



NOTE BY THE TECHNICAL SECRETARIAT

**REPORT OF THE FORTY-EIGHTH MEETING OF THE VALIDATION GROUP
FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE
19 – 20 MARCH 2019**

1. The Validation Group met on 19 and 20 March 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 acting 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

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. The Validation Group accepted the resignation of Mr Hugh Gregg (United States of America). He was acknowledged and thanked for his contributions to the Group and as Head of the OPCW Laboratory.
5. The Validation Group welcomed Mr Arcady Braun (Russian Federation) as a new member of the MS subgroup and Mr Ethan Alex Jestel (United States of America) as a new member of the MS and GC(RI) subgroups.
6. Considerations relating to the evaluation of high-resolution data were discussed (S/1686/2018, dated 13 November 2018) in a presentation given by Mr Arne Ficks (Germany). He spoke on the potential development of a high-resolution GC-MS



database. The Group encouraged a round robin analysis across several laboratories to assess how such a database might be both developed and applied in practice. It was also recommended that—in light of developments in new Orbitrap/high-resolution instrumentation—the Group revisit language in S/1686/2018, which specifically excludes ion-trap data.

7. The MS subgroup recommended re-evaluating wording in the MS/MS section of S/1686/2018.
8. The Group additionally agreed to begin drafting conditions for the collection and submission of high-resolution MS data.
9. Mr Timothy Wood (OPCW Laboratory) gave a presentation on the development of a curated high-resolution LC Orbitrap MS database of chemical warfare agent and related compounds. He shared results of an OPCW Laboratory survey, which indicated interest by a number of laboratories to submit data for inclusion in such a database.
10. Mr Armando Alcaraz recommended that the Group consider the collection and use of Raman data on portable platforms considering the needs of both on-site and off-site analyses.
11. The Validation Group elected Mr Brian Mayer (United States of America) to be its new Chairperson.
12. This report presents the sets of validated analytical data on scheduled and non-scheduled chemicals (Annexes 1 and 2, respectively), to be forwarded to the Director-General for appropriate action.
13. Annex 3 to this report lists the members and evaluators of the Validation Group.
14. 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 17 and 18 September 2019. The evaluators agreed to send their evaluation reports to the appointed coordinators no later than 3 September 2019. 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 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
04-2-0592	2,2-Dimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0593	1-Ethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0594	1,1,2-Trimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0595a	Pinacolyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0595b	Pinacolyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0596	tert-Butyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0597a	1,4-Dimethylpentyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0597b	1,4-Dimethylpentyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0598	1-Isopropyl-2-methylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0600a	2,6-Dimethylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0600b	2,6-Dimethylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	A
04-2-0601a	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)	RI(d)	Decision
04-4-0401	2,2-Dimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1438				A
04-4-0402	1-Ethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1482				A
04-4-0403	1,1,2-Trimethylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1452				A
04-4-0404	Pinacolyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1510	1516			A
04-4-0405	tert-Butyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1338				A
04-4-0406	1,4-Dimethylpentyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1605	1611			A
04-4-0407	1-Isopropyl-2-methylpropyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1601				A
04-4-0408	2-Methylcyclopentyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1630	1639			A
04-4-0409	2,6-Dimethylcyclohexyl N,N-diethylphosphoramidocyanidate	1.A.02	1	1779	1791			A
15-4-0094r	Decahydronaphthalen-2-yl methylphosphonofluoridate	1.A.01	1	1636	1665	1670		A
15-4-0101r	Bis(2-cyclohexylpropyl) methylphosphonate	2.B.04	1	2457				A
15-4-0106r	Bicyclo[2.2.1]hept-2-yl methylphosphonofluoridate	1.A.01	1	1305				A
15-4-0124r	Dicyclohexyl dimethylpyrophosphonate	2.B.04	1	2290				A
15-4-0129r	Hexyl N,N-diethyl-P-isopropylphosphonamidate	2.B.04	1	1711				A
15-4-0130r	3-Methylpentyl N,N-diethyl-P-isopropylphosphonamidate	2.B.04	1	1796				A
15-4-0134r	4-Methylcyclohexyl N,N-diethyl-P-propylphosphonamidate	2.B.04	1	1818	1847			A
15-4-0136r	Cyclopropylmethyl ethyl ethylphosphonate	2.B.04	1	1314				A
15-4-0137r	Diisobutyl diisopropylpyrophosphonate	2.B.04	1	1849	1861			A
15-4-0139r	sec-Butyl N,N-diethyl-P,P'-diisopropylidiphosphono-P-amidate	2.B.04	1	1903	1922	1937		A
15-4-0141r	Isobutyl N,N-diethyl-P,P'-diisopropylidiphosphono-P-amidate	2.B.04	1	1934	1951			A
15-4-0144r	Pinacolyl N,N-diethyl-P,P'-dimethylidiphosphono-P-amidate	2.B.04	1	1848	1865	1876	1888	A
17-4-0142	Isopropylphosphonothionic dichloride	2.B.04	1	1072				A
17-4-0185	2-Ethyl-5-methyl-1,3,2-benzoxathiaphosphole-2-oxide	2.B.04	1	1715				A
17-4-0430	trans-Hex-4-enyl trimethylsilyl propylphosphonate	2.B.04	1	1589				A

