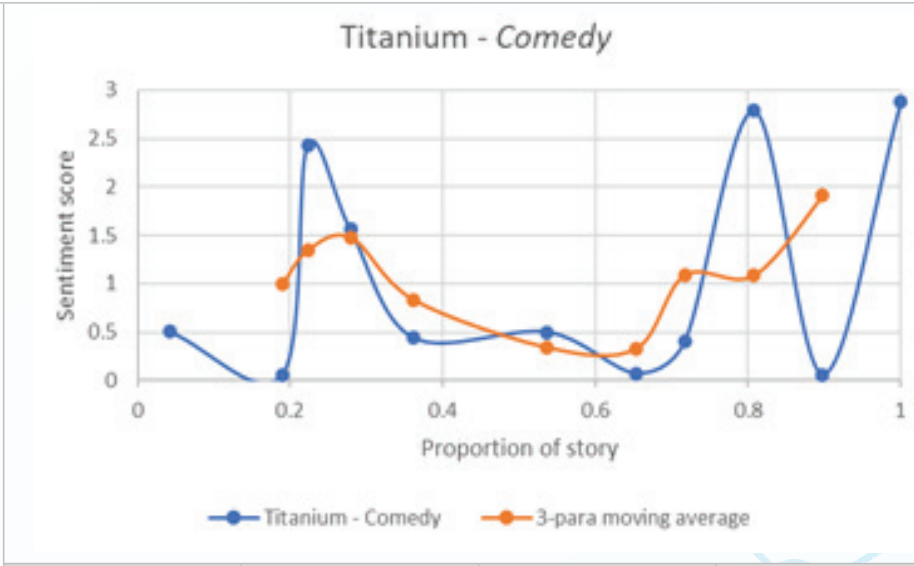
Application of sentiment analysis to Primo Levi's stories

The simplest type of plot is comedy (which, incidentally, is not necessarily amusing), a three-stage plot rather similar to the generic plot described above. 'Titanium', a simple story about a painter restraining a girl's interest in drying paint (Fig. 2), and 'Sulfur' (not shown: a simple story about keeping a potentially exploding industrial boiler under control) are characterised by a confused or confusing activity at the mid-point of the story, but there is a 'happy ending'.

The plot for 'Arsenic' (Fig. 3) broadly resembles that for comedy, but in this instance because the storyline is concerned with Levi's successful initiation into being a consulting chemist, it is here assigned to the rags to riches category. The high sentiment score (i.e. more positive sentiment score) at the

I - COMEDY
(Booker, p. 150)

1. a little world with a shadow of confusion, uncertainty and frustration, people are shut off from each other
2. confusion gets worse; everyone in a nightmarish tangle
3. perceptions dramatically changed, shadows destroyed, and a joyful union results

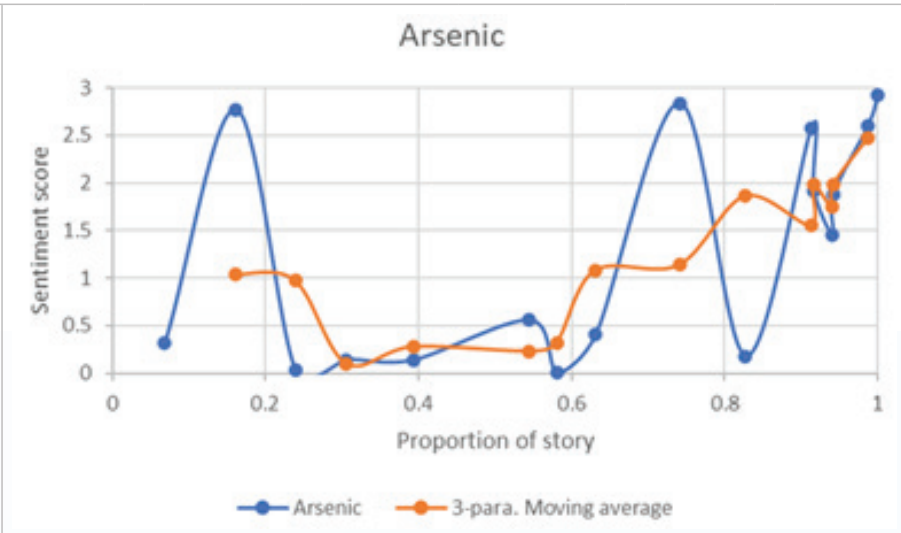


STAGES	1	2	3

Fig. 2. Variation of sentiment plots for Levi's 'Titanium' story as stages of comedy

II - RAGS TO RICHES
(Booker, pp. 65-66)

1. initial wretchedness at home and the 'call'
2. out into the world, initial success
3. the central crisis: everything suddenly goes wrong
4. Independence and the final ordeal
5. final union, completion and fulfilment ('living happily ever after')



STAGES	1	2	3	4	5

Fig. 3. Variation of sentiment plot for Levi's 'Arsenic' story and inferred stages of rags to riches plot

II - RAGS TO RICHES
(Booker, p.156)

1. anticipation stage
2. dream stage
3. frustration
4. nightmare stage (things out of control)
5. destruction or death wish stage

STAGES	1	2	3	4	5

Fig. 4A. Variation of sentiment plot for Levi's 'Zinc' story and inferred stages of tragedy

end of this story suggests a greater satisfaction with its outcome than with either the drying of paint in the 'Titanium' comedy or the gaining control of a potentially malfunctioning boiler in the 'Sulfur' comedy!

Tragedies, i.e. stories where the outcome is disappointing or unfavourable (but not death in these particular stories), are represented in Levi's book by the stories for 'Zinc', 'Nitrogen', 'Hydrogen', 'Nickel' and 'Tin' (Fig. 4). As expected, the sentiment scores are low at the end of the stories, but – interestingly, and unexpectedly – the sentiment scores are sometimes high at the height of the crisis.

It might be inferred that, at least in these stories, Levi the chemist revels in the challenges that the chemical crises bring. The 'Hydrogen' and 'Nickel' stories are similar in that both involve a failed experiment (because of incompetence in handling potassium metal and because of a lack of knowledge of the bonding of nickel in silicate minerals respectively) which could have had adverse consequences for Primo Levi's continued employment, but which did not occur.

