VOLUME 2 NUMBER 11

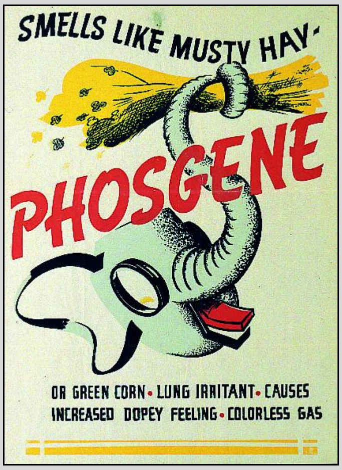
The OPCW Science & Technology Monitor

A sampling of Science & Technology Relevant to the Chemical Weapons Convention

10 December 2015

In This Issue

Featured content



Schedule 3 Chemicals; Phosgene identification poster from World War II.

Image from *allelopathylisacooley*.
Allelopathy

Image from *Pixapay*.
The Internet of Things

Welcome

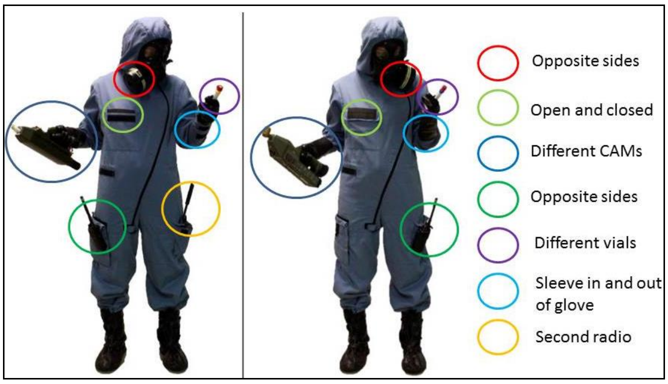
Welcome to the *OPCW Science and Technology Monitor*, an occasional bulletin to provide updates on developments in science and technology across a broad spectrum of topics relevant to the CWC. Past issues are available from the Science and Technology section of the OPCW website.

We begin this last newsletter of 2015 with an acknowledgement of the people who have contributed all of the time, ideas, and effort that makes the *S&T Monitor* possible. Our intern staff continues to raise the bar on both form and substance and we wish them the best of luck as they move onward in their careers. We have been lucky to have such a talented group of individuals choosing to spend time in our office this year. Thank you: Edoxie Allier-Gagneur, Wesam Alwan, Wardah Amir, Natalie Childress, Thomas Faria, Beatrice Maneshi, Johannes Niemeier and Inam Siraj.

Today marks the one-hundred fourteenth anniversary of the first Nobel Prize Award ceremony held in 1901 in accordance with Alfred Nobel's will. This day, 10 December is also the anniversary of Nobel's death in 1896. In 1901, the physics prize was awarded to to Wilhelm Röntgen for the discovery of X-rays; the chemistry prize went to Jacobus Henricus van 't Hoffwork for work on chemical dynamics and osmotic pressure; the physiology or medicine prize was given to Emil von Behring for his work on serum therapy, particularly for its use in the treatment of diphtheria; poet Sully Prudhomme was awarded the prize in literature; and the very first Nobel Peace Prize was jointly awarded to Jean Henry Dunant and Frédéric Passy.

The S&T Puzzle

We once again congratulation our friends at CTBTO, the first to spot the differences in the photos of our masked colleague Edoxie Allier-Gagneur (who was not identified for the bonus prize).



The main differences (aside from subtle changes in body position) are illustrated above. Puzzle statistics now stand at: VER 5, OSP 2, OCS 1, INS 1 and CTBTO 6.

Science Fun:

In our last issue of *Science Fun* we learned about [the secrets of honey and why it does not go bad](). That was fifteen days before Halloween 2015, a day known amongst many of us for candy! Now, with more sweets to be consumed for the upcoming end of year holidays (for which we hope you are fully recovered from any October [candy induced stomach pains]()), we explore the chemistry of [candy]() (and taste a few [cookies]() too).

