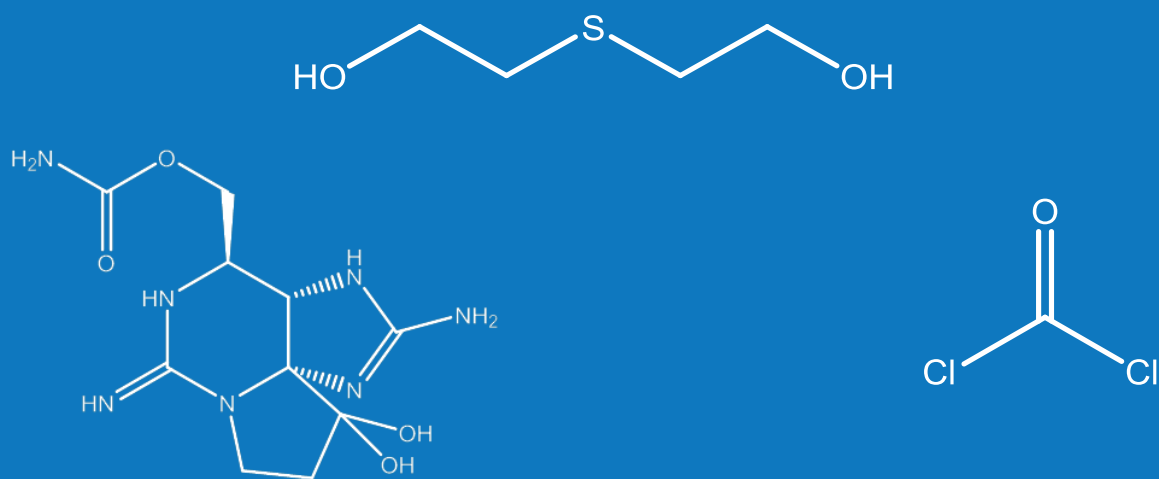


ORGANISATION FOR THE PROHIBITION OF THE CHEMICAL WEAPONS

THE SCIENCE FOR DIPLOMATS ANNEX ON CHEMICALS

*A user friendly and scientifically annotated version of the
Chemical Weapons Convention annex on chemicals*



OPCW

THE SCIENCE FOR DIPLOMATS ANNEX ON CHEMICALS

*A user friendly and scientifically annotated version of
the Chemical Weapons Convention Annex on Chemicals¹*

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- A. GUIDELINES FOR SCHEDULES OF CHEMICALS
- B. VISUALISING AND READING MOLECULAR STRUCTURES
- C. SCHEDULES OF CHEMICALS

¹ An official version of the Annex on Chemicals can be obtained from the OPCW public website, www.opcw.org/chemical-weapons-convention/annexes/annex-chemicals/annex-chemicals.



A. GUIDELINES FOR SCHEDULES OF CHEMICALS

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.

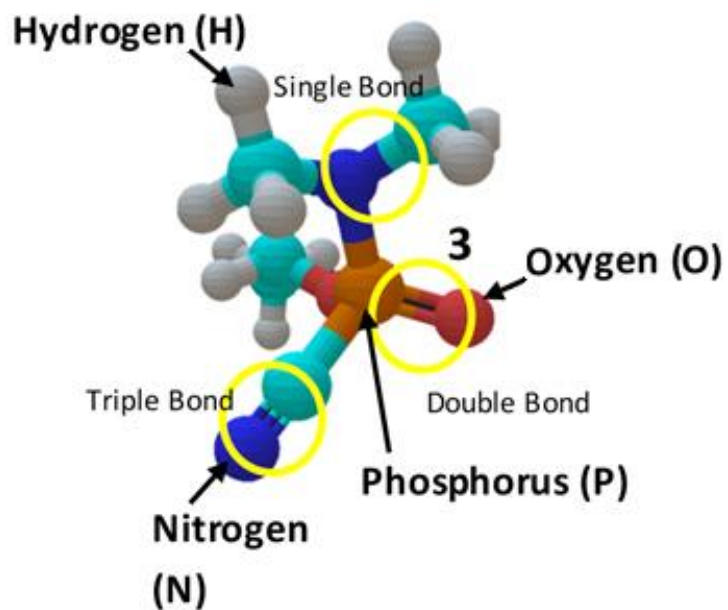
B. VISUALISING AND READING MOLECULAR STRUCTURES

Colour Code for Chemical Elements in 3D representations of this Annex

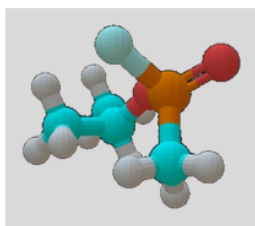
Carbon (C)		Hydrogen (H)		Sulfur (S)	
Nitrogen (N)		Phosphorus (P)		Arsenic (As)	
Chlorine (Cl)		Fluorine (F)		Oxygen (O)	

3D Models

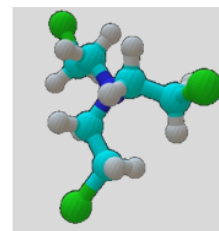
Representation of chemical structures as 3D ball and stick models. Each “ball” represents an atom of a chemical element identified by colour. The atoms are linked by chemical bonds, where a single line represents a “single bond”, two lines represent a “double bond” and three lines represent a “triple bond”.



