OPCW

Technical Secretariat

Verification Division
S/725/2008
17 December 2008
ENGLISH only

REPORT OF THE TWENTY-EIGHTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 18 AND 19 NOVEMBER 2008

1. The Validation Group (hereinafter "the Group") met for the twenty-eighth time on 18 and 19 November 2008 to discuss the evaluation of new analytical data for possible inclusion in the OPCW Central Analytical Database (OCAD), and to consider matters related to it. Mr Hugh Gregg of the United States of America chaired the Meeting.

2. The evaluators for the analytical techniques evaluated new data and sent their written reports to the coordinators for each analytical technique. The names of the coordinators who were present at the meeting, along with the technique for which each is responsible, are listed below:

Gas chromatography (retention index) GC(RI)	Mr Martin Söderström (Finland)
Mass spectrometry (MS)	Mr Sten-Åke Fredriksson (Sweden)

3. These coordinators provided an evaluation summary to the Group for discussion at the meeting. The evaluators finalised the evaluation of the analytical data and confirmed that the data approved is technically valid.

4. The Group forwarded lists of the validated analytical data to the Director-General for appropriate action (see Annex 1).

5. The Group reviewed some mass spectral data in the OCAD, and recommended the removal of the data listed in Annex 2 for two reasons: In accordance with subparagraph 5.2(b) of S/373/2003, dated 18 August 2003, "Spectra that have been obtained on ion trap instruments will not be accepted", and hence the ion trap mass spectral data listed in Table 1 of that Annex should not be in the OCAD. In terms of Table 2, listed mass spectra contain excessive hydrocarbon fragments for which higher quality data are available in the OCAD.

6. The Group updated the Rules for Naming Compounds in the OCAD (see paragraph 2.14 of Annex 3). Using these new rules, a set of data validated at the

Twenty-Seventh Meeting of the Group was renamed, and is being forwarded to the Director-General for appropriate action (see Tables 4 and 5 of Annex 1).

7. The Technical Secretariat (hereinafter "the Secretariat") reported that all the data on scheduled chemicals submitted by the Group up to and including its Twenty-Seventh Meeting has been approved by the Executive Council, and will be incorporated into the next release of the OCAD v.11_2008. This version will be released in December 2008.

8. The Secretariat reported that a Validation Group Working Database (VGWD), containing all data validated by the Group up to and including its Twenty-Eighth Meeting will be prepared in early 2009 and will be available from the Secretariat on request.

9. The Group continued to discuss the possibility of establishing a liquid chromatography-mass spectrometry (LC-MS) database for potential inclusion in the OCAD. The Group noted little progress on this activity, and agreed to continue to consider data from this technique for inclusion in the OCAD.

10. The Secretariat inquired about the status of predicting GC(RI) data for those compounds for which only MS data is available in the OCAD. The Group noted that little progress has been made. The Group decided to include subsets of this group of missing data for evaluation by the Group during forthcoming meetings. Predicted GC(RI) data shall include a description of the predication method and a minimum of three predicated values of chemicals that justify the GC(RI) data being in the OCAD.

11. The Group noted that the GC(RI) subgroup is down to a minimum number of members. It is critical that the GC(RI) group remain strong, and the Group urgently requests Member States to nominate colleagues to join the GC(RI) subgroup. Additionally, the Group decided that, if former Group members from the OPCW Laboratory were willing to participate in any of the validation subgroups for which they have the scientific expertise, the Group would welcome these additional members.

12. The following new analytical data is available for evaluation at the next meeting:

IR[1]	New data	04-1-0294v through 04-1-0303v
GC(RI)	New data	04-4-0281 through 04-4-0290
NMR[2]	Resubmission	25-3-0001r through 25-3-0040r
MS	New data	04-2-0472 through 04-2-0481

13. Additional NMR, MS, GC(RI), and IR data could be expected before the next meeting.

14. The evaluators agreed to send their written evaluation reports to the appointed coordinators **no later than 23 February 2009**. The next meeting is scheduled to take place on 3 and 4 March 2009. The evaluator has agreed to come that meeting

[1] IR = infrared
[2] NMR = nuclear magnetic resonance spectrometry

prepared to finalise the evaluation of the analytical data referred to in paragraphs 11 and 12.

