



The OPCW Science & Technology Monitor

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

14 November 2014

Volume 1, Number 5

Featured Content:

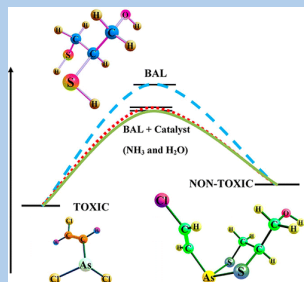


Image from [J. Phys. Chem. A, 2013, 117 \(16\), 3496–3506](#).

Understanding the mechanism of chemical agent detoxification using computational chemistry



Image from [Chem. Rev., 2014, 114 \(11\), 5695–5727](#).

Air purification by metal-organic frameworks with gas mask applications

Science Fun:

Previously we pointed out how saxitoxin can be used to stop itching, and here we suggest [why such a seemingly drastic approach may be required](#) ([technical details here](#)).

Welcome

Welcome to our fifth issue of *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.

We begin with well deserved congratulations to the recipients of this year's inaugural [OPCW-Hague Award](#), jointly awarded to [Dr Robert Mathews of Australia](#) and the [Finnish Institute for the Verification of the Chemical Weapons Convention \(VERIFIN\)](#). [Dr Mathews](#) made significant contributions to the drafting of the CWC and served on the OPCW SAB and many of the TWGs. [VERIFIN](#) is one of the OPCW designated laboratories that provided off-site analysis in the August [2013 UN lead investigation of alleged use of chemical agents in Syria](#).

The S&T Puzzle

The *S&T Monitor* puzzle has a winner: Hans de Jong confirmed that 0.07 is indeed the coefficient of friction on the surface beneath a banana peel; congratulations Hans! Honourable mention goes to Philippe Denier for his valiant search efforts (going through all our links); we thank Philippe for finding [an invention which could be combined with the banana peel to improve effectiveness by reducing friction!](#)

For this issues puzzle we ask, what do you call a molecule that is the lowest-energy structure for a certain sum formula? The answer can be found in one of our links.

To the first person to solve the puzzle, we once again offer your choice of choosing our next featured topic or a gift of a special beverage hand selected by the Science Policy Adviser. Good luck!

In this issue:

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[101 Years of Mass Spectrometry and a Comet](#)

With so much worry about the Zombie Apocalypse, we want to ensure our readers are fully informed on [how to survive it using science \(more information here\)](#). The special chemistry involved is explained in this [infographic](#).

A look at the problem of [chemical warfare in your swimming pool](#) (technical details can be found [here](#)). In fact, [a multitude of chemical species can collect and form in swimming pools](#) if you are not careful (full report can be found [here](#)).

For those of you who like pictures, check out the [science images of October](#) and try your luck in the Science Net Links [mystery image contest](#) (see image below from AAAS).



Finally, don't forget to vote for your favourite [Vizzie](#).

Crowdsourcing:

This week the crowd is asked to inspire science excitement in kindergarten through grade 12 students. If you have a science related job, please [answer these 5 questions!](#)

And while you are inspiring students, let science inspire you by voting for the [science breakthrough of 2014](#).

News and Updates

We introduce this section in effort to keep readers informed on recent reports and scientific developments that don't fit into the featured content.

Recently published reports:

CEFIC report on [the European chemical industry's commitment to Sustainability](#).

AAAS, FBI, and UNICRI report on [National and Transnational Security Implications of Big Data in the Life Sciences](#).

Department of Defense, Defense Science Board Task Force Report on [Assessment of Nuclear Monitoring and Verification Technologies](#).

Biochemical Security 2030 study of [contemporary dual-use chemical and life-science research potentially applicable to incapacitating chemical agent weapons](#).

Making news in chemistry:

[From the week of 6 October to 1 November](#)

[From the week of 2-8 November](#)

Computational Chemistry

Computational methods are employed in nearly all fields of chemistry to explore and predict chemical properties as well as to design new chemicals ([this is particularly useful for pharmaceuticals](#)). The power of these methods has moved far beyond small molecules as demonstrated by studies of complex [biological macromolecules](#). The impact on science from these methods was recognised by the [2013 Chemistry Nobel Prize for the development of multiscale models for complex chemical systems](#) ([click here for an informative introductory article](#)).

Computational methods can aid in identifying conditions and components of chemical reactions, including designing [enzymes](#) and [catalysts](#) for detoxification of chemical warfare agents. Computation also provides insight into the processes by which chemical agents [adsorb onto surfaces](#); valuable information for informing the development of decontamination methods and protocols.

For the production of chemicals, computational methods can identify ["winning" molecules for fermentation](#). The full technical report can be found [here](#).

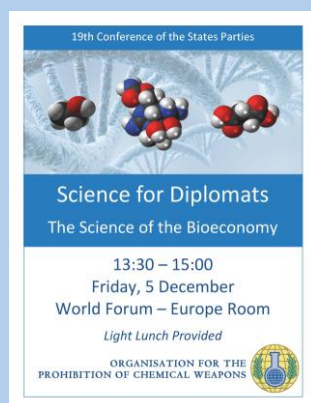
Upcoming S&T Related Events:

19 - 21 November 2014
[Biological and Chemical Security in an Age of Responsible Innovation](#);
Organised by the Biochemical Security 2030 Project at the Royal Society, London

28 November 2014
Science and Technology Breakout Discussion as part of the 16th Annual Meeting of National Authorities, The Hague, 9:00 - 12:30.

