OPCW

Technical Secretariat

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NOTE BY THE TECHNICAL SECRETARIAT

REPORT OF THE FORTY-NINTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 17 – 18 SEPTEMBER 2019

1. The Validation Group met on 17 and 18 September 2019 to discuss the evaluation of new analytical data for possible inclusion in the OPCW Central Analytical Database (OCAD) and to consider matters related to this database. Mr Brian Mayer (United States of America) served as Chairperson of 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 was responsible, are listed below.

Mr Ferdinand Visser (South Africa)	Gas chromatography (retention index) (GC(RI))
Ms Karin Höjer Holmgren (Sweden)	Mass spectrometry (MS)
Mr Armando Alcaraz (United States of America)	Infrared (IR) spectroscopy
Mr Damian Magiera (Germany)	Nuclear magnetic resonance (NMR) spectroscopy

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

4. Mr Timothy Wood (OPCW Laboratory) gave a presentation updating Validation Group members on the development of a curated high-resolution liquid chromatography Orbitrap MS database of chemical warfare agents and related compounds. He reminded the Group of results of an OPCW Laboratory survey, which indicated interest by a number of laboratories to submit data to such a database. Mr Wood then provided a demonstration of the ownCloud platform for the collection and evaluation of Orbitrap data. He encouraged laboratories to contact him if they were interested in contributing to this effort.

5. The MS subgroup recommended as a submission criterion that the mass of the base peak of any high resolution spectra agree with its theoretical mass to within ±2.5 parts per million.

6. The MS subgroup decided to delay the review of the first sets of GC high resolution (HR) electron ionisation MS data after discussion of criteria for GC-HRMS data submission and evaluation. They also recommended that a survey be performed at the next proficiency test meeting to determine interest in the development and use of a GC-HRMS database.

7. The IR subgroup was still considering the feasibility of a Raman database for use at on-site inspections.

8. This report presents the sets of validated analytical data on scheduled chemicals (Annex 1) and non-scheduled chemicals (Annex 2), to be forwarded to the Director-General for appropriate action. The Group also validated data from relevant derivatives (see Annex 3).

9. Annex 4 to this report lists the members and evaluators of the Validation Group.

10. Available data from all analytical techniques will be sent to the Validation Group at least six weeks before its next scheduled meeting, which is scheduled to take place on 31 March and 1 April 2020. The evaluators agreed to send their evaluation reports to the appointed coordinators no later than 17 March 2020. The evaluators agreed to come to the meeting prepared to finalise the evaluation of the analytical data provided to the Group.

Annexes:

Annex 1: Lists of Approved Data on Scheduled Chemicals Recommended for Inclusion in the OPCW Central Analytical Database

Annex 2: Lists of Approved Data on Non-Scheduled Chemicals Relevant to the Chemical Weapons Convention and Recommended for Inclusion in the OPCW Central Analytical Database

Annex 3: List of Approved Data of Derivatives Relevant to the Chemical Weapons Convention

Annex 4: List of Members of the Validation Group

Annex 1

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

Note: In the "Decision" column of the tables that follow, "A" means "accepted" and "B" means "accepted subject to minor corrections".

TABLE 1: LIST OF APPROVED MS DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
04-2-0599ar	2-Methylcyclopentyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0599br	2-Methylcyclopentyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0600c	2,6-Dimethylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0601b	4-tert-Butylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	A

TABLE 2: LIST OF APPROVED GC(RI) DATA ON SCHEDULED CHEMICALS

Note: Under the "Column" heading for GC(RI) data, a "1" means an HP5 or an SE54 column and a "2" means a DB-5MS column.