15. The Group is pleased to announce that Mr Sten-Åke Fredriksson (Sweden) was elected as the coordinator of the MS subgroup. Ms Sarah Chinn (United States of America) was welcomed as a new member of the NMR subgroup (taking over from Robert Maxwell) (United States of America). Annex 4 to this report lists the evaluators by analytical technique.

Annexes:

Annex 1: Lists of Approved Data Recommended for Inclusion in the OPCW Central Analytical Database
Annex 2: Lists of Recommended Changes to the OPCW Central Analytical Database
Annex 3: Rules for Naming Compounds in the OPCW Central Analytical Database
Annex 4: List of Members of the Validation Group

Annex 1

LISTS OF APPROVED DATA RECOMMENDED FOR INCLUSION IN THE OPCW CENTRAL ANALYTICAL DATABASE

Note: In the last column of the tables that follow in this and the next Annex, "A" means "accepted"; "B", "accepted subject to minor corrections". A "1" under the "Column" heading means an HP5 or an SE54 column.

TABLE 1: LIST OF APPROVED MS DATA

OPCW Code	Chemical Name	Schedule	Decision
15-2-0067r	2-Isopropyl-5-methylcyclohexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0122r	2-Isopropyl-5-methylcyclohexyl ethylphosphonofluoridate	1.A.01	B
15-2-0124r	2-Isopropyl-5-methylcyclohexyl propylphosphonofluoridate	1.A.01	B
15-2-0126	N,N-Diethyl-P-isopropylphosphonamidic chloride	2.B.04	B
15-2-0150	3,3,5,5-Tetramethylcyclohexyl methylphosphonofluoridate	1.A.01	B
15-2-0151	3,3,5,5-Tetramethylcyclohexyl ethylphosphonofluoridate	1.A.01	B
15-2-0152	3,3,5,5-Tetramethylcyclohexyl propylphosphonofluoridate	1.A.01	B
15-2-0155	1-Propylcyclohexyl ethylphosphonofluoridate	1.A.01	B
15-2-0156	1-Propylcyclohexyl methylphosphonofluoridate	1.A.01	B
15-2-0159	4-Methylcyclohexyl N,N-diethyl-P-propylphosphonamidate	2.B.04	B
15-2-0162	2-Cyclohexylpropyl methylphosphonofluoridate	1.A.01	B
15-2-0163	Bis(2-cyclohexylpropyl) methylphosphonate	2.B.04	B
15-2-0165	Bis(cyclopropylmethyl) ethylphosphonate	2.B.04	B
15-2-0166	Bis(cyclopropylmethyl) methylphosphonate	2.B.04	B
15-2-0167	Bis(cyclopropylmethyl) propylphosphonate	2.B.04	B
15-2-0168	Dicyclohexyl dimethylpyrophosphonate	2.B.04	B
15-2-0170	Cyclopropylmethyl ethyl ethylphosphonate	2.B.04	B
15-2-0171	Cyclopropylmethyl propylphosphonofluoridate	1.A.01	B
15-2-0172	Decahydronaphthalen-2-yl methylphosphonofluoridate	1.A.01	B
15-2-0173	Bicyclo[2.2.1]hept-2-yl ethylphosphonofluoridate	1.A.01	B
15-2-0174	Bicyclo[2.2.1]hept-2-yl methylphosphonofluoridate	1.A.01	B
15-2-0175	Bicyclo[2.2.1]hept-2-yl propylphosphonofluoridate	1.A.01	B
15-2-0176	Bis(bicyclo[2.2.1]hept-2-yl) ethylphosphonate	2.B.04	B
15-2-0177	Bis(bicyclo[2.2.1]hept-2-yl) methylphosphonate	2.B.04	B
15-2-0179	Diisobutyl diisopropylpyrophosphonate	2.B.04	B
15-2-0180	Diisobutyl dimethylpyrophosphonate	2.B.04	B
15-2-0181	N,N,N´,N´-Tetraethyl-P-ethylphosphonic diamide	2.B.04	B
15-2-0182	sec-Butyl N,N-diethyl-P,P´-diisopropyldiphosphonamidate	2.B.04	B
15-2-0183	Hexyl N,N-diethyl-P-isopropylphosphonamidate	2.B.04	B
15-2-0184	Isobutyl N,N-diethyl-P-methylphosphonamidate	2.B.04	B
15-2-0185	Isobutyl N,N-diethyl-P,P´-diisopropyldiphosphonamidate	2.B.04	B
15-2-0186	Cyclohexyl N,N-diethyl-P-ethylphosphonamidate	2.B.04	B
15-2-0187	Cyclohexyl N,N-diethyl-P,P´-diethyldiphosphonamidate	2.B.04	B
15-2-0188	Hexyl N,N-diethyl-P-ethylphosphonamidate	2.B.04	B
15-2-0190	Pinacolyl N,N-diethyl-P,P´-dimethyldiphosphonamidate	2.B.04	B

