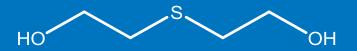
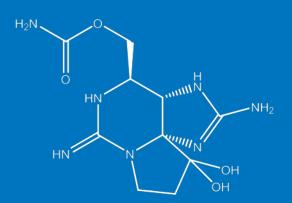
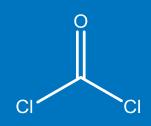
ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS

THE "SCIENCE FOR DIPLOMATS" ANNEX ON CHEMICALS

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









THE "SCIENCE FOR DIPLOMATS" ANNEX ON CHEMICALS

*A user friendly and scientifically annotated version of the Chemical Weapons Convention Annex on Chemicals*¹

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1

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

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.

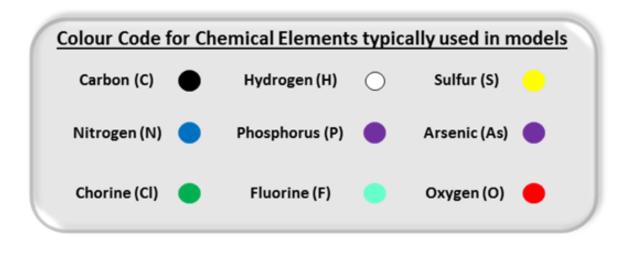
Guidelines for Schedule 2

- 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

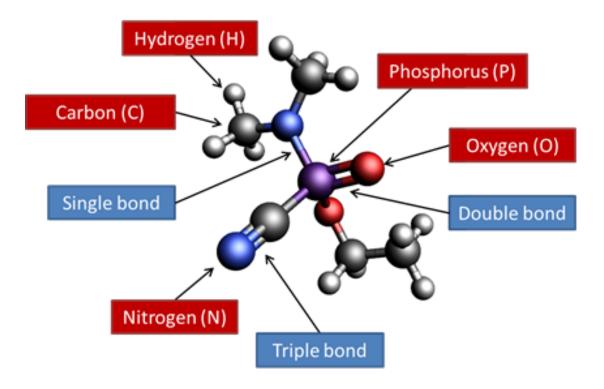
- 3. The following criteria shall be taken into account in considering whether a toxic chemical or precursor, not listed in other Schedules, should be included in Schedule 3:
 - (a) It has been produced, stockpiled or used as a chemical weapon;
 - (b) It poses otherwise a risk to the object and purpose 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.

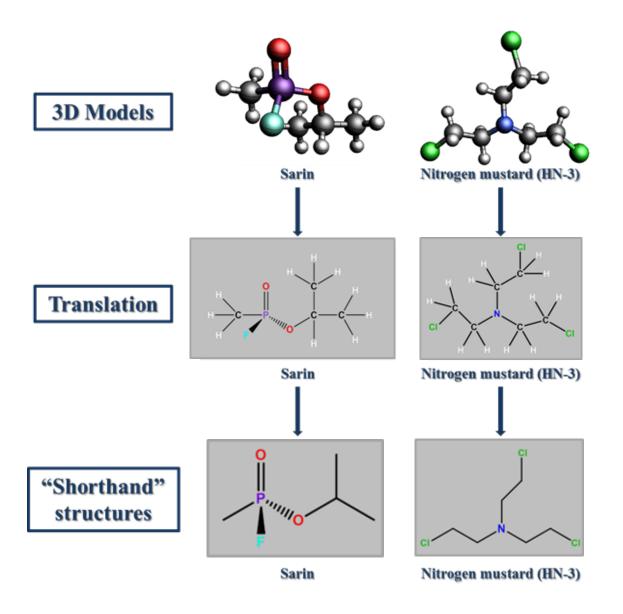
B. VISUALISING AND READING MOLECULAR STRUCTURES





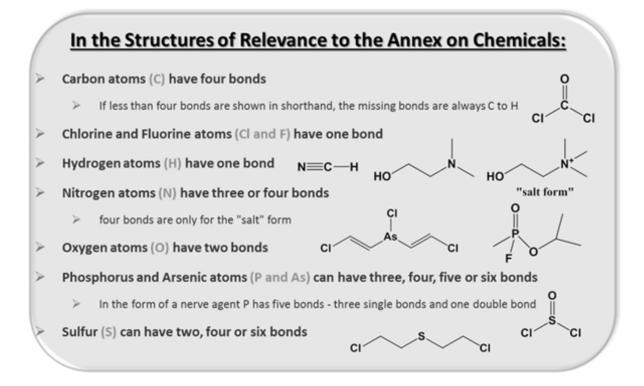
Representation of chemical structures as 3D ball and stick models. Each "ball" represents an atom of a chemical element identified by colour. The atoms are linked by chemical bonds, where a single line represents a "single bond", two lines represent a "double bond" and three lines represent a "triple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





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.



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. Specific chemical examples are provided with associated interactive 3D molecular structures. These structures are activated by clicking on the graphic to enable 3D Content.³ Once activated, click on the image again and use the mouse to rotate (left button) or resize (right button).

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 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}

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 April 2016). Available at: <u>www.opcw.org/sites/default/files/documents/SAB/en/sab-23-wp01_e_.pdf</u>.



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.

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 In order to use the interactive molecular structure feature, you may be prompted to enable the 3D Content by labelling the document as "trusted" (there will be an option to select for this).

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

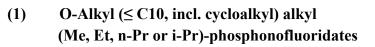
⁶ For further information see *Report of the Scientific Advisory Board on Developments in Science and Technology for the Fourth Special Session of the Conference of the States Parties to Review the Operation of the Chemical Weapons Convention* (RC-4/DG.1, dated 30 April 2018). Available at: <u>www.opcw.org/sites/default/files/documents/CSP/RC-4/en/rc4dg01_e_.pdf</u>.

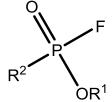


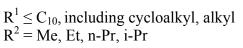
Schedule 1

(2)

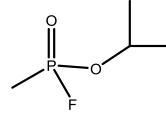
A. Toxic chemicals:

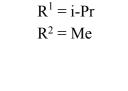






e.g. Sarin: O-Isopropyl methylphosphonofluoridate (*IUPAC Name: 2-[fluoro(methyl)phosphoryl]oxypropane*)

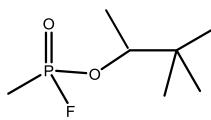




(107-44-8)

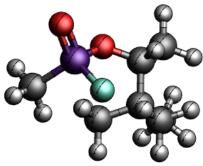
(96-64-0)

e.g Soman: O-Pinacolyl methylphosphonofluoridate (IUPAC Name: 3-[fluoro(methyl)phosphoryl]oxy-2,2-dimethylbutane)

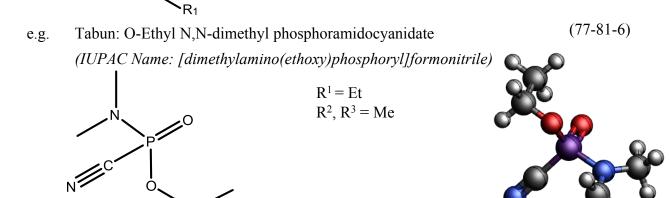


O-Alkyl ($\leq C_{10}$, incl. cycloalkyl) *N*,*N*-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidocyanidates

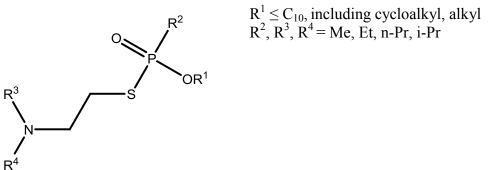
 R^1 = Pinacolyl (3,3-dimethyl-2-butyl) R^2 = Me



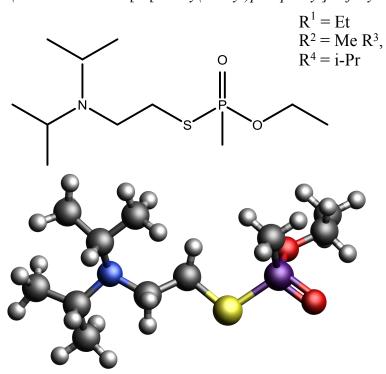
 $R^1 \leq C_{10}$, including cycloalkyl, alkyl R^2 , $R^3 = Me$, Et, n-Pr, i-Pr



(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.



e.g. VX: O-Ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (50782-69-9) (*IUPAC Name: N-[2-[ethoxy(methyl]phosphoryl]sulfanylethyl]-N-propan-2-ylpropan-2-amine*)

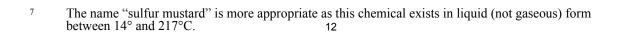


(4) Sulfur mustards:

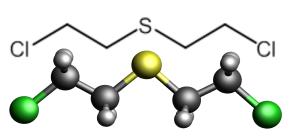
(IUPAC Name: 1-chloro-2-(2-chloroethylsulfanyl)ethane)

Bis(2-chloroethylthio)methane (*IUPAC Name: 1-chloro-2-(2-chloroethylsulfanylmethylsulfanyl)ethane*)

(3563-36-8)



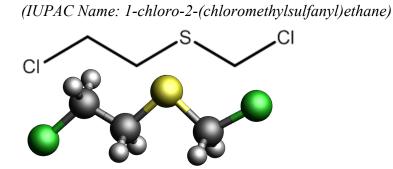
CI



Sesquimustard: 1,2-Bis(2-chloroethylthio)ethane (IUPAC Name: 1,2-bis(2-chloroethylsulfanyl)ethane)

C

С



Mustard gas7: Bis(2-chloroethyl)sulphide

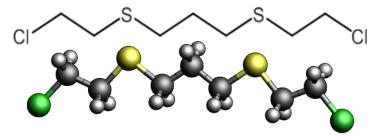
2-Chloroethylchloromethylsulfide

(2625-76-5)

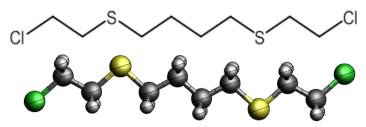
(505-60-2)

(63869-13-6)

1,3-Bis(2-chloroethylthio)-n-propane (IUPAC Name: 1,3-bis(2-chloroethylsulfanyl)propane)



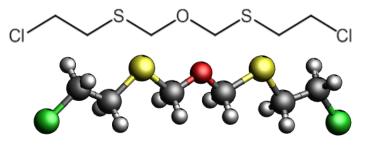
1,4-Bis(2-chloroethylthio)-n-butane (*IUPAC Name: 1,4-bis(2-chloroethylsulfanyl)*butane)



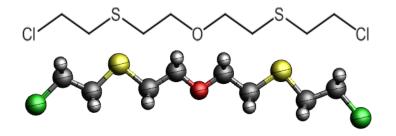
1,5-Bis(2-chloroethylthio)-n-pentane (IUPAC Name: 1,5-bis(2-chloroethylsulfanyl)pentane)

S CI CI

Bis(2-chloroethylthiomethyl)ether (IUPAC Name: 1,4-bis[(2-chloroethyl)sulfanyl]butane)



O-Mustard: Bis(2-chloroethylthioethyl)ether (IUPAC Name: 1-chloro-2-(2-chloroethylsulfanylmethoxymethylsulfanyl)ethane)



(142868-94-8)

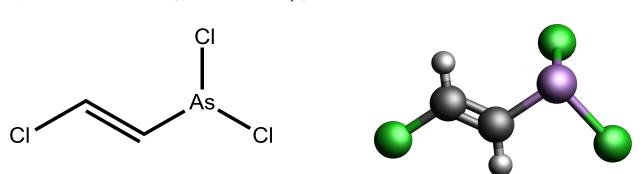
(142868-93-7)

(63918-89-8)

(63918-90-1)

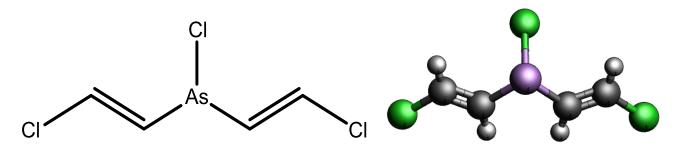
(5) Lewisites:

Lewisite 1: 2-Chlorovinyldichloroarsine (*IUPAC Name: dichloro-[(E)-2-chloroethenyl]arsane*) (541-25-3)

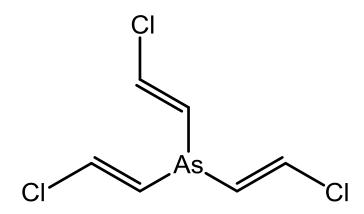


Lewisite 2: Bis(2-chlorovinyl)chloroarsine (IUPAC Name: chloro-bis[(E)-2-chloroethenyl]arsane)

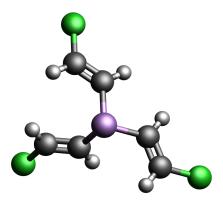
(40334-69-8)



Lewisite 3: Tris(2-chlorovinyl)arsine (*IUPAC Name: tris[(E)-2-chloroethenyl]arsane*)



(40334-70-1)



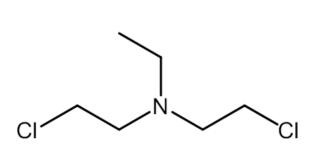
(6) Nitrogen mustards:

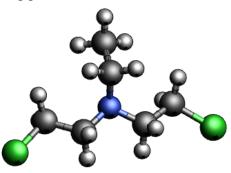
HN1: Bis(2-chloroethyl)ethylamine

(538-07-8)

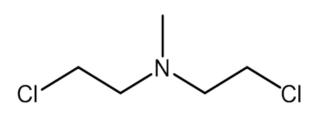
(*IUPAC Name: 2-chloro-N-(2-chloroethyl)-N-ethylethanamine*)

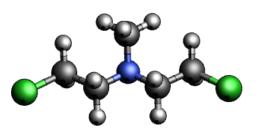
Scientific Advisory Board recommendation: including corresponding protonated salts.



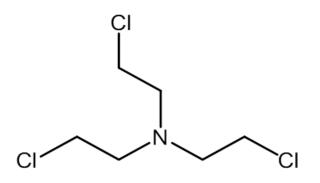


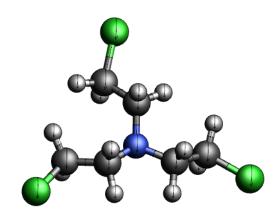
HN2:Bis(2-chloroethyl)methylamine(51-75-2)(IUPAC Name: 2-chloro-N-(2-chloroethyl)-N-methylethanamine)Scientific Advisory Board recommendation: including corresponding protonated salts.





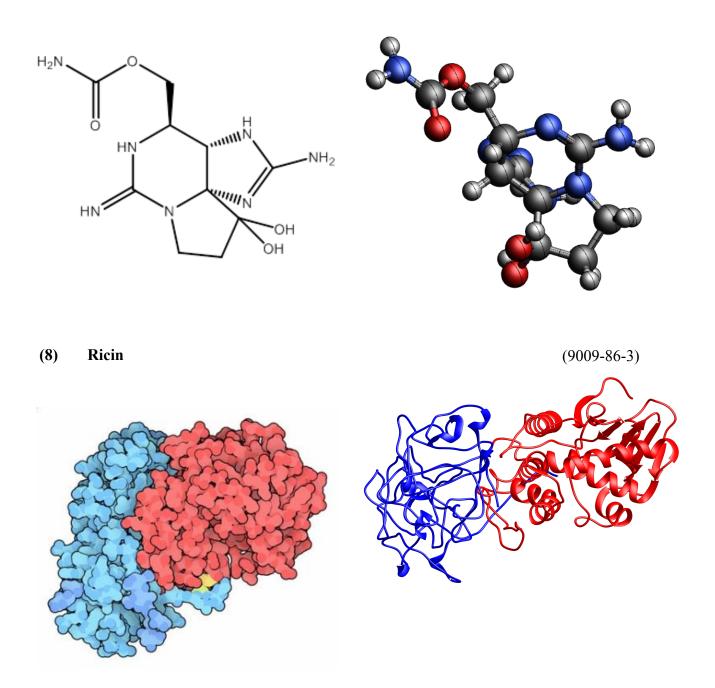
HN3: Tris(2-chloroethyl)amine(555-77-1)(IUPAC Name: 2-chloro-N,N-bis(2-chloroethyl)ethanamine)Scientific Advisory Board recommendation: including corresponding protonated salts.





