



OPCW

Technical Secretariat

Verification Division

S/687/2008

10 April 2008

ENGLISH only

**REPORT OF THE TWENTY-SEVENTH MEETING OF THE VALIDATION GROUP
FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE
11 AND 12 MARCH 2008**

1. The Validation Group (hereinafter “the Group”) met for the 27th time on 11 and 12 March 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)
Infrared spectroscopy (IR)	Mr Colin Pottage (United Kingdom of Great Britain and Northern Ireland)
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 are 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 validated some analytical data for which the Group could not come to a consensus on how to consistently name the compounds (see Annex 2). The Technical Secretariat (hereinafter “the Secretariat”) will consult with interested members of the Group and then distribute a proposal for naming to the Group who will work on additions to the Rules for Naming Compounds in the OPCW Central Analytical Database. The Group will finalize these rules at the next meeting of the Group. Once the naming rules are updated, the Group will recommend that these data be forwarded to the Director-General for appropriate action.



6. The Information Services Branch of the Secretariat presented a prototype of a web-view access of the analytical data in the OCAD for the use of the Group.
7. The Secretariat reported that the data on scheduled chemicals submitted by the Group through its 23rd meeting and approved by the Executive Council (hereinafter “the Council”) have been incorporated into the latest release of the OCAD (PDF-OCAD v.10 and e-OCAD v.8). This version was released in December 2007.
8. The Secretariat reported that the data on scheduled chemicals submitted by the Group at its 24th meeting to the Council for a decision at its Forty-Ninth Session have been approved. The data from the Group’s 25th meeting were approved at the Fifty-First Session of the Council. The data from the Group’s 26th meeting were considered at the Fifty-Second Session of the Council, and the Council decided to consider them further at its next regular session.
9. The Secretariat reported that a Validation Group Working Database (VGWD), containing all data validated by the group through its 26th meeting, has been prepared and is available on request to the Secretariat.
10. The IR evaluation group discussed requirements for submission of data for its evaluation. The Group requests that the original pdf files, submitted by laboratories, be supplied to the evaluators together with the electronic versions of the data. This will provide additional verification of the data.
11. The Group continued to discuss the possibility of establishing a liquid chromatography-mass spectrometry (LC-MS) database for potential inclusion in the OCAD. Mr Martin Söderström summarised the efforts that had been made so far: data from four laboratories have been collected and initial review indicates that defining standard conditions may be problematic. The Group agreed to continue to consider data from this technique for inclusion in the OCAD.
12. The Secretariat inquired about the status of predicting GC(RI) data for those compounds for which only MS data are available in the OCAD. The Group noted that little progress has been made. The Group decided to include subsets of these missing data for evaluation in the forthcoming Group meetings.
13. The Group reviewed existing data in the OCAD, and recommended the removal of the ion trap MS data listed in Annex 4, since data of higher quality are available in the OCAD. Additionally, the Group requested that appropriate action be taken for data validated at earlier meetings, which were inadvertently not included in earlier reports (Annex 1, Table 4 and Annex 3).

14. The Group, when recommending changes to or removal of data from the OCAD, shall make a note of the reason in the Group's reports. The Group recommends that the Secretariat include these notes when preparing papers for the Council.
15. The Group remains without a permanent MS sub-group coordinator and encourages members to consider this responsibility. Additionally, Mr Armando Alcaraz has kindly agreed to take over the responsibilities of IR coordinator from Mr Colin Pottage.
16. The following new analytical data are available for evaluation at the next meeting:

GC(RI)	New Data	28-4-0001 through 28-4-0012
NMR	Resubmission	25-3-0001r through 25-3-0040r
MS	Postponed	04-2-0463, 04-2-0464, 17-2-0177, 17-2-0178
17. Additional data are expected for NMR, MS, GC(RI), and IR before the next meeting.
18. Annex 5 to this report lists the evaluators by analytical technique. The evaluators agreed to send their written evaluation reports to the appointed coordinators **no later than 10 November 2008**. The next meeting is scheduled to take place on **18 and 19 November 2008**. The evaluators agreed to come to that meeting prepared to finalise the evaluation of the analytical data referred to in paragraphs 16 and 17.
19. The Group welcomed Mr Wei Chongxi (China) and Mr James Riches (United Kingdom of Great Britain and Northern Ireland) as new evaluators for MS data.
20. The Group notes its regret that Mr Shigeyuki Hanaoka and Mr Luis Ramalho have resigned from the Group, and expresses its appreciation for their work as members of the MS group.

