

**NOTE BY THE TECHNICAL SECRETARIAT****REPORT OF THE FIFTIETH MEETING OF THE VALIDATION GROUP
FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE
16 SEPTEMBER 2020**

1. The Validation Group met on 16 September 2020 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. Due to travel challenges related to the COVID-19 pandemic, the meeting was held remotely via video conference; subgroup meetings addressing data review were held prior to the main Validation Group meeting.
2. The evaluators for the analytical techniques evaluated new data and reported 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 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. The Validation Group accepted the resignation of Mr Vesa Häkkinen (Finland). He was acknowledged and deeply thanked for his longstanding contributions to the Validation Group. The Group also welcomed to the IR subgroup Mr Adam Bosák and Mr Jan Dědič from the National Institute for Nuclear, Chemical and Biological Protection, Czech Republic, and to the MS subgroup Ms Hanna Hakulinen from VERIFIN (Finland).



5. 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).
6. The Validation Group made some changes to the OCAD naming rules (version 8), copies of which can be obtained from the Technical Secretariat. The changes were made in an effort to clarify the naming rules in the new schedules.
7. Annex 4 to this report lists the members and evaluators of the Validation Group.
8. Available data from all analytical techniques will be sent to the Validation Group at least six weeks before its next scheduled meeting, which is set to take place on 31 March and 1 April 2021. The evaluators agreed to send their evaluation reports to the appointed coordinators no later than 17 March 2021. 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
04-2-0603	1-Ethylpropyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-2-0607a	1,4-Dimethylpentyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-2-0607b	1,4-Dimethylpentyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-2-0609a	2-Methylcyclopentyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-2-0611	4-tert-Butylcyclohexyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
07-2-3598	N-(1-(Diethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	B
07-2-3599	N-(1-(Diethylamino)ethylidene)-P-ethylphosphonamidic fluoride	1.A.13	B
07-2-3600r	N-(1-(Diethylamino)ethylidene)-P-propylphosphonamidic fluoride	1.A.13	A
07-2-3601	N-(1-(Diethylamino)ethylidene)-P-isopropylphosphonamidic fluoride	1.A.13	B
07-2-3602	Methyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
07-2-3603	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
07-2-3604	Propyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
07-2-3605	Isopropyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
07-2-3606r	N-(Bis(diethylamino)methylene)-P-methylphosphonamidic fluoride	1.A.15	A
28-2-0294	N-(Bis(dimethylamino)methylidene)-P-methylphosphonamidoseleonic fluoride	2.B.04	B
28-2-0295	Methyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleonoate	2.B.04	B
28-2-0296	Methyl-d3 N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleonoate	2.B.04	B
28-2-0297	Ethyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleonoate	2.B.04	B
28-2-0298	Ethyl-d5 N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleonoate	2.B.04	B

OPCW Code	Chemical Name	Schedule	Decision
28-2-0299	Isopropyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleate	2.B.04	B
28-2-0300	Propyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleate	2.B.04	B
28-2-0302	Butyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleate	2.B.04	B
28-2-0303	2-Methylbutyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleate	2.B.04	B
28-2-0304	Cyclopentyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleate	2.B.04	B
28-2-0305	Hexyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleate	2.B.04	B
28-2-0306	Phenyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleate	2.B.04	B

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	Schedule	Column	RI(a)	RI(b)	Decision
04-4-0414	Pinacolyl N,N-dipropylphosphoramidocyanidate	1.A.02	1	1677	1682	A
04-4-0416	1,4-Dimethylpentyl N,N-dipropylphosphoramidocyanidate	1.A.02	1	1779	1786	A
04-4-0418	2-Methylcyclopentyl N,N-dipropylphosphoramidocyanidate	1.A.02	1	1792	1797	A
04-4-0420	4-tert-Butylcyclohexyl N,N-dipropylphosphoramidocyanidate	1.A.02	1	2209		A
07-4-3461	N-(1-(Diethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	2	1503		B
07-4-3462	N-(1-(Diethylamino)ethylidene)-P-ethylphosphonamidic fluoride	1.A.13	2	1605		B
07-4-3463	N-(1-(Diethylamino)ethylidene)-P-propylphosphonamidic fluoride	1.A.13	2	1689		B
07-4-3464	N-(1-(Diethylamino)ethylidene)-P-isopropylphosphonamidic fluoride	1.A.13	2	1657		B
07-4-3465	Methyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	2	1581		B
07-4-3466	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	2	1639		B
07-4-3467	Propyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	2	1728		B
07-4-3468	Isopropyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	2	1658		B
07-4-3469	N-(Bis(diethylamino)methylene)-P-methylphosphonamidic fluoride	1.A.15	2	1652		B
28-4-0297	N-(Bis(dimethylamino)methylidene)-P-methylphosphonamidoseleenoic fluoride	2.B.04	1	1707		B
28-4-0298	Methyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleenoate	2.B.04	1	1822		B
28-4-0299	Methyl-d3 N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleenoate	2.B.04	1	1820		B
28-4-0300	Ethyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleenoate	2.B.04	1	1864		B
28-4-0301	Ethyl-d5 N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleenoate	2.B.04	1	1861		B
28-4-0302	Isopropyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleenoate	2.B.04	1	1890		B
28-4-0303	Propyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidoseleenoate	2.B.04	1	1956		B