OPCW Code	Chemical Name	Sched	Column	RI(a)	RI(b)	RI(c)	Decision
04-4-0401r	2,2-Dimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1438			A
04-4-0402r	1-Ethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1482			A
04-4-0403r	1,1,2-Trimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1452			A
04-4-0404r	Pinacolyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1510	1516		A
04-4-0405r	tert-Butyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1338			A
04-4-0406r	1,4-Dimethylpentyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1605	1611		A
04-4-0407r	1-Isopropyl-2-methylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1601			A
04-4-0408r	2-Methylcyclopentyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1630	1639		A
04-4-0409r	2,6-Dimethylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	2	1779	1791	1815	A
04-4-0325r	2-Methylpentyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	2	2012			A
04-4-0327r	1-Methylhexyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	2	2045	2050		A
09-4-0040	N,N-Diisopropylphosphoramidic dichloride	2.B.05	2	1254			A
09-4-0064	S-Methyl methylphosphonothiolochloridate	2.B.04	2	2122	2129		A
15-4-0138r	4-Methylcyclohexyl 1-(4-methylcyclohexyloxy)ethyl ethylphosphonate	2.B.04	2	2236			A
15-4-0143r	4-Methylcyclohexyl 1-(4-methylcyclohexyloxy)ethyl methylphosphonate	2.B.04	2	2162			A
16-4-0337	3-Methoxybutyl 2-diisopropylaminoethyl methylphosphonate	2.B.04	2	1897			A
16-4-0341	Cyclobutylmethyl 2-diisopropylaminoethyl methylphosphonate	2.B.04	2	1904			A
16-4-0342	4-Methylpentyl 2-diisopropylaminoethyl methylphosphonate	2.B.04	2	1900			A
16-4-0348	Cyclobutyl 2-diisopropylaminoethyl ethylphosphonate	2.B.04	2	1861			A
16-4-0351	1-Methylbutyl 2-diisopropylaminoethyl ethylphosphonate	2.B.04	2	1820	1834		A
16-4-0355	4-Methoxybutyl 2-diisopropylaminoethyl ethylphosphonate	2.B.04	2	2028			A
17-4-0081	Methyl bis(chlorovinyl)arsinite	DS*	2	1240			A
17-4-0082	Dimethyl 2-chlorovinylarsonite	DS	2	1330			A
17-4-0083	Trimethyl arsenite	DS	2	825			A
17-4-0084	Bis(trimethylsilyl) 2-chlorovinylarsonite	DS	2	1240			A
17-4-0085	Trimethylsilyl bis(2-chlorovinyl)arsinite	DS	2	1330			A

OPCW Code	Chemical Name	Sched	Column	RI(a)	RI(b)	RI(c)	Decision
17-4-0098	2-Isopropyl-5-methylcyclohexyl methylphosphonochloridate	2.B.04	2	1614	1621		A
17-4-0099	Bis(2-isopropyl-5-methylcyclohexyl) methylphosphonate	2.B.04	2	2295			A
17-4-0235	Trimethylsilyl 2-(trimethylsilyloxy)cyclohexyl propylphosphonate	2.B.04	2	1817			A
17-4-0450	N,N,N',N'-Tetrapropyl-P-ethylphosphondiamidate	2.B.04	2	1832			A

*DS: These compounds are analytical derivatives (using approved on-site derivatising agents) of schedule 1.A.05 chemicals.

