OPCW

Scientific Advisory Board

SAB-IV/1
6 February 2001
Original: ENGLISH

REPORT OF THE FOURTH SESSION OF THE SCIENTIFIC ADVISORY BOARD

1. Introduction

1.1 The Scientific Advisory Board (hereinafter the "Board") met for its fourth session from 5 - 6 February 2001 in The Hague.

1.2 The proceedings of the Board were directed by its chairman, Claude Eon of France.

1.3 The list of participants is contained in annex 1 to this report.

1.4 The Board adopted the following agenda:

(a) Opening and adoption of the agenda

(b) Information on the status of the Board's recommendations submitted during its third session in 2000

(c) Analytical procedures

(d) Low concentration limits for Schedule 2A and 2A* chemicals

(e) Biomedical samples

(f) Information on the status of work of the other temporary working groups

(g) Preparations for the 2003 Review Conference

(h) Extension of the terms of office of Board members

(i) Any other business

(j) Adoption of the report and closure of the fourth session of the Board

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2. Results of the work of the Board's temporary working groups - recommendations and observations

Concentration limits for Schedule 2A and 2A* chemicals

2.1 The issue of low concentration limits for Schedule 2A and 2A* chemicals was referred to the Board by the Conference of the States Parties, in its decision C-V/DEC.19, dated 19 May 2000. A temporary working group was accordingly formed, which met in The Hague from 30 - 31 August 2000. The group's recommendations were recorded in the report contained in annex 2 to this report.

2.2 The Board discussed the findings of the above-mentioned temporary working group. It observed that the issue at stake is not in fact of a scientific nature, but is regulatory, and commented that scientific advice can indicate to the decision-makers which concentration limits would be appropriate for what regulatory purpose, and that any decision on this issue remains outside the realm of science.

2.3 With this consideration in mind, the Board endorsed the following conclusions of the temporary working group:

(a) in relation to amiton, any decision on a concentration limit for mixtures containing that chemical in a low concentration can be based on regulatory considerations only. No specific concentration limit was proposed;

(b) in relation to BZ, if the objective of the regulator was to have the production of BZ as an intermediate and its subsequent in situ consumption declared and inspected - if the quantities of BZ exceed the relevant threshold, the concentration level should be set below 1%. Alternatively, no production of BZ as an intermediate would be declarable and inspectable unless the quantity of the raw materials used, which are listed in Schedule 2B, exceeded the thresholds for declaration or inspection respectively; and

(c) in relation to PFIB, the decision on a concentration limit has to be based on regulatory purposes, and not on scientific considerations per se. If the intention of the regulator is to regulate materials that could be diverted for CW purposes as they are, the concentration limit should be set somewhere above 10%. If, however, the intention of the regulator is to address the potential for diverting the material in order to *recover* PFIB for chemical weapons purposes, there should either be no concentration limit, or it should be set below 1%. The recovery of PFIB at that concentration level is, however, not normally considered feasible from an industrial point of view.

Analytical procedures

2.4 From 28 – 29 August 2000 the Board's temporary working group on analytical procedures met to discuss the issue of the possible inclusion in the OPCW Central Analytical Database of unscheduled chemicals. It had been requested to address this issue by the Director-General, who was following up on a recommendation made by

the Board during its third session. The recommendations of the temporary working group have been submitted to the Board in the report contained in annex 2 to this report.

2.5 The Board reviewed these recommendations and endorsed in principle the inclusion of the spectra of certain unscheduled chemicals. The Board submitted the following conclusions to the Director-General:

(a) the spectra of certain non-scheduled chemicals should be incorporated into the Central OPCW Analytical Database, primarily to assist analysis in challenge inspections or for investigations of alleged use. The selection of data for on-site analysis should be done in accordance with the purpose of sampling and analysis during an inspection. The addition of such data could also expand the analytical capabilities of the designated laboratories. The following groups of non-scheduled chemicals, prioritised in the following sequence, should be considered for inclusion:

(i) non-scheduled degradation products of scheduled chemicals;

(ii) riot control agents and old/abandoned chemical weapons;

(iii) salts of scheduled chemicals; and

(iv) non-scheduled precursors and byproducts of the synthesis of scheduled chemicals;

(b) the general principles for the possible inclusion of non-scheduled chemicals in the Central OPCW Analytical Database for the various groups of non-scheduled chemicals and riot control agents should be those contained in paragraphs 5 and 6 of the report of the temporary working group. In addition, the Board recommended that only spectra of unscheduled chemicals that are not widely used in the chemical industry should be incorporated, in order to facilitate the protection of confidentiality, and also in order to avoid false-positive detection; and

(c) the lists of chemicals proposed by the temporary working group were reviewed. The Board endorsed them in principle, and identified those compounds that should be incorporated into the OPCW Central Analytical Database with the highest priority. These compounds are contained in annex 4 to this report.

Other temporary working groups

2.6 The Board continued its consideration of issues related to CW destruction technologies, inspection equipment, and biomedical samples.

2.7 In relation to equipment, the Board noted that the survey conducted by the chairman of the temporary working group in relation to instrumentation for on-site analysis that is currently available confirms that the OPCW-approved equipment is state of the art.

