

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

# IMPACT OF SCIENTIFIC DEVELOPMENTS ON THE CHEMICAL WEAPONS CONVENTION

## (IUPAC Technical Report)

Prepared for publication by  
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# Impact of scientific developments on the Chemical Weapons Convention

## (IUPAC Technical Report)

*Abstract:* This document was prepared as a report from IUPAC to the Organisation for the Prohibition of Chemical Weapons (OPCW) to provide an evaluation of scientific and technological advances in the chemical sciences relevant to the Chemical Weapons Convention (CWC). The report is intended to assist OPCW and its Member States in preparation for the First Review Conference to be held on 28 April 2003. The CWC, now ratified by 145 nations and in effect since 1997, totally prohibits the production, storage, or use of toxic chemicals as weapons of war. This report is based on an IUPAC Workshop held in Bergen, Norway, 30 June to 3 July 2002.

The report highlights developments in organic synthesis and changes in chemical plant design that will pose new challenges to the Convention, but it also describes recent and probable future developments in analytical chemistry that should assist in implementation of the Convention. The key issues identified at the Workshop are listed, and the findings and observations are summarized in 18 points.

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## INTRODUCTION

The International Union of Pure and Applied Chemistry (IUPAC) has undertaken an evaluation of scientific and technological advances in the chemical sciences that might have an impact on the implementation of the CWC. This is one of the efforts by IUPAC to provide a sound scientific foundation for decision makers to address important global issues. Such an evaluation is timely in view of the forthcoming First Review Conference of the CWC to be held on 28 April 2003. The Director-General informed the Member States of OPCW of both the IUPAC initiative and of his acceptance of this at the Sixth Session of the Conference of States Parties on 14 May 2001. In his opening statement, the Director-General said:

*An important aspect of the preparations for the review conference is an assessment of the scientific foundations of the Convention. Does the present verification regime under Article VI, and the Schedules contained in the Annex on Chemicals, adequately reflect the scientific and technological progress that has been made over the past decade, and the current trends in science and technology? Much has changed, as is evidenced by the completion of the human genome project and the emergence of genomics, as well as by advances in chemical production technologies, a better understanding of the functioning of certain biomolecules and receptors, etc. The International Union of Pure and Applied Chemistry has proposed to the Secretariat that it undertake a review of key areas of science, with a view to identifying developments and trends that are relevant to the CWC. We welcome this offer and look forward to the results of this international scientific review. Its results will, of course, be passed on to Member States for advice and action well before the review conference.*

As the only independent, nongovernmental, international organization devoted to the chemical sciences and their applications, IUPAC was regarded as very well placed to conduct this review. Formed in 1919, IUPAC is an association of bodies—National Adhering Organizations—that represent the chemists of different member countries. IUPAC has 44 National Adhering Organizations, and 20 other countries are also linked to IUPAC in the status of Associate National Adhering Organizations. Appendix 1 provides further background information about IUPAC.

The negotiators of the CWC were farsighted in calling for periodic “reviews of the operation of this Convention. Such reviews shall take into account any relevant scientific and technological developments.” The progress in the chemical sciences and technology over the past decade has been impressive. The research community—academic, industrial, governmental—has made dramatic progress toward treatment of diseases such as HIV infection and cancer and in developing new materials for electronic and optical devices for communications and information technology. New analytical techniques have made possible analysis of minute quantities of material, even single molecules in some instances. The chemical and allied industries have brought these discoveries to fruition and benefited the lives of millions. In addition, these industries have developed new process technologies that enable production of chemical products more efficiently, more safely, and with increased protection of the environment. In the context of chemical weapons issues, the rapid advances in science and technology have the potential both to challenge and to assist in implementation of the CWC. Some advances in process technology could be misappropriated to provide easier access to chemical weapons. On the other hand, advances in analytical methods and instrumentation have the potential to assist OPCW and National Authorities in the effective implementation of the CWC so as to ensure the total prohibition of chemical weapons.

Director-General Pfirter emphasized in an address on 20 September 2002 that the development of technological innovations offers promise as a future means of increasing cost-efficiency in the inspections carried out by OPCW.

## THE WORKSHOP

IUPAC organized a Workshop entitled Impact of Scientific Developments on the Chemical Weapons Convention in Bergen, Norway on 30 June to 3 July 2002. Financial support was provided by the John D. and Catherine T. MacArthur Foundation, NATO, the Ploughshares Fund, the U.S. National Academies, the Ministry of Foreign Affairs of Norway, Amersham Health AS, the University of Bergen, the Royal Society (London), and the International Council of Chemical Associations.

There were 79 participants from 34 countries.\* Twenty-seven of the participants from 17 countries were representatives of governments coming from National Authorities and government laboratories. Leading international scientists and engineers presented lectures that described recent technical developments and assessed the state of the art in several areas of organic synthesis, industrial chemical processing, and analytical chemistry methodologies. The Workshop successfully brought together the collective knowledge of academia, industry, government, and OPCW in order to address how the implementation of the Convention could reflect the leading edge of chemistry. This exciting new information provided background for three discussion sessions in which participants in small groups identified principal issues in the application of new technologies to problems in the implementation of the CWC.

The findings by the Workshop participants form the basis for this report. The report is presented in four sections, as follows:

- A. Presentations and discussions in the Workshop
- B. Key issues that emerged from the deliberations at the Workshop
- C. Summary findings and observations
- D. Rationale for the findings and observations

## A. PRESENTATIONS AND DISCUSSIONS

The Workshop lectures were divided into five sessions, as follows:

- **Background and Context for the Workshop: The First Review Conference**  
In this session, the speakers—primarily present and former officials of the OPCW Secretariat—provided information on the Convention and how it is being implemented by the Secretariat. They focused particularly on inspections, verification procedures, costs, lessons from current experience, and unresolved issues. The important issue of the Convention in the context of chemical terrorism was also reviewed. A representative of the chemical industry reported on voluntary steps taken by the industry in some countries to enhance national security.
- **New Developments in Chemical Synthesis**  
Over recent years, many new procedures have been developed to speed up the synthesis of new chemicals required in particular for biological evaluation by the pharmaceutical industry. Combinatorial chemical techniques were described together with other methods for rapid synthesis and screening. This enabled participants to assess whether such advances posed new problems for the Convention.
- **New Methods in Biological Synthesis of Chemical Compounds**  
As the molecular basis of biology becomes better understood, it is becoming easier to use that knowledge both to design new biologically active chemicals and to synthesize chemicals using enzymes or cell-based systems. In some areas, this leads to considerable overlap between the

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\*Participants came from the following countries: Australia, Austria, Canada, Chile, China, Croatia, Czech Republic, Estonia, Ethiopia, Finland, France, Germany, Hungary, India, Italy, Ivory Coast, Japan, Kazakhstan, Kenya, Korea, Moldova, Netherlands, Norway, Russia, Singapore, Slovakia, South Africa, Spain, Sweden, Switzerland, Tunisia, UK, USA, and Vietnam.

CWC and the Biological and Toxin Weapons Convention (BTWC). These advances have the potential to change the nature of the way chemicals are synthesized and to make practical the synthesis on reasonable scales of chemicals that previously were little more than curiosities.

- **New Developments in Processing and Manufacturing**

There has been a vast increase in the types of techniques available to facilitate chemical production, for example, new catalysts, phase-transfer techniques, photochemistry, ultrasonic, microwave-assisted reactions, biocatalysis, solid supported reagents, membrane reactors, microreactors, electrochemical processes, and many more. In addition, the increasingly global nature of chemical industry means that knowledge of these advances is becoming widespread. The Workshop considered the implications on the inspection procedures of OPCW, of the changing nature of manufacturing facilities. Concepts such as “just-in-time” synthesis are changing plant design in ways that must be understood by the OPCW inspectorate.

- **Analytical Techniques**

A wide range of analytical techniques were reviewed, starting with those currently employed or under consideration as chemical agent detectors as well as instruments and techniques for agent identification. Topics also covered included NMR-based metabonomics, immunoassay, and biosensors for toxins, new clean-up and separation techniques, and “lab-on-a-chip” technology, along with the high costs of converting laboratory techniques to robust field-usable equipment. These reviews provided the background necessary to enable participants to consider the options for on- and off-site analysis needed by the Technical Secretariat of OPCW in carrying out the various inspection and verification roles required by the Convention.

A summary program for the Workshop, together with a list of participants, is given in Appendix 2.

## **B. KEY ISSUES**

All participants were assigned to one of four discussion groups, which examined and discussed in detail the relevant scientific and technological developments. Reports from the discussion groups were presented in the final session of the Workshop, which identified and discussed the key issues to be addressed in the IUPAC Report.