TABLE 3: LIST OF APPROVED MS/MS DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
02-5-0103	sec-Butyl methylphosphonate	2.B.04	A
02-5-0104	sec-Butyl methylphosphonate	2.B.04	A
02-5-0105	sec-Butyl methylphosphonate	2.B.04	A
02-5-0106	Cyclohexyl methylphosphonate	2.B.04	A
02-5-0107	Cyclohexyl methylphosphonate	2.B.04	A
02-5-0108	Cyclohexyl methylphosphonate	2.B.04	A
02-5-0109	Propylphosphonic acid	2.B.04	A
02-5-0110	Propylphosphonic acid	2.B.04	A
02-5-0111	Propylphosphonic acid	2.B.04	A
02-5-0112	Butyl methylphosphonate	2.B.04	A
02-5-0113	Butyl methylphosphonate	2.B.04	A
02-5-0114	Butyl methylphosphonate	2.B.04	A
02-5-0115	Butyl methylphosphonate	2.B.04	A
02-5-0116	Butyl methylphosphonate	2.B.04	A
02-5-0117	Butyl methylphosphonate	2.B.04	A
02-5-0118	2-(N,N-Diisopropylamino)ethanethiol	2.B.12	A
02-5-0119	2-(N,N-Diisopropylamino)ethanethiol	2.B.12	A
02-5-0120	2-(N,N-Diisopropylamino)ethanethiol	2.B.12	A
02-5-0124	Ethyl 2-diisopropylaminoethyl methylphosphonate	2.B.04	A
02-5-0125	Ethyl 2-diisopropylaminoethyl methylphosphonate	2.B.04	A
02-5-0126	Ethyl 2-diisopropylaminoethyl methylphosphonate	2.B.04	A
18-5-0007	Methyl methylphosphonate	2.B.04	A
18-5-0008	Methyl methylphosphonate	2.B.04	A
18-5-0009	Methyl methylphosphonate	2.B.04	A
18-5-0010	Methyl methylphosphonate	2.B.04	A
18-5-0011	Methyl methylphosphonate	2.B.04	A
18-5-0012	Methyl methylphosphonate	2.B.04	A
18-5-0013	Propyl methylphosphonate	2.B.04	A
18-5-0014	Propyl methylphosphonate	2.B.04	A
18-5-0015	Propyl methylphosphonate	2.B.04	A
18-5-0016	Propyl methylphosphonate	2.B.04	A
18-5-0017	Propyl methylphosphonate	2.B.04	A
18-5-0018	Propyl methylphosphonate	2.B.04	A
18-5-0019	Butyl methylphosphonate	2.B.04	A
18-5-0020	Butyl methylphosphonate	2.B.04	A
18-5-0021	Butyl methylphosphonate	2.B.04	A
18-5-0022	Butyl methylphosphonate	2.B.04	A
18-5-0023	Butyl methylphosphonate	2.B.04	A
18-5-0024	Butyl methylphosphonate	2.B.04	A
18-5-0028	Isobutyl methylphosphonate	2.B.04	A
18-5-0029	Isobutyl methylphosphonate	2.B.04	A