On the issue of reducing the numbers of inspectors required for permanent monitoring at CW destruction sites, the approach developed within the Secretariat was considered sound. The temporary working group will continue monitoring developments in relation to available instrumentation, but will not in the near future address any specific additional tasks. It will be involved at a later stage when additional CW destruction facilities come on line.

2.8 In relation to destruction technologies, the Board was informed that a comprehensive review of presently available and proven CW destruction technologies has almost been completed, in the context of the respective IUPAC working group. When available, this review will provide a sound basis for the future work of the temporary working group. As far as the preparation by members of the temporary working group is concerned of a brochure on CW destruction technologies, the Board was informed that this is by and large completed, short of some final discussions, as well as editing and arrangements for publishing it. In relation to the meeting on the destruction of ACW proposed by the temporary working group, no final decisions on time and venue have been taken, but it appears highly unlikely that the meeting can be convened during this year.

2.9 In relation to biomedical samples, the Board received a briefing on the background of the issue, as well as on the results of an expert meeting that took place in December 1999, and on the proposed content of a questionnaire that the Secretariat intends to send to Member States regarding their current abilities for the handling and analysis of biomedical samples.

2.10 A temporary working group of the Board will be established by the Director-General soon, to address the following issues:

(a) provide an assessment of the OPCW's current ability to provide meaningful results from samples of biomedical origin in the context of an investigation of alleged use of chemical weapons; and

(b) provide an estimate of the resource implications that would be involved in establishing an ability for the handling and analysis of biomedical samples that is comparable with the current ability for handling and analysing environmental and chemical samples.

2.11 The members of the Board will discuss the issues raised in relation to biomedical samples with the appropriate experts in their countries, and will propose suitable candidates for possible appointment as members of this new temporary working group.

First CWC Review Conference

2.12 The Board continued discussing its involvement in the preparations for the First CWC Review Conference to be convened in accordance with paragraph 22 of Article VIII of the Convention. It was informed of the contacts in this respect with the Secretary-General and the President of the International Union of Pure and Applied Chemistry (IUPAC), and of the wish of IUPAC to contribute to the review of relevant

scientific and technical developments in preparation for the Review Conference. The Board discussed the procedural side of this cooperation, and asked both Thomas Inch and Will Carpenter to liaise on its behalf with the IUPAC leadership. It also discussed how National Academies of Sciences may be involved in this process, and agreed that Board members will have to play a crucial role in involving and assisting these academies.

2.13 In relation to the kinds of scientific developments that should be looked into in preparation for the Review Conference, the Board considered it particularly relevant to identify scientific developments that could have a bearing on the scope of the Convention, or that would affect its effective implementation. The Board noted that, in terms of methodology, it will assess developments in science and technology over the past decade or so, in relation to how they impact on the main provisions of the Convention.

2.14 In relation to the Convention's scope, and in this context also to both the definition of chemical weapons and the problem of potential new threats, the Board felt that it was important for developments in, inter alia, the following areas of science to be reviewed: toxicology, pharmacology, molecular genetics, genetic engineering, and receptor research. While research in these areas is being conducted with the aim of improving human health, it may also lead to scientific insight that could have a direct bearing on the scope of the Convention. The Board also felt that some of the issues that it had addressed in the past might be taken up again in this context, for example in relation to the coverage of salts of scheduled chemicals.

2.15 As far as chemical production methods are concerned, the Board agreed that biosynthesis and process technology including some emerging methods of chemical synthesis (e.g. solid phase chemistry) should be reviewed. In this context, it will also be important to study whether and how scientific developments affect the interface between the Convention and the Biological and Toxin Weapons Convention, for example with respect to toxins and related molecules.

2.16 In relation to the effective implementation of the Convention, such areas as destruction technologies, analytical chemistry, bioassays, remote sensing, and the miniaturisation of instrumental analysis, including the use of biosensors and nano-technology, should be included in the review.

3. Other matters

3.1 During the Board's proceedings the question of whether and how depleted uranium relates to the provisions of the Chemical Weapons Convention was raised.

3.2 The Board confirmed Claude Eon of France as its Chairman and Will Carpenter of the United States of America as its Vice-Chairman.

3.3 The first term of office of the present members of the Scientific Advisory Board will expire in the summer of 2001. In accordance with the terms of reference of the Scientific Advisory Board (Conference decision C-II/DEC.10, dated 5 December 1997), it is possible to renew the membership of a Board member once.

The Board was informed that, in the interest of continuity, and in particular bearing in mind that the preparations for the 2003 Review Conference will require a significant contribution by the Board, the Director-General has decided to offer a second term to all those current members of the Board who are willing to continue. The Director-General will soon initiate the process of identifying candidates for the seats on the Board that will become vacant in mid-2001.

4. Closure of the meeting and adoption of the report

The Board adopted this report, and closed its meeting at 15:45 on 6 February 2001.

