# Science for Diplomats

# Scheduled chemicals and riot control agents: a visual guide

November 2024



This visual guide to scheduled chemicals and riot control agents has been designed as a useful resource under the Science for Diplomats initiative. The aim of its simplified content is to provide an enhanced understanding of these Convention-relevant chemicals and a visualisation of some of their structures. **It is not part of the official Annex on Chemicals**.

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# Contents

I.	Introduction	2
	1. Schedules of chemicals	3
	1.1 Alkyl groups	4
	1.2 CAS Registry Numbers	5
	2. Visualising molecular structures	5
	2.1 Examples 2D structures	6
	2.2 Interpreting 3D ball-and-stick models	7
	2.3 Translating 3D models to 2D structures	8
	2.4 Chemical identifiers	8
	3. Guidelines for Schedules of chemicals	9
	3.1 Guidelines for Schedule 1	9
	3.2 Guidelines for Schedule 2	10
	3.3 Guidelines for Schedule 3	10
	4. Schedules summary	11
II.	Annex on Chemicals	12
	Schedule 1.A – Toxic chemicals	14
	Schedule 1.B – Precursors	20
	Schedule 2.A – Toxic chemicals	22
	Schedule 2.B – Precursors	24
	Schedule 3.A – Toxic chemicals	30
	Schedule 3.B – Precursors	32
III.	Riot control agents	40
IV.	Glossary	47

# INTRODUCTION

# 1. Schedules of chemicals

The **three Schedules** of chemicals list **toxic chemicals** and their **precursors** and are found in the Annex on Chemicals to the Chemical Weapons Convention. For the purpose of implementing the Convention, the Schedules identify chemicals for the application of verification measures according to the provisions of the Verification Annex. Pursuant to Article II, subparagraph 1 (a), these Schedules do not constitute a definition of chemical weapons.

Each of the three Schedules is divided into two sections, A and B. Section A lists the toxic chemicals and Section B lists precursors (see Glossary for definitions). Entries in the Schedules may refer to a specific single chemical or may refer to a family of chemicals, such as Schedule 1.A.1 shown below.



# Illustrative examples

Chemicals are grouped into families based on their structural similarities. This grouping helps identify chemicals that might have similar effects. By organising chemicals into families, a wide range of substances can be more effectively monitored and regulated, including ones that might not be specifically listed but still pose similar risks due to their related structures and functions. **This approach allows for broader control over potentially dangerous chemicals without needing to list every single substance individually**.

# 1.2 Alkyl groups

In a family of scheduled chemicals, the alkyl group(s) typically vary. An alkyl group is not a specific chemical but rather a generic term for a type of chemical structure made up exclusively of carbon and hydrogen atoms. The carbon atoms are joined by single bonds and may be in a chain (linear or branched) or in a ring.

Alkyl groups with " $\leq$ C10 incl. cycloalkyl" means that there may be up to 10 carbon atoms in the group and these may be in a chain or in a ring (cyclic). In the case of entry 1.A.1, the second alkyl group may be a methyl (Me), ethyl (Et), normal propyl (*n*-Pr), or *iso*-propyl (*i*-Pr) group **only** and their structures are shown below.



Examples of "≤C10 incl. cycloalkyl":





C<sub>5</sub> – cyclopentyl

Whenever reference is made to groups of dialkylated chemicals with two alkyl groups in parentheses, all chemicals containing any possible combination of these alkyl groups are considered as listed in the respective Schedule unless explicitly exempted.

# **1.3 CAS Registry Numbers**

The OPCW Scientific Advisory Board (SAB) has advised that CAS Registry Numbers (see Glossary) should not solely be relied upon to define chemicals covered by the Schedules.<sup>a</sup> Although relevant as aids to declaration and verification, CAS numbers are not the only means to identify a chemical or to determine whether a chemical is included in, or excluded from, a Schedule.

# 2. Visualising molecular structures

Chemists use structures to represent chemical molecules because these drawings show how the atoms are connected and arranged. This is important because the structure of a molecule determines how it behaves, reacts with other substances, and what properties it has.