Stories that involve discoveries, ei-

ther related to the self or to material goods, often fit Booker's (2004) criteria for quests. Examples include the discovery of the structure of DNA and the history of the periodic table of the elements, the most diagnostic features being two distinct minima in sentiment, corresponding to early frustrations and final ordeals, respectively.

In these respects, in Primo Levi's book, the stories 'Cerium', 'Uranium' and 'Silver' fit the stages of a quest well (Fig. 5).

On occasion, the combination of biography and science has the potential to complicate sentiment analysis because effectively the chapter may actually comprise more than one story; for example, a story related to the investigation of a chemical process may be intertwined with a story related to an experience earlier in Levi's life.

Although the 'Potassium' and 'Uranium' stories are examples of such a combination, the quest's characteristic features remain visible on their sentiment plots.

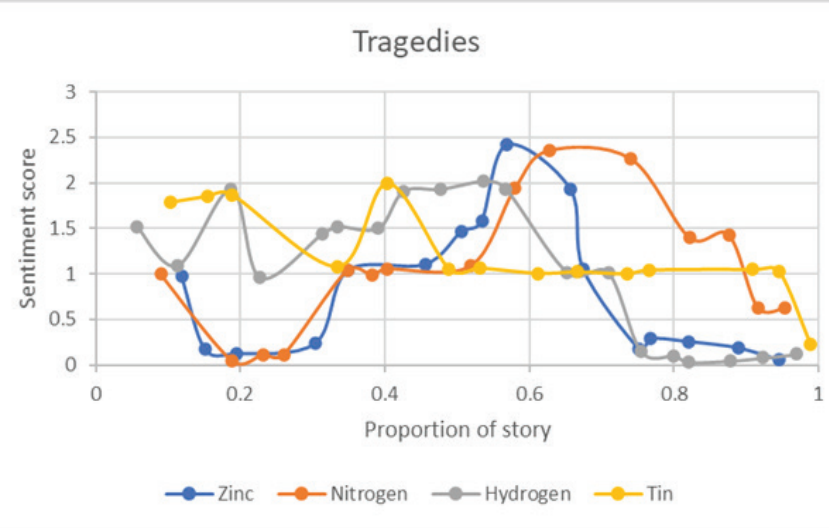
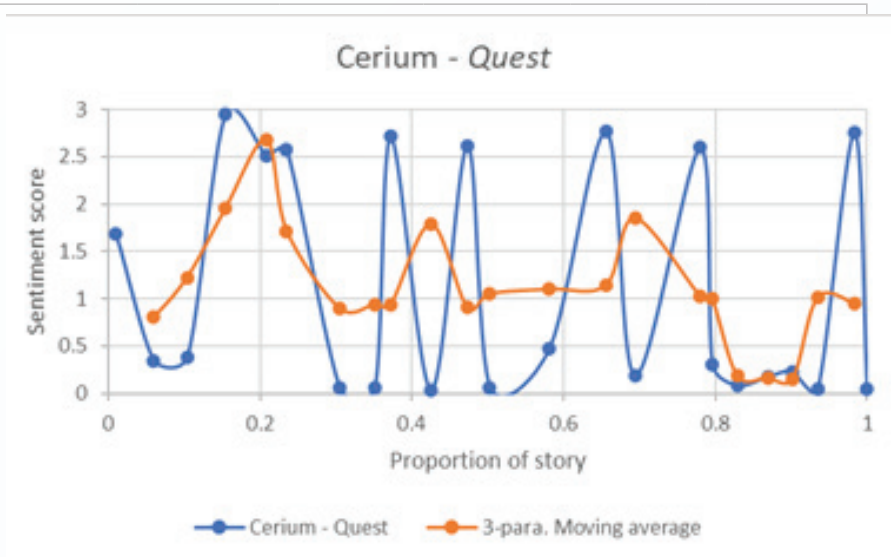


Fig. 4B. Variation of 3-paragraph moving average sentiment plot for Levi's 'Zinc' (see also Fig. 4A), 'Nitrogen', Hydrogen', and 'Tin' stories. Typically, the dream stage (Stage 2) occurs at about 0.2 proportion of story; the frustration stage (Stage 3) at about 0.3-0.5 proportion of story, and the nightmare stage (Stage 4) at about 0.6 proportion of story. At the nightmare stage, sentiment seems moderately high despite "things [being] out of control." Of these stories, that for 'Tin' seems to fit the tragedy trend least well; in fact, the story is a continuous series of misfortunes leading to Levi's decision to abandon chemical consultancy as an occupation, in part because: 'Nothing of the generous good nature of tin, Jove's metal, survives in its chloride… This salt is an energetic reducing agent, that is to say, it is eager to free itself of its two electrons and does so at the slightest pretext, sometimes with disastrous results'.

The final two types of plot are similar in that they involve a form of recycling. Voyage and return (Fig. 6) takes the element carbon on a biological journey, but in this story, it does not return to its original entity in CO_2: there is, thus, no 'thrilling return', and the story just trails off. A similar voyage and return type of story for a chemical element in a historic context can be given for gold:

IV- QUEST
(Booker, pp. 83-84)

1. the call
2. the journey
3. arrival and frustration
4. the final ordeals (a last eries of tests)
5. the goal (achieved after 'thrilling escape from death'; treasure is won)



STAGES	1	2	3	4	5

Fig. 5A. Variation of sentiment plot for 'Cerium' and inferred stages of quest. Of all the stories in Levi's *The Periodic Table*, this one – requiring Levi's combination of chemical and entrepreneurial skills in a prison environment – matches most closely the criteria for a quest.[16]

"We can imagine the life of a gold coin two millennia ago, struck perhaps in a provincial mint and used by a young soldier as part of his pay to buy goods on the northern frontier of England and finding its way back to Roe in the coffers of an imperial official sent to collect taxes, before passing into the hands of a trader heading east, and then being used to pay for produce bought from traders who had come to sell their provisions at Barygaza.

There it was admired and presented to leaders in the Hindu Kush, who marvelled at its design, shape and size and then gave over to be copied by an engraver – himself perhaps from Persia, or from India or China, or perhaps even someone local who had been taught the skills of striking. This was a world that was connected, complex and hungry for exchange."