The participants identified the following key scientific and technological issues that should be taken into account at the First Review Conference:

- I. Technical challenges to the Convention
- II. Analytical techniques for routine inspections, challenge inspections, and investigations of alleged use
- III. Technical capability of the Secretariat
- IV. Education and outreach

In addition, although the Bergen Workshop did not address the technologies for chemical weapons destruction, some aspects relating to the procedures used for verification of chemical weapons destruction facilities were believed by the participants to merit attention:

- V. Destruction of chemical weapons

## **C. SUMMARY FINDINGS AND OBSERVATIONS**

The findings and observations made by IUPAC on the basis of discussions at the Workshop are summarized in this section under the key issues identified above. The following section provides a more detailed discussion and rationale for each finding.

## I. Technical challenges to the Convention

1. In recent years, there have been major advances in synthetic and manufacturing technologies that have improved the ability of the chemical industry to supply a wide range of consumer products. However, the general review of these advances at the Workshop demonstrates that there is much potential for new methods to be misused to manufacture both scheduled and other toxic chemicals and their precursors and intermediates.
2. The CWC includes three Schedules of chemicals that were regarded when the Convention was negotiated as presenting a particular risk to the Convention. Although the Schedules are far from comprehensive, they have provided a common context for initiating declarations and verification procedures. On balance, it does not appear necessary to change the Schedules at this time. However, it would be desirable to clarify issues in relation to salts, where the scientific fact is that acid salts and the parent compounds from which they are derived exist in equilibrium in most environments.
3. The rapid pace of developments in biomolecular science (e.g., genomics and proteomics), coupled with advances in chemical synthesis (e.g., combinatorial chemistry), certainly increases the possibility that new toxic chemicals will be found that could be misused as chemical weapons. However, these advances do not significantly change the situation in view of the large numbers of already known toxic chemicals, many of which are not listed in the Schedules. Moreover, the general-purpose criterion of the CWC covers all toxic chemicals intended for nonpeaceful purposes, both known and new, irrespective of whether or not they are included on the Schedules.
4. New methods of synthesis and manufacture will have an impact on the ability to produce either scheduled chemicals or other toxic chemicals by new routes, thereby changing the situation regarding the potential for breakout.
5. Many parts of the chemical industry around the world operate with multipurpose batch facilities, which can readily be switched from one product to another. This versatility is needed to produce the wide variety of chemicals on which the world depends to sustain a modern way of life, but it could be misdirected to produce chemical warfare agents. This potential threat is enhanced by technological developments in the use of automated microreactors to produce substantial quantities of chemicals in a relatively small plant. With the increasing globalization of industry, there is a need to review the verification regime for "other chemical production facilities" (OCPF) to ensure that it is effective. Inspectors should remain knowledgeable about these developments, and there may be a need in terms of resource allocation to emphasize the OCPF regime more strongly.
6. The ever-increasing range of toxic chemicals and the new processes that make it easier to synthesize such chemicals, including the scheduled chemicals, on scales of a few tens of kilograms make it easier for terrorist groups to engage in chemical terrorism. States Parties should be aware of the scope of this problem in considering relevant national penal legislation that fully implements the CWC.

## II. Analytical techniques for routine inspections, challenge inspections, and investigations of alleged use

7. The general review of analytical methodology clearly demonstrated the strengths and limitations of current technologies. The power of modern analytical science is such that, if it were used to the full extent of its capabilities, all the analytical requirements of the Convention probably could be achieved.
8. On-site inspections can be effective with presently available gas chromatography/mass spectrometry (GC/MS) equipment provided that time is available to set up and validate the equipment and to do all the necessary sample preparation. Such time appears to be available for Schedule 2 inspections (96 h), but not for Schedule 3 and OCPF inspections. There are advantages when the

chromatographic and spectroscopic data from the analyses can be compared with specific commercial databases as well as the OPCW database, as this can clarify some interpretations.

9. Some of the analytical equipment held by the OPCW Technical Secretariat is no longer supported by service agreements. More versatile and mobile equipment of the types now available might better meet the requirements for efficient analysis and could be considered for approval by States Parties.
10. At present, there is no explicit agreement on the level of detection required to demonstrate the absence of a toxic chemical. Such agreement is desirable in order to avoid differing interpretations of data and to provide guidance in developing specifications for new analytical instruments for the Technical Secretariat. It may be that if trace analysis is required, off-site analysis will be the only option.
11. Advances in technology offer great promise for improved analyses, but they seem unlikely to solve on-site sample preparation and analysis problems in the near term (less than 5–10 years) since many of the problems appear to be procedural and logistical.
12. It appears that for analysis of samples obtained during routine inspections, challenge inspections, or allegations of use of chemical weapons the designated laboratories are well practiced to analyze environmental samples, at least for scheduled chemicals, but less experienced if toxins or other unscheduled chemicals are involved. However, few of the designated labs could carry out analyses of biological samples from incidents of alleged use. There may be a need for the OPCW Technical Secretariat and the States Parties to review the options available for accurate unequivocal analyses of unscheduled chemicals and of biological samples. Consideration might be given to enlisting help from appropriate laboratories that possess the necessary analytical skills and for monitoring advances in new techniques for analyzing biological samples.

### **III. Technical capability of the Secretariat**

13. Given the rapid pace of developments in the screening of new unscheduled chemicals and in the development of new, more flexible production processes for chemicals, attention needs to be given to ensuring that the Technical Secretariat is kept up to date and has the necessary competence to take such developments into account in the implementation of the Convention.
14. For sampling and analysis, only the highest standards are acceptable because of the importance of accurate results. Such standards, both in the OPCW Technical Secretariat and in the designated laboratories that support the OPCW analytical activities, cannot be achieved and sustained without all the staff involved being well trained and well practiced. There is a need to review what training is provided, how it is provided and whether sufficient resources are available to sustain the process.
15. Consideration should be given to the organization of periodic workshops to review relevant scientific and technological developments. Such workshops should be part of the ongoing training of staff members but could also benefit States Parties. Planning for such workshops is principally the responsibility of the Technical Secretariat and the OPCW Scientific Advisory Board, but IUPAC and other appropriate international scientific bodies might be consulted as appropriate.

### **IV. Education and outreach**

16. Greater efforts on education and outreach to the worldwide scientific and technical community are needed in order to increase awareness of the CWC and its benefits. An informed scientific community within each country can be helpful in providing advice to States Parties and in disseminating unbiased information to the public.

17. Education of and outreach to Signatory States and non-Signatory States could be helpful in increasing awareness of the importance of universal adherence to the Convention, thereby enhancing safety and security for all States.

## V. Destruction of chemical weapons

18. As the number of destruction facilities increases, the demands on inspectorate resources for on-site monitoring of the destruction of declared chemical weapons may become overwhelming. To alleviate this situation while maintaining an adequate level of confidence, OPCW should consider the introduction of remote monitoring procedures and/or less manpower-intensive verification of chemical weapon destruction facilities.

## D. RATIONALE FOR THE FINDINGS

In the opening session of the Workshop, representatives of OPCW set the context by discussing the successes and the challenges in bringing the CWC into force over the past five years. They also discussed potential problems facing them over the next few years. One new challenge is the threat of terrorism by organizations with global reach, sometimes with support from so-called rogue nations. OPCW outlined some aspects of its response to this challenge. However, much of the response to potential threats from terrorists using chemical or biological weapons must come from responsible nations, international alliances, and nongovernmental partners such as industry associations. A representative of one industry association outlined the voluntary steps being taken by its members to prevent the facilities of the U.S. chemical industry from being misappropriated by terrorists. Similar industry initiatives are under way in Europe.

This section highlights the major results presented in the 21 formal talks and provides a summary of the wide-ranging deliberations by the discussion groups. The discussions were guided by the underlying requirements specified in the CWC. Appendix 3 provides extracts from relevant sections of the Convention.

## I. Technical challenges to the Convention

The lectures presented at the Workshop and the subsequent working group discussions identified two particular technical challenges to the Convention:

- New toxic chemicals that are not listed on the Schedules may be discovered or used for purposes prohibited under the Convention.
- New methods of synthesis/manufacture may be used to hide illegal activities or be used for rapid breakout from the Convention by a nation that chooses to breach the Convention and produce chemical weapons.

These two topics are considered below, together with reference to the fact that many toxic chemicals already exist that are not listed on the Schedules but could be used as chemical weapon agents. The question of whether our current knowledge of new toxic chemicals or existing toxic chemicals that are not listed on the Schedules calls for revision of the Schedules is also considered.

### *New toxic chemicals*

Advances in biomolecular science (e.g., genomics and proteomics), coupled with advances in chemical synthesis (e.g., combinatorial chemistry) make it possible to identify very large numbers of biologically active chemicals at increasing rates.