Structures are useful because they make it easier to understand and communicate details about a molecule. Instead of describing each part of a molecule in words, a structure provides a quick, visual way to see the molecule's shape, size, and potential reaction points.

Molecules can be shown in simplified two-dimensional (2D) structures (most common) or rendered in three dimensions (3D), often as "balland-stick" models that help illustrate the spatial arrangement of the atoms. Chemists also frequently use "shorthand" 2D structures for speed and simplicity, which are described in Section 2.3.

The following table provides example 2D structures and shows how the atoms are connected and represented. For clarity, it includes only the atoms most commonly found in scheduled chemicals and riot control agents.

<sup>&</sup>lt;sup>a</sup> Response to the Director-General's Request to the Scientific Advisory Board to Provide Further Advice on Scheduled Chemicals (SAB-23/WP.1, dated 28 April 2016). Available at: <u>www.</u> <u>opcw.org/sites/default/files/documents/SAB/en/sab-23-wp01\_e\_.pdf</u>

#### 2.1 Example 2D structures

6



# 2.2 Interpreting 3D ball-and-stick models



Each "ball" represents an atom of a chemical element identified by colour. The atoms are linked by chemical bonds, where a single line represents a single bond, two lines represent a double bond and three lines (not shown above) represent a triple bond.



# 2.3 Translating 3D models to 2D structures

The 3D model is "translated" to a 2D molecular structure, where the type of atom is indicated by its chemical symbol. This 2D structure illustrates the connections between the atoms. This is an intermediate representation to the shorthand structures.

Shorthand structures are a format often used by chemists to simplify the structural representation. They illustrate the bonds between atoms as connecting lines. Each point where a line intersects with another line or where a line terminates, but has no element symbol, represents a carbon (C) atom. Bonds between carbon and hydrogen (H) atoms are omitted completely. All other elements are indicated by their chemical symbol and bonds between a hydrogen atom and any type of atom other than carbon are shown. A worked example for sarin is shown below.



# 2.4 Chemical identifiers

The 2D structures and 3D models display the spatial arrangement of atoms and bonds in a molecule. Chemical identifiers, on the other

hand, use text-based encodings to represent molecules in a compact, linear format while conveying their connectivity and, in some cases, spatial arrangement. Two common chemical identifiers are **SMILES** (Simplified Molecular Input Line Entry System) and **InChI** (International Chemical Identifier). Both are primarily used for the storage, retrieval, and unique identification of chemical structures in databases and software systems. The encoding for sarin is shown below for comparison.

InChI: InChI=1S/C4H10F02P/c1-4(2)7-8(3,5)6/h4H,1-3H3 SMILES: CC(C)O[P@](=O)(C)F

# 3. Guidelines for Schedules of Chemicals

The following guidelines are listed verbatim from the Annex on Chemicals and explain how the Schedules are derived.

# 3.1 Guidelines for Schedule 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.

# 3.2 Guidelines for Schedule 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.

# 3.3 Guidelines for Schedule 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.

# 4. Schedules summary

	Schedule 1	Schedule 2	Schedule 3
Number of entries for families of chemicals			
Number of entries for specific chemicals			
Production quantity for peaceful purposes			
Reaction steps to a chemical weapon			





# ANNEX ON CHEMICALS

# Key to symbols and explanatory notes



Schedule entry relates to a family of chemicals



Schedule entry is for a single specified chemical

In the official Annex on Chemicals, the different types of alkyl groups and salts are defined for every entry relating to a family of chemicals listed in Schedule 1 or 2. For readability, the family-related entries have been abbreviated in this visual guide. The entries for 1.A.1 and 1.A.3 are shown below as examples.

