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.

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

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

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

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¹ The number listed is the CWC schedule

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

Unsaturated Vinyl, Allyl, Isopropenyl.

3-((Dimethylcarbamoyl)oxy)-2-picolinyl is to be used instead of (3-((dimethylcarbamoyl)oxy)pyridin-2-yl)methyl

$$\begin{array}{c|c}
N \\
O \\
O \\
N \\
Br \\
OH
\end{array}$$

 N^{1} -(3-((Dimethylcarbamoyl)oxy)-2-picolinyl)- N^{10} -hydroxymethyl- N^{1} -ethyl- N^{10} -methyl- N^{1} , N^{10} -dipropyldecane-1,10-diammonium dibromide 1.A.16

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.

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.

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 "2-dialkylaminoethyl" moiety.

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.

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:

Bis(S-tert-butyl) propylphosphonodithiolate

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

2.B.04

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

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

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



Diethyl methylphosphonodithiolothionate 2.B.0

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 nain nalkyli
- (a) the n- in n-alkyl; O Butyl ethyl phosphonate 2.B.04
- (b) the 1- before 1-alkyl, in case of a normal alkyl chain;
- (c) the O in O-Alkyl alkylphosphonohalidates;

(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)arsinothiolite

(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:

(ii) Dibutyl 2-chlorovinylarsonodithiolite of As ;

(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.

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

(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'.

- (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

DS

N-Ethyl-N-heptafluorobutyryloxyethyl-N-methylamine

2.18 For chemicals other than those listed in the Convention and chemicals with the same configuration around the phosphorus atom, trivalent phosphorus chemicals shall be named according to the IUPAC naming rule that classifies these chemicals as phosphines.

² Derivative of scheduled chemical

2.19 Compounds containing deuterium atoms shall be named as follows:

For structure and formula -- use capital **D**;

For names -- use lowercase d.

 H_3C

2.20 1.A.13 and 1.A.15 chemicals are to be named as phosphonamidic fluoride because the halide takes priority in naming.

N-(Bis(diethylamino)methylidene)-P-methylphosphonamidic fluoride 1.A.15

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2.21 The order in which to write the various groups for 1.A.16 chemicals should be: N¹-(3-((dimethylcarbamoyl)oxy)-2-picolinyl)) comes first, then the hydroxyl/cyano/acetoxy group, then the alkyl groups in alphabetical order, then finally decane or dioxoalkane.

 $N^1-(3-((Dimethylcarbamoyl)oxy)-2-picolinyl)-N^{10}-hydroxymethyl-N^1-ethyl-N^{10}-methyl-N^1,N^{10}-dipropyldecane-1,10-diammonium dibromide$

 $N^1-(3-((Dimethylcarbamoyl)oxy)-2-picolinyl)-N^{10}-(2-cyanoethyl)-N^1-butyl-N^1,\\N^{10}-diethyl-N^{10}-methyldecane-1,\\10-diammonium dibromide$

$$\begin{array}{c|c}
O & N \\
O & N \\
O & Br
\end{array}$$

 $N^1,N^8-Bis(3-((dimethylcarbamoyl)oxy)-2-picolinyl)-N^1,N^8-diethyl-N^1,N^8-dimethyl-2,7-dioxooctane-1,8-diammonium dibromide$

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

Examples of Names of Scheduled Compounds

Schedule	Name	Structure
1.A.01	Alkyl alkylphosphonofluoridate	R O R' F
1.A.02	Alkyl N,N-dialkylphosphoramidocyanidate	R-N O O-R'
1.A.03	Alkyl S-2-dialkylaminoethyl alkylphosphonothiolate	R R"-0 R N S R'
	Alkyl S-trialkylammoniumethyl alkylphosphonothiolate halide (i.e. chloride, iodide)	R R R' R"
1.A.04	2-Chloroethylchloromethylsulfide	CISCI
	Bis(2-chloroethyl)sulfide	Cl
	Bis(2-chloroethylthio)methane	CI
İ	1,2-Bis(2-chloroethylthio)ethane	CI S S CI
	1,3-Bis(2-chloroethylthio)propane	CI S CI
	1,4-Bis(2-chloroethylthio)butane	CI S CI
	1,5-Bis(2-chloroethylthio)pentane	CISCI
	Bis(2-chloroethylthiomethyl)ether	CI S CI
	Bis(2-chloroethylthioethyl)ether	a s o s
1.A.05	2-Chlorovinyldichloroarsine	CI————————————————————————————————————
	Bis(2-chlorovinyl)chloroarsine	CI————————————————————————————————————
	Tris(2-chlorovinyl)arsine	CI————————————————————————————————————