(7) Saxitoxin

(*IUPAC Name:* [(3aS,4R,10aS)-2,6-diamino-10,10-dihydroxy-3a,4,8,9-tetrahydro-1Hpyrrolo[1,2-c]purin-4-yl]methyl carbamate) Scientific Advisory Board recommendation: including corresponding protonated salts.



Ricin is a protein composed of toxic (A-chain) and cell-targeting (B-chain) subunits, illustrated in red (A-chain) and blue (B-chain) in the structure on the left. The right structure is an interactive ribbon model of the ricin molecule.⁸

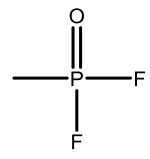
 ⁸ E. Rutenber, B. J. Katzin, S. Ernst, E. J. Collins, M. P. Ready, J. D. Robertus; Crystallographic refinement of ricin to 2.5 Angstroms; *Proteins*; 1991, 10, 240-250. DOI: 10.1002/prot.340100308. Protein Data Bank structure 2AA1. Available at: https://www.rcsb.org/structure/2AAI.

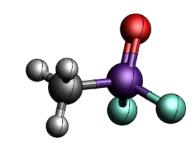
B. Precursors:

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



e.g DF: Methylphosphonyldifluoride (IUPAC Name: difluorophosphorylmethane)

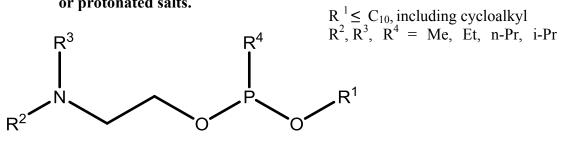




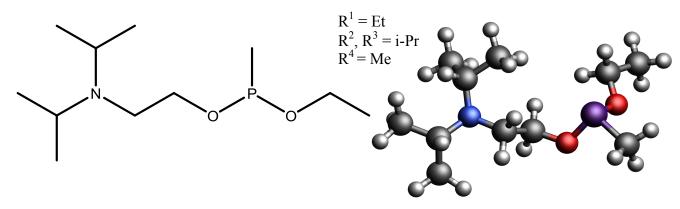
(676 - 99 - 3)

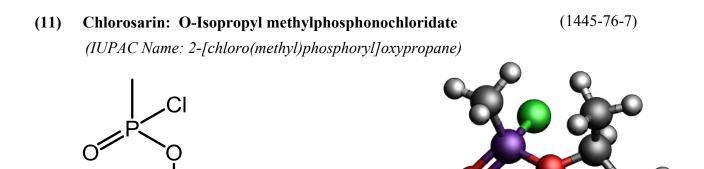
(10) O-Alkyl (H or ≤ C₁₀, incl. cycloalkyl) *O*-2-dialkyl
(Me, Et, n-Pr or i-Pr)-aminoethyl alkyl
(Me, Et, n-Pr or i-Pr) phosphonites and corresponding alkylated or protonated salts.

 $R^1 = Me$

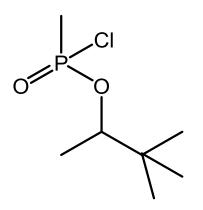


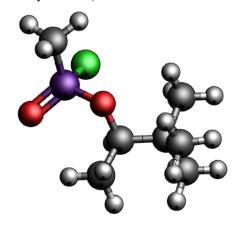
e.g. QL: O-Ethyl O-2-diisopropylaminoethyl methylphosphonite (57856-11-8) (*IUPAC Name: N-[2-[ethoxy(methyl)phosphanyl]oxyethyl]-N-propan-2-ylpropan-2-amine*)





(12) Chlorosoman: O-Pinacolyl methylphosphonochloridate (7040-57-5) (IUPAC Name: 3-[chloro(methyl)phosphoryl]oxy-2,2-dimethylbutane)

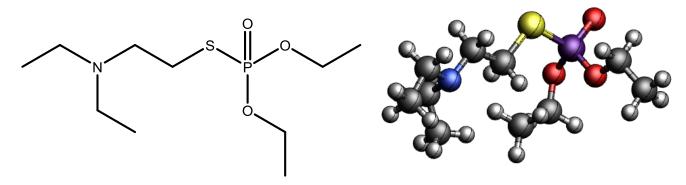




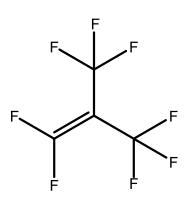
Schedule 2

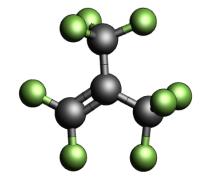
A. Toxic chemicals:

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

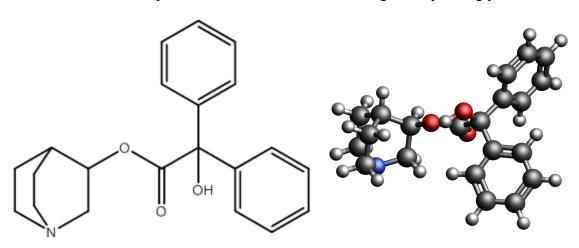


(2) **PFIB: 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene** (382-21-8) (*IUPAC Name: 1,1,3,3,3-pentafluoro-2-(trifluoromethyl)prop-1-ene*)

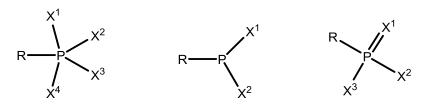




(3) BZ: 3-Quinuclidinyl benzilate (*) (6581-06-2) (*IUPAC Name: 1-azabicyclo*[2.2.2]octan-3-yl 2-hydroxy-2,2-diphenylacetate) Scientific Advisory Board recommendation: including corresponding protonated salts.

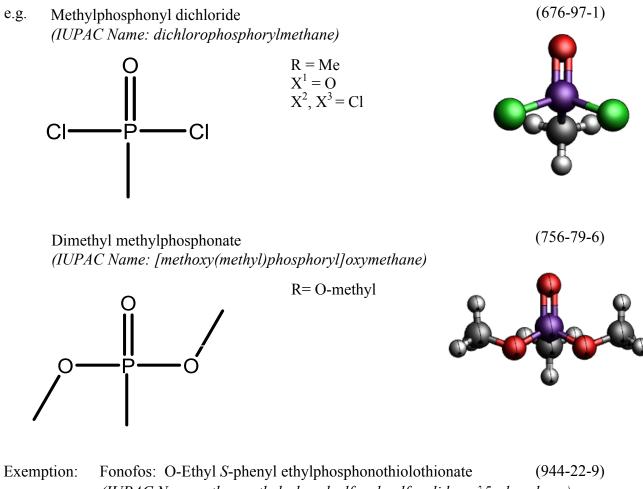


- B. Precursors:
- (4) Chemicals, except for those listed in Schedule 1, containing a phosphorus atom to which is bonded one methyl, ethyl or propyl (normal or iso) group but not further carbon atoms. The following structures are possible:

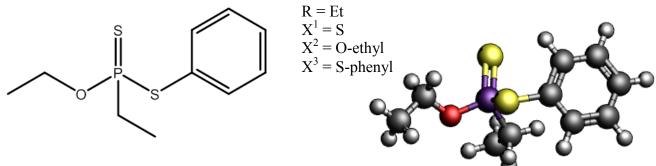


R = Me, Et, n-Pr, i-Pr

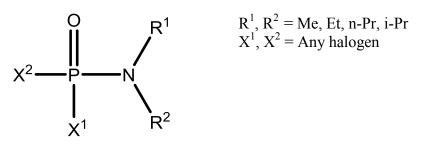
 X_1, X_2, X_3, X_4 = Any group not attached to the phosphorus atom through a carbon.

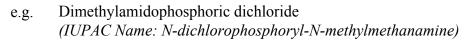


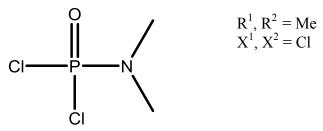
(IUPAC Name: ethoxy-ethyl-phenylsulfanyl-sulfanylidene- λ 5-phosphane)

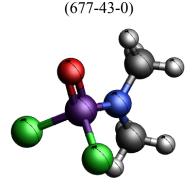


(5) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) phosphoramidic dihalides

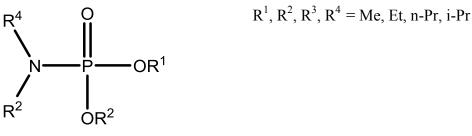






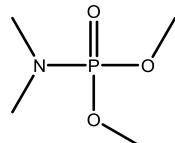


(6) Dialkyl (Me, Et, n-Pr or i-Pr) N,N-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoramidates (Me, Et, n-Pr or i-Pr)-phosphoramidates

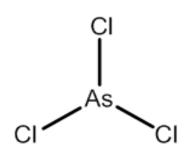


e.g. Dimethyl dimethylphosphoramidate (597-07-9) (IUPAC Name: N-dimethoxyphosphoryl-N-methylmethanamine)

 $R^{1}, R^{2}, R^{3}, R^{4} = Me$

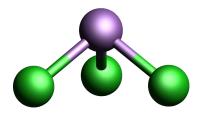


(7) Arsenic trichloride (IUPAC Name: trichloroarsane)



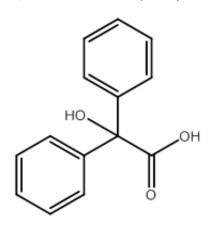


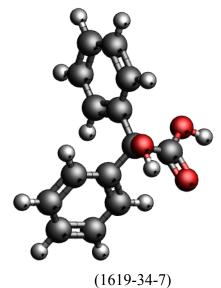
(7784 - 34 - 1)



(8) 2,2-Diphenyl-2-hydroxyacetic acid (IUPAC Name: 2-hydroxy-2,2-diphenylacetic acid)

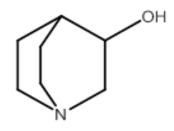
(76-93-7)

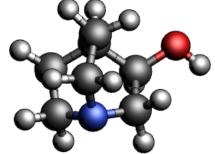




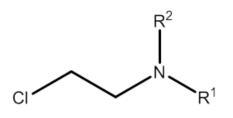
(9) Quinuclidin-3-ol

(IUPAC Name: 1-azabicyclo[2.2.2]octan-3-ol) Scientific Advisory Board recommendation: including corresponding protonated salts.



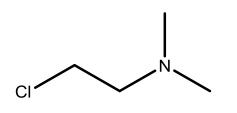


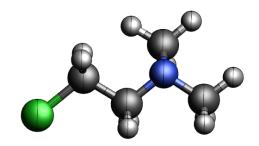
(10) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethyl-2-chlorides and corresponding protonated salts.



 R^1 , R^2 = Me, Et, n-Pr, i-Pr

e.g. 2-chloro-N,N-dimethylethan-1-amine (IUPAC Name: 2-chloro-N,N-dimethylethanamine)





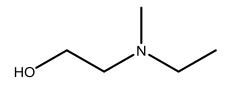
(4684 - 46 - 7)

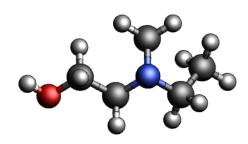
 $R^1, R^2 = Me$

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



e.g. 2-(ethylmethylamino)ethanol (IUPAC Name: 2-[ethyl(methyl)amino]ethanol)





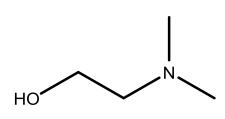
(2893-43-8)

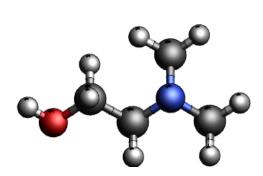
Exemptions: N,N-Dimethylaminoethanol and corresponding protonated salts (108-01-0) (IUPAC Name: 2-(dimethylamino)ethanol)

 $R^1, R^2 = Me$

 R^1 , $R^2 = Et$

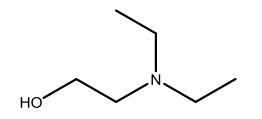
 $R^{1} = Et$ $R^{2} = Me$

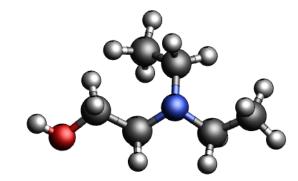




N,N-Diethylaminoethanol and corresponding salts (*IUPAC Name: 2-(diethylamino)ethanol*)





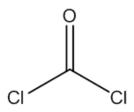


and corresponding protonated salts. R^1 R^1 , $R^2 = Me$, Et, n-Pr, i-Pr R^2 HS 2-(dimethylamino)ethan-1-thiol (108-02-01)e.g. (IUPAC Name: 2-(dimethylamino)ethanethiol) $R^1, R^2 = Me$ HS (111-48-8)Thiodiglycol: Bis(2-hydroxyethyl)sulfide (13) (IUPAC Name: 2-(2-hydroxyethylsulfanyl)ethanol) HO OH Pinacolyl alcohol: 3,3-Dimethylbutan-2-ol (464-07-3)(14) (IUPAC Name: 3,3-dimethylbutan-2-ol) OH

(12) N,N-Dialkyl (Me, Et, n-Pr or i-Pr) aminoethane-2-thiols

Schedule 3

- A. Toxic chemicals:
- (1) Phosgene: Carbonyl dichloride (IUPAC Name: carbonyl dichloride)



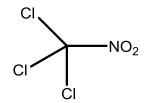
(2) Cyanogen chloride (IUPAC Name: Cyanic chloride)



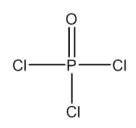
(3) Hydrogen cyanide (IUPAC Name: carbononitridic chloride)



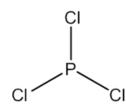
(4) Chloropicrin: Trichloronitromethane (*IUPAC Name: trichloro(nitro)methane*)

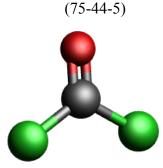


- B. Precursors:
- (5) Phosphorus oxychloride (IUPAC Name: phosphoryl trichloride)



(6) Phosphorus trichloride (IUPAC Name: trichlorophosphane)

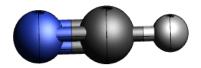




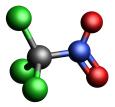




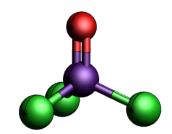
(74-90-8)



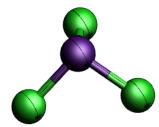
(76-06-2)

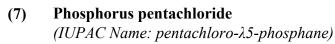


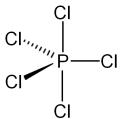
(10025-87-3)

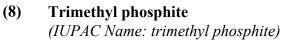


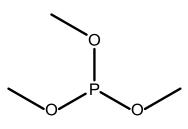
(7719-12-2)

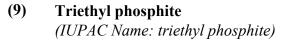


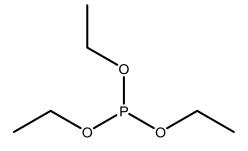




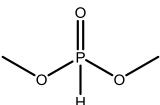


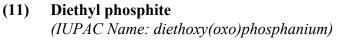


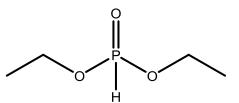




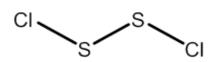


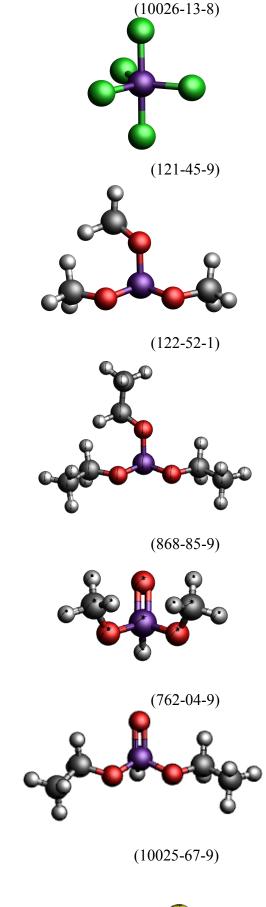




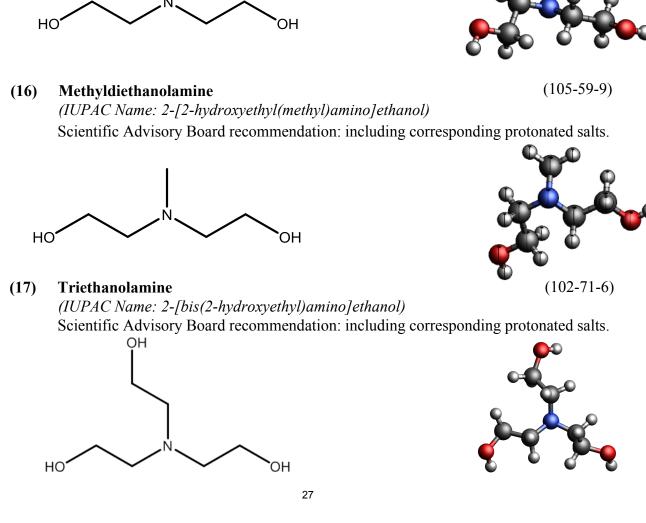


(12) Sulfur monochloride (IUPAC Name: chlorosulfanyl thiohypochlorite)



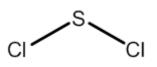






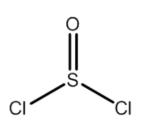
Scientific Advisory Board recommendation: including corresponding protonated salts.