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	Decision
28-4-0304	sec-Butyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidosenoate	2.B.04	1	1987	1990	B
28-4-0305	Butyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidosenoate	2.B.04	1	2055		B
28-4-0306	2-Methylbutyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidosenoate	2.B.04	1	2112		B
28-4-0307	Cyclopentyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidosenoate	2.B.04	1	2215		B
28-4-0308	Hexyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidosenoate	2.B.04	1	2262		B
28-4-0309	Phenyl N-(bis(dimethylamino)methylidene)-P-methylphosphonamidosenoate	2.B.04	1	2388		B

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

OPCW Code	Chemical Name	Schedule	Decision
18-5-0130	Methylphosphonic acid	2.B.04	A
18-5-0131	Methylphosphonic acid	2.B.04	A
18-5-0132	Methylphosphonic acid	2.B.04	A
18-5-0133	Methylphosphonic acid	2.B.04	A
18-5-0134	Methylphosphonic acid	2.B.04	A
18-5-0135	Methylphosphonic acid	2.B.04	A
18-5-0136	Ethylphosphonic acid	2.B.04	A
18-5-0137	Ethylphosphonic acid	2.B.04	A
18-5-0138	Ethylphosphonic acid	2.B.04	A
18-5-0139	Ethylphosphonic acid	2.B.04	A
18-5-0140	Ethylphosphonic acid	2.B.04	A
18-5-0141	Ethylphosphonic acid	2.B.04	A
18-5-0142	Propylphosphonic acid	2.B.04	A
18-5-0143	Propylphosphonic acid	2.B.04	A
18-5-0144	Propylphosphonic acid	2.B.04	A
18-5-0148	Isopropylphosphonic acid	2.B.04	A
18-5-0149	Isopropylphosphonic acid	2.B.04	A
18-5-0150	Isopropylphosphonic acid	2.B.04	A
18-5-0151	Methylphosphonic dichloride	2.B.04	A
18-5-0152	Methylphosphonic dichloride	2.B.04	A
18-5-0153	Methylphosphonic dichloride	2.B.04	A
18-5-0154	Ethylphosphonic dichloride	2.B.04	A
18-5-0155	Ethylphosphonic dichloride	2.B.04	A
18-5-0156	Ethylphosphonic dichloride	2.B.04	A
18-5-0157	Propylphosphonic dichloride	2.B.04	A
18-5-0158	Propylphosphonic dichloride	2.B.04	A
18-5-0159	Propylphosphonic dichloride	2.B.04	A
18-5-0160	Isopropylphosphonic dichloride	2.B.04	A
18-5-0161	Isopropylphosphonic dichloride	2.B.04	A
18-5-0162	Isopropylphosphonic dichloride	2.B.04	A
18-5-0163	Methyl ethylphosphonate	2.B.04	A
18-5-0164	Methyl ethylphosphonate	2.B.04	A
18-5-0165	Methyl ethylphosphonate	2.B.04	A
18-5-0166	O-Methyl ethylphosphonothionate	2.B.04	A
18-5-0167	O-Methyl ethylphosphonothionate	2.B.04	A
18-5-0168	O-Methyl ethylphosphonothionate	2.B.04	A
18-5-0169	Isopropyl methylphosphonate	2.B.04	A
18-5-0170	Isopropyl methylphosphonate	2.B.04	A
18-5-0171	Isopropyl methylphosphonate	2.B.04	A
18-5-0172	Isobutyl methylphosphonate	2.B.04	A
18-5-0173	Isobutyl methylphosphonate	2.B.04	A
18-5-0174	Isobutyl methylphosphonate	2.B.04	A

TABLE 4: LIST OF APPROVED IR DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
04-1-0414v	2,2-Dimethylpropyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0415v	1-Ethylpropyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0416v	1,1,2-Trimethylpropyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0417v	Pinacolyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0418v	tert-Butyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0419v	1,4-Dimethylpentyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0420v	1-Isopropyl-2-methylpropyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0421v	2-Methylcyclopentyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0422v	2,6-Dimethylcyclohexyl N,N-dipropylphosphoramidocyanidate	1.A.02	A
04-1-0423v	4-tert-Butylcyclohexyl N,N-dipropylphosphoramidocyanidate	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: LIST OF APPROVED MS/MS DATA ON NON-SCHEDULED CHEMICALS RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

OPCW Code	Chemical Name	Schedule	Decision	Justification¹
18-5-0175	1,4-Oxathiane	NS	A	Potential reaction by-product of 1.A.04
18-5-0176	1,4-Oxathiane	NS	A	
18-5-0177	1,4-Oxathiane	NS	A	

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.

Annex 3

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

TABLE 1: LIST OF APPROVED MS DATA OF DERIVATIVES RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

OPCW Code	Chemical Name	Schedule	Decision
31-2-0001	Bis(2-(tert-butylidimethylsilyloxy)ethylthioethyl)ether	NS	A
31-2-0002	Bis(2-(tert-butylidimethylsilyloxy)ethylthiomethyl)ether	NS	A

TABLE 2: LIST OF APPROVED GC(RI) DATA OF DERIVATIVES RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

OPCW Code	Chemical Name	Schedule	Column	RI(a)	Decision
31-4-0001	Bis(2-(tert-butylidimethylsilyloxy)ethylthioethyl)ether	NS	2	2627	A
31-4-0002	Bis(2-(tert-butylidimethylsilyloxy)ethylthiomethyl)ether	NS	2	2388	A

Annex 4

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