OPCW Scientific Advisory Board Briefing to States Parties

Thursday 11 June 2015
13:30 - 15:00
Ooms Room

The Chair and Vice-Chair of the SAB will report on activities of the Board including the report of the TWG on Verification

Light lunch provided (available at 13:00)

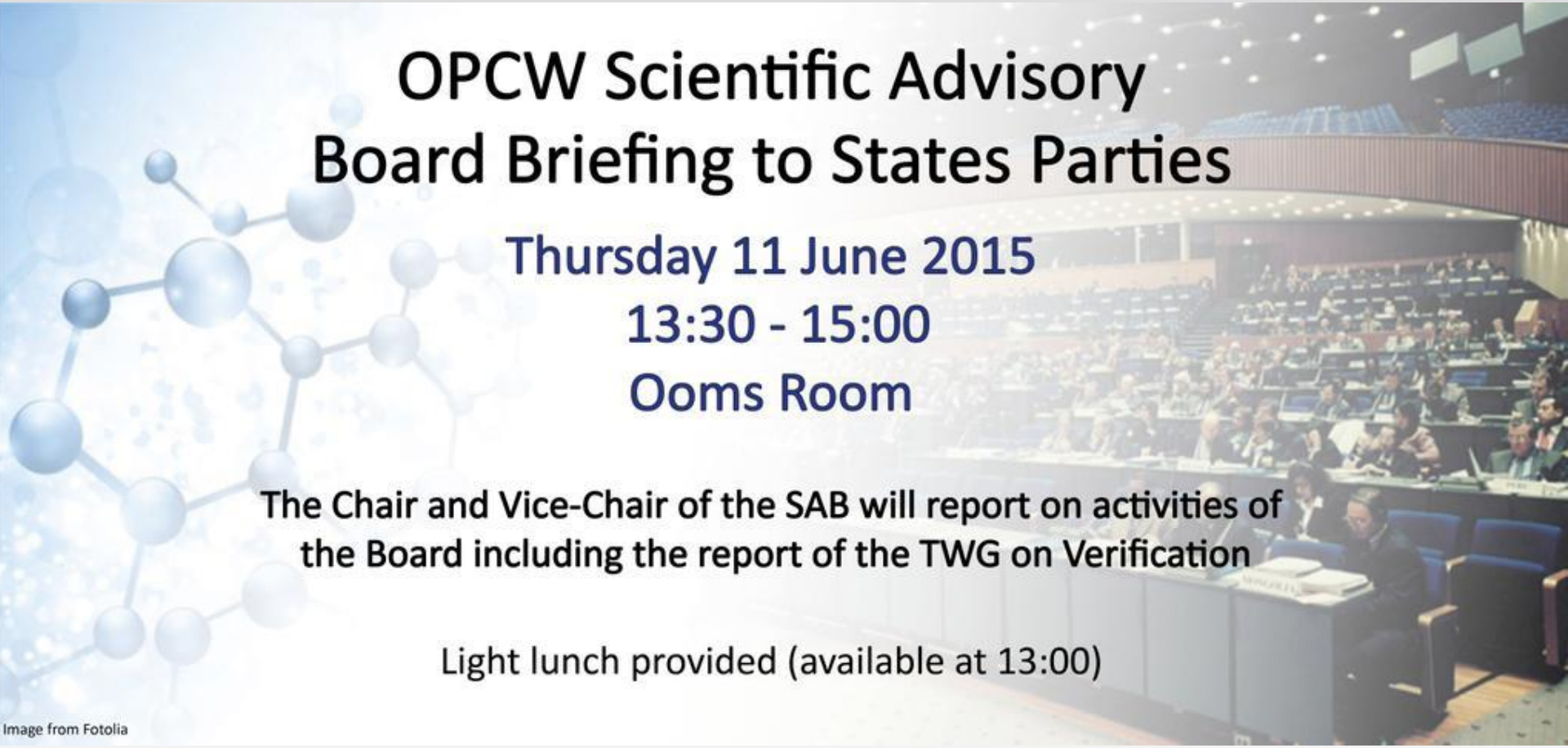
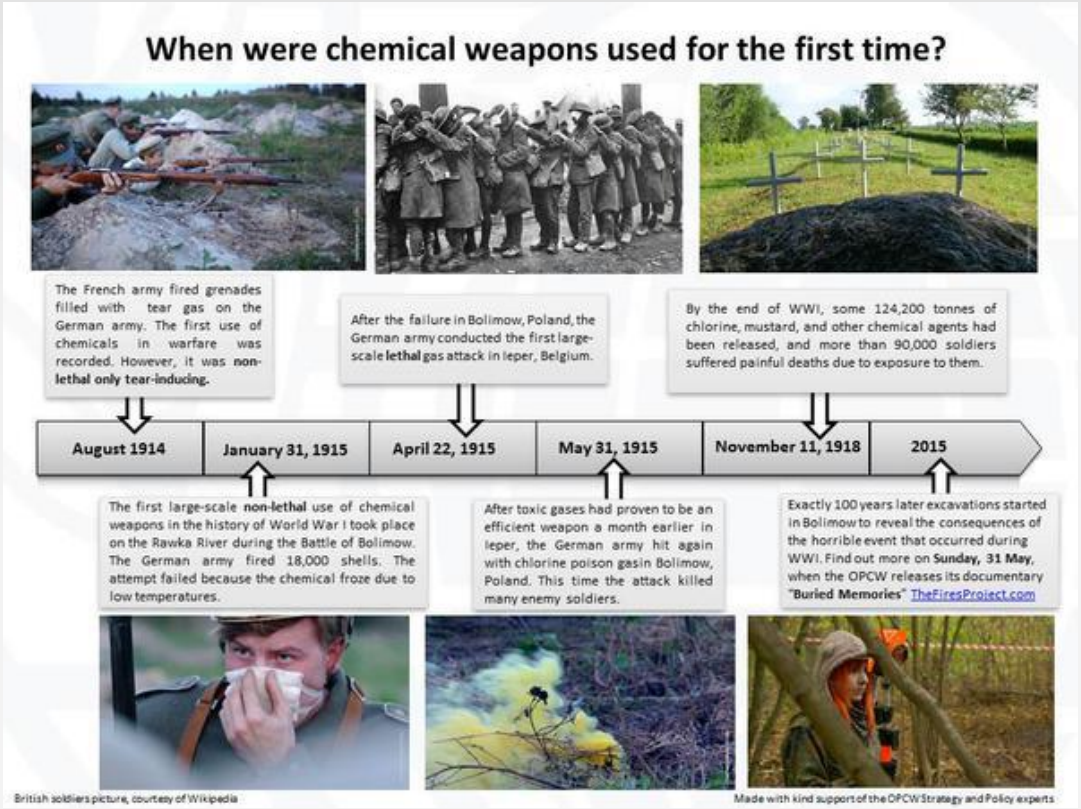
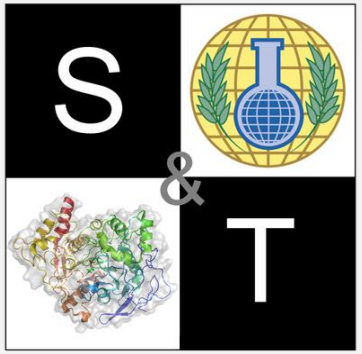


Image from Fotolia

100 years of chemical weapons





Science and the CWC

Science and technology underpins many Articles of the CWC

Art II	**definitions**
Art III	**declarations (accurate and complete)**
Art IV	**destruction methodologies**
Art VI	**verification methodologies such as sampling & analysis**
Art VII	**effective national implementation depends in part on S&T knowledge/awareness/outreach**
Art IX/X	**investigations, assistance, challenge, inspections**
Art XI	**peaceful use (e.g. outreach)**

Science and technology is central to OPCW's future priorities

SAB composition

Chair

Dr Christopher Timperley (United Kingdom and Northern Ireland)

Vice-chair

Mr Cheng Tang (Peoples Republic of China)

Departing members

Alejandra Suarez (Argentina)
Djafer Benachour (Algeria)
Michael Geist (Germany)
Muhammad Zafar-Uz Zaman (Pakistan)
Slavica Vucinic (Serbia)
Bill Kane (USA)

Outline

SAB activities since Review Conference-3 (RC-3)

SAB and its Temporary Working Groups (TWGs)

SAB and the OPCW future strategy up to 2025

SAB and its science and technology initiatives

SAB plans and future activities

RC-3 recommendations

Monitor science and technology developments

Build extra laboratory and analysis capabilities

Build expertise, training/knowledge management

Become more active in education and outreach

Examine developments and advise on verification

Provide support to assistance and protection

ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

Working together for a world free of chemical weapons

FACT SHEET 11

The Scientific Advisory Board

The states that negotiated the Convention on Chemical Weapons (CWC) knew that in order for the Convention to remain relevant and avoid the problems of earlier chemical weapon treaties, the CWC would have to be adaptable. Both the Convention and its implementing body, the Organisation for the Prohibition of Chemical Weapons (OPCW), are intended to adapt not only to shifts in the international environment and the changing needs of States Parties, but also to respond to scientific and technological developments. To this end, the Convention foresees that the States Parties should 'review scientific and technological developments that could affect the operation of this Convention'. To provide States Parties with the expertise needed for such a review, Article VIII, paragraph 21 (h) of the CWC mandates the establishment of a Scientific Advisory Board (SAB) to monitor developments in science and technology and assess their impact on CWC implementation. The OPCW Conference of the States Parties (see Factsheet 3 on OPCW structure) addressed this issue at its second session in December 1997 when it instructed the Director-General to establish such a body.

Structure and Function of the Scientific Advisory Board

The SAB is a subsidiary body of the OPCW, enabling the Director-General to provide specialised advice in science and technology to OPCW policy-making bodies and Member States. The SAB reports to the Director-General, who then makes the Board's reports available, alongside his own response, to the Executive Council and the public. Every five years, the SAB prepares a comprehensive report for submission to the review conference. The SAB held its first meeting in 1998 and meets once or twice per year at the OPCW's headquarters in The Hague.