OPCW Code	Chemical Name	Schedule	Decision
15-2-0191	3-Methylpentyl N,N-diethyl-P-isopropylphosphonamidate	2.B.04	B
09-2-0123	O-Ethyl S-ethyl methylphosphonothiolate	2.B.04	A
09-2-0124	S-Ethyl O-propyl methylphosphonothiolate	2.B.04	B
09-2-0125	O-Cyclohexyl O-isopropyl methylphosphonothionate	2.B.04	A
09-2-0126	O-Cyclohexyl O-methyl methylphosphonothionate	2.B.04	A
09-2-0127	O-Cyclohexyl O-pinacolyl methylphosphonothionate	2.B.04	A
09-2-0128	O-Isopropyl O-methyl methylphosphonothionate	2.B.04	A
09-2-0129	1-Ethylpropyl propylphosphonofluoridate	1.A.01	A
09-2-0130	1-Isobutyl-3-methylbutyl propylphosphonofluoridate	1.A.01	A
09-2-0131	Methyl methylphosphonofluoridate	1.A.01	A
09-2-0132	1-Methylbutyl N,N-diisopropylphosphoramidocyanidate	1.A.02	A
09-2-0133	1-Methylheptyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
09-2-0134	1-Methylpentyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
09-2-0135	2-Cyclohexylethyl N,N-diisopropylphosphoramidocyanidate	1.A.02	A
09-2-0136	2-Cyclohexylethyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
09-2-0137	2-Ethylhexyl N,N-diethylphosphoramidocyanidate	1.A.02	A
09-2-0138	2-Ethylhexyl N,N-dimethylphosphoramidocyanidate	1.A.02	A
09-2-0139	3-Methylbutyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	A
09-2-0140	3-Methylbutyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0141	Cyclohexyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
09-2-0142	Cyclohexyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
09-2-0143	Pentyl N-isopropyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0144	Propylphosphonic difluoride	1.B.09	A
09-2-0145	2-Diisopropylaminoethyl methylphosphinate	2.B.04	A
09-2-0146	Benzyl butyl methylphosphonate	2.B.04	A
09-2-0147	Benzyl methylphosphonofluoridate	2.B.04	A
09-2-0148	Bis(1-isobutyl-3-methylbutyl) propylphosphonate	2.B.04	A
09-2-0149	Bis(2-methoxyethyl) propylphosphonate	2.B.04	A
09-2-0150	Bis(tert-butyldimethylsilyl) ethylphosphonate	2.B.04	A
09-2-0151	Bis(tert-butyldimethylsilyl) isopropylphosphonate	2.B.04	A
09-2-0152	Bis(tert-butyldimethylsilyl) methylphosphonate	2.B.04	A
09-2-0153	Bis(tert-butyldimethylsilyl) propylphosphonate	2.B.04	A
09-2-0154	Butyl ethyl methylphosphonodithiolothionate	2.B.04	A
09-2-0155	Dibutyl methylphosphonodithiolothionate	2.B.04	A
09-2-0156	Dipinacolyl dimethylpyrophosphonate	2.B.04	A
09-2-0157	Isopropyl methylphosphonazidate	2.B.04	A
09-2-0158	N,N-Diisopropylphosphoramidic dichloride	2.B.05	A
09-2-0159	2-(N,N-Dimethylamino)ethylchloride	2.B.10	A
09-2-0160	2-(N-Isopropyl-N-methylamino)ethylchloride	2.B.10	A
09-2-0161	2-(N-Methyl-N-propylamino)ethylchloride	2.B.10	A
09-2-0162	2-(N-Isopropyl-N-methylamino)ethanol	2.B.11	A
09-2-0163	2-(N-Methyl-N-propylamino)ethanol	2.B.11	A
09-2-0164	Dimethyl phosphite	2.B.10	A
17-2-0177	(5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl methyl methylphosphonate	2.B.04	A