1 - 5 December 2014
Biological Weapons Convention Meeting of States Parties;
Geneva, Switzerland

5 December 2014
Science for Diplomats (3)
- The Science of the Bioeconomy. World Forum, Europe Room, 13:30-15:00 (with light lunch provided)



11 - 12 December 2014
New Technologies and Approaches for Information Analysis to Support Non-Proliferation and Disarmament Verification;

Vienna Center for Disarmament and Non-Proliferation (VCDNP) and the James Martin Center for Non-proliferation Studies (CNS), Vienna, Austria

Computational methods can be based on both fundamental scientific theory and empirical observations. As with the human brain, predictive power can be improved by observation and learning. Predictive tools for molecular design benefit from the input of many brains. To harness all this intelligence, [scientists have created online video games \(which do not require players to be scientists\)](#), to help [solve complex molecular structural questions](#) and produce [improved predictive tools](#). An added benefit is that some studies suggest [playing video games may make you smarter](#) (technical details can be found [here](#)).

Computational tools are valuable in research and development, however, any robust and fieldable technology requires experimental validation. An example of the interplay between computational design and real-world function is nicely illustrated in the ability to use [folding rules to design stable unnatural proteins](#).

Nanotechnology and Materials for Neutralisation and Protection

Methods for the destruction and neutralisation of chemical agents have been described in [many publications](#). [New discoveries in nanotechnology may also have applications in this regard](#) and may also provide a mechanism [to incorporate neutralisation capabilities into wearable protective equipment](#) (technical information [here](#)).

Examples include, [Self-propelled microstirrers that can degrade organophosphorus compounds](#) (technical details [here](#)) and [water fuelled photocatalytic "microrockets"](#) (technical details [here](#)).

Photocatalytic [nanoparticles that can degrade pollutants](#) and even [nerve agents](#) are known and can be [incorporated into material coatings](#).

For air purification the [catalytic properties and high surface area of metal-organic frameworks \(MOFs\)](#) can be used for gas masks. There are also surprisingly simple ways to keep [gas masks](#) functional (technical details [here](#)). Nanomaterials are another means to remove odour producing chemicals [from the air in confined spaces](#).

It is very encouraging to see the emerging technologies for protection from chemical agents. Some reports suggest that in the future, perhaps [a cup of tea](#) may be an effective countermeasure.

Pesticides

[Pesticides](#) are substances or mixtures of substances intended to prevent, destroy, repel or mitigate any pest. We normally think of pesticides as [insecticides](#), however, [herbicides](#), [fungicides](#) and various other substances used to control pests are also classified as pesticides.

28 - 29 January 2015
5th Meeting of the Scientific Advisory Board's Temporary Working Group on Verification. The Hague

21 - 26 March 2015
[249th American Chemical Society \(ACS\) National Meeting & Exposition](#).
Denver, Colorado, USA.

During the open session of the ACS Board of Directors meeting, the 2013 Nobel Peace Prize recipient, the OPCW will be honoured for its work in finding peaceful applications of chemical sciences worldwide.

22 - 26 June 2015
[CTBT Science and Technology Conference \(SnT2015\)](#)
Vienna, Austria

6 - 13 August 2015
[IUPAC 2015](#)
48th General Assembly
45th World Chemistry Congress
Busan, Republic of Korea

27 September - 1 October 2015
[ECCE10 \(10th European Congress of Chemical Engineering\)](#)

[ECAB3 \(3rd European Congress of Applied Biotechnology\)](#)

[EPIC5 \(5th European Process Intensification Conference\)](#)

Nice, France.

Contact:

Questions, comments, suggestions, contributions? Or to be added to the mailing list, please contact the [Science Policy Adviser](#) in the Office of Strategy and Policy

[Organophosphorus pesticides \(OPs\)](#) are notorious as observations of their insecticidal properties were the inspiration for G-Agents such as [soman](#), [sarin](#) and [tabun](#). There are concerns about use of OPs as described in recent studies suggesting that exposure can effect both [cognitive](#) and [neurological](#) development. For these reasons, there is much interest in [engineering proteins to prevent brain damage from exposure to OPs](#) (technical report can be found [here](#)) .

OPs and G-type nerve agents can be detected using common analytical methods. New analytical tools for these purposes are continually being developed; some recent examples include the use of [Raman spectroscopy](#) for detecting OPs in fruit and point of care [biosensors](#).

[Neonicotinoids represent another class of insecticides](#). There has been controversy over their use due to concerns about the effect these chemicals may have on [bee](#) and [bird](#) populations (see the following technical reports on [neuronal inactivation](#) and [olfactory learning and memory impairment](#) in bees; and [declining bird populations](#)).

101 Years of Mass Spectrometry and a Comet

Last year marked the beginning of the [second century for mass spectrometry \(MS\)](#), a method that comes from the ground-breaking work of Nobel laureate Sir Joseph John Thomson in 1913 and has [advanced significantly since over time](#). MS is an extremely important analytical tool for [verification](#). [A special open access issue of the International Journal of Mass Spectrometry dedicated to the 100th anniversary is available online](#). Here is a [video showing how MS works](#).

We see daily reports of new developments in MS, including applications for [simultaneous detection of multiple chemical warfare agent exposure in biomedical samples](#), [quantitation of target analytes in complex sample matrices](#) and for [determination of size and chemical composition of nanoparticles](#) (technical details can be found [here](#)).

Of course, we cannot end this issue of the *S&T Monitor* without mentioning the historical comet landing of the [Rosetta Mission](#). Critical to the purpose of the Rosetta Mission is an array of [analytical instrumentation](#) that includes the [ROSINA mass spectrometer](#). Mass spectrometry determined that comet 67P/Churyumov-Gerasimenko has a [foul odour and emits a schedule 3 chemical](#).

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