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

OPCW Code	Chemical Name	Schedule	Decision
02-5-0052	Ethyl S-2-diisopropylaminoethyl methylphosphonothiolate	1.A.03	A
02-5-0053	Ethyl S-2-diisopropylaminoethyl methylphosphonothiolate	1.A.03	A
02-5-0054	Ethyl S-2-diisopropylaminoethyl methylphosphonothiolate	1.A.03	A
02-5-0055	Diethyl P,P'-dimethylphosphono-P-thionate	2.B.04	A
02-5-0056	Diethyl P,P'-dimethylphosphono-P-thionate	2.B.04	A
02-5-0057	Diethyl P,P'-dimethylphosphono-P-thionate	2.B.04	A
02-5-0058	Diethyl dimethylpyrophosphonate	2.B.04	A
02-5-0059	Diethyl dimethylpyrophosphonate	2.B.04	A
02-5-0060	Diethyl dimethylpyrophosphonate	2.B.04	A
02-5-0061	Ethyl S-2-isopropylaminoethyl methylphosphonothiolate	2.B.04	A
02-5-0062	Ethyl S-2-isopropylaminoethyl methylphosphonothiolate	2.B.04	A
02-5-0063	Ethyl S-2-isopropylaminoethyl methylphosphonothiolate	2.B.04	A
02-5-0064	Tris(2-chloroethyl)amine	1.A.06	A
02-5-0065	Tris(2-chloroethyl)amine	1.A.06	A
02-5-0066	Tris(2-chloroethyl)amine	1.A.06	B
02-5-0070	Dipinacolyl methylphosphonate	2.B.04	A
02-5-0071	Dipinacolyl methylphosphonate	2.B.04	A
02-5-0072	Dipinacolyl methylphosphonate	2.B.04	A
02-5-0073	Pinacolyl methylphosphonate	2.B.04	A
02-5-0074	Pinacolyl methylphosphonate	2.B.04	A
02-5-0075	Pinacolyl methylphosphonate	2.B.04	A
02-5-0076	3-Quinuclidinyl benzilate	2.A.03	A
02-5-0077	3-Quinuclidinyl benzilate	2.A.03	A
02-5-0078	3-Quinuclidinyl benzilate	2.A.03	A
02-5-0079	Diethyl ethylphosphonate	2.B.04	A
02-5-0080	Diethyl ethylphosphonate	2.B.04	A
02-5-0081	Diethyl ethylphosphonate	2.B.04	A
02-5-0082	Dicyclohexyl diethylpyrophosphonate	2.B.04	A
02-5-0083	Dicyclohexyl diethylpyrophosphonate	2.B.04	A
02-5-0084	Dicyclohexyl diethylpyrophosphonate	2.B.04	B
02-5-0085	Diethyl N,N-diethylphosphoramidate	2.B.06	A
02-5-0086	Diethyl N,N-diethylphosphoramidate	2.B.06	A
02-5-0087	Diethyl N,N-diethylphosphoramidate	2.B.06	A
02-5-0094	Isobutyl methylphosphonate	2.B.04	A
02-5-0095	Isobutyl methylphosphonate	2.B.04	A
02-5-0096	Isobutyl methylphosphonate	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, an “A” means “accepted” and a “B” means “accepted subject to minor corrections”.

TABLE 4: LIST OF APPROVED MS/MS DATA ON NON-SCHEDULED CHEMICALS RELEVANT TO THE CHEMICAL WEAPONS CONVENTION

OPCW Code	Chemical Name	Schedule	Decision	Justification ¹
02-5-0067	(2-N,N-Diisopropylaminoethyl)(2-N-isopropylaminoethyl)disulfide	NS	A	Known impurity/degradation product associated with 1.A.03 synthesis
02-5-0068	(2-N,N-Diisopropylaminoethyl)(2-N-isopropylaminoethyl)disulfide	NS	A	
02-5-0069	(2-N,N-Diisopropylaminoethyl)(2-N-isopropylaminoethyl)disulfide	NS	A	
02-5-0088	Ethyl N,N-diethylphosphoramidofluoridate	NS	A	Potential reaction byproducts of 1.A.01 and 1.A.02
02-5-0089	Ethyl N,N-diethylphosphoramidofluoridate	NS	A	
02-5-0090	Ethyl N,N-diethylphosphoramidofluoridate	NS	A	
02-5-0091	Tetraethylphosphorodiamidic fluoride	NS	A	
02-5-0092	Tetraethylphosphorodiamidic fluoride	NS	A	
02-5-0093	Tetraethylphosphorodiamidic fluoride	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.

Annex 3

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