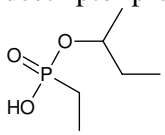
PROTOCOL FOR NAMING COMPOUNDS IN THE OPCW CENTRAL ANALYTICAL DATABASE

ANY CHANGES TO THIS PROTOCOL SHALL BE APPROVED BY THE VALIDATION GROUP. A NEW VERSION OF THIS PROTOCOL WILL BE DISTRIBUTED TO ALL VALIDATION GROUP MEMBERS.

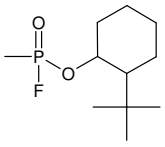
1. In general, the name (spelling, punctuation, spaces, and so on) is to be based on the name given in the Annex on Chemicals to the Chemical Weapons Convention (hereinafter "the Convention").

2. The following additional rules should be followed in cases where the information in the Schedules of Chemicals is insufficient to designate only one name.

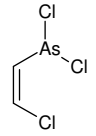
2.1 The name is to be capitalised—the only exceptions being the structural and stereo-descriptors, sec-, tert-, *cis*-, and *trans*-. In cases where a structural or stereo-descriptor prefixes a name, the name is to be capitalised.



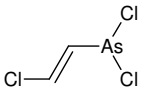
sec-Butyl ethylphosphonate 2.B.04[1]



2-tert-Butylcyclohexyl methylphosphonofluoridate 1.A.01



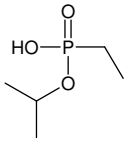
cis-2-Chlorovinyldichloroarsine 1.A.05



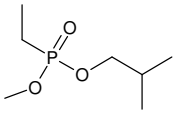
trans-2-Chlorovinyldichloroarsine 1.A.05

2.2 The trivial names for the following radicals are to be used:

Saturated branched Isopropyl, Isobutyl, sec-Butyl, tert-Butyl.

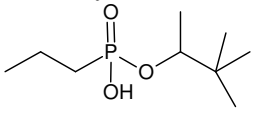


Isopropyl ethylphosphonate 2.B.04



Isobutyl methyl ethylphosphonate 2.B.04

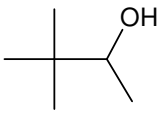
Pinacolyl is to be used instead of 1,2,2-trimethylpropyl.



Pinacolyl propylphosphonate 2.B.04

[1] The number listed is the CWC schedule

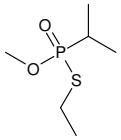
However, pinacolyl alcohol should be referred to as 3,3-dimethylbutan-2-ol.



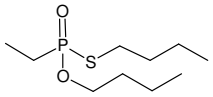
3,3-Dimethylbutan-2-ol 2.B.14

Unsaturated Vinyl, Allyl, Isopropenyl.

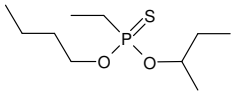
2.3 When a compound has several substituents, they are to be listed in alphabetical order, irrespective of the presence of N-, O-, or S- prefixes, and of the descriptors, sec-, tert-, cis- or trans-; but see rule 2.5 below.



S-Ethyl O-methyl isopropylphosphonothiolate 2.B.04

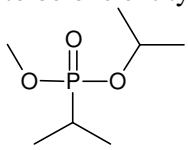


O-Butyl S-butyl ethylphosphonothiolate 2.B.04

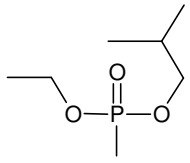


O-Butyl O-sec-butyl ethylphosphonothionate 2.B.04

2.4 The radicals beginning with iso e.g. isobutyl, isopropenyl, and isopropyl are considered to be one entity and are to be listed in alphabetical order starting from “iso” e.g.

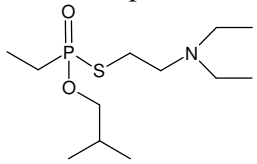


Isopropyl methyl isopropylphosphonate 2.B.04



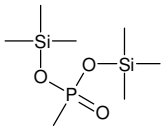
Ethyl isobutyl methylphosphonate 2.B.04

2.5 The substituents in Schedule 1.A.03 and 1.B.10 compounds are to be listed in the order “alkyl 2-dialkylaminoethyl”, in line with the names given in the Convention, but constituting an exception to rule 2.3 above. The same exception applies to Schedule 2.B.4 compounds containing the “alkyl 2-dialkylaminoethyl” moieties.