Combinatorial chemistry now plays an important role in the discovery and optimization processes in the pharmaceutical industry and increasingly in agrochemicals and other areas of discovery chem-

istry. Solid-phase synthesis holds a dominant position in combinatorial synthesis as more chemistries are adapted for this medium. The increasing use of supported reagents, catalysts, and scavengers enable reactions to take place efficiently in a parallel mode. Increasing levels of automation allow new synthetic processes and synthetic routes to be developed rapidly. The new synthetic methods permit synthesis of families of compounds at a rate of thousands per year. To keep pace with the new synthetic methods, automated procedures for high-throughput screening have been developed to test the new compounds for biological activity at a comparable rate. These methods often rely on enhanced understanding of physiological processes so that researchers can test minute amounts of material by interaction with enzyme or tissue cultures rather than intact plants or animals.

Many recent developments in laboratory automation and microwave chemistry are relevant to CWC issues. They make possible toxic chemical synthesis without extensive safety precautions and facilitate the synthesis of sophisticated toxic chemicals.

The application of automated syntheses and high-throughput screening by pharmaceutical and agrochemical companies has produced databases of physiological properties associated with millions of chemical compounds. While the industries have been primarily interested in biological properties of commercial interest (e.g., anticancer drugs, selective pesticides, etc.), the databases contain large amounts of information on toxicity of chemicals to plants, animals, and humans. In such applications, work on a compound normally stops when it becomes clear that it is too toxic for the planned application. Database “mining” could uncover potential chemical warfare agents based on toxic chemicals with possibly appropriate physical properties. A useful indicator might be that work has continued on compounds that are too toxic for legitimate purposes. Extrapolation from current data could also predict new toxic chemicals with potential lethal applications.

Some new chemicals found by database mining will have toxicity characteristics that could lead to their being considered as chemical weapon agents. Since there have been active searches for new biologically active molecules for many decades in defense laboratories, industries, and universities, the key question is how these new technologies may challenge the ability of the CWC verification regime to confidently assure that the purpose and object of the Convention continue to be met. It would appear that suitable procedures for declaration and verification, particularly of chemical defense facilities, where the primary knowledge and understanding relating to chemical weapons is held, will provide the principal basis to counter such threats.

Extensive and highly sophisticated laboratories are currently required for the synthesis and rapid screening of biologically active compounds. Such capabilities are becoming available in universities and research centers around the world and will not be limited to a few developed countries. Unless the compounds are simple and of low molecular weight, considerable effort will be required to devise practical methods to produce sufficient quantities to constitute a threat. Such quantities are likely to be a few tens of kilograms for research and development (or terror applications) and tens or hundreds of tons for military use. Further, unless the new compounds are gases or liquids with suitable volatility characteristics, all the usual problems of dispersing solids so that they could be used effectively as chemical weapons will apply.

In discussions at the Workshop, it was argued that a systematic search for new chemical weapon agents with the new technologies now favored by pharmaceutical and biotechnology companies would be an ineffective procedure when considered in relation to already known toxic chemicals that are not listed on the Schedules and which could be used as chemical weapons. One cannot rule out the possibility that the new technologies as used in industrial and university laboratories could lead to the accidental discovery of toxic chemicals attractive as chemical weapon agents, particularly for smaller-scale or terrorist-type activities.

This analysis of the possible discovery of new toxic chemicals and the recognition that many toxic compounds already exist (e.g., carbamates and novichoks) that are not on the Schedules, serves as a reminder of a central strength of the Convention. The CWC embraces all such chemicals under the *general-purpose criterion*, which prohibits any toxic chemical not intended for peaceful purposes, as

described in more detail in Appendix 3. The Convention does not prohibit the production or use of any chemical per se. In fact, in an enumeration of the principal features of the CWC on 30 September 2002, the Director-General pointed out:

*It also encourages international cooperation in the development of chemistry and chemical technology, and aims at fostering trade in chemicals, chemical manufacturing equipment and technology for peaceful purposes.*

The Convention prohibits the production and use of toxic chemicals only when the intent or *purpose* of such production or use is not related to peaceful applications. Consequently, both legislation and implementation measures should not be limited to scheduled chemicals, but need to take into account this wider remit for toxic chemicals. Thus far, both within the OPCW Technical Secretariat and in National Authorities, there appear to have been few steps taken to monitor compliance for unscheduled toxic chemicals. Since this aspect is likely to assume greater importance, the issue of how best to implement the general-purpose criterion should be addressed by each State Party.

The above analysis suggests that, although the newer technologies, such as the advances in bio-molecular science and in chemical synthesis, must be kept under regular review, they do not materially change the situation regarding the risks posed to the Convention by toxic chemicals that are not listed in the Schedules.

#### *Processing and manufacturing*

Many think of the chemical industry as being composed of giant single-purpose plants with continuous production in easily recognizable process elements. This picture is true for manufacture of commodity chemicals such as plastics and fertilizers by large chemical and petrochemical firms. However, there is another part of the industry characterized by smaller batch facilities that can easily be switched from one product to another. Fine chemicals such as pesticides, pharmaceutical intermediates, fragrances, inks, and specialty coatings tend to be made in multipurpose facilities. Such versatile facilities—OCPFs in CWC terms—that could readily be switched from making commercial chemicals to making chemical weapon agents present a greater risk than single-purpose plants. OPCW inspectors should remain knowledgeable of various processing methods and alert to any subversion for prohibited purposes.

Looking ahead, industry is reducing costs and producing chemicals by cleaner (greener) processes using a wide range of new technologies. Presentations at the Workshop described many of the new developments.

New homogeneous catalysts are providing processes that entail fewer waste products, thus contributing to a cleaner environment. Enantioselective catalysts can produce specific optical isomers of chiral compounds desired for pharmaceutical and agrochemical applications. An interesting example presented at the Workshop was the catalytic synthesis of the phosphonic acid analog of the analgesic naproxen with great selectivity. Other new developments reported were catalytic reactions in water and in supercritical CO<sub>2</sub> as ways to avoid the use of organic reaction solvents. In fact, solventless reactions between solids have the potential to eliminate solvents altogether. While the elimination of solvents and reduction in waste products is usually beneficial ecologically, such changes may make it harder to detect illicit chemical production.

New developments in heterogeneous catalysis have yielded commercial technology that may challenge the effectiveness of the chemical weapon verification regime. In response to the Bhopal incident involving a release of methyl isocyanate, new catalytic technology was developed that facilitates “just-in-time” production of methyl isocyanate, thus eliminating the need to store large quantities of this highly toxic, volatile chemical intermediate. The new process is based on *N*-methylformamide, a widely available chemical, rather than the Schedule 3 chemical, phosgene, used in the conventional process. New catalytic processes have also been developed for cleaner processes to make the Schedule 3 chemicals phosgene and thionyl chloride.

A wide range of new reactor technologies including phase-transfer catalysis, microwave reactors, and electrochemistry were described. It was pointed out that some of these process technologies are capable of being scaled down to sizes that could be operated inconspicuously outside a normal chemical production setting. The potential use by terror organizations seemed obvious, but subsequent discussions pointed out some difficulties in producing chemical weapon agents in a “backyard” setting.

One new development that spurred much discussion concerned the development of automated microreactors. Small reactors fabricated by technology adapted from the electronics industry can be surprisingly productive when operated continuously. It was pointed out that a fist-sized reactor with a flow rate of 1 ml/s can potentially produce 30 tons of material per year when run continuously under computer control. The teaming of several such reactors in parallel has been well demonstrated. Several types of microreactors are now available commercially. In one pharmaceutical process, economic advantages have been noted. The production of toxic chemicals such as hydrogen cyanide (HCN), phosgene, and methyl isocyanate in such reactors appears to offer advantages in terms of safety. The potential of such reactors for clandestine synthesis of chemical weapon agents was the subject of much discussion in the working groups. It is evident that, with technologies such as microreactors becoming more widely utilized in industry, the scaling up of production processes from laboratory scale to industrial scale is much easier and faster.

Enzyme-catalyzed reactions as well as reactions in more complex biological media are alternatives to more conventional synthesis either alone or in conjunction with conventional synthetic methods. For example, the use of an enzyme-catalyzed trigger to initiate a series of conventional reactions was demonstrated to have advantages for enantioselective synthesis. It is evident from the definitions in Article II of the Convention that the term “toxic chemicals” includes *all such chemicals, regardless of their origin or of their method of production*. Consequently, production of toxic chemicals for illicit purposes is prohibited by synthetic routes that include biochemical steps, as well as those that do not. The significance of this concept should be fully understood as plant design moves toward greater incorporation of biochemically based syntheses.