Annexes:

- Annex 1: Lists of Approved Data Recommended for Inclusion in the OPCW Central Analytical Database
- Annex 2: Lists of Technically Valid Data Requiring a Name Change before Inclusion in the OPCW Central Analytical Database
- Annex 3: List of Technically Valid Data Not Recommended for Inclusion in the OPCW Central Analytical Database
- Annex 4: List of Recommended Changes to the OPCW Central Analytical Database
- Annex 5: 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
04-2-0415r	2-Ethylhexyl S-2-diethylaminoethyl methylphosphonothiolate	1.A.03	A
04-2-0449r	2-Ethylhexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0462	2,4-Dimethyl-3-pentyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	B
04-2-0465	Propyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0466	Isopropyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0467	Butyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0468	Pentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0469	2-Methylbutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0470	Ethyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0471	sec-Butyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
09-2-0121	Sulfur monochloride	3.B.12	B
14-2-0110	O-Isopropyl O-trimethylsilyl isopropylphosphonothionate	2.B.04	A
14-2-0111	O-Propyl O-trimethylsilyl isopropylphosphonothionate	2.B.04	A
15-2-0040	Isobutyl isopropylphosphonofluoridate	1.A.01	B
15-2-0041	Cyclobutyl isopropylphosphonofluoridate	1.A.01	B
15-2-0042	Cyclopentyl isopropylphosphonofluoridate	1.A.01	B
15-2-0043	Cyclohexyl ethylphosphonofluoridate	1.A.01	B
15-2-0044	Cyclohexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0046	1,3-Dimethylbutyl isopropylphosphonofluoridate	1.A.01	B
15-2-0047	1-Ethyl-2,2-dimethylpropyl isopropylphosphonofluoridate	1.A.01	B
15-2-0049	2-Methylcyclohexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0051	2-Ethylhexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0052	2-Ethylhexyl propylphosphonofluoridate	1.A.01	B
15-2-0054	Cyclooctyl isopropylphosphonofluoridate	1.A.01	B
15-2-0055	Cyclooctyl propylphosphonofluoridate	1.A.01	B
15-2-0056	Ethyl isopropylphosphonofluoridate	1.A.01	B
15-2-0057	1-Isopropyl-2-methylpropyl isopropylphosphonofluoridate	1.A.01	B
15-2-0058	Cycloheptyl isopropylphosphonofluoridate	1.A.01	B
15-2-0059	3,5,5-Trimethylcyclohexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0061	3,7-Dimethyloctyl isopropylphosphonofluoridate	1.A.01	B
15-2-0062	2-tert-Butyl cyclohexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0063	Bis(3,3,5,5-tetramethylcyclohexyl) ethylphosphonate	2.B.04	B
15-2-0064	1-Isopropylbutyl isopropylphosphonofluoridate	1.A.01	B