3D Models

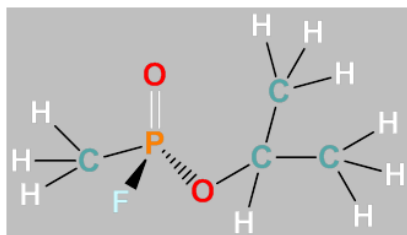


Sarin

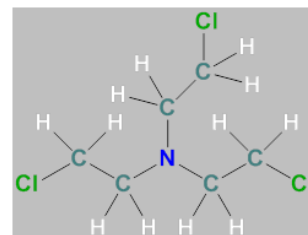


Nitrogen mustard (HN-3)

Translation

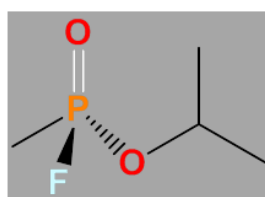


Sarin

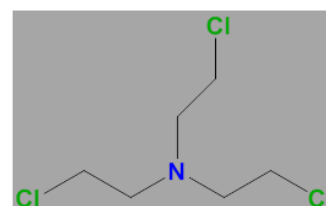


Nitrogen mustard (HN-3)

“Shorthand” structures



Sarin



Nitrogen mustard (HN-3)

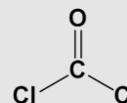
The 3D model is **translated** to a 2D molecular structure, where the type of atom is indicated by its chemical symbol. This 2D structure illustrates the connections between the atoms. This is an intermediate representation to the “shorthand” structures.

“**Shorthand**” structures are a format often used by chemists to simplify the structural representation. It illustrates 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 C and hydrogen (H) are not displayed. All other elements are indicated by their chemical symbol and bonds between an H atom and any type of atom other than C are displayed.

In the Structures of Relevance to the Annex on Chemicals:

➤ **Carbon atoms (C) have four bonds**

- If less than four bonds are shown in shorthand, the missing bonds are always C to H



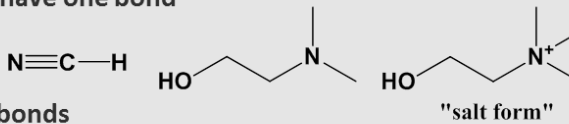
➤ **Chlorine and Fluorine atoms (Cl and F) have one bond**

➤ **Hydrogen atoms (H) have one bond**



➤ **Nitrogen atoms (N) have three or four bonds**

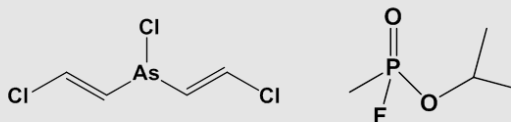
- four bonds are only for the "salt" form



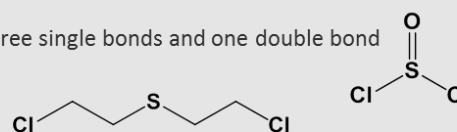
➤ **Oxygen atoms (O) have two bonds**

➤ **Phosphorus and Arsenic atoms (P and As) can have three, four, five or six bonds**

- In the form of a nerve agent P has five bonds - three single bonds and one double bond



➤ **Sulfur (S) can have two, four or six bonds**



C. SCHEDULES OF CHEMICALS

The following Schedules list toxic chemicals and their precursors. For the purpose of implementing this Convention, these 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.

Individual Schedules are defined by a general formula for a chemical family and/or specific chemical compounds. Associated chemical structures² and Chemical Abstracts Service (CAS) numbers are also included. Some of the chemicals have an associated 3D structure in “augmented reality” that can be viewed by scanning a QR code.^{2,3} Augmented reality QR codes are identified by ‘(A)’.

Whenever reference is made to groups of dialkylated chemicals, followed by a list of alkyl groups in parentheses, all chemicals possible by all possible combinations of alkyl groups listed in the parentheses are considered as listed in the respective Schedule as long as they are not explicitly exempted. A chemical marked "*" on Schedule 2, part A, is subject to special thresholds for declaration and verification, as specified in Part VII of the Verification Annex.

Scientific Advisory Board (SAB) Recommendations

Chemical Abstract Service (CAS) numbers should not solely be relied upon to define chemicals covered by the schedules. 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.^{4,5}

² These have been added to provide additional information to the contents of the Annex on Chemicals, it is not part of the official Annex on Chemicals of the Chemical Weapons Convention.

³ Viewing 3D molecular structures in augmented reality requires the use of the “Augment” App. The App is available for download to a mobile device from the “Play Store” (Android) or the “App Store” (iOS).



⁴ See: *Response to the Direction-General's Request to the Scientific Advisory Board to Provide Further Advice on Scheduled Chemicals* (SAB-23/WP.1, dated 28 of April 2016). Available at: www.opcw.org/sites/default/files/documents/SAB/en/sab-23-wp01_e_.pdf.