(13) Sulfur dichloride (IUPAC Name: chloro thiohypochlorite)

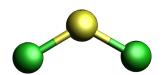


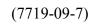
(14) **Thionyl chloride** (IUPAC Name: thionyl dichloride)

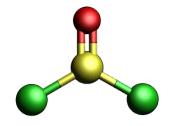
Ethyldiethanolamine



(IUPAC Name: 2-[ethyl(2-hydroxyethyl)amino]ethanol)







(139-87-7)



(15)

(10545-99-0)

D. RIOT CONTROL AGENTS

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".⁹

RCAs are subject to declaration in accordance with subparagraph 1(e) of Article III of the Chemical Weapons Convention.¹⁰

Scientific Advisory Board Advice

The SAB considered a list of 60 chemicals that included 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 Chemical Agent Database (OCAD) that had been drafted by the SAB's Temporary Working Group (TWG) on Analytical Procedures in 2001;¹¹ 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.^{12,13}



The SAB advised that the following set of 17 chemicals would be consistent with the definition of an RCA under the Chemical Weapons Convention:¹⁴

- See paragraph 7 of Article II of the *Chemical Weapons Convention*. Available at: <u>www.opcw.org/chemical-weapons-convention/articles/article-ii-definitions-and-criteria</u>.
- See subparagraph 1(e) of Article III of the *Chemical Weapons Convention*. Available at: www.opcw.org/chemical-weapons-convention/articles/article-iii-declarations.



See paragraph 2.5 of *Report of the Fourth Session of the Scientific Advisory Board* (SAB-IV/1, dated 6 February 2001), Available at: www.opcw.org/sites/default/files/documents/SAB/en/SABIV1 e .pdf.



13

12

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11

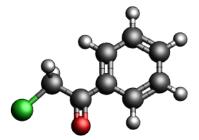
See: Response to the Direction-General's Request to the Scientific Advisory Board to Provide Consideration On Which Riot Control Agents are Subject to Declaration Under the Chemical Weapons Convention (SAB-25/WP.1, dated 27 March 2017). Available at: www.opcw.org/sites/default/files/documents/SAB/en/sab25wp01 e .pdf.

For further information see: "Advice from Scientific Advisory Board of the Organisation for the Prohibition of Chemical Weapons on riot control agents in connection with the Chemical Weapons Convention". C. Timperley, J. Forman, P. Aas, M. Abdollahi, D. Benachour, A. Al-Amri, A. Baulig, R. Becker-Arnold, V. Borrett, F. Carino, C. Curty, D. Gonzalez, M. Geist, Michael; B. Kane, Z. Kovarik, R. Martinez-Alvarez, B. Mikulak, N. Mourao, S. Neffe, E. Noguiera, P. Ramasami, Ponnadurai; S. Raza, V. Rubaylo, A. Saeed, K. Takeuchi, C. Tang, F. Trifiro, F. van Straten, A. Suarez, F. Waqar, P. Vanninen, M. Zafar-Uz-Zamen, S. Vucinic, V. Zaitsev, M. Zina, S. Holen, F. Izzati; RSC Adv, 2018, 8, 41731-41739. DOI: 10.1039/c8ra08273a.

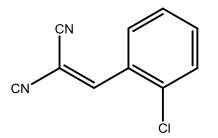


See: Note by the Technical Secretariat - Declaration of Riot Control Agents: Advice From the Scientific Advisory Board (S/1177/2014, dated 1 May 2014). Available at: www.opcw.org/sites/default/files/documents/S series/2014/en/s-1177-2014 e .pdf.

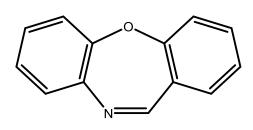
(1) 2-Chloroacetophenone (CN) (IUPAC Name: 2-chloro-1-phenylethanone) (532-27-4)

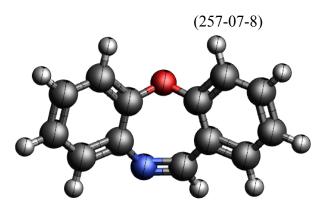


(2) 2-Chlorobenzylidenemalononitrile (CS) (2698-41-1) (IUPAC Name: 2-[(2-chlorophenyl)methylidene]propanedinitrile)

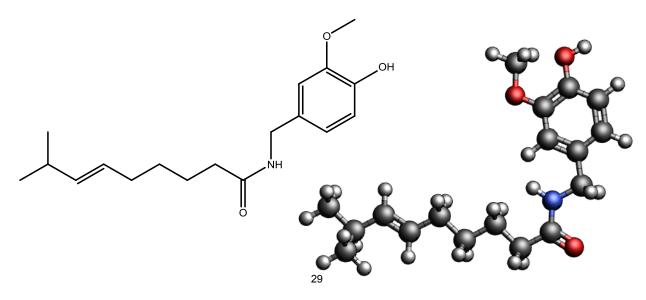


(3) **Dibenzo[b,f][1,4]oxazepine (CR)** (IUPAC Name: benzo[b][1,4]benzoxazepine)

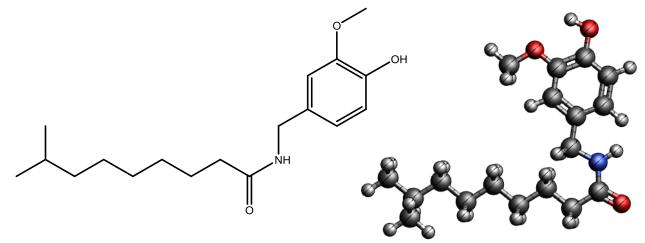




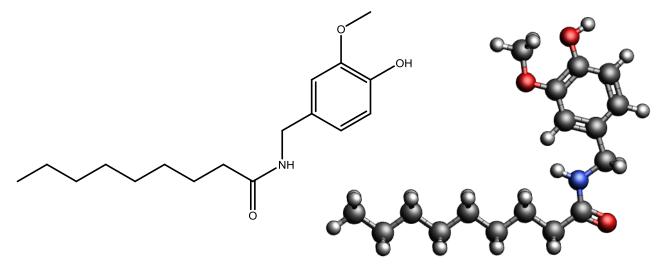
(4)8-Methyl-N-vanillyl-trans-6-nonenamide (capsaicin)(404-86-4)(IUPAC Name: (E)-N-[(4-hydroxy-3-methoxyphenyl)methyl]-8-methylnon-6-enamide)



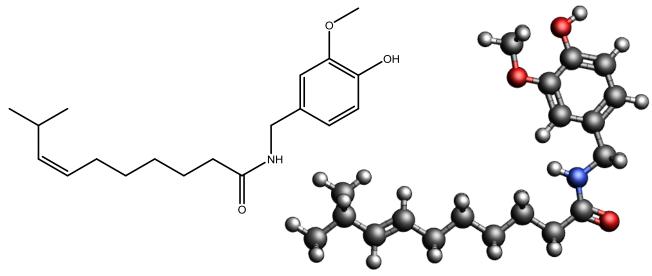
(5) **8-Methyl-N-vanillylnonamide (dihydrocapsaicin)** (19408-84-5) (*IUPAC Name: N-[(4-hydroxy-3-methoxyphenyl)methyl]-8-methylnonanamide*)



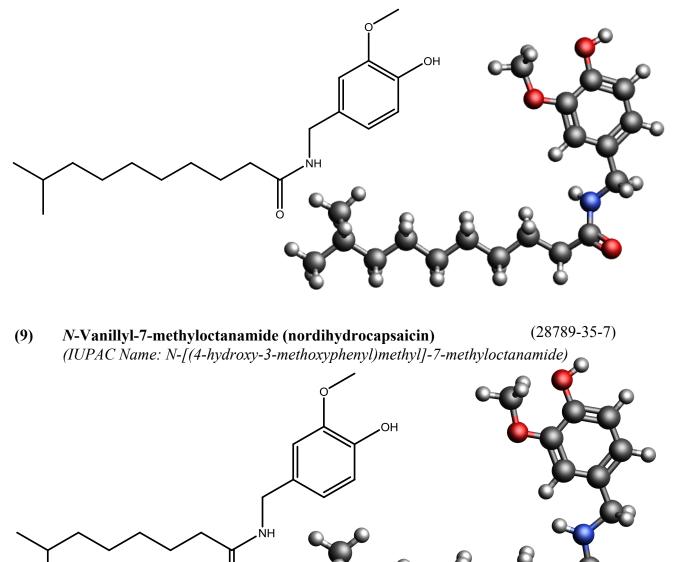
(6) *N*-VanillyInonamide (pseudocapsaicin, PAVA) (2444-46-4) (*IUPAC: N-[(4-hydroxy-3-methoxyphenyl)methyl]nonanamide*)

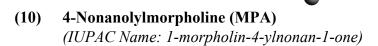


(7) *N*-Vanillyl-9-methyldec-7-(*E*)-enamide (homocapsaicin) (58493-48-4) (*IUPAC Name: (E)-N-[(4-hydroxy-3-methoxyphenyl)methyl]-9-methyldec-7-enamide*)



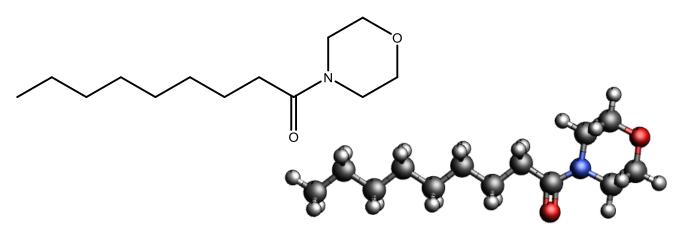
(8) *N*-Vanillyl-9-methyldecanamide (homodihydrocapsaicin) (20279-06-5) (*IUPAC Name: N-[(4-hydroxy-3-methoxyphenyl)methyl]-9-methyldecanamide*)



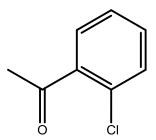


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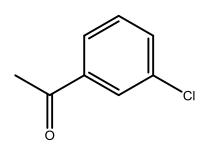
(5299-64-9)

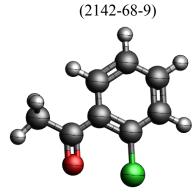


(11) 2'-Chloroacetophenone (IUPAC Name: 1-(2-chlorophenyl)ethanone)

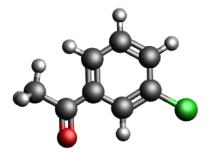


(12) **3'-Chloroacetophenone** (*IUPAC Name: 1-(3-chlorophenyl)ethanone*)



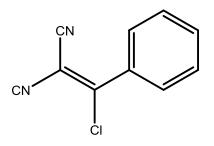


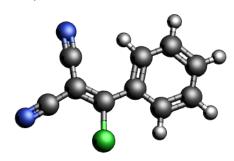
(99-02-5)



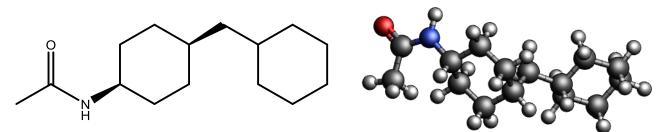
(13) α-Chlorobenzylidenemalononitrile (IUPAC Name: 2-[chloro(phenyl)methylidene]propanedinitrile)

(18270-61-6)





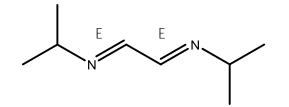
(14 *Cis*-4-acetylaminodicyclohexylmethane (37794-87-9) (*IUPAC Name: N-[trans-4-(Cyclopentylmethyl)cyclohexyl]acetamide*)

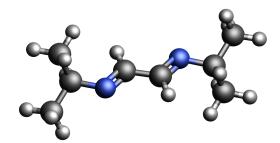


(15) *N*,*N*'-Bis(isopropyl)ethylenediimine

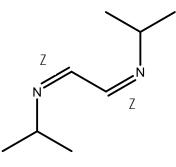
(a) (*E*,*E*')- *N*,*N'*-Bis(isopropyl)ethylenediimine (*IUAPC Name: N/A*) (28227 - 41 - 0)

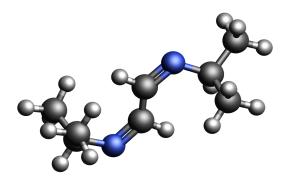
(185245-09-4)



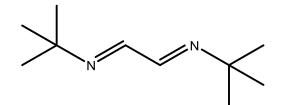


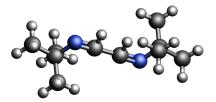
(b) (*Z*,*Z*)- *N*,*N*'-Bis(isopropyl)ethylenediimine (*IUAPC Name: N/A*)



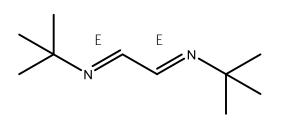


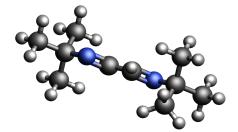
(16)N,N'-Bis(tert-butyl)ethylenediimine(30834-74-3)This CAS number does not specify geometric isomers.
(IUPAC Name: [1E,2E]or[(1Z,2Z)]-N,N'-Bis(2-methyl-2-propanyl)-1,2-ethanediimine)





(a) (*E,E'*)-*N,N'*-Bis(tert-butyl)ethylenediimine (28227-42-1) (*IUPAC Name: 1E,2E*)-*N,N'*-Bis(2-methyl-2-propanyl)-1,2-ethanediimine)





(8023-77-6)

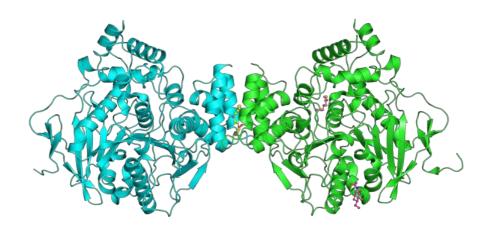
(17) Oleoresin capsicum (OC)

Oleoresin capsicum (OC) is a mixture containing $\geq 8\%$ capsaicins: capsaicin, dihydrocapsaicin and nordihydrocapsaicin dissolved in an organic solvent.

E. GLOSSARY

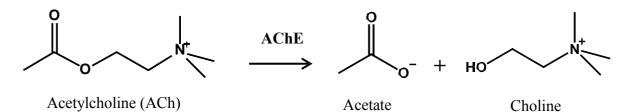
Acetylcholinesterase (AChE)

Acetylcholinesterase (AChE) is an enzyme [see also] responsible for breaking down the neurotransmitter acetylcholine (ACh) into choline and acetate. AChE is inhibited by the action of nerve agents [see also].