Although the 'Nickel' story includes elements of the tragedy type of story, both the uneconomic nickel mine and Levi's lack of understanding of the characteristics of nickel in silicate minerals are effectively unchanged at the end of the story from their status at the beginning, despite tumultuous sentiment variations between those points, as Levi suggests unlikely – and unsuccessful – means of concentrating the nickel to economic grade; this suggests assignment of the voyage and return type of plot is more appropriate.

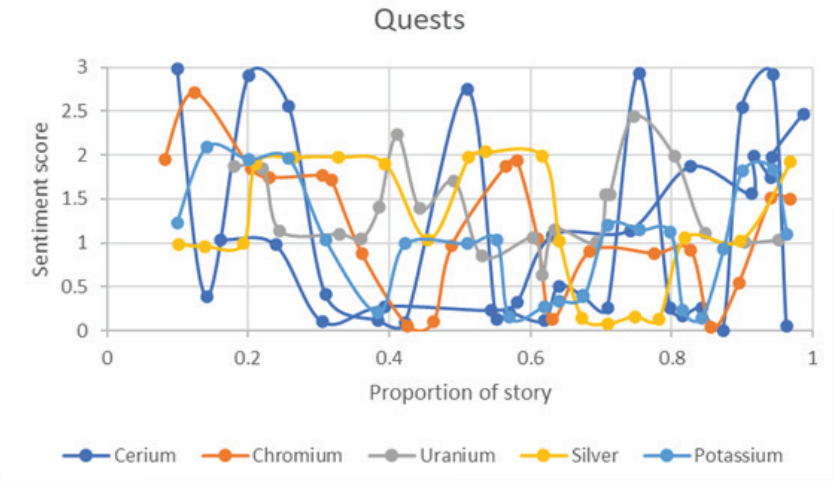


Fig. 5B. Variation of 3-paragraph moving average sentiment plot for Levi's 'Cerium' (see also Fig. 5A), 'Chromium', 'Uranium', 'Silver', and 'Potassium' stories. All show a "call' at the start of the story, and all show at least two excursions into low sentiment scores indicating early frustrations and later ordeals before the final up-swing in sentiment associated with the achievement of the quest.

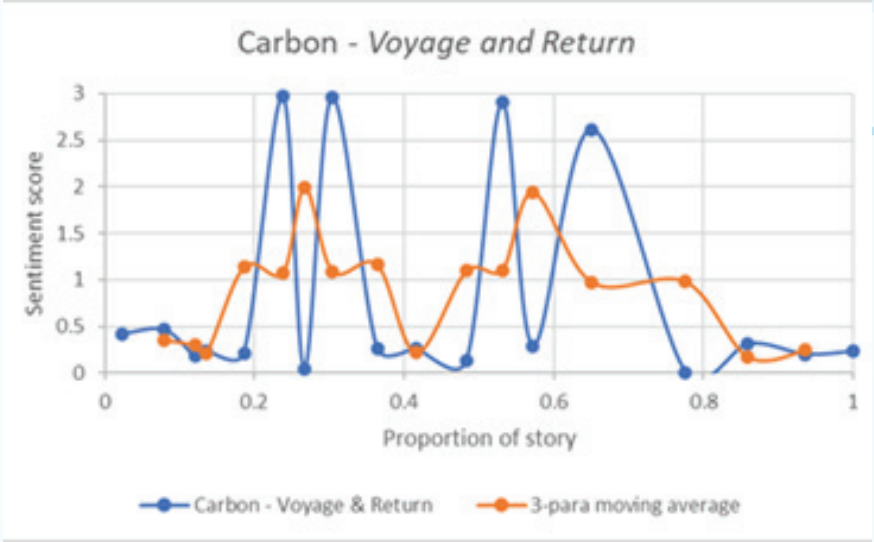
Rebirth is a darker version of voyage and return but ends on a more positive note (i.e., higher sentiment score); in Levi's book, only the 'Vanadium' story matches this form (Fig. 7).

Fig. 7. Variation of sentiment plot for Levi's story 'Vanadium' and inferred stages of rebirth. Although vanadium is the chemical theme of this chapter, the chapter's equally important storyline is Levi's interaction with a former associate at Auschwitz (a Dr Müller) which is reactivated by the appearance of Müller as an employee of the firm responsible for the problem with the purity of the vanadium that Levi seeks to solve.

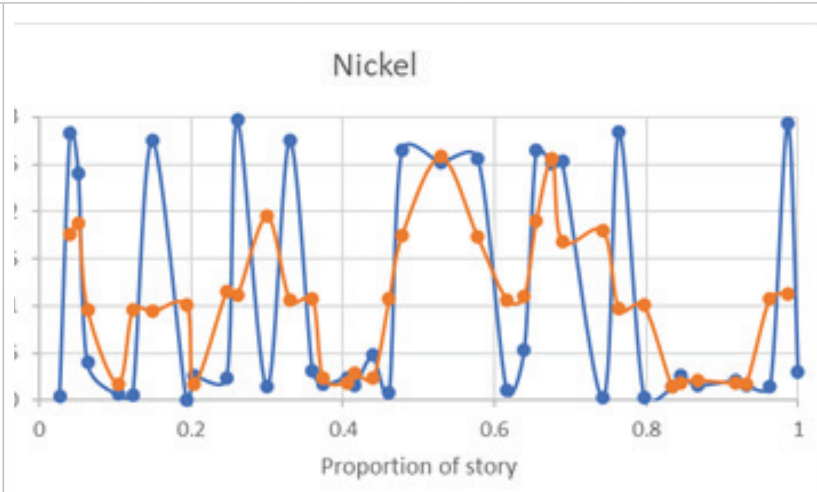
The 'all-the-story' sentiment scores

V - VOYAGE AND RETURN
(Booker, p. 105-106)

1. anticipation stage and 'fall' into the other world
2. initial fascination or dream stage (exhilaration)
3. frustration stage (adventure changes to difficulty and oppression)
4. nightmare stage (survival threatened)
5. thrilling escape and return



STAGES	1	2	3	4	5



STAGES	1	2	3	4	5

Fig. 6. Variation of sentiment plot for Levi's 'Carbon' and 'Nickel' stories and inferred stages of voyage and return