The SAB consists of 25 members, each of whom is an expert in one or more technical fields relevant to the Convention. SAB members serve in their individual capacity as independent experts. States Parties nominate candidates, and the Director-General makes the final selection, keeping in mind the need for geographical balance. Members are appointed for three years and can serve two consecutive terms. Members are drawn from universities, industry, defence organisations and other institutions. Only citizens of OPCW member states are eligible for SAB membership. Every year the SAB elects a Chair and Vice-Chair from its members.

Cooperation is important. The SAB coordinates with the OPCW Technical Secretariat, which provides support for SAB activities. The board invites experts from other international organisations, scientific institutes and industry associations to make presentations at meetings of the SAB and its temporary working groups (TWGs). Members of the SAB and its working groups also share their views with the scientific and industry communities by presenting at conferences.

Members of the Scientific Advisory Board in 2014

Funding for SAB activities comes from the OPCW's regular budget and voluntary contributions. A trust fund for the Board was set up in 2006. 14 States Parties and the European Union have contributed.

Past and Present Temporary Working Groups	
Chemical Weapons Destruction Technologies	1999 – 2000
Reviewed technologies for the destruction of chemical weapons.	
Equipment Issues	1999 – 2000
Examined issues related to equipment for inspections and on-site monitoring of chemical weapon destruction operations.	
Analytical Procedures	1999 – 2000
Addressed alternative inspection methods, the use of analytical equipment belonging to the inspected State Party and possible inclusion of non-Scheduled chemicals in the Central OPCW Analytical Database.	
Ricin Production	1999 – 1999
Examined how and at what stage production of ricin should be reported.	
Adamsite	1999 – 1999
Determine whether adamsite is an acceptable riot control agent and criteria to be taken into account when declaring holdings of adamsite.	
Low Concentration Limits for Schedule 2A and 2A* Chemicals	2000 – 2000
Examined the concentration level at which mixtures of chemicals containing Schedule 2A and 2A* chemicals should be regulated.	
Biomedical Samples	2004 – 2007
Examined whether the OPCW Laboratory and designated laboratory network can develop the capacity to analyze biomedical samples.	
Sampling and Analysis	2007 – 2012
Examined issues relating to the collection and analysis of samples for verification purposes.	
Convergence of Chemistry and Biology	2011 – 2013
Examined the risks and benefits that rapid advances in life sciences pose to the Convention.	
Education and Outreach	2012 – 2014
Examined how to raise awareness of the Convention and build relationships between the OPCW and the scientific community, the academic community, chemical industry, international organisations and other groups.	
Verification	2013 – 2015
Examined verification technologies, methodologies and equipment.	

Issues for the SAB

Science and technology underpin almost every aspect of the Convention, from complex verification procedures to the CWC's most fundamental definitions. Science, technology and world events can change rapidly, requiring new insights and understandings to ensure the OPCW and the Convention can respond. Therefore, the SAB is called upon to provide guidance on a wide range of issues. Some of the topics on which the Director-General has recently asked the SAB for advice include medical treatment for blister and nerve agents, riot control agents (RCAs), new approaches to verification, and education and outreach in science and technology. The SAB also provides expert advice on any proposed changes to the Schedules of Chemicals (see Factsheet 7).

In addition to its ongoing activities, the SAB has temporary working groups to provide recommendations on specific issues within specific timeframes. The Director-General establishes these working groups in consultation with the SAB. The SAB Chairperson appoints one member of the SAB to chair each TWG, and the Director-General appoints additional experts to serve as members of the group based on suggestions from OPCW member states and the SAB. Only citizens of member states are eligible to be members of a working group. At the end of the group's mandate, it submits a report of its findings to the SAB and Director-General.

Since its creation, the SAB has had eleven TWGs on the following topics: the convergence of chemistry and biology; verification; education and outreach; sampling and analysis; ricin production; analytical procedures; on-site monitoring equipment; chemical weapon destruction technologies; adamsite; low concentration limits for Schedule 2A chemicals; and biomedical samples. See the summary table on the left for details.

As of October 2014, the Board has one active temporary working group, on Verification. Two other temporary working groups, on the Convergence of Biology and Chemistry and on Education and Outreach, ended their mandate in 2013 and 2014, respectively. TWG and SAB reports are publically available on the SAB website at www.opcw.org/about-opcw/subsidiary-bodies/scientific-advisory-board.

OPCW
Johan de Wittlaan 32
2517 JR The Hague
The Netherlands
Tel: +31 70 416 3300
media@opcw.org
www.opcw.org

Revised: 31 October 2014

/opcwonline
/opcw
/opcwonline
/opcw

Temporary Working Groups

Convergence

14 experts; chair Mr. Bill Kane

Report published in June 2014

Education and Outreach

11 experts; chair Prof. Djafer Benachour

Report published in November 2014

Convergence TWG

Chemicals being produced increasingly by biomediated processes (e.g. fermentation)

Estimated ~10% of chemical production volume will use such processes by 2012

Have been rapid advances in chemical synthesis of molecules of biological origin

SAB recommended that 'produced by synthesis' describes any process for producing a chemical (as applies to Part IX of the Verification Annex, in the context of declarations required for OCPFs)

Findings

New production processes, combined with developments in drug discovery and delivery, could be exploited to produce toxic chemicals

Increasing overlap between topics of interest to both the CWC and BWC (e.g. toxins) and contacts should be maintained with the BWC

Convergence is being used for improved chemical and biological warfare medical countermeasures, new decontamination and detection/diagnostics methods, and for improving protective clothing

Recommended that science at the crossroads of chemistry and biology is tracked closely to pick up any step changes that might impact on the CWC and BWC, including on verification of the CWC

Spiez CONVERGENCE

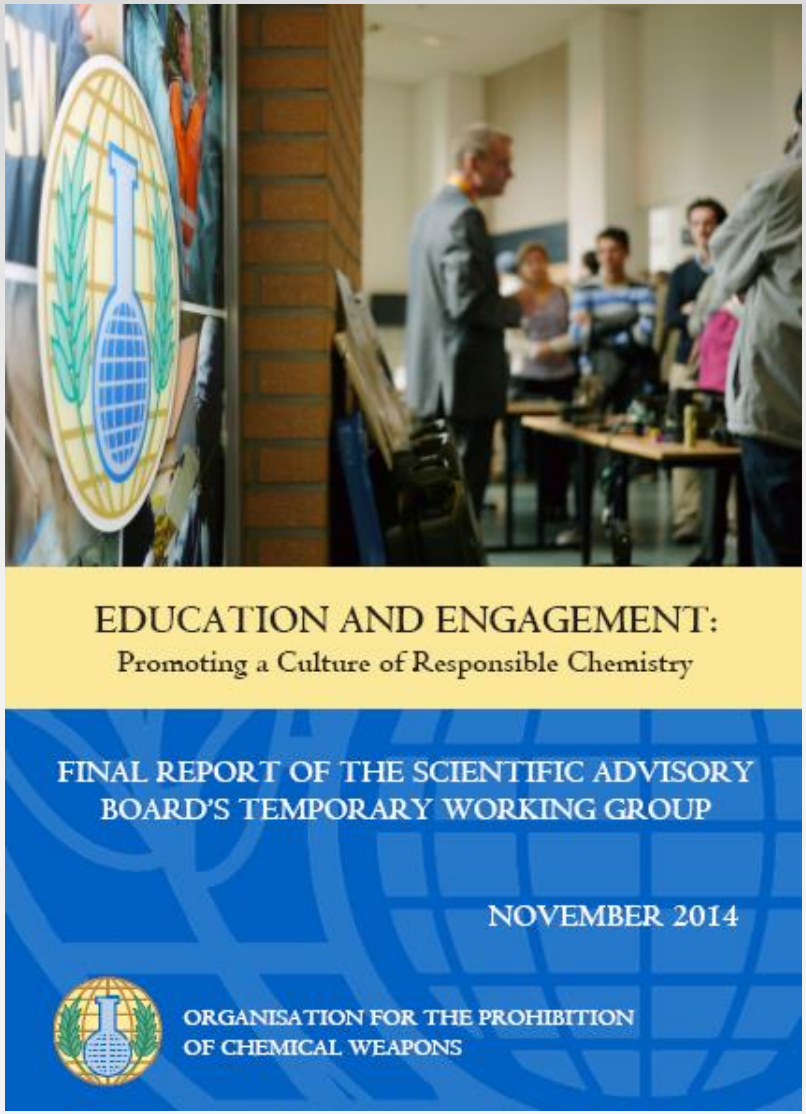
Involved experts from NGOs, the SAB, academia, industry and policy sphere

Invited experts presented on 12 topics

Concluded that the life sciences are advancing at an unprecedented pace

And that the expansion of data and knowledge will lead to non-linear progress in future, which will outpace CWC and BWC treaty review cycles

Recommended that advances in the life sciences should be monitored constantly



Education and outreach TWG

Recommendations

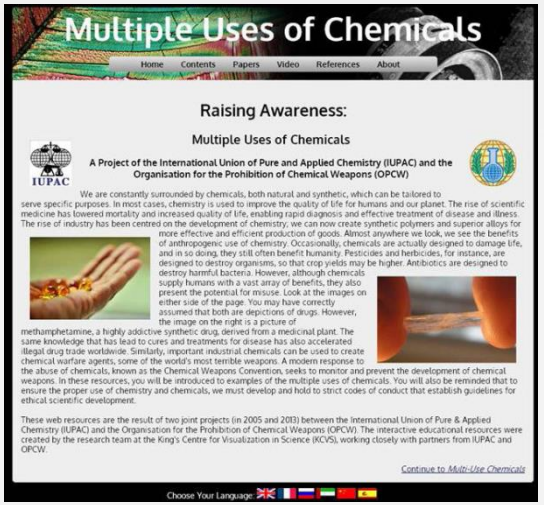
E&O with respect to responsible use of science relevant to the CWC should remain a core activity of OPCW