Crystal structure of the dimer of acetylcholinesterase (AChE) in complex with Xenon (Protein Data Bank 3M3D).¹⁵

Break down of ACh to acetate and choline by AChE:





15

34

Behnen, J., Brumshtein, B., Toker, L., Silman, I., Sussman, J., Klebe, G. and Heine, A., Crystal structure of Acetylcholinesterase in complex with Xenon. RCSB Protein Data Bank, 2011, DOI: 10.2210/pdb3M3D/pdb; www.rcsb.org/structure/3m3d

Acid

A molecule that can release a proton (a positively charged hydrogen atom, H^+ , often referred to as a "hydrogen ion"). A common example is the gas hydrogen chloride (HCl), that when dissolved in water generates protons and produces an acidic solution (hydrochloric acid).

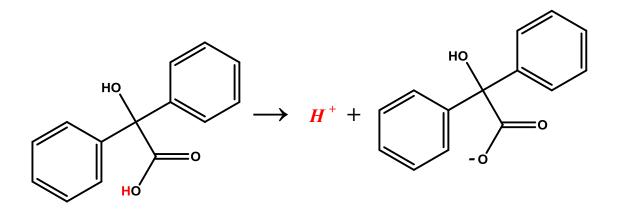
The dissociation of HCl:

$$HCl \rightarrow H^+ + Cl^-$$

In water, H^+ couples with a water molecule (H₂O) to produce hydronium ion (H₃O⁺). For simplicity H^+ is generally written in place of H₃O⁺ when illustrating chemical reactions.

$$HCl + H_2O \rightarrow H_3O^+ + Cl^-$$

Examples of acids listed in the Annex on Chemicals include 2,2-diphenyl-2-hydroxyacetic acid (Schedule 2B.08) and hydrogen cyanide (Schedule 3A.03). Their dissociation reactions are shown below:



2,2-diphenyl-2-hydroxyacetic acid

 $H \longrightarrow C \equiv N \longrightarrow H^+ + C \equiv N^-$

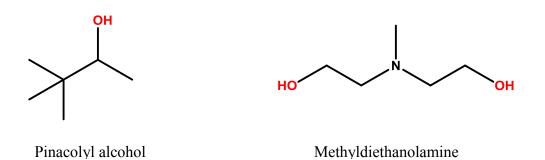
Hydrogen cyanide

Alcohol

An organic compound containing a hydroxyl group (OH) attached to a primary, secondary or tertiary carbon atom (C) in an alkane or alkyl group [see also]. A familiar example is ethanol (ethyl alcohol):



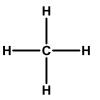
Examples of alcohols listed in the Annex on Chemicals include 3,3-dimethylbutan-2-ol (pinacolyl alcohol) (Schedule 2B.14) and methyldiethanolamine (Schedule 3B.16).



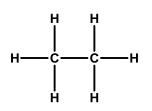
Alkane

Alkanes are chemicals that consist entirely of carbon (C) and hydrogen (H) atoms. The atoms are connected through single bonds. In an alkane molecule, each C has bonds to four other atoms (this can be any combination of C or H atoms) and each H is connected to a single C atom. When an alkane structure contains no rings of C atoms (cycles) the molecular formula is C_nH_{2n+2} (where n = the number of C atoms in the molecule). Methane, ethane and propane are examples of simple alkanes:

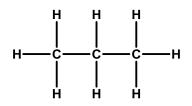
(a) Methane (1 carbon atom with the formula CH₄)



(b) Ethane (2 carbon atoms with the formula C_2H_6)

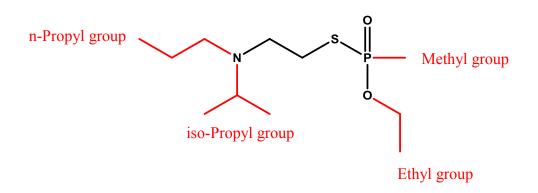


(c) Propane (3 carbon atoms with the formula C_3H_8)



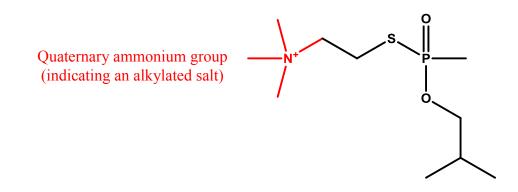
Alkyl group

An alkyl group is a molecular substructure derived from a parent alkane [see also] molecule. The alkyl group structure replaces one or more hydrogen atoms (H) from the parent alkane structure with a non-alkane functional group [see also] or an atom that is not carbon or hydrogen. Methyl [see also], ethyl [see also], iso-propyl [see also] and n-propyl [see also] are examples of alkyl groups derived from the alkanes methane, ethane and propane. The Schedule 1A.03 molecular structure illustrated below contains four alkyl groups: methyl, ethyl, iso-propyl and n-propyl.



Alkylated salts

Alkyklated salts are amino group containing molecules where the amine nitrogen atom (N) is connected to four alkyl groups [see also] (a quaternary ammonium group) [see also]. The quaternary ammonium group bears a positive charge (indicated by a "+" next to the N atom) and acts as the positive component (the "cation" [see also]) of the salt [see also]. There are no specific examples of alkylated salts in the Annex on Chemicals, however, alkylated salts are covered under certain Schedules including Schedule 1A.03. For example, N,N-diethyl-2-[methyl(2-methylpropoxy)phosphoryl]sulfanylethanamine:

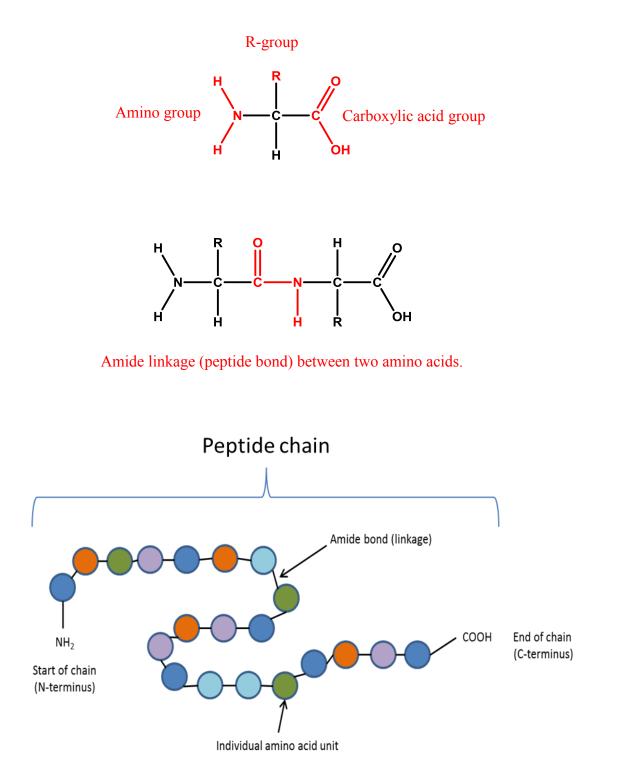


Amide

An amide is a functional group [see also] consisting of a carbon atom (C) connected to an oxygen atom (O) through a double bond, and to a nitrogen atom (N) through a single bond. The N atom is connected to any combination of two H atoms and/or alkyl groups [see also]. If the C atom is replaced with a phosphorus atom (P), the functional group is a "phosphonamide" [see also] (when there is an alkyl group also attached to the P atom) or "phosphoramide" [see also] (when there are only oxygen (O), N or halogen (X) atoms attached to the P atom).

Amino acid

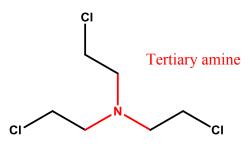
An amino acid (short for α -amino acid) is a molecule that contains an amino group [see also] and a carboxylic acid group [see also] bound to a common carbon atom that is also connected to a variable R-group [see also]. The R-group is unique to each individual amino acid. Proteins [see also] are made up of chains of amino acids that are connected through amide linkages (referred to as peptide bonds) formed between the amine and acid groups of sequential amino acids along the chain. Short chains of amino acids linked in this way are often referred to as peptides.



Amino Group

An amino group consists of a nitrogen atom (N) attached to at least one alkyl group [see also] with two additional connections to hydrogen atoms (H) and/or alkyl groups. Compounds containing amino groups are referred to as amines. If the amine has two H atoms and one alkyl group it is called a primary (1°) amine; if it has one H atom and two alkyl groups it is a secondary (2°) amine and; if it has three alkyl groups it is called a tertiary (3°) amine.

Examples of amines listed in the Annex on Chemicals include the nitrogen mustard tris(2-chloroethyl)amine (HN3) (Schedule 1A.06):



Methylamine and diethylamine are examples of primary and secondary amines (these are unscheduled chemicals):



Methylamine (primary amine)

н

Diethylamine (secondary amine)

Anion

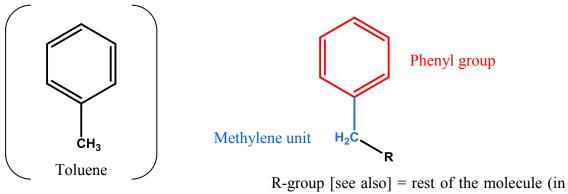
An anion is an ion [see also] that carries a negative charge.

Atom

An atom is the smallest particle of matter that retains the properties of an element. Atoms are composed of a nucleus containing protons [see also] (positively charged subatomic particles) and neutrons [see also] (subatomic particle with no electrical charge), as well as electrons [see also] (negatively charged subatomic particles) that are found outside the nucleus. The arrangement of an atom's electrons determines its chemical behaviour. Chemical bonds (connections) form between atoms through the sharing of electrons to produce molecules.

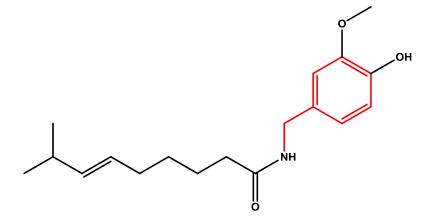
Benzyl Group

The benzyl group is derived from the hydrocarbon toluene, it consists of a phenyl group [see also] connected to a methylene unit (a carbon atom connected to two hydrogen atoms and a variable functional group [see also]. The methylene serves as the point of attachment of the benzyl group to a larger molecular structure (the R-group).



this case it is not limited to alkyl groups).

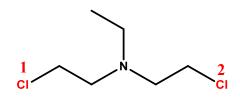
The riot control agent [see also] capsaicin is an example of a chemical structure that contains a (substituted) benzyl group:



Bis

A prefix in a chemical name indicating "two". It is used as an alternate prefix to "di" [see also] for the attachment of two identical substructures to a specific atom within a molecular structure.

Examples of chemicals that have the term "bis" within their names in the Annex on Chemicals include Bis(2-chloroethyl)ethylamine (HN1) (Schedule 1A.06):



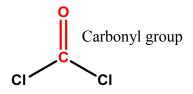
Blister agent

See entry for vesicant.

Carbonyl Group

A carbonyl group (C=O) is a functional group [see also] that consists of a carbon atom (C) connected to an oxygen atom (O) through a double bond.

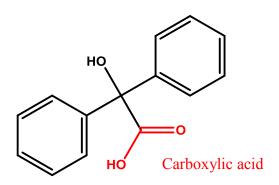
Examples of carbonyl group containing chemicals listed in the Annex on Chemicals include carbonyl dichloride (phosgene) (Schedule 3A.01):



Carboxylic acid group

A carboxylic acid group (-COOH) is a functional group [see also] that consists of a carbon atom (C) connected to two oxygen atoms (O), one through a double bond and the other through a single bond. There is a hydrogen atom connected to the single-bonded O atom, this is the acidic proton [see also acid].

Examples of carboxylic acid containing chemicals listed in the Annex on Chemicals include 2,2-diphenyl-2-hydroxyacetic acid (Schedule 2B.08):



CAS (Chemical Abstracts Service) Registry Number

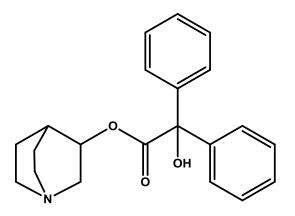
A Chemical Abstracts Service (CAS) Registry Number is a unique numeric identifier. It contains up to 10 digits, divided into three parts by hyphens and has no chemical significance. While each CAS Number is an identifier for a unique chemical substance, a given chemical can have multiple CAS Numbers assigned to it (representing stereoisomers, defined purity, isotopic enrichment, the form in which it was studied and other noteworthy properties from a scientific report or publication). The Chemical Registry System was developed by CAS from work initiated in the early 1960s after the perfection of an algorithm for generating a unique and unambiguous computer language representation of the molecular configuration of each chemical (www.cas.org). Since January 1965 the structures, names and molecular formulas of all substances indexed for chemical abstracts have been recorded in computer files that constitute the Chemical Registry System. Each substance is assigned a permanent computer checkable registry number that identifies it in the CAS database and links it to the structure record, the various names used for the chemical in the literature and its Chemical Abstracts index name.

Cation

A cation is an ion [see also] that carries a positive charge.

Central Nervous System (CNS) Acting Chemical

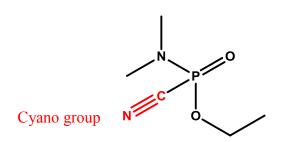
A central nervous system (CNS) acting chemical is a toxic chemical that targets the central nervous system. CNS-acting chemicals are sometimes referred to as "incapacitating chemical agents (ICAs). Chemicals that can act as anaesthetics, sedatives and analgesics are CNS-acting. Specific CNS-acting chemicals that are commonly discussed in the context of the Chemical Weapons Convention include $\alpha 2$ adrenergic receptor agonists, inhaled anaesthetics, fentanils and the Schedule 2A.03* chemical BZ (below).



Cyano Group

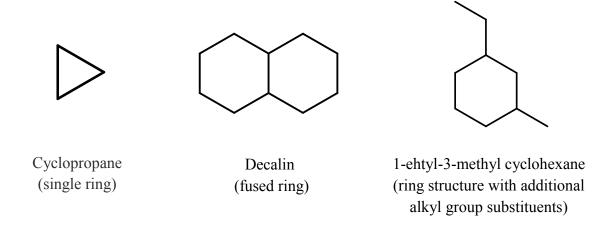
A cyano group is a functional group [see also], which consists of a carbon atom (C) connected to a nitrogen atom (N) through a triple bond (C=N). When the cyano group is connected to an alkyl chain, the chemical is commonly referred to as a nitrile [see also]. A negatively charged cyano group is referred to as the cyanide ion [see also], the anionic component of inorganic cyanide salts.

Examples of cyano group containing chemicals listed in the Annex on Chemicals include Tabun (Schedule 1A.02):



Cycloalkane

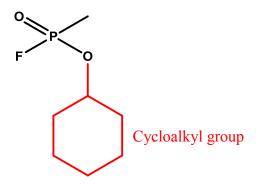
A cycloalkane is an alkane [see also] possessing a molecular structure that includes carbon atoms (C) arranged in the form of a "cycle" (the smallest cycloalkane being "cyclopropane" with three C atoms arranged in a triangular ring). When an alkane contains one or more rings of carbon atoms, the molecular formula is $C_nH_{\{2n-[(m-1) \times 2]\}}$ (where n = the number of C atoms and m = the number of ring structures in the molecule). Examples of cycloalkanes are found in the following molecular structures:



Cycloalkyl

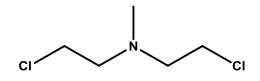
An alkyl group [see also] derived from a cycloalkane [see also] parent molecule.

Examples of chemicals that contain cycloalkyl groups covered under the Annex on Chemicals include cyclosarin (Schedule 1.A.01), which contains a "cyclohexyl" group.



