Chapter 1
Introduction

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Chemical Weapons Convention Chemicals Analysis

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CHAPTER 1
Introduction

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1 THE CHEMICAL WEAPONS CONVENTION (CWC)

The Convention on the prohibition of the development, production, stockpiling, and use of chemical weapons and of their destruction (the Chemical Weapons Convention, CWC) was signed on January 13, 1993, and entered into force on April 29, 1997. The CWC includes 24 Articles, the Annex on Chemicals, the Annex on Implementation and Verification (so-called Verification Annex), and the Confidentiality Annex. The Verification Annex, which by the length occupies the majority of the CWC, is written in 11 parts. Article I lists the general obligations of the CWC as shown in Figure 1.

2 DEFINITIONS

The terms used in the CWC need to be explained, and for this reason, the terms used in the Articles are defined in Article II, Definitions and Criteria. The terms used in the Verification Annex are defined in its first part. In general, a chemical weapon may be understood as munition filled with toxic chemical, but the definition of the CWC gives a larger perspective. Also, from the point of view of analytical chemistry, it is necessary to have an idea about what kind of chemicals we are aiming at. Also related to chemicals are a whole set of terms that need to be defined, that is, 'Chemical Weapons', 'Toxic Chemical', 'Precursor', and, in addition, 'key component'. The definitions are as follows.

'Chemical Weapons' means 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; (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

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ARTICLE I
GENERAL OBLIGATIONS

Each State Party to this Convention undertakes never under any circumstances:

to develop, produce, otherwise acquire, stockpile or retain chemical weapons, or transfer, directly or indirectly, chemical weapons to anyone;

to use chemical weapons;

to engage in any military preparations to use chemical weapons;

to assist, encourage or induce, in any way, anyone to engage in any activity prohibited to a State Party under this Convention.

Each State Party undertakes to destroy chemical weapons it owns or possesses, or that are located in any place under its jurisdiction or control, in accordance with the provisions of this Convention.

Each State Party undertakes to destroy all chemical weapons it abandoned on the territory of another State Party, in accordance with the provisions of this Convention.

Each State Party undertakes to destroy any chemical weapons production facilities it owns or possesses, or that are located in any place under its jurisdiction or control, in accordance with the provisions of this Convention.

Each State Party undertakes not to use riot control agents as a method of warfare.

Figure 1. Article I of the Chemical Weapons Convention

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 (b).

'Toxic Chemical' means 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.

'Precursor' means any chemical reactant that takes part at any stage in the production, by whatever method, of a toxic chemical. This includes any key component of a binary or multicomponent chemical system.

'Key Component of Binary or Multicomponent Chemical Systems' (hereinafter referred to as 'key component') means any precursor, which plays the most important role in determining the toxic properties of the final product and reacts rapidly with other chemicals in the binary or multicomponent system.

3 SCHEDULES OF CHEMICALS

For the purpose of implementing the CWC, toxic chemicals and precursors, which have been identified for the application of verification measures, are listed in Schedules contained in the Annex on Chemicals (for the Schedules, *see* **Chapter 2**). Schedule 1 includes chemicals developed, produced, stockpiled, or used as a chemical weapon as defined above, and chemicals structurally close to them. Schedule 2 lists three toxic chemicals not included in Schedule 1 and the degradation products and precursors of these toxic chemicals as well as of those of Schedule 1. Schedule 3 lists four toxic chemicals and precursors not listed in the other Schedules. The Schedules contain mainly organic chemicals with different chemical and physical properties, being neutral chemicals, acids, bases, volatiles, and nonvolatiles, where phosphorus, fluorine, sulfur, chlorine, nitrogen, and oxygen occur frequently. Riot control agents are not included in the Schedules.

