OPCW

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NOTE BY THE TECHNICAL SECRETARIAT

REPORT OF THE FIFTY-EIGHTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 18 AND 19 SEPTEMBER 2024

1. The Validation Group met on 18 and 19 September 2024 to discuss the evaluation of 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 the Chairperson of the meeting. The meeting was held in a hybrid format, with some members attending in person and others joining via videoconference. Meetings addressing data review were held in accordance with the subgroup coordinators' preferences.

2. The evaluators for the analytical techniques evaluated new data and reported to the coordinators for each analytical technique. The names of the coordinators, along with the technique for which each was responsible, are listed below:

Mr Marc-Michael Blum (Germany)	Gas chromatography (retention index) (GC(RI))
Ms Karin Höjer Holmgren (Sweden)	Mass spectrometry (MS)
Mr Damian Magiera (Germany)	Nuclear magnetic resonance (NMR) spectroscopy

3. Ms Havva Bekiroğlu Ataş (Türkiye), Mr Patrick Mornane (Australia), and Mr Soumya Singha Roy (United Kingdom of Great Britain and Northern Ireland) joined the Validation Group and were acknowledged and welcomed by the existing members. Mr Alex Balboa (United States of America), Ms Hoe Chee Chua (Singapore), Mr John Cort (United States), Mr Brian Crow (United States), Mr Johannes Heikkinen (Finland), and Mr Petrus Hemström (Sweden) were present as observers (either in person or virtually).

4. Mr Gary Mallard (United States of America) resigned as GC(RI) subgroup coordinator and was thanked for his leadership and service in this role. Ms Anne Puustinen (Finland) resigned from the Validation Group due to retirement and was also thanked for her service.

5. The Validation Group continues to actively recruit new members. Nominations for membership are welcomed by any member of the chemical sciences community with recognised expertise in the field of analytical chemistry. Prospective members are not

required to work for an OPCW designated laboratory. Nominations are provided to the OPCW Technical Secretariat by the nominee's National Authority and must include a curriculum vitae confirming their expertise.

6. The Validation Group has decided to review approximately 350 previously evaluated data sets on non-scheduled chemicals not yet sent for approval by the OPCW Executive Council. This review process will happen over time, with the first batch relating to infrared (IR) spectroscopy and NMR data. Additional data will be reviewed as part of future Group meetings. Data deemed appropriate by the Group will be recommended for inclusion in the OCAD.

7. The Validation Group discussed making recommendations regarding what schedules of the Chemical Weapons Convention (the Convention) should be prioritised by submitting laboratories. While the Group encourages submissions of all data relevant to the OCAD, it recommends that submitting laboratories, if able, focus on chemicals in Schedules 1.A.13, 1.A.14, 1.A.15, and 1.A.16 and related compounds, particularly MS and GC(RI) data. The Group will continue these discussions at future meetings.

8. To aid the evaluation process, the Validation Group recommended that laboratories submitting GC high-resolution MS data (such as, from orbitrap or quadrupole time-of-flight (QTOF) mass detectors) also submit corresponding single quadrupole MS data of the same compound for comparative purposes, if not already present in the OCAD.

9. The Validation Group agreed that in order to enhance validation of MS and GC(RI) data, the two relevant subgroups would begin holding a joint meeting after concluding their individual subgroup evaluations to holistically evaluate the data, as necessary.

10. To streamline the data submission and evaluation processes and encourage the involvement of new submission laboratories, Validation Group members decided to work within their subgroups to develop data submission templates for use by laboratories. Once finalised, these templates will be included as part of the guidelines for data submission.

11. Consistent with previous evaluations conducted at the forty-fourth Validation Group meeting (S/1433/2016, dated 7 November 2016), the Validation Group suspended GC(RI) data entry 09-4-0058 and recommended that it be removed from the OCAD, particularly because the corresponding MS data (09-2-0176) for this compound was already suspended and recommended for removal from the OCAD.

12. A number of GC(RI) data sets that have duplicate entries in the OCAD have been suspended (status "S") and recommended for removal from the OCAD. A summary of these recommendations is provided in Annex 3 hereto.