Annexes (English only):

Annex 1: List of participants in the fourth session of the Scientific Advisory Board
Annex 2: Report of the temporary working group of the OPCW Scientific Advisory Board on low concentration limits for Schedule 2A and 2A* chemicals
Annex 3: Third report of the temporary working group of the OPCW Scientific Advisory Board on analytical procedures
Annex 4: Priority of data to be obtained for the Central OPCW Analytical Database

Annex 1

LIST OF PARTICIPANTS IN THE FOURTH SESSION OF THE SCIENTIFIC ADVISORY BOARD

Claudio **Costa Neto**	Brazil
A. K. **Datta**	India
Claude **Eon**	France
Alfred **Frey**	Switzerland
Shintaro **Furusaki**	Japan
Tom. D. **Inch**	UK
Li Weimin	China
Consuelo **Lopez-Zumel**	Spain
Gerhard **Matz**	Germany
Brahim Youcef **Meklati**	Algeria
Giorgio **Mondena**	Italy
Erno **Pungör**	Hungary
Marjatta **Rautio**	Finland
Burkhard **Seeger**	Chile
Abbas **Shafiee**	Iran
Theodoros **Solomon**	Ethiopia
Branko **Stanovnik**	Slovenia
Eric **Wils** (observer)	The Netherlands Chairman, Validation Group for the OPCW Central Analytical Database

Annex 2

REPORT OF THE TEMPORARY WORKING GROUP OF THE OPCW SCIENTIFIC ADVISORY BOARD ON LOW CONCENTRATION LIMITS FOR SCHEDULE 2A AND 2A* CHEMICALS

31 August 2000

1. Introduction

1.1 The Temporary Working Group on low concentration limits for Schedule 2A and Schedule 2A* chemicals of the OPCW Scientific Advisory Board (hereinafter "the group") met from 30 - 31 August 2000 in The Hague to discuss "all relevant aspects of the applicable concentration limits for mixtures of chemicals containing Schedule 2A and 2A* chemicals". This is the report on its deliberations and conclusions.

1.2 Dr Will Carpenter of the United States of America chaired the proceedings of the group.

1.3 The list of participants is contained in the appendix to this report.

2. Background

2.1 The Director-General, following the decision of the Conference of the States Parties as contained in document C-V/DEC.19 dated 19 May 2000, requested the SAB to study "all relevant aspects of the applicable concentration limits for mixtures of chemicals containing Schedule 2A and 2A* chemicals and to report the results for his submission to the Executive Council for consideration with a view to a decision being submitted for the consideration of States Parties at the Sixth Session of the Conference of the States Parties". Following this request, the temporary working group was formed.

2.2 The temporary working group was aware of the view taken by chemical industry associations worldwide that there is a preference in industry to regulate all mixtures containing Schedule 2 chemicals or Schedule 3 chemicals in the same way (i.e., setting the concentration limit at 30 per cent) unless there is scientific evidence that mixtures with a lower concentration of such a chemical pose a risk to the object and purpose of the Convention.

2.3 As there are only three chemicals listed in Part A of Schedule 2, the group was in a position to discuss them one by one. The group, in particular, addressed the actual situation in relation the manufacturing and uses, if any, of these chemicals. The group did not attempt to develop proposals that would be strictly in the regulatory domain, but instead limited its deliberations to issues that are of a scientific or technical nature.

3. Amiton

3.1 Amiton (chemical name O,O-diethyl S-[2-diethylamino)ethyl] phosphorothiolate, CAS registry number 78-53-5) is a compound which inhibits the cholinesterase, thus showing insecticide properties as well as being toxic to mammals. It was developed as an insecticide during the 1950ies, but given its high acute toxicity to man, to the best knowledge of the group it is no longer in commercial production or use. It's lethal dose is given as 0.5 mg/kg (oral, human) and 5.4 mg/kg (oral, rat).[1]

3.2 Amiton appears to be available through commercial channels in small quantities, apparently for research purposes. The group was, however, not aware of any production or uses of this chemical that would exceed quantities typical for research purposes, or that would exceed the declaration threshold stipulated in Part VII of the VA.

3.3 The group thus concluded that, from a strict scientific or industrial perspective, a decision on the concentration limit for Amiton would have no impact in practice, whatever the chosen concentration limit would be. A decision can thus be based exclusively on regulatory considerations.

4. BZ

4.1 BZ (chemical name 3-Quinuclidinyl benzilate, CAS registry number 6581-06-2) is a chemical compound with anticholinergic properties acting on the CNS. It has been weaponised in the past as an incapacitating agent. At dosages of 0.01 mg/kg or higher, it causes severe psychic disorders that can last for several days. Air dispersions at very low concentrations cause perception disorder, visual and auditory hallucinations, and temporary incapacitation. At high dosages, BZ intoxication can be fatal (above 10 mg/kg). BZ is easily absorbed by inhalation, through the skin or orally.[2] Its LD_{50} in mice is given as 25 mg/kg.[3]

4.2 BZ is an intermediate in the manufacturing of Clidinium Bromide, an active pharmaceutical ingredient with anticholinergic activity at the peripheral nervous system. The group is not aware of any other commercial-scale production of BZ, whether as an intermediate or final product.