⁵ For further information see: “Advice from the Scientific Advisory Board of the Organisation for the Prohibition of Chemical Weapons on Isotopically Labelled Chemicals and Stereoisomers in Relation to the Chemical Weapon Convention”, C. M. Timperley, J. E. Forman, M. Abdollahi, A.S. Al-Amri, I. P. Alonso, A. Baulig, V. Borrett, Veronica Borrett, F. A. Cariño, C. Curty, D. Gonzalez, Z. Kovarik, R. Martínez-Álvarez, R. Mikulak, N. M. Fusaro Mourão, P. Ramasami, S. Neffe, S. K. Raza, V. Rubaylo, K. Takeuchi, C. Tang, F. Trifirò, F. Mauritz van Straten, P. S. Vanninen, V. Zaitsev, F. Waqar, M. Saïd Zina, S. Holen, H. A. Weinstein; *Pure Appl. Chem.*, 2018, *90*(10), 1647-1670. DOI: 10.1515/pac-2018-0803.

In order to ensure the consistency of declarations, if a chemical is included within a schedule, then all possible isotopically-labelled forms and stereoisomers of that chemical should be included, irrespective of whether or not they have been assigned a CAS number or have CAS numbers different to those shown in the Annex on Chemicals to the Convention. The isotopically-labelled compound or stereoisomer related to the parent chemical specified in the schedule should be interpreted belonging to the same schedule.^{4,5}

In regard to protonated salts of Scheduled chemicals, on scientific grounds, there should be no differentiation between the treatment of the free base and corresponding salt. Relevant Schedules are annotated to reflect this.⁶

⁶ For further information see *Report of the Scientific Advisory Board on Developments in Science and Technology for the Fourth Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention* (RC-4/DG.1, dated 30 April 2018). Available at: www.opcw.org/sites/default/files/documents/CSP/RC-4/en/rc4dg01_e.pdf.



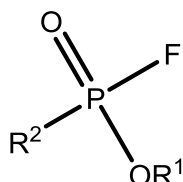
Schedule 1

(CAS registry number)

A. Toxic chemicals:

(1) O-Alkyl ($\leq C_{10}$, incl. cycloalkyl) alkyl

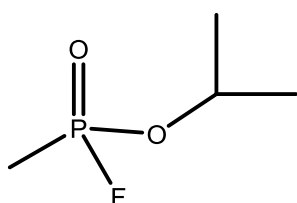
(Me, Et, n-Pr or i-Pr)-phosphonofluoridates



$R^1 \leq C_{10}$, including cycloalkyl, alkyl
 $R^2 = \text{Me, Et, n-Pr, i-Pr}$

e.g. Sarin: O-Isopropyl methylphosphonofluoridate

(107-44-8)



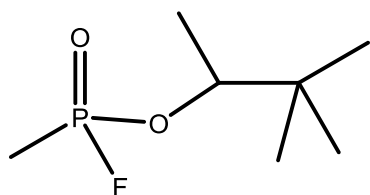
$R^1 = \text{i-Pr}$
 $R^2 = \text{Me}$



(A)

Soman: O-Pinacolyl methylphosphonofluoridate

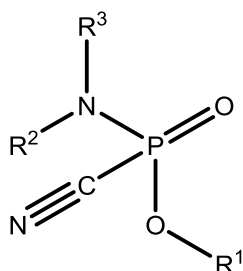
(96-64-0)



$R^1 = \text{Pinacolyl (3,3-dimethyl-2-butyl)}$
 $R^2 = \text{Me}$

(2) O-Alkyl ($\leq C_{10}$, incl. cycloalkyl) N,N-dialkyl

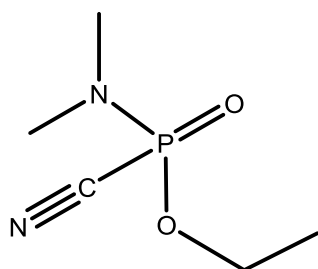
(Me, Et, n-Pr or i-Pr)-phosphoramidocyanidates



$R^1 \leq C_{10}$, including cycloalkyl, alkyl
 $R^2, R^3 = \text{Me, Et, n-Pr, i-Pr}$

e.g. Tabun: O-Ethyl N,N-dimethyl phosphoramidocyanidate

(77-81-6)



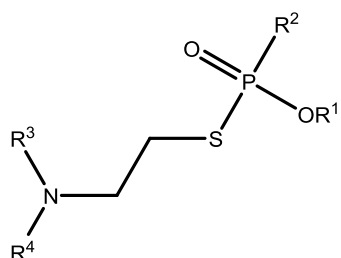
$R^1 = \text{Et}$
 $R^2, R^3 = \text{Me}$



(A)

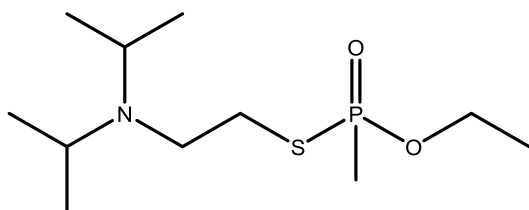
(3) O-Alkyl (H or $\leq C_{10}$, incl. cycloalkyl) S-2-dialkyl

(Me, Et, n-Pr or i-Pr)-aminoethyl alkyl
(Me, Et, n-Pr or i-Pr) phosphonothiolates and
corresponding alkylated or protonated salts.



