



Verification Division
S/634/2007
28 March 2007
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**REPORT OF THE TWENTY-FIFTH MEETING OF THE VALIDATION GROUP FOR
THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE
27 AND 28 MARCH 2007**

1. The Validation Group (hereinafter “the Group”) met for the 25th time on 27 and 28 March 2007 to discuss the evaluation of new analytical data for possible inclusion in the OPCW Central Analytical Database (OCAD), and to consider related matters. 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 table below lists the names of the coordinators who were present at the Meeting, along with the technique for which each is responsible.

Technique	Coordinator
Mass spectrometry (MS)	Mr Edward White (United States of America)
Gas chromatography (retention index) GC(RI)	Mr Martin Söderström (Finland)
Infrared (IR) spectrometry	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 approved data are technically valid.
4. The Group forwarded lists of the validated analytical data to the Director-General for appropriate action (see Annexes 1 and 2).
5. The Technical Secretariat (hereinafter “the Secretariat”) requested that the Group discuss the data on several chemicals, already in the OCAD, that are neither from scheduled chemicals nor are they analytical derivatives of scheduled chemicals. The Group recommends that the Secretariat seek further guidance on the possible inclusion in the OCAD of data on non-scheduled chemicals that may be relevant in the analysis of chemical weapons-related samples. The Group recognised that technically valid data of some non-scheduled chemicals are already included in the OCAD (see Annex 3).



6. The Group, after obtaining more information regarding IR spectrum 04-1-0242v, which was initially evaluated at the 23rd meeting of the Group, recommends that this spectrum now be accepted.
7. The Secretariat reported that the decision concerning data on scheduled chemicals, submitted to the Executive Council (hereinafter “the Council”) at its Forty-Eighth Session, was postponed to the next Session.
8. The Secretariat reported that the PDF Version 10 (Electronic Version 8) of the OCAD should be ready for release by the end of 2007.
9. The Secretariat informed the Group that the OCAD project involving the creation of a relational database is ongoing, and that work is continuing on the creation of a working database that contains analytical data on relevant non-scheduled chemicals. The Group will also request that the Secretariat submit this database to the Group’s coordinators as part of the authentication process.
10. The naming rules for several analytical derivatives of lewisites (Schedule 1.A.05) were discussed, and names for specific analytical derivatives of lewisites were established. The “Rules for Naming Compounds in the OPCW Central Analytical Database” were updated (see Annex 4, paragraph 2.13).
11. Following the discussion on this matter that took place at the Ninth Meeting of the Scientific Advisory Board (subparagraph 3.3(c) of SAB-9/1, dated 14 February 2007), the Group discussed the possibility of establishing a liquid chromatography-mass spectrometry (LC-MS) database for potential inclusion in the OCAD. Mr Martin Söderström agreed to lead an effort to poll several laboratories and create a proposal for the Group to consider at its next Meeting.
12. The following analytical data are available for evaluation:

MS	16-2-0028 to 16-2-0059, 04-2-0071, 07-2-1930, 07-2-1931, 07-2-2385, 18-2-0073, 07-2-2350
GC(RI)	16-4-0067 to 16-4-0095

13. Additional data are expected for nuclear magnetic resonance spectrometry (NMR), MS, GC(RI), and IR.
14. The Group appointed evaluators for the analytical techniques. 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 4 September 2007. The coordinators agreed to send evaluation summary reports to the Group’s Chairperson and to the evaluators no later than 11 September 2007, so that the reports can be discussed at the Group’s next Meeting, which is scheduled for 18 and 19 September 2007. The evaluators agreed to come to that meeting prepared to finalise the evaluation of the analytical data referred to in paragraphs 12 and 13.
15. The Group would like to welcome Mr R. S. Verma (India) as the new evaluator for MS data.