[Candy has a rich history in human societies](), starting from tree sap in prehistoric times (not so strange if you think about [maple syrup]()) to figs and dates and on to the introduction in Europe of a new spice called "sugar" in 1000 AD. There is a rich [chemistry to be found across the world of candy](). Did you know that chocolate contains [more than 600 chemicals](), [is toxic to dogs]() and [tastes better when prepared with beer yeast]()? Did you know that understanding crystal structures and crystallisation methods is important for preparing [rock candy]() (and [other candies](), even [chocolate]())? Did you know that Candy can [store significant amounts of energy]()? Or that [Candy Canes contain chemicals that bind to TRPM8 receptors]()? For those who like lab work, you might want to try your own [candy chemistry experiments]().

Image from [Wikipedia]().

Making candy is a scientific process that relies heavily on [technology]() as illustrated by the need for an industrial revolution, before it became [possible to make cotton candy]()!

			2	6		7		1
6	8			7			9	
1	9				4	5		
8	2		1				4	
		4	6		2	9		
	5				3		2	8
		9	3				7	4
	4			5			3	6
7		3		1	8			

In this edition of the puzzle, we ask you to first complete the Sudoko puzzle on the left, then use the sum of the numbers in each coloured section to find the symbol of an element in the periodic table. The element symbols can be arranged to spell the name of a Schedule 1 chemical. Be the first to tell us the chemical and you win the prize: your choice of requesting a featured topic, designing a puzzle or receiving a beverage hand selected by the Science Policy Adviser. Send answers by [email](). Good luck!

News and Updates

Recent reports and publications:

The OPCWs *[Practical Guide for Medical Management of Chemical Warfare Casualties]()*.

A *[Handbook on chemical and biological waste management]()*.

[Tear gassing by remote control: The development and promotion of remotely operated means of delivering or dispersing riot control agents]().

Wilson Center report on *[U.S. Trends in Synthetic Biology Research Funding]()*.

The [report of the Blue Ribbon Study Panel on Biodefense]().

CNS Occasional Paper *[#21 Biotechnology E-commerce: A Disruptive Challenge to Biological Arms Control]()*.

Wilton Park Report, *[Compliance with the BTWC: strategies towards the 2016 Review Conference]()*.

WHO *[World Health Statistics 2015]()* and [Antibiotic resistance: Multi-country public awareness survey]().

[2015 World Intellectual Property Report]() and a *[Guide to Using Patent Information]()* from the World Intellectual Property Organisation (WIPO).

Report on the *[Top 10 Urban Innovations of 2015]()*.

[UNESCO Science Report: Towards 2030]().

The *[Nature Index 2015]()* looks at [global scientific collaborations]().

OCED Policy Paper, *[Scientific Advice for Policy Making: The Role and Responsibility of Expert Bodies and Individual Scientists]()*.

Industrialisation also gave us the modern lollipop, which when studied with lasers can generate knowledge of shape dynamics and scaling laws for bodies dissolving in fluid flow. Our readers however, might be more interested in knowing how many licks it takes to get to the chewy chocolate center of a Tootsie pop (a question that requires statistics to answer)! Technological development in candy making continues marching forward with 3D printing now enabling production of visually interesting and tasty treats! Candy not only uses technology, it helps to advance it; as demonstrated by a contribution to the field of soft silicon microstructures (although it took a failure in the kitchen in order to make this discovery).

Science is also important for making that perfect cookie (3D printing helps too, and there are open source recipes). As for chemistry, did you know that baking gingerbread cookies produces a chemical called zingerone? This chemical is not actually present in ginger until it is cooked!

Maybe candy and cookies are not your thing? Not to worry, ice cream also has interesting (and complicated) chemistry to explore! We'll have to come back to that one next summer!

Crowdsourcing:

Compete for the Open Science Prize and enable discoveries for health by harnessing the innovative power of open data.

An app to allow your smartphone to process data and advance cancer research while you sleep.

Have any ideas for a minimally invasive skin biopsy technique for gene expression measurements? Take a look at this reduction-to-practice challenge.

Interested in initiating a citizen science project? Take a look a CitSci.org: a platform for

National Science Foundation special report, *Cybersecurity: Tech, Tools, and Training to safeguard the future*.

October 2015 issue of Dstl's *inSIGHT*.

November 2015 issue of PNNL's *Currents*.

October 2015 issue of *Biocoder*.

September 2015 issue of ICSU Newsletter.

UN Security Council report on OPCW Fact Finding Missions.

Science, education and industry resources:

Creative Technologies in the Classroom.

Presentation files from the Science and Technology for Nonproliferation and Terrorism Studies course at the Middlebury Institute of International Studies at Monterey.