OPCW Code	Chemical Name	Schedule	Decision
15-2-0065	3,3,5,5-Tetramethylcyclohexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0066	4-tert-Butylcyclohexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0068	2-Isopropyl-4-methylcyclohexyl isopropylphosphonofluoridate	1.A.01	B
15-2-0070	Isobutyl propylphosphonofluoridate	1.A.01	B
15-2-0071	Bis(2-methylpropyl) propylphosphonate	2.B.04	B
15-2-0072	Cyclobutyl propylphosphonofluoridate	1.A.01	B
15-2-0073	Cyclopentyl propylphosphonofluoridate	1.A.01	B
15-2-0074	Bis(1,3-dimethylbutyl) dipropylpyrophosphonate	2.B.04	B
15-2-0079	1,3-Dimethylbutyl propylphosphonofluoridate	1.A.01	B
15-2-0083	2-Methylcyclopentyl propylphosphonofluoridate	1.A.01	B
15-2-0084	1-Isopropylbutyl propylphosphonofluoridate	1.A.01	B
15-2-0085	2-tert-Butylcyclohexyl propylphosphonofluoridate	1.A.01	B
15-2-0087	1-Ethyl-2-methylpropyl propylphosphonofluoridate	1.A.01	B
15-2-0088	Ethyl propylphosphonofluoridate	1.A.01	B
15-2-0089	Diisobutyl ethylphosphonate	2.B.04	B
15-2-0090	Isobutyl ethylphosphonofluoridate	1.A.01	B
15-2-0091	Bis(3-methylpentyl) dimethylpyrophosphonate	2.B.04	B
15-2-0093	Ethyl ethylphosphonofluoridate	1.A.01	B
15-2-0094	Cyclopentyl ethylphosphonofluoridate	1.A.01	B
15-2-0095	1-Ethyl-2-methylpropyl ethylphosphonofluoridate	1.A.01	B
15-2-0096	Dicyclobutyl ethylphosphonate	2.B.04	B
15-2-0098	4-tert-Butylcyclohexyl methyl ethylphosphonate	2.B.04	B
15-2-0099	4-tert-Butylcyclohexyl ethylphosphonofluoridate	1.A.01	B
15-2-0100	2-tert-Butylcyclohexyl ethylphosphonofluoridate	1.A.01	B
15-2-0102	Bis(2-ethylhexyl) methylphosphonate	2.B.04	B
15-2-0103	1-Ethyl-2,2-dimethylpropyl methylphosphonofluoridate	1.A.01	B
15-2-0105	sec-Butyl methylphosphonofluoridate	1.A.01	B
15-2-0106	Cyclobutyl methylphosphonofluoridate	1.A.01	B
15-2-0107	1,3-Dimethylbutyl ethyl methylphosphonate	2.B.04	B
15-2-0108	Bis(1,3-dimethylbutyl) methylphosphonate	2.B.04	B
15-2-0109	Bis(1,3-dimethylbutyl) dimethylpyrophosphonate	2.B.04	B
15-2-0110	1,3-Dimethylbutyl methylphosphonofluoridate	1.A.01	B
15-2-0111	Cyclooctyl ethyl methylphosphonate	2.B.04	B
15-2-0112	Dicyclooctyl methylphosphonate	2.B.04	B
15-2-0113	Diisobutyl methylphosphonate	2.B.04	B
15-2-0114	Ethyl 2-ethylhexyl methylphosphonate	2.B.04	B
15-2-0115	4-tert-Butylcyclohexyl methylphosphonofluoridate	1.A.01	B
15-2-0117	2-Methylcyclopentyl methylphosphonofluoridate	1.A.01	B
15-2-0118	Bis(sec-butyl) diethylpyrophosphonate	2.B.04	B
15-2-0121	2-Isopropyl-5-methylcyclohexyl methylphosphonofluoridate	1.A.01	B
15-2-0122	2-Isopropyl-4-methylcyclohexyl ethylphosphonofluoridate	1.A.01	B
15-2-0124	2-Isopropyl-4-methylcyclohexyl propylphosphonofluoridate	1.A.01	B
15-2-0130	Bis(N,N-diethylamino) diisopropylpyrophosphonate	2.B.04	B
15-2-0142	Bis(N,N-diethylamino) dimethylpyrophosphonate	2.B.04	B