Annexes:

- Annex 1: List of Approved Data Recommended for Inclusion in the OPCW Central Analytical Database
- Annex 2: List of Technically Valid Data Not Recommended for Inclusion in the OPCW Central Analytical Database
- Annex 3: Non-scheduled Chemicals in the OPCW Central Analytical Database
- Annex 4: Rules for Naming Compounds in the OPCW Central Analytical Database
- Annex 5: List of Evaluators by Analytical Technique

Annex 1

**LIST 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
04-2-0374r	Diisopropyl methylphosphonate	2.B.04	A
04-2-0450	Nonyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0452	Decyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0453	1-Methylnonyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0454	Cyclopentyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0455	Cyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0456	Cycloheptyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0457	2-Methylcyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0458	Cyclooctyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0459	tert-Butyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0460	3-Methylbutyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0461	1,1-Dimethylpropyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
08-2-0117	O-Cyclopentyl S-ethyl methylphosphonothiolate	2.B.04	A
09-2-0013r	Butyl N,N-diethylphosphoramidocyanidate	1.A.02	A
09-2-0015r	Cyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	A
09-2-0023r	Cyclohexyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
09-2-0024r	2-Ethylhexyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
09-2-0028r	Propyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
09-2-0029r	sec-Butyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
09-2-0038r	Methyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0039r	Ethyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0040r	Propyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0041r	Butyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0042r	Pentyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0043r	Hexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0044r	Isopropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0045r	Isobutyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0046r	1-Ethylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0047r	3-Methylbutyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0048r	Cyclohexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0049r	sec-Butyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0051r	Octyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0061r	3-Methylbutyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
09-2-0064r	Hexyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
09-2-0066r	Octyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	A
09-2-0074r	3-Methylbutyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0075r	Hexyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	A

OPCW Code	Chemical Name	Schedule	Decision
09-2-0079r	Isopropyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0080r	1-Ethylpropyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0081r	Octyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	A
09-2-0086r	Pentyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	A
09-2-0089r	Isobutyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	A
09-2-0090r	1-Ethylpropyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	A
09-2-0092r	Octyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	A
09-2-0094r	Hexyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	A
09-2-0099r	Butyl N-isopropyl-N-propylphosphoramidocyanidate	1.A.02	A
14-2-0024	Octyl methylphosphonochloridate	2.B.04	B
14-2-0025	1-Methylheptyl methylphosphonochloridate	2.B.04	B
14-2-0026	1-Ethylpropyl ethylphosphonochloridate	2.B.04	B
14-2-0027	3-Methylbutyl ethylphosphonochloridate	2.B.04	B
14-2-0028	1,2-Dimethylbutyl ethylphosphonochloridate	2.B.04	B
14-2-0029	Cyclohexyl isopropylphosphonochloridate	2.B.04	B
14-2-0030	4,4-Dimethylcyclohexyl methylphosphonofluoridate	1.A.01	B
14-2-0031	Cyclopropylmethyl isopropylphosphonofluoridate	1.A.01	B
14-2-0033	2-Dipropylaminoethyl methylphosphonofluoridate	2.B.04	B
14-2-0034	2-Diisopropylaminoethyl methylphosphonofluoridate	2.B.04	B
14-2-0036	Octyl S-2-diethylaminoethyl methylphosphonothiolate	1.A.03	B
14-2-0037	Nonyl S-2-diethylaminoethyl methylphosphonothiolate	1.A.03	B
14-2-0039	Hexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	B
14-2-0041	Decyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	B
14-2-0042	1,2-Dimethylpropyl S-2-diisopropylaminoethyl ethylphosphonothiolate	1.A.03	B
14-2-0044	2-Methylcyclopentyl S-2-diisopropylaminoethyl ethylphosphonothiolate	1.A.03	B
14-2-0046	3,5,5-Trimethylhexyl S-2-dimethylaminoethyl propylphosphonothiolate	1.A.03	B
14-2-0047	1-Isopropyl-2-methylpropyl N,N-dimethylphosphoramidocyanidate	1.A.02	B
14-2-0048	1-Methylpentyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B
14-2-0049	Pentyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	B
14-2-0050	Hexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	B
14-2-0051	Octyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	B
14-2-0052	Nonyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	B
14-2-0053	Decyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	B
14-2-0054	Ethyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
14-2-0055	Methyl trimethylsilyl methylphosphonate	2.B.04	B
14-2-0056	tert-Butyldimethylsilyl methyl methylphosphonate	2.B.04	B
14-2-0057	tert-Butyldimethylsilyl isobutyl methylphosphonate	2.B.04	B
14-2-0058	tert-Butyldimethylsilyl 2-methylbutyl methylphosphonate	2.B.04	B
14-2-0059	tert-Butyldimethylsilyl 3-methylbutyl methylphosphonate	2.B.04	B
14-2-0060	tert-Butyldimethylsilyl hexyl methylphosphonate	2.B.04	B
14-2-0061	tert-Butyldimethylsilyl 3-methylpentyl methylphosphonate	2.B.04	B
14-2-0062	tert-Butyldimethylsilyl 2-ethylhexyl methylphosphonate	2.B.04	B
14-2-0063	tert-Butyldimethylsilyl 2-methylcyclohexyl methylphosphonate	2.B.04	B
14-2-0064	tert-Butyldimethylsilyl 2-methoxyethyl methylphosphonate	2.B.04	B
14-2-0065	Isopropyl methyl ethylphosphonate	2.B.04	B
14-2-0066	Hexyl methyl ethylphosphonate	2.B.04	B