The advances in chemistry cited in the presentations offer new types of synthetic processes. Such processes open the possibility of new routes to well-known scheduled chemicals that would not start from the expected precursors. It is also evident that versatile multipurpose facilities are common in much of the fine chemicals business around the world and that batch facilities are potentially much more adaptable for the production of undeclared scheduled chemicals or other chemicals for use as chemical weapons than are the continuous processes used for commodity chemicals. These multipurpose facilities, due to requirements such as those for the purity of the product and minimizing maintenance costs, are using more expensive stainless steels, high-nickel steels, and enamel or glass-lined reactors—and, consequently, such corrosion-resistant equipment has some potential for chemical weapon agent production.

It is important that OPCW inspectors be aware of these rapidly changing process technologies and be alert to the implications. These technologies are more likely to appear in OCPFs around the world than in Schedule 2 and 3 facilities. “Walk-and-talk” inspections will be effective only if the inspectors are fully familiar with new technologies and what they look like. The inspectors also need to be fully aware of the ways in which scheduled and other toxic chemicals can be prepared in versatile multipurpose manufacturing facilities. It might be desirable to conduct training courses in The Hague that would update the Technical Secretariat and its inspectors on the developments in technologies seen by the States Parties as being important.

It is not an easy task in such a rapidly developing field to anticipate how and where new types of chemical plants will appear and for what purposes. It is, however, clear that the review of the overall verification regime for the chemical industry, including that for OCPFs, to be carried out at the First CWC Review Conference needs to take these new developments fully into account when recommending improvements.

In view of the rapid pace of developments in synthesis and production, there could be benefit from the OPCW convening a panel of experts, perhaps biennially, to review whether the new technologies could significantly increase the risks that prohibited activities could elude capture by the declaration and inspection procedures of the Convention.

#### *Do the Schedules require change?*

The discussions on new toxic chemicals and existing toxic chemicals that are not on the Schedules leads to questions about the need for modifications to the Schedules. Although there was some sentiment expressed at the Workshop toward adding substances, the participants recognized the many practical difficulties in obtaining agreement to make changes in the Schedules. Moreover, the potential for synthesis of new toxic materials will make it impossible to list all chemicals that might pose a threat. We believe, therefore, that with the scientific information now available, it may be too soon for the consideration of *broad* changes to the Schedules at the Review Conference.

Some specific changes in understandings relating to the Schedules might be desirable. In particular, one issue that was discussed at the Workshop was the current practice of regarding salts and their parent chemicals as totally different compounds. Thus, for example, saxitoxin is a Schedule 1 chemical defined by its Chemical Abstracts Services (CAS) number. Current practice is to regard the salts of saxitoxin as not being Schedule 1 chemicals because they do not have this CAS number, and, therefore, such salts do not need to be declared in the same way and transfer restrictions need not be applied. There is little chemical rationale for this distinction. In solution, a salt and its free base are both present, with equilibrium concentrations depending on the acidity of the solution. It seems inevitable that the distinction between the free base and the salt will cause anomalies among States Parties in the way they report such materials. There is a need to clarify the way in which the Schedules are interpreted in this respect.

## **II. Analytical techniques for routine inspections, challenge inspections, and investigations of alleged use**

### *Introduction*

A series of presentations at the Bergen Workshop reported on current developments in analytical science to enable the Workshop participants to discuss whether the application of such developments would be of value to the verification requirements of the Convention. Some of these dealt with current methodology, where modern instruments and data handling might permit almost immediate upgrades to the analytical capabilities of the Technical Secretariat. Other presentations focused on very promising technology that is still under development but might, over a longer period of probably more than 5–10 years, provide greatly improved sensitivity and specificity for analyses that could be important, particularly in challenge inspections or in instances of alleged use of chemical weapons.

### *Current and projected analytical instruments and techniques*

Several presentations at the Workshop pointed out that advances in GC/MS equipment since the specification of the OPCW instrument was approved by the States Parties have made it smaller and more portable. Flame photometric detectors for new GC equipment can be specific for chemicals containing certain elements (e.g., phosphorus or sulfur), thus facilitating the identification of scheduled chemicals even in the presence of other materials. The combination of liquid chromatography with flame photometric detection appears promising for analysis of soil samples. Micromulticapillary chromatography with ion-coupled plasma detection also affords element-specific detection even with nanogram quantities of chemical weapon agents. The portable isotopic neutron spectrometer (PINS) also permits element identification, but without the need for intrusive sampling. However, unlike GC/MS, it does not identify specific compounds. Advances in mass spectrometry have made the equipment more versatile, especially in dealing with relatively nonvolatile samples. Even proteins of moderate molecular weight are now characterized by matrix-assisted laser desorption into a mass spectrometer.

Looking ahead, several new spectroscopies are being tested for the identification of chemical weapon agents. These include polymer-based lanthanide fluorescence spectroscopy, surface acoustic wave (SAW) spectroscopy, and ion mobility spectroscopy. A portable version of the latter coupled with mass spectroscopy is being developed for characterization of agents and their identification products. Nuclear magnetic resonance (NMR) studies of intact cells using state-of-the-art spectrometers and new experimental protocols have shown NMR to be a valuable tool for understanding biological processes at a fundamental level. At some time in the future, it may be useful for detecting disruption of physiological processes by chemical weapon agents.

While many new chromatographic and spectroscopic methods show promise for detection of chemical weapon agents at low levels or in difficult sample matrices, the transition of such developments from the laboratory to rugged, field-portable instruments suitable for use by OPCW inspectors is a slow, expensive process. In two specific examples, development of field-ready instruments from already proven components cost about \$3 million and almost two years development time. Although the market for equipment specifically designed for OPCW use is too small to warrant commercial investment, national defense organizations are supporting a large amount of relevant development work. Instruments resulting from these efforts may or may not be adaptable to OPCW needs.

The topic of biosensors and immunoassays for both scheduled chemicals and new neurotoxins received much attention as a means for highly specific detection of chemical and biological weapon agents with simple portable devices. Immunoassays based on the immune response to proteins and glycoproteins are quick and very sensitive once the analytical system is set up, but the set-up time in the situations described was about four months. Detection by lanthanide fluorescence techniques is gradually replacing the use of radiolabels in this methodology. An immunoassay for the nerve agent sarin has been developed.

Other types of biosensors have been in use for some time in a national program and have been studied elsewhere. Typically in the detection of nerve agents, a specific enzyme such as an organophosphate hydrolase is used to hydrolyze the chemical weapon agent. The hydrolysis products such as acid may be quantified potentiometrically. Recently, the system has been adapted to a “lab-on-a-chip” device by coupling an enzyme such as acetylcholinesterase to a semiconductor-based detector. The detection is simple and rapid, but not exceptionally sensitive. In contrast, the use of an atomic force microscope as a detector for interactions with a surface-bound ligand has permitted the detection of even a single bacterium when applied to biological weapon agent detection.

Lab-on-a-chip devices are being developed for a great variety of applications because they offer exceptional sensitivity and can be used to characterize the minute quantities of products arising from combinatorial syntheses carried out on solid matrices. Sensitivities down the attomolar scale have been demonstrated with laser fluorescence detection or thermal lens microscopy. Practical use of these devices in the chemical weapon arena was estimated to be more than 10 years in the future. However, lab-on-a-chip developments merit careful monitoring by OPCW and other organizations with a requirement to identify chemical and biological weapon agents at very low levels.

### *General observations*

The following points were raised during wide-ranging discussions following the presentations:

- As new instruments and techniques are considered, it is important to recognize the very high sensitivity now available—in some techniques, the ultimate sensitivity of detecting a single molecule. At present, there appears to be no clear understanding of what is meant by “the absence of scheduled chemicals”. “Absence” cannot scientifically really mean “zero”. In practice, it presumably means that there is effectively no scheduled chemical present above some data point, usually an analytical detection limit. Also, a decision on an allowable limit can have considerable impact on the sensitivity required in the equipment used for carrying out the analysis. For on-site analysis, the requirement to use equipment that is easily deployed and is simple to use may mean that some sensitivity has to be sacrificed compared with some dedicated laboratory equipment.

The specifications for analytical technologies that would really make a difference are onerous in that the analytical equipment needs to be light and easily portable and be such that preliminary sample preparation and clean-up are not necessary to avoid transporting reagents and ancillary equipment and to reduce the time for analysis of each sample.

An appreciation of what absence means in different scenarios is critical to setting the analytical protocol. For example, for routine inspections of production facilities where the main purpose is to confirm the absence of scheduled chemicals that have not been declared, it is reasonable to assume that background levels of the scheduled chemicals, their precursors, by-products, or degradation products will be sufficiently high to permit identification in appropriately selected samples. This means that it is not necessary to resort to the procedures needed if the object was trace analysis to the limits of sensitivity for any particular technique. On the other hand, for example, where the samples could be of biological origin or have been obtained for analysis long after an alleged use, there may be a requirement to exploit the most sensitive of methods with very carefully controlled protocols.