4.3 In the manufacture of Clidinium Bromide, the intermediate BZ is produced from 3-hydroxy quinuclidine and methyl benzilate. The concentration of BZ in the process mixture reaches a maximum of approximately 10 weight per cent. It is the primary component in the process solution. BZ is not isolated, however, but used captively. The BZ solution remains in the reaction vessel and is *in situ* reacted with methyl bromide to form the final product (Clidinium Bromide). The final product is then separated from the solution and purified. The concentration of BZ in the final product after purification is less than 0.03 %.

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1 Chemical Weapons Convention Verification: Handbook on Chemicals, Canada August 1993.

2 Information taken from BZ Technical Sheet, Laboratori MAG Milano Italy, BZ MSDS.

3 Chemical Weapons Convention Verification: Handbook on Chemicals, Canada August 1993.

4.4 It appears from declarations received from those States Parties which have regulated concentration limits for mixtures containing BZ below a few % that the quantities of BZ manufactured and subsequently consumed are in the order of tonnes per year on average, clearly in excess of the declaration threshold of 1 kg per annum.

4.5 The group noted that BZ is produced from another Schedule 2 chemical, quinuclidin-3-ol, which is reacted with methyl benzilate (2,2-Diphenyl-2-hydroxyacetic acid methylester). The latter is usually made from 2,2-Diphenyl-2-hydroxyacetic acid, also a Schedule 2B chemical. The group also noted, however, that the applicable declaration and verification thresholds for BZ on the one hand, and for quinuclidin-3-ol as well as 2,2-Diphenyl-2-hydroxyacetic acid on the other, vary by a factors of one thousand.

4.6 A decision on the concentration limit for BZ should be driven by the regulatory purpose as established under the Convention. If a concentration level of 30 % would be set, any BZ production as an intermediate in the manufacture of Clidinium Bromide would remain outside the requirements for declaration and inspection unless the quantities of the precursor chemicals used would exceed the respective thresholds for Schedule 2B chemicals. Alternatively, the regulatory objective could be to have the total production of BZ as an intermediate in the manufacture of Clidinium Bromide declared and inspected (when exceeding the respective threshold amounts), taking into account that BZ is the principle component in the process solution at the intermediate stage and could be removed from the reaction vessel and the solvent distilled off. If that were the regulatory purpose, any such solution containing BZ should be declared if the amount of BZ exceeds the declaration threshold, irrespective of its concentration. For practical reasons, it may still be necessary to set a concentration limit, which should then be below 1 %.

5. PFIB

5.1 PFIB (chemical name 1,1,3,3,3-pentafluoro-2-(trifuoromethyl)-1-propene, CAS registry number 382-21-8) is a chemical that is formed as an unavoidable byproduct in the production of tetrafluoroethene (TFE) and hexafluoropropene (HFP), both monomers used for the synthesis of flourocarbon polymers such as PTFE. Its acute (inhalative) toxicity is comparable to hydrogen cyanide.[4] An LCt_{50} of 0.5 ppm was reported for rats (single exposure). The 15-second LC_{50} was given as 361 ppm, the 10-minute LC_{50} as 17 ppm. Similarly high acute toxicity was also observed in other test animals (mice, rabbits, guinea pigs, cats), for additional data see the literature.[5]

5.2 PFIB itself has no uses. It is destroyed, either by thermal oxidation or by reacting it with methanol. The reaction product formed with methanol is then also destroyed by incineration. Occasionally, however, this reaction product is used in the manufacture of other chemical products. Plants producing TFE and/or HFP and generating PFIB as

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4 Chemical Weapons Convention Verification: Handbook on Chemicals, Canada August 1993

5 A review with these and other data was published by J Patocka and J Bajgar, "Toxicology of Perfluoroisobutene", The ASA Newsletter 1998, available at www.asanltr/ASANews-98/pfib.html

a byproduct are equipped with a dedicated incinerator (which however may also be used to destroy other materials from the plant site).

5.3 There are different processes in use for the production of TFE and HFP but essentially, they can be grouped into the following three categories:

(a) TFE production only, resulting in fairly low PFIB concentrations in the waste streams (the concentration at the outlet of the reactor is less than 0.1 per cent, the maximum concentration reached in the system may reach in the order of a few per cent);

(b) production of TFE and HFP and detoxification of PFIB with methanol: concentrations of PFIB at the reactor outlet are typically around 4 % but this concentration depends on a variety of factors and may be as high as 7-8 %. PFIB is removed by reaction with methanol. If that detoxification reaction is carried out after the separation of the monomer from the mixture, the PFIB concentration in the waste stream would temporarily increase. Upon completion of the reaction between PFIB and MeOH, its concentration can be neglected. The reaction product is normally incinerated;

(c) production of TFE and HFP without detoxification of the PFIB with methanol: the product is separated from the waste stream containing PFIB, which leads to an increase of the PFIB concentration in the waste stream that may reach as high as 55 weight %. This waste effluent is not stored or further treated but fed directly into an incinerator where PFIB is destroyed.