OPCW Code	Chemical Name	Schedule	Decision
15-2-0143	Bis(N,N-diethylamino) methylphosphonate	2.B.04	B
15-2-0145	Bis(N,N-diethylamino) diethylpyrophosphonate	2.B.04	B
17-2-0113	4-tert-Butylcyclohexyl methylphosphonochloridate	2.B.04	A
17-2-0114	4-tert-Butylcyclohexyl methylphosphonofluoridate	1.A.01	A
17-2-0115	3-Cyclopentylpropyl methylphosphonofluoridate	1.A.01	A
17-2-0116	Bis(3-cyclopentylpropyl) methylphosphonate	2.B.04	A
17-2-0118	1-Methylnonyl methylphosphonofluoridate	1.A.01	A
17-2-0119	Bis(1-methylnonyl) methylphosphonate	2.B.04	A
17-2-0120	1-Methylnonyl methylphosphonochloridate	2.B.04	A
17-2-0122	3,5,5-Trimethylhexyl methylphosphonofluoridate	1.A.01	A
17-2-0123	Bis(3,5,5-trimethylhexyl) methylphosphonate	2.B.04	A
17-2-0124	Bis(3-cyclohexylpropyl) methylphosphonate	2.B.04	A
17-2-0125	3-Cyclohexylpropyl methylphosphonofluoridate	1.A.01	A
17-2-0126	Cyclooctyl methylphosphonofluoridate	1.A.01	A
17-2-0127	Dicyclooctyl methylphosphonate	2.B.04	A
17-2-0128	4-Cyclohexylbutyl methylphosphonofluoridate	1.A.01	A
17-2-0129	Bis(4-cyclohexylbutyl) methylphosphonate	2.B.04	A
17-2-0130	2-Isopropyl-5-methylcyclohexyl methylphosphonochloridate	2.B.04	A
17-2-0132	2-Isopropyl-5-methylcyclohexyl methylphosphonofluoridate	1.A.01	A
17-2-0134	Dicycloheptylmethyl methylphosphonate	2.B.04	B
17-2-0135	Cycloheptylmethyl methylphosphonofluoridate	1.A.01	A
17-2-0136	1-Propylheptyl methylphosphonofluoridate	1.A.01	A
17-2-0137	1-Propylheptyl methylphosphonochloridate	2.B.04	A
17-2-0138	Diisobutyl dimethylpyrophosphonate	2.B.04	A
17-2-0139	Bis(1-propylheptyl) methylphosphonate	2.B.04	A
17-2-0140	Ethyl 1-propylheptyl methylphosphonate	2.B.04	A
17-2-0141	Ethyl 1-propylheptyl dimethylpyrophosphonate	2.B.04	A
17-2-0142	2-Methyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	A
17-2-0143	2-Propyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	A
17-2-0144	2-Ethyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	A
17-2-0145	2-Isopropyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	A
17-2-0146	Dihexyl diisopropylpyrophosphonate	2.B.04	A
17-2-0147	Pinacolyl propyl methylphosphonate	2.B.04	A
17-2-0148	3-Quinuclidinol	2.B.09	A
17-2-0149	Bis(2-chloroethylthiomethyl)ether	1.A.04	A
17-2-0150	1,5-Bis(2-chloroethylthio)pentane	1.A.04	A
17-2-0151	Diisopropyl dimethylpyrophosphonate	2.B.04	A
17-2-0152	Ethyl 2-methoxyethyl methylphosphonate	2.B.04	A
17-2-0153	2-Methoxyethyl pinacolyl methylphosphonate	2.B.04	A
17-2-0154	Diethyl dimethylpyrophosphonate	2.B.04	A
17-2-0155	Pinacolyl propyl dimethylpyrophosphonate	2.B.04	A
17-2-0156	N,N-Dimethylphosphoramidic dichloride	2.B.05	A
17-2-0157	6-Methyl-2-propyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0158	6-Butyl-2-methyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0159	6-Ethyl-2-methyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A

OPCW Code	Chemical Name	Schedule	Decision
17-2-0160	2,6-Dimethyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0161	6-Butyl-2-isopropyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0162	6-Ethyl-2-isopropyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0163	2-Isopropyl-6-methyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	B
17-2-0164	6-Butyl-2-ethyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0165	2,6-Diethyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0166	2-Ethyl-6-methyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0167	6-Butyl-2-propyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0168	6-Ethyl-2-propyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	A
17-2-0169	Isopropylphosphonic dichloride	2.B.04	A
17-2-0170	Bis(2-isopropyl-5-methylcyclohexyl) methylphosphonate	2.B.04	B
17-2-0171	Bis(4-tert-butylcyclohexyl) methylphosphonate	2.B.04	B
17-2-0172	4-tert-Butylcyclohexyl methylphosphonofluoridate	1.A.01	A
17-2-0173	1-Isobutyl-3-methylbutyl methylphosphonofluoridate	1.A.01	A
17-2-0174	1-Isobutyl-3-methylbutyl methylphosphonochloridate	2.B.04	A
17-2-0175	Bis(1-isobutyl-3-methylbutyl) methylphosphonate	2.B.04	A
28-2-0001	2,5,5-Trimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
28-2-0002	2,4,4,6-Tetramethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
28-2-0003	2-Ethyl-4,4,6-trimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
28-2-0004	2-Ethyl-5,5-dimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
28-2-0005	4,4,6-Trimethyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
28-2-0006	5,5-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
28-2-0007	5,5-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
28-2-0008	4,4,6-Trimethyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
28-2-0009	2,5,5-Trimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
28-2-0010	2,4,4,6-Tetramethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
28-2-0011	2-Ethyl-5,5-dimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
28-2-0012	2-Ethyl-4,4,6-trimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B

TABLE 2: LIST OF APPROVED GC(RI) DATA

OPCW Code	Chemical Name	Sched	Column	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	RI(f)	Decision
04-4-0271	1-Isopropyl-2-methylpropyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	1975						B
04-4-0273	3,5-Dimethylcyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2180						A
04-4-0274	Propyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	1831						A
04-4-0275	Isopropyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	1751						A
04-4-0276	Butyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	1921						A