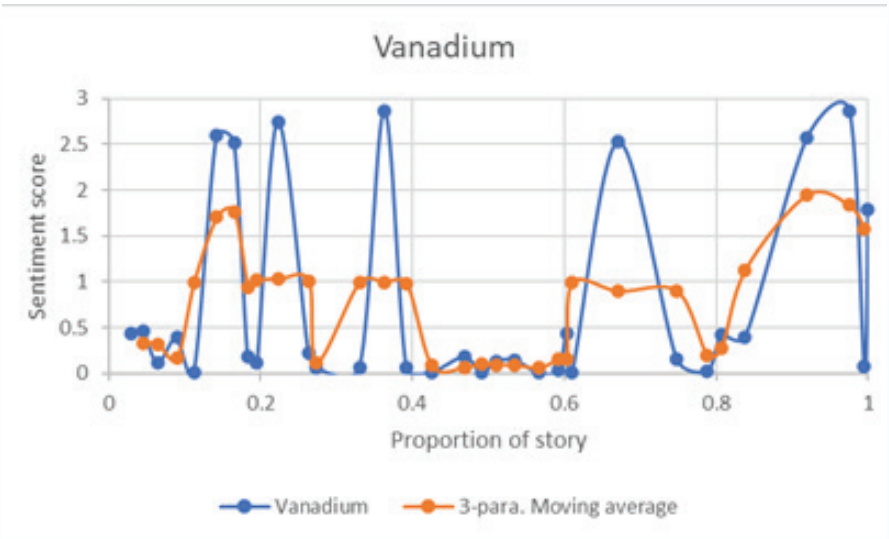
(Table 2 and Fig. 8) are within the range of neutral to negative polarity. While this might imply that these are not necessarily 'likable' stories for the reader, the variation in sentiment scores is not only a measure of Levi's frustrations but also his determination to rise to the challenges of the real experiences portrayed in the stories.

From the inferred dates of some of the stories (Table 2), there is an overall decreasing sentiment score over time, as shown in Fig. 9, with a particularly pronounced 'dip' in the early 1940s. As expected from the earlier plots (Figs. 2-7), the 'all-the-story' sentiment scores are low – mostly within the range of neutral sentiment, i.e., 1.0 – 2.0. Fig. 9 also shows that the sentiment scores for Levi's poems (see Appendix 2) - always higher than his non-fiction prose – show a dramatic increase in the mid-1940, followed by a modest decline through the 1960s.

In comparison, the poems written in Levi's later life show large variations in sentiment score – ranging from

VI - REBIRTH
(Booker, p. 204)

1. hero/heroine falls under shadow of a dark power
2. for a while all goes reasonably well, the threat may even have receded
3. shadow returns; hero/heroine imprisoned in a state of living death
4. continues for a long time
5. a miraculous redemption



STAGES	1	2	3	4	5

Fig. 7. Variation of sentiment plot for Levi's story 'Vanadium' and inferred stages of rebirth. Although vanadium is the chemical theme of this chapter, the chapter's equally important storyline is Levi's interaction with a former associate at Auschwitz (a Dr Müller) which is reactivated by the appearance of Müller as an employee of the firm responsible for the problem with the purity of the vanadium that Levi seeks to solve.

Table 2. Sentiment scores for Levi's Periodic Table stories

Chapter	Type of plot						Exempt*	Inferred year of story's occurrence†
	Rags to riches	Quest	Voyage & return	Comedy	Tragedy	Rebirth		
	'All the story' sentiment score ‡							
Argon							1.442	1930
Hydrogen					0.877			
Zinc					0.88			
Iron							1.478	1939
Potassium		1.956						
Nickel			0.92					
Lead §							0.994	
Mercury §							1.083	
Phosphorus							1.359	1942
Gold							0.931	1942
Cerium		1.227						1944
Chronium		1.352						1946
Sulphur				0.645				
Titanium				0.909				
Arsenic	1.552							
Nitrogen					1.022			
Tin					1.639			
Uranium		1.482						
Silver		1.428						
Vanadium						0.948		1967
Carbon			0.778					

*'Exempt' stories are those that do not involve analytical chemistry techniques and/or inorganic chemistry processes and reactions.

† Where feasible, the approximate date of the story is inferred from the text.
‡The 'all-the-story' sentiment score (S) is calculated as S = Σi=n i=1 (si x pi), where si is the sentiment score for a given paragraph of the story (determined as described earlier) and pi is the proportion of words in the total story that comprise the paragraph; the summation (Σ) being carried out for all n paragraphs of the story. The scores are also shown in Appendix 1, together with their corresponding sentiment percentages and polarities.

§ A fictional story.

highly positive to highly negative sentiment. This seems consistent with Levi's own motivation for writing the poems, expressed in 1984 as:

"In every civilization, even those without writing, many renowned and unknown alike, feel the need to express themselves on poetry; and give in to it; so they secrete poetic matter, spirited or lifeless, eternal or ephemeral, and address it to themselves, to their neighbour or to the universe…

"Occasionally, 'at an uncertain hour', I too have surrendered to this impulse: apparently it is encoded in our DNA. At certain moments, poetry felt to me more suitable than prose to communicate an idea or an image. I can't explain why, and it never concerned me: I know little of theories of poetics, I read little of other people's poetry, I don't believe in the sacredness of art, nor do I believe that these poems of mine are great. I can only assure any prospective reader that seldom (usually no more than once again), on the spur of the moment, particular motives have spontaneously come to take a certain form, which my rational half continues to regard as unnatural"

Fig. 9. Variation over time of the sentiment scores for Primo Levi's Periodic Table stories, related to his chemistry experiences, and for his poems (which address a wider range of experiences and topics).

Conclusion

In his story 'Silver', Levi revealed his "kind of story" as one:

"in which you thrash about in the dark for a week or a month, it seems that it will be dark forever, and you feel like throwing it all up and changing your trade; then in the dark you espy a glimmer, proceed groping in that direction, and the light grows, and finally order follows chaos."

This description of the story concurs with either Booker's generic story or with his comedy variant. In the next paragraph of 'Silver', Levi's one-time student colleague (Cerrato) is reported by Levi to have considered that stories based on his experience:

"... sometimes things went like that {i.e., as in previous quotation] ... but in general it was really dark all the time. You couldn't see the glimmer, you beat your head again and again against an ever lower ceiling, and ended by coming out of the cave on your hands and knees and backward, a little older than when you went in."