5.4 When addressing the issue of low concentration limits that should be applied to PFIB, the group concluded that any decision on this matter must be guided by the regulatory objectives. The decision should take scientific and technical aspects into account, and must be taken in the full knowledge of the implications, but can itself not be driven by scientific or technical considerations.

5.5 The group noted that while concentration levels of PFIB vary depending on the process used, the quantities of PFIB generated by the different producers of either TFE or HFP (or both) are in the same order of magnitude for equal amounts of monomer production. These PFIB amounts clearly exceed the declaration and inspection thresholds established in the Convention for Schedule 2A chemicals.

5.6 The group also noted that for CW purposes, quite large amounts of PFIB would be needed given its properties, and in concentrations clearly higher than a few per cent. If PFIB is contained in a process stream at a level of a few per cent or even less, further concentration would not normally be considered feasible from an industrial point of view.

5.7 If the objective of the regulator was to address the potential of *diverting process streams* containing PFIB in order to *directly* weaponise that material for CW purpose, concentrations of PFIB as they are reached in the production of HFP without the removal of PFIB with methanol would have to be considered relevant. Facilities using

this type of process, or facilities using other processes but with similar concentration levels of PFIB in the waste stream (around 50 % in weight) should be declared and inspected when the PFIB quantities exceed the respective threshold. There would, however, be little justification to declare and inspect facilities using the other types of processes, or facilities that only manufacture TFE, because the maximum concentration levels of PFIB in the process streams would still remain well below a level that would pose a risk to the object and purpose of the Convention. With this objective in mind, the concentration limit could be set anywhere above 10-15 %, and other considerations (e.g., risk perceptions, regulatory harmony, administrative impact) could drive the decision making process.

5.8 If, however, the regulatory objective was to address the potential of diverting process streams containing PFIB in order to *recover* PFIB and *then* weaponise it for CW purposes, it would be prudent not to establish a concentration limit at all (or to set it below 1 %), in order to capture all relevant facilities for declaration and inspection.

6. Summary and conclusions

6.1 In relation to Amiton, the group concluded that any decision on a concentration limit for mixtures containing that chemical in a low concentration can be based on regulatory considerations only. No specific concentration limit is proposed by the group.

6.2 In relation to BZ, the group concluded that if the objective of the regulator was to have the production of BZ as an intermediate and its subsequent in situ consumption declared and inspected, if the BZ quantities exceed the respective threshold, the concentration level should be set below 1 per cent. Alternatively, no production of BZ as an intermediate would be declarable and inspectable unless the quantity of the raw materials used, which are listed in Schedule 2B, would exceed the respective declaration threshold for declaration or inspection.

6.3 In relation to PFIB, the group wishes to stress that the decision on a concentration limit has to be based on the regulatory purposes, not on scientific considerations per se. If the intention of the regulator is to regulate materials that could be diverted for CW purposes as they are, the concentration limit should be set somewhere above 10 per cent. If, however, the intention of the regulator is to address the potential of diverting the material in order to *recover* PFIB for weapons purposes, there should be no concentration limit or it should be set below 1 %. The recovery of PFIB at that concentration level is, however, not normally considered feasible from an industrial point of view.

Appendix

LIST OF PARTICIPANTS

Will D. **Carpenter** Chairman of the TWG	USA
Claude **Eon** Chairman of the SAB	France
Marjatta **Rautio**	Finland
Abbas **Shafiee**	Iran
Claudio **Costa Neto**	Brazil
Alfred **Frey**	Switzerland
Tom. D. **Inch**	UK
Tom **Spoormaker**	The Netherlands
Masaaki **Okabe**	Japan
Hans-Josef **Staudt**	Germany
Paolo Luigi Biagio **Ricci**	Italy
Detlef **Männig**	Germany

* Theo Juurlink Verification Division, OPCW attended as observer

Annex 3

THIRD REPORT OF THE TEMPORARY WORKING GROUP OF THE OPCW SCIENTIFIC ADVISORY BOARD ON ANALYTICAL PROCEDURES
29 August 2000

1. The Temporary Working Group (hereinafter TWG) on Analytical Procedures of the Scientific Advisory Board met in The Hague on the 28 and 29 August 2000 to develop a list of non-scheduled chemicals whose spectra should be incorporated into the Central OPCW Analytical Database as a matter of priority. The meeting was chaired by Dr Marjatta Rautio of Finland. The list of participants is contained in appendix 1 to this report.

2. The TWG considered the following groups of non-scheduled chemicals and prioritised them in the following order:

   (a) non-scheduled degradation products of scheduled chemicals;
   (b) riot control agents and old/abandoned chemical weapons;
   (c) salts of scheduled chemicals;
   (d) non-scheduled precursors and by-products of synthesis of scheduled chemicals.

3. The extension of the Central OPCW Analytical Database with data on the above-mentioned chemicals is primarily to assist analysis in challenge inspections or for investigations of alleged use. Selection of data for on-site analysis should be done in accordance with the purpose of sampling and analysis during an inspection. The addition of these data could also expand the analytical capabilities of the designated laboratories.