The American Chemical Society Division of Chemistry Education Committee on Computers in Chemistry Education (ACS CHED CCCE) fall newsletter features articles on 21st Century Chemical Education, the use of Google Forms for lab reports, the PubChem Laboratory Chemical Safety Summary, online science and education resources from the OPCW, the Marvin Live application for online chemistry collaboration, Conservation and Art Materials Encyclopedia Online, the ChemWiki, the online biochemical and life sciences collection published by Henry Stewart, MolView, and a look back at 20 Years of the MOLECULE OF THE MONTH Website.

Some news from world of science and technology:

From the weeks of 11 – 17, 18 – 24, and 25 – 31 October; 1 – 6, 7 – 14, 15 – 21 and 22 - 28 November; and 29 November – 5 December; in chemistry.

Schedule 3 Chemicals

We began 2015 with a look at Schedule 1 chemicals in patents, provided statistics on Schedule 2 chemicals in scientific publications in August and now we leave 2015 with a look at the chemicals of Schedule 3.

From the Chemical Weapons Convention, the following criteria are taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:

(a) It has been produced, stockpiled or used as a chemical weapon;

(b) It poses otherwise a risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that might enable it to be used as a chemical weapon;

managing, documenting, and sharing citizen science data.

Upcoming S&T Related Events:

OPCW Calendar of Events October to December 2015.

14 – 18 December 2015
Biological Weapons Convention Meeting of States Parties
Geneva, Switzerland.

15 – 20 December 2015
Pacifichem 2015.
Honolulu, Hawaii
United States of America

25 January - 4 February 2016
Science and Diplomacy for Peace and Security: The CTBT @ 20
Vienna, Austria

2 – 4 February 2016
The Unmanned Systems Expo (TUSE)
The World Forum, The Hague
The Netherlands

16 – 18 February 2016
7th International Conference on Drug Discovery and Therapy
University of Sharjah, Sharjah, UAE

23 - 25 February 2016
NCT CBRNe Europe
Amsterdam, The Netherlands

6 – 10 March 2016
Pittconn 2016
Atlanta, GA
United States of America

13 – 17 March 2016
251st American Chemical Society National Meeting & Exposition
San Diego, CA, USA.
United States of America

16 – 19 March 2016
16th Asian Chemical Congress
Dhaka, Bangladesh.

21 - 23 March 2016
Biomarker Summit 2016
San Diego, CA, USA.

6 – 8 April 2016
XXI IUPAC CHEMRAWN Conference Solid Urban Waste Management
Rome, Italy.

(**c**) It poses a risk to the object and purpose of this Convention by virtue of its importance in the production of one or more chemicals listed in Schedule 1 or Schedule 2, part B;

(**d**) It may be produced in large commercial quantities for purposes not prohibited under this Convention.

Figure 1 illustrates the relationship between the three Schedules, showing how sulphur mustard (a Schedule 1 chemical warfare agent) is formed by treating its Schedule 2 pre-cursor (thiodiglycol) with a Schedule 3 reagent (thionyl chloride, a commonly used chlorinating agent for organic chemistry).

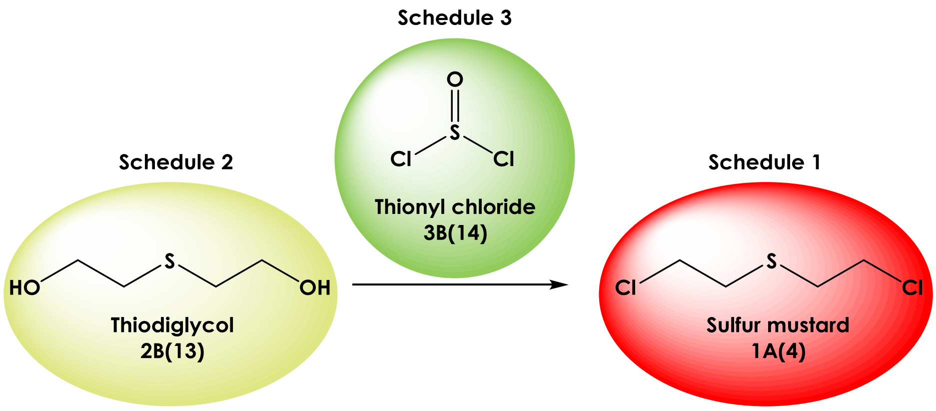


Figure 1: Illustration of the relationship between Schedule 1, 2 and 3 chemicals in the preparation of sulphur mustard.