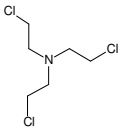


Isobutyl S-2-diethylaminoethyl ethylphosphonothiolate 1.A.03

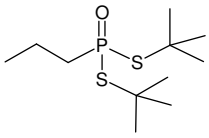
2.6 Parentheses are to be used in the following cases around prefixes defining substituted substituents—after the numerical multiplicative prefixes “bis”, “tris”, and so on; around simple substituent prefixes to separate locants of the same type referring to different structural elements; and to avoid ambiguity.



Bis(trimethylsilyl) methylphosphonate 2.B.04



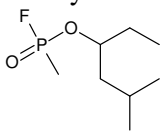
Tris(2-chloroethyl)amine 1.A.06



Bis(S-tert-butyl) propylphosphonodithiolate 2.B.04

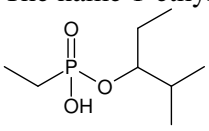
2.7 For radicals with a branching structure, the name should be derived from the longest continuous chain starting (position 1) at the conjunction with the parent structure. Examples:

(a) The methylphosphonofluoridate made using 5-methyl-3-hexanol is 1-Ethyl-3-methylbutyl methylphosphonofluoridate.



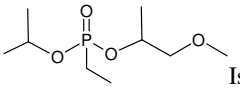
1-Ethyl-3-methylbutyl methylphosphonofluoridate 1.A.01

(b) The name 1-ethyl-2-methylpropyl is to be used instead of 1-isopropylpropyl.



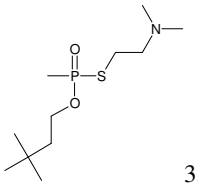
1-Ethyl-2-methylpropyl ethylphosphonate 2.B.04

(c) Substituted chains are to be alphabetical as well.

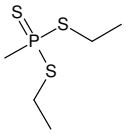


Isopropyl 2-methoxy-1-methylethyl ethylphosphonate 2.B.04

2.8 Thiolate and thionate are to be differentiated according to whether the S-atom is single- or double-bonded to the phosphorus atom.

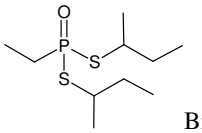


3,3-Dimethylbutyl S-2-dimethylaminoethyl methylphosphonothiolate 1.A.03

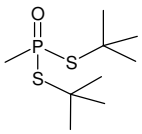


Diethyl methylphosphonodithiolothionate 2.B.04

2.9 For phosphorus compounds containing two S-sec-butyl or S-tert-butyl groups linked to phosphorus, the name has to start with Bis(S-sec-butyl) or Bis(S-tert-butyl).

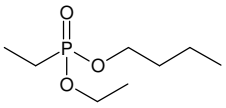


Bis(S-sec-butyl) ethylphosphonodithiolate 2.B.04



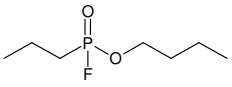
Bis(S-tert-butyl) methylphosphonodithiolate 2.B.04

2.10 The name is to be as short as possible, and unnecessary characters such as the following are to be left out

(a) the n- in n-alkyl;  Butyl ethyl ethylphosphonate 2.B.04

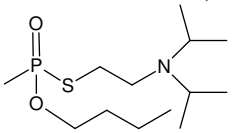
(b) the 1- before 1-alkyl, in case of a normal alkyl chain;

(c) the O in O-Alkyl alkylphosphonohalidates;



Butyl propylphosphonofluoridate 1.A.01

(d) the O in O-Alkyl S-2-dialkylaminoethyl alkylphosphonothiolates belonging to Schedule 1.A.03; and



Butyl S-2-diisopropylaminoethyl methylphosphonothiolate 1.A.03

(e) unnecessary brackets and parentheses.

2.11 Hydrochloride salts of schedule 2.B.10, 2.B.11 and 2.B.12 chemicals are to be named as free amines with the addition of hydrochloride.