4. The TWG elaborated on general principles for the possible inclusion of non-scheduled chemicals in the Central OPCW Analytical Database. These principles are presented here for the various groups of the non-scheduled chemicals and riot control agents.

5. Non-scheduled chemicals

5.1 For the non-scheduled degradation products, salts of scheduled chemicals, and non-scheduled precursors and by-products, the relation between these chemicals and the scheduled chemicals from which they are derived should be incorporated in the Central OPCW Analytical Database.

5.2 Non-scheduled degradation products of scheduled chemicals

5.2.1 The following principles are recommended for adding a non-scheduled degradation product of a scheduled chemical:

(a) the addition of non-scheduled degradation products must be limited to products derived from Schedule 1 and Schedule 2.A chemicals; and
(b) there must be a link through a chemical pathway between the degradation product and the scheduled chemical. This link is based on chemical reactions such as hydrolysis, oxidation or elimination; and
(c) the degradation product must still contain key structure elements of the scheduled chemical; and
(d) the degradation product of the scheduled chemical must have been detected and reported.

5.2.2 In addition to the degradation product its analytical derivatives, if applicable, should be added.

5.2.3 Based on these principles a number of chemicals listed in appendix 2 to this report were recommended for inclusion in the Central OPCW Analytical Database. The list should not be considered as exhaustive and should be expanded when new degradation products are reported.

5.3 Salts of scheduled chemicals

As many nitrogen containing scheduled chemicals are stored or used as their salts, data on protonated and alkylated salts are important to the analyst and therefore should be added to the database when they are not included in the schedule list. The salts are listed in appendix 3 to this report.

5.4 Non-scheduled precursors and by-products of synthesis of scheduled chemicals

During the synthesis of scheduled chemicals characteristic by-products may be formed. These by-products could be more stable than the original scheduled chemical and therefore may give a long-term indicator of the presence of the scheduled chemical. In addition, for the production of Schedule 1 and 2.A chemicals characteristic non-scheduled precursors could be used. The TWG discussed this item and recommends the inclusion of a number of these chemicals which are listed in appendix 4 to this report. The list should not be considered as exhaustive and should be expanded when new synthetic routes involving characteristic non-scheduled precursors are reported.

6. Riot control agents and old/abandoned chemical weapons

6.1 Riot control agents

6.1.1 The following principles are recommended for adding riot control agents (as defined in the Convention):

(a) the chemicals must have been used as riot control agents; or
(b) have been declared by a State Party as a riot control agent.

6.1.2 In addition to the riot control agent its analytical derivatives, if applicable, should be added.

6.1.3 Based on these principles a number of chemicals is recommended which are contained in appendix 5 to this report. The list should not be considered as exhaustive and should be expanded when new riot control agents are declared.

6.1.4 The TWG considered the addition of degradation products of riot control agents on the same principles explained in paragraph 5.2.1, but decided that at the moment, this was not of a high priority.

6.2 Old/abandoned chemical weapons

Analytical data on chemicals which have been used in the past as chemical weapons should be included in the OPCW Central Analytical Database. Some of these chemicals have also been used as riot control agents. Therefore, a combined list of recommended chemicals is contained in appendix 5 to this report. There may also be a need to expand this list with characteristic degradation products based on the same principles as stated in paragraph 5.2.1.

Appendix 1

LIST OF PARTICIPANTS

Marjatta **Rautio** Chairperson of the TWG	Finland
Claude **Eon** Chairman of the SAB	France
Brahim Youcef **Meklati**	Algeria
Ernõ **Pungor**	Hungary
Abbas **Shafiee**	Iran
Theodros **Solomon**	Ethiopia
Claudio **Costa Neto**	Brazil
Andreas **Niederhauser**	Switzerland
Collin **Pottage**	UK
Margo **Jackisch**	USA
Eric **Wils** - observer	The Netherlands

Appendix 2

NON-SCHEDULED DEGRADATION PRODUCTS OF SCHEDULED CHEMICALS

1. Schedule 1.A.2 (Tabun family)

Data on various representatives of N,N-dialkyl O-alkyl phosphoramidates, the primary hydrolysis products of the Schedule 1.A.2 chemicals should be added. As a first priority compounds with the N,N-dimethyl and N,N-diethyl moieties should be selected. The list of alcohols should also be limited to those readily available in large quantities.

2. Schedule 1.A.3 (VX-family)

Most of the degradation products of the VX family are scheduled compounds falling under Schedule 2.B.4. However, the well-known degradation products related to the S-2-dialkylaminoethyl side chain are not covered. The addition of the following degradation products is recommended:

Bis(dimethylaminoethyl)sulfide
Bis(dimethylaminoethyl)disulfide
Bis(diethylaminoethyl)sulfide
Bis(diethylaminoethyl)disulfide
Bis(dipropylaminoethyl)sulfide
Bis(dipropylaminoethyl)disulfide
Bis(diisopropylaminoethyl)sulfide
Bis(diisopropylaminoethyl)disulfide

Data on protonated and/or alkylated salts should be added as well.