$R^1 \leq C_{10}$, including cycloalkyl, alkyl
 $R^2, R^3, R^4 = \text{Me, Et, n-Pr, i-Pr}$

e.g. VX: O-Ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (50782-69-9)



$R^1 = \text{Et}$
 $R^2 = \text{Me}$
 $R^3, R^4 = \text{i-Pr}$

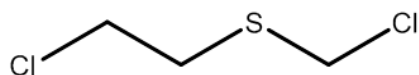


(A)

(4) Sulfur mustards:

2-Chloroethylchloromethylsulfide

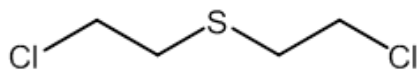
(2625-76-5)



(A)

Mustard gas: Bis(2-chloroethyl)sulphide

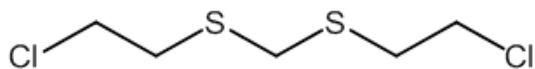
(505-60-2)



(A)

Bis(2-chloroethylthio)methane

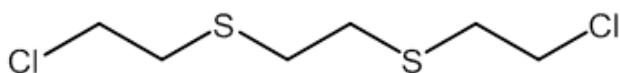
(63869-13-6)



(A)

Sesquimustard: 1,2-Bis(2-chloroethylthio)ethane

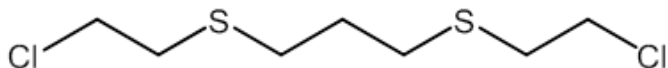
(3563-36-8)



(A)

1,3-Bis(2-chloroethylthio)-n-propane

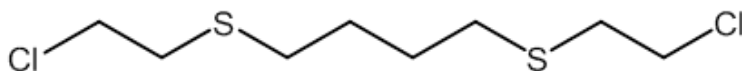
(63905-10-2)



(A)

1,4-Bis(2-chloroethylthio)-n-butane

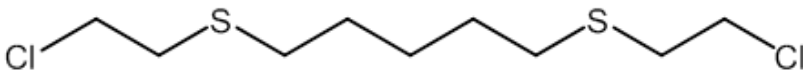
(142868-93-7)



(A)

1,5-Bis(2-chloroethylthio)-n-pentane

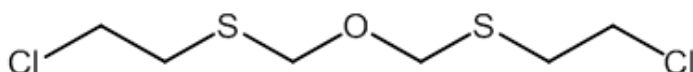
(142868-94-8)



(A)

Bis(2-chloroethylthiomethyl)ether

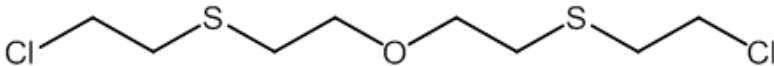
(63918-90-1)



(A)

O-Mustard: Bis(2-chloroethylthioethyl)ether

(63918-90-1)

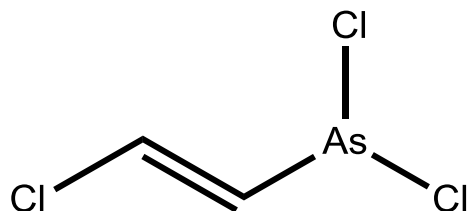


(A)

(5) **Lewisites:**

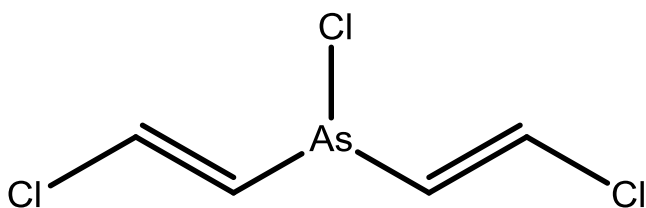
Lewisite 1: 2-Chlorovinylchloroarsine

(541-25-3)



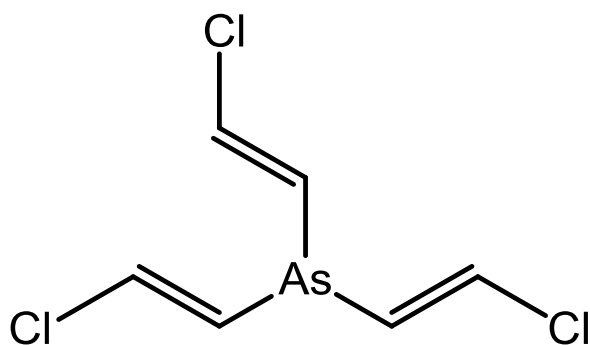
Lewisite 2: Bis(2-chlorovinyl)chloroarsine

(40334-69-8)



Lewisite 3: Tris(2-chlorovinyl)arsine

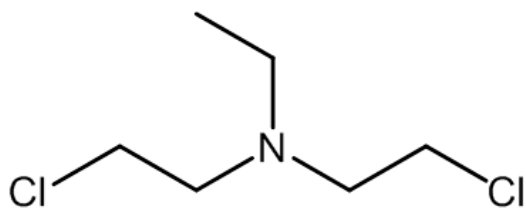
(40334-70-1)



(6) Nitrogen mustards:

HN1: Bis(2-chloroethyl)ethylamine

(538-07-8)

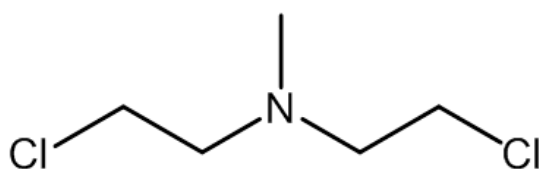


(A)

Including corresponding protonated salts (SAB recommendation).