Schedule 3 is the smallest of the Schedules (only 17 chemicals are listed), yet Schedule 3 chemicals, most notably hydrogen cyanide and triethanolamine, appear in more scientific reports (journal articles and patents) than both Schedule 1 and 2 chemicals combined. As of 3 November 2015, we identified over 330,000 journal articles and patents published from 1900 – 2014 that make reference to Schedule 3 chemicals using SciFinder® (see Figure 2). Figure 3 shows a breakdown of the individual Schedules appearing in publications in 2014.

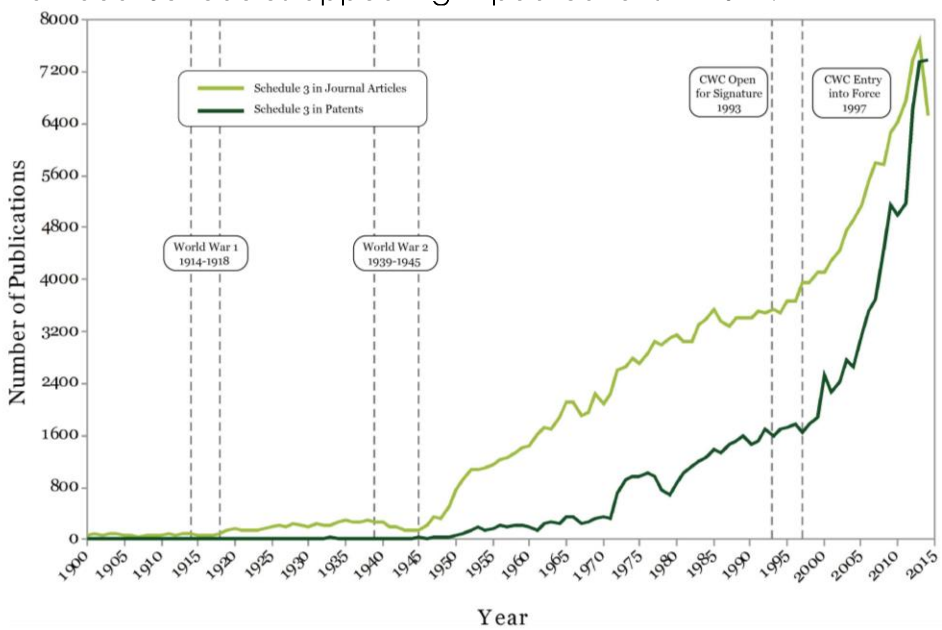


Figure 2: Number of journal articles and patents referencing Schedule 3 Chemicals from 1900-2014 (from SciFinder® as of 3 November 2015).

2 – 4 May 2016
The International Day for the 19th Anniversary of the Foundation of the OPCW.
2016 theme: *"Chemical Safety and Security in a Technologically Evolving World"*
OPCW Headquarters, The Hague
The Netherlands

6 May 2016
2016 Spring ConfChem
Science, Disarmament, and Diplomacy in Chemical Education: The Example of the Organisation for the Prohibition of Chemical Weapons.

24 – 26 May 2016
Innorobo 2016
Paris, France

26 - 28 May 2016
23rd Symposium on Chemical and Science Education
TU Dortmund University, Germany

6 – 9 June 2016
2016 BIO International Convention
San Francisco, California, USA

18 – 22 July 2016
The International Conference on Pure and Applied Chemistry (ICPAC 2016)
"Emerging Trends in Chemical Sciences" Mauritius

15 – 20 August 2016
24th IUPAC International Conference on Chemistry Education (ICCE 2016)
Kuching, Sarawak.
Malaysia

4 – 7 September 2016
52nd Congress of the European Societies of Toxicology (EUROTOX2016)
Istanbul, Turkey

4 – 8 September 2016
6th IUPAC Green Conference (ICGC 2016)
Venice, Italy

7 – 10 September 2016
European Conference on Research in Chemistry Education (ECRICE 2016)
Barcelona, Spain