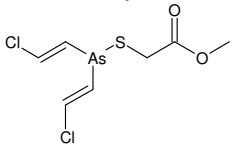
2-(N,N-Dipropylamino)ethylchloride hydrochloride	2.B.10
2-(N,N-Dipropylamino)ethanol hydrochloride	2.B.11
2-(N,N-Diethylamino)ethanethiol hydrochloride	2.B.12

2.12 Substituents to an aromatic ring are to be numbered numerically.

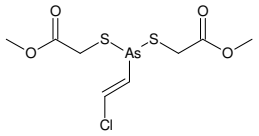
2.13 Arsenic-containing derivatives or decomposition products of the Lewisites (Schedule 1.A.05) shall be named as follows:

(a) Derivatives with alkyl thioglycolates shall be named per the following examples:

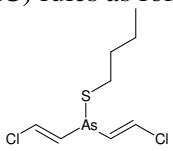
(i) 2-Methoxy-2-oxoethyl bis(2-chlorovinyl)arsinothiolate

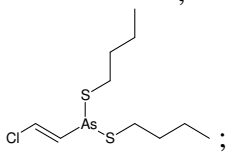


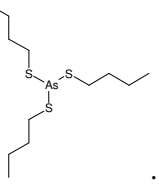
(ii) Bis(2-methoxy-2-oxoethyl) 2-chlorovinylarsonodithiolite.



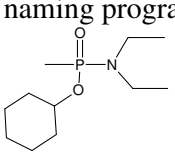
(b) Derivatives with butanethiol shall be named in accordance with the International Union of Pure and Applied Chemistry (IUPAC) rules as follows:

(i) Butyl bis(2-chlorovinyl)arsinothiolite  ;

(ii) Dibutyl 2-chlorovinylarsonodithiolite  ;

(iii) Tributyl arsenotrithiolite  .

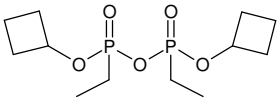
2.14 Amidate shall be used instead of amidoate (a term used by some commercial chemical naming programs)



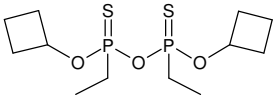
Cyclohexyl N,N-diethyl-P-methylphosphonamidate 2.B.04

2.15 Compounds with multiple phosphorus atoms shall be named as follows:

(a) A symmetrical phosphonate dimer with an oxygen linkage shall be called a pyrophosphonate.

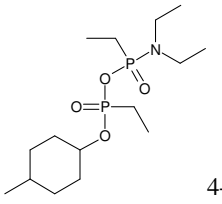


Dicyclobutyl diethylpyrophosphonate 2.B.04



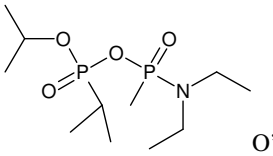
Dicyclobutyl diethylpyrophosphonodithionate 2.B.04

(b) Multiple phosphorus atoms shall be identified as P, P', etc.



4-Methylcyclohexyl N,N-diethyl-P,P'-diethyldiphosphono-P-amidate 2.B.04

(c) Groups attached to the phosphorus shall be indicated by corresponding prime marks (e.g. "-S-methyl" or "-N',N'-diethyl-", etc.), with P listed before P'.



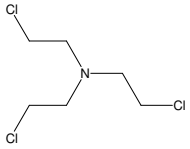
O'-Isopropyl N,N-diethyl-P-methyl-P'-isopropylphosphono-P-amidate 2.B.04

(d) Otherwise, IUPAC names shall be used.

2.16 Compounds based on amines shall be named as follows:

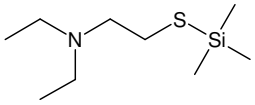
(a) Amines named in the Convention shall use the Convention names.

(b) Amines with three identical groups shall be named without using the N- prefix.



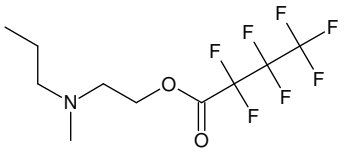
Tris(2-chloroethyl)amine

(c) All other amines shall be named with the N positions explicitly identified.