HN2: Bis(2-chloroethyl)methylamine

(51-75-2)

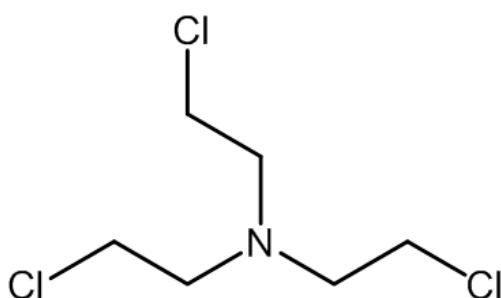


(A)

Including corresponding protonated salts (SAB recommendation).

HN3: Tris(2-chloroethyl)amine

(555-77-1)

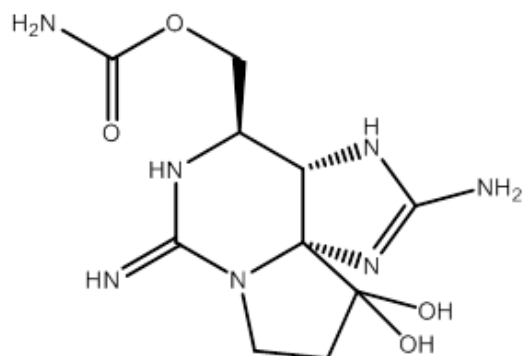


(A)

Including corresponding protonated salts (SAB recommendation).

(7) **Saxitoxin**

(35523-89-8)

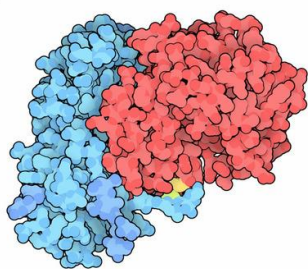


Including corresponding protonated salts (SAB recommendation).



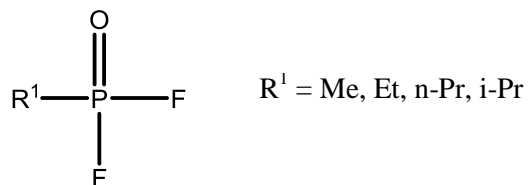
(8) **Ricin**

(9009-86-3)



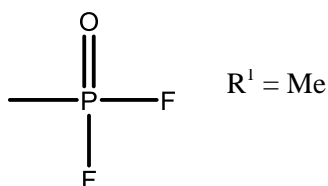
B. Precursors:

(9) Alkyl (Me, Et, n-Pr or i-Pr) phosphonyldifluorides



e.g. DF: Methylphosphonyldifluoride

(676-99-3)



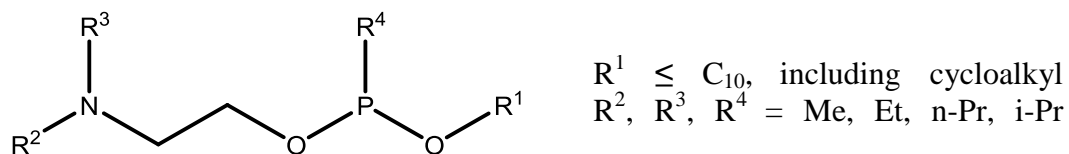
(A)

(10) O-Alkyl (H or $\leq \text{C}_{10}$, incl. cycloalkyl) O-2-dialkyl

(Me, Et, n-Pr or i-Pr)-aminoethyl alkyl

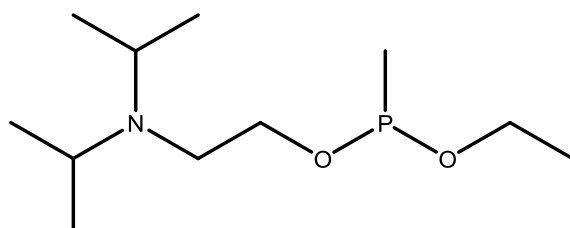
(Me, Et, n-Pr or i-Pr) phosphonites and

corresponding alkylated or protonated salts.



e.g. QL: O-Ethyl O-2-diisopropylaminoethyl methylphosphonite

(57856-11-8)



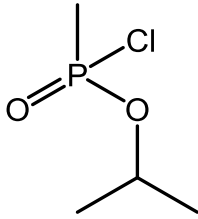
$\text{R}^1 = \text{Et}$
 $\text{R}^2, \text{R}^3 = \text{i-Pr}$
 $\text{R}^4 = \text{Me}$



(A)

(11) Chlorosarin: O-Isopropyl methylphosphonochloridate

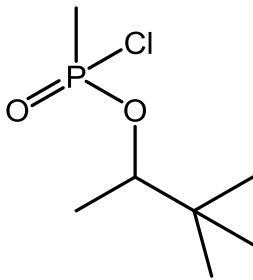
(1445-76-7)



(A)

(12) Chlorosoman: O-Pinacolyl methylphosphonochloridate

(7040-57-5)

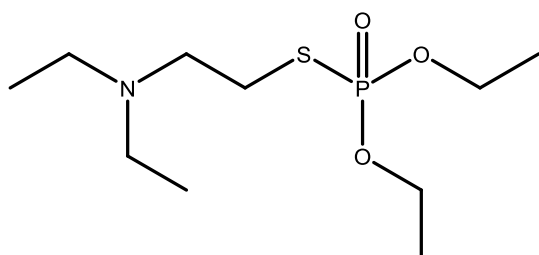


(A)