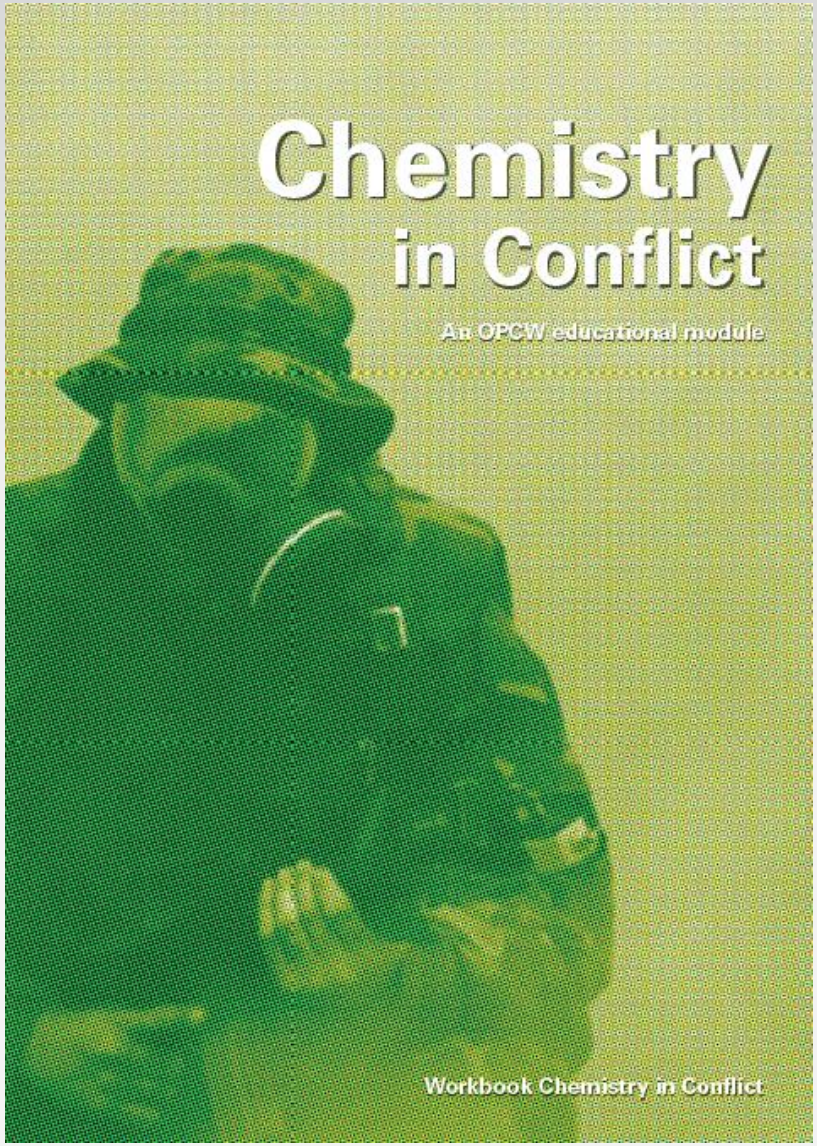
An ongoing expert advisory group on E&O should be established to help OPCW fulfil its mandate for E&O

Until such time as the expert advisory group is appointed, the current TWG should continue its work

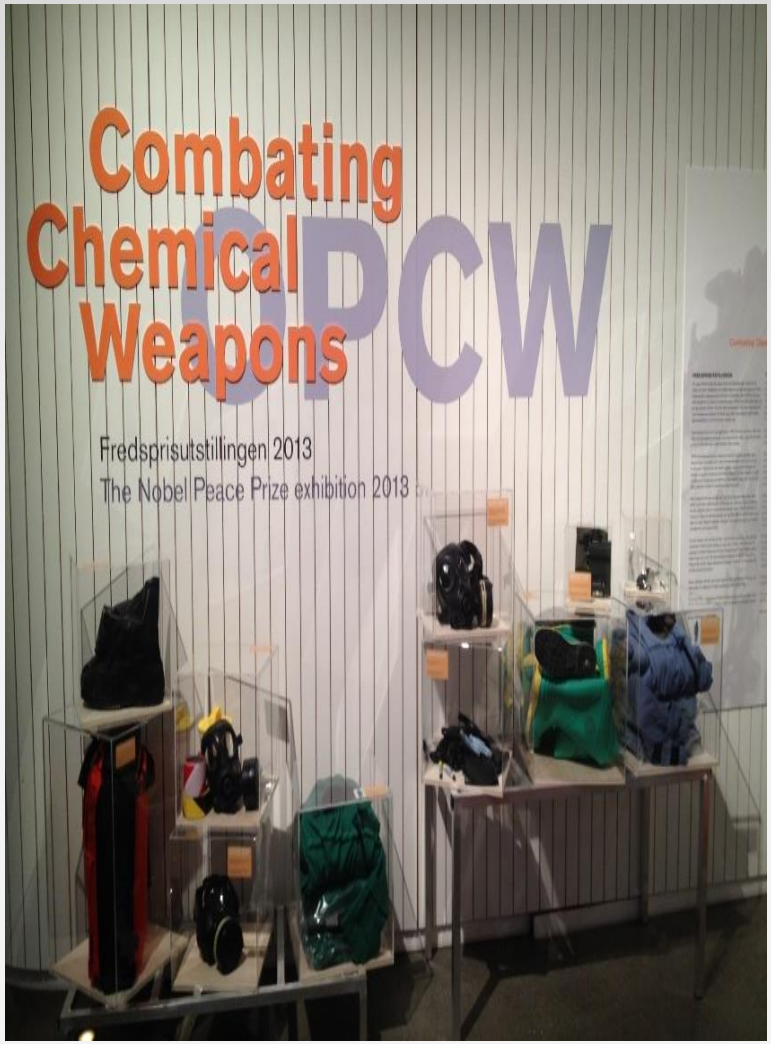
Education and outreach TWG

"Education for peace: new pathways for securing chemical disarmament"
22-23 September 2014





Contents


Combating
Chemical
Weapons
OPCW
Fredsprisutstillingen 2013
The Nobel Peace Prize exhibition 2013


WERKEN AAN VREDE
GIVE PEACE A CHANCE
TM 2 NOV 2014

5th IUPAC International Conference on Green Chemistry ~ 2014

OPCW EVENTS

Wednesday 20 August

Plenary Lecture: Educating for a Sustainable and Secure Planet — 8:30
Peter Mahaffy — Great Ilanga Room

Keynote: Green Chemistry Education in Africa — 9:30
Engida Temechegn — Suites 1-3

OPCW Sustainability & Security Symposium

Security Dimensions of Sustainable Technology Development — 9:30
Jonathan E. Forman — Great Ilanga Room

A Three-Legged Stool: IUPAC and OPCW Working Together to Promote Sustainability and Security — 9:45
Peter Mahaffy & Alistair Hay — Great Ilanga Room

Sustainability, Security and Ethics — 10:00
Liliana Mammino — Great Ilanga Room

OPCW Capacity Building Programmes for the Peaceful and Sustainable Applications of Chemistry — 10:15
Sergey Zinoviev — Great Ilanga Room

Workshop: Multiple Uses of Chemicals — 13:30
Peter Mahaffy & Alistair Hay — Great Ilanga Room

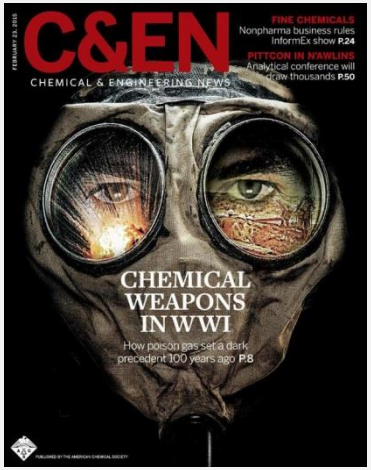
ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

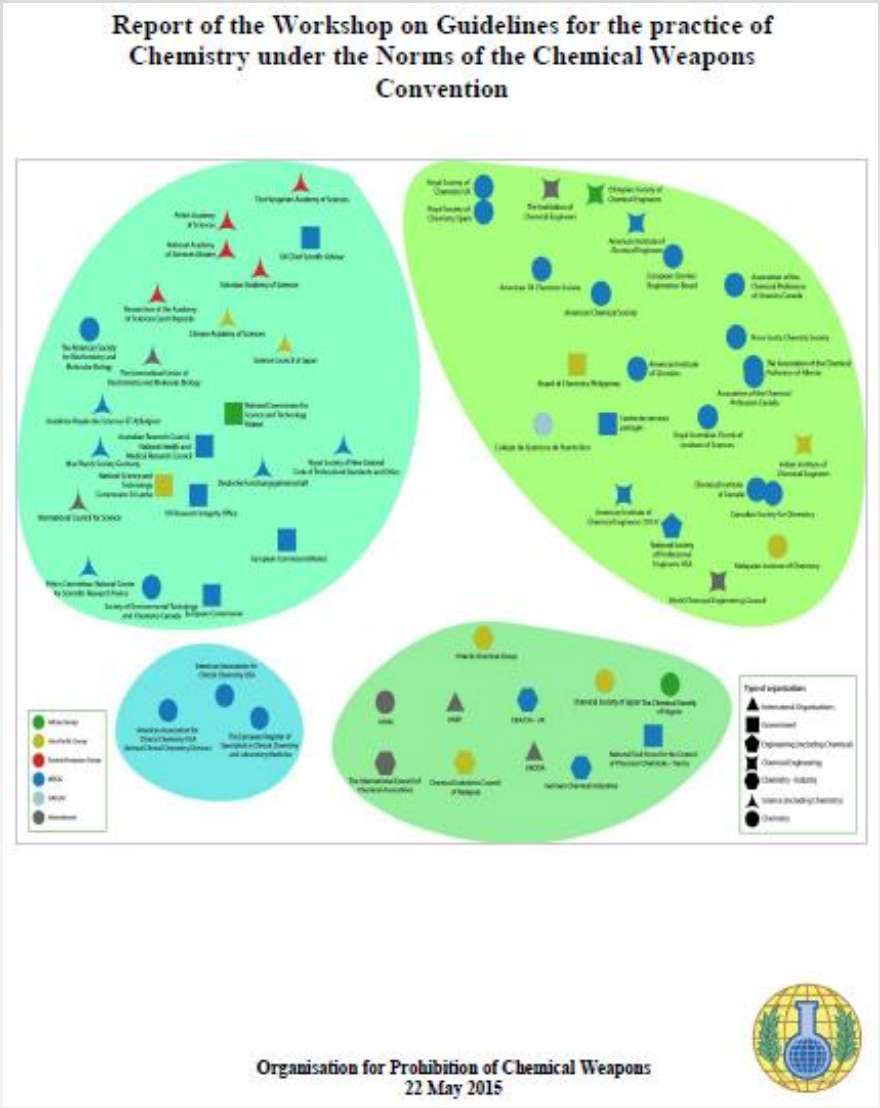
National societies

American Chemical Society
Recognised OPCW for promoting chemistry in service of peace