# Official Annex of Chemicals entry 1.A.1:

O-Alkyl (≤C10, incl. cycloalkyl) alkyl (Me, Et, *n*-Pr or *i*-Pr)-phosphono-fluoridates

# Visual guide entry 1.A.1:

O-Alkyl<sup>1</sup> alkyl<sup>2</sup>-phosphonofluoridates

# Official Annex of Chemicals entry 1.A.3:

O-Alkyl (H or ≤C10, incl. cycloalkyl) S-2-dialkyl (Me, Et, *n*-Pr or *i*-Pr) -aminoethyl alkyl (Me, Et, *n*-Pr or *i*-Pr) phosphonothiolates and corresponding alkylated or protonated salts

# Visual guide entry 1.A.3:

O-Alkyl<sup>3</sup> S-2-dialkyl<sup>2</sup>-aminoethyl alkyl<sup>2</sup> phosphonothiolates <sup>4</sup>

- $^{1} \leq$  C10, incl. cycloalkyl
- <sup>2</sup> Me, Et, *n*-Pr or *i*-Pr
- <sup>3</sup> H or  $\leq$  C10, incl. cycloalkyl
- <sup>4</sup> Incl. corresponding alkylated or protonated salts



Scan the QR code for more information about the chemical

# 1.A.1 28

# O-Alkyl<sup>1</sup> alkyl<sup>2</sup>-phosphonofluoridates

Agent type	Chemical family
Nerve agent	Organophosphorus compounds

1.A.2

# O-Alkyl<sup>1</sup> N,N-dialkyl<sup>2</sup>phosphoramidocyanidates

Agent type	Chemical family
Nerve agent	Organophosphorus compounds

1.A.3

# O-Alkyl<sup>3</sup> S-2-dialkyl<sup>2</sup>-aminoethyl alkyl<sup>2</sup> phosphono-thiolates <sup>4</sup>

Agent type	Chemical family
Nerve agent	Organophosphorus compounds

1.A.4 202

#### Sulfur mustards

Agent type	Chemical family
Blister agent	Organosulfur compounds

# Family group example



# 1.A.5 28

# Lewisites

Agent type	Chemical family
Blister agent	Arsenicals
1.A.6 <u>28</u> 2	:
Nitrogen mustards	
Agent type	Chemical family
Blister agent	Haloalkyl amines
1.A.7 <mark>8</mark>	; 
Saxitoxin	
Agent type	Origin
Biotoxin	Algae
1.A.8 <mark>8</mark> Ricin	;
Agent type	Origin
Biotoxin	Castor beans

# Family group example or specific entry



ricin is typically illustrated with 3D

and shape as a protein.

models that capture its detailed folding

# 1.A.13 22

# *P*-alkyl<sup>3</sup> *N*-(1-(dialkyl<sup>1</sup>amino))alkylidene<sup>3</sup>phosphonamidic fluorides <sup>4</sup>

Agent type	Chemical family
Nerve agent	Organophosphorus compounds

1.A.14 28

O-alkyl<sup>3</sup> N-(1-(dialkyl<sup>1</sup>amino))alkylidene<sup>3</sup>phosphoramidofluoridates <sup>4</sup>

Agent type	Chemical family
Nerve agent	Organophosphorus compounds

# 1.A.15 💧

# Methyl-(bis(diethylamino)methylene)phosphonamidofluoridate

Agent type	Chemical family
Nerve agent	Organophosphorus compounds

1.A.16

#### Quaternaries and bisquaternaries of dimethylcarbamoyloxypyridines

Agent type	Chemical family
Nerve agent	Carbamates

Methyl-(1-(diethylamino)ethylidene)phosphonamidofluoridate









N1-(3-((Dimethylcarbamoyl)oxy)-2-picolinyl)-N10-(2-hydroxyethyl)-N1-ethyl-N1,N10,N10-trimethyldecane-1,10- diammonium dibromide