3. Schedule 1.A.4 (sulfur mustards)

Sulfur mustard agents decompose by hydrolysis and by oxidation of the sulfur atom. Of the many possible degradation products, only thiodiglycol (Schedule 2.B.13) is a scheduled chemical. The addition of the following degradation products is recommended:

(a) Oxidised products of mustard gas

Bis(2-chloroethyl)sulfoxide
Bis(2-chloroethyl)sulfone

(b) Hydrolysis products:

bis(2-hydroxyethylthio)methane
1,2-bis(2-hydroxyethylthio)ethane
1,3-bis(2-hydroxyethylthio)propane
1,4-bis(2-hydroxyethylthio)butane

1,5-bis(2-hydroxyethylthio)pentane
bis(2-hydroxyethylthiomethyl)ether
bis(2-hydroxyethylthioethyl)ether

(c) Oxidised hydrolysis products:

bis(2-hydroxyethylsulfinyl)methane
bis(2-hydroxyethyl)sulfoxide
1,2-bis(2-hydroxyethylsulfinyl)ethane
1,3-bis(2-hydroxyethylsulfinyl)propane
1,4-bis(2-hydroxyethylsulfinyl)butane
1,5-bis(2-hydroxyethylsulfinyl)pentane
bis(2-hydroxyethylsulfinylmethyl)ether
bis(2-hydroxyethylsulfinylethyl)ether

bis(2-hydroxyethylsulfonyl)methane
bis(2-hydroxyethyl)sulfone
1,2-bis(2-hydroxyethylsulfonyl)ethane
1,3-bis(2-hydroxyethylsulfonyl)propane
1,4-bis(2-hydroxyethylsulfonyl)butane
1,5-bis(2-hydroxyethylsulfonyl)pentane
bis(2-hydroxyethylsulfonylmethyl)ether
bis(2-hydroxyethylsulfonylethyl)ether

In addition data on divinylsulfide and other vinyl analogues, formed by elimination, and of the analytical derivatives, if applicable, should be obtained.

4. Schedule 1.A.5 (lewisites)

The addition of the following lewisite degradation products and their analytical derivatives are recommended:
2-chlorovinylarsine oxide
2-chlorovinylarsonic acid
bis(2-chlorovinyl)arsinic acid
tris(2-chlorovinyl)arsine oxide

5. Schedule 2.A.1

Although the primary hydrolysis products of Amiton, diethylphosphate and diethylthiophosphate, are rather unspecific compounds, they may serve as indicators for the presence of Amiton when other degradation products derived from the S-2-diethylaminoethyl moiety are found. Therefore these chemicals and their analytical derivatives should be added to the database.

Appendix 3

SALTS OF SCHEDULED CHEMICALS

Bis(2-chloroethyl)ethylamine hydrochloride
Bis(2-chloroethyl)methylamine hydrochloride
Tris(2-chloroethyl)amine hydrochloride
3-Quinuclidinyl benzilate hydrochloride
3-Quinuclidin-3-ol hydrochloride
Ethyldiethanolamine hydrochloride
Methyldiethanolamine hydrochloride
Triethanolamine hydrochloride

Appendix 4

NON-SCHEDULED PRECURSORS AND BYPRODUCTS OF THE SYNTHESIS OF SCHEDULED CHEMICALS

1. Non-scheduled precursors:

Methyl benzilate
Ethyl benzilate
Alkyl N,N-dimethylphosphoramidochloridates

2. Byproducts:

Bis(2-chloroethyl)disulfide
1,4-Dithiane
1,4-Thioxane

Appendix 5

RIOT CONTROL AGENTS AND OLD/ABANDONED CHEMICAL WEAPONS

Name (code)	CAS number
Methyldichloroarsine (MD)	593-89-5
Ethyldichloroarsine (ED)	598-14-1
Phenyldichloroarsine (PD)	696-28-6
Diphenylchloroarsine (Clark I)	712-48-1
Diphenylcyanoarsine (Clark II)	23525-22-6
10-Chloro-5,10-dihydrophenarsazine (Adamsite)	578-94-9
Alpha-bromobenzyl cyanide (CA)	5798-79-8
Omega-chloroacetophenone (CN)	532-27-4
2-Chlorobenzylidenemalonitrile (CS)	2698-41-1
Dibenzoxazepine (CR)	257-07-8
Capsaicin	404-86-4
4-Nonanoylmorpholine	5299-64-9
Pelargonic acid vanillylamide	2444-46-4
Ethyl iodoacetate	623-48-3
Ethyl bromoacetate	105-36-2
Phosgene oxime (CX)	1794-86-1
Xylyl bromide	ortho: 89-92-9
	meta: 620-13-3
	para: 104-81-4
Benzyl bromide	100-39-0
Diphosgene	503-38-8
Triphosgene	32315-10-9

Annex 4

PRIORITY OF DATA TO BE OBTAINED FOR THE CENTRAL OPCW ANALYTICAL DATABASE

Non-scheduled degradation products of scheduled chemicals

1. Schedule 1.A.2 (Tabun family)

High priority:

O-ethyl N,N-dimethylphosphoramidate
O-isopropyl N,N-dimethylphosphoramidate

and their analytical derivatives (trimethylsilylesters).