National Academy of Sciences USA
Collaborating on workshops on S&T developments relevant to CWC/BWC

Royal Society of Chemistry UK
Interest in Article XI programmes (through OPCW International Cooperation Branch)





Ethical guidelines

Workshop on Guidelines for Practice of Chemistry under the Norms of the CWC held on 11 March 2015 (24 experts)

Team involving SAB members is working on text of ethical guidelines for chemical professionals (C-19/5, dated 5 December 2014, para 23.3)

Contributors to workshop

ACS Chemistry for Life®

IUPAC

ICC Indian Chemical Council

EuCheMS

EUROPEAN CHEMICAL SCIENCES EuCheMS

NATIONAL ACADEMY OF SCIENCES

GESELLSCHAFT DEUTSCHER CHEMIKER

FACS FEDERATION OF ASIAN CHEMICAL SOCIETIES

cefic

中华人民共和国工业和信息化部
Ministry of Industry and Information Technology of the People's Republic of China

Bangladesh Chemical Society

Culture of responsible chemistry

SAB Vice-Chair accepted invitation to attend two meetings on CBRN security culture at side-events of the Global Partnership Against the Spread of WMD

G7 GERMANY

UNODA United Nations Office for Disarmament Affairs

**SIDE EVENT G7 GLOBAL PARTNERSHIP:
COMPREHENSIVE CBRN SECURITY CULTURE:
MOVING FORWARD TO ADDRESS NEW CHALLENGES**

**April 24, 2015
United States Consulate
Munich, Germany
Königinstraße 5**

Hosted by the U.S. Consulate in Munichunder the auspices of Germany's Presidency of the G7 Global Partnership and in cooperation with the United Nations Office for Disarmament Affairsand the Global Partnership Sub-Working Group on Centers of Excellence and CBRN Security, using funds from the UN Trust Fund for Global and Regional Disarmament Activities donated by the Governments of Norway, the United States of America and the European Union

"A Road Map for Comprehensive and Sustainable CBRN Security Culture"
Berlin, 3 November 2014

"Comprehensive CBRN Security Culture: Moving Forward to Address New Challenges"
Munich, 24 April 2015

OPCW recognised as an interface among States Parties and different stakeholders on chemical security culture

Verification

S/1252/2015
6 March 2015
Original: ENGLISH

NOTE BY THE TECHNICAL SECRETARIAT

THE OPCW IN 2025: ENSURING A WORLD FREE OF CHEMICAL WEAPONS

OPCW in 2025

2. Verification to ensure continued confidence in compliance will remain at the heart of the Organisation's work. But its methods and practices will need to be adapted to changing realities. In addition to maintaining a viable industry verification regime and preparedness for non-routine inspections, greater emphasis will be placed on enhancing the Organisation's analytical capabilities.

10. The missions in the Syrian Arab Republic provide important lessons to learn for the future of the Organisation. These range from the conduct at short notice of an investigation of use in adverse conditions, to the collaboration with the United Nations and other international organisations, to the in-depth involvement with a chemical demilitarisation programme. Identifying and learning lessons from these missions will help further increase the resilience of the Organisation and help it to continue to fulfil its mission under the Convention.

14. In order to prevent the re-emergence of chemical weapons, an effective industry verification regime will have to be sustained. This needs to be supported by the augmented data monitoring and transfer controls provided for in the Convention. In addition, full and effective national implementation of the Convention is vitally important for preventing the re-emergence of chemical weapons, as is the continued problem resolution and deterrent value of the provisions for consultation, cooperation, and fact-finding, including the capability to conduct non-routine verification activities such as challenge inspections and investigations of potential use at any point in time.

21. However, the Organisation will devote fewer resources to chemical weapons inspection-related activities as the destruction of currently declared stockpiles of chemical weapons nears completion. Approaching this major milestone provides the opportunity to re-examine the routine verification system of the Convention in order to adapt the Organisation's permanent mandate to changing circumstances. Emphasis will be placed on the following areas:

(a) While the evaluation of declaration data and the conduct of inspections will remain an essential part of the Organisation's verification work, the Organisation will need to enhance its analytical capabilities, putting in place processes that are more robustly geared towards a process of gathering, validating, and evaluating information befitting an independent and more holistic assessment of how the treaty is implemented. Developing and maintaining such an analytical capability within the Secretariat will contribute to the goal of maintaining confidence in compliance. An augmented capability to use reliable publicly available information will form part of this process, which will build upon efforts already under way in conjunction with States Parties.

(b) The Organisation will also require enhanced capabilities to monitor the full spectrum of relevant toxic chemicals falling within its mandate, ranging from toxic industrial chemicals to chemicals used for example in medicine or law enforcement, including those acting on the central nervous system. In this regard, developments in science and technology and relevant advice from the Scientific Advisory Board (SAB), as well as in-house scientific resources, will inform the Organisation's course of action.

45. In order to continue achieving the goals of the Convention, the transition process will require that the Organisation's verification system be further developed to enhance its monitoring and analytical capabilities while retaining core expertise, and that its capacity development and engagement efforts be strengthened through enhanced capacities to analyse and respond to the implementation needs of States Parties. Combined with the improvements in organisational governance outlined above, this will enable the Organisation to remain fit for purpose, and to lead the way in preventing the re-emergence of chemical weapons.

Verification TWG

15 experts; chair Prof. Roberto Martinez-Alvarez

TWG structure

Six meetings held, started March 2013 and finished in May 2015

Briefings received from experts from international organisations

And from members of OPCW Technical Secretariat on current practices and future plans

TWG conducted a gap analysis by interviewing Secretariat members

UNOG
THE UNITED NATIONS OFFICE AT GENEVA

VCDNP Vienna Center for Disarmament and Non-Proliferation

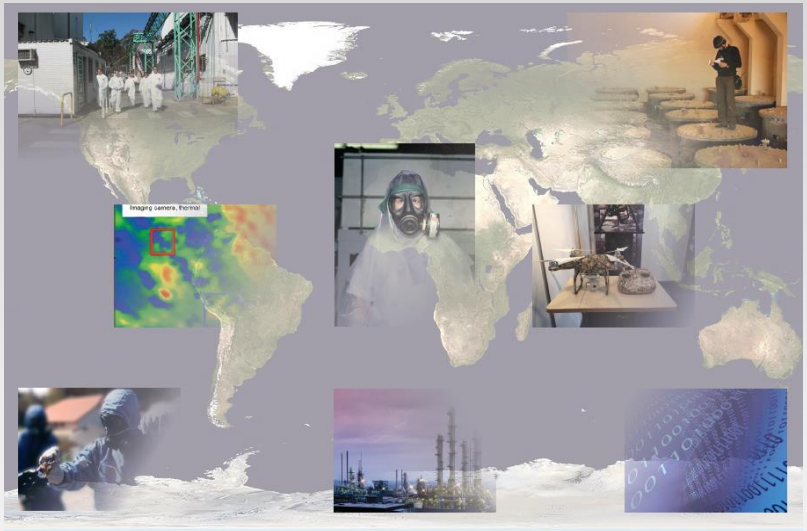
World Health Organization

IAEA International Atomic Energy Agency

AAAS
ADVANCING SCIENCE, SERVING SOCIETY

EUROPOL

Office of International and Security Affairs



VERIFICATION

REPORT OF THE SCIENTIFIC ADVISORY BOARD'S TEMPORARY WORKING GROUP

June 2015

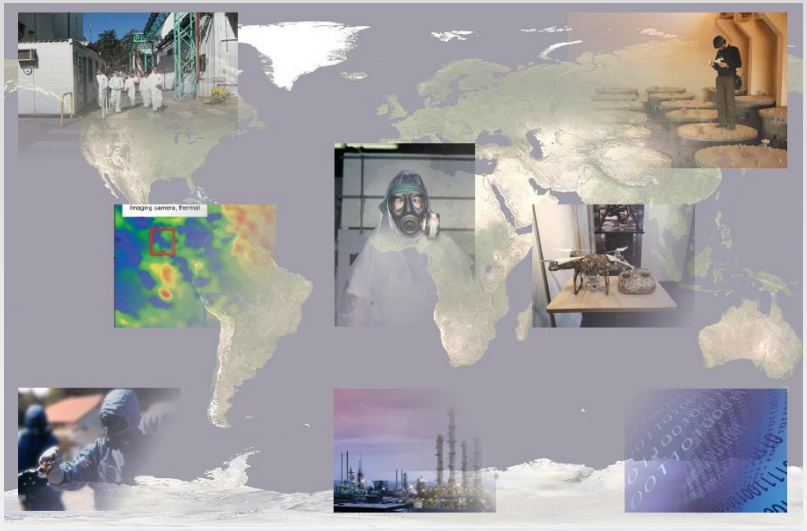
ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

What are the technologies/methodologies used for verification purposes in other international treaties that could benefit the verification regime of the CWC?

Systematic use of information collected from multiple sources by the Secretariat could, e.g. assist States Parties identify declarable activities and the Secretariat to follow global trends relevant to verification

Recommendation

Secretariat should consider adopting a comprehensive more analytical approach to verification utilising all available and verifiable information



Which methodologies (whether existing or new) could assist States Parties to ensure that all declarable plant sites are identified for declaration?

Effective use of open-source information could help the Secretariat identify and understand the wider development and trends of the chemical industry

This could help OPCW to be able to address future developments/evolving challenges

Recommendation

Secretariat should acquire the capability to use open-source information routinely

Which new or emerging technologies may add value to existing capabilities for verification purposes (such as data analysis/data mining, statistical analysis, attribution analysis)?

A more analytical approach to verification using all available information would require improved information management support within OPCW

Recommendations

Secretariat should put in place an information management structure that can provide the support required for the verification process

Remote/automated monitoring technologies should be added to the list of approved inspection equipment

Secretariat should look into the option of using satellite imagery for the planning of non-routine missions, in particular for investigations of alleged use (IAU) and challenge inspections

Which new or emerging technologies may add value to existing capabilities for verification purposes (such as data analysis/data mining, statistical analysis, attribution analysis)?