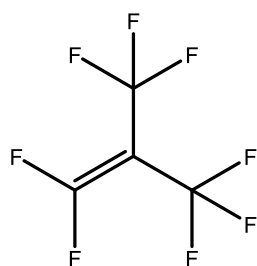
Schedule 2

A. Toxic chemicals:

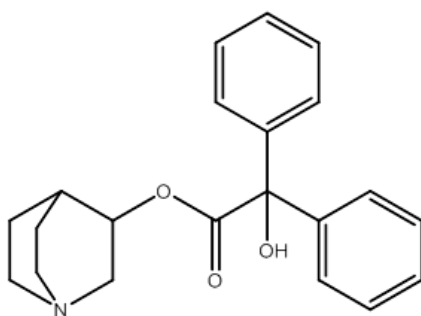
- (1) **Amiton: O,O-Diethyl S-[2-(diethylamino)ethyl]** phosphorothiolate and corresponding alkylated or protonated salts. (78-53-5)



- (2) **PFIB: 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene** (382-21-8)



- (3) **BZ: 3-Quinuclidinyl benzilate (*)** (6581-06-2)

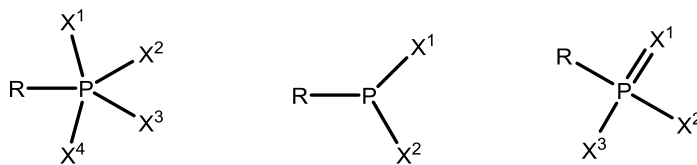


Including corresponding protonated salts (SAB recommendation).



B. Precursors:

- (4) 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. The following structures are possible:

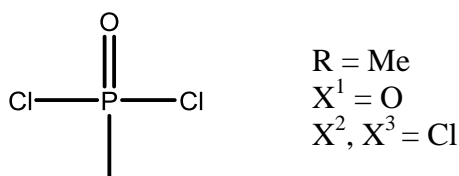


R = Me, Et, n-Pr, i-Pr

X₁, X₂, X₃, X₄ = Any group not attached to the phosphorus atom through a carbon.

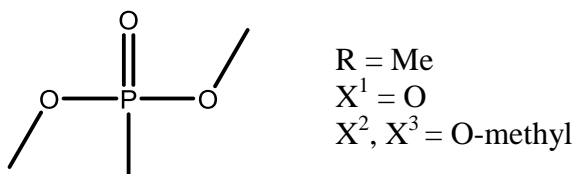
e.g. Methylphosphonyl dichloride

(676-97-1)



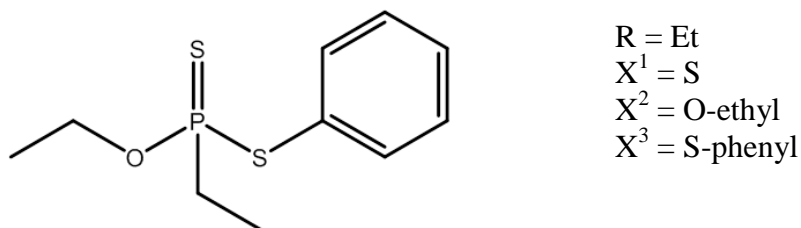
Dimethyl methylphosphonate

(756-79-6)

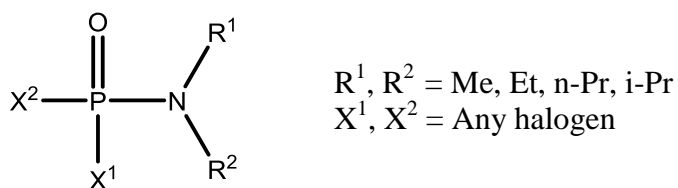


Exemption: Fonofos: O-Ethyl S-phenyl ethylphosphonothiolothionate

(944-22-9)

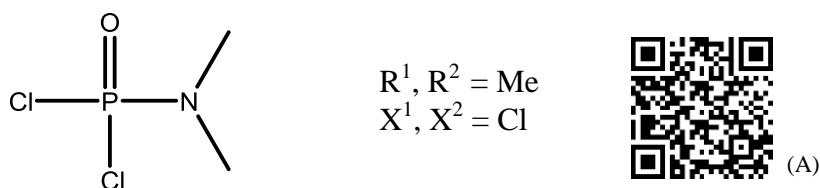


(5) **N,N-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidic dihalides**

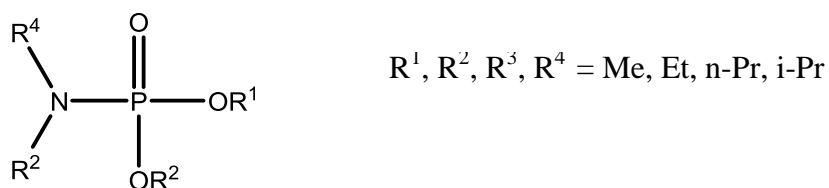


e.g. Dimethylamidophosphoric dichloride

(1499-29-2)