Lower priority:

Data on other representatives of N,N-dialkyl O-alkyl phosphoramidates and their analytical derivatives (trimethylsilylesters).

2. Schedule 1.A.3 (VX-family)

High priority:

Bis(diethylaminoethyl)sulfide
Bis(diethylaminoethyl)disulfide
Bis(diisopropylaminoethyl)sulfide
Bis(diisopropylaminoethyl)disulfide

and their protonated salts.

Lower priority:

Bis(dimethylaminoethyl)sulfide
Bis(dimethylaminoethyl)disulfide
Bis(dipropylaminoethyl)sulfide
Bis(dipropylaminoethyl)disulfide

and their protonated salts.

3. Schedule 1.A.4 (sulfur mustards)

(a) Oxidised products of mustard gas:

High priority:

Bis(2-chloroethyl)sulfoxide
Bis(2-chloroethyl)sulfone

(b) Hydrolysis products:

High priority:

1,2-bis(2-hydroxyethylthio)ethane
bis(2-hydroxyethylthioethyl)ether

Low priority:

bis(2-hydroxyethylthio)methane
1,3-bis(2-hydroxyethylthio)propane
1,4-bis(2-hydroxyethylthio)butane
1,5-bis(2-hydroxyethylthio)pentane
bis(2-hydroxyethylthiomethyl)ether

(c) Oxidised hydrolysis products:

High priority:

bis(2-hydroxyethyl)sulfoxide
bis(2-hydroxyethyl)sulfone
1,2-bis(2-hydroxyethylsulfinyl)ethane
1,2-bis(2-hydroxyethylsulfonyl)ethane
bis(2-hydroxyethylsulfinylethyl)ether
bis(2-hydroxyethylsulfonylethyl)ether

Low priority:

bis(2-hydroxyethylsulfinyl)methane
bis(2-hydroxyethylsulfonyl)methane
1,3-bis(2-hydroxyethylsulfinyl)propane
1,3-bis(2-hydroxyethylsulfonyl)propane
1,4-bis(2-hydroxyethylsulfinyl)butane
1,4-bis(2-hydroxyethylsulfonyl)butane
1,5-bis(2-hydroxyethylsulfinyl)pentane
1,5-bis(2-hydroxyethylsulfonyl)pentane
bis(2-hydroxyethylsulfinylmethyl)ether
bis(2-hydroxyethylsulfonylmethyl)ether

In addition data on divinylsulfide and other vinyl analogues, formed by elimination, and of the analytical derivatives, if applicable, should be obtained.

4. Schedule 1.A.5 (lewisites)

High priority:

2-chlorovinylarsine oxide
2-chlorovinylarsonic acid
bis(2-chlorovinyl)arsinic acid
tris(2-chlorovinyl)arsine oxide

5. Schedule 2.A.1

Low priority:

diethylphosphate
diethylthiophosphate

Salts of scheduled chemicals

Priority depends on the analytical technique. For GC-MS there is a low priority, whereas for IR data the priority is high.

Bis(2-chloroethyl)ethylamine hydrochloride
Bis(2-chloroethyl)methylamine hydrochloride
Tris(2-chloroethyl)amine hydrochloride
3-Quinuclidinyl benzilate hydrochloride
3-Quinuclidin-3-ol hydrochloride
Ethyldiethanolamine hydrochloride
Methyldiethanolamine hydrochloride
Triethanolamine hydrochloride

Non-scheduled precursors and byproducts of the synthesis of scheduled chemicals

1. Non-scheduled precursors:

High priority:

Methyl benzilate
Ethyl benzilate
O-ethyl N,N-dimethylphosphoramidochloridates
O-isopropyl N,N-dimethylphosphoramidatochloridates

Low priority:

Other alkyl N,N-dimethylphosphoramidochloridates

2. Byproducts:

High priority:

Bis(2-chloroethyl)disulfide
1,4-Dithiane
1,4-Thioxane

Riot control agents and old/abandoned chemical weapons

High priority:

Name (code)	CAS number
Methyldichloroarsine (MD)	593-89-5
Ethyldichloroarsine (ED)	598-14-1
Phenyldichloroarsine (PD)	696-28-6
Diphenylchloroarsine (Clark I)	712-48-1
Diphenylcyanoarsine (Clark II)	23525-22-6
10-Chloro-5,10-dihydrophenarsazine (Adamsite)	578-94-9
Alpha-bromobenzyl cyanide (CA)	5798-79-8
Omega-chloroacetophenone (CN)	532-27-4
2-Chlorobenzylidenemalonitrile (CS)	2698-41-1
Dibenzoxazepine (CR)	257-07-8
Capsaicin	404-86-4
4-Nonanoylmorpholine	5299-64-9
Pelargonic acid vanillylamide	2444-46-4
Ethyl iodoacetate	623-48-3
Ethyl bromoacetate	105-36-2
Phosgene oxime (CX)	1794-86-1
Xylyl bromide	ortho: 89-92-9
	meta: 620-13-3
	para: 104-81-4
Benzyl bromide	100-39-0
Diphosgene	503-38-8
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