Recommendations

Secretariat should visit the National Authorities to obtain assurance on the accuracy and completeness of declarations; outcome of such visits may impact on the inspection frequency

Secretariat must commission an independent review of all activities pertaining to the missions carried out in the Syrian Arab Republic


14/03/2015 15:13


06/03/2015 12:28


06/03/2015 12:18


30/03/2015 10:10

What are the key technical components of a consistent approach to declaring complex mixtures of discrete organic chemicals (DOCs)?

Part IX of the Verification Annex puts the focus on the plant sites that produce DOCs, rather than on the chemicals.

CWC does not exempt facilities producing mixtures containing low concentrations of DOCs from declaration requirements, nor does it define a purity level for DOCs

Recommendation

List of declarable OPCFs submitted by States Parties should include all facilities that fall under the requirement of para. 1 of Part IX of Verification Annex, regardless of the purity level of a DOC or DOC mixtures produced

What are the verification aspects of the meaning of "produced by synthesis"?

Recommendations

Not all facilities that fall under Part IX of the Verification Annex should be considered of the same relevance to the object and purpose of the CWC

(TWG has recommended a practical approach for enhancing the utilisation of verification resources for OCPF declaration and on-site processes)

Verification thresholds for OCPFs producing highly relevant chemicals, and the possibility of revision of the product codes should be addressed by SAB as well as the industry cluster

How can sampling and analysis be utilised most effectively for verification purposes?

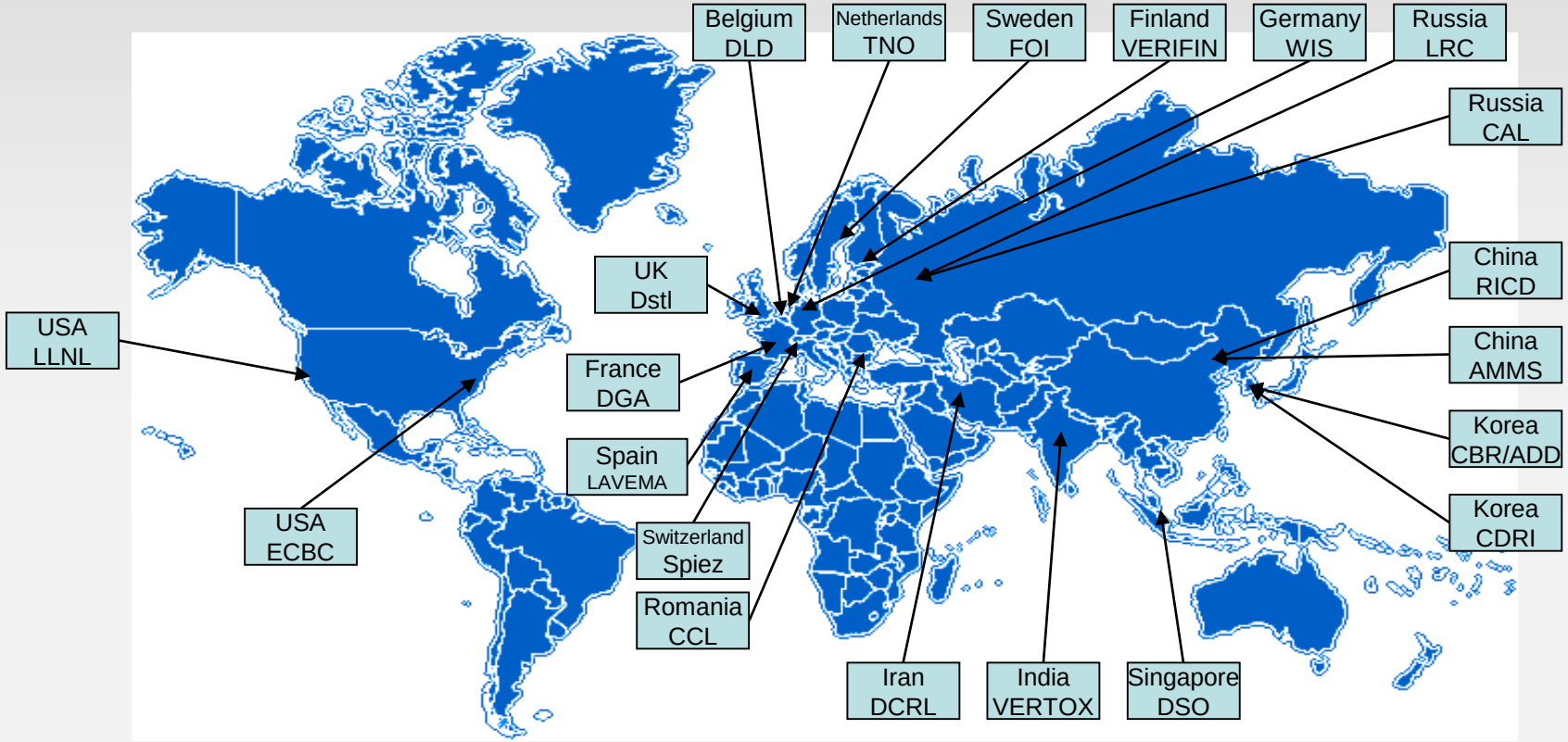
Recommendations

OPCW should increase staff of OPCW Laboratory to cope with:

- various aspects of IAU
- biomedical samples
- trace environmental analysis
- toxins
- on-site analysis

Establishing a network of Designated Labs for biomedical sample analysis should be a high priority

OPCW Designated Laboratories (environmental)



21 Designated Laboratories (7 suspended) in 17 countries

as of March 2015

How can sampling and analysis be utilised most effectively for verification purposes?

Recommendations

Lessons on chemical sampling and analysis form the OPCW's support to the UN Mission to investigate the use of CW in the Syrian Arab Republic, and all subsequent OPCW activities in relation to the Syrian Arab Republic must be identified and implemented

Proficiency Tests should incorporate a broader range of chemicals and at a wider range of concentrations to prepare laboratories for IAU scenarios

How can sampling and analysis be utilised most effectively for verification purposes?

Recommendations

Secretariat should expedite toxin identification exercises

Continuous additions to OCAD are recommended to allow the OPCW to meet all its mandated inspection aims, including IAU

Developments in analytical instrument portability, miniaturisation and disposable biosensors should be reviewed periodically by the Secretariat and SAB for potential applicability for on-site analysis

Secretariat should monitor developments in attribution analysis/chemical forensics

Which methodologies might be helpful for the Secretariat to keep abreast of developments in science and technology of relevance to the CWC verification regime?

Recommendation

Secretariat should augment its capability to monitor and forecast developments in science and technology of relevance to the Convention and its verification regime

Invited speakers at SAB-22

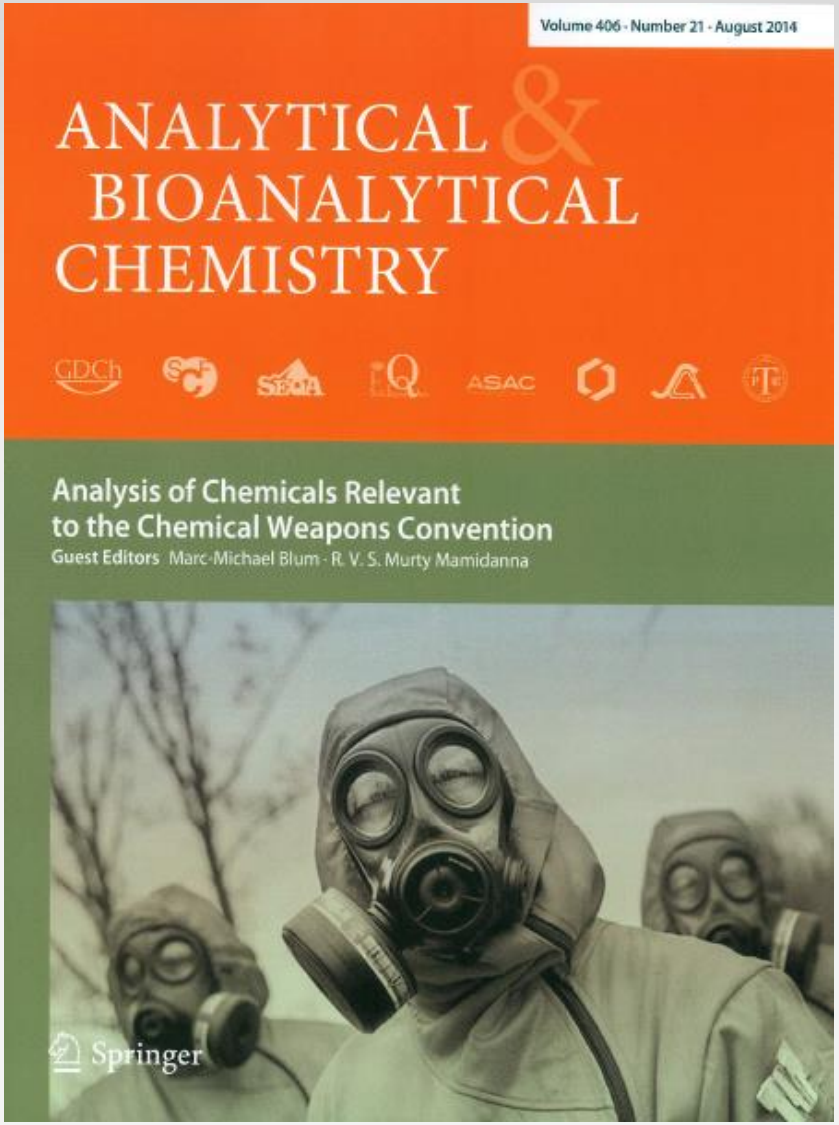
Prof. Ake Sellstrom
Leader of the UN mission to investigate the use of chemical weapons in the Syrian Arab Republic

Dr. Daan Noort
Principal scientist at the Netherlands Organisation for Applied Scientific Research (TNO) Defence, Safety and Security

Ambassador Istvan Gyarmati
Chair of Advisory Board to the UN Secretary-General on Disarmament Matters

Science and technology


THE SCIENCE OF DESTRUCTION AND VERIFICATION
THE CONVERGENCE OF CHEMISTRY AND BIOLOGY
Feature Article:
Plants as Nerve Agent Detectors
SCIENCE AND INTERNATIONAL COLLABORATION
OPCW Today
Volume 3 No. 1 • Aug 2014
www.opcw.org
SCIENCE AND TECHNOLOGY
ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS


Volume 406 · Number 21 · August 2014
ANALYTICAL & BIOANALYTICAL CHEMISTRY
GDCh
SEQA
ASAC
Analysis of Chemicals Relevant to the Chemical Weapons Convention
Guest Editors Marc-Michael Blum · R. V. S. Murty Mamidanna
Springer

METAL–ORGANIC FRAMEWORKS

Breaking bad chemicals down

A metal–organic framework with large pores catalytically destroys chemical warfare agents.