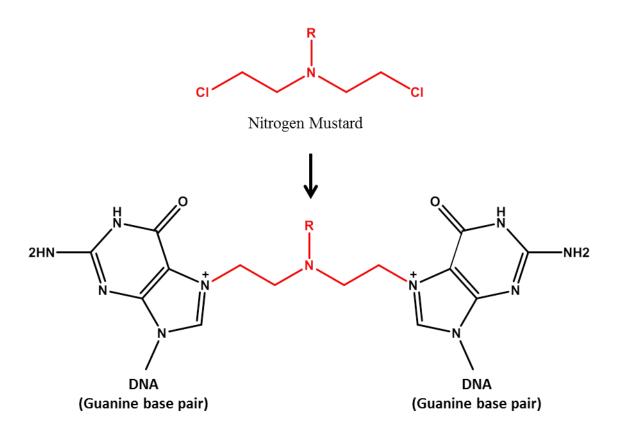
Cytotoxic Chemotherapy Agents

Cytotoxic chemotherapy agents are drugs used for the purpose of destroying cancer cells by inhibiting cellular division. The dialkylating agent HN2, a nitrogen mustard (Schedule 1A.06) [see also] was one of the first compounds to be taken through clinical trials and approved for use as a chemotherapy drug (Mustergen). It works through a mechanism of action that crosslinks and damages DNA strands to prevent tumour cells from replicating.



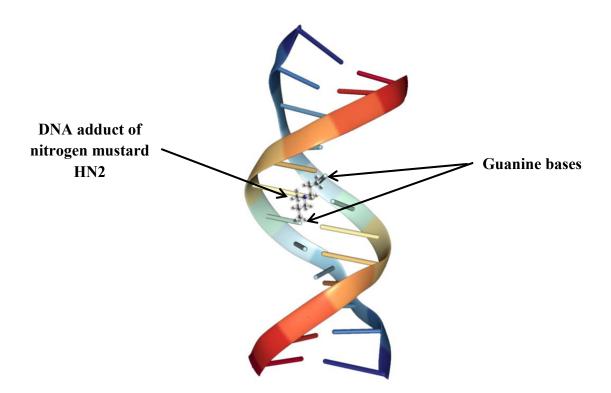
Bis(2-chloroethyl)methyl amine (HN2)

Interaction of nitrogen mustard with double-stranded DNA, leads to the formation of interstrand crosslinks through the alkylation of guanine bases in the DNA as illustrated below (sulfur mustard produces analogous DNA adducts).



DNA adduct of nitrogen mustard

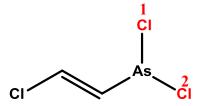
The schematic below illustrates the interstrand crosslink between two guanine base pairs in a double-stranded DNA molecule.



Di

A prefix used in chemical names meaning "two". It is used to indicate the presence of two identical substructures (or specific atoms) within a molecular structure.

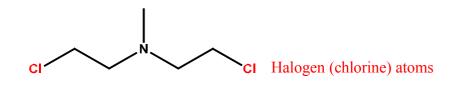
Examples of chemicals that have the term "di" within their names in the Annex on Chemicals include the Lewesite 2-chlorovinyldichloroarsine (Lewisite 1) (Schedule 1A.05):



Dihalides

A dihalide is a compound containing two halogen atoms [see also].

Examples of dihalides listed in the Annex on Chemicals include the nitrogen mustard bis(2-chloroethyl)methylamine (HN2) (Schedule 1A.06):



Discrete Organic Chemical (DOC)

For purposes of implementation of the Chemical Weapons Convention a Discrete Organic Chemical (DOC) is any chemical belonging to the class of chemical compounds consisting of all compounds of carbon except for its oxides, sufides and metal carbonates. See the Annex on Verification, Part I, paragraph 4 of the Chemical Weapons Convention (<u>www.opcw.org/chemical-weapons-convention/annexes/verification-annex/part-i-definitions</u>). For examples of oxides (e.g. carbon monoxide and carbon dioxide), sulfides (e.g. carbon disulfide) and metal carbonates (e.g. M_nCO_3) see the entry for inorganic chemical.



Electron

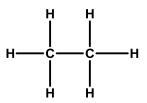
The electron is a stable subatomic particle found outside the nucleus of an atom [see also] that carries a negative charge. It is commonly indicated by the symbol e⁻. Atoms form bonds (connections) to one another through the sharing of electrons.

Enzyme

Enzymes are protein molecules that function as biomolecular catalysts. They serve to accelerate chemical reactions, converting substrates (the chemicals undergoing conversion) into "products" (the outcome of the chemical conversion). Acetylcholinesterase (AChE) [see also] is an enzyme whose substrate is the neurotransmitter acetylcholine (ACh) and "products" are acetate and choline as illustrated in the AChE entry of this glossary.

Ethane

A two carbon atom (C) alkane [see also] of molecular formula C_2H_6 . Ethane is a colourless and odourless natural gas.



Ether

An ether is a compound that contains two alkyl [see also] or substituted alkyl [see also] groups connected through a bridging oxygen atom (O).

Examples of ethers listed in the Annex on Chemicals include the sulfur mustard bis(2-chloroethylthioethyl)ether (O-Mustard) (Schedule 1A.04):

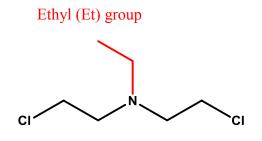


Ether linkage between substituted alkyl groups [see also].

Ethyl (Et)

Ethyl ("Et") is a two carbon (C) alkyl group [see also] derived from the parent alkane [see also] ethane [see also].

Examples of chemicals containing an Et group listed in the Annex on Chemicals include the nitrogen mustard bis(2-chloroethyl)ethylamine (HN1) (Schedule 1A.06):



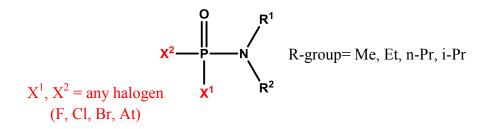
Functional Group

A functional group is a particular group of atoms [see also] on a molecule [see also] that defines its reactivity and influences its chemical properties and behaviour. A table of functional groups is provided in part F of this Annex on Chemicals.

Halogen

Halogens are the elements of Group VIIA of the Periodic Table. These include fluorine (F), chlorine (Cl), bromine (Br), iodine (I) and astatine (At). In a molecular structure, halogen atoms can act as leaving groups [see also] which allows the molecules to undergo substitution reactions (this can be a key aspect of how a toxic chemical causes harm to life processes). The term "halogen" means "salt-former" and "salts" are commonly encountered compounds containing halogen atoms (e.g: table salt – NaCl). The letter "X" is often used to signify a variable group in a molecular structure that can be a halogen atom.

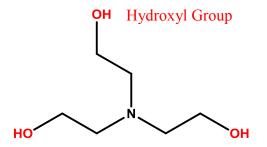
N,N-dialkyl (Me, Et, n-Pr or i-PR) phosphoramidic dihalides (Schedule 2B.05) are examples of a family of chemicals with halogen atoms in their molecular structures:



Hydroxyl Group

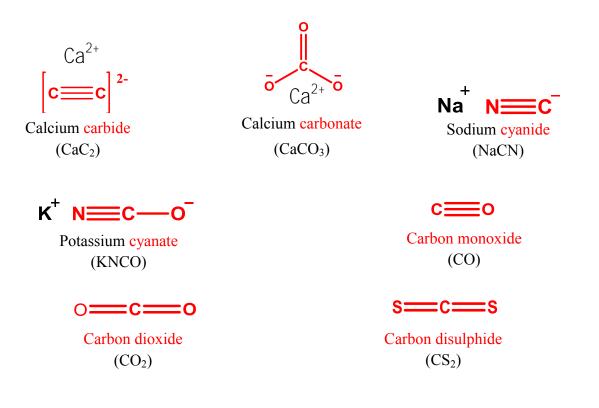
A hydroxyl group consists of an oxygen atom (O) connected to a hydrogen atom (H) with the O atom acting as the point of attachment to a larger molecular structure (attached through an alkyl group carbon atom (C)). Alkanes [see also] substituted with a hydroxyl group are referred to as alcohols [see also].

Examples of hydroxyl group containing chemicals listed in the Annex on Chemicals include triethanolamine (Schedule 3B.17):



Inorganic Chemical

A broad class of substances encompassing all chemicals that do not include carbon (C) and its derivatives as their principal elements. Additionally, carbides, carbonates, cyanides, cyanates, carbon monoxide, carbon dioxide and carbon disulfide are considered to be inorganic chemicals. Examples include:



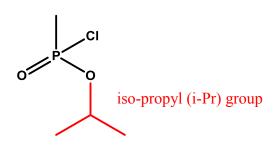
Ion

An ion is an atom [see also] or molecule [see also] with a net electric charge (positive or negative) due to the loss or gain of one or more electrons or protons [see also acid]. Ions are the component atoms and molecules of a salt [see also]. Cations [see also] possess a positive charge, anions [see also] possess a negative charge.

iso-Propyl Group (i-Pr)

An iso-propyl (i-propyl or "i-Pr)" is a three carbon alkyl group [see also] derived from the alkane propane. It has as its point of attachment the middle carbon atom (C) of the 3 carbon propyl [see also] chain.

Examples of chemicals listed in the Annex on Chemicals that contain an *i-Pr* group include O-Isopropyl methylphosphonochloridate (chlorosarin) (Schedule 1B.11):



Leaving Group

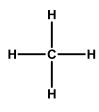
A leaving group is an atom [see also] or a molecular substructure that breaks away from the rest of the molecule, taking with it a pair of electrons [see also]. The reactivity (ease of bond breaking) of a leaving group will influence the toxicity of any chemical that requires the leaving group to break away in order to effect life processes.

Lewisite

Lewisites are organoarsenic compounds [see also] found in Schedule 1A.05 that act as vesicants (blistering agents) [see also]. Lewisite (Lewisite 1) itself is an oily, colourless liquid with an odour similar to geraniums that was used as a chemical warfare agent in the First World War.

Methane

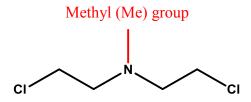
Methane is the simplest organic compound [see also] and hydrocarbon [see also], with the chemical formula CH₄. It is a colourless and odourless natural gas that is mainly used as a fuel for heating, cooking and generating electricity.



Methyl (Me)

A Methyl group ("Me") is an alkyl group [see also] containing one carbon (C) derived from the alkane [see also] methane [see also].

Examples of methyl group containing chemicals listed in the Annex on Chemicals include Bis(2-chloroethyl)methylamine (HN2) (Schedule 1A.6):



Moiety

Refers to a "part" (a substructure) of a molecule. This can be a specific substructure or a functional group [see also] found within the molecules structure.

Molecule

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

Nerve Agent

Nerve agents are chemicals that block impulses between nerve cells (across synapses) through the inhibition of the enzyme acetylcholinesterase [see also]. They are highly toxic and act primarily by absorption through the skin and lungs. The most well-known nerve agents are organophosphorus compounds that fall into two main groups: G-series (examples of which are found in Schedules 1A.01 and 1A.02) and V-series agents (examples of which are found in Schedules 1A.03.

Neutron

The neutron is a stable subatomic particle found in the nucleus of an atom [see also]. Unlike protons [see also] or electrons [see also] it does not carry a charge.

Nitrile

A nitrile is an organic compound that contains a cyano group [see also] connected to an alkyl group [see also].

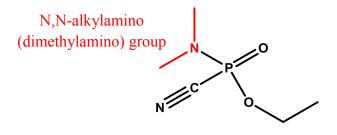
Nitrogen Mustards

Nitrogen mustards are alkylating agents [see also] found in Schedule 1A.06 that were produced in the 1920s and 1930s as potential chemical warfare agents. Nitrogen mustards are vesicants (blister agents) [see also] similar to the sulfur mustards [see also]. The nitrogen mustard HN2 also finds use as a cytotoxic chemotherapy agent [see also].

N,N-dialkyl

This term in a chemical name indicates a molecular structure that possesses a nitrogen atom (N) to which two alkyl groups [see also] are attached. An example from the Annex on Chemicals is seen with N,N-dialkylamino groups. Unless specified otherwise by a given Schedule, the two alkyl groups attached to the N atom do not need to be identical.

Examples of N,N-dialkyl containing chemicals listed in the Annex on Chemicals include O-Ethyl N,N-dimethyl phosphoramidocyanidate (Tabun) (Schedule 1A.02):



n-Propyl Group (n-Pr)

An n-propyl group ("n-Pr") is a three carbon alkyl group [see also] derived from the alkane propane [see also]. Its point of attachment is a terminal carbon atom (C) of the 3 C propyl chain.

Examples of n-Pr containing chemicals covered under Schedule 1A.01 of the Annex on Chemicals is methyl propylphosphonofluodridate:



O-alkyl (alkoxy)

An O-alkyl (or "alkoxy") group is a molecular substructure in which an oxygen atom (O) connects an alkyl group [see also] to another molecular structure.

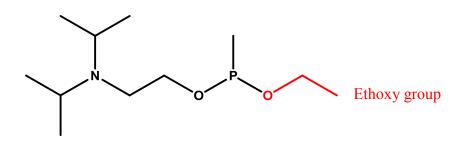
Examples of O-alkyl containing chemicals listed in the Annex on Chemicals include O-Pinacolyl methylphophonofluoridate (Soman) (Schedule 1A.01):



O-ethyl (ethoxy)

An O-ethyl (or "ethoxy") group is an O-alkyl group [see also] where the alkyl group [see also] is ethyl [see also].

Examples of chemicals listed in the Annex on Chemicals that possess O-ethyl groups include O-ethyl O-2-diisopropylaminoethyl methylphosphonite (QL) (Schedule 1B.10):



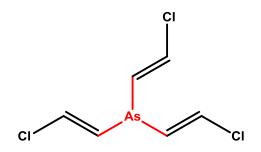
Organic Chemical

A broad class of substances based on molecular scaffolds that are made up of carbon (C) and hydrogen (H) atoms. These chemicals frequently contain functional groups [see also] that include oxygen (O), nitrogen (N), sulfur (S), phosphorus (P) and other atoms. The molecular structures of organic compounds can also contain chains or rings (cycles) of C atoms. See also the entry for inorganic chemical.

Organoarsenic Compound

Organoarsenic compounds are chemicals whose molecular structures contain arsenic atoms (As) connected to organic chemical substructures.

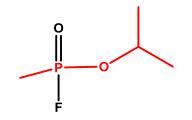
Examples of organoarsenic compounds listed in the Annex on Chemicals include the Lewisite tris(2-chlorovinyl)arsine (Lewisite 3) (Schedule 1A.05):

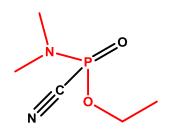


Organophosphorus Compound

Organophosphorus compounds are chemicals whose molecular structures contain phosphorus atoms (P) connected to organic chemical substructures.

Examples of organophosphorus compounds listed in the Annex on Chemicals include Oisopropyl methylphosphonofluoridate (Sarin) (Schedule 1A.01) and O-Ethyl N,N-dimethyl phosphoroamidocyanidate (Tabun) (Schedule 1A.02):





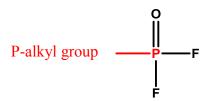
O-isopropyl methylphosphonofluoridate (Sarin)

O-Ethyl N,N-dimethyl phosphoroamidocyanidate (Tabun)

P-alkyl

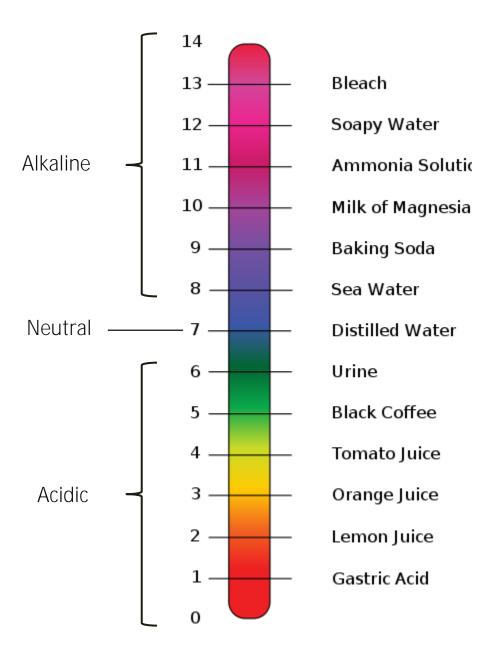
A P-alkyl group indicates a molecular structure that contains a phosphorus atom (P) to which an alkyl group [see also] is attached.