# 1.B.9 22

# Alkyl<sup>2</sup>phosphonyldifluoride

Precursor to	Manufacture of
Sarin, soman	Nothing

1.B.10 28

# O-Alkyl<sup>3</sup> O-2-dialkyl<sup>2</sup>-aminoethyl alkyl<sup>2</sup>-phosphonites <sup>4</sup>

Precursor to	Manufacture of
VX	Nothing

# 1.B.11 🔒

#### O-Isopropyl methylphosphonochloridate

Precursor to	Manufacture of
Sarin	Nothing

# 1.B.12 🔒

#### O-Pinacolyl methylphosphonochloridate

Precursor to	Manufacture of
Soman	Nothing



# 2.A.1 22

# 0,0-Diethyl S-[2-(diethylamino)ethyl]phosphorothiolate <sup>4</sup>

Agent type	Chemical family
Nerve agent	Organophosphorus compounds

2.A.2

# 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene

Agent type	Chemical family
Choking agent	Fluorocarbons

2.A.3

## **3-Quinuclidinyl benzilate**

Agent type	Chemical family
Central nervous system-acting chemical	Glycolates

# Family group example or specific entry



1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene (PFIB)









#### දිදුදු 2.B.4

# Chemicals containing *P*-alkyl<sup>2</sup>

Precursor to	Manufacture of
Sarin, soman	Flame retardants

2.B.5 28

# N,N-Dialkyl<sup>2</sup>phosphoramidic dihalide

Precursor to	Manufacture of
Tabun	Other chemicals

2.B.6

# Dialkyl<sup>2</sup> N,N-dialkyl<sup>2</sup>-phosphoramidates

Precursor to	Manufacture of
Tabun	Other chemicals

2.B.7 🔗

# Arsenic trichloride

Precursor to	Manufacture of
Lewisites and other arsenicals	Pharmaceuticals, pesticides, and ceramics



# 2.B.8 🖁

# 2,2-Diphenyl-2-hydroxyacetic acid

Precursor to	Manufacture of
BZ	Pharmaceuticals

# 2.B.9

# Quinuclidin-3-ol

Precursor to	Manufacture of
BZ	Pharmaceuticals

# 2.B.10 28

#### N,N-Dialkyl<sup>2</sup>aminoethyl-2-chlorides <sup>4</sup>

Precursor to	Manufacture of
VX	Other chemicals

# 2.B.11 28

# N,N-Dialkyl<sup>2</sup>aminoethane-2-ols <sup>4</sup>

Precursor to	Manufacture of
VX	Other chemicals

# Family group example or specific entry



# 2.B.12 28

# N,N-Dialkyl<sup>2</sup>aminoethane-2-thiols <sup>4</sup>

Precursor to	Manufacture of
VX	Other chemicals

# 2.B.13 🛛

# Bis(2-hydroxyethyl)sulfide

Precursor to	Manufacture of
Sulfur mustard	Water-based inks/dyes, and plastics

2.B.14 🛛

# 3,3-Dimethylbutan-2-ol

Precursor to	Manufacture of
Soman	Flavouring agents



# 3.A.1 8

# Carbonyl dichloride

Agent type	Manufacture of
Choking agent	Foams, coatings, plastics, and pharmaceuticals

# 3.A.2 🔗

# Cyanogen chloride

Agent type	Manufacture of
Blood agent	Nylon, rubber, pigments, and dyes

3.A.3 🖁

# Hydrogen cyanide

Agent type	Manufacture of
Blood agent	Plastics, synthetic fibres, and other chemicals

3.A.4 👌

# Trichloronitromethane

Agent type	Manufacture of
Choking agent	Soil fumigants





# 3.B.5 🛛 🖁

# Phosphorus oxychloride

Precursor to	Manufacture of
Various nerve agents	Plastics, pesticides, and other chemicals
3.B.6 <u>8</u>	

# **Phosphorus trichloride**

Precursor to	Manufacture of
Sulfur mustard and various nerve agents	Pesticides, plasticisers, lubricants, and other chemicals