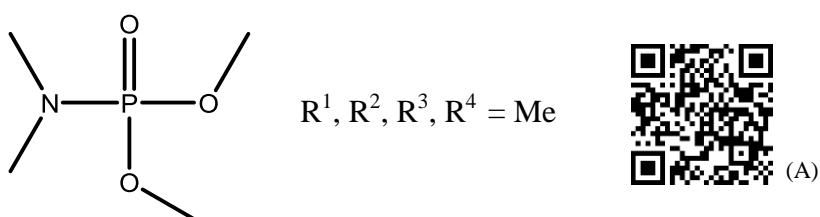


(6) **Dialkyl (Me, Et, n-Pr or i-Pr) N,N-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidates**



e.g. Dimethyl dimethylphosphoramidate

(597-07-9)



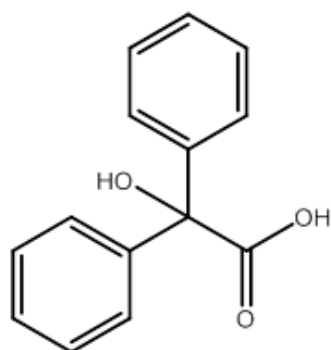
(7) **Arsenic trichloride**

(7784-34-1)



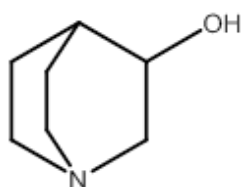
(8) 2,2-Diphenyl-2-hydroxyacetic acid

(76-93-7)



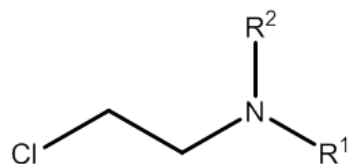
(9) Quinuclidin-3-ol

(1619-34-7)



Including corresponding protonated salts (SAB recommendation).

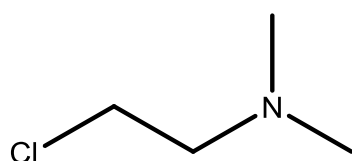
(10) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethyl-2-chlorides and corresponding protonated salts.



R¹, R² = Me, Et, n-Pr, i-Pr

e.g. 2-chloro-N,N-dimethylethan-1-amine

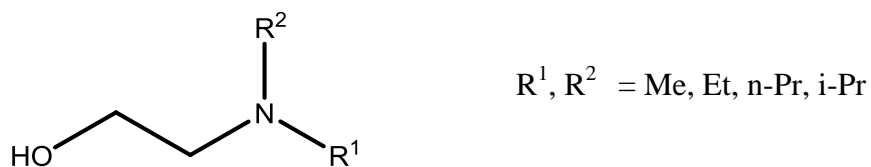
(4684-46-7)



R¹, R² = Me

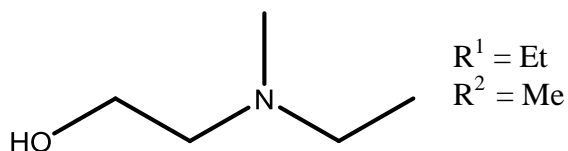


(11) **N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-ols**
and corresponding protonated salts.



e.g. 2-(ethylmethylamino)ethanol

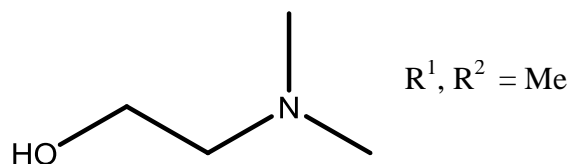
(2893-43-8)



(A)

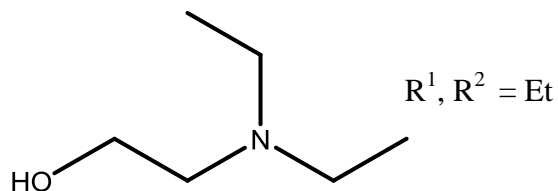
Exemptions: N,N-Dimethylaminoethanol
and corresponding protonated salts

(108-01-0)

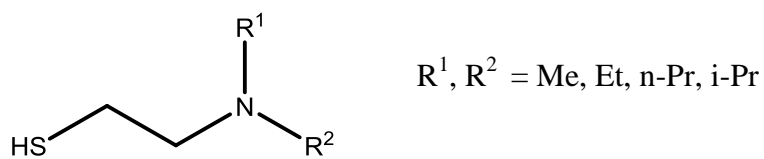


N,N-Diethylaminoethanol
and corresponding salts

(100-37-8)

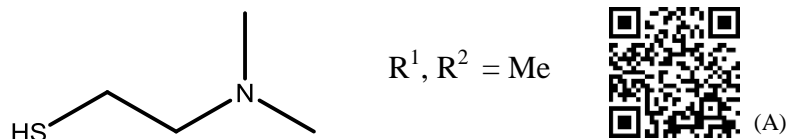


(12) **N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-thiols**
and corresponding protonated salts.