Examples of P-alkyl containing chemicals listed in the Annex on Chemicals include methylphophonyldifluoride (DF) (Schedule 1B.09):



pН

pH is a measure of hydrogen (H) ion concentration [see also entry for acid], which describes the acidity of a solution. The pH scale is normally used to describe aqueous (water based) solutions and ranges from 0 to 14. A pH of 7 is "neutral", while a pH less than 7 is considered acidic, and a pH greater than 7 is considered basic or alkaline.

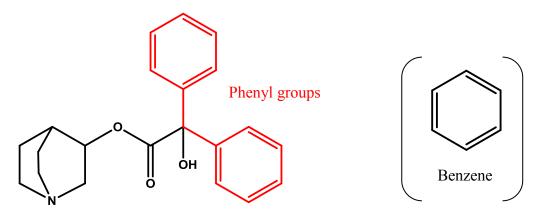




Phenyl Group

A phenyl group is a molecular substructure derived from the benzene molecule. The structure is made up of a ring formed by six carbon atoms (C) that is drawn as having alternating single and double bonds between the adjacent C atoms (shifting the position of the double bonds by one C atom and keeping the alternating pattern is a chemically equivalent structure). The benzene structure is a special kind of hydrocarbon, commonly referred to as an "aromatic" compound, and a phenyl group is an "aryl" (as opposed to an "alkyl" [see also]) substituent in a molecular structure. In an unsubstituted phenyl group, five of the C atoms are each connected to a single hydrogen atom (H) and the remaining C atom serves as the point of attachment to another molecular structure.

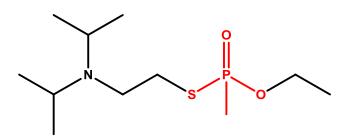
Examples of chemicals that contain phenyl groups listed in the Annex on Chemicals include 3-quinuclidinyl benzilate (BZ) (Schedule 2A.03):



Phosphonate

Phosphonates are compounds with molecular structures that contain a phosphorus atom (P) connected to an oxygen atom (O) through a double bond, and an alkyl group [see also]. All further connections to the P atom attach from an O and/or a sulfur (S) atoms that serve as a bridges to other alkyl groups, and/or halogen atoms (X).

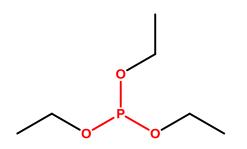
Examples of phosphonate compounds listed in the Annex on Chemicals include O-ethyl S-2diisopropylaminoethyl methyl phosphonothiolate (VX) (Schedule 1A.03):



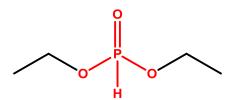
Phosphite Ester

Phosphite esters have molecular structures in which a phosphorus atom (P) is connected to three oxygen atoms (O). The general structure for a phosphite ester is $P(OR)_3$, where at least one of the variable R groups [see also] is an alkyl group [see also], with the remaining R groups being alkyl groups or hydrogen atoms (H). In the situation where only two of the O atoms are linked to alkyl groups and the third O atom is connected to an H, the chemical structure is commonly shown as having a double bond between the third O and the P atoms with the H atom connected directly to the P.

Examples of phosphite ester compounds listed in the Annex on Chemicals include triethyl phosphite (Schedule 3B.09) and diethyl phosphite (Schedule 3B.11):



Triethyl phosphite

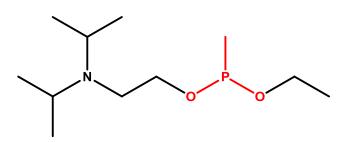


Diethyl phosphite

Phosphonite

Phosphonites are compounds with molecular structures that contain a phosphorus atom (P) connected to an alkyl group [see also], and two oxygen atoms (O) which serve as bridges to additional alkyl groups. Phosphonite compounds have the general structure $P(OR)_2R$, where each R group [see also] is an alkyl group.

Examples of phosphonite compounds listed in the Annex on Chemicals include O-ethyl O-2diisopropylaminoethyl methylphosphonite (QL) (Schedule 1B.10):



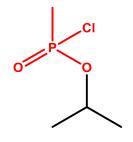
Phosphonamide (phosphonamidate)

Phosphonamides are compounds with molecular structures that contain a phosphorus atom (P) connected to an alkyl group [see also], an oxygen atom (O) through a double bond, an amino (or alkyl amino) group through the nitrogen (N) atom, and a second O atom that acts as a bridge to another molecular substructure, such as an alkyl group or a chlorine atom (Cl). See also entry for amide.

Phosphonochloridate

Phosphonochloridates are compounds with molecular structures that contain a phosphorus atom (P) connected to an alkyl group [see also], an oxygen atom (O) through a double bond, a second O atom that acts as a bridge to another molecular substructure (such as an alkyl group) and a chlorine atom (Cl). These compounds can serve as final stage precursors [see also] for the preparation of phosphonofluoridates [see also].

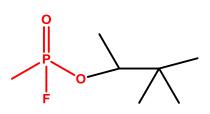
Examples of phosphonochloridates listed in the Annex on Chemicals include O-isopropyl methylphosphonochloridate (chlorosarin) (Schedule 1B.11):



Phosphonofluoridate

Phosphonofluoridates are compounds with molecular structures that contain a phosphorus atom (P) connected to an alkyl group [see also], an oxygen atom (O) through a double bond, an O atom that acts as a bridge to another molecular substructure (such as an alkyl group) and a fluorine atom (F).

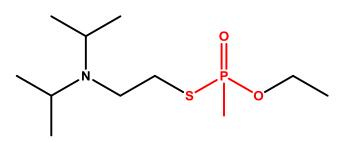
Examples of phosphonofluoridates listed in the Annex on Chemicals include O-pinacolyl methylphosphonofluoridate (Soman) (Schedule 1A.01):



Phosphonothiolate

Phosphonothiolates are compounds with molecular structures that contain a phosphorus atom (P) connected to an oxygen atom (O) through a double bond, as well as single bonds to an alkyl group [see also], and to O and sulfur (S) atoms that serve as bridges to other alkyl groups.

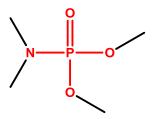
Examples of phosphonothiolates listed in the Annex on Chemicals include O-ethyl S-2diisopropylaminoethyl methyl phosphonothiolate (VX) (Schedule 1A.03):



Phosphoramide (phosphoroamidate)

Phosphoramidates are compounds with molecular structures that contain a phosphorus atom (P) connected to an oxygen atom (O) through a double bond, an amino group [see also] (or alkylamino group) through the nitrogen atom (N), and two additional connections that can be to oxygen atoms (O) that serve as bridges to alkyl groups [see also] and/or to a halogen [see also] (or pseudo-halogen [see also]). See also entry for amide.

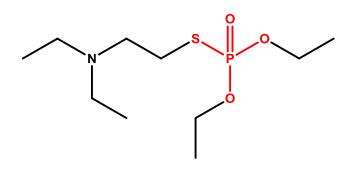
Examples of phosphoramidates listed in the Annex on Chemicals include dimethyl dimethylphosphoroamidate (Schedule 2B.06):



Phosphorothiolate

Phosphorothiolates are compounds with molecular structures that contain a phosphorus atom (P) connected to an oxygen atom (O) through a double bond, and has further connections to two O atoms and one sulfur atom (S) that serve as bridges to alkyl groups [see also].

Examples of phosphorothiolates listed in the Annex on Chemicals include O,O-diethyl S-[2-(diethylamino)ethyl] phosphorothiolate (Amiton) (Schedule 2A.01):



Precursor

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. For chemicals of relevance to the Chemical Weapons Convention, this definition applies to precursors of toxic chemicals [see also] as per paragraph 3 of Article II (www.opcw.org/chemical-weapons-convention/articles/article-ii-definitions-and-criteria).



Bis(2-hydroethyl)sulphide (Thiodiglycol) Precursor (Schedule 2B.13)

Thionyl chloride Precursor (Schedule 3B.14)

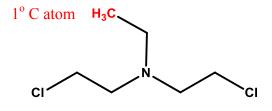
CI

Bis(2-chloroethyl)sulphide (Sulfur mustard) Toxic chemical (Schedule 1A.04)

Primary (1°) Carbon Atom

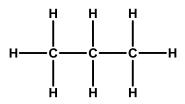
A primary (1°) carbon (C) is a C atom in an alkane [see also] or alkyl group [see also] that is connected to only one other C atom.

Examples of chemicals with molecular structures containing 1° C atoms listed in the Annex on Chemicals include the nitrogen mustard bis(2-chloroethyl)ethylamine (HN1) (Schedule 1A.06):



Propane

A three carbon atom (C) alkane [see also] of molecular formula C₃H₈.



Protein

Proteins are large, complex, biological molecules composed of sequences of amino acids [see also]. Proteins play many critical roles as essential components for biomolecular and cellular function, including cellular structure and regulation of life processes. Proteins can also be toxic chemicals [see also].

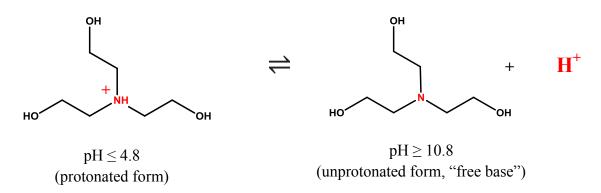
There is only one protein specifically listed in the Annex on Chemicals, ricin (Schedule 1A.08) [see also].

Proton

The proton is a stable subatomic particle found in the nucleus of the atom [see also] that carries a positive charge of +1. Protons are commonly indicated by the symbols p or p^+ . A hydrogen atom which has lost an electron (e.g. H^+), is also referred to as a proton, as it has a single proton in its nucleus and bears a net positive charge [see also entry for acid].

Protonated Salts

Protonated salts are molecules with structures that contain a protonated amino group (e.g: a nitrogen atom (N) attached to a hydrogen ion (H^+) and any combination of three alkyl groups [see also] and/or H atoms. The protonated amino group bears a positive charge (indicated by a "+" next to the N atom) and acts as the positive component (the "cation") of a salt. Protonated salts can be de-protonated (removal of the H^+) to provide the parent ("free base") amino compound through control of pH. For example, the protonation and de-protonation of triethanolamine (Schedule 3B.17) in aqueous solution:¹⁶



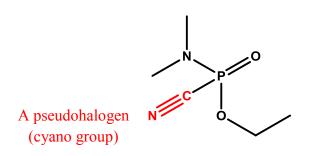
In the pH range from 4.8 to 10.8, triethanolamine will exist as a mixture of protonated and unprotonated forms (at pH 7.8 there is a 1:1 ratio of the two forms). Each unique amino compound that can form a protonated salt will have its own specific pH transition values for protonation/deprotonation.

¹⁶ Based on an ionization constant (pKa) of 7.8 for protonated triethanolamine

Pseudohalogen

Pseudohalogens are functional groups [see also] that show chemical behaviour similar to a halogen [see also] in a molecular structure (in particular they can act as leaving groups [see also]). The cyano group ($C \equiv N$) is a common pseudohalogen.

Examples of chemicals containing a cyano group listed in the Annex on Chemicals include O-ethyl N,N-dimethyl phosphoramidocyanidate (Tabun) (Schedule 1A.02):



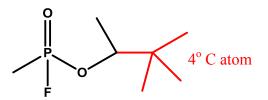
PSF-chemical

For the purposes of the Chemical Weapons Convention a PSF-chemical is an unscheduled Discrete Organic Chemical (DOC) [see also] containing the elements phosphorus (P), sulfur (S) and/or fluorine (F).

Quaternary (4°) Carbon Atom

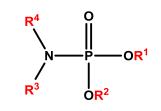
A quaternary (4°) carbon (C) is a C atom in an alkane [see also] or alkyl group [see also] that is connected to four other alkyl C atoms.

Examples of chemicals with molecular structures containing 4° C atoms listed in the Annex on Chemicals include O-pinacolyl methylphosphonofluoridate (Soman) (Schedule 1A.01):



R-Group

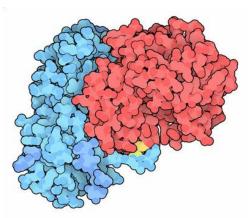
The letter "R", for "rest of the molecule", is used to identify a variable substructure at a given position of a molecular structure. R is most commonly used to indicate variable alkyl groups [see also]. For example, in the family description of Schedule 2B.06: dialkyl (Me, Et, n-Pr, or i-Pr) N,N-dialkyl (Me, Et, n-Pr or i-Pr)-phosphoroamidates, where each R-group can be methyl [see also], ethyl [see also], n-Propyl [see also] or i-Propyl [see also].



 R^1 , R^2 , R^3 , R^4 = Me, Et, n-pr or i-Pr

Ricin

Ricin (Schedule 1A.08) is a type 2 ribosome-inactivating protein (RIP) toxin [see also] found in the seed of the castor bean plant. It inhibits protein synthesis in eukaryotic cells through deactivation of ribosomal protein synthesis. Ricin is the only protein [see also] toxin listed in the Annex on Chemicals.



The structure of Ricin is composed of two subunits: the A-chain, which is responsible for intracellular toxicity (shown in red) and a cell-targeting B-chain (shown in blue).¹⁷

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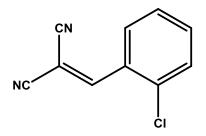
D. Goodsell, PBD-101, Molecule of the Month, Protein Data Bank Education Portal, May 2013. DOI: 10.2210/rcsb pdb/mom 2013 5.



Riot Control Agent (RCA)

A Riot Control Agent (RCA) is 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. See also Chemical Weapons Convention, Article II, paragraph 7 (www.opcw.org/chemical-weapons-convention/articles/article-ii-definitions-and-criteria).

Section D of this annotated Annex on Chemicals provides a list of chemicals that when used under appropriate circumstances might conform with the definition of an RCA, for example 2-chlorobenzylidenemalononitrile (CS):

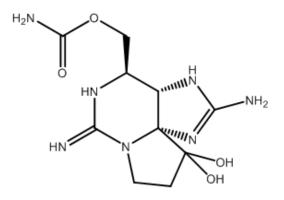


Salt

A salt is an ionic chemical compound (composed of ions [see also]) that contains positively charged ("cation" [see also]) and negatively charged ("anion" [see also]) components. The ions [see also] can be charged molecular structures or charged atoms [see also]. The Annex on Chemicals refers to alkylated and protonated salts [see also] of some types of chemicals, these specifically refer to the cation. When an anion is not specified, it suggests that any possible anion associated with the cationic structure of interest would fall under the relevant schedule. Negatively charged halogen [see also] atoms represent anions commonly found in salts.

Saxitoxin

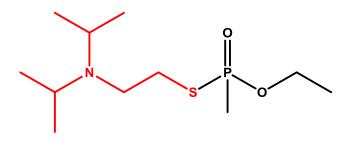
Saxitoxin (Schedule 1A.07) is a small molecule toxin [see also] produced in cyanobacteria (especially red algae) in fresh water and marine environments. It is a neurotoxic sodium ion channel inhibitor that blocks the initiation and propagation of action potentials in nerve and muscle cells. Saxitoxin is one of two toxins that are specifically listed in the Annex on Chemicals.



S-alkyl

An S-alkyl group indicates a molecular structure that contains a sulfur atom (S) to which an alkyl group [see also] is attached.