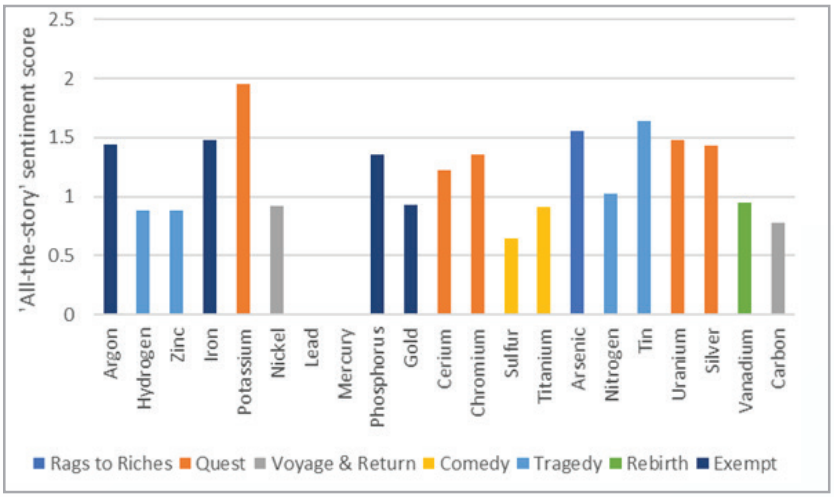


Fig. 8. Variation of 'all-the-story' sentiment score with position of chapter in Levi's The Periodic Table (the first chapter is entitled 'Argon'; the last chapter is entitled 'Carbon'). Sentiment scores are not included on this plot for the fictional stories, viz, 'Lead' and 'Mercury'.

This description more closely resembles that tragedy plot. However, this paper illustrates that Levi's stories show variations in sentiment that are collectively indicative of the full range of plots established for fictional works.

This has been achieved by the appropriation of sentiment analysis from market research, albeit modified for application to fiction (including poetry – see Fig. 9), combined with a typology of literary fiction. The approach has provided a new way of looking at stories written about science, in particular the periodic table of the chemical elements (Fig. 10).

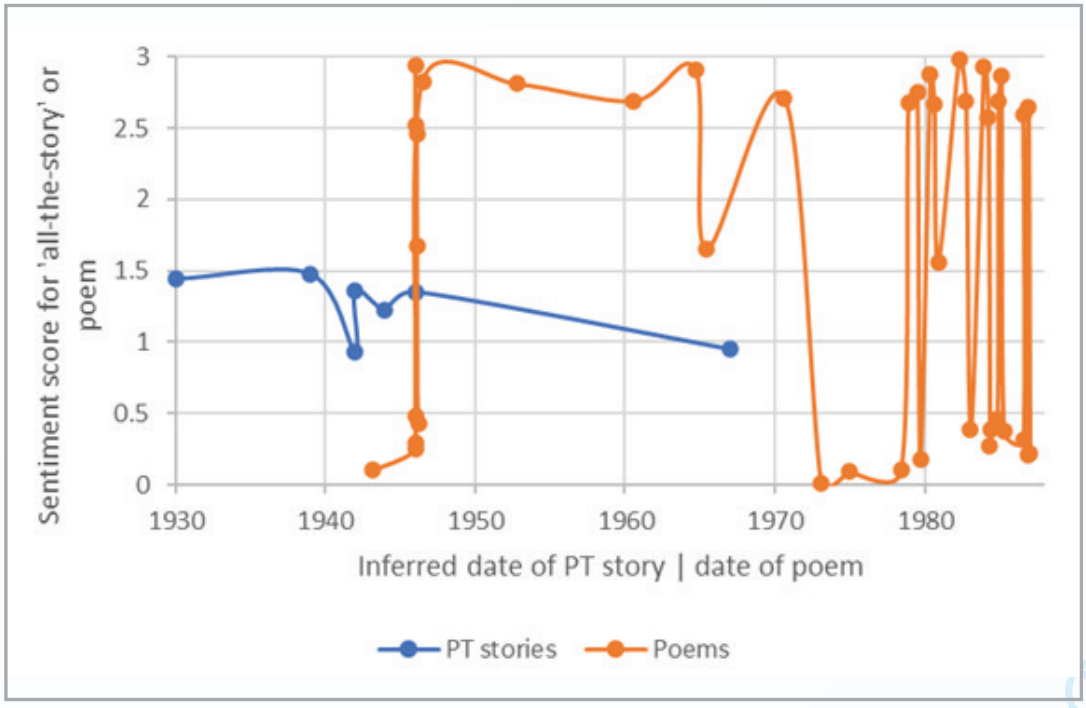


Fig. 9. Variation over time of the sentiment scores for Primo Levi's Periodic Table stories, related to his chemistry experiences, and for his poems (which address a wider range of experiences and topics)