- Currently, the principal items of analytical equipment approved for on-site routine inspections consist only of infrared spectroscopy and GC/MS, and these are usually to be used well within their sensitivity limits. The specifications of these particular approved instruments are probably still adequate for the purpose, but some of the equipment held by OPCW is becoming increasingly expensive to service, and these methods may not be the most appropriate for the analysis required.
- Although many new methods have good potential for application to the verification regime, they require careful validation for laboratory use. To develop them into robust and practical equipment for field use will require much time, effort, and money.
- There is a particular problem with samples of biological origin, which may arise from investigations of incidents of alleged use, since neither the OPCW Technical Secretariat nor many of the designated laboratories are capable of analyzing such samples for which the methodology may be highly specialized.
- There is little prospect in the short term of advances in analytical techniques changing the current situation, since many of the problems are procedural and logistical but providing newer GC/MS instrumentation to OPCW inspectors could facilitate their work.
- A particular problem is that methods for sample preparation and derivatization need improving.
- There is potential—but only in the longer term, probably 5–10 years—for lab-on-a-chip technology, perhaps with multiarray chip detectors based on immunoassay. Equally, immunoassays for a whole range of chemicals could be developed. Further, there remains some scope for miniaturization of mass spectrometric procedures. Some of these may reduce the requirement for clean-up and derivatization of samples.

The collection, handling, and analysis of samples form a central element of the Convention, and detailed requirements are included in the Convention itself or in the Verification Annex. Appendix 4 provides a number of extracts and comments regarding the criteria and limitations for the collection, handling, and analysis of samples under the CWC, many of which are based on the need for commercial confidentiality and national security. Differing requirements are applicable for routine inspections of facilities dealing with scheduled chemicals and for OCPFs. Challenge inspections and investigations of alleged use of chemical weapons trigger totally different approaches. Relevant points are summarized in the following sections.

#### *Routine inspections*

Although there are some specific requirements depending on the type of site being inspected, in general terms, inspectors are required to show that the facility activities they inspect are consistent with declarations. Only on Schedule 2 sites, however, is analysis specifically mandated to check for the absence (or presence) of undeclared scheduled chemicals. For Schedule 3 and OCPF sites, on-site

analysis is at the discretion of the inspectors, but removal of samples to a designated off-site laboratory requires the consent of the State Party being inspected.

The options open to inspectors for performing analyses are:

- **On-site analysis using equipment and facilities already present on-site.** Although OPCW believes that some Schedule 2 facility agreements may include provisions for use of on-site equipment, many will not, as many sites do not possess the necessary equipment since they are equipped only for process and quality control.
- **On-site analysis using equipment approved by States Parties.** The States Parties last approved the list of equipment in 1997, less than a month after entry into force of the Convention. Most of the approved analytical equipment held by the OPCW Technical Secretariat can no longer be considered state-of-the-art.

On-site sample preparation and clean-up is routinely required, which takes time and reagents and also requires appropriate ancillary equipment that also needs to be transported.

On Schedule 2 facilities, the Convention allows 96 h for the inspection, which is adequate time for analysis. However, for Schedule 3 facilities and OCPF's, only 24 h is allowed for inspections. This is insufficient time to carry out analysis without improvements in analytical methods and procedures.

For on-site analysis using GC/MS, the equipment is fitted with software that identifies any scheduled chemicals, precursors, side products, or breakdown products by reference to the OPCW database, which holds data on over 1000 compounds. There would seem to be advantages in using the equipment not only with the OPCW database, which could be extended as required, but also with some commercial databases that include agreed targeted substances. This procedure represents a very nonintrusive method of analysis that meets the purposes of the CWC without compromising commercial confidentiality.

Some scheduled chemicals, such as the toxins ricin and saxitoxin, are not so easily detected by GC/MS. Other potentially convenient methods for such toxins, such as immunoassay, are not currently on the list of approved equipment and may require further development and validation before they could be accepted.

- **Removal of samples for off-site laboratory analysis.** In situations where the inspectors deem it necessary to resolve an ambiguity, the Convention provides for samples to be sent off-site for analysis. (For inspections at Schedule 3 and OCPF sites, the agreement of the State Party is required.) There are many practical and logistical problems in selecting samples and perhaps in transporting them to designated laboratories. In addition, there are political problems since some countries are reluctant to allow samples off-site or out of the country. Also, once samples are sent to laboratories in several countries, there will always be concerns by industry that the analysis could be too intrusive and reveal information that is commercially confidential. For OCPF's, where the precise inventory of chemicals produced is not declared, off-site analysis is specifically included for addressing unresolved ambiguities, but this procedure is subject to approval by the inspected State Party.

Workshop participants noted that there is considerable question as to the importance of being able to carry out analyses on-site during routine inspections. The right of inspectors to take and analyze samples during routine inspections is an essential component of the Convention. It allows confidence to be gained that the activities being inspected are consistent with declarations and provides an incentive that declarations must be accurate. On the other hand, it appears that on bona fide sites any ambiguities found by inspectors appear to be readily clarified by cooperative site personnel. In practice, it appears that the inspectors rarely see the need for analysis since they are able in nearly all cases to satisfy themselves that the declarations are accurate by inspection of facilities and records. However, there will presumably be occasions, although perhaps not very frequent, when there are ambiguities that will require analysis for their resolution.

The power of modern analytical science is such that if it is used in such a way that its capabilities are fully utilized there is a high probability that all the requirements of the Convention could be achieved. However, particularly for routine inspections, the restrictions currently imposed because of concerns for national security and commercial confidentiality means that the full use of analytical capabilities will rarely be possible. Presumably, more comprehensive analyses could be done on-site if the limitations were altered to allow sufficient time to set up whatever equipment is deemed necessary and to deploy a team of analysts. Alternatively, sample removal with subsequent analyses in designated laboratories could achieve the same purpose, but this introduces more problems in relation to the chain of custody of samples, their transport, and the maintenance of confidentiality of results.

### *Challenge inspections*

Although the provisions for sampling and analysis are to some extent clearer than for routine inspections, since the inspection team has the right to take wipes, air, soil, or effluent samples as part of their perimeter activities, it is still necessary to negotiate with the inspected State Party what sampling and analysis is carried out within the agreed inspection perimeter. As no challenge inspections have yet been carried out, there is no past experience to guide the Technical Secretariat.

As the purpose of a challenge inspection is to clarify and resolve any questions concerning possible noncompliance with the provisions of the Convention, it would be expected in purely scientific terms that the inspecting team would be able to collect samples as necessary and have them analyzed as comprehensively as necessary. This almost certainly would require off-site analysis in at least two designated laboratories since the on-site equipment available to inspectors is limited to the equipment such as GC/MS used in routine inspections and mainly suitable for the scheduled chemicals except for the two toxins. Since equipment and protocols may differ between the designated laboratories, all the OPCW agreed standards of good laboratory practice need to be applied, and final identification may need to be by comparison with authentic compounds.

The area of challenge inspection is one in which some of the possible techniques such as immunoassay or multiarray sensors have much to offer since use of these devices could meet the needs of the challenge inspection without compromising security or commercial confidentiality. Were they to become available in the future, it would be valuable to consider protocols for their use in all forms of inspection.

### *Allegations of use*

In investigations of the alleged use of chemical weapons, the scenarios may vary from cases such as the Iran/Iraq conflict in the 1980s, when Iran invited UN experts to carry out investigations, to cases such as those in Laos and Cambodia in the early 1980s, where reports of suspicious attacks led to samples being collected and analyzed in several countries and the subsequent "Yellow Rain" hypothesis and controversy.

In the former situation, where there were clear indications and evidence from the attacks, OPCW teams of investigators would certainly be equipped with the latest monitoring equipment for chemical weapon agents. Some indication of the nature of agents used could be provided by medical observations. Mainly for confirmation purposes, environmental samples (from soil, water, and vegetation) and biological samples (such as urine, saliva, blood, and tissue) from victims of the attack would be taken for laboratory confirmation. In cases like the latter, where there was little indication or evidence of the nature of the attack, samples might be obtained for forensic-type laboratory analysis some significant time after the alleged attack took place.

We understand that the designated analytical laboratories, which have been taking part in OPCW proficiency exercises, are currently well placed to check environmental samples for scheduled chemicals and their degradation products. The situation is more problematic if toxins or other unscheduled chemicals are to be analyzed. Moreover, it appears that there are currently no laboratories set up to carry out broad-based general analyses of biological samples of the types indicated above. Several broadly applicable generic techniques were described at the Workshop, which may have considerable potential

but are still being developed. For example, NMR metabonomics (a technique that uses pattern recognition methods to compare normal and abnormal magnetic resonance spectra of biological samples) has been very successful with test samples, while immunoassay techniques for a small number of chemical weapon agents are beginning to appear. There could be an advantage in addressing in advance of any investigation precisely what data would be considered an unequivocal identification.