Examples of S-alkyl containing chemicals listed in the Annex on Chemicals include O-ethyl S-2-diisopropylaminoethyl methyl phosphonothiolate (VX) (Schedule 1A.03):

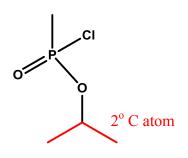


S-alkyl group (which also has an amino group substituent)

Secondary (2°) Carbon Atom

A secondary (2°) carbon (C) is a C atom in an alkane [see also] or alkyl group [see also] that is connected to two other C atoms.

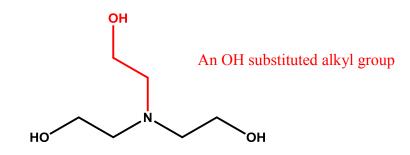
Examples of chemicals with molecular structures containing 2° C atoms listed in the Annex on Chemicals include O-isopropyl methylphosphonochloridate (Chlorosarin) (Schedule 1B.11):



Substituted alkyl group

A substituted alkyl group is an alkyl group [see also] with one or more non-alkane functional groups [see also] connected to it.

Examples of chemicals with molecular structures containing a substituted alkyl group listed in the Annex on Chemicals include triethanolamine (Schedule 3B.17), where the alkyl group also contains a hydroxyl group [see also]:



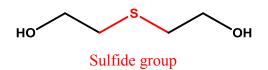
Sulfur Mustard

Sulfur mustards are alkylating agents found in Schedule 1A.04. They act as vesicants (blistering agents) [see also] similar to the nitrogen mustards [see also].

Sulfide

A sulfide is a chemical structure that contains a sulfur atom (S) that acts as a bridge between two alkyl groups [see also]. Sulfides are sometimes referred to as thioethers, analogous to the ether group [see also] with an oxygen atom.

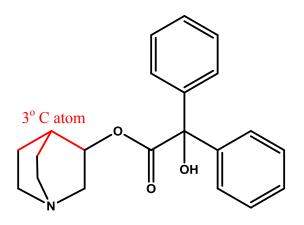
Examples of sulfide containing chemicals listed in the Annex on Chemicals include bis(2-hydroxyethyl)sulphide (thiodiglycol) (Schedule 2B.13):



Tertiary (3°) Carbon Atom

A tertiary (3°) carbon (C) is a C atom in an alkane [see also] or alkyl group [see also] that is connected to three other C atoms.

Examples of chemicals with molecular structures containing 3° C atoms listed in the Annex on Chemicals include 3-quinuclidinyl benzilate (*) (BZ) (Schedule 2A.03):



Tetra

A prefix used in chemical names meaning "four". It is used to indicate the presence of four identical substructures (or types of atoms) within a molecular structure.

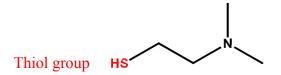
Tetrakis

A prefix used in a chemical name indicating "four". It is used as an alternate prefix to "tetra" [see also] for the attachment of four identical substructures to a specific atom within a molecular structure.

Thiol

A thiol group (SH) consists of a sulfur atom (S) connected to a hydrogen atom (H), with the S atom acting as the point of attachment to a larger molecular structure.

Examples of chemicals containing thiol groups that are listed in the Annex on Chemicals include 2-(dimethylamino)ethan-1-thiol (Schedule 2B.12):



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. See also Chemical Weapons Convention Article II, paragraph 2 (www.opcw.org/chemical-weapons-convention/articles/article-ii-definitions-and-criteria).



Toxin

Toxins are toxic chemicals produced by living organisms (e.g. plants, bacteria, animals, fungi). Toxins can be small molecules or complex proteins. While only two toxins are listed in the Annex on Chemicals, the use of toxins for purposes prohibited by the Chemical Weapons Convention would be covered under the general purpose criterion of Article II of the Chemical Weapons Convention (www.opcw.org/chemical-weapons-convention/articles/ article-ii-definitions-and-criteria).



The possession and use of toxins as weapons is also a violation of the Biological Weapons Convention under Article I, section A, paragraph 1 due to toxins being of biological origin.

(https://bit.ly/2HEz0mK).

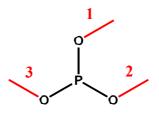


The two toxins explicitly listed in Schedule 1 of the Annex on Chemicals are ricin [see also] (Schedule 1A.08) and saxitoxin [see also] (Schedule 1A.07).

Tri

A prefix used in chemical names meaning "three". It is used to indicate the presence of three identical substructures (or types of atoms) within a molecular structure.

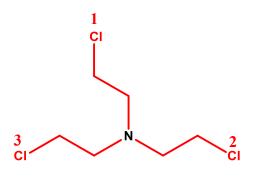
Examples of chemicals that have the term "tri" within their names that are listed in the Annex of Chemicals include trimethyl phosphite (Schedule 3B.08):



Tris

A prefix in a chemical name indicating "three". It is used as an alternate prefix to "tri" [see also] for the attachment of three identical substructures to a specific atom within a molecular structure.

Examples of chemicals that have the term "tris" within their names that are listed in the Annex on Chemicals include the nitrogen mustard Tris(2-chloroethyl)amine (HN3) (Schedule 1A.06):



Vesicant

Vesicants, also referred to as blister agents, are oily substances that act via inhalation and contact, affecting the eyes, respiratory tract and skin, first as an irritant and then as a cytotoxic poison. Exposure to vesicants results in large and potentially life-threatening skin blisters which resemble severe burns. Exposure can also result in blindness and permanent damage to the respiratory system.

The chemicals found within Schedules 1A.04 (sulfur mustards), 1A.05 (Lewsities) and 1A.06 (nitrogen mustards) provide examples of vesicants.

F. ORGANIC CHEMICAL FUNCTIONAL GROUPS

Chemicals are defined by the functional groups they contain within their molecular structures. A functional group is a particular group of atoms in a molecule that defines reactivity, and influences chemical properties and behaviour. Complex molecules can contain multiple types of functional groups. This table provides descriptions of many of the types of functional groups found in organic chemistry, it is not intended to be comprehensive.

Functional Group Nomenclature	General Structure	Substructures	Description
Acetal [substructure: -al dialkyl acetal]	$R^3 \longrightarrow 0 \longrightarrow H$ $R^2 \longrightarrow R^1$	R^1 = hydrogen atom or alkyl group R^2 , R^3 = alkyl group	Acetals are chemical structures containing a carbon atom connected to two oxygen atoms (which serve as bridges to alkyl groups), and to either two hydrogen atoms or to a hydrogen atom and an alkyl group.
Acid Anhydride [substructure: -oic anhydride]	$R^1 \xrightarrow{O} O \xrightarrow{O} R^2$	R ¹ , R ² = hydrogen atom or alkyl group	Acid anhydrides are chemical structures in which an oxygen atom serves as a bridge between two carbonyl groups (a carbon connected to an oxygen atom through a double bond), each of which is further connected to a hydrogen atom or alkyl group.
Acyl Halide [substructure: -oyl halide (e.g. fluoride, chloride, bromide, iodide, astatide)]		R = hydrogen atom or alkyl group X = halogen atom	Acyl Halides are chemical structures containing a carbon atom connected to a hydrogen atom or an alkyl group, a halogen and an oxygen atom through a double bond.
Alcohol [substructure: <i>-ol</i>]	R—OH	R = alkyl group	Alcohols are chemical structures that contain a hydroxyl group (an oxygen atom attached to a hydrogen atom) connected to an alkyl group, and has no other oxygen atoms connected to the carbon to which the hydroxyl is attached.

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Functional Group Nomenclature	General Structure	Substructures	Description
Aldehyde [substructure: -al]		R = alkyl group	Aldehydes are chemical structures containing a carbon atom connected to an oxygen atom through a double bond. The carbon atom is further connected to either two hydrogen atoms, or a hydrogen atom and an alkyl group.
Alkane [substructure: -alkyl or -ane]	$ \mathbb{R}^{4} \xrightarrow{\qquad C \\ \qquad C \\ \qquad R^{3}}^{R^{1}} \mathbb{R}^{2} $	$\mathbf{R}^{1}, \mathbf{R}^{2}, \mathbf{R}^{3}, \mathbf{R}^{4} =$ hydrogen atom or alkyl group	Alkanes are chemical structures composed entirely of carbon and hydrogen atoms connected by single bonds (each carbon is connected to four other atoms – these can be carbon or hydrogen, and each hydrogen atom is connected to one carbon).
Alkene [substructure: -alkenyl or -ene]	R^1 R^2 R^2 R^3	R^1 , R^2 , R^3 , R^4 = hydrogen atom, alkyl group and/or other functional group	Alkenes are chemical structures containing a double bond connecting two carbon atoms. Each carbon is connected to two other groups through single bonds.
Alkyl Halide [Substructure = halo- or (alkyl) halide (e.g. fluoride, chloride, bromide, iodide, astatide)]	R—X	R = alkyl group X = halogen atom	Alkyl halides (also called haloalkanes) are chemical structures containing a halogen atom connected to an alkyl group.
Alkyne [substructure: -alkynyl or -yne]	R ¹ —C <u></u> C—R ²	R ¹ , R ² = hydrogen atom, alkyl group and/or other functional group	Alkynes are chemical structures containing a triple bond connecting two carbon atoms. Each carbon is connected to one other group through a single bond.
Amide [substructure: -amide or -amido]	R^1 R^2 R^3	R ¹ = alkyl group R ² , R ³ = hydrogen atom or alkyl group	Amides are chemical structures containing a carbon atom connected to an oxygen atom through a double bond, with a nitrogen atom and an alkyl group or hydrogen atom through single bonds. The nitrogen atom is connected to additional hydrogen atoms and/or alkyl groups.

Functional Group Nomenclature	General Structure	Substructures	Description
Amidine [substructure: amidinyl or -amidine]	R^2 N C N R^4 R^4	R^1 = alkyl group R^2 = hydrogen atom, alkyl group and/or other functional group R^3 , R^4 = hydrogen atom or alkyl group	Amidines are chemical structures containing a carbon atom connected to a nitrogen atom through a double bond, and to a second nitrogen atom and an alkyl group through single bonds. The nitrogen atom attached through a double bond serves as a bridge to other functional groups (typically alkyl), and the nitrogen atom attached through a single bond has two additional connections to either hydrogen atoms or alkyl groups.
Amine [substructure: amino or -amine]	$R^1 \longrightarrow N$ R^3 R^3	R^1 = alkyl group R^2 , R^3 = hydrogen atom or alkyl group	Amines are chemical structures containing amino groups connected to an alkyl group. An amino group consist of a nitrogen atom connected to two groups (which can be hydrogen atoms or alkyl groups) through single bonds.
Arene [substructure: <i>-arenyl</i>]	$R^{6} \xrightarrow{C} C \xrightarrow{C} R^{2}$ $R^{5} \xrightarrow{C} \xrightarrow{C} R^{3}$	R ¹ , R ² , R ³ , R ⁴ , R ⁵ , R ⁶ = hydrogen atom, alkyl group and/or other functional group	Arenes are "aromatic compounds" containing rings of six carbon atoms with alternating single and double bonds. The six- membered ring structure imparts unique chemical properties and reactivity as compared to an alkene. Each carbon atom is connected to one other group through a single bond (when all six R groups are hydrogen atoms, the structure is called "benzene"). When the ring is connected to a single alkyl carbon atom, the substructure is referred to as "phenyl". Arenes can be present in place of alkyl groups in many of the functional groups described in this table.

Functional Group Nomenclature	General Structure	Substructures	Description
Azide [substructure: azide]	RNNN RNNN	R = alkyl group	Azides are chemical structures containing a linear arrangement of three nitrogen atoms, with one "end" connected to an alkyl group through a single bond. The three atoms can be represented as either a central nitrogen bridging the two other nitrogen atoms through double bonds, or as a nitrogen atom connected through a single bond to a triple bonded pair of nitrogen atoms.
Azo Compound [substructure: -diazene]	R ¹	R^1 , R^2 = alkyl group	Azo compounds are chemical structures containing a double bond connecting two nitrogen atoms. Each of the nitrogen atoms are connected to an alkyl group through a single bond.
Carbamate [substructure: <i>-carbamate</i>]	R^1 C N R^2 R^3	R^1 = alkyl group R^2 , R^3 = hydrogen atom or alkyl group	Carbamates are molecular structures containing a carbon atom connected to an oxygen atom through a double bond, to a nitrogen atom (which serves as a bridge to two hydrogen atoms and/or alkyl groups) and to a second oxygen atom (which serves as a bridge to a hydrogen atom or an alkyl group) through single bonds.
Carbonate [substructure: carbonate]	R^1 C R^2	R^1 , R^2 = hydrogen atom or alkyl group	Carbonates are molecular structures containing a carbon atom connected to an oxygen atom through a double bond, and two oxygen atoms (which serve as bridges to hydrogen atoms or alkyl groups) through single bonds.

Functional Group Nomenclature	General Structure	Substructures	Description
Carboxylate [substructure: -oate]		R = hydrogen atom or alkyl group	Carboxylates are the deprotonated (anionic) form of a carboxylic acid. The molecular structure contains a carbon atom connected to an oxygen atom through a double bond, with connections to a second oxygen atom (which carries a negative charge) and an alkyl group or hydrogen atom through single bonds.
Carboxylic Acid [substructure: -oic acid]		R = hydrogen atom or alkyl group	Carboxylic acids are chemical structures containing a carbon atom connected to an oxygen atom through a double bond, with connections to a second oxygen atom (connected to a hydrogen atom) and an alkyl group or hydrogen atom through single bonds.
Cycloalkane [substructure: <i>-cycloalkyl</i>]	$ \begin{pmatrix} R^{1} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$	R^1 , R^2 = hydrogen atom or alkyl group $n \ge 3$	Cycloalkanes are chemical structures composed entirely of carbon and hydrogen atoms. The carbon atoms are arranged in the form of a ring (a "cycle"). Each atom in the molecular structure is connected by single bonds (each carbon connected to four other atoms – these can be carbon or hydrogen, and each hydrogen atom is connected to one carbon). Cycloalkanes can be considered as alkanes/alkyls for purposes of the functional group definitions in this table.
Disulfide [substructure: -disulfide]	R ¹ —S—S—R ²	R ¹ , R ² = hydrogen atom or alkyl group	Disulfides are chemical structures composed of two sulfur atoms connected through a single bond that are each connected to an alkyl group.

Functional Group Nomenclature	General Structure	Substructures	Description
Di- thiocarboxylic Acid (Carbodithioic Acid) [substructure: -dithioic acid]	R SH	R = hydrogen atom or alkyl group	Dithiocarboxylic acids are chemical structures containing a carbon atom connected to a sulfur atom through a double bond, with connections to a second sulfur atom (connected to a hydrogen atom) and an alkyl group or hydrogen atom through single bonds.
Di- thiocarboxylic Acid Ester (Carbodithio) [substructure: -dithioate]	R^{1} C S R^{2}	R^1 = hydrogen atom or alkyl group R^2 = alkyl group	Carbodithio esters are chemical structures containing a carbon atom connected to a sulfur atom through a double bond, a second sulfur atom through a single bond (this sulfur serves as a bridge to an alkyl group), and an alkyl group or hydrogen atom through a single bond.
Epoxide [substructure: <i>-ene oxide</i>]	R^1 C C R^3 R^2 R^4	R^1 , R^2 , R^3 , R^4 = hydrogen atom or alkyl group	Epoxides are chemical structures containing a three membered ring ("cycle") of two carbon atoms and one oxygen atom. Each carbon atom has two additional connections to hydrogen atoms and/or alkyl groups.
Ester [substructure: <i>-yl -oate</i>]	$R^1 \xrightarrow{O} O = R^2$	R ¹ = hydrogen atom or alkyl group R ² = alkyl group	Esters are chemical structures containing a carbon atom connected to an oxygen atom through a double bond, a second oxygen atom through a single bond (this oxygen serves as a bridge to an alkyl group), and an alkyl group or hydrogen atom.
Ether [substructure: -oxy -ane]	R ¹ R ²	R^1 , R^2 = alkyl group	Ethers are chemical structures containing an oxygen atom that acts as a bridge between two alkyl groups.