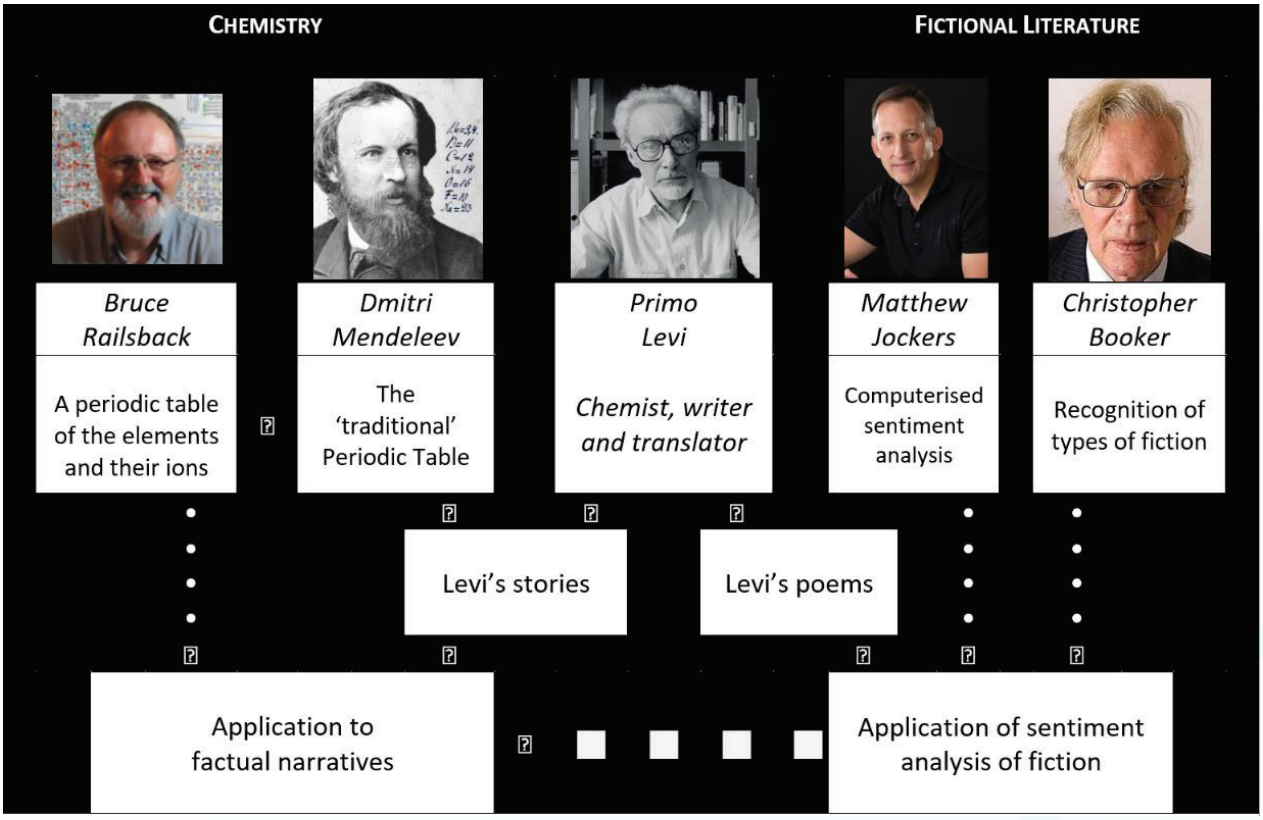
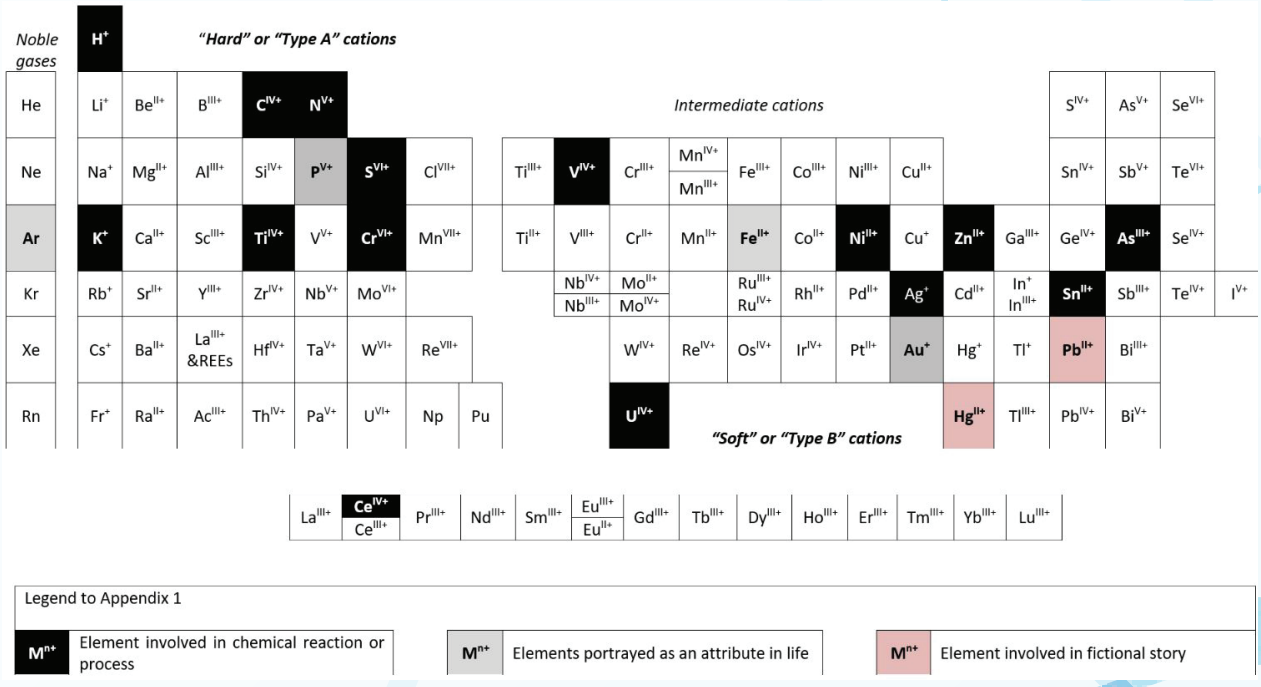


Fig. 10. Dramatis personae and process flow chart for 'Sentiment analysis of Primo Levi's The Periodic Table'

Appendix 1. Chemical elements from stories in Primo Levi's *The Periodic Table*, highlighted on the skeletal framework of the 'cation' side of the 'Earth Scientist's Periodic Table of the Elements and their Ions'



Notes to Appendix 1.