Schedule	Name	Structure
1.A.06	Bis(2-chloroethyl)ethylamine	N CI
	Bis(2-chloroethyl)methylamine	N CI
	Tris(2-chloroethyl)amine	CI C
1.A.07	Saxitoxin	H ₂ N O O H NH NH NH OHOHOH
1.A.08	Ricin	
1.A.13	N-(1-(Dialkylamino)alkylidene)-P-alkylphosphonamidic fluoride	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
1.A.14	Alkyl N-(1- (dialkylamino)alkylidene)phosphoramidofluor idate	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
1.A.15	N-(Bis(diethylamino)methylidene)-P-methylphosphonamidic fluoride	H_3C N CH_3 CH_3 CH_3 N O $ $ N P CH_3 $ $ P

Schedule	Name	Structure
1.A.16	N¹-(3-((Dimethylcarbamoyl)oxy)-2-picolinyl)-N¹0-((hydroxy, cyano, acetoxy)alkyl)-N¹-alkyl-N¹-alkyl-N¹0-alkyl-N¹0-alkyldecane-1,10-diammonium dibromide	R_1 R_2 R_3 R_4 R_5 R_4 R_5 R_4 R_5 R_5 R_4 R_5
	N ¹ ,N ⁿ -Bis(3-((dimethylcarbamoyl)oxy)-2-picolinyl)-N ¹ ,N ⁿ -dialkyl-N ¹ ,N ⁿ -dialkyl-2,(n-1)-dioxoalkane-1,n-diammonium dibromide	H_3C CH_3 R_2 R_2 R_2 R_3 R_4 R_5 R_5 R_5 R_7
1.B.09	Alkylphosphonic difluoride	Br Br F R—P==0 F
1.B.10	Alkyl 2-dialkylaminoethyl alkylphosphonite	N R" R—P O—R'
1.B.11	Isopropyl methylphosphonochloridate	CI
1.B.12	Pinacolyl methylphosphonochloridate	
2.A.01	O,O-Diethyl S-2-diethylaminoethyl phosphorothiolate	

Schedule	Name	Structure
2.A.02	1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-	F
	propene	
		f f
2 4 02	2.0 : 1:1: 11 :1.4	F´ F
2.A.03	3-Quinuclidinyl benzilate	N OH
2.B.04	To avoid any confusion, the O and S groups sho	uld be indicated in esters when sulfur is present.
	Methylphosphonothionic acid	OH
		—Þ=S
	O.F.d. 1	ÓН ОН
	O-Ethyl methylphosphonothionate	—P=s
		0 /
	O,O-Diethyl methylphosphonothionate	
		0 0-P=s
	O-Propyl O-trimethylsilyl	
	propylphosphonothionate	\right\).
		0′ 0、 Si
	O-Ethyl S-ethyl methylphosphonothiolate	
		s
		Ö—P=0
	S-Ethyl O-methyl methylphosphonothiolate	
)
		// 0/
	O-Ethyl S-2-methylthioethyl	0, ,
	methylphosphonothiolate	0-\bar{p}-3\cdots
		5 \ 5

Schedule	Name	Structure
	O-Ethyl S-ethyl methylphosphonothiolothionate	O—P=S
	Bis(S-sec-butyl) methylphosphonodithiolate	O S S
	O-Ethyl methylphosphonothionochloridate	CI 0-P=s
	S-(4-Mercaptobutyl) isopropylphosphonothiolothionochloridate	HS S P S
	Methylphosphonous dichloride	CI
	Methylphosphonic dichloride	CI CI P
	Methylphosphonothionic dichloride	CI CI S
	Dimethyl methylphosphonate	
	Bis(1,2-dimethylpropyl) methylphosphonate	
	N-(Bis(dimethylamino)methylidene)-P-methylphosphonamidic fluoride	H ₃ C CH ₃ F CH ₃ CH ₃ CH ₃
	Methyl N-(bis(dimethylamino)methylidene)- P-methylphosphonamidate	H ₃ C O P CH ₃ CH ₃ CH ₃ CH ₃