3.B.7 🔒

#### Phosphorus pentachloride

Precursor to	Manufacture of
Various nerve agents	Plastics and pesticides

3.B.8 8

# **Trimethyl phosphite**

Precursor to	Manufacture of
Various nerve agents	Pesticides and paints

# **Specific entry**



# 3.B.9 8

# **Triethyl phosphite**

Precursor to	Manufacture of
Various nerve agents	Lubricants and plasticisers
3.B.10 <u>8</u>	·

# **Dimethyl phosphite**

Precursor to	Manufacture of
Sarin	Herbicides and flame retardants

# 3.B.11 🛛

#### **Diethyl phosphite**

Precursor to	Manufacture of
Various nerve agents	Agrochemicals, flame retardants, and pharmaceuticals

# 3.B.12 🛛

# Sulfur monochloride

Precursor to	Manufacture of
Sulfur mustard	Insecticides, dyes, and pharmaceuticals

# Specific entry



# 3.B.13 🛛

# Sulfur dichloride

Precursor to	Manufacture of
Sulfur mustard	Vulcanised oils/rubbers and pesticides

# 3.B.14 💧

# Thionyl chloride

Precursor to	Manufacture of
Various nerve and blister agents	Plastics, pharmaceuticals, and pesticides

# 3.B.15 💧

# Ethyldiethanolamine

Precursor to	Manufacture of
Nitrogen mustard (HN1)	Detergents

# 3.B.16 💧

# Methyldiethanolamine

Precursor to	Manufacture of
Nitrogen mustard (HN2)	Pharmaceuticals and coatings

# Specific entry



# 3.B.17 8

# Triethanolamine

Precursor to	Manufacture of
Nitrogen mustard (HN3)	Personal care, home maintenance, and automotive products

# Specific entry



# RIOT CONTROL AGENTS

# Definition

For the purpose of implementing the Chemical Weapons Convention, riot control agents (RCAs) are defined as: "Any chemical not listed in a Schedule, which can produce rapidly in humans sensory irritation or disabling physical effects which disappear within a short time following termination of exposure" (Article II, paragraph 7).

RCAs are subject to declaration in accordance with subparagraph 1(e) of Article III of the Chemical Weapons Convention.

# SAB advice

In response to a request by the Director-General at the Board's Twentieth Session in June 2013, the SAB considered a list of 60 chemicals to provide advice on which RCAs would be subject to declaration under the Convention.<sup>b</sup> These chemicals comprised:

- 14 chemicals declared as RCAs since entry into force of the Convention;
- chemicals identified as potential RCAs from a list of "riot control agents and old/abandoned chemical weapons" to be considered for inclusion in the OPCW Central Analytical Database (OCAD) that had been drafted by the SAB's Temporary Working Group on Analytical Procedures in 2001;
- an initial survey conducted by the Technical Secretariat in 2013 of RCAs that have been researched or are available for purchase, beyond those that are already declared; and
- 13 additional chemicals recognised by the SAB as having potential RCA applications.

The SAB advised that the following set of **17 chemicals** would be consistent with the definition of an RCA under the Chemical Weapons Convention.

<sup>b</sup> Response to the Director-General's Request to the Scientific Advisory Board to Provide Consideration on Which Riot Control Agents Are Subject to Declaration under the Chemical Weapons Convention (SAB-25/WP.1, dated 17 March 2017). Available at: <u>www.opcw.org/</u> <u>sites/default/files/documents/SAB/en/sab25wp01\_e\_.pdf</u>

# 2-Chloroacetophenone (CN)















Dibenzo[b,f][1,4]oxazepine (CR)













<sup>+</sup>Note: Due to the double bonds in these molecules, there can be different forms (isomers) of each compound. The structure shown is just one possible form of each RCA.

# Oleoresin capsicum (OC)

The structure of oleoresin capsicum is not available as this is not a discrete chemical but a mixture of various compounds. It's a naturally occuring oily, resin-like substance containing capsaicin compounds and is the chemical that gives chili peppers their heat.





# **Biotoxins**

Biotoxins are toxic chemicals usually obtained from biological source materials. Two specific biotoxins are listed in Schedule 1: saxitoxin, which is a small molecule, and ricin, which is a large protein.