13. The NMR subgroup discussed enhancing the corresponding portion of the OCAD database with a tool that can perform direct searches of NMR data based on chemical shifts, coupling constants, and metadata embedded in PDF files in the OCAD. Observer Mr John Cort (United States of America) presented work that his organisation had conducted to create a digital database from data mined from OCAD PDF files. The subgroup will work with Mr Cort to investigate ways to share this tool with the Validation Group and the OPCW Laboratory.

14. The coordinators provided an evaluation summary of the data submitted to the Validation Group for discussion at the meeting. The evaluators finalised their evaluation of the analytical data and confirmed that the approved data were technically valid.

15. This document presents the sets of validated analytical data on scheduled chemicals recommended for inclusion in the OCAD (Annex 1). Validated analytical data on non-scheduled chemicals relevant to the Convention are found in Annex 2 to this Note. Annex 3 summarises the GC(RI) and MS data entries recommended for removal from the OCAD. Annex 4 lists the members and evaluators of the Validation Group.

16. The available data from all analytical techniques will be sent to the Validation Group at least six weeks before its next scheduled meeting, which is proposed to take place on 9 and 10 April 2025 at the OPCW Centre for Chemistry and Technology (ChemTech Centre). The evaluators agreed to send their evaluation reports to the appointed coordinators no later than 28 March 2025. The evaluators agreed to provide their individual data evaluations prior to the meeting and to come to the meeting prepared to finalise the evaluation of the analytical data provided to the Group. If travel to the ChemTech Centre is not possible, the evaluators may meet virtually.

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: Lists of Data Entries Recommended for Removal from the OPCW Central Analytical Database

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
29-2-0011	N-(1-(Dimethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-2-0012	N-(1-(Ethylmethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-2-0013	N-(1-(Methylpropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-2-0014	N-(1-(Isopropylmethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-2-0015	N-(1-(Diethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-2-0016	N-(1-(Dipropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-2-0017	N-(1-(Diisopropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-2-0018	N-(1-(Dibutylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-2-0020	Methyl N-(1-(dipropylamino)butylidene)phosphoramidofluoridate	1.A.14	A
29-2-0021	Methyl N-(1-(dibutylamino)butylidene)phosphoramidofluoridate	1.A.14	A
29-2-0022	Ethyl N-(1-(ethylmethylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
29-2-0023	Ethyl N-(1-(methylpropylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
29-2-0024	Ethyl N-(1-(diisopropylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
29-2-0025	O-Methyl S-propyl methylphosphonothiolate	2.B.04	A
29-2-0026	O-Methyl S-isopropyl methylphosphonothiolate	2.B.04	A
29-2-0027	O-Methyl S-butyl methylphosphonothiolate	2.B.04	A
29-2-0028	O-Methyl S-cyclohexyl methylphosphonothiolate	2.B.04	A
29-2-0029	O-Methyl S-hexyl methylphosphonothiolate	2.B.04	A
29-2-0030	O-Methyl S-heptyl methylphosphonothiolate	2.B.04	A
29-2-0031	O-Ethyl S-propyl methylphosphonothiolate	2.B.04	A
29-2-0032	O-Ethyl S-isopropyl methylphosphonothiolate	2.B.04	A

OPCW Code	Chemical Name	Schedule	Decision
29-2-0033	O-Ethyl S-butyl methylphosphonothiolate	2.B.04	A
29-2-0034	O-Ethyl S-cyclohexyl methylphosphonothiolate	2.B.04	A
29-2-0035	O-Ethyl S-hexyl methylphosphonothiolate	2.B.04	A
29-2-0036	O-Ethyl S-heptyl methylphosphonothiolate	2.B.04	A
36-2-0001r	Diisopropyl methylphosphonate	2.B.04	B
36-2-0005	N-(1-(Dipropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	B