Functional Group Nomenclature	General Structure	Substructures	Description
Guanidine [substructure: guanidino or -guanidine]	$R^{5} \qquad \qquad$	R^1 = hydrogen atom, alkyl group and/or other functional group R^2 , R^3 , R^4 , R^5 = hydrogen atom or alkyl group	The guanidine functional group contains a carbon atom connected to a nitrogen atom through a double bond, and two additional nitrogen atoms through single bonds. The nitrogen atoms have connections to additional groups (hydrogen atoms or alkyl groups). The single bonded nitrogen atoms have two additional connections, and the double bonded nitrogen atom has a single additional connection.
Hemiacetal [substructure: -al alkyl hemiacetal]	R ² —O R ¹ C H	R ¹ = hydrogen atom or alkyl group R ² = alkyl group	Hemiacetals are chemical structures containing a carbon atom connected to two oxygen atoms (one serving as a bridge to a hydrogen atom, and the other as a bridge to an alkyl group), and to either two hydrogen atoms or to a hydrogen atom and an alkyl group.
Hemiketal [substructure: -one alkyl hemiketal]	$R^3 \longrightarrow OH$ $R^2 \longrightarrow C$ R^1	R^1 , R^2 , R^3 = alkyl group	Hemiketals are chemical structures containing a carbon atom connected to two oxygen atoms (one serving as a bridge to a hydrogen atom, and the other as a bridge to an alkyl group), and to two alkyl groups.
Hydroperoxide [substructure: hydroperoxide]	ROH	R = alkyl group	Hydroperoxides are chemical structures containing an oxygen atom connected to a hydrogen atom, and to a second oxygen atom which serves as a bridge to an alkyl group.

Functional Group Nomenclature	General Structure	Substructures	Description
Imide [substructure: imido- or -imide]	$O = \begin{bmatrix} R^3 \\ I \\ N \\ C \\ R^2 \end{bmatrix} = \begin{bmatrix} R^3 \\ R^1 \end{bmatrix} O$	R^1 , R^2 , $R^3 =$ hydrogen atom or alkyl group	Imides are chemical structures containing a nitrogen atom that serves as a bridge between two carbon atoms (each connected to an oxygen atom through a double bond and to either a hydrogen atom or alkyl group through a single bond). The nitrogen atom has an additional connection to either a hydrogen atom or alkyl group through a single bond.
Imine [substructure: imino- or -imine]	R^3 R^2 R^1	R ¹ , R ² , R ³ = hydrogen atom or alkyl group	Imines are chemical structures containing a double bond connecting a carbon atom and a nitrogen atom. The carbon atom is connected to two other groups (hydrogen atoms or alkyl groups) through single bonds, and the nitrogen atom connects to either a hydrogen atom or alkyl group through a single bond.
Isocyanate [substructure: <i>isocyanate</i>]	R—_NCO	R = alkyl group	Isocyanates are molecular structures containing a carbon atom connected to a nitrogen atom and an oxygen atom through double bonds. The nitrogen atom is connected to an additional group (a hydrogen atom or alkyl group) through a single bond.
Isothiocyanate [substructure: thiocyanate]	R—N—C—S	R = alkyl group	Isothiocyanates are molecular structures containing a carbon atom connected to a nitrogen atom and a sulfur atom through double bonds. The nitrogen atom is connected to an additional group (a hydrogen atom or alkyl group) through a single bond.

Functional Group Nomenclature	General Structure	Substructures	Description
Ketal [substructure: -one dialkyl ketal]	$R^3 \longrightarrow C \longrightarrow C^4$ $R^2 \longrightarrow R^4$	R^1 , R^2 , R^3 , R^4 = alkyl group	Ketals are chemical structures containing a carbon atom connected to two oxygen atoms (which serve as bridges to alkyl groups), and to two additional alkyl groups.
Ketone [substructure: one]		R^1 , R^2 = alkyl group	Ketones are chemical structures containing a carbon atom connected to an oxygen atom through a double bond, and to two alkyl groups through single bonds.
Nitrate (Ester) [substructure: nitrate]		R = alkyl group	Nitrate esters are chemical structures containing a positively charged nitrogen atom connected to an oxygen atom through a double bond, and to two additional oxygen atoms through single bonds. One of the additional oxygen atoms serves as a bridge to an alkyl group, and the second additional oxygen atom carries a negative charge.
Nitrile [substructure: <i>-nitrile</i>]	R—C ≡ N	R = alkyl group	Nitriles are chemical structures containing a carbon atom connected to a nitrogen atom through a triple bond, where the carbon atom has an additional connection to an alkyl group through a single bond. When the carbon atom is not connected to an alkyl group, the functional group is referred to as a cyano group.
Nitrite [substructure: nitrite]	R—0—N—0	R = alkyl group	Nitrites are chemical structures containing a nitrogen atom connected to an oxygen atom through a double bond and to an additional oxygen atom (which serves a bridge to an alkyl group) through a single bond.

Functional Group Nomenclature	General Structure	Substructures	Description
Nitro Compound [Substructure = nitro-]	$ \begin{array}{c} $	R = alkyl group	Nitro compounds are chemical structures containing a positively charged nitrogen atom connected to an alkyl group, and two oxygen atoms, one through a double bond and the other through a single bond, which contains a negative charge. The structure is often shown with the two oxygen atoms being equivalent and having a "mixed" double/single bond character (and the negative charge shared between the two oxygen atoms).
Nitroso Compound [Substructure = nitroso- or nitrosyl]	RN===0	R = alkyl group	Nitroso compounds are chemical structures containing a nitrogen atom connected to an oxygen atom through a double bond, and to an alkyl group through a single bond.
Oxime [Substructure = oxime]	R^3 N R^2 R^1	R^1 , R^2 = hydrogen atom or alkyl group R^3 = hydrogen atom, alkyl group and/or other functional group	Oximes are chemical structures containing a nitrogen atom connected to a carbon atom through a double bond, and to an oxygen atom that serves as a bridge to a hydrogen atom (a hydroxyl group). The carbon atom has two additional single bonds to hydrogen atoms or alkyl groups. The oxygen of the hydroxyl group also serves as an additional point to connect the oxime to a larger molecular structure as a substitute for the hydrogen atom.
Peroxide [Substructure = peroxy- or peroxide]	R ¹ OR ²	R^1 , R^2 = alkyl group	Peroxides are chemical structures composed of two oxygen atoms connected through a single bond that are each connected to an alkyl group.

Functional Group Nomenclature	General Structure	Substructures	Description
Phosphate [Substructure = <i>phosphate</i>]	$R^2 \xrightarrow{O} \xrightarrow{O} \xrightarrow{O} \xrightarrow{O} \xrightarrow{O} \xrightarrow{R^3}$	R^1 , R^2 , $R^3 =$ hydrogen atom or alkyl group	Phosphates are chemical structures derived from phosphoric acid. The molecular structure contains a phosphorus atom connected to an oxygen atom through a double bond, and three additional oxygen atoms through single bonds. The single bonded oxygens serve as bridges to hydrogen atoms or alkyl groups. Also referred to as phosphate esters.
Phosphine [Substructure = phosphanyl- or -phosphane]		R = alkyl group	Phosphines are chemical structures containing a phosphorus atom connected to an alkyl group and to two hydrogen atoms through single bonds.
Phosphite Ester [Substructure = phosphite]	$R^2 \xrightarrow{O} P \xrightarrow{O} R^3$ $R^1 \xrightarrow{O} R^3$	R ¹ , R ² , R ³ = hydrogen atom or alkyl group	Phosphite esters are chemical structures containing a phosphorus atom connected to three oxygen atoms through single bonds. The oxygen atoms serve as bridges to hydrogen atoms and/or alkyl groups. When two of the oxygen atoms bridge alkyl groups and the third a hydrogen atom, the phosphorus atom is often shown as having a double bond to the oxygen and single bond connect to the hydrogen atom (which is no longer shown connected to the oxygen atom).
Phosphon- amide [Substructure = -phosphonamide]	$X \xrightarrow{\mathbf{P}}_{\mathbf{R}^{1}} \overset{\mathbf{N}}{\mathbf{R}^{2}} \overset{\mathbf{R}^{2}}{\overset{\mathbf{R}^{2}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}}{\overset{\mathbf{R}^{3}}{\overset{1}}{\overset{1}}{\overset{1}}{\overset{1}}{\overset{1}}{\overset{1}}{\overset{1}}{\overset{1}}{\overset{1}}$	R^1 = alkyl group R^2 , R^3 = hydrogen atom or alkyl group X = O-alkyl or halogen	Phosphonamides are chemical structures containing a phosphorus atom connected to an alkyl group, a nitrogen atom (with two connections to hydrogen atoms or alkyl groups), an oxygen atom through a double bond, and to either a second oxygen atom that bridges an alkyl group or to a halogen.

Functional Group Nomenclature	General Structure	Substructures	Description
Phosphonate [Substructure = phosphonate]	XPX X R^1	R = alkyl group X = O-alkyl, S-alkyl or halogen	Phosphonates are chemical structures containing a phosphorus atom connected to an alkyl group, an oxygen atom through a double bond and to two additional groups that can be oxygen or sulfur atoms (which serve as bridges to an additional alkyl groups and/or halogen atoms).
Phosphonite [Substructure = phosphonite]	P^2 O P $OR^1 R^3$	R^1 , R^2 , R^3 = alkyl group	Phosphonites are chemical structures containing a phosphorus atom connected to an alkyl group, and to two oxygen atoms through single bonds (each serving as a bridge to additional alkyl groups).
Phosphono- halodate [Substructure = phosphono halide (e.g. fluoro, chloro, bromo, iodo, astato)]	$x \xrightarrow{P}_{R^1} x \xrightarrow{R^2}$	R ¹ , R ² = alkyl group X = halogen	Phosphonohalodates are chemical structures containing a phosphorus atom connected to an oxygen atom through a double bond, and an alkyl group, a halogen atom, and an additional oxygen atom (which serves as a bridge to an alkyl group) through a single bond.
Phosphono- thiolate [Substructure = -phosphono- thiolate]	$ \begin{array}{c} $	R^1 , R^2 , R^3 = alkyl group	Phosphonothiolates are chemical structures containing a phosphorus atom connected to an oxygen atom through a double bond, and an alkyl group and oxygen and sulfur atoms (each serving as a bridge to additional alkyl groups) through single bonds.

Functional Group Nomenclature	General Structure	Substructures	Description
Phosphor- amide [Substructure = -phosphoramide]	$X \xrightarrow{0}_{R^2} X$ $R^2 \xrightarrow{N}_{R^1}$	R^1 , R^2 = hydrogen atom or alkyl group X = O-alkyl halogen or psuedohalogen	Phosphoroamidates are chemical structures containing a phosphorus atom connected to an oxygen atom through a double bond, with two single bond connections to oxygen atoms (which serve as bridges to additional alkyl groups) and/or to halogen atoms (or pseudohalogens), and an additional single bond connecting the phosphorus atom to a nitrogen atom. The nitrogen atom has two single bond connections to hydrogen atoms and/or alkyl groups.
Protonated Ammonium Salt [substructure: -ammonium]		R^1 = alkyl group R^2 , R^3 = hydrogen atom or alkyl group	Protonated ammonium salts are chemical structures containing a nitrogen atom (which carries a positive charge) connected to an alkyl group, with three additional connections to either alkyl groups or hydrogen atoms through single bonds.
Quaternary Ammonium Salt [substructure: -ammonium]	$R^{2} \xrightarrow{\qquad N \atop }{} R_{4}$	R^1 , R^2 , R^3 , R^4 = alkyl group	Quaternary ammonium salts are chemical structures containing a nitrogen atom (which carries a positive charge) connected to four alkyl groups through single bonds.
Sulfide [Substructure = di- (substituent) sulfide]	R ¹ —S—R ²	R^1 , R^2 = alkyl group	Sulfides are chemical structures containing a sulfur atom that acts as a bridge between two alkyl (or substituted alkyl) groups.

Functional Group Nomenclature	General Structure	Substructures	Description
Sulfinic Acid [Substructure: <i>-sulfinic acid</i>]		R = hydrogen atom or alkyl group	Sulfinic acids are chemical structures containing a sulfur atom connected to an oxygen atom through a double bond, with connections to a second oxygen atom (connected to a hydrogen atom) and an alkyl group or hydrogen atom through single bonds.
Sulfonate Ester [Substructure = (-sulfonyl)oxy or -sulfonate]	R^1 O R^2	R^1 , R^2 = alkyl group	Sulfonate esters are chemical structures containing a sulfur atom connected to an alkyl group and three oxygen atoms. Two oxygen atoms are connected through double bonds and the other (which serves as a bridge to an alkyl group) is connected through a single bond.
Sulfone [Substructure = di- (substitutent) sulfone]	R ¹ R ²	R^1 , R^2 = alkyl group	Sulfones are chemical structures containing a sulfur atom connected to two oxygen atoms through double bonds, and two alkyl groups through single bonds.
Sulfonic Acid [Substructure: -sulfonic acid]	R OH	R = alkyl group	Sulfonic acids are chemical structures containing a sulfur atom connected to an alkyl group and three oxygen atoms. Two oxygen atoms are connected through double bonds and the other (which serves as a bridge to a hydrogen atom) is connected through a single bond.
Sulfoxide [Substructure = di- (substituent) sulfoxide]	R^1 R^2	R^1 , R^2 = alkyl group	Sulfoxides are chemical structures containing a sulfur atom connected to an oxygen atom through a double bond and to two alkyl groups through single bonds.

Functional Group Nomenclature	General Structure	Substructures	Description
Thial [Substructure: <i>-thial</i>]	R H	R = hydrogen atom or alkyl group	Thials are chemical structures containing a carbon atom connected to a sulfur atom through a double bond, and to either two hydrogen atoms or a hydrogen atom and an alkyl group through single bonds.
Thiocarboxylic acid (Carbothoic S- acid) [Substructure: - <i>thioic S-acid</i>]		R = hydrogen atom or alkyl group	Carbothoic S-acids are chemical structures containing a carbon atom connected to an oxygen atom through a double bond, with connections to a sulfur atom (connected to a hydrogen atom) and to an alkyl group or hydrogen atom through single bonds.
Thiocarboxylic acid (Carbothoic O- acid) [Substructure: - <i>thioic O-acid</i>]	R C OH	R = hydrogen atom or alkyl group	Carbothoic O-acids are chemical structures containing a carbon atom connected to a sulfur atom through a double bond, with connections to an oxygen atom (connected to a hydrogen atom) and an alkyl group or hydrogen atom through single bonds
Thiocyanate [Substructure: <i>thiocyanate</i>]	R—S—C <mark>—</mark> N	R = hydrogen atom or alkyl group	Thiocyanates are chemical structures containing a carbon atom connected to a nitrogen atom through a triple bond and to a sulfur atom through a single bond. The sulfur atom is connected to an additional group (hydrogen atom or alkyl group) through a single bond.
Thiolester [Substructure: S-alkyl-alkane- <i>thioate</i>]	R^1 S R^2	R^1 , R^2 = alkyl group	Thiolesters are chemical structures containing a carbon atom connected to an oxygen atom through a double bond, an alkyl group and a sulfur atom (which serves as a bridge to an alkyl group).

Functional Group Nomenclature	General Structure	Substructures	Description
Thionoester [Substructure: O-alkyl-alkane- thioate]	$R^1 \xrightarrow{C} O \xrightarrow{R^2}$	R^1 , R^2 = alkyl group	Thionoesters are chemical structures containing a carbon atom connected to a sulfur atom through a double bond, an alkyl group and an oxygen atom (which serves as a bridge to an alkyl group).
Thioketone [Substructure: <i>-thione</i>]		R^1 , R^2 = alkyl group	Thioketones are chemical structures containing a carbon atom connected to a sulfur atom through a double bond and to two alkyl groups through single bonds.
Thiol [Substructure: <i>-thiol</i>]	RSH	R = alkyl group	Thiols are chemical structures that contain thiol groups (a sulfur atom and a hydrogen atom) connected to an alkyl group.