OPCW Code	Chemical Name	Schedule	Decision
18-5-0030	Isobutyl methylphosphonate	2.B.04	A
18-5-0031	Pentyl methylphosphonate	2.B.04	A
18-5-0032	Pentyl methylphosphonate	2.B.04	A
18-5-0033	Pentyl methylphosphonate	2.B.04	A
18-5-0034	Pentyl methylphosphonate	2.B.04	A
18-5-0035	Pentyl methylphosphonate	2.B.04	A
18-5-0036	Pentyl methylphosphonate	2.B.04	A
18-5-0037	3-Methylbutyl methylphosphonate	2.B.04	A
18-5-0038	3-Methylbutyl methylphosphonate	2.B.04	A
18-5-0039	3-Methylbutyl methylphosphonate	2.B.04	A
18-5-0040	3-Methylbutyl methylphosphonate	2.B.04	A
18-5-0041	3-Methylbutyl methylphosphonate	2.B.04	A
18-5-0042	3-Methylbutyl methylphosphonate	2.B.04	A
18-5-0043	Pinacolyl methylphosphonate	2.B.04	A
18-5-0044	Pinacolyl methylphosphonate	2.B.04	A
18-5-0045	Pinacolyl methylphosphonate	2.B.04	A
18-5-0046	Dimethyl methylphosphonate	2.B.04	A
18-5-0047	Dimethyl methylphosphonate	2.B.04	A
18-5-0048	Dimethyl methylphosphonate	2.B.04	A
18-5-0049	Dipropyl methylphosphonate	2.B.04	A
18-5-0050	Dipropyl methylphosphonate	2.B.04	A
18-5-0051	Dipropyl methylphosphonate	2.B.04	A
18-5-0052	Dibutyl methylphosphonate	2.B.04	A
18-5-0053	Dibutyl methylphosphonate	2.B.04	A
18-5-0054	Dibutyl methylphosphonate	2.B.04	A
18-5-0055	Diisobutyl methylphosphonate	2.B.04	A
18-5-0056	Diisobutyl methylphosphonate	2.B.04	A
18-5-0057	Diisobutyl methylphosphonate	2.B.04	A
18-5-0058	Dipentyl methylphosphonate	2.B.04	A
18-5-0059	Dipentyl methylphosphonate	2.B.04	A
18-5-0060	Dipentyl methylphosphonate	2.B.04	A
18-5-0061	Bis(3-methylbutyl) methylphosphonate	2.B.04	A
18-5-0062	Bis(3-methylbutyl) methylphosphonate	2.B.04	A
18-5-0063	Bis(3-methylbutyl) methylphosphonate	2.B.04	A
18-5-0064	Dipinacolyl methylphosphonate	2.B.04	A
18-5-0065	Dipinacolyl methylphosphonate	2.B.04	A
18-5-0066	Dipinacolyl methylphosphonate	2.B.04	A
18-5-0073	Ethyl methylphosphonate	2.B.04	A
18-5-0074	Ethyl methylphosphonate	2.B.04	A
18-5-0075	Ethyl methylphosphonate	2.B.04	A
18-5-0076	Ethyl methylphosphonate	2.B.04	A
18-5-0077	Ethyl methylphosphonate	2.B.04	A
18-5-0078	Ethyl methylphosphonate	2.B.04	A
18-5-0082	Isopropyl methylphosphonate	2.B.04	A
18-5-0083	Isopropyl methylphosphonate	2.B.04	A
18-5-0084	Isopropyl methylphosphonate	2.B.04	A

OPCW Code	Chemical Name	Schedule	Decision
18-5-0085	Diethyl methylphosphonate	2.B.04	A
18-5-0086	Diethyl methylphosphonate	2.B.04	A
18-5-0087	Diethyl methylphosphonate	2.B.04	A
18-5-0088	Diisopropyl methylphosphonate	2.B.04	A
18-5-0089	Diisopropyl methylphosphonate	2.B.04	A
18-5-0090	Diisopropyl methylphosphonate	2.B.04	A
18-5-0091	Cyclohexyl methylphosphonate	2.B.04	A
18-5-0092	Cyclohexyl methylphosphonate	2.B.04	A
18-5-0093	Cyclohexyl methylphosphonate	2.B.04	A
18-5-0094	Dicyclohexyl methylphosphonate	2.B.04	A
18-5-0095	Dicyclohexyl methylphosphonate	2.B.04	A
18-5-0096	Dicyclohexyl methylphosphonate	2.B.04	A
18-5-0103	2-(N,N-Dipropylamino)ethanol	2.B.11	A
18-5-0104	2-(N,N-Dipropylamino)ethanol	2.B.11	A
18-5-0105	2-(N,N-Dipropylamino)ethanol	2.B.11	A
18-5-0106	2-(N,N-Diisopropylamino)ethanol	2.B.11	A
18-5-0107	2-(N,N-Diisopropylamino)ethanol	2.B.11	A
18-5-0108	2-(N,N-Diisopropylamino)ethanol	2.B.11	A
18-5-0109	2-(N,N-Diisopropylamino)ethanethiol	2.B.12	A
18-5-0110	2-(N,N-Diisopropylamino)ethanethiol	2.B.12	A
18-5-0111	2-(N,N-Diisopropylamino)ethanethiol	2.B.12	A
18-5-0121	Bis(2-hydroxyethyl)sulfide	2.B.13	A
18-5-0122	Bis(2-hydroxyethyl)sulfide	2.B.13	A
18-5-0123	Bis(2-hydroxyethyl)sulfide	2.B.13	A