Matthew J. Rosseinsky, Martin

Organisation for the Prohibition of Chemical Weapons (OPCW; www.opcw.org), winner of the 2013 Nobel Peace Prize for "its extensive efforts to eliminate chemical weapons"[2], was

This year marks the centennial of the large-scale use of chemical weapons. The response then — during the First World War — was to equip personnel with mouth pads, and later with gas masks whose canisters contained activated carbon. Today, this carbon-based material takes the form of a highly porous granular solid with a typical surface area of 1,000 $m^2 g^{-1}$. For military use, the carbon is impregnated with metal salts, which improve protection against volatile toxic chemicals, such as hydrogen cyanide. Such canisters save lives (Fig. 1) and without them personnel can succumb quickly to chemical warfare, for example, in the Ghouta attack on 21 August 2013, where the organophosphorus nerve agent sarin[1] caused around 1,500 deaths. The Organisation for the Prohibition of Chemical Weapons (OPCW; www.opcw.org), winner of the 2013 Nobel Peace Prize for "its extensive efforts to eliminate chemical weapons"[2], was able to coordinate the destruction thereafter, with international partners, of the chemical stockpile of the Syrian Arab Republic. This episode emphasized the global need for rapid, efficient systems to neutralize and destroy chemical warfare agents, provide personal and collective protection, and eliminate chemical stockpiles.

Writing in *Nature Materials*, Joseph Mondloch and co-workers now report a way to destroy chemical warfare agents using a porous metal–organic framework (MOF) called NU-1000 with a specific arrangement of Lewis acid metal–oxo units[3]. These acidic units catalyse the hydrolytic destruction of nerve agents, in this case soman (also known as GD), which is a more toxic relative of sarin, with similar physical and chemical properties[4].

Metal–organic frameworks consist of metal-based units (which can be mononuclear or clusters) connected by coordinate bonds to polydentate organic ligands[5]. By combining the metal and ligand chemistry to determine the geometry of the resulting extended structure, large-pore crystalline open frameworks can be synthesized with a high degree of control. Such large-pore ordered materials have exciting properties and can be used in areas such as sorption of fuel gases[6], separation of economically important molecules with low energy inputs[7] and in components can have catalytic activity, there is considerable interest in the application of MOFs in catalysis[9], as their pore dimensions may allow them to process larger molecules compared with currently available crystalline open frameworks. Stable framework-forming chemistries are available that can enable catalytic applications in demanding environments such as water[10]. One of the most promising MOF families is based on the oxygen-bridged Zr_6 cation clusters[11], where water-stable crystalline materials with surface areas of over 4,000 $m^2 g^{-1}$ are available[12]. The Lewis acidity of the Zr^{4+} metal species, which attracts electron density from molecules that bind to its centre, is known to enable catalytic destruction of nerve agent analogues, but this has so far only been observed in materials that are non-porous or whose pores restrict this catalytic chemistry to the external surface.

The NU-1000 MOF catalyst studied by Mondloch and co-workers[13] uses a multidentate organic ligand[14] that organizes these metal–oxo clusters to produce 3-nm-diameter one-dimensional channels. This allows it to adsorb the nerve agent molecules rapidly and exposes all the reactive clusters to them, not simply those on the external surface of the material. The chemical structure of the nerve agents makes them moderately stable in water, so a potential catalyst must offer a low-energy pathway to accelerate their decomposition. The

Figure 1 | A British S10 respirator with a replaceable charcoal canister shown on the right. Image reproduced with permission from: © Zaid Meherali; www.defencephotos.com.

all, highly charged Zr^{4+} cations bind to negatively charged regions of the nerve agent, in particular to the P=O bond of the phosphonate group. This interaction activates the nerve agents so that they can be cleaved more readily by water. By controlling the cluster chemistry through changing the bridging species from hydroxide (OH^-) to oxo (O^{2-}), the authors reduced the number of oxide-based species binding to the Zr^{4+} centres (that is, their coordination number) from 8 to 6 and thus enhanced their Lewis acidity for binding and activating the nerve agents. The selection of a porous structure that both stably connects the metal centres while retaining low metal coordination numbers for high catalytic activity is key to the success of the method. The solid-state structure of the MOF is essential for its activity, which is not displayed by an isolated molecular cluster.

The mode of action of the catalyst is revealed by computational studies that show the precise atomic-scale matching of the weak points in the nerve agent molecules to the active sections of the cluster, coupling hydrogen bonding and electrostatic interactions at the Lewis acid centres to lower the energy barrier (Fig. 2) to scission of the P–F bond that defines the nerve agent structure and thus its lethal *in vivo* function (which is inhibition of the enzyme acetylcholinesterase). This detailed understanding opens up new opportunities to design more active MOF catalysts, for example with several pre-arranged catalytic and activating groups that might act simultaneously on multiple parts of a target molecule. These endeavours will be assisted by identifying the role of defects in the extended structure in the amplification of catalytic activity over that deduced from the average structure: defects such as missing organic linker molecules are known in this class of MOF, and zeolite catalysts, such as those used in the fluid catalytic cracking processes that produce all the gasoline used today, are optimized by control of defects within their structures. *In operando* spectroscopic studies may also reveal important details of how the catalyst of Mondloch and colleagues functions.

The MOFs designed by these authors could potentially be used in some filters

to supplement activated carbon (which physically adsorbs volatile toxic vapours weakly) and catalyse agent destruction.

The opportunity to harness stable MOF chemistries and optimize active catalytic units through their controlled positioning within regular open-framework structures for chemical agent destruction is clearly set as an exciting challenge by this study. The transition of MOFs from the laboratory to the field — which are tolerant to temperature and humidity fluctuations, dust, rough-handling and other real-world conditions — will require experts in materials science, adsorption, and security and defence to work together to examine the degradation of a range of chemical warfare agents. This collaboration could provide ready destruction of stockpiles of such agents, and affordable, broad-spectrum respiratory protection that may deter the use of chemicals in conflict and aid the OPCW in its goal of a world free of chemical weapons. ❐

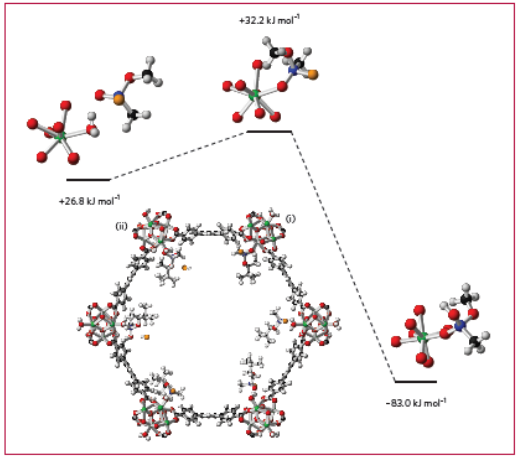


Figure 2 | The Lewis acidic Zr^{4+} centres in NU-1000 provide a low-energy pathway for the decomposition of a structurally simplified analogue of the nerve agent soman by activation of the molecule through coordination of the P=O bond. These interactions are enabled by the large internal surface and chemical functionality of the 3-nm channels of the MOF, formed by coordination of a tetradentate carboxylate ligand to a $Zr_6O_8^{8+}$ cluster (bottom left). A hydrated Zr^{4+} centre in NU-1000 (top left) binds to the analogue $CH_3O(CH_3)P(O)F$ to yield a high-energy intermediate (top middle). Water reacts with this intermediate with loss of hydrogen fluoride (not shown) to generate the bound, non-toxic phosphonic acid (bottom right). The computed Gibbs free energies of each reaction step are shown. A schematic catalytic cycle is depicted within a representative pore and proceeds clockwise: the analogue binds (i) and hydrolyses to the phosphonic acid and hydrogen fluoride (ii). Zr, green; O, red; H, grey; P, blue; F, orange; C, black. Figure courtesy of J. E. Mondloch.

Matthew J. Rosseinsky is in the Department of Chemistry, University of Liverpool, Crown Street, Liverpool L69 7ZD, UK. Martin W. Smith and Christopher M. Timperley are in the Defence Science and Technology Laboratory (Dstl), Porton Down, Salisbury, Wiltshire SP4 0JQ, UK.
e-mail: m.j.rosseinsky@liverpool.ac.uk; mwsmith@dstl.gov.uk; cmtimperley@dstl.gov.uk

References
1. Gravett, M. R. *et al. Proc. R. Soc. A* 470, 20140076 (2014).
2. Üzümcü, A. *Organisation for the Prohibition of Chemical Weapons (OPCW) — Nobel Lecture: Working Together for a World Free of Chemical Weapons, and Beyond* (2013); http://www.nobelprize.org/nobel_prizes/peace/laureates/2013/opcw-lecture.html
3. Mondloch, J. E. *et al. Nature Mater.* 14, 512–516 (2015).
4. Timperley, C. M. *Best Synthetic Methods: Organophosphorus (V) Chemistry* Ch. 1, 13–17 (Elsevier, 2015).
5. Furukawa, H., Cordova, K. E., O'Keeffe, M. & Yaghi, O. M. *Science* 341, 1230444 (2013).
6. Yan, Y., Yang, S., Blake, A. J. & Schröder, M. *Acc. Chem. Res.* 47, 296–307 (2014).
7. Horn, Z. R. *et al. Science* 340, 960–964 (2013).
8. Millar, S. R. *et al. Chem. Commun.* 49, 7773–7775 (2013).
9. Gascon, J., Corma, A., Kapteijn, F. & Llabrés i Xamena, F. X. *ACS Catal.* 4, 361–378 (2014).
10. Dhakshinamoorthy, A., Asiri, A. M. & Garcia, H. *Chem. Commun.* 50, 12800–12814 (2014).
11. Cavka, J. H. *et al. J. Am. Chem. Soc.* 130, 13850–13851 (2008).
12. Kalidindi, S. B. *et al. Angew. Chem. Int. Ed.* 54, 221–226 (2015).
13. Mondloch, J. E. *et al. J. Am. Chem. Soc.* 135, 10294–10297 (2013).
14. Stylianou, K. C. *et al. J. Am. Chem. Soc.* 132, 4119–4130 (2010).