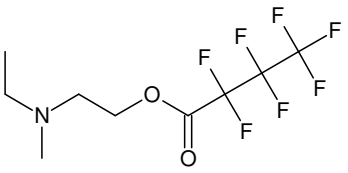


N,N-Diethyl-N-(2-trimethylsilylthioethyl)amine

2.17 Analytical derivatives of amines shall be named on the basis of the original compounds before derivatization.

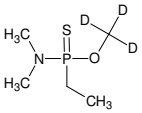


N-Heptafluorobutyryloxyethyl-N-methyl-N-propylamine DS[2]

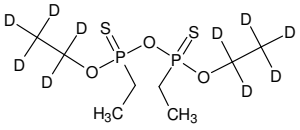


N-Ethyl-N-heptafluorobutyryloxyethyl-N-methylamine DS

2.18 Compounds containing deuterium atoms shall be named as follows:
For structure and formula -- use capital **D**;
For names -- use lowercase **d**.



Methyl-d3 N,N-dimethyl-P-ethylphosphonamidothionate 2.B.04

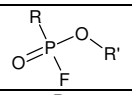
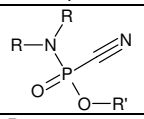
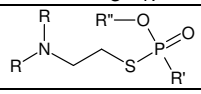
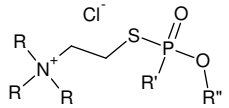
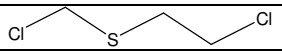
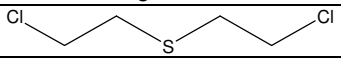
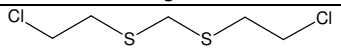
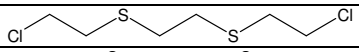
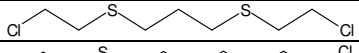
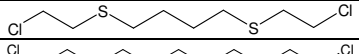
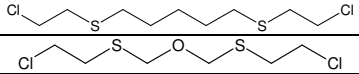
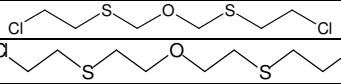
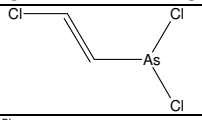
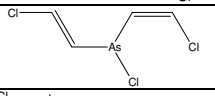
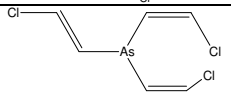
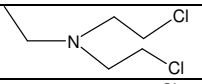
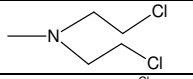
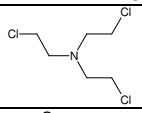
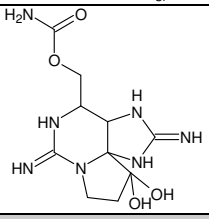
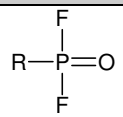


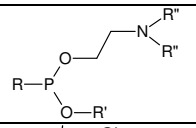
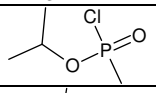
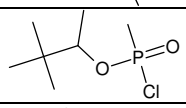
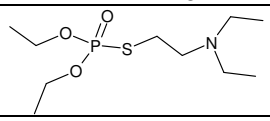
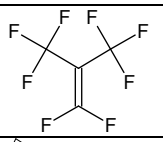
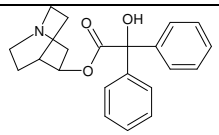
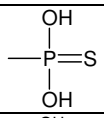
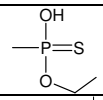
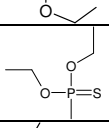
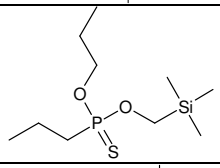
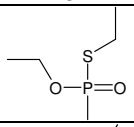
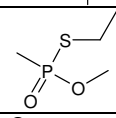
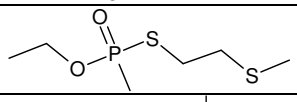
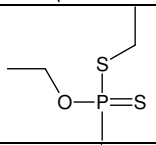
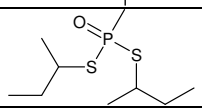
Bis(ethyl-d5) P,P'-diethylpyrophosphonodithionate 2.B.04