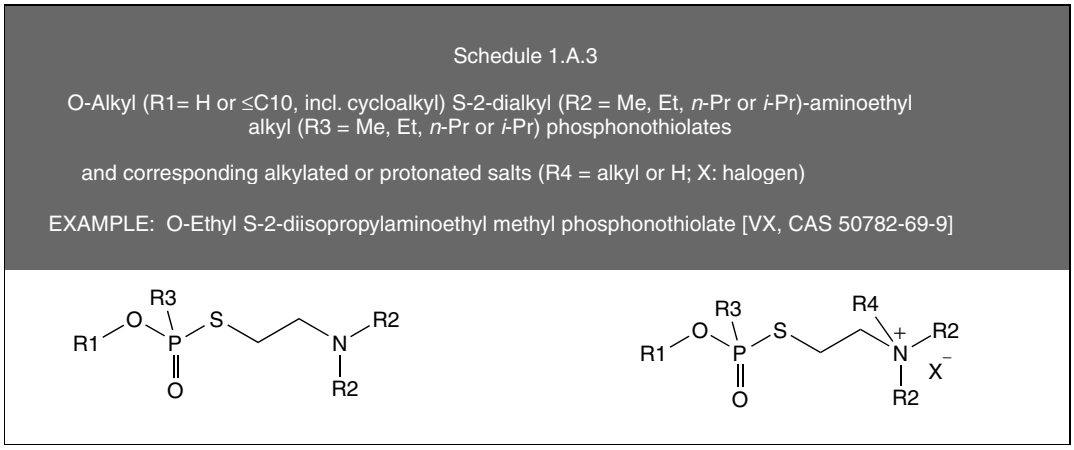

Figure 2. Definition and structures of Schedule 1.A.3 chemicals

The three Schedules contain altogether 57 list items from which 42 are individual chemicals and 15 are families of chemicals with a common structural backbone. Such families in the Schedules make the number of chemicals that are subject to verification very large. An idea of the number of chemicals in the Schedules may be obtained when considering, for example, the family of VX (Schedule 1.A.3), including its salts (Figure 2).

Another example is found in Schedule 2.B.4, which contains an even larger number of chemicals defined in the following way: 'Chemicals, except for those listed in Schedule 1, containing a phosphorus atom to which is bonded one methyl, ethyl or propyl (normal or iso) group but not further carbon atoms [exemption: Fonofos, CAS 944-22-9]'.

4 ORGANIZATION FOR THE PROHIBITION OF CHEMICAL WEAPONS (OPCW)

The States Parties to the CWC have established the Organization for the Prohibition of Chemical Weapons (OPCW; www.opcw.org) to achieve the object and purpose of the CWC, to ensure the implementation of its provisions, including those for international verification of compliance with it, and to provide a forum for consultation and cooperation among States Parties (SPs). All SPs to the CWC are members of the OPCW. The Organization shall conduct its verification activities provided under the CWC in the least intrusive manner possible, consistent with the timely and efficient accomplishment of their objectives. It shall request only the information and data necessary to fulfill its responsibilities under the CWC. It shall take every precaution to protect the confidentiality of information on civil and military activities and facilities coming to its knowledge in the implementation of the CWC and, in particular, shall abide by the provisions set forth in the Confidentiality Annex. In undertaking its verification activities, the OPCW shall consider measures to make use of advances in science and technology.

5 VERIFICATION

The OPCW performs verification activities on a regular basis and can conduct challenge inspections. The purpose is to verify that the SPs fulfill their obligations under the CWC. Regular verification includes assessment of the declarations made by the SPs by conducting on-site inspections of declared sites.

The general rules for verification (Verification Annex, Part II, paragraphs 52–54) describe sample taking (sampling, sample collection) and analysis. By way of example, sampling and analysis shall be undertaken to check for the absence of undeclared scheduled chemicals during inspections under

regime of Schedule 2 chemicals and facilities related to such chemicals. Also, sampling and on-site analysis may be undertaken to check for the absence of undeclared scheduled chemicals during inspections under regime of Schedule 3 chemicals and facilities related to such chemicals. In case of unresolved ambiguities, samples may be analyzed in a designated off-site laboratory, subject to the inspected SPs agreement. (For the summary on the sampling and analysis in the CWC, *see* Annex 1 in **Chapter 2**.)

