OPCW

Technical Secretariat

S/2062/2022
23 May 2022
ENGLISH only

NOTE BY THE TECHNICAL SECRETARIAT

REPORT OF THE FIFTY-THIRD MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 30 MARCH 2022

1. The Validation Group met on 30 March 2022 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 the Chairperson of the meeting. The meeting was held remotely via video conference, due to travel challenges related to the COVID-19 pandemic. The 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 Gary Mallard (United States of America)	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. Mr Armando Alcaraz provided an update on the discussions that the IR subgroup had about hand-held, portable Raman devices. Under discussion was the topic of instrument vendors, specifically whether or not the subgroup should recommend a single vendor or allow for the possible use of instruments from multiple vendors. The subgroup decided to assist in supporting systems currently approved for on-site use, focusing only on scheduled chemicals of relevance to on-site inspections.

5. Ms Karin Holmgren provided a summary of the MS subgroup's discussion on the development of a dedicated GC high-resolution mass spectrometry (GC-HRMS) database for off-site analysis. It was noted that high-resolution instrumentation has been

used more widely in recent years, particularly regarding trace analysis and chemical attribution. To support this work, the subgroup will schedule a meeting this summer to further discuss criteria for HRMS data submission and evaluation and will report back to the Group in September 2022.

6. The Validation Group had a conversation about clarifying the nomenclature for derivatised chemicals in the Validation Group Working Database. It was recommended that a new designation in addition to "DS" be created for chemicals derivatised in a single-step process with compounds that are not approved for use during on-site inspections. It was suggested that this designation should be "DSX", which would be exclusively contained within the Working Database. The recommendation was circulated to the Validation Group and it was supported unanimously by those members who responded.

7. The Validation Group considered if MS and GCRI data for the same chemical should be accepted together to avoid inconsistencies in data submission, review, and acceptance. It was recommended that reviews of this data would be performed by currently established subgroups, but that the MS and GCRI subgroups would have a meeting prior to the main Validation Group meeting to coordinate a joint final review of submitted data.

8. Mr Jiří Čermák (Czech Republic) announced his retirement, and the Group recognised and thanked him for his long-standing service to the Group and the OPCW mission. The Group also welcomed to the MS subgroup Ms Karen Jacques from Defence Science and Technology Laboratory (DSTL, the United Kingdom of Great Britain and Northern Ireland).

9. This document presents the sets of validated analytical data on scheduled chemicals (Annex 1) recommended for inclusion in the OCAD. No data for non-scheduled or derivatised chemicals relevant to the Chemical Weapons Convention were evaluated in this cycle.

10. Annex 2 to this Note lists the members and evaluators from the Validation Group.

11. 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 set to take place on 21 and 22 September 2022. The evaluators agreed to send their evaluation reports to the appointed coordinators no later than 7 September 2022. The evaluators agreed to come to the meeting prepared to finalise the evaluation of the analytical data provided to the Group. If travel to the OPCW Headquarters is still not possible at that time, the evaluators agreed to meet virtually on 21 September 2022, and to ensure that the data evaluation by the subgroups is completed prior to the meeting.

Annexes:

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

Annex 2: 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
04-2-0612r	2,2-Dimethylpropyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0614r	1,1,2-Trimethylpropyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0615ar	Pinacolyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0617ar	1,4-Dimethylpentyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0617br	1,4-Dimethylpentyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
04-2-0622	2,2-Dimethylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0623	1-Ethylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0624a	2,6-Dimethylcyclohexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0624b	2,6-Dimethylcyclohexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0626	2-Ethylhexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0627a	1,4-Dimethylpentyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0627b	1,4-Dimethylpentyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0630a	3,5-Dimethylcyclohexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-2-0631	4-tert-Butylcyclohexyl N-methyl-N-propylphosphoramidocyanidate	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	Schedule	Column	RI(a)	RI(b)	RI(c)	Decision
04-4-0427r	1-Isopropyl-2-methylpropyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	1	1523			A
04-4-0429r	2,6-Dimethylcyclohexyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	1	1691	1704	1716	A
04-4-0431	2,2-Dimethylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	1	1458			A
04-4-0432	1-Ethylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	1	1506			A
04-4-0434	Pinacolyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	1	1535	1549		A
04-4-0435	2-Ethylhexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	1	1778			A
04-4-0436	1,4-Dimethylpentyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	1	1629	1637		A
04-4-0437	1-Isopropyl-2-methylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	1	1632			A
04-4-0438	2-Methylcyclopentyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	1	1642	1646		A

TABLE 3: LIST OF APPROVED IR DATA ON SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
04-1-0431rv	2-Methylcyclopentyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	A
04-1-0434v	2,2-Dimethylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0435v	1-Ethylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0436v	2,6-Dimethylcyclohexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0437v	Pinacolyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0438v	2-Ethylhexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0439v	1,4-Dimethylpentyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0440v	1-Isopropyl-2-methylpropyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0441v	2-Methylcyclopentyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0442v	3,5-Dimethylcyclohexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A
04-1-0443v	4-tert-Butylcyclohexyl N-methyl-N-propylphosphoramidocyanidate	1.A.02	A