There are also some encouraging developments for identifying some biomarkers for scheduled chemicals such as sulfur mustards and nerve agents. Possible biomarkers have also been identified for phosgene, nitrogen mustards, and lewisite. At present, there are no laboratories accredited by OPCW for biomedical sample analysis. Care will need to be given to the criteria required for unequivocal identification.

Planning and preparations for investigations of alleged use of chemical weapons would probably benefit from closer links between the Technical Secretariat and public health services that are preparing contingency plans for countering terrorist attacks using chemicals in order to share information on best practices.

### **III. Technical capability of the Secretariat**

The Convention specifically directs that the paramount consideration for employment of staff is to secure the highest standards of efficiency, competence, and integrity. This competence must be assiduously maintained through study and practical experience. For example, routine inspections serve to maintain and enhance the capability of the Technical Secretariat.

Continuing priority attention should be devoted to the professional development of the Technical Secretariat. Given the rapid pace worldwide of developments in the screening of new unscheduled chemicals and in the development of new, more flexible production processes for chemicals, the Technical Secretariat must be kept up to date and have the necessary competence to take such developments into account in the implementation of the Convention. The pace of developments in information technology and the ability to handle large quantities of data will become increasingly relevant and important because the ability to detect trends in the development and production of chemicals will contribute to the strengthening of the CWC regime.

This professional development of the Technical Secretariat should extend also to having a knowledge and awareness of the developments in analytical equipment capabilities and techniques, notably in sampling and analysis relevant to the Convention. Regular use of these techniques during routine inspections can serve to maintain the competence of the inspectorate.

It is important that the States Parties also are kept up to date with new developments so they can understand the need for adopting a very flexible approach to the implementation of the Convention.

Providing an appropriate level of professional development and current awareness will require the allocation of adequate resources by OPCW. Virtually all organizations heavily dependent on science and technology—industrial, academic, and governmental—have learned over decades that such investments are essential and usually pay large dividends in performance and output. Consideration should be given to drawing up a plan for ongoing training for Secretariat staff and for organizing periodic workshops for OPCW and States Parties to review the relevant scientific and technological developments. The OPCW Scientific Advisory Board represents a valuable international scientific resource that could be used to plan and organize such activities. IUPAC and other relevant international organizations might be consulted for advice and technical assistance as appropriate.

### **IV. Education and outreach**

At the Workshop, all discussion groups independently reached the conclusion that greater efforts should be made in education and outreach to various audiences, ranging from the States Parties and their National Authorities to non-States Parties and to the worldwide scientific community. In this respect,

an informed scientific and technical community within each country can be very helpful in providing advice and disseminating information to the public. IUPAC, together with its National Adhering Organizations, can play an important role in this education and outreach program by working in cooperation with the National Authorities within the individual States Parties to enhance awareness by chemists of the obligations and undertakings of the Convention. A parallel approach could usefully be taken worldwide by chemical industry associations in cooperation with National Authorities. In due course, chemical weapon prohibition and nonproliferation considerations may even be incorporated into university and school curricula as part of chemistry education in a similar way to that in which environmental issues, ethics of genetics, and similar issues have been incorporated into chemistry and biology education in the recent past.

Education and outreach is also important in the context of the promotion of the universality of the Convention. The CWC currently has 145 States Parties, 29 Signatory States—who have signed the Convention but have yet to ratify the Convention and thus implement it—and 20 non-Signatory States. Some of the Signatory and non-Signatory States may not have ratified or acceded to the Convention because of a lack of awareness of the benefits that the Convention brings.

## V. Destruction of chemical weapons

During the first five years of CWC implementation, the resources of the Technical Secretariat have been predominantly devoted to the monitoring and verification of the destruction of chemical weapons and of chemical weapon production facilities in the four States Parties that have declared the possession of chemical weapons. The prediction is that the number of continuously operating chemical weapon destruction facilities will rise from the current 1–2 facilities to 12 by 2006, and that the current non-continuous chemical weapon destruction facilities will also rise from the current 4–6 facilities to 12 by 2006. It is likely to be impossible to carry out the verification of chemical weapons destruction using the current verification procedures with the current size of the inspectorate.

Although chemical weapon destruction technology was not a specific topic of the Workshop, the participants noted during the general discussion that advances in automation technology, coupled with the use of remote monitoring techniques, or approaches in which the destruction facility was effectively contained, enabling inputs and outputs to be monitored, appear to offer the potential of providing the same level of confidence in verification with the use of less manpower. Also, it was suggested that the risk to the Convention posed by less frequently monitored destruction of the declared chemical weapons stockpiles in the four States Parties may be sufficiently low as not to merit the current intensive verification regime. For example, analytical chemists, as well as others responsible for quality control measures, are familiar with the use of random sampling techniques, coupled with follow-up that targets areas that proved deficient. Another approach might be material balance verification. Although not examined in detail at the Workshop, less manpower-intensive verification of chemical weapon destruction facilities may be desirable.

The Workshop did not examine technologies for the destruction of chemical weapons, as IUPAC had recently published a 130-page technical report\* entitled “Critical Evaluation of Proven Chemical Weapon Destruction Technologies” in the February 2002 issue of *Pure and Applied Chemistry*. Copies of this report had been sent to OPCW and to each of the States Parties and were distributed to Workshop participants.

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\*G. S. Pearson and R. S. Magee. “Critical evaluation of proven chemical weapon destruction technologies”, *Pure Appl. Chem.* **74** (2), 187–316 (2002). Available at <<http://www.iupac.org/publications/pac/2002/pdf/7402x0187.pdf>>

**APPENDIX 1. INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY (IUPAC)**

IUPAC\* serves to advance the worldwide aspects of the chemical sciences and to contribute to the application of chemistry in the service of mankind. As a scientific, international, nongovernmental, and objective body, IUPAC is able to and does address many global issues involving the chemical sciences. IUPAC was formed in 1919 by chemists from industry and academia. Over nearly eight decades, the Union has succeeded in fostering worldwide communications in the chemical sciences and in uniting academic, industrial, and public-sector chemistry in a common language. IUPAC has long been recognized as the world authority on chemical nomenclature, terminology, standardized methods for measurement, atomic weights, and many other critically evaluated data. The Union sponsors major international meetings that range from specialized scientific symposia to meetings with societal impact. IUPAC is an association of bodies, National Adhering Organizations, which represent the chemists of different member countries. There are 44 National Adhering Organizations\*\*, and 20 other countries are also linked to IUPAC in the status of Associate National Adhering Organizations‡.

IUPAC is the largest of 26 Scientific Unions associated with the International Council for Science (ICSU). Other unions include a number of general and specialized fields, but IUPAC is the only union dealing with chemistry as an overall science and in myriad applications.

**APPENDIX 2. IUPAC WORKSHOP: IMPACT OF SCIENTIFIC DEVELOPMENTS ON THE CHEMICAL WEAPONS CONVENTION****Summary Program****Sunday Evening, 30 June: Opening of the Workshop—Edwin D. Becker, Chairman**

John Gee, Acting Director-General, OPCW  
 Pieter Steyn, President, IUPAC  
 Leiv Sydnes, University of Bergen  
 Welcome Reception

**Monday Morning, 1 July: Claude Eon, Chairman*****Background and Context for the Workshop: The First Review Conference***

Background to the CWC and OPCW—John Gee, OPCW  
 Verification procedures—Ron Manley, OPCW, Retired  
 Responding to Chemical Terrorism: The Role of States Parties—Ralf Trapp, OPCW  
 Industry Changes for Enhanced Security—Marybeth Kelliher, American Chemistry Council

**Monday Afternoon, 1 July: George Parshall, Chairman*****New Developments in Chemical Synthesis***

Supported Synthesis and Improved Experimental Design—Mark Bradley, Southampton University  
 Chemical Crop Protection Research—Urs Müller, Syngenta  
 Catalysis for Organic Synthesis—Irina Beletskaya, Russian Academy of Sciences

\*About IUPAC. Available at <http://www.iupac.org/general/about.html>

\*\*The countries of the 44 National Adhering Organizations are: Argentina, Australia, Austria, Belgium, Brazil, Bulgaria, Canada, Chile, China, Croatia, Czech Republic, Denmark, Egypt, Finland, France, Germany, Greece, Hungary, India, Ireland, Israel, Italy, Japan, Korea, Kuwait, Netherlands, New Zealand, Norway, Pakistan, Poland, Portugal, Puerto Rico, Russia, Slovakia, Slovenia, South Africa, Spain, Sweden, Switzerland, Turkey, UK, USA, and Yugoslavia.