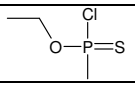
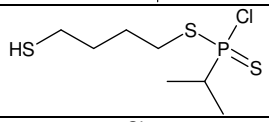
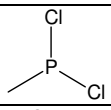
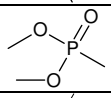
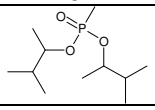
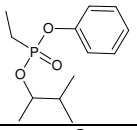
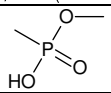
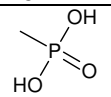
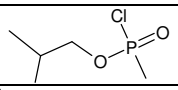
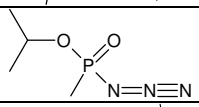
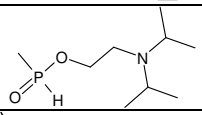
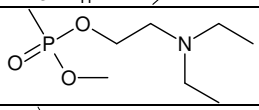
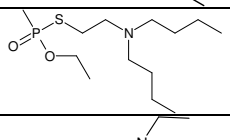
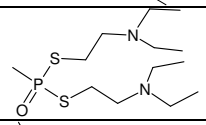
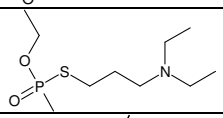
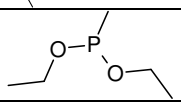
3. These rules are illustrated below by examples of scheduled compounds, derivatives associated with the scheduled compounds, and non-scheduled reportable chemicals.

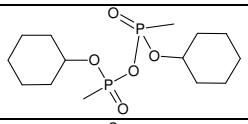
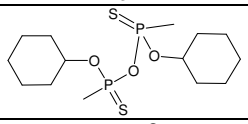
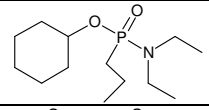
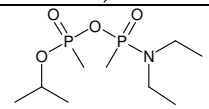
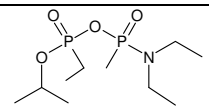
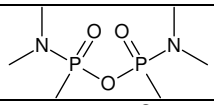
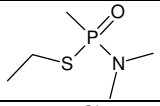
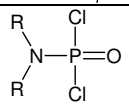
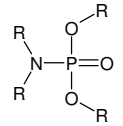
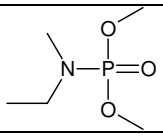
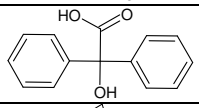
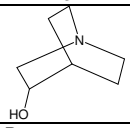
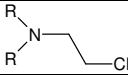
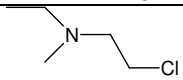
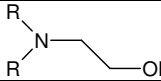
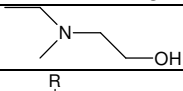
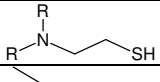
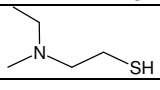
[2] Derivative of scheduled chemical

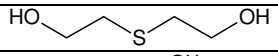
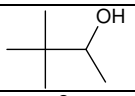
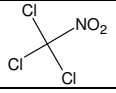
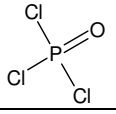
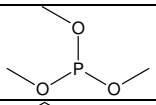
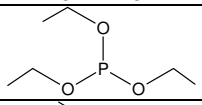
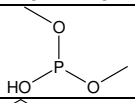
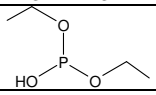
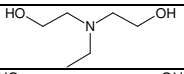
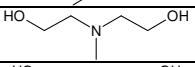
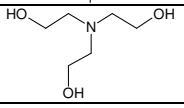
Examples of Names of Scheduled Compounds

Schedule	Name	Structure
1.A.01	Alkyl alkylphosphonofluoridate	
1.A.02	Alkyl N,N-dialkylphosphoramidocyanidate	
1.A.03	Alkyl S-2-dialkylaminoethyl alkylphosphonothiolate	
	Alkyl S-trialkylammoniumethyl alkylphosphonothiolate halide (i.e. chloride, iodide)	
1.A.04	2-Chloroethylchloromethylsulfide	
	Bis(2-chloroethyl)sulfide	
	Bis(2-chloroethylthio)methane	
	1,2-Bis(2-chloroethylthio)ethane	
	1,3-Bis(2-chloroethylthio)propane	
	1,4-Bis(2-chloroethylthio)butane	
	1,5-Bis(2-chloroethylthio)pentane	
	Bis(2-chloroethylthiomethyl)ether	
	Bis(2-chloroethylthioethyl)ether	
1.A.05	2-Chlorovinyldichloroarsine	
	Bis(2-chlorovinyl)chloroarsine	
	Tris(2-chlorovinyl)arsine	
1.A.06	Bis(2-chloroethyl)ethylamine	
	Bis(2-chloroethyl)methylamine	
	Tris(2-chloroethyl)amine	
1.A.07	Saxitoxin	
1.A.08	Ricin	
1.B.09	Alkylphosphonic difluoride	