OPCW Code	Chemical Name	Schedule	Decision
14-2-0067	1-Ethylbutyl methyl ethylphosphonate	2.B.04	B
14-2-0068	1-Ethylpropyl trimethylsilyl ethylphosphonate	2.B.04	B
14-2-0069	tert-Butyldimethylsilyl methyl ethylphosphonate	2.B.04	B
14-2-0070	tert-Butyldimethylsilyl ethyl ethylphosphonate	2.B.04	B
14-2-0071	tert-Butyldimethylsilyl 1,2-dimethylpropyl ethylphosphonate	2.B.04	B
14-2-0072	tert-Butyldimethylsilyl 2-methoxyethyl ethylphosphonate	2.B.04	B
14-2-0073	1-Ethyl-2-methylpropyl methyl propylphosphonate	2.B.04	B
14-2-0074	1-Ethyl-2,2-dimethylpropyl methyl propylphosphonate	2.B.04	B
14-2-0075	1,5-Dimethylhexyl methyl propylphosphonate	2.B.04	B
14-2-0077	3,5-Dimethylcyclohexyl methyl propylphosphonate	2.B.04	B
14-2-0078	tert-Butyldimethylsilyl methyl propylphosphonate	2.B.04	B
14-2-0080	Cyclopropylmethyl methyl isopropylphosphonate	2.B.04	B
14-2-0081	1-Ethylbutyl trimethylsilyl isopropylphosphonate	2.B.04	B
14-2-0084	Bis(1-ethylpropyl) methylphosphonate	2.B.04	B
14-2-0085	2,3-Dimethylcyclohexyl ethyl methylphosphonate	2.B.04	B
14-2-0086	Bis(1,3-dimethylbutyl) ethylphosphonate	2.B.04	B
14-2-0087	2-Ethylbutyl propyl ethylphosphonate	2.B.04	B
14-2-0088	Ethyl octyl ethylphosphonate	2.B.04	B
14-2-0089	Bis(1-methylbutyl) propylphosphonate	2.B.04	B
14-2-0090	Butyl propyl propylphosphonate	2.B.04	B
14-2-0091	Dihexyl isopropylphosphonate	2.B.04	B
14-2-0092	Bis(3,3-dimethylbutyl) isopropylphosphonate	2.B.04	B
14-2-0093	Bis(2,4,4-trimethylpentyl) isopropylphosphonate	2.B.04	B
14-2-0094	O-Cyclobutyl methylphosphonothionochloridate	2.B.04	B
14-2-0095	N,N-Dipropylphosphoramidic difluoride	2.B.05	B
14-2-0096	Propylphosphonous dichloride	2.B.04	B

TABLE 2. LIST OF APPROVED MS DATA

OPCW Code	Chemical Name	Schedule	Decision
08-2-0088	2-(2-Chlorovinyl)-1,3,2-dithiarsolane	DS	A
08-2-0090	2-(2-Chlorovinyl)-5-methyl-1,3,2-benzodithiarsole	DS	A
14-2-0097	N-Ethyl-N-methyl-N-(2-trimethylsilyloxyethyl)amine	DS	B
17-2-0103	Butyl bis(2-chlorovinyl)arsinothiolite	DS	B
25-2-0014	Dibutyl 2-chlorovinylarsonodithiolite	DS	B