‡The 20 countries linked to IUPAC as Associate National Adhering Associations are: Albania, Bangladesh, Cuba, Cyprus, Estonia, Hong Kong, Latvia, Malaysia, Mexico, Peru, Philippines, Romania, Singapore, Sri Lanka, Tanzania, Thailand, Tunisia, Ukraine, Uruguay, and Vietnam.

***New Methods in Biological Synthesis of Chemical Compounds***

Biotechnology and Biochemical Weapons Development—Mark L. Wheelis, University of California, Davis  
Advances in Biocatalytic Synthesis—Kurt Faber, University of Graz

**Tuesday Morning, 2 July: Detlev Maennig, Chairman*****New Developments in Processing and Manufacturing***

Manufacturing and Processing: An Overview—George Parshall, DuPont (retired)  
Chemical Processing Technologies—M. M. Sharma, University of Mumbai  
Advances in Microreactors—Holger Löwe, University of Mainz

***Breakout Session #1***

Discussion Group Chairmen / Co-chairmen: Graham S. Pearson / Krystin Kee; Claude Eon / Philip C. Coleman; Thomas D. Inch / Hector Paz; George W. Parshall / Minbo Chen

**Tuesday Afternoon, 2 July*****Analytical Techniques—Tom Inch, Chairman***

Current Conventional Analytical Methods—Herbert Hill, Washington State University  
Parameters for Field-Portable Trace Detection Equipment: Transitioning Analytical Instrumentation from the Lab to Harsh Environments—Robert Turner, Graseby Dynamics  
NMR-Based Metabonomic Approaches to the Investigation of Toxic Processes—Jeremy Nicholson, Imperial College  
Possible Use of System Analysis and Knowledge-based Tools for Monitoring Advanced Chemical Activities Potentially Challenging the Chemical Weapons Convention—Ferenc Darvas, ComGenex, Inc.

***Breakout Session #2*****Wednesday Morning, 3 July: Boris Myasoedov, Chairman*****Analytical Techniques, Continued***

Organic Mass Spectrometric Techniques—Johanna Szpunar, CNRS EP 132  
Clean-up Methods and Separations—Maria Luque de Castro, University of Cordova  
Immunoassay/Biological Analytical Techniques—Richard Venn, Pfizer  
Biosensors for Quantitation of Neurotoxins of Various Classes, Including Chemical War Agents, and Biocatalytic Technologies for Their Destruction—S. D. Varfolomeyev, Lomonosov Moscow State University  
Lab on a Chip—Takehiko Kitamori, University of Tokyo

**Wednesday Afternoon, 3 July: Issues for the IUPAC Report to OPCW and the First Review Conference*****Breakout Session #3******Reports from Discussion Groups******Final Discussion, Conclusions, and Recommendations—Alan Hayes, Chairman***

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## APPENDIX 3. THE CHEMICAL WEAPONS CONVENTION

### Introduction

The Chemical Weapons Convention (CWC)\* totally prohibits the development, production, acquisition, stockpiling, or retention of chemical weapons. It defines chemical weapons as meaning the following, together or separately:

- (a) *Toxic chemicals and their precursors, **except where intended for purposes not prohibited under this Convention, as long as the types and quantities are consistent with such purposes;** [Emphasis added]*
- (b) *Munitions and devices, specifically designed to cause death or other harm through the toxic properties of those toxic chemicals specified in subparagraph (a), which would be released as a result of the employment of such munitions and devices;*
- (c) *Any equipment specifically designed for use directly in connection with the employment of munitions and devices specified in subparagraph (b).*

The text in bold is referred to as the **general-purpose criterion**, which ensures that all toxic chemicals and their precursors are embraced by the Convention *except where intended for purposes not prohibited under the Convention*. Toxic chemicals are defined in the Convention as meaning:

*Any chemical which through its chemical action on life processes can cause death, temporary incapacitation or permanent harm to humans or animals. This includes all such chemicals, regardless of their origin or of their method of production, and regardless of whether they are produced in facilities, in munitions or elsewhere.*

All chemicals that can cause death, temporary incapacitation, or permanent harm to humans or animals are thus prohibited unless they are in types and quantities consistent with their intended uses for purposes not prohibited under the Convention, which are defined in the Convention as:

- (a) *Industrial, agricultural, research, medical, pharmaceutical or other peaceful purposes;*
- (b) *Protective purposes, namely those purposes directly related to protection against toxic chemicals and to protection against chemical weapons;*
- (c) *Military purposes not connected with the use of chemical weapons and not dependent on the use of the toxic properties of chemicals as a method of warfare;*
- (d) *Law enforcement including domestic riot control purposes.*

The CWC was opened for signature in January 1993 and entered into force on 29 April 1997, which was 180 days after the 65<sup>th</sup> State Party had deposited its instrument of ratification. In July 2002, the Convention has 145 States Parties\*\*.

Article VIII of the Convention, which establishes the Organization to achieve the object and purpose of the Convention, includes the requirement to undertake periodic reviews of the operation of the Convention:

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\*United Nations, *Convention on the Prohibition of the Development, Production, Stockpiling and Use of Chemical Weapons and on Their Destruction*, Corrected version in accordance with Depository Notification C.N.246.1994.Treaties-5 and the corresponding Process-Verbal of Rectification of the Original of the Convention, issued on 8 April 1994. Available at <<http://www.opcw.org/cwc/cwc-eng.htm>>

\*\*Organisation for the Prohibition of Chemical Weapons, *States Parties to the Chemical Weapons Convention*. Available at <[http://www.opcw.org/html/db/members\\_ratifyer.html](http://www.opcw.org/html/db/members_ratifyer.html)>

22. *The Conference shall not later than one year after the expiry of the fifth and the tenth year after the entry into force of this Convention, and at such other times within that time period as may be decided upon, convene in special sessions to undertake reviews of the operation of this Convention. Such reviews shall take into account any relevant scientific and technological developments. At intervals of five years thereafter, unless otherwise decided upon, further sessions of the Conference shall be convened with the same objective.*

It will be noted that such reviews are required to take into account “any relevant scientific and technological developments”.

In addition, Part IX of the Verification Annex to the Convention, which addresses the regime for other chemical production facilities, includes a requirement that:

26. *At the first special session of the Conference convened pursuant to Article VIII, paragraph 22, the provisions of this Part of the Verification Annex shall be re-examined in the light of a comprehensive review of the overall verification regime for the chemical industry (Article VI, Parts VII to IX of this Annex) on the basis of the experience gained. The Conference shall then make recommendations so as to improve the effectiveness of the verification regime.*

It is consequently evident that the First Review Conference is required to carry out a comprehensive review of the overall verification regime for the chemical industry in order to re-examine the provisions for other chemical production facilities and to make recommendations so as to improve the effectiveness of the verification regime.

The regime for the chemical industry is specified in Article VI of the Convention, which addresses “Activities Not Prohibited under this Convention”. The key requirement is stated in paragraph 2 that:

2. *Each State Party shall adopt the necessary measures to ensure that toxic chemicals and their precursors are only developed, produced, otherwise acquired, retained, transferred, or used within its territory or in any other place under its jurisdiction or control for purposes not prohibited under this Convention. To this end, and in order to verify that activities are in accordance with obligations under this Convention, each State Party shall subject toxic chemicals and their precursors listed in Schedules 1, 2 and 3 of the Annex on Chemicals, facilities related to such chemicals, and other facilities as specified in the Verification Annex, that are located on its territory or in any other place under its jurisdiction or control, to verification measures as provided in the Verification Annex.*

The Convention in its Annex on Chemicals assigns chemicals judged to present a risk to the Convention into three Schedules according to the following criteria:

#### **Guidelines for Schedule 1**

1. *The following criteria shall be taken into account in considering whether a toxic chemical or precursor should be included in Schedule 1:*
  - (a) *It has been developed, produced, stockpiled or used as a chemical weapon as defined in Article II;*
  - (b) *It poses otherwise a high risk to the object and purpose of this Convention by virtue of its high potential for use in activities prohibited under this Convention because one or more of the following conditions are met:*

- (i) *It possesses a chemical structure closely related to that of other toxic chemicals listed in Schedule 1, and has, or can be expected to have, comparable properties;*
  - (ii) *It possesses such lethal or incapacitating toxicity as well as other properties that would enable it to be used as a chemical weapon;*
  - (iii) *It may be used as a precursor in the final single technological stage of production of a toxic chemical listed in Schedule 1, regardless of whether this stage takes place in facilities, in munitions or elsewhere;*
- (c) *It has little or no use for purposes not prohibited under this Convention.*