OPCW Code	Chemical Name	Schedule	Decision
17-2-0178	(5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl methyl methylphosphonate	2.B.04	A
23-2-0002	(5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl methyl methylphosphonate	2.B.04	B
23-2-0003	5-Ethyl-5-methoxymethyl-2-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
09-2-0165	N,N-Diisopropyl-N-(2-tert-butyldimethylsilyloxyethyl)amine	DS	A
09-2-0166	N,N-Dipropyl-N-(2-trimethylsilyloxyethyl)amine	DS	A

TABLE 2: LIST OF APPROVED GC(RI) DATA

OPCW Code	Chemical Name	Schedule	Column	Average	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	Decision
09-4-0005	O-Ethyl S-ethyl methylphosphonothiolate	2.B.04	1	1176	1176					B
09-4-0006	S-Ethyl O-propyl methylphosphonothiolate	2.B.04	1	1270	1270					A
09-4-0007	O-Cyclohexyl O-isopropyl methylphosphonothionate	2.B.04	1	1505	1505					A
09-4-0008	O-Cyclohexyl O-methyl methylphosphonothionate	2.B.04	1	1421	1421					A
09-4-0009	O-Cyclohexyl O-pinacolyl methylphosphonothionate	2.B.04	1	1732	1728	1735				A
09-4-0010	O-Isopropyl O-methyl methylphosphonothionate	2.B.04	1	1033	1033					A
09-4-0011	1-Ethylpropyl propylphosphonofluoridate	1.A.01	1	1192	1192					A
09-4-0012	1-Isobutyl-3-methylbutyl propylphosphonofluoridate	1.A.01	1	1413	1413					A
09-4-0013	Methyl methylphosphonofluoridate	1.A.01	1	704	704					A
09-4-0014	1-Methylbutyl N,N-diisopropylphosphoramidocyanidate	1.A.02	1	1544	1544					A
09-4-0015	1-Methylheptyl N,N-dipropylphosphoramidocyanidate	1.A.02	1	1895	1890	1899				A
09-4-0016	1-Methylpentyl N,N-dipropylphosphoramidocyanidate	1.A.02	1	1707	1703	1710				A
09-4-0017	2-Cyclohexylethyl N,N-diisopropylphosphoramidocyanidate	1.A.02	1	1983	1983					A
09-4-0018	2-Cyclohexylethyl N,N-dipropylphosphoramidocyanidate	1.A.02	1	2058	2058					A
09-4-0019	2-Ethylhexyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1756	1756					A
09-4-0020	2-Ethylhexyl N,N-dimethylphosphoramidocyanidate	1.A.02	1	1623	1623					A
09-4-0021	3-Methylbutyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	1	1549	1549					A
09-4-0022	3-Methylbutyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	1	1522	1522					A

OPCW Code	Chemical Name	Schedule	Column	Average	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	Decision
09-4-0023	Cyclohexyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	1	1629	1629					A
09-4-0024	Cyclohexyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	1	1691	1691					A
09-4-0025	Pentyl N-isopropyl-N-propylphosphoramidocyanidate	1.A.02	1	1664	1664					A
09-4-0026	Propylphosphonic difluoride	1.B.09	1	673	673					A
09-4-0030	Bis(1-isobutyl-3-methylbutyl) propylphosphonate	2.B.04	1	1922	1922					A
09-4-0031	Bis(2-methoxyethyl) propylphosphonate	2.B.04	1	1573	1573					A
09-4-0036	Butyl ethyl methylphosphonodithiolothionate	2.B.04	1	1661	1661					A
09-4-0037	Dibutyl methylphosphonodithiolothionate	2.B.04	1	1843	1843					A
09-4-0038	Dipinacolyl dimethylpyrophosphonate	2.B.04	1	1871	1841	1859	1873	1880	1900	A
09-4-0041	2-(N,N-Dimethylamino)ethylchloride	2.B.10	1	750	750					A
09-4-0042	2-(N-Isopropyl-N-methylamino)ethylchloride	2.B.10	1	922	922					A
09-4-0043	2-(N-Methyl-N-propylamino)ethylchloride	2.B.10	1	924	924					A
09-4-0044	2-(N-Isopropyl-N-methylamino)ethanol	2.B.11	1	907	907					A
09-4-0045	2-(N-Methyl-N-propylamino)ethanol	2.B.11	1	908	908					A
09-4-0046	Dimethyl phosphite	3.B.10	1	808	808					A
09-4-0048	N,N-Dipropyl-N-(2-trimethylsilyloxyethyl)amine	DS	1	1190	1190					A

TABLE 3: LIST OF APPROVED IR DATA FROM THE TWENTY-SEVENTH MEETING*

OPCW Code	Chemical Name	Schedule	Decision
04-1-0291v	2-Methylbutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A

* This spectrum was inadvertently left out of the report of the Group's Twenty-Seventh Meeting.