TABLE 3. LIST OF APPROVED GC(RI) DATA

OPCW Code	Chemical Name	Schedule	Column	a	b	Decision
04-4-0259	Nonyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2348		A
04-4-0260	1-Methyloctyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2221	2229	A
04-4-0261	Decyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2451		A
04-4-0262	1-Methylnonyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2325	2334	A

OPCW Code	Chemical Name	Schedule	Column	a	b	Decision
04-4-0263	Cyclopentyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	1995		A
04-4-0264	Cyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2104		A
04-4-0265	Cycloheptyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2234		A
04-4-0266	2-Methylcyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2138	2146	A
04-4-0267	Cyclooctyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	2357		A
04-4-0268	tert-Butyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	1725		A
04-4-0269	3-Methylbutyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	1907		A
04-4-0270	1,1-Dimethylpropyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	1	1836		A
08-4-0093	O-Cyclopentyl S-ethyl methylphosphonothiolate	2.B.04	1	1504		A
08-4-0094	O-Methyl S-pentyl methylphosphonothiolate	2.B.04	1	1403		A

TABLE 4. LIST OF APPROVED IR DATA

OPCW Code	Chemical Name	Schedule	Decision
04-1-0272v	Nonyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0273v	1-Methyloctyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0274v	Decyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0275v	1-Methylnonyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0276v	Cyclopentyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0277v	Cyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0278v	Cycloheptyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0279v	2-Methylcyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0280v	Cyclooctyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0282v	3-Methylbutyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-1-0283v	1,1-Dimethylpropyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
02-1-0225	<i>cis</i> -2-Chlorovinyl dichloroarsine	1.A.05	B
02-1-0226	<i>trans</i> -2-Chlorovinyl dichloroarsine	1.A.05	B
02-1-0227	<i>cis</i> -2-Chlorovinyl(<i>trans</i> -2-chlorovinyl)chloroarsine	1.A.05	B
02-1-0228	Bis(<i>cis</i> -2-chlorovinyl)chloroarsine	1.A.05	B

OPCW Code	Chemical Name	Schedule	Decision
02-1-0229	Tris(2-chlorovinyl)arsine	1.A.05	B
02-1-0017r	4-Methylcyclohexyl methylphosphonofluoridate	1.A.01	A
04-1-0242v	Cyclopentyl S-2-diethylaminoethyl methylphosphonothiolate	1.A.03	A