OPCW Code	Chemical Name	Sched	Column	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	RI(f)	Decision
04-4-0280	sec-Butyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	1856	1860					A
15-4-0001	1,1-Dimethylpropyl ethylphosphonofluoridate	1.A.01	1	1068						A
15-4-0002	1,1-Dimethylpropyl methylphosphonofluoridate	1.A.01	1	975						A
15-4-0003	1,3-Dimethylbutyl ethylphosphonofluoridate	1.A.01	1	1140	1150					A
15-4-0004	1,3-Dimethylbutyl methylphosphonofluoridate	1.A.01	1	1050	1059					A
15-4-0005	1,3-Dimethylbutyl propylphosphonofluoridate	1.A.01	1	1218	1232					A
15-4-0006	1-Ethyl-2,2-dimethylpropyl ethylphosphonofluoridate	1.A.01	1	1228	1230					B
15-4-0007	1-Ethyl-2,2-dimethylpropyl methylphosphonofluoridate	1.A.01	1	1136	1138					A
15-4-0008	1-Ethyl-2-methylpropyl ethylphosphonofluoridate	1.A.01	1	1175						B
15-4-0009	1-Ethyl-2-methylpropyl methylphosphonofluoridate	1.A.01	1	1084						A
15-4-0010	1-Ethyl-2-methylpropyl propylphosphonofluoridate	1.A.01	1	1259	1261					A
15-4-0011	1-Isopropylbutyl methylphosphonofluoridate	1.A.01	1	1159	1161					A
15-4-0012	1-Isopropylbutyl propylphosphonofluoridate	1.A.01	1	1333						A
15-4-0013	sec-Butyl propylphosphonofluoridate	1.A.01	1	1101						B
15-4-0014	sec-Butyl ethylphosphonofluoridate	1.A.01	1	1015						B
15-4-0015	sec-Butyl methylphosphonofluoridate	1.A.01	1	923	925					B
15-4-0016	2,2-Dimethylpropyl methylphosphonofluoridate	1.A.01	1	974						A
15-4-0017	2,2-Dimethylpropyl propylphosphonofluoridate	1.A.01	1	1148						A
15-4-0018	2-Ethylhexyl ethylphosphonofluoridate	1.A.01	1	1392						A
15-4-0019	2-Ethylhexyl methylphosphonofluoridate	1.A.01	1	1303						A
15-4-0020	2-Ethylhexyl propylphosphonofluoridate	1.A.01	1	1475						A
15-4-0021	2-Methylcyclohexyl methylphosphonofluoridate	1.A.01	1	1260	1262					A
15-4-0022	2-Methylcyclopentyl methylphosphonofluoridate	1.A.01	1	1161	1165					A
15-4-0023	3,3,5-Trimethylcyclohexyl ethylphosphonofluoridate	1.A.01	1	1432	1445	1446				B
15-4-0024	3,3,5-Trimethylcyclohexyl methylphosphonofluoridate	1.A.01	1	1338	1340	1351				B
15-4-0025	3,3,5-Trimethylcyclohexyl propylphosphonofluoridate	1.A.01	1	1514	1516	1532	1534			B