TABLE 4: LIST OF MS DATA APPROVED DURING THE TWENTY-SEVENTH MEETING *

OPCW Code	Chemical Name	Schedule	Decision
15-2-0127	Isobutyl N,N-diethyl-P-isopropylphosphonamidate	2.B.04	B
15-2-0128	Isopropyl N,N-diethyl-P,P'-diisopropyldiphosphonamidate	2.B.04	B
15-2-0129	Isopropyl N,N-diethyl-P-isopropylphosphonamidate	2.B.04	B
15-2-0131	Isobutyl N,N-diethyl-P,P'-dimethyldiphosphonamidate	2.B.04	B
15-2-0132	4-Methylcyclohexyl N,N-diethyl-P,P'-dimethyldiphosphonamidate	2.B.04	B

OPCW Code	Chemical Name	Schedule	Decision
15-2-0133	4-Methylcyclohexyl N,N-diethyl-P-methylphosphonamidate	2.B.04	B
15-2-0134	Cyclohexyl N,N-diethyl-P,P'-dimethyldiphosphonamidate	2.B.04	B
15-2-0135	Cyclohexyl N,N-diethyl-P-methylphosphonamidate	2.B.04	B
15-2-0136	3-Methylpentyl N,N-diethyl-P,P'-dimethyldiphosphonamidate	2.B.04	B
15-2-0137	3-Methylpentyl N,N-diethyl-P-methylphosphonamidate	2.B.04	B
15-2-0138	sec-Butyl N,N-diethyl-P,P'-dimethyldiphosphonamidate	2.B.04	B
15-2-0139	sec-Butyl N,N-diethyl-P-methylphosphonamidate	2.B.04	B
15-2-0140	Pinacolyl N,N-diethyl-P-methylphosphonamidate	2.B.04	B
15-2-0141	N,N-Diethyl-P-methylphosphonamidic chloride	2.B.04	B
15-2-0144	4-Methylcyclohexyl N,N-diethyl-P-ethylphosphonamidate	2.B.04	B
15-2-0146	3,3,5,5-Tetramethylcyclohexyl N,N-diethyl-P,P'-diethyldiphosphonamidate	2.B.04	B
15-2-0147	Pinacolyl N,N-diethyl-P-ethylphosphonamidate	2.B.04	B
15-2-0148	Pinacolyl N,N-diethyl-P,P'-diethyldiphosphonamidate	2.B.04	B
15-2-0149	3,3,5,5-Tetramethylcyclohexyl N,N-diethyl-P-ethylphosphonamidate	2.B.04	B

* The new naming rules applied to these spectra were previously approved during the Group's Twenty-Seventh Meeting.

TABLE 5: LIST OF GC(RI) DATA APPROVED DURING THE GROUP'S TWENTY-SEVENTH MEETING *

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	Decision
17-4-0090	Ethyl 1-propylheptyl P,P'-dimethyldiphosphonate	2.B.04	1	2004	2015	B
17-4-0156	Pinacolyl propyl P,P'-dimethyldiphosphonate	2.B.04	1	1711	1736	B

* The new naming rules applied to these spectra were previously approved at the Group's Twenty-Seventh Meeting.