TABLE 2: LIST OF APPROVED NMR DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
23-3-0011r	Methyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
23-3-0012r	Methyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
23-3-0015r	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B
23-3-0016r	Ethyl N-(1-(diethylamino)ethylidene)phosphoramidofluoridate	1.A.14	B

TABLE 3: LIST OF APPROVED GC(RI) DATA ON SCHEDULED CHEMICALS

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

OPCW Code	Chemical Name	Schedule	Column	RI(a)	Decision
29-4-0011	N-(1-(Dimethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1427	A
29-4-0012	N-(1-(Ethylmethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1481	A
29-4-0013	N-(1-(Methylpropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1562	A
29-4-0014	N-(1-(Isopropylmethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1539	A
29-4-0015	N-(1-(Diethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1530	A
29-4-0016	N-(1-(Dipropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1677	A
29-4-0017	N-(1-(Diisopropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1634	A
29-4-0018	N-(1-(Dibutylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1859	A
29-4-0022	Ethyl N-(1-(ethylmethylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1621	A
29-4-0023	Ethyl N-(1-(methylpropylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1698	A
29-4-0024	Ethyl N-(1-(diisopropylamino)ethylidene)phosphoramidofluoridate	1.A.14	1	1737	A
29-4-0025	O-Methyl S-propyl methylphosphonothiolate	2.B.04	1	1205	A
29-4-0026	O-Methyl S-isopropyl methylphosphonothiolate	2.B.04	1	1143	A
29-4-0027	O-Methyl S-butyl methylphosphonothiolate	2.B.04	1	1303	A
29-4-0028	O-Methyl S-cyclohexyl methylphosphonothiolate	2.B.04	1	1549	A
29-4-0029	O-Methyl S-hexyl methylphosphonothiolate	2.B.04	1	1508	A
29-4-0030	O-Methyl S-heptyl methylphosphonothiolate	2.B.04	1	1612	A
29-4-0031	O-Ethyl S-propyl methylphosphonothiolate	2.B.04	1	1266	A
29-4-0032	O-Ethyl S-isopropyl methylphosphonothiolate	2.B.04	1	1202	A

OPCW Code	Chemical Name	Schedule	Column	RI(a)	Decision
29-4-0033	O-Ethyl S-butyl methylphosphonothiolate	2.B.04	1	1361	A
29-4-0034	O-Ethyl S-cyclohexyl methylphosphonothiolate	2.B.04	1	1603	A
29-4-0035	O-Ethyl S-hexyl methylphosphonothiolate	2.B.04	1	1563	A
29-4-0036	O-Ethyl S-heptyl methylphosphonothiolate	2.B.04	1	1665	A
36-4-0005	N-(1-(Dipropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	1	1678	A

TABLE 4: LIST OF APPROVED GC-HRMS DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
29-7-0001	N-(1-(Dimethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-7-0002	N-(1-(Ethylmethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-7-0003	N-(1-(Methylpropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-7-0004	N-(1-(Isopropylmethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-7-0005	N-(1-(Diethylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-7-0007	N-(1-(Diisopropylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-7-0008	N-(1-(Dibutylamino)ethylidene)-P-methylphosphonamidic fluoride	1.A.13	A
29-7-0009	Methyl N-(1-(dibutylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
29-7-0010	Methyl N-(1-(dipropylamino)butylidene)phosphoramidofluoridate	1.A.14	A
29-7-0011	Methyl N-(1-(dibutylamino)butylidene)phosphoramidofluoridate	1.A.14	A
29-7-0013	Ethyl N-(1-(methylpropylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
29-7-0014	Ethyl N-(1-(diisopropylamino)ethylidene)phosphoramidofluoridate	1.A.14	A
29-7-0015	O-Methyl S-propyl methylphosphonothiolate	2.B.04	A
29-7-0016	O-Methyl S-isopropyl methylphosphonothiolate	2.B.04	A
29-7-0017	O-Methyl S-butyl methylphosphonothiolate	2.B.04	A
29-7-0021	O-Ethyl S-propyl methylphosphonothiolate	2.B.04	A
29-7-0022	O-Ethyl S-isopropyl methylphosphonothiolate	2.B.04	A
29-7-0023	O-Ethyl S-butyl methylphosphonothiolate	2.B.04	A
29-7-0024	O-Ethyl S-cyclohexyl methylphosphonothiolate	2.B.04	A
29-7-0025	O-Ethyl S-hexyl methylphosphonothiolate	2.B.04	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, "A" means "accepted," and "B" means "accepted subject to minor corrections".