OPCW Code	Chemical Name	Sched	Column	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	RI(f)	Decision
15-4-0026	Butyl ethylphosphonofluoridate	1.A.01	1	1068						A
15-4-0027	Cyclobutyl ethylphosphonofluoridate	1.A.01	1	1099						A
15-4-0028	Cyclobutyl propylphosphonofluoridate	1.A.01	1	1183						A
15-4-0029	Cycloheptyl ethylphosphonofluoridate	1.A.01	1	1437						A
15-4-0030	Cycloheptyl propylphosphonofluoridate	1.A.01	1	1528						A
15-4-0031	Cyclooctyl ethylphosphonofluoridate	1.A.01	1	1562						A
15-4-0032	Cyclopentyl ethylphosphonofluoridate	1.A.01	1	1199						A
15-4-0033	Cyclopentyl propylphosphonofluoridate	1.A.01	1	1289						A
15-4-0034	1-Isopropyl 2-methylpropyl methylphosphonofluoridate	1.A.01	1	1153						B
15-4-0035	Ethyl ethylphosphonofluoridate	1.A.01	1	880						A
15-4-0036	Ethyl methylphosphonofluoridate	1.A.01	1	802						A
15-4-0037	Ethyl propylphosphonofluoridate	1.A.01	1	962						A
15-4-0038	Isobutyl ethylphosphonofluoridate	1.A.01	1	1029						B
15-4-0039	Isobutyl methylphosphonofluoridate	1.A.01	1	937						A
15-4-0040	Isobutyl propylphosphonofluoridate	1.A.01	1	1114						A
15-4-0042	Nonyl ethylphosphonofluoridate	1.A.01	1	1566						A
15-4-0045	1,3-Dimethylbutyl methyl propylphosphonate	2.B.04	1	1359	1363					A
15-4-0053	4-tert-Butylcyclohexyl methyl ethylphosphonate	2.B.04	1	1814						A
15-4-0054	Bis(2-ethylhexyl) ethylphosphonate	2.B.04	1	2052						B
15-4-0055	Diisobutyl propylphosphonate	2.B.04	1	1448						B
15-4-0061	Cyclobutyl ethyl ethylphosphonate	2.B.04	1	1312						A
15-4-0064	Dicyclobutyl ethylphosphonate	2.B.04	1	1537						A
15-4-0065	Diethyl ethylphosphonate	2.B.04	1	1096						A
15-4-0066	Diethyl methylphosphonate	2.B.04	1	1015						A
15-4-0067	Diisobutyl ethylphosphonate	2.B.04	1	1374						A
15-4-0068	Diisobutyl methylphosphonate	2.B.04	1	1300						A
15-4-0069	Dimethyl methylphosphonate	2.B.04	1	893						A
15-4-0070	3,7-Dimethyloctyl ethyl methylphosphonate	2.B.04	1	1693						A
15-4-0072	Ethyl methyl ethylphosphonate	2.B.04	1	1036						A
15-4-0073	Ethyl methyl methylphosphonate	2.B.04	1	956						A
15-4-0081	Diethyl propylphosphonate	2.B.04	1	1174						B
17-4-0088	Ethyl methylphosphonofluoridate	1.A.01	1	795						A

OPCW Code	Chemical Name	Sched	Column	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	RI(f)	Decision
17-4-0089	Ethyl 1-propylheptyl methylphosphonate	2.B.04	1	1651	1652					A
17-4-0091	1-Propylheptyl methylphosphonofluoridate	1.A.01	1	1459	1467					A
17-4-0092	1-Propylheptyl methylphosphonochloridate	2.B.04	1	1617	1618					B
17-4-0093	Bis(1-propylheptyl) methylphosphonate	2.B.04	1	2211	2229	2247				A
17-4-0094	Bis(1-propylheptyl) dimethylpyrophosphonate	2.B.04	1	2540	2546	2563	2567	2582		A
17-4-0095	Bis(1-methylnonyl) methylphosphonate	2.B.04	1	2315	2350	2383				A
17-4-0096	1-Methylnonyl methylphosphonofluoridate	1.A.01	1	1490	1501					A
17-4-0097	1-Methylnonyl methylphosphonochloridate	2.B.04	1	1654	1661					B
17-4-0100	2-tert-Butylcyclohexyl methylphosphonofluoridate	1.A.01	1	1475	1485	1502	1509			A
17-4-0101	4-tert-Butylcyclohexyl methylphosphonochloridate	2.B.04	1	1733						A
17-4-0103	4-tert-Butylcyclohexyl methylphosphonofluoridate	1.A.01	1	1509	1554					A
17-4-0105	4-Cyclohexylbutyl methylphosphonofluoridate	1.A.01	1	1629						B
17-4-0106	Bis(3-cyclopentylpropyl) methylphosphonate	2.B.04	1	2329						A
17-4-0107	3-Cyclopentylpropyl methylphosphonofluoridate	1.A.01	1	1423						A
17-4-0108	Bis(3-cyclohexylpropyl) methylphosphonate	2.B.04	1	2550						A
17-4-0109	3-Cyclohexylpropyl methylphosphonofluoridate	1.A.01	1	1528						A
17-4-0110	Cyclooctyl methylphosphonofluoridate	1.A.01	1	1464						A
17-4-0111	Dicyclooctyl methylphosphonate	2.B.04	1	2408						A
17-4-0112	Cycloheptylmethyl methylphosphonofluoridate	1.A.01	1	1460						A
17-4-0113	Bis(cycloheptylmethyl) methylphosphonate	2.B.04	1	2422						A
17-4-0114	Bis(3,5,5-trimethylhexyl) dimethylpyrophosphonate	2.B.04	1	2452						A
17-4-0115	Bis(3,5,5-trimethylhexyl) methylphosphonate	2.B.04	1	2084						A
17-4-0116	3,5,5-Trimethylhexyl methylphosphonofluoridate	1.A.01	1	1332						A
17-4-0117	1-Isobutyl-3-methylbutyl methylphosphonofluoridate	1.A.01	1	1250						A
17-4-0118	Bis(1-isobutyl-3-methylbutyl) dimethylpyrophosphonate	2.B.04	1	2170	2173					B
17-4-0119	Bis(1-isobutyl-3-methylbutyl) methylphosphonate	2.B.04	1	1828						A