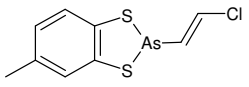
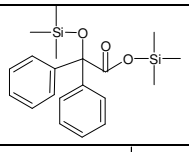
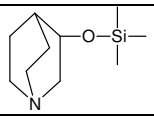
Schedule	Name	Structure
1.B.10	Alkyl 2-dialkylaminoethyl alkylphosphonite	
1.B.11	Isopropyl methylphosphonochloridate	
1.B.12	Pinacolyl methylphosphonochloridate	
2.A.01	O,O-Diethyl S-2-diethylaminoethyl phosphorothiolate	
2.A.02	1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene	
2.A.03	3-Quinuclidinyl benzilate	
2.B.04	To avoid any confusion, the O and S groups should be indicated in esters when sulfur is present.	
	Methylphosphonothionic acid	
	O-Ethyl methylphosphonothionate	
	O,O-Diethyl methylphosphonothionate	
	O-Propyl O-trimethylsilyl propylphosphonothionate	
	O-Ethyl S-ethyl methylphosphonothiolate	
	S-Ethyl O-methyl methylphosphonothiolate	
	O-Ethyl S-2-methylthioethyl methylphosphonothiolate	
	O-Ethyl S-ethyl methylphosphonothiolothionate	
	Bis(S-sec-butyl) methylphosphonodithiolate	

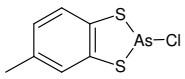
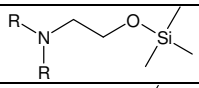
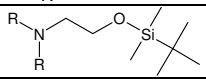
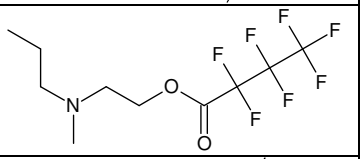
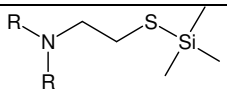
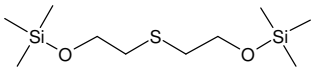
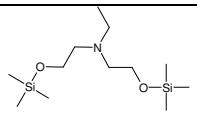
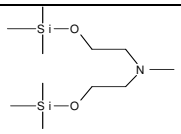
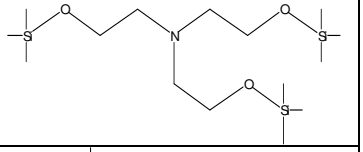
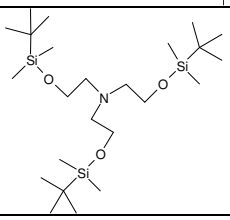
Schedule	Name	Structure
	O-Ethyl methylphosphonothionochloridate	
	S-(4-Mercaptobutyl) isopropylphosphonothiolothionochloridate	
	Methylphosphonous dichloride	
	Methylphosphonic dichloride	
	Methylphosphonothionic dichloride	
	Dimethyl methylphosphonate	
	Bis(1,2-dimethylpropyl) methylphosphonate	
	1,2-Dimethylpropyl phenyl ethylphosphonate	
	Methyl methylphosphonate instead of methyl methylphosphonic acid	
	Methylphosphonic acid	
	Isobutyl methylphosphonochloridate	
	Isopropyl methylphosphonoazidate	
	2-Diisopropylaminoethyl methylphosphinate	
	Methyl 2-diethylaminoethyl methylphosphonate	
	O-Ethyl S-2-dibutylaminoethyl methylphosphonothiolate	
	Bis(S-2-diethylaminoethyl) methylphosphonodithiolate	
	O-Ethyl S-3-diethylaminopropyl methylphosphonothiolate	
	Diethyl methylphosphonite	