Annex 2

LIST OF RECOMMENDED CHANGES TO THE OPCW CENTRAL ANALYTICAL DATABASE

TABLE 1: LIST OF DATA TO BE REMOVED FROM THE OCAD: ION TRAP MASS SPECTRA*

OPCW Code	Chemical Name	Schedule
18-2-0006	Propyl isopropylphosphonofluoridate	1.A.01
18-2-0007	Isopropyl isopropylphosphonofluoridate	1.A.01
18-2-0008	sec-Butyl isopropylphosphonofluoridate	1.A.01
18-2-0009	Isobutyl isopropylphosphonofluoridate	1.A.01
18-2-0010	Butyl isopropylphosphonofluoridate	1.A.01
18-2-0011	Pentyl isopropylphosphonofluoridate	1.A.01
18-2-0012	3-Methylbutyl isopropylphosphonofluoridate	1.A.01
18-2-0013	Cyclopentyl isopropylphosphonofluoridate	1.A.01
18-2-0016	Isobutyl methyl isopropylphosphonate	2.B.04
18-2-0017	sec-Butyl methyl isopropylphosphonate	2.B.04
18-2-0018	Butyl methyl isopropylphosphonate	2.B.04
18-2-0020	Methyl 3-methylbutyl isopropylphosphonate	2.B.04
18-2-0021	Cyclopentyl methyl isopropylphosphonate	2.B.04
18-2-0025	Butyl isopropylphosphonochloridate	2.B.04
18-2-0026	Pentyl isopropylphosphonochloridate	2.B.04
18-2-0027	3-Methylbutyl isopropylphosphonochloridate	2.B.04
18-2-0028	Cyclopentyl isopropylphosphonochloridate	2.B.04
18-2-0029	Dipropyl isopropylphosphonate	2.B.04
18-2-0030	Dibutyl isopropylphosphonate	2.B.04
18-2-0031	Dipentyl isopropylphosphonate	2.B.04
18-2-0032	Bis(3-methylbutyl) isopropylphosphonate	2.B.04
18-2-0033	Cyclopropylmethyl methylphosphonofluoridate	1.A.01
18-2-0049	Cyclohexyl isopropylphosphonofluoridate	1.A.01
18-2-0053	2-Methylcyclohexyl isopropylphosphonofluoridate	1.A.01

* Ion-trap mass spectral data should not be in the OCAD, as per paragraph 5.2(b) of S/373/2003.

TABLE 2: LIST OF DATA TO BE REMOVED FROM THE OCAD: SPECTRA CONTAIN EXCESSIVE HYDROCARBON FRAGMENTATION FOR WHICH ALTERNATIVE SPECTRA EXIST

OPCW Code	Chemical Name	Schedule
06-2-0013	2,2-Dimethylpropyl methylphosphonofluoridate	1.A.01
06-2-0028	Diisopropyl dimethylpyrophosphonate	2.B.04
06-2-0259	1,4-Dimethylpentyl methylphosphonofluoridate	1.A.01
06-2-0266	1,5-Dimethylhexyl methylphosphonofluoridate	1.A.01
06-2-0267	2,4,4-Trimethylpentyl methylphosphonofluoridate	1.A.01
06-2-0270	3,5,5-Trimethylhexyl methylphosphonofluoridate	1.A.01
06-2-0273	1-Methylnonyl methylphosphonofluoridate	1.A.01
06-2-0274	3,7-Dimethyloctyl methylphosphonofluoridate	1.A.01

OPCW Code	Chemical Name	Schedule
06-2-0275	1-Propylheptyl methylphosphonofluoridate	1.A.01
06-2-0287	4-tert-Butylcyclohexyl methylphosphonofluoridate	1.A.01
06-2-0290	2,2-Dimethylhexyl methylphosphonofluoridate	1.A.01
06-2-0291	1-Ethyl-2,2-dimethylpropyl methylphosphonofluoridate	1.A.01
06-2-0371	Isopropylphosphonic dichloride	2.B.04

Annex 3

RULES FOR NAMING COMPOUNDS IN THE OPCW CENTRAL ANALYTICAL DATABASE

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.
However, pinacolyl alcohol should be referred to as 3,3-dimethyl-2-butanol.
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.

2.4 The radicals isobutyl, isopropenyl, and isopropyl are considered to be one entity and are to be listed in alphabetical order starting from "iso".

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.

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:

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

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

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

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).

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;

(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

(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.

2.12 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; and
(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; and
(iii) Tributyl arsenotrithiolite.

2.14 Compounds with multiple phosphorus atoms shall be named as follows (examples below under 2.B.04):

(a) A symmetrical phosphonate dimer with an oxygen linkage shall be called a pyrophosphonate.
(b) Amidate shall be used instead of amidoate.
(c) Otherwise, IUPAC names shall be used.

3. These rules are illustrated below by examples of scheduled compounds and by derivatives associated with the scheduled compounds.