OPCW Code	Chemical Name	Sched	Column	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	RI(f)	Decision
17-4-0120	1-Isobutyl-3-methylbutyl methylphosphonochloridate	2.B.04	1	1401						A
17-4-0121	6-Butyl-2-ethyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1697						B
17-4-0122	2,6-Diethyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1516						B
17-4-0123	2-Ethyl-6-methyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1421						B
17-4-0124	6-Butyl-2-isopropyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1727						B
17-4-0125	6-Ethyl-2-isopropyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1548						B
17-4-0126	2-Isopropyl-6-methyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1461						B
17-4-0127	6-Butyl-2-methyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1611						B
17-4-0128	6-Ethyl-2-methyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1427						B
17-4-0129	2,6-Dimethyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1338						B
17-4-0130	6-Butyl-2-propyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1792						B
17-4-0131	6-Ethyl-2-propyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1604						B
17-4-0132	6-Methyl-2-propyl-1,3,6,2-dioxazaphosphocane-2-oxide	2.B.04	1	1519						B
17-4-0133	2-Methyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	1	1519						B
17-4-0134	2-Ethyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	1	1597						B
17-4-0135	2-Isopropyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	1	1630						B
17-4-0136	2-Propyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	1	1690						B
17-4-0137	3-Quinuclidinol	2.B.09	1	1186						A
17-4-0138	Dihexyl diisopropylpyrophosphonate	2.B.04	1	2300	2310					A
17-4-0139	Diisopropyl dimethylpyrophosphonate	2.B.04	1	1439						A
17-4-0140	Methylphosphonothioic dichloride	2.B.04	1	898						A
17-4-0141	Ethylphosphonothioic dichloride	2.B.04	1	998						A
17-4-0143	Propylphosphonothioic dichloride	2.B.04	1	1087						A
17-4-0144	Bis(2-chloroethylthiomethyl) ether	1.A.04	1	1744						B
17-4-0145	1,5-Bis(2-chloroethylthio) pentane	1.A.04	1	2045						B
17-4-0146	Ethyl 2-methoxyethyl methylphosphonate	2.B.04	1	1215						A

OPCW Code	Chemical Name	Sched	Column	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	RI(f)	Decision
17-4-0147	2-Methoxyethyl pinacolyl methylphosphonate	2.B.04	1	1447	1461					A
17-4-0148	Isopropylphosphonic dichloride	2.B.04	1	1000						A
17-4-0149	N,N-Dimethylphosphoramidic dichloride	2.B.05	1	1014						A
17-4-0151	Diethyl dimethylpyrophosphonate	2.B.04	1	1402	1404					A
17-4-0154	Pinacolyl propyl methylphosphonate	2.B.04	1	1343	1353					A
17-4-0155	Dipinacolyl dimethylpyrophosphonate	2.B.04	1	1840	1857	1870	1876	1897	1899	A
17-4-0157	Diisobutyl dimethylpyrophosphonate	2.B.04	1	1660						A

TABLE 3: LIST OF APPROVED IR DATA

OPCW Code	Chemical Name	Schedule	Decision
04-1-0284v	1-Isopropyl-3-methylpropyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	B
04-1-0285v	4-tert-Butylcyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0286v	3,5-Dimethylcyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0288v	Isopropyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0289v	Butyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0290v	Pentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0292v	Ethyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0293v	sec-Butyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A

TABLE 4: LIST OF APPROVED MS DATA FROM 22ND MEETING OF THE VALIDATION GROUP

OPCW Code	Chemical Name	Schedule	Decision
24-2-0037	2-Chloroethyl 2-hydroxyethyl sulfide	NS	B