#### **Central nervous system-acting chemical**

A central nervous system (CNS)-acting chemical is a toxic substance that targets the central nervous system. These chemicals, sometimes called "incapacitating agents", include substances that can act as anesthetics, sedatives, or analgesics. Specific CNS-acting chemicals that are commonly discussed in the context of the Chemical Weapons Convention include inhaled anaesthetics, fentanils and the Schedule 2.A.3 chemical BZ.

# Chemical Abstracts Service Registry Number ("CAS number")

A CAS number is a unique numeric identifier assigned to a chemical substance. It contains up to 10 digits, divided into three parts by

hyphens, and has no inherent chemical meaning. While each CAS number uniquely identifies a specific substance, a single chemical can have multiple CAS numbers depending on differences in form, purity, or structure that were reported.

The CAS Chemical Registry System was developed in the early 1960s by CAS, following the creation There are (at least) 17 CAS numbers for substances containing the sarin structure

of an algorithm capable of generating a unique, unambiguous representation of each chemical's molecular structure for use in a computerised system (CAS.org). Since January 1965, CAS has recorded the structures, names, and molecular formulas of all substances indexed for Chemical Abstracts in computer files, creating the Chemical Registry System. Each substance is assigned a unique, permanent registry number that allows easy computer checking and links to its structure, alternative names used in the literature, and its official Chemical Abstracts index name.

# Discrete organic chemical (DOC)

For purposes of implementation of the Chemical Weapons Convention a DOC is defined as "any chemical belonging to the class of chemical compounds consisting of all compounds of carbon except for its oxides, sufides and metal carbonates". While these exceptions contain carbon, they are classified as inorganic rather than organic.

## **Inorganic chemical**

Inorganic chemicals refer to a broad class of substances that primarily do not contain carbon as their main element. However, certain carboncontaining compounds are classified as inorganic. These include carbides, carbonates, cyanides, cyanates, carbon monoxide, carbon dioxide, and carbon disulfide.

#### Molecule

A molecule is a chemical structure consisting of two or more atoms that are chemically bonded together.

#### **Organic chemical**

Organic chemicals refer to broad class of substances based on molecular structures that are made up of carbon (C) and hydrogen (H) atoms. These compounds often also include other elements, such as oxygen (O), nitrogen (N), sulfur (S), and phosphorus (P). The molecular structures of organic compounds can feature chains or rings (cycles) of carbon atoms.

#### Organophosphorus compound

Organophosphorus compounds are chemicals that contain phosphorus (P) atoms connected to organic structures. Examples of organophosphorus compounds listed in the Schedules include sarin (1.A.1) and tabun (1.A.2).

#### Precursor

Put simply, a precursor is any chemical that is involved at any stage in the process of making another chemical. The Chemical Weapons Convention defines a precursor as "any chemical reactant which takes part at any stage in the production by whatever method of a chemical. This includes any key component of a binary or multicomponent chemical system."

#### Protein

Proteins are large, complex molecules made up of smaller building blocks called amino acids. They are essential for many important functions in the body, including providing structure to cells and helping to regulate various life processes. Some proteins can also be toxic. There is only one protein specifically listed in the Schedules, ricin (1.A.8).

# **Protonated salts**

Nitrogen atoms typically form three bonds, resulting in a neutrally charged molecule like ammonia (NH<sub>3</sub>). In some cases, a nitrogen atom can form a fourth bond with a positively charged atom or molecule, such as a hydrogen ion (also known as a proton). This creates a positively charged nitrogen-containing species, such as NH<sub>4</sub><sup>+</sup> (ammonium), which requires a negatively charged chemical species to form a stable compound. This stable combination is called a protonated salt. An example is  $NH_4^+$  combined with  $Cl^-$  (chloride). Protonated salts can be de-protonated (removal of the hydrogen ion) to provide the parent compound, which is often referred to as the free base.

# **Toxic chemical**

A toxic chemical is 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.