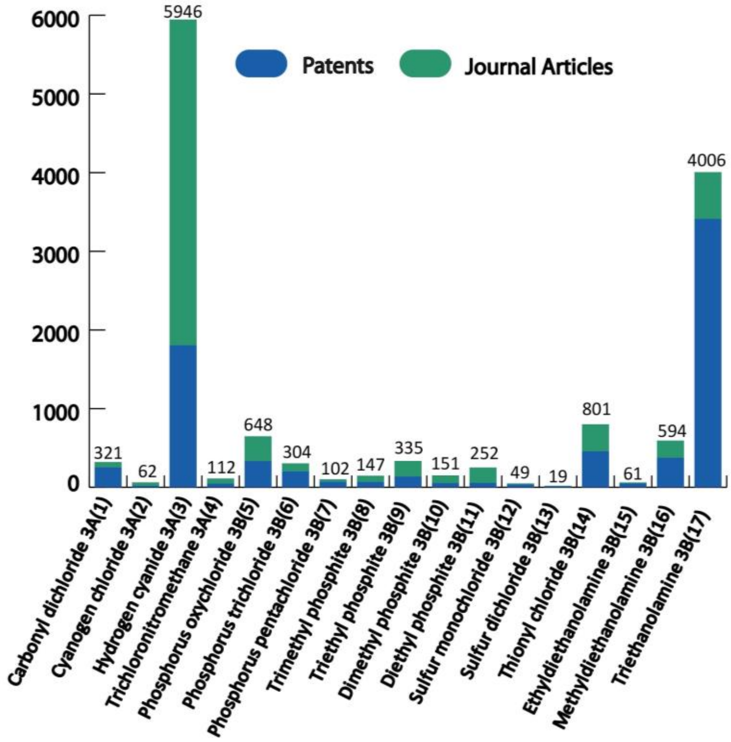
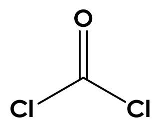


Figure 3: The number of publications (journal articles and patents) referencing Schedule 3 chemicals in 2014 (from SciFinder® as of 3 November 2015).

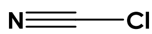
We continue this feature with a look at the chemicals of Schedule 3, parts A (Toxic Chemicals) and B (Precursors), in regard to uses of these chemicals for purposes not prohibited under the Chemical Weapons Convention:

Schedule 3 Part A, Toxic Chemicals



Phosgene:
Carbonyl dichloride 3A(1)

Schedule 3A(1): Phosgene (Carbonyl dichloride) was used as a chemical weapon in World War 1. Today, phosgene plays a role in the manufacture of a variety of products found in everyday life. These include flexible and rigid foam materials, thermoplastic polyurethanes, coatings, adhesives, sealants, elastomers, polycarbonate plastics, and a wide variety of pharmaceuticals, agricultural chemicals, and specialty chemical intermediates. A set of safe practice guidelines is available for those who work with phosgene.



Cyanogen chloride
3A(2)

Schedule 3A(2): Cyanogen chloride (CK) is volatile liquid and a highly toxic blood agent. The chemical has a number of uses in organic synthesis that include formation of aliphatic carbamates and addition of cyano groups to double bonds double bonds. Trace amounts of cyanogen chloride can actually form if uric acid is introduced into a swimming pool (details here).

Hydrogen cyanide
3A(3)

Schedule 3A(3): Hydrogen cyanide (prussic acid) is a colourless, extremely poisonous liquid that boils slightly above room temperature. The chemical is industrially

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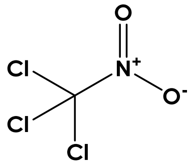
important as precursor to chemical compounds ranging from polymers to pharmaceuticals. It is also used to produce cyanide salts for mining and electroplating. The chemical is known to exist in interstellar space and can actually be found in seeds and nuts that contain cyanogenic glycosides (bitter almonds for example).

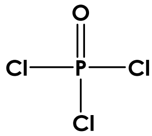
Schedule 3A(4): Chloropicrin (trichloronitromethane) is used as a soil fumigant where it acts on a wide range of species that include fungi, bacteria, nematodes and insects.



Chloropicrin: Trichloronitromethane
3A(4)

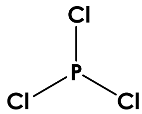
Schedule 3 Part B, Precursors

Schedule 3B(5): Phosphorus oxychloride is a colourless liquid mainly used to produce triarylphosphate esters. These are compounds that find use in flame retardants and plasticisers.