VOLUME 2 NUMBER 7

The OPCW Science & Technology Monitor

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

1 June 2015

In This Issue

Featured content

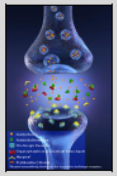
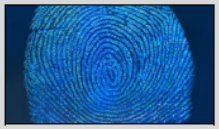


Image from DuoDote®
Medical countermeasures at work in a synapse.



Fingerprinting chemicals.

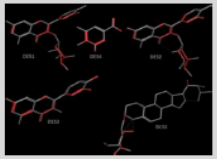


Image from PLoS One. 2013 Nov. 8(11)
Drug discovery research in OPCW Supported Research Projects

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.

Thanks to all of you who have taken our survey. For those who have not yet responded, the survey is still open (click here). There are only six questions, all easier than the puzzle (we promise) and all responses are anonymous. Your feedback is highly appreciated!

Today marks the 25th anniversary of the signing of the 1990 Chemical Weapons Accord by the United States of America and the Soviet Union. This agreement, which pre-dated the CWC, marks one of many steps taken in the journey toward a world free of chemical weapons. Steps taken in chemical disarmament have been supported by the science of chemistry itself; a scientific field that provides opportunities for international collaborations and brings forth new developments with peaceful economic and technological benefits. As we move into the future, we look forward to a wealth of new discoveries from this evolving scientific field.

The S&T Puzzle

We once again congratulate our colleagues at the CTBTO, whose entry correctly recognized four of the top five spoken words of the Director-General in the eight statements delivered from 22 January to 29 April 2015 (in case you were wondering, they missed "States"). The prize for best visualisation of the words of the Director-General, however, goes unclaimed as no submissions (except our own, below) were received. Puzzle statistics now stand at: VER 4, OSP 2, OCS 1, INS 1 and CTBTO 3.

For this edition of the puzzle, we look at the multiple uses of a cup of coffee. Can you tell us the identity and LD_{50} (that's right, the median lethal dose) of the most abundant chemical in the cup; the molarity (M) of caffeine (molecule above); and the LD_{50} of coffee itself? To keep this simple, assume this coffee is made with Arabica beans and brewed by a certified procedure (for

Monitoring latest S&T

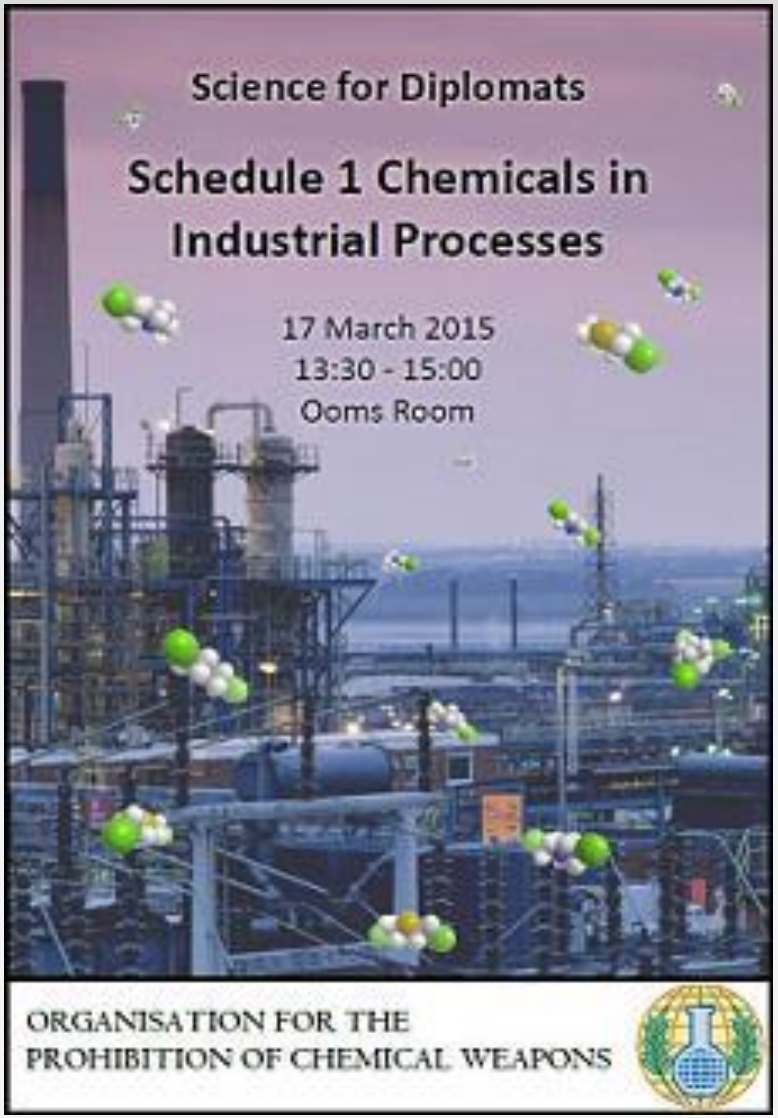
Monthly newsletter in popular science format on topics relevant to the CWC

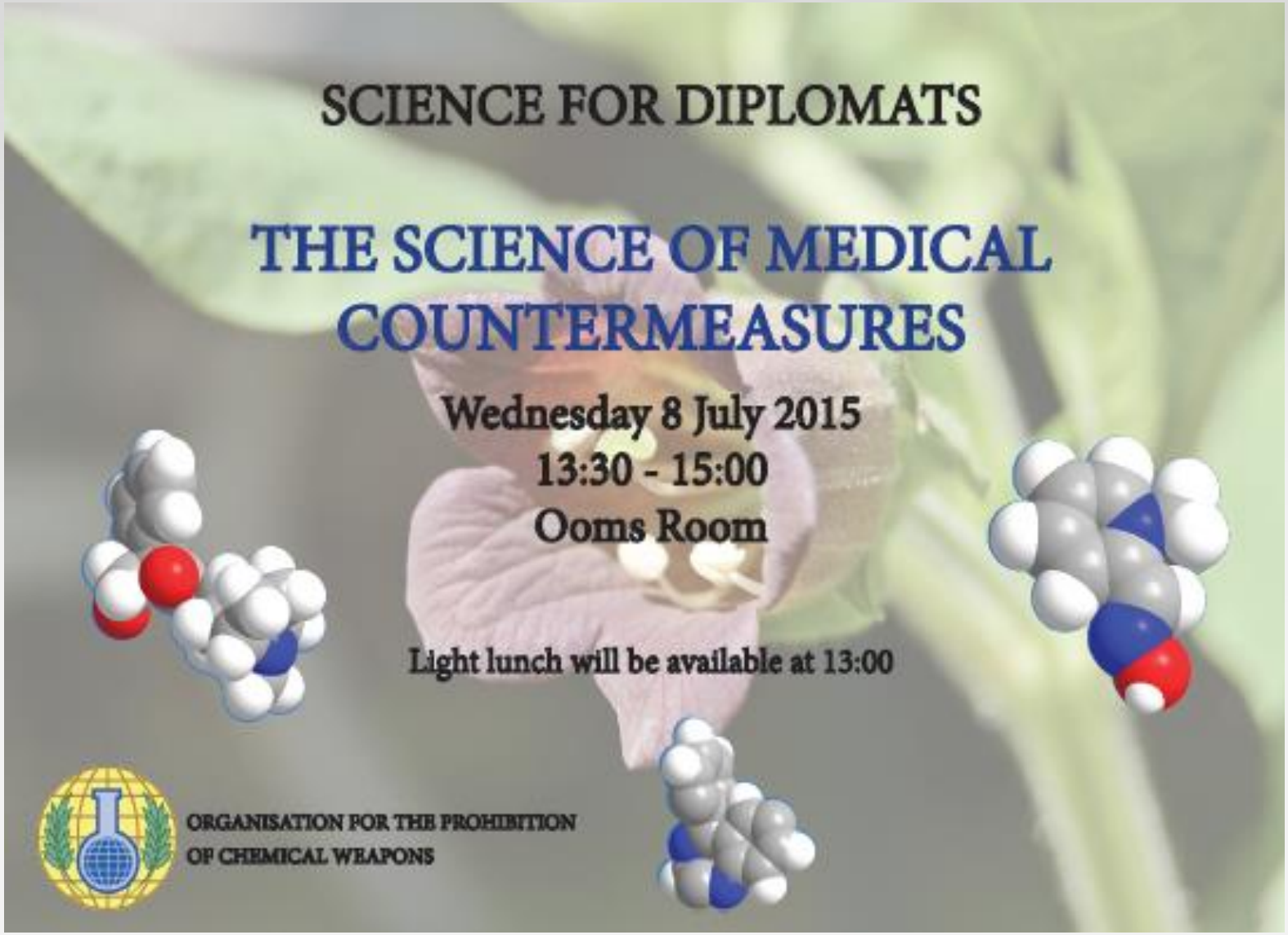
Chemical Forensics

We thank our colleagues from the OPCW Laboratory for their major contribution and input to this feature

The ability to obtain unique signatures such as fingerprints and DNA to identify individuals or the marks left on a fired bullet to identify the firearm that shot it, to compare with reference materials (such as a fingerprint obtained from a suspect) are among the most powerful forensic tools available to law enforcement. Chemical signatures that indicate drug use or gender can even be collected from fingerprints.