**Guidelines for Schedule 2**

2. *The following criteria shall be taken into account in considering whether a toxic chemical not listed in Schedule 1 or a precursor to a Schedule 1 chemical or to a chemical listed in Schedule 2, part A, should be included in Schedule 2:*
- (a) *It poses a significant risk to the object and purpose of this Convention because it possesses such lethal or incapacitating toxicity as well as other properties that could enable it to be used as a chemical weapon;*
  - (b) *It may be used as a precursor in one of the chemical reactions at the final stage of formation of a chemical listed in Schedule 1 or Schedule 2, part A;*
  - (c) *It poses a significant risk to the object and purpose of this Convention by virtue of its importance in the production of a chemical listed in Schedule 1 or Schedule 2, part A;*
  - (d) *It is not produced in large commercial quantities for purposes not prohibited under this Convention.*

**Guidelines for Schedule 3**

3. *The following criteria shall be 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;*
  - (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.*

#### APPENDIX 4. CONVENTION REQUIREMENTS FOR SAMPLING AND ANALYSIS

The collection, handling, and analysis of samples form a central element of the CWC. In the Verification Annex, Part II General Rules of Verification, seven paragraphs set out the general rules relating to collection, handling, and analysis of samples. These include the following:

52. *Representatives of the inspected State Party or of the inspected facility shall take samples at the request of the inspection team in the presence of inspectors. If so agreed in advance with the representatives of the inspected State Party or of the inspected facility, the inspection team may take samples itself.*
53. *Where possible, the analysis of samples shall be performed on-site. The inspection team shall have the right to perform on-site analysis of samples using approved equipment brought by it. At the request of the inspection team, the inspected State Party shall, in accordance with agreed procedures, provide assistance for the analysis of samples on-site. Alternatively, the inspection team may request that appropriate analysis on-site be performed in its presence.*
54. *The inspected State Party has the right to retain portions of all samples taken or take duplicate samples and be present when samples are analysed on-site.*
55. *The inspection team shall, if it deems it necessary, transfer samples for analysis off-site at laboratories designated by the Organization.*
56. *The Director-General shall have the primary responsibility for the security, integrity and preservation of samples and for ensuring that the confidentiality of samples transferred for analysis off-site is protected.... He shall:*
  - (a) *Establish a stringent regime governing the collection, handling, transport and analysis of samples;*
  - (b) *Certify the laboratories designated to perform different types of analysis;*
  - (c) *Oversee the standardization of equipment and procedures at these designated laboratories, mobile analytical equipment and procedures, and monitor quality control and overall standards in relation to the certification of these laboratories, mobile equipment and procedures; and*
  - (d) *Select from among the designated laboratories those which shall perform analytical or other functions in relation to specific investigations.*
57. *When off-site analysis is to be performed, samples shall be analysed in at least two designated laboratories....*
58. *The Technical Secretariat shall compile the results of the laboratory analysis of samples relevant to compliance with this Convention and include them in the final inspection report....*

It is important to note that these general provisions take precedence unless specifically modified by the provisions governing the individual types of inspections.

Sampling and analysis has a specific role to play in regard to the verification activities relating to the activities not prohibited under the Convention in accordance with Article VI. The provisions are different depending on the inspection being carried out:

- a. **The regime for Schedule 2 chemicals.** Part VII of the Verification Annex in a section on *Inspection procedures* states that:

27. *Sampling and analysis shall be undertaken to check for the absence of undeclared scheduled chemicals.*
- b. **The regime for Schedule 3 chemicals.** Part VIII of the Verification Annex in a section on *Inspection procedures* states that:
27. *Sampling and on-site analysis may be undertaken to check for the absence of undeclared scheduled chemicals. In case of unresolved ambiguities, samples may be analyzed in a designated off-site laboratory, subject to the inspected State Party's agreement.*
- c. **The regime for other chemical production facilities.** Part IX of the Verification Annex in a section on *Inspection procedures* states that:
19. *Sampling and on-site analysis may be undertaken to check for the absence of undeclared scheduled chemicals. In case of unresolved ambiguities, samples may be analysed in a designated off-site laboratory, subject to the inspected State Party's agreement.*
- d. **The regime for challenge inspections.** Part X of the Verification Annex includes several provisions for the use of sampling and analysis that include:
- i. Exit monitoring procedures, as agreed by the inspection team and the inspected State Party may include, inter alia:
- (c) *Sample analysis.*
- ii. In conducting perimeter activities, the inspection team shall have the right to:
- (b) *Take wipes, air, soil or effluent samples;*
- iii. The particular inspection activities, *including sampling*, within the site shall be negotiated by the inspection team and the inspected State Party. In addition, the inspected State Party shall have the right to take measures to protect sensitive installation and prevent disclosure of confidential information and data not related to chemical weapons. Such measures may include, inter alia:
- (e) *Restriction of sample analysis to the presence or absence of chemicals listed in Schedules 1, 2 and 3 or appropriate degradation products.*
- e. **The regime for investigations in cases of alleged use of chemical weapons.** Part XI of the Verification Annex includes a section on sampling which states that:
16. *The inspection team shall have the right to collect samples of types, and in quantities it considers necessary. If the inspection team deems it necessary, and if so requested by it, the inspected State Party shall assist in the collection of samples under the supervision of inspectors or inspection assistants. The inspected State Party shall also permit and cooperate in the collection of appropriate control samples from areas neighbouring the site of the alleged use and from other areas as requested by the inspection team.*
17. *Samples of importance in the investigation of alleged use include toxic chemicals, munitions and devices, remnants of munitions and devices, environmental samples (air, soil, vegetation, water, snow, etc.) and biomedical samples from human or animal sources (blood, urine, excreta, tissue etc.).*

18. *If duplicate samples cannot be taken and the analysis is performed at off-site laboratories, any remaining sample shall, if so requested, be returned to the inspected State Party after the completion of the analysis.*

It is consequently widely accepted that sampling and analysis have an important role to play in implementing the CWC. However, to date, with the exception of inspections at chemical destruction facilities, analytical results have only infrequently been obtained and used by OPCW in routine inspections although there have been trials of some procedures. Therefore, as there have also been no investigations of alleged use or challenge inspections there is little case history to help define current needs.

Consideration of the above paragraphs of the Convention and other related paragraphs such as those on general rules for collecting and analyzing samples in paragraphs 52 to 58 of Part II of the Verification Annex leads to the following summary of the provisions in the Convention:

- a. **For routine inspections**, sampling and analysis **shall** (for Schedule 2 facilities) and **may** (for Schedule 3 and OCPF facilities) be undertaken to check for the absence of undeclared scheduled chemicals. Should there be unresolved ambiguities, then samples may be analyzed in a designated off-site laboratory. However, for Schedule 3 and OCPF facilities, such off-site analysis is subject to the inspected State Party's agreement. Routine inspection sampling and analysis may be carried out on-site either using approved equipment brought by the inspection team, or, if so requested by the inspection team, carried out by the inspected facility. Off-site analysis at a designated laboratory is not explicitly ruled out by the Convention—although the Convention does state that *where possible, the analysis of samples shall be performed on-site*— and off-site analysis is specifically included for addressing unresolved ambiguities.
- b. **For challenge inspections**, sampling and analysis within the agreed perimeter is to be negotiated by the inspection team and the inspected State Party. It is evident that sampling may include the taking of samples as well as wipes, air, soil, or effluent samples. Although not explicitly stated, the expectation would be that samples would be analyzed off-site by at least two designated laboratories because of the importance to the Convention regime of obtaining accurate analytical results and ensuring freedom from possible cross-contamination.
- c. **For investigation of alleged use**, samples can be collected in the types and quantities as considered necessary by the inspection team, recognizing that samples may include toxic chemicals, munitions and devices, remnants of munitions and devices, environmental samples (air, soil, vegetation, water, snow, etc.) and biomedical samples from human or animal sources (blood, urine, excreta, tissue, etc.). Although not explicitly stated, the expectation would be that samples would be analyzed off-site by at least two designated laboratories because of the importance to the Convention regime of obtaining accurate analytical results and ensuring freedom from possible cross-contamination.

Sampling and analysis are part of the on-site verification provisions in the Convention, which are required under Article VI to be carried out in accordance with the following provisions:

9. *For the purpose of on-site verification, each State Party shall grant to the inspectors access to facilities as required in the Verification Annex.*
10. *In conducting verification activities, the Technical Secretariat shall avoid undue intrusion into the State Party's chemical activities for purposes not prohibited under this Convention and, in particular, abide by the provisions set forth in the Annex on the Protection of Confidential Information (hereinafter referred to as "Confidentiality Annex").*