Annex 2

**LISTS OF TECHNICALLY VALID DATA REQUIRING A NAME CHANGE
BEFORE INCLUSION IN THE OPCW CENTRAL ANALYTICAL DATABASE**

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

TABLE 1: LIST OF TECHNICALLY VALID MS DATA

OPCW Code	Chemical Name	Schedule	Decision
15-2-0127	Isobutyl N,N-diethylamino isopropylphosphonate	2.B.04	B
15-2-0128	Isopropyl N,N-diethylamino diisopropylpyrophosphonate	2.B.04	B
15-2-0129	Isopropyl N,N-diethylamino isopropylphosphonate	2.B.04	B
15-2-0131	Isobutyl N,N-diethylamino dimethylpyrophosphonate	2.B.04	B
15-2-0132	4-Methylcyclohexyl N,N-diethylamino dimethylpyrophosphonate	2.B.04	B
15-2-0133	4-Methylcyclohexyl N,N-diethylamino methylphosphonate	2.B.04	B
15-2-0134	Cyclohexyl N,N-diethylamino dimethylpyrophosphonate	2.B.04	B
15-2-0135	Cyclohexyl N,N-diethylamino methylphosphonate	2.B.04	B
15-2-0136	3-Methylpentyl N,N-diethylamino dimethylpyrophosphonate	2.B.04	B
15-2-0137	3-Methylpentyl N,N-diethylamino methylphosphonate	2.B.04	B
15-2-0138	sec-Butyl N,N-diethylamino dimethylpyrophosphonate	2.B.04	B
15-2-0139	sec-Butyl N,N-diethylamino methylphosphonate	2.B.04	B
15-2-0140	Pinacolyl N,N-diethylamino methylphosphonate	2.B.04	B
15-2-0141	N,N-Diethyl methylphosphoramidic chloride	2.B.04	B
15-2-0144	4-Methylcyclohexyl N,N-diethylamino ethylphosphonate	2.B.04	B
15-2-0146	3,3,5,5-Tetramethylcyclohexyl N,N-diethylamino diethylpyrophosphonate	2.B.04	B
15-2-0147	Pinacolyl N,N-diethylamino ethylphosphonate	2.B.04	B
15-2-0148	Pinacolyl N,N-diethylamino diethylpyrophosphonate	2.B.04	B
15-2-0149	3,3,5,5-Tetramethylcyclohexyl N,N-diethylamino ethylphosphonate	2.B.04	B

TABLE 2: LIST OF TECHNICALLY VALID GC(RI) DATA

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

Annex 3**LIST OF TECHNICALLY VALID DATA NOT RECOMMENDED FOR INCLUSION
IN THE OPCW CENTRAL ANALYTICAL DATABASE**

Note: In the last column of the tables that follow in this Annex, “B” indicates “accepted subject to minor corrections”.

**LIST OF TECHNICALLY VALID MS DATA FROM
THE 20TH MEETING OF THE VALIDATION GROUP**

OPCW Code	Chemical Name	Schedule	Decision
16-2-0024	Diphenyl propylthioarsine	NS	B
16-2-0025	Diphenyl ethylthioarsine	NS	B
16-2-0026	Methyl (diphenylarsino)thioacetate	NS	B
16-2-0027	Bis(diphenylarsine)oxide	NS	B

Annex 4**LIST OF RECOMMENDED CHANGES TO THE OPCW CENTRAL
ANALYTICAL DATABASE****LIST OF DATA TO BE REMOVED FROM THE OCAD
DUE TO THE PRESENCE OF OTHER HIGHER QUALITY MS DATA
FOR THESE CHEMICALS IN THE OCAD***

OPCW Code	Chemical Name	Schedule
18-2-0044	Methyl isopropylphosphonofluoridate	2.B.04
18-2-0054	Dimethyl isopropylphosphonate	2.B.04
18-2-0056	Hexyl methyl isopropylphosphonate	2.B.04
18-2-0059	Methyl 3-methylcyclopentyl isopropylphosphonate	2.B.04
18-2-0062	Methyl octyl isopropylphosphonate	2.B.04
18-2-0063	2-Ethylhexyl methyl isopropylphosphonate	2.B.04
18-2-0064	Methyl 2-methylcyclohexyl isopropylphosphonate	2.B.04
18-2-0069	Cyclohexyl isopropylphosphonochloridate	2.B.04
18-2-0076	Bis(2-ethylhexyl) isopropylphosphonate	2.B.04
18-2-0077	Bis(2-methylcyclopentyl) isopropylphosphonate	2.B.04

* Ion-trap mass spectral data should not be in the OCAD, as per paragraph 5.2(b) of S/373/2003 (dated 18 August 2003).

Annex 5

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