TABLE 4: LIST OF APPROVED IR DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
04-1-0404v	2,2-Dimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-1-0405v	1-Ethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-1-0406rv	1,1,2-Trimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-1-0408v	tert-Butyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-1-0409v	1,4-Dimethylpentyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-1-0410rv	1-Isopropyl-2-methylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-1-0411rv	2-Methylcyclopentyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-1-0412rv	2,6-Dimethylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-1-0413rv	4-tert-Butylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	A

Annex 2

LISTS OF APPROVED DATA ON NON-SCHEDULED CHEMICALS RELEVANT TO THE CHEMICAL WEAPONS CONVENTION AND RECOMMENDED FOR INCLUSION IN THE OPCW CENTRAL ANALYTICAL DATABASE

Note: In the "Decision" column of the tables that follow, an "A" means "accepted" and a "B" means "accepted subject to minor corrections".

TABLE 1: LIST OF APPROVED MS/MS DATA ON NON-SCHEDULED CHEMICALS RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

OPCW Code	Chemical Name	Schedule	Decision	Justification[1]
02-5-0121	Bis(2-N,N-diisopropylaminoethyl)sulfide	NS	A	Potential reaction byproduct of 1.A.03
02-5-0122	Bis(2-N,N-diisopropylaminoethyl)sulfide	NS	A	
02-5-0123	Bis(2-N,N-diisopropylaminoethyl)sulfide	NS	A	
18-5-0097	2-(N,N-Dimethylamino)ethanol	NS	B	Potential reaction byproduct of 1.A.03
18-5-0098	2-(N,N-Dimethylamino)ethanol	NS	B	
18-5-0099	2-(N,N-Dimethylamino)ethanol	NS	B	
18-5-0100	2-(N,N-Diethylamino)ethanol	NS	B	Potential reaction byproduct of 1.A.03
18-5-0101	2-(N,N-Diethylamino)ethanol	NS	B	
18-5-0102	2-(N,N-Diethylamino)ethanol	NS	B	

[1] A classification, as used for non-scheduled GC/MS data used for on-site analysis, is not necessary for MS/MS data as it is only used by off-site laboratories.

TABLE 2: LIST OF APPROVED GC(RI) DATA ON NON-SCHEDULED CHEMICALS RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

Note: Under the "Column" heading for GC(RI) data, a "1" means an HP5 or an SE54 column and a "2" means a DB-5MS column.

OPCW Code	Chemical Name	Sched	Column	RI(a)	Decision	Justification	Classification
08-4-0067	Dimethyl trimethylsilyl phosphate	NS	2	1081	A	Derivatised potential reaction byproduct of 1.A.01	NDP(1A01)*
16-4-0051	Bis(2-chloroethyl)sulfone	NS	2	1425	A	Potential reaction byproduct/degradation product of 1.A.04	NDP(1A04)†
16-4-0052	Bis(2-chloroethyl)sulfoxide	NS	2	1446	A		
24-4-0005r	Bis(2-N,N-dimethylaminoethyl)sulfide	NS	2	1295	A	Potential reaction byproduct of 1.A.03	NDP(1A03) ‡

*Non-scheduled degradation products and/or known synthesis impurities or by-products related to schedule 1.A.01.
†Non-scheduled degradation products and/or known synthesis impurities or by-products related to schedule 1.A.04.
‡Non-scheduled degradation products and/or known synthesis impurities or by-products related to schedule 1.A.03.

Annex 3

LIST OF APPROVED DATA OF DERIVATIVES RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

TABLE 1: LIST OF APPROVED GC(RI) DATA OF DERIVATIVES RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

OPCW Code	Chemical Name	Sched	Column	RI(a)	Decision
08-4-0069	Dimethyl tert-butyldimethylsilyl phosphate	NS	2	1283	A
09-4-0047	N,N-Diisopropyl-N-(2-tert-butyldimethylsilyloxyethyl)amine	DS	2	1378	A

Annex 4

LIST OF MEMBERS OF THE VALIDATION GROUP

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