Chapter	Ion	Brief chemistry notes	'All of story' ...	
			Sentiment % and polarity*	Sentiment score †
1	Ar	Argon (Ar^0) is portrayed as metaphor for 'relegation to the margins of the great river of life'.	N44.2%	1.442
2	**H+**	Electrolysis of water yields H^2 and O^2 in explosive proportions.	-12.3%	0.877
3	**ZnII+**	A simple synthesis of zinc sulfate.	-12%	0.88
4	FeII+	Iron is portrayed as a metaphor for strength.	N47.8%	1.478
5	**K+**	Another ill-fated experiment, with potassium 'in contact with water not only develops hydrogen but also ignites' (Levi, p. [49]).	N95.6%	1.956
6	**NiII+**	The fictional story concerns asbestos, in which minor amounts of NiII+ replace FeII+ in minerals such as anthophyllite $(Mg, Fe)^7(Si^8O^{22})(OH, F)^2$.	-7.7%	0.923
7	PbII+	In this fictional story, the un-named mineral that is crudely smelted is likely to have been galena (PbS).	-0.6%	0.994
8	HgII+	In this improbable fictional story metallic mercury (Hg^0) is recovered from an active volcano and purified by distillation.	N8.3%	1.083
9	PV+	The story recognises that inadequate distinction is made between 'inorganic P', 'organic P', and 'total P' resulting in the failure of a primitive experiment in diabetes research.	N35.9%	1.359
10	Au+	This story about alluvial gold (Au^0) asserts that wisdom and skills are more desirable than gold.‡	-6.9%	0.931
11	**CeIV+**	This story relates to cerium metal (Ce^0), which tarnishes readily in the air; it oxidises slowly in cold water and rapidly in hot water. It dissolves in acids. It can burn when heated or scratched with a knife.	N22.7%	1.227
12	**CrVI+**	This story features chromate-based anti-rust paint.	N35.2%	1.352
13	**SVI+**	The behaviour of naptha and sulfodiene in a furnace.	-35.5%	0.645
14	**TiIV+**	The whitening agent in paint is TiO^2.	-9.1%	0.909
15	**AsIII+**	This story features arsenious sulfide As^2S^3; and arsenious anhydride (arsenic trioxide, As^2O^3).	N55.2%	1.552
16	**NV+**	Actually, the story is not about NV+ at all; rather, it is about the purification of alloxan, which itself can be derived from uric acid, a significant component of avian and reptilian excrement.	N2.2%	1.022
17	**SnII+**	The story features stannous chloride.	N63.9%	1.639
18	**UIV+**	Material provided to Levi was mistaken as uranium metal; the ore from which U would have been derived is uraninite (UO^2); the material probably contained cadmium metal.	N48.2%	1.482
19	**Ag+**	Reduction of silver bromide to silver by phenols.	N42.8%	1.428
20	**V^{IV+}**	Vanadium is tetravalent in vanadium napthenate.	-5.2%	0.948
[21]	**CIV+**	Effectively a description of a natural carbon cycle.	-22.2%	0.778

* Sentiment polarity (negative [-], neutral [N], or positive [+]) and percentage determined from: https://monkeylearn.com/sentiment-analysis/

† Sentiment score (S) is: 1-(negative %/100), giving a range of scores from 0-0.99; or 1+(neutral %/100), giving a range of scores from 0-1.99; or 2+(positive %/100), giving a range of scores from 2.00-3.00. On this basis sentiment scores will be between 0 and 3.

‡ In essence, this is the translation of the motto associated with the original coat of arms of Victoria University of Wellington, which read in Latin: "Sapientia magis auro desideranda" (Barrownan, R., Victoria University of Wellington 1899—1999. A History. Victoria University Press: Wellington, 1999, p. 19)

Appendix 2. Selected poems by Primo Levi (data used in Fig. 9)

Date of poem	Title of poem		Sentiment % and polarity*	Sentiment score †
	Italian	*English*		
February, 1943	Crescenzago	Crescenzago	-89.6%	0.104
3 January, 1946	Cantare	Singing	-75.3%	0.247
9 January, 1946	25 febbraio 1944	25 February, 1944	-51.4%	0.486
10 January, 1946	Shemà	Shema	+93.4%	2.934
17 January, 1946	Lunedi	Monday	-70.3%	0.297
28 January, 1946	Un altro lunedi	Another Monday	+52.2%	2.522
7 February, 1946	Il tramonto di Fossoli	Sunset at Fossoli	N67.6%	1.676
11 February, 1946	11 febbraio 1946	11 February 1946	+45.9%	2.459
15 March, 1946	Il ghiacciaio	The glacier	-56.8%	0.432
28 June, 1946	Avigliana	Avigliana	+82.5%	2.825
6 October, 1952	Epigrafe	Epitah	+80.9%	2.809
20 July, 1960	Per Adolf Eichmann	For Adolf Eichmann	+68.9%	2.689
10 September, 1964	Approdo	Sundown	+90.7%	2.907
23 May, 1965	lilit	Lilith	N65.2%	1.652
13 August, 1970	Nel principio	In the Beginning	+71.4%	2.714
2 February, 1973	Via Cigna	Via Cigna	-99.1%	0.009
30 November, 1974	Le stella nere	The Black Stars	-90.7%	0.093
23 May, 1978	Plinio	Pliny	-89.6%	0.104
20 November, 1978	La bambina di Pompeii	The Little Girl From Pompeii	+67.3%	2.673
22 June, 1979	Annunciazione	Annunciation	+75%	2.750
5 September, 1979	Verso valle	Down to the Valley	-81.9%	0.181
10 May, 1980	Core di legno	Wooden Heart	+79.4%	2.794
13 August, 1980	Schiera bruna	Brown Battalion	+66.7%	2.667
12 November, 1980	Autobiografia	Autobiography	N56.1%	1.561
9 August, 1982	Pasqua	Passover	+97.7%	2.977
22 September. 1982	Vecchia talpa	Old Mole	+68.7%	2.687
15 January, 1983	Un topo	The Mouse	-61.1%	0.389
7 December 1983	La chiocciola	The Snail	+92.4%	2.924
23 March, 1984	L'elefante	The Elephant	+57.2%	2.572
3 May, 1984	Casa Galvani	At Galvani's	-72.7%	0.273
18 May, 1984	Pio	Pious	-61.4%	0.386
29 October, 1984	Una valle	A Valley	-53.7%	0.463
24 November, 1984	Agenda	Agenda	+68.9%	2.689
2 February, 1985	Il disgelo	The Thaw	+87.0%	2.870
5 April, 1985	Delila	Delilah	-62.2%	0.378
5 April, 1985	Sansone	Samson	-68.9%	0.311
22 July, 1986	Agosto	August	+95.2%	2.952
24 November, 1986	Il domedario	The Dromedary	-78.5%	0.215
25 November, 1986	Un ponte	A Bridge	+65.1%	2.651
2 January, 1987	Almanacco	Almanac	-78.3%	0.217

* Sentiment polarity (negative [-], neutral [N], or positive [+]) and percentage determined from: https://monkeylearn.com/sentiment-analysis/

† Sentiment score (S) is: ^{1}-(negative %/$_{100}$), giving a range of scores from ^{0}-$^{0.99}$; or ^{1}+(neutral %/$_{100}$), giving a range of scores from ^{0}-$^{1.99}$; or ^{2}+(positive %/$_{100}$), giving a range of scores from $^{2.00}$-$^{3.00}$. On this basis sentiment scores will be between ^{0} and ^{3}.