Schedule	Name	Structure
	S,S-Diethyl methylphosphonodithioloselenoate	H ₃ C Se CH ₃
	O-Isobutyl methylphosphonothionate, sodium salt	H_3C O
	1,2-Dimethylpropyl phenyl ethylphosphonate	
	Methyl methylphosphonate instead of methyl methylphosphonic acid	O— HO
	Methylphosphonic acid	OH P HO
	Isobutyl methylphosphonochloridate	CI O_P_O
	Isopropyl methylphosphonoazidate	$N = N \equiv N$
	2-Diisopropylaminoethyl methylphosphinate	H O O
	Methyl 2-diethylaminoethyl methylphosphonate	0 N N
	O-Ethyl S-2-dibutylaminoethyl methylphosphonothiolate	OZP S N
	Bis(S-2-diethylaminoethyl) methylphosphonodithiolate	S N

Schedule	Name	Structure
	O-Ethyl S-3-diethylaminopropyl methylphosphonothiolate	op s N
	Diethyl methylphosphonite	O-P, O-
	Bis(ethylthio)methylphosphine	H ₃ C—P S——CH ₃
	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	N P O P N
	S-Ethyl N,N-dimethyl-P- methylphosphonamidothiolate	S P N

Schedule	Name	Structure
2.B.05	N,N-Dialkylphosphoramidic dichloride	R CI N—P==0 R CI
2.B.06	Dialkyl N,N-dialkylphosphoramidate	R O R N—P=O R O R
	Dimethyl N-ethyl-N-methylphosphoramidate	N-P=0 0
2.B.07	Arsenic trichloride	AsCl ₃
2.B.08	2,2-Diphenyl-2-hydroxyacetic acid	HO OH
2.B.09	3-Quinuclidinol	HO
2.B.10	2-(N,N-Dialkylamino)ethylchloride	R N—CI
	2-(N-Ethyl-N-methylamino)ethylchloride	N———CI
2.B.11	2-(N,N-Dialkylamino)ethanol	R N—OH
	2-(N-Ethyl-N-methylamino)ethanol	N——OH
2.B.12	2-(N,N-Dialkylamino)ethanethiol	R SH
	2-(N-Ethyl-N-methylamino)ethanethiol	N
2.B.13	Bis(2-hydroxyethyl)sulfide	HO

Schedule	Name	Structure	
2.B.14	3,3-Dimethyl-2-butanol	OH	
3.A.01	Carbonyl dichloride	0	
		CI CI	
3.A.02	Cyanogen chloride	CI	
3.A.03	Hydrogen cyanide	H-CN	
3.A.04	Trichloronitromethane	CI NO2	
		CI NO2	
3.B.05	Phosphorus oxychloride	Qi Qi	
0.2.00	The spheros enjements	P	
		Cl Cl	
3.B.06	Phosphorus trichloride	P-Cl ₃	
3.B.07	Phosphorus pentachloride	P-Cl ₅	
3.B.08	Trimethyl phosphite	o	
3.B.09	Triethyl phosphite	, o	
2 D 10	Di di li li li	0 0	
3.B.10	Dimethyl phosphite	\odol	
		HO P O	
3.B.11	Diethyl phosphite	· O	
		HOPO	
3.B.12	Sulfur monochloride	S ₂ Cl ₂	
3.B.13	Sulfur dichloride	SCl ₂	
3.B.14	Thionyl chloride	S(O)Cl ₂	
3.B.15	Ethyldiethanolamine	HO	
A D 16		HO, A OH	
3.B.16	Methyldiethanolamine	N VON	

Schedule	Name	Structure
3.B.17	Triethanolamine	НО
		OH

Examples of Names for Derivatives of Scheduled Compounds

Associated	Chemical Name	Structure
Schedule 1.A.05	2-(2-Chlorovinyl)-5-methyl-1,3,2- benzodithiarsole	S As—CI
2.B.08	Bis(trimethylsilyl)benzilate	-Si-O O -Si-
2.B.09	3-Quinuclidinyl trimethylsilyl ether	0-Si-
2.B.07	2-Chloro-5-methyl-1,3,2-benzodithiarsole	S As-Cl
2.B.11	N,N-Dialkyl-N-(2-trimethylsilyloxyethyl)amine	R N O Si
	N,N-Dialkyl-N-(2-tert-butyldimethylsilyloxyethyl)amine	R N O Si
	N-Heptafluorobutyryloxyethyl-N-methyl-N-propylamine	N O F F
2.B.12	N,N-Dialkyl-N-(2-trimethylsilylthioethyl)amine	R S Si

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Associated Schedule	Chemical Name	Structure
2.B.13	Bis(2-trimethylsilyloxyethyl)sulfide	Si o Si
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	S-S