Examples of Names of Scheduled Compounds

Schedule	Name
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
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.
	Examples
	Methylphosphonothioic acid [$(CH_3P(=S)(OH)_2$]
	O-Ethyl methylphosphonothionate [$(C_2H_5O)P(=S)(CH_3)(OH)$]
	O,O-Diethyl methylphosphonothionate [$(C_2H_5O)_2P(=S)(CH_3)$]
	O-Propyl O-trimethylsilyl propylphosphonothionate
	O-Ethyl S-ethyl methylphosphonothiolate [$(C_2H_5O)P(=O)(CH_3)(SC_2H_5)$]
	S-Ethyl O-methyl methylphosphonothiolate
	O-Ethyl S-2-methylthioethyl methylphosphonothiolate
	O-Ethyl S-ethyl methylphosphonothiolothionate [$(C_2H_5O)P(=S)(CH_3)(SC_2H_5)$]
	Bis(S-sec-butyl) methylphosphonodithiolate

Schedule	Name
	O-Ethyl methylphosphonothionochloridate [$(C_2H_5O)P(=S)(CH_3)(Cl)$]
	Methylphosphonous dichloride ($CH_3P\text{-}Cl_2$)
	Methylphosphonic dichloride [$(CH_3P(=O)\text{-}Cl_2)$]
	Methylphosphonothioic dichloride [$(CH_3P(=S)\text{-}Cl_2)$]
	Dimethyl methylphosphonate
	Bis(1,2-dimethylpropyl) methylphosphonate
	Benzyl 1,2-dimethylpropyl ethylphosphonate
	Methyl methylphosphonate instead of methyl methylphosphonic acid
	Methylphosphonic acid
	Isobutyl methylphosphonochloridate
	Isopropyl methylphosphonoazidate
	2-Diisopropylaminoethyl methylphosphinate [$(i\text{-}C_3H_7)_2N\text{-}CH_2CH_2\text{-}O\text{-}P(=O)(H)(CH_3)$]
	Methyl 2-diethylaminoethyl methylphosphonate
	O-Ethyl S-2-dibutylaminoethyl methylphosphonothiolate
	Bis(S-2-diethylaminoethyl) methylphosphonodithiolate
	O-Ethyl S-3-dimethylaminopropyl methylphosphonothiolate
	Diethyl methylphosphonite [$(C_2H_5O)_2P(CH_3)$]
	Dicyclohexyl dimethylpyrophosphonate [$(C_6H_{11}O)(CH_3)P(=O)\text{-}O\text{-}P(=O)(CH_3)(C_6H_{11}O)$]
	Dicyclohexyl dimethylpyrophosphonodithionate [$(C_6H_{11}O)(CH_3)P(=S)\text{-}O\text{-}P(=S)(CH_3)(C_6H_{11}O)$]
	Cyclohexyl N,N-diethyl-P-propylphosphonamidate [$(C_6H_{11}O)(C_3H_7)P(=O)N(C_2H_5)_2$]
	Isopropyl N,N-diethyl-P,P'-dimethyldiphosphonamidate [$(i\text{-}C_3H_7O)(CH_3)P(=O)\text{-}O\text{-}P(=O)(CH_3)N(C_2H_5)_2$]
2.B.05	N,N-Dialkylphosphoramidic dihalide
2.B.06	Dialkyl N,N-dialkylphosphoramidate
	Dimethyl N-ethyl-N-methylphosphoramidate
2.B.07	Arsenic trichloride
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
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
3.A.04	Trichloronitromethane
3.B.05	Phosphorus oxychloride

Schedule	Name
3.B.06	Phosphorus trichloride
3.B.07	Phosphorus pentachloride
3.B.08	Trimethyl phosphate
3.B.09	Triethyl phosphate
3.B.10	Dimethyl phosphate
3.B.11	Diethyl phosphate
3.B.12	Sulfur monochloride
3.B.13	Sulfur dichloride
3.B.14	Thionyl chloride
3.B.15	Ethyldiethanolamine
3.B.16	Methyldiethanolamine
3.B.17	Triethanolamine

Examples of Names for Derivatives

D.S.	Type of Name
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
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
2.B.12	N,N-Dialkyl-N-(2-trimethylsilylthioethyl)amine
2.B.13	Bis(2-trimethylsilyloxyethyl)sulphide
3.B.15	Bis(2-trimethylsilyloxyethyl)ethylamine
3.B.16	Bis(2-trimethylsilyloxyethyl)methylamine
3.B.17	Tris(2-trimethylsilyloxyethyl)amine
	Tris(2-tert-butyldimethylsilyloxyethyl)amine

Annex 4

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