Annex 2

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

TABLE 1. LIST OF TECHNICALLY VALID MS DATA

OPCW Code	Chemical Name	Schedule	Decision
08-2-0086	O,O-Diethyl S-methyl phosphorothiolate	NS	A
08-2-0087	Diethyl methyl phosphate	NS	A
08-2-0089	O,O-Diethyl O-methyl phosphorothionate	NS	A
08-2-0091	Diethyl O-trimethylsilyl phosphorothionate	NS	A
08-2-0093	Diethyl trimethylsilyl phosphate	NS	A
08-2-0095	Diethyl tert-butyltrimethylsilyl phosphate	NS	A
08-2-0096	tert-Butyltrimethylsilyl N,N-dimethylaminoethyl-2-sulfonate	NS	B
08-2-0100	Trimethylsilyl N,N-dimethylaminoethyl-2-sulfonate	NS	B
08-2-0103	Methyl trimethylsilyl N,N-dipropylphosphoramidate	NS	B
08-2-0104	Methyl N,N-dimethylaminoethyl-2-sulfonate	NS	B
08-2-0105	Methyl N,N-diethylaminoethyl-2-sulfonate	NS	B
08-2-0108	Methyl trimethylsilyl N,N-diethylphosphoramidate	NS	B
08-2-0109	Isopropyl trimethylsilyl N,N-diethylphosphoramidate	NS	B
08-2-0110	Isopropyl trimethylsilyl N,N-dipropylphosphoramidate	NS	B
08-2-0111	Methyl tert-butyltrimethylsilyl N,N-diethylphosphoramidate	NS	B
08-2-0113	Methyl tert-butyltrimethylsilyl N,N-dipropylphosphoramidate	NS	B
08-2-0115	Ethyl trimethylsilyl N,N-diethylphosphoramidate	NS	B
08-2-0116	Ethyl tert-butyltrimethylsilyl N,N-diethylphosphoramidate	NS	B
09-2-0057r	2-Methoxyethyl N-isopropyl-N-methylphosphoramidocyanidate	NS	B
09-2-0101r	2-Methoxyethyl N-isopropyl-N-propylphosphoramidocyanidate	NS	B
24-2-0033	Bis(2-N,N-dimethylaminoethyl)sulfide	NS	A
24-2-0036	Bis(2-N,N-dipropylaminoethyl)disulfide	NS	A
24-2-0043	2-Chloroethyl vinyl sulfoxide	NS	A
24-2-0044	2-Chloroethyl vinyl sulfone	NS	A
24-2-0045	2-Hydroxyethyl vinyl sulfide	NS	A
24-2-0052	Bis(2-trimethylsilyloxyethylthiomethyl)ether	NS	A
24-2-0054	1,2-Bis(2-trimethylsilyloxyethylsulfonyl)ethane	NS	A
24-2-0069	Methyldichloroarsine	NS	B
24-2-0070	Ethyldichloroarsine	NS	B
24-2-0073	Diphenylcyanoarsine	NS	B
24-2-0074	10-Chloro-5,10-dihydrophenarsazine	NS	B
24-2-0078	Phosgene oxime	NS	B
08-2-0086	O,O-Diethyl S-methyl phosphorothiolate	NS	A

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

OPCW Code	Chemical Name	Schedule	Column	RI	Decision
08-4-0061	O,O-Diethyl S-methyl phosphorothiolate	NS	1	1229	A
08-4-0062	Diethyl methyl phosphate	NS	1	1066	A
08-4-0064	O,O-Diethyl O-methyl phosphorothionate	NS	1	1112	A
08-4-0066	O,O-Diethyl O-trimethylsilyl phosphorothionate	NS	1	1229	A
08-4-0068	Diethyl trimethylsilyl phosphate	NS	1	1184	A
08-4-0070	Diethyl tert-butyldimethylsilyl phosphate	NS	1	1386	A
08-4-0071	tert-Butyldimethylsilyl N,N-dimethylaminoethyl-2-sulfonate	NS	1	1565	B
08-4-0072	tert-Butyldimethylsilyl N,N-diethylaminoethyl-2-sulfonate	NS	1	1717	B
08-4-0073	tert-Butyldimethylsilyl N,N-diisopropylaminoethyl-2-sulfonate	NS	1	1833	B
08-4-0074	tert-Butyldimethylsilyl N,N-dipropylaminoethyl-2-sulfonate	NS	1	1865	B
08-4-0075	Trimethylsilyl N,N-dimethylaminoethyl-2-sulfonate	NS	1	1349	B
08-4-0076	Trimethylsilyl N,N-diethylaminoethyl-2-sulfonate	NS	1	1497	B
08-4-0077	Trimethylsilyl N,N-diisopropylaminoethyl-2-sulfonate	NS	1	1612	B
08-4-0079	Methyl trimethylsilyl N,N-dipropylphosphoramidate	NS	1	1407	B
08-4-0080	Methyl N,N-dimethylaminoethyl-2-sulfonate	NS	1	1218	B
08-4-0081	Methyl N,N-diethylaminoethyl-2-sulfonate	NS	1	1372	B
08-4-0082	Methyl N,N-diisopropylaminoethyl-2-sulfonate	NS	1	1497	B
08-4-0083	Methyl N,N-dipropylaminoethyl-2-sulfonate	NS	1	1532	B
08-4-0084	Methyl trimethylsilyl N,N-diethylphosphoramidate	NS	1	1262	B
08-4-0085	Isopropyl trimethylsilyl N,N-diethylphosphoramidate	NS	1	1320	B
08-4-0086	Isopropyl trimethylsilyl N,N-dipropylphosphoramidate	NS	1	1456	B
08-4-0087	Methyl tert-butyldimethylsilyl N,N-diethylphosphoramidate	NS	1	1475	B
08-4-0089	Methyl tert-butyldimethylsilyl N,N-dipropylphosphoramidate	NS	1	1616	B
08-4-0090	Isopropyl tert-butyldimethylsilyl N,N-dipropylphosphoramidate	NS	1	1664	B
08-4-0091	Ethyl trimethylsilyl N,N-diethylphosphoramidate	NS	1	1307	B
08-4-0092	Ethyl tert-butyldimethylsilyl N,N-diethylphosphoramidate	NS	1	1516	B
24-4-0001r	Bis(2-N,N-diethylaminoethyl)sulfide	NS	1	1589	A
24-4-0002r	Bis(2-N,N-diethylaminoethyl)disulfide	NS	1	1811	A
24-4-0003r	Bis(2-N,N-diisopropylaminoethyl)sulfide	NS	1	1844	A
24-4-0004r	Bis(2-N,N-diisopropylaminoethyl)disulfide	NS	1	2066	A
24-4-0006r	Bis(2-N,N-dimethylaminoethyl)disulfide	NS	1	1513	A
24-4-0007r	Bis(2-N,N-dipropylaminoethyl)sulfide	NS	1	1892	A
24-4-0008r	Bis(2-N,N-dipropylaminoethyl)disulfide	NS	1	2116	A