For the on-site analysis, the inspectors bring with them mobile instrumentation capable of performing the analysis in the least intrusive manner where the chemicals are revealed only according to the purpose of the inspection and the information on nonscheduled chemicals will remain confidential (for so-called blinded analysis, *see* **Chapter 4**).

For the off-site analysis, the designated laboratories are used. These laboratories have instrumental capability, preparedness, and analytical methods to analyze the samples taken by the inspectors or by the inspected SP representatives. The samples sent (after the agreement of the inspected SP) to the off-site laboratory are coded, and therefore the laboratory receiving the samples will not know their origin. The laboratories are capable of confirming the presence or absence of CWC-related chemicals and other chemicals, but must report only data relevant to the purpose of the analysis as defined by the OPCW. The laboratory's work on the OPCW samples is confidential, which is a normal practice when regarding the work with laboratory's other collaborators and commercial business partners. The work is reported only to the OPCW.

6 THIS BOOK

Chemical Weapons Convention Chemicals Analysis discusses sample collection, sample preparation and analysis, and concentrates on verification that takes place on site, analyses off site, and methods and procedures used. In the first part of the book is discussed the mobile laboratory of the OPCW and instrumentation and software used therein, as well as other on-site analysis equipment, procedures, and strategies. The OPCW gas chromatograph–mass spectrometer for on-site analysis is described and an introduction to Automated Mass Spectrometry Deconvolution and Identification System (AMDIS) software is given. Various monitoring methods of hazardous substances are viewed. A comprehensive review to 10 OPCW proficiency tests has been done. The topics related to the OPCW Central Analytical Database (OCAD) are discussed.

The second part of the book begins with a discussion of the analysis strategy employed in an OPCW-designated laboratory and continues with a discussion on sample preparation methods in an off-site laboratory and concludes with discussion on the various analytical techniques used for analysis of CWC-related chemicals in (designated) laboratories worldwide. The analytical techniques are gas chromatography (GC), gas chromatography/mass spectrometry (GC/MS), liquid chromatography/mass spectrometry (LC/MS), nuclear magnetic resonance (NMR) spectroscopy, gas chromatography/Fourier transform infrared spectroscopy (GC/FTIR), and capillary electrophoresis (CE). The methods included in this part provide the best off-site performance for unambiguous identification of CWC-related chemicals. The success of these off-site analysis techniques has been unequivocally confirmed in the international proficiency tests. Other examples in the literature exist from excellent performance from 'real samples', for example, the detection of intact sarin by mass spectrometry from a painted metal fragment after four years of contamination.

In the third part, methods for retrospective detection of exposure to toxic scheduled chemicals using mass spectrometric and immunochemical analysis methods are discussed. The described methods are applied to human origin samples. These methods are essential when in cases of use, or allegations of use, previous presence or absence of toxic chemicals need to be confirmed. Identification of CWC-related chemicals provides key supporting evidence of noncompliance with the CWC.

ABBREVIATIONS AND ACRONYMS

AMDIS	Automated Mass Spectrometry Deconvolution and Identification System
CAS	Chemical Abstracts Service

CE	Capillary Electrophoresis
CWC	Chemical Weapons Convention
GC	Gas Chromatography
GC/FTIR	Gas Chromatography/Fourier Transform Infrared Spectroscopy
GC/MS	Gas Chromatography/Mass Spectrometry
LC/MS	Liquid Chromatography/Mass Spectrometry
NMR	Nuclear Magnetic Resonance
OCAD	OPCW Central Analytical Database
OPCW	Organization for the Prohibition of Chemical Weapons
SPs	States Parties
VX	*O*-Ethyl *S*-2-diisopropylaminoethyl methylphosphonothiolate