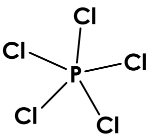
Phosphorus oxychloride
3B(5)

Schedule 3B(6): Phosphorus trichloride is an important industrial chemical used in the synthesis of organophosphorus compounds.

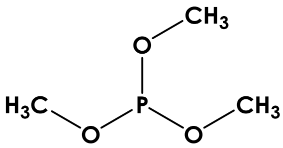


Phosphorus trichloride
3B(6)

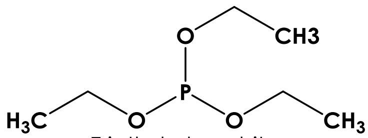
Schedule 3B(7): Phosphorus pentachloride finds use as a chlorinating agent in organic chemistry. **Schedules 3B(8)** trimethyl phosphite and **3B(9)** triethyl phosphite are compounds that are often used as ligands in organometallic chemistry. These trialkylphopshates can also be used in organic synthesis of phosphate esters.



Phosphorus pentachloride
3B(7)

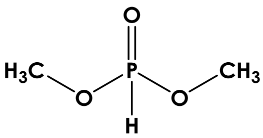


Trimethyl phosphite
3B(8)

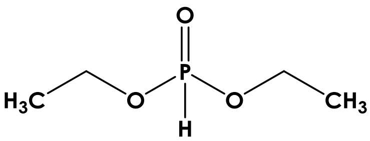


Triethyl phosphite
3B(9)

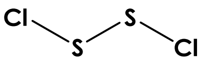
Schedules 3B(10) dimethyl phosphite and **3B(11)** diethyl phosphite are compounds that can be used to produce phosphate esters. **Schedules 3B(12)** sulphur monochloride, **3B(13)** sulphur dichloride and **3B(14)** thionyl chloride are chlorinating agents with many applications in organic chemistry.



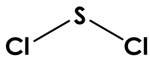
Dimethyl phosphite
3B(10)



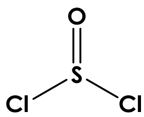
Diethyl phosphite
3B(11)



Sulfur monochloride
3B(12)

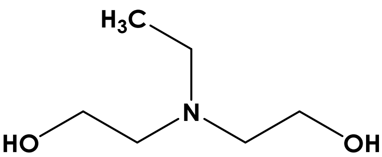


Sulfur dichloride
3B(13)

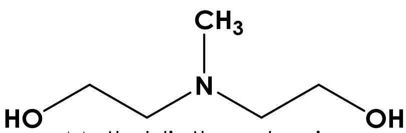


Thionyl chloride
3B(14)

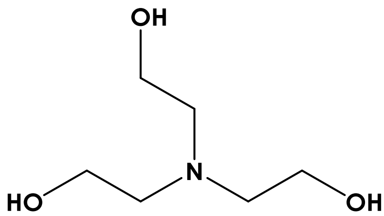
Schedule 3B(15): Ethyldiethanolamine, has applications in CO_2 capture. **Schedule 3B(16):** Methyldiethanolamine is broadly used as a sweetening agent to remove hydrogen sulfide from natural gas. **Schedule 3B(17):** Triethanolamine (TEA) is widely used as an emulsifier in personal care products.



Ethyldiethanolamine
3B(15)



Methyldiethanolamine
3B(16)



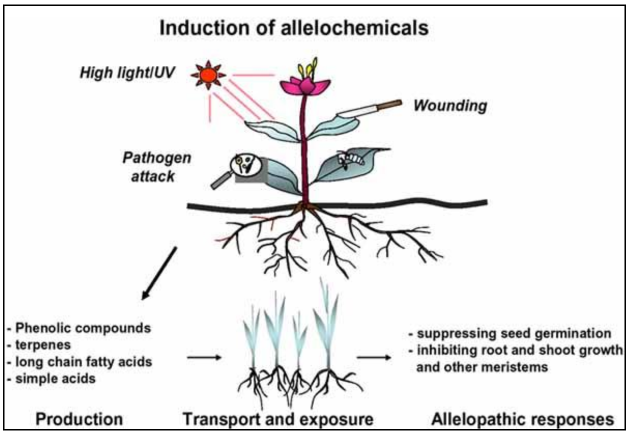
Triethanolamine
3B(17)

Allelopathy

Chemicals emitted by plants are familiar to us from the scents and smells of flowers. The volatile chemicals that produce these scents play an important role in plant reproduction and not surprisingly, this has inspired biotechnological engineering projects. Plant biochemistry has many more dimensions than insect attracting scent chemicals, including potential to produce economically valuable chemicals and the ability to produce and deploy bioregulatory chemicals that influence other plants around them. The release of biochemicals to produce both harmful and beneficial effects on other plants, is called allelopathy; one could think about allelopathy as a botanical use of chemical agents and a potential chemical defence against invasive species!