OPCW Code	Chemical Name	Schedule	Column	RI	Decision
24-4-0009r	2-Chloroethyl 2-hydroxyethyl sulfide	NS	1	1186	A
24-4-0010r	1,4-Dithiane	NS	1	1071	A
24-4-0011r	1,4-Oxathiane	NS	1	890	A
24-4-0012r	N-(2-Hydroxyethyl)thiomorpholine	NS	1	1302	A
24-4-0013r	N-(2-Trimethylsilyloxyethyl)thiomorpholine	NS	1	1435	A
24-4-0014r	Bis(2-chloroethyl)disulfide	NS	1	1401	A
24-4-0015r	Bis(2-chloroethyl)sulfoxide	NS	1	1451	A
24-4-0016r	Bis(2-chloroethyl)sulfone	NS	1	1430	A
24-4-0017r	Divinylsulfoxide	NS	1	918	A
24-4-0018r	Divinylsulfone	NS	1	1001	A
24-4-0019r	2-Chloroethyl vinyl sulfide	NS	1	911	A
24-4-0020r	2-Chloroethyl vinyl sulfoxide	NS	1	1172	A
24-4-0021r	2-Chloroethyl vinyl sulfone	NS	1	1212	A
24-4-0022r	2-Hydroxyethyl vinyl sulfide	NS	1	927	A
24-4-0024r	2-Hydroxyethyl vinyl sulfone	NS	1	1039	A
24-4-0026r	Bis(2-trimethylsilyloxyethylthioethyl)ether	NS	1	2164	A
24-4-0027r	Bis(2-trimethylsilyloxyethylthio)methane	NS	1	1769	A
24-4-0028r	1,3-Bis(2-trimethylsilyloxyethylthio)propane	NS	1	1993	A
24-4-0029r	1,4-Bis(2-trimethylsilyloxyethylthio)butane	NS	1	2105	A
24-4-0030r	1,5-Bis(2-trimethylsilyloxyethylthio)pentane	NS	1	2209	A
24-4-0031r	Bis(2-trimethylsilyloxyethylthiomethyl)ether	NS	1	1931	B
24-4-0032r	Bis(2-trimethylsilyloxyethyl)sulfoxide	NS	1	1672	A
24-4-0033r	Bis(2-trimethylsilyloxyethyl)sulfone	NS	1	1694	A
24-4-0034r	1,2-Bis(2-trimethylsilyloxyethylsulfanyl)ethane	NS	1	1860	A
24-4-0035r	1,2-Bis(2-trimethylsilyloxyethylsulfonyl)ethane	NS	1	2357	A
24-4-0037r	1,2-Bis(2-trimethylsilyloxyethylsulfonyl)ethyl)ether	NS	1	2743	A
24-4-0038r	Bis(2-trimethylsilyloxyethylsulfanyl)methane	NS	1	1818	B
24-4-0039r	Bis(2-trimethylsilyloxyethylsulfonyl)methane	NS	1	2094	B
24-4-0040r	1,3-Bis(2-trimethylsilyloxyethylsulfanyl)propane	NS	1	1991	A
24-4-0041r	1,3-Bis(2-trimethylsilyloxyethylsulfonyl)propane	NS	1	2557	A
24-4-0042r	1,4-Bis(2-trimethylsilyloxyethylsulfanyl)butane	NS	1	2104	A
24-4-0043r	1,4-Bis(2-trimethylsilyloxyethylsulfonyl)butane	NS	1	2713	A
24-4-0044r	1,5-Bis(2-trimethylsilyloxyethylsulfanyl)pentane	NS	1	2208	A
24-4-0045r	1,5-Bis(2-trimethylsilyloxyethylsulfonyl)pentane	NS	1	2853	A
24-4-0046r	Bis(2-trimethylsilyloxyethylsulfanylmethyl)ether	NS	1	2198	A
24-4-0047r	Bis(2-trimethylsilyloxyethylsulfonylmethyl)ether	NS	1	2400	A
24-4-0048r	Diethyl trimethylsilyl phosphate	NS	1	1186	A
24-4-0049r	Diethyl methyl phosphate	NS	1	1069	A
24-4-0051r	O,O-Diethyl S-methyl phosphorothiolate	NS	1	1229	A
24-4-0052r	Methyldichloroarsine	NS	1	802	A
24-4-0053r	Ethyldichloroarsine	NS	1	900	A
24-4-0054r	Phenyldichloroarsine	NS	1	1347	A
24-4-0055r	10-Chloro-5,10-dihydrophenarsazine	NS	1	2412	A
24-4-0056r	Capsaicin	NS	1	2580	A
24-4-0057r	Pelargonic acid vanillylamide	NS	1	2537	A