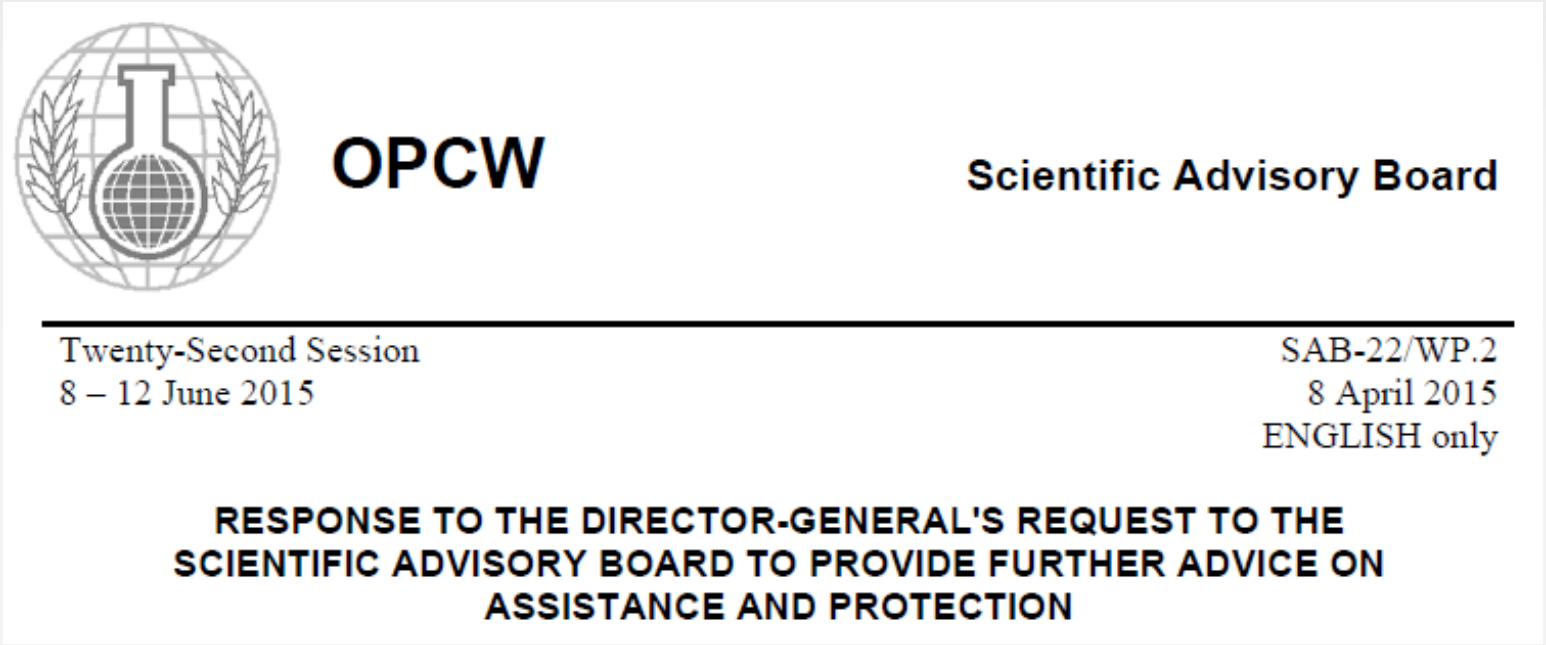
Chemical samples can also have unique signatures that might reflect how and where they originated. For the Chemical Weapons Convention, one might ask, questions such as: What kind of molecular signatures exists for chemical warfare agents and toxic chemicals that may have been used in an incident under investigation, what kind of reference samples are required for comparison and what kind of forensic information can be obtained with such information?


Science for Diplomats
Schedule 1 Chemicals in Industrial Processes
17 March 2015
13:30 - 15:00
Ooms Room
ORGANISATION FOR THE
PROHIBITION OF CHEMICAL WEAPONS


SCIENCE FOR DIPLOMATS
THE SCIENCE OF MEDICAL COUNTERMEASURES
Wednesday 8 July 2015
13:30 - 15:00
Ooms Room
Light lunch will be available at 13:00
ORGANISATION FOR THE PROHIBITION
OF CHEMICAL WEAPONS

Assistance and protection

SAB has provided further advice on nerve agent medical countermeasures



OPCW

Scientific Advisory Board

Twenty-Second Session
8 – 12 June 2015

SAB-22/WP.2
8 April 2015
ENGLISH only

RESPONSE TO THE DIRECTOR-GENERAL'S REQUEST TO THE SCIENTIFIC ADVISORY BOARD TO PROVIDE FURTHER ADVICE ON ASSISTANCE AND PROTECTION

Future activities of SAB

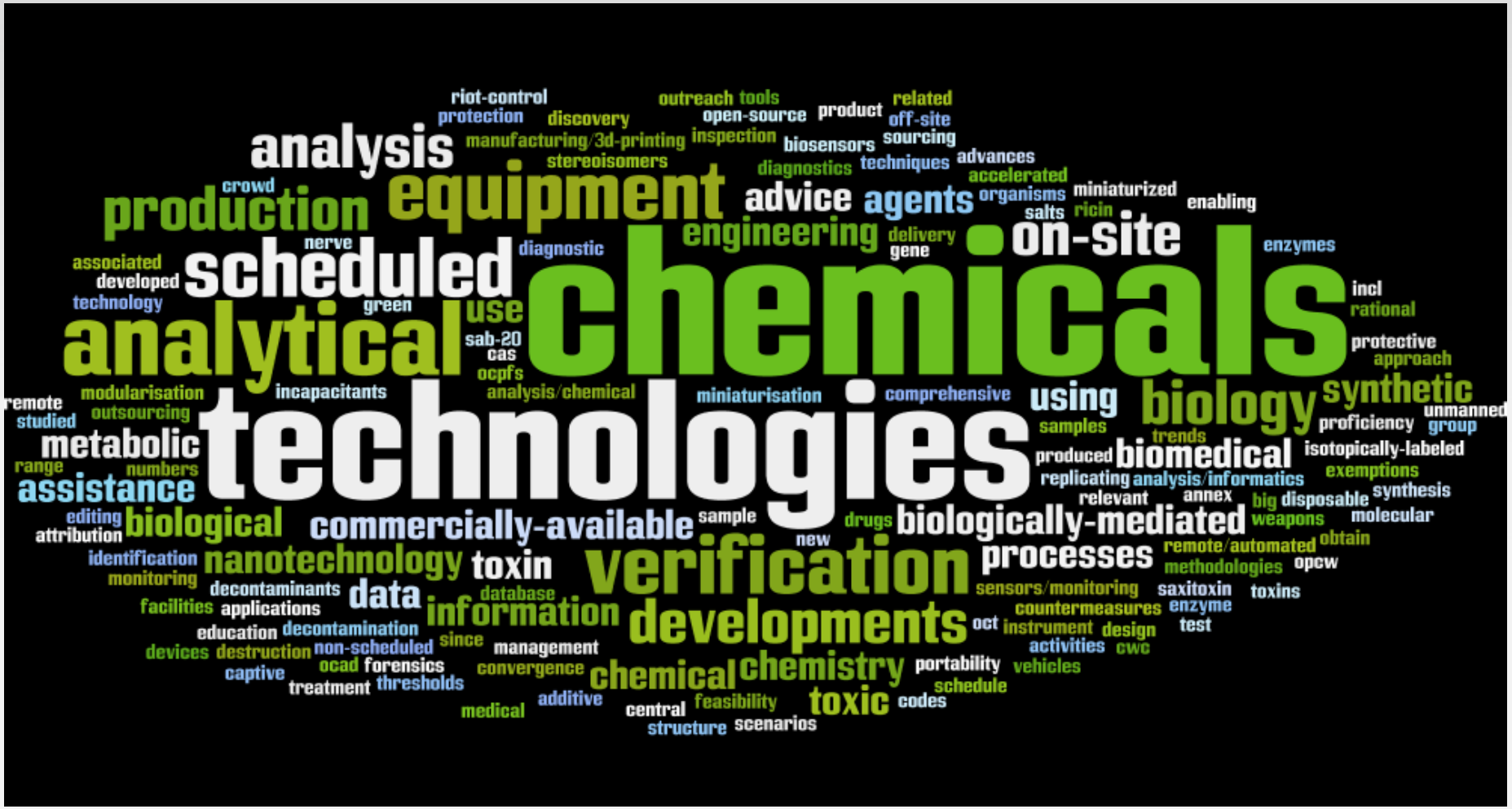
Request from Director General to provide advice on isotopically labelled scheduled chemicals and stereoisomers of scheduled chemicals

Planning by SAB and Secretariat for the S&T report to 4th Review Conference has started

Education and outreach activities will continue

Attend SAB item at EC-80 on 7 October 2015

Briefing of SAB verification report to the BWC Meeting of Experts in Geneva, 11-14 August 2015


riot-control
protection
discovery
outreach tools
open-source
product
related
off-site
analysis
manufacturing/3d-printing
inspection
biosensors
sourcing
stereoisomers
diagnostics
techniques
advances
accelerated
crowd
production
equipment
advice
agents
organisms
miniaturized
salts
ricin
enabling
engineering
delivery
gene
on-site
nerve
diagnostic
enzymes
associated
developed
scheduled
chemicals
technology
green
use
incl
rational
analytical
sab-20
cas
ocpfs
protective
approach
modularisation
incapacitants
analysis/chemical
miniaturisation
comprehensive
using
biology
synthetic
remote
studied
outsourcing
samples
trends
proficiency
unmanned
group
metabolic
technologies
produced
biomedical
isotopically-labeled
range
numbers
replicating
analysis/informatics
exemptions
assistance
relevant
annex
big disposable
synthesis
editing
attribution
biological
commercially-available
sample
drugs
biologically-mediated
weapons
molecular
identification
nanotechnology
toxin
new
verification
processes
remote/automated
obtain
monitoring
methodologies
opcw
decontaminants
data
database
sensors/monitoring
saxitoxin
toxins
facilities
applications
information
developments
countermeasures
enzyme
education
decontamination
oct
instrument
design
test
since
activities
cwc
devices
destruction
non-scheduled
management
ocad
forensics
chemical
chemistry
portability
vehicles
captive
convergence
treatment
thresholds
schedule
medical
additive
central
feasibility
toxic
codes
structure
scenarios

SAB-22


Any questions?