Allelopathy involves the release of "allelochemicals" into the environment through a variety of processes such as leaching, root extraction, residue decomposition and volatilization. Plants employ volatile chemicals to fend off herbivores, mobilize insects (or parasitic species to insects) in response to herbivore infestations and to inhibit other plant species competing for resources! Allelopathy has also been observed in fungi and marine organisms that include diatoms and sponges (fresh water sponges too).

As the complexity of the biochemical interactions of plants and their ecological systems is better understood, scientists have recognized opportunities to breed plants that use naturally produced chemicals as pesticides (details here) or herbicides ("organic weed management"). This has relevance for the reduction of use of more toxic and/or environmentally persistent agricultural chemicals. There is much work to be done in this field, as the complexity of plant interaction with environment can be influenced by adverse environmental conditions or soil additives.



Inducing allelochemcials (from "The importance of allelopathy in breeding new cultivars").

The Internet of Things (IoT)

Have you ever considered how many devices are currently connected to the internet? Current estimates are about 15 billion (and that's only 1% of what is possible) with 50 billion devices expected to be online by 2020! What we now refer to as the Internet of Things (IoT) is the continually growing network of connected devices that began to emerge in 2008. Who would have imagined that the few connected nodes of ARPANET gave way to the possibility of 1.5 trillion connected devices; potentially revolutionizing how we approach menial and complicated tasks, transforming businesses, daily activities and even our personal health management.

For businesses, the IoT can help to optimize the working environment in real-time, making offices more efficient. Take for example, the Edge building in Amsterdam, which can give individual workers different daily working environments according to their needs and schedules (including temperature preferences throughout the building), while at the same time producing and conserving energy through smart management of the buildings solar panels and climatic controls. Shopping districts could potentially track consumer bounce rates (how long customers stay in a store and which stores they visit) and contribute to security monitoring.

Urban infrastructure can be fitted with sensors to generate data that helps make cities "smarter". For example, "smart parking" can reduce congestion and vehicle exhaust emissions; and, "smart street lamps" can guide citizens out for a nightly stroll to well-lit areas. We have also seen solar and wind powered lamppost concepts in developing countries that trap dengue fever carrying mosquitoes (more details here)!

Sensors that analyse microbes and chemicals can measure sewer water to generate data relevant to public health. In a hospital, IoT devices can more accurately predict the location of patients and the amount of services they receive. This will provide more accurate analysis of drug application, immediate response to emergency situations and external monitoring systems that can trigger immediate response. There are already a wealth of health tracking wearable devices; going forward we can expect these sensors to improve rates of data retrieval and incorporate more functions.

For your home, the same sensors that make buildings smart can be applied to household needs. The concept of a "Smart Fridge" is often brought up, that is a refrigerator that will order food items from a store as they are consumed. However, it may be a while before fridges are indeed smart since the IoT is not about one connected object, but a wide network of objects with sensors. For those interested, there are many DIY home smartsensors available.

Other applications of the IoT may surprise you, for example the connected cow (with both ear and gut connected to the internet). What purpose does connecting a cow serve? It allows one to detect when an animal is sick, when it is in heat and allows the monitoring of its gut microbiome to ensure production of good quality milk! In regard to chemical security, the IoT is a potentially valuable tool for sniffing out hazardous substances.

As incredible as it all sounds, there are still issues to solve, especially in regard to the capacity to handle the incredible amount of data that would be generated (and consider the size of a daily internet scan) and a need for "the cloud" for worldwide communication. Many solutions have been proposed, such as the use of fog computing, mobile devices as temporary data gateways and the use of data fusion techniques.

What we can expect from all of these developments is a rethinking of our relationship to tools, consumption, services, manufacturing and perhaps even governance. In the meantime, we are privileged to be able to watch this new connected world evolve and perhaps make our own contributions to it!

Did You Know?

There are over 45,000 journal articles and patents published between 1900 and 2014 that make reference to Schedule 1 and Schedule 2 chemicals.