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21. Portrait credits for Fig. 10: Bruce Railsback, https://geology.uga.edu/directory/people/bruce-railsback ; Dmitri Mendeleev, https://www.chemistryworld.com/features/the-father-of-the-periodic-table/3009828.article ; Primo Levi, https://www.chemistryworld.com/features/primo-levi-and-the-other-periodic-table/3010512.article ; Matthew Jockers, https://cdrh.unl.edu/about/faculty/jockers ; Christopher Booker, https://alchetron.com/Christopher-Booker.
22. Railsback, 2018, *op. cit*., p. 209 (fig. 11.1).

Article

Diabetic foot ulcers: an unmet challenge in medicinal chemistry

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Keywords: *diabetes, foot ulcers, COVID-19, insulin, medicinal chemistry*

Introduction

There are currently close to half a billion people in the world living with diabetes. The great majority of them (90%) have type 2 diabetes. The countries with the largest number of diabetics (in millions) are China (116.4), India (77), the United States (31), Pakistan (19.4), Brazil (16.8), Mexico (12.8), Indonesia (10.7), Germany (9.5), Egypt (8.9) and Bangladesh (8.4).[1-2]

It is our Pacific Island neighbours who have the largest number of diabetes sufferers as a percentage of the total population, with Kiribati, Tuvalu, Mauritius, New Caledonia, Solomon Islands and Papua New Guinea at roughly 20%, while Tonga and Fiji have a rate of 14-16%.[1-2]

In New Zealand, we have close to 250,000 diagnosed cases of diabetes in the country. 90% of these cases are type 2 diabetes.[1-3] Although this number would appear relatively small (at the moment only 6% of the population is affected), we have a high prevalence of people with pre-diabetes, i.e. people with high blood sugar levels.

A 2008/2009 nutrition survey found that high blood sugar levels affect close to 19% of the population, equating to approximately 930,000 people.[4] In 2019, it was estimated that 100,000 Kiwis suffering from type 2 diabetes were yet to be diagnosed.[5-6]

If current trends continue, in 20 years we can expect to see an increase of 70-90% in the number of people suffering from type 2 diabetes in New Zealand, i.e. approximately 407,000 patients).[3] Māori, Pasifika and Asian communities are predicted to be the worst affected. Current projections are an 18-25% prevalence of type 2 diabetes in Pasifika; 9.3-10.5% for Asian communities; 9.5-10.5% for Māori, and less than 5% for other communities.[3]

"Evidence shows that Kiwis from lower socio-economic backgrounds and living in more deprived areas have higher rates of diagnosed diabetes."

Evidence shows that Kiwis from lower socioeconomic backgrounds and living in more deprived areas have higher rates of diagnosed diabetes.[7-8] The median reported age of diagnosis of diabetes is 50 years; however, the age of diagnosis varies across different communities, with Māori and Pasifika being diagnosed at a younger age.

Diagnosis at a younger age is associated with a higher risk of chronic kidney disease, cardiovascular disease and early mortality.[9-10] Diabetes is more prevalent in males than in females. However, female diabetic patients often suffer from more serious complications compared to men (heart disease, vascular disease and kidney disease), and this often results in a higher risk of death.[11-12]

Diabetes places a large mental, physical and financial strain on the individual and his/her family. Financially, the economic cost for treating type 2 diabetes is currently NZD 2.1 billion p.a. (0.67% of GDP). If present trends continue, in 20 years' time this figure will increase by 63% to 3.5 billion NZD p.a. (in current NZD).[3, 13]

Diabetic foot ulcers

Diabetes complications include poor vascularisation and can result in the formation of diabetic foot ulcers (DFU). DFU is a major complication of diabetes, affecting 3-13% of all diabetic patients annually. DFU is expected to affect up to 34% of all diabetic patients during their lifetime, with a high chance of recurrence (40% within one year, and 65% within five years).[14-22]

DFU is the main cause of hospitalisation among people with diabetes and is responsible for over 80% of all lower leg amputations. The current cost of treatment for a wound resulting in an amputation is approximately NZD 42,774, whilst the median cost of a wound episode not requiring an amputation is NZD 27,385.[23]

Amputations also result in higher mortality and morbidity, poor quality of life and mental health issues. Additionally, 50% of amputees are rendered functionally dependent – placing strain on whānau, community and carers.[3] Five-year mortality rates after new onset of DFU are 43-55% and up to 74% for patients who had an amputation.[21] Amputations occur at a higher rate for Māori and Pasifika populations, those living in socio-economic deprivation, and males.[3]

DFU is largely preventable, and the frequency of amputations can be lowered significantly (49-87%) by preventing DFU.[24-25] Current treatments for DFU are largely ineffective and expensive, with best clinical practice effective in less than 40% of cases. The overall success rate of so-called "advanced" wound healing therapies is low, typically providing less than a 20% added benefit over best clinical practice protocols, whilst their cost is disproportionately high.

Diabetes and COVID-19

In November 2020, a global analysis published in the journal Diabetes, Obesity and Metabolism found that up to 14.4% of people who were hospitalised with severe SARS-CoV-2 went on to develop diabetes.[26-27] It appears that SARS-CoV-2 can target and impair the body's insulin-producing cells, raising the possibility that the coronavirus may preferentially infect the insulin-producing beta cells.

In addition to the loss of beta cells, SARS-CoV-2 infection also appears to change the fate of the surviving cells. Studies showed that beta cells go through a process of transdifferentiation, in which they appeared to be reprogrammed to produce less insulin. Although the full consequences of this transdifferentiation of beta cells are not yet clear, they are likely to result in higher insulin deficiency and raised blood glucose levels. More studies are needed to understand how SARS-CoV-2 reaches the pancreas and what role the immune system might play in the resulting damage.[28-29]

In conclusion, we are in the middle of a worldwide diabetes epidemic whose effects and impacts are only going to increase, particularly if we consider the negative effect of SARS-Cov-2 on beta cells. Chemistry has the unique opportunity and responsibility to design and develop solutions that are effective, safe and affordable and that can work in and out of the clinic.

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