Schedule	Name	Structure
	Dicyclohexyl dimethylpyrophosphonate	
	Dicyclohexyl dimethylpyrophosphonodithionate	
	Cyclohexyl N,N-diethyl-P-propylphosphonamidate	
	Isopropyl N,N-diethyl-P,P'-dimethyldiphosphono-P-amidate	
	O'-Isopropyl N,N-diethyl-P-methyl-P'-ethyldiphosphono-P-amidate	
	N,N,N',N'-Tetramethyl-P,P'-dimethylpyrophosphonic diamide	
	S-Ethyl N,N-dimethyl-P-methylphosphonamidothiolate	
2.B.05	N,N-Dialkylphosphoramidic dichloride	
2.B.06	Dialkyl N,N-dialkylphosphoramidate	
	Dimethyl N-ethyl-N-methylphosphoramidate	
2.B.07	Arsenic trichloride	$AsCl_3$
2.B.08	2,2-Diphenyl-2-hydroxyacetic acid	
2.B.09	3-Quinuclidinol	
2.B.10	2-(N,N-Dialkylamino)ethylchloride	
	2-(N-Ethyl-N-methylamino)ethylchloride	
2.B.11	2-(N,N-Dialkylamino)ethanol	
	2-(N-Ethyl-N-methylamino)ethanol	
2.B.12	2-(N,N-Dialkylamino)ethanethiol	
	2-(N-Ethyl-N-methylamino)ethanethiol	

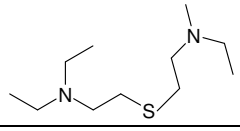
Schedule	Name	Structure
2.B.13	Bis(2-hydroxyethyl)sulfide	
2.B.14	3,3-Dimethyl-2-butanol	
3.A.01	Carbonyl dichloride	
3.A.02	Cyanogen chloride	
3.A.03	Hydrogen cyanide	H-CN
3.A.04	Trichloronitromethane	
3.B.05	Phosphorus oxychloride	
3.B.06	Phosphorus trichloride	$P\text{-}Cl_3$
3.B.07	Phosphorus pentachloride	$P\text{-}Cl_5$
3.B.08	Trimethyl phosphite	
3.B.09	Triethyl phosphite	
3.B.10	Dimethyl phosphite	
3.B.11	Diethyl phosphite	
3.B.12	Sulfur monochloride	S_2Cl_2
3.B.13	Sulfur dichloride	SCl_2
3.B.14	Thionyl chloride	$S(O)Cl_2$
3.B.15	Ethyldiethanolamine	
3.B.16	Methyldiethanolamine	
3.B.17	Triethanolamine	

Examples of Names for Derivatives of Scheduled Compounds

Associated Schedule	Chemical Name	Structure
1.A.05	2-(2-Chlorovinyl)-5-methyl-1,3,2-benzodithiarsole	
2.B.08	Bis(trimethylsilyl)benzilate	
2.B.09	3-Quinuclidinyl trimethylsilyl ether	

Associated Schedule	Chemical Name	Structure
2.B.07	2-Chloro-5-methyl-1,3,2-benzodithiarsole	
2.B.11	N,N-Dialkyl-N-(2-trimethylsilyloxyethyl)amine	
	N,N-Dialkyl-N-(2-tert-butyldimethylsilyloxyethyl)amine	
	N-Heptafluorobutyryloxyethyl-N-methyl-N-propylamine	
2.B.12	N,N-Dialkyl-N-(2-trimethylsilylthioethyl)amine	
2.B.13	Bis(2-trimethylsilyloxyethyl)sulfide	
3.B.15	N-Ethyl-N,N-bis(2-trimethylsilyloxyethyl)amine	
3.B.16	N-Methyl-N,N-bis(2-trimethylsilyloxyethyl)amine	
3.B.17	Tris(2-trimethylsilyloxyethyl)amine	
	Tris(2-tert-butyldimethylsilyloxyethyl)amine	

Examples of Names for Relevant Non-Scheduled Chemicals

Schedule	Chemical Name	Structure
N.S.	(2-N,N-Diethylaminoethyl)(2-N-ethyl-N-methylaminoethyl)sulfide	
N.S.	(2-N,N-Diethylaminoethyl)(2-N-ethyl-N-methylaminoethyl)disulfide