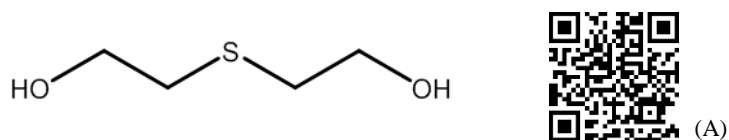
e.g. 2-(dimethylamino)ethan-1-thiol

(108-01-0)



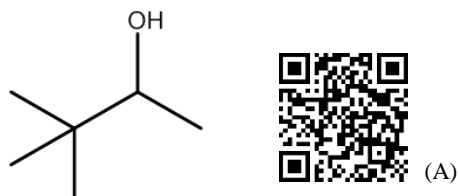
(13) **Thiodiglycol: Bis(2-hydroxyethyl)sulfide**

(111-48-8)



(14) **Pinacolyl alcohol: 3,3-Dimethylbutan-2-ol**

(464-07-3)



Schedule 3

A. Toxic chemicals:

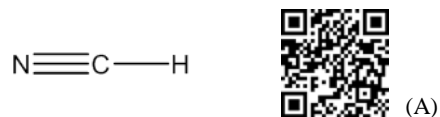
- (1) **Phosgene: Carbonyl dichloride** (75-44-5)



- (2) **Cyanogen chloride** (506-77-4)



- (3) **Hydrogen cyanide** (74-90-8)

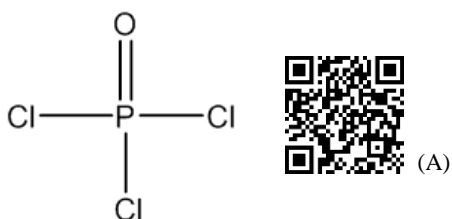


- (4) **Chloropicrin: Trichloronitromethane** (76-06-2)



B. Precursors:

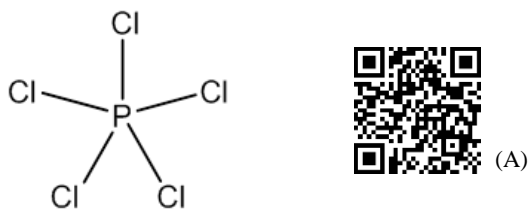
- (5) **Phosphorus oxychloride** (10025-87-3)



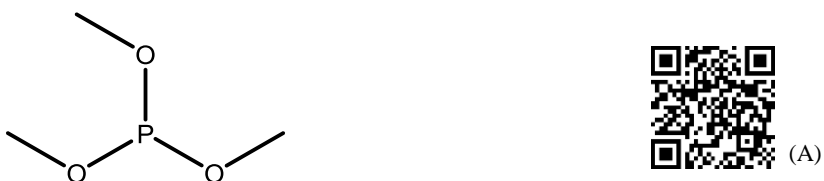
- (6) **Phosphorus trichloride** (7719-12-2)



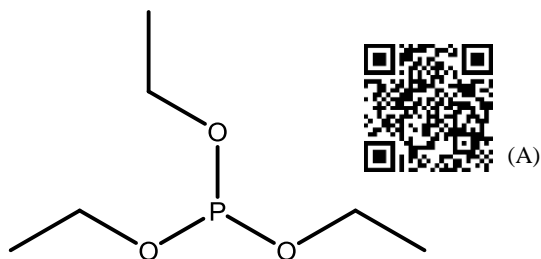
(7) **Phosphorus pentachloride** (10026-13-8)



(8) **Trimethyl phosphite** (121-45-9)



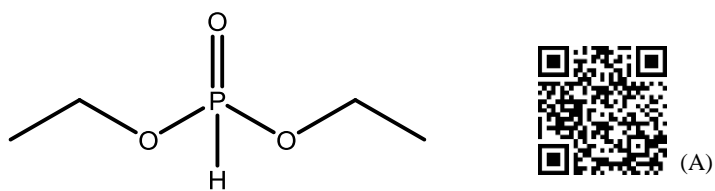
(9) **Triethyl phosphite** (122-52-1)



(10) **Dimethyl phosphite** (868-85-9)



(11) **Diethyl phosphite** (762-04-9)

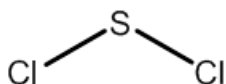


(12) **Sulfur monochloride** (10025-67-9)



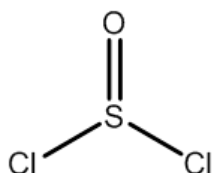
(13) Sulfur dichloride

(10545-99-0)



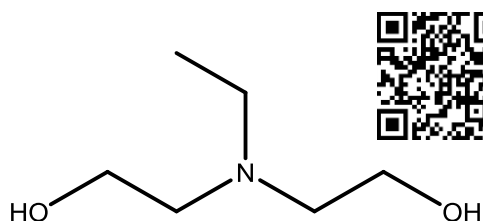
(14) Thionyl chloride

(7719-09-7)



(15) Ethyldiethanolamine

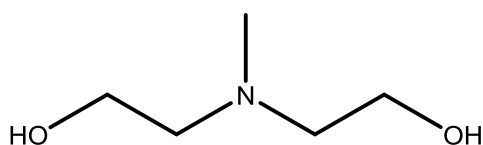
(139-87-7)



Including corresponding protonated salts (SAB recommendation).

(16) Methyldiethanolamine

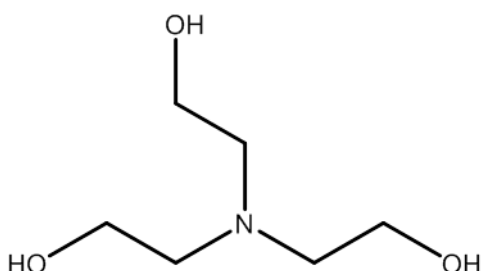
(105-59-9)



Including corresponding protonated salts (SAB recommendation).

(17) Triethanolamine

(102-71-6)



Including corresponding protonated salts (SAB recommendation).