OPCW Code	Chemical Name	Schedule	Column	RI	Decision
24-4-0058r	Ethyl iodoacetate	NS	1	993	A
24-4-0059r	Ethyl bromoacetate	NS	1	910	A
24-4-0060r	Phosgene oxime	NS	1	1060	A
24-4-0061r	o-Xylyl bromide	NS	1	1209	A
24-4-0062r	m-Xylyl bromide	NS	1	1206	A
24-4-0063r	p-Xylyl bromide	NS	1	1213	A

TABLE 3. LIST OF TECHNICALLY VALID IR DATA

OPCW Code	Chemical Name	Schedule	Decision
02-1-0230	Tetrakis(2-chlorovinyl)diarsoxane	NS	B
02-1-0231	Dimethyl 2-chlorovinylarsonite	NS	B
02-1-0232	Diethyl 2-chlorovinylarsonite	NS	B
02-1-0233	Methyl 2-chlorovinylarsonochloridite	NS	B
02-1-0234	Dipropyl 2-chlorovinylarsonodithiolite	NS	B
02-1-0235	Propyl bis(2-chlorovinyl)arsinothiolite	NS	B
02-1-0236	Pinacolyl 2-chlorovinylarsonochloridite	NS	B
02-1-0237	Diisopropyl 2-chlorovinylarsonodithiolite	NS	B
02-1-0238	Isopropyl bis(2-chlorovinyl)arsinothiolite	NS	B
02-1-0240	Dimethyl 2-chlorovinylarsonite	NS	B
02-1-0241	Octyl bis(2-chlorovinyl)arsinite	NS	B
02-1-0242	Octyl 2-chlorovinylarsonochloridite	NS	B
02-1-0243	Diocetyl 2-chlorovinylarsonite	NS	B
02-1-0244	Decyl 2-chlorovinylarsonochloridite	NS	B
02-1-0245	2-Methoxy-2-oxoethyl bis(2-chlorovinyl)arsinothiolite	NS	B
02-1-0246	Bis(2-methoxy-2-oxoethyl) 2-chlorovinylarsonodithiolite	NS	B
02-1-0247	2-(2-Chlorovinyl)-5-methyl-1,3,2-benzodithiarsole	NS	B