TABLE 1: LIST OF APPROVED MS DATA ON NON-SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision	Justification	Classification
02-2-0087	2-Hydroxyethyl vinyl sulfone	NS	A	Reaction by-product or degradation product of 1.A.04	NDP-H[1]
02-2-0088	2-(2-Chloroethanesulfonyl)ethan-1-ol	NS	A		

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

OPCW Code	Chemical Name	Schedule	Column	RI(a)	Decision	Justification	Classification
02-4-0001	2-Hydroxyethyl vinyl sulfone	NS	1	1228	A	Reaction by-product or degradation product of 1.A.04	NDP-H[1]
02-4-0002	2-(2-Chloroethanesulfonyl)ethan-1-ol	NS	1	1472	A		
36-4-0004	N,N-Dipropylethanimidamide	NS	1	1149	A	Precursor of 1.A.13 and 1.A.14	NDP-N[2]

[1] Non-scheduled precursors, degradation products, known synthesis impurities, or by-products related to Schedule 1.A.04.

[2] Non-scheduled precursors, degradation products, known synthesis impurities, or by-products related to Schedules 1.A.13, 1.A.14, 1.A.15, and 1.A.16.

Annex 3

LISTS OF DATA ENTRIES RECOMMENDED FOR REMOVAL FROM THE OPCW CENTRAL ANALYTICAL DATABASE

TABLE 1: LIST OF DUPLICATE GC(RI) DATA RECOMMENDED FOR REMOVAL FROM THE OCAD

OPCW Code	Chemical Name	Schedule
04-4-0401	2,2-Dimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02
04-4-0402	1-Ethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02
04-4-0403	1,1,2-Trimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02
04-4-0404	Pinacolyl N,N-diethylphosphoramidocyanidate	1.A.02
04-4-0405	tert-Butyl N,N-diethylphosphoramidocyanidate	1.A.02
04-4-0406	1,4-Dimethylpentyl N,N-diethylphosphoramidocyanidate	1.A.02
04-4-0407	1-Isopropyl-2-methylpropyl N,N-diethylphosphoramidocyanidate	1.A.02
04-4-0408	2-Methylcyclopentyl N,N-diethylphosphoramidocyanidate	1.A.02
04-4-0409	2,6-Dimethylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02
28-4-0107	O-Ethyl-d5 N,N-dimethyl-P-methylphosphonamidothionate	2.B.04
28-4-0114	O-Allyl N,N-dimethyl-P-methylphosphonamidothionate	2.B.04
28-4-0123	N,N,N',N'-Tetramethyl-P-methylphosphonothionic diamide	2.B.04
28-4-0164	O-Methyl-d3 N,N-dimethyl-P-ethylphosphonamidothionate	2.B.04
28-4-0166r	O-Ethyl-d5 N,N-dimethyl-P-ethylphosphonamidothionate	2.B.04

TABLE 2: LIST OF GC(RI) AND MS DATA RECOMMENDED FOR REMOVAL FROM THE OCAD DUE TO INCORRECT NAME AND STRUCTURE[3]

OPCW Code	Chemical Name	Schedule
09-2-0176	O-Isobutyl O-trimethylsilyl methylphosphonothionate	NS
09-4-0058		

[3] Consistent with previous evaluations conducted at the forty-fourth Validation Group meeting (S/1433/2016).

Annex 4

LIST OF MEMBERS OF THE VALIDATION GROUP

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* The evaluator was present at this meeting of the Validation Group (either in person or virtually) and provided a written evaluation.
† The evaluator provided a written evaluation but did not attend the meeting.
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