Annex 2

LIST OF MEMBERS OF THE VALIDATION GROUP

Name	Country	Address	Phone/Fax/Email	Speciality
Christine Albaret	France	DGA Maîtrise NRBC BP-3 91710 Vert-le-Petit, France	+33 1 69908224 +33 1 64935266 christine.albaret@intradef.gouv.fr	NMR
Armando Alcaraz*	United States of America	Lawrence Livermore National Laboratory Forensic Science Center P.O. Box 808, L-090 Livermore, CA 94550, United States of America	+1 925 423 6889 +1 925 423 9014 (fax) alcaraz1@llnl.gov	MS, IR Coordinator of the IR subgroup
Mehran Babri	Iran (Islamic Republic of)	Defence Chemical Research Lab (DCRL) P.O. Box 31585-1461 Karaj, Islamic Republic of Iran	+98 263 2313442 +98 263 2313447 (fax) dcrl.mod@gmail.com	MS
Adam Bosák*	Czech Republic	National Institute for NBC Protection (SÚJCHBO, v.v.i.) Chemical Protection Department Kamenná 71, 262 31 Milín, Czech Republic	+420 318 600 235 +420 318 626 055 (fax) bosak@sujchbo.cz	IR
Arkady Braun*	Russian Federation	LCAC 27th Research Centre of the Ministry of Defense, Russian Federation	+7 915 4558009 avbraun@yandex.ru	MS
Jiří Čermák*	Czech Republic	Výzkumný ústav organických syntéz a.s (Research Institute for Organic Syntheses) c.p. 296 53354 Rybitví, Czech Republic	+420 724400614 +420 466 823 900 (fax) jiri.cermak@vuos.com	MS

* The evaluator was present at this meeting of the Group.

Name	Country	Address	Phone/Fax/Email	Speciality
Jan Dědič*	Czech Republic	National Institute for NBC Protection (SÚJCHBO, v.v.i.) Chemical Protection Department Kamenná 71, 262 31 Milín, Czech Republic	+420 318 600 235 +420 318 626 055 (fax) dedic@sujchbo.cz	IR
Devendra K. Dubey	India	Defence R&D Establishment VERTOX Laboratory Jhansi Road, Gwalior 474002, India	+91 751 223 3488 +91 751 234 1148 dkdubey@rediffmail.com	MS
Zdeňka Fabiánová*	Czech Republic	State Office for Nuclear Safety Division of Chemical Weapons Prohibition Senovážné nám. 9, 110 00 Praha 1, Czech Republic	+420 226 514 372 zdenka.fabianova@sujb.cz	IR
Arne Ficks*	Germany	Wehrwissenschaftliches Institut für Schutztechnologien – ABC-Schutz (WIS) 29633 Munster, Germany	+49 5192 136 428 +49 5192 136 355 (fax) arneficks@bundeswehr.org	MS
Hanna Hakulinen*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki, Finland	+358 5037 67914 hanna.hakulinen@helsinki.fi	MS
Harri August Heikkinen*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki, Finland	+358 2 94150448 harri.a.heikkinen@helsinki.fi	NMR
Karin Höjer Holmgren*	Sweden	FOI CBRN Defence and Security Cementvagen 20, SE-90182 Umeå, Sweden	+46 90 106665 +46 72 5709234 karin.hojer@foi.se	MS Coordinator of the MS subgroup

Name	Country	Address	Phone/Fax/Email	Speciality
Karen Jacques*	United Kingdom of Great Britain and Northern Ireland	DSTL Porton Down, Salisbury, SP4 0JQ, United Kingdom of Great Britain and Northern Ireland	+44 (0)1980 956645 | kajacques@dstl.gov.uk	MS
Ethan Alex Jestel*	United States of America	DEVCOM CBC Forensic Analytical Center Maryland, United States of America	+1 410 436 0306 ethan.a.jestel.civ@army.mil	GC
Shilei Liu*	China	RICD Yangfang Town, Changping District P.O. Box 1043, 102205 Beijing, China	+86 10 69760259 liushilei402@263.net	MS
Damian Magiera*	Germany	Wehrwissenschaftliches Institut für Schutztechnologien - ABC-Schutz (WIS) 29633 Munster, Germany	+49 5192 136 402 +49 5192 136 355 (fax) damianmagiera@bundeswehr.org	NMR, IR Coordinator of the NMR subgroup
Gary Mallard*	United States of America	Teal Consulting Chevy Chase, MD 20815, United States of America	+1 301 656-0402 gary.mallard@gmail.com	GC Acting Coordinator of the GC subgroup
Brian Mayer*	United States of America	Lawrence Livermore National Laboratory 7000 East Avenue, L-091 Livermore, CA 94550, United States of America	+1 925 423 1128 +1 925 423 9014 (fax) mayer22@llnl.gov	NMR Chairperson of the Validation Group
Urs Meier*	Switzerland	Spiez Laboratory CH-3700 Spiez, Switzerland	+41 33228 1713 +41 33228 1402 urs.meier@babs.admin.ch	NMR

Name	Country	Address	Phone/Fax/Email	Speciality
Mohammad Taghi Naseri	Iran (Islamic Republic of)	Defence Chemical Research Lab (DCRL) P.O. Box 31585-1461, Karaj, Islamic Republic of Iran	+98 263 2313442 +98 263 2313447 (fax) dcrl.mod@gmail.com	GC
Daan Noort	Netherlands	TNO Defence, Security and Safety Lange Kleiweg 137, 2288GJ Rijswijk, Netherlands	+31 888 661307 daan.noort@tno.nl	NMR
Deepak Pardasani	India	Defence Research & Development Establishment Gwalior, India	+91 751 2341148 +91 751 2233488 dkpardasani@drde.drdo.in	GC
Leo de Reuver*	Netherlands	TNO Defence, Security and Safety Lange Kleiweg 137, 2288GJ Rijswijk, Netherlands	+31 88 8661339 leo.dereuver@tno.nl	GC
Jijun Tang	China	AMMS 27 Taiping Road, Haidian District, Beijing, China	+8610 13810338946 