Annex 3

**NON-SCHEDULED CHEMICALS IN THE OPCW CENTRAL
ANALYTICAL DATABASE**

TABLE 1. NON-SCHEDULED CHEMICALS IN THE OCAD

OPCW Code	Chemical Name
02-1-0092	Dioctyl N,N-dimethylphosphoramidate
02-1-0094	Dihexyl N,N-dimethylphosphoramidate
02-2-0076	Dibutyl N,N-dimethylphosphoramidate
02-2-0077	Dipentyl N,N-dimethylphosphoramidate
02-2-0082	Dioctyl N,N-dimethylphosphoramidate
02-2-0084	Dihexyl N,N-dimethylphosphoramidate
02-2-0086	Diheptyl N,N-dimethylphosphoramidate

Annex 4

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.
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 first letter of the name is to be capitalised; the only exceptions to this rule are the following structural and stereo-descriptors: “sec-”, “tert-”, “cis-”, and “trans-”. In cases where a structural or stereo-descriptor prefixes a name, the first letter of 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. 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 include the following:
 - (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 must begin 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 the 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 lewisites (Schedule 1.A.05) shall be named as follows:
- (a) derivatives with alkyl thioglycolates shall be named similarly to the following examples:
 - (i) 2-Methoxy-2-oxoethyl bis(2-chlorovinyl)arsinothiolite;
 - (ii) Bis(2-methoxy-2-oxoethyl) 2-chlorovinylarsonodithiolite; and
 - (b) derivatives with butanethiol shall be named in accordance with the rules of the International Union and Pure and Applied Chemistry:
 - (i) butyl bis(2-chlorovinyl)arsinothiolite;
 - (ii) dibutyl 2-chlorovinylarsonodithiolite; and
 - (iii) tributyl arsenotrithiolite.

3. The examples below of scheduled compounds and derivatives associated with the scheduled compounds illustrate all of the rules stated above.

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-trialkylammoniummethyl 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-Chlorovinylchloroarsine
	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 ₃ P(=S)(OH) ₂]
	O-Ethyl methylphosphonothionate [(C ₂ H ₅ O)P(=S)(CH ₃)(OH)]
	O,O-Diethyl methylphosphonothionate [(C ₂ H ₅ O) ₂ P(=S)(CH ₃)]
	O-Propyl O-trimethylsilyl propylphosphonothionate
	O-Ethyl S-ethyl methylphosphonothiolate [(C ₂ H ₅ O)P(=O)(CH ₃)(SC ₂ H ₅)]
	S-Ethyl O-methyl methylphosphonothiolate
	O-Ethyl S-2-methylthioethyl methylphosphonothiolate
	O-Ethyl S-ethyl methylphosphonothiolothionate [(C ₂ H ₅ O)P(=S)(CH ₃)(SC ₂ H ₅)]

Schedule	Name
	Bis(S-sec-butyl) methylphosphonodithiolate
	O-Ethyl methylphosphonothionochloridate $[(C_2H_5O)P(=S)(CH_3)(Cl)]$
	Methylphosphonous dichloride (CH_3P-Cl_2)
	Methylphosphonic dichloride $[(CH_3P(=O)-Cl_2)]$
	Methylphosphonothioic dichloride $[(CH_3P(=S)-Cl_2)]$
	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 $[(i-C_3H_7)_2N-CH_2CH_2-O-P(=O)(H)(CH_3)]$
	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 $[(C_6H_{11}O)(CH_3)P(=O)-O-P(=O)(CH_3)(C_6H_{11}O)]$
	Dicyclohexyl dimethylpyrophosphonodithionate $[(C_6H_{11}O)(CH_3)P(=S)-O-P(=S)(CH_3)(C_6H_{11}O)]$
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
3.B.06	Phosphorus trichloride
3.B.07	Phosphorus pentachloride
3.B.08	Trimethyl phosphate

Schedule	Name
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.)

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-butyl dimethylsilyloxyethyl)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-butyl dimethylsilyloxyethyl)amine

Annex 5

LIST OF EVALUATORS BY ANALYTICAL TECHNIQUE¹

TABLE 1: IR EVALUATORS

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¹ An asterisk indicates that the evaluator in question was present at the Twenty-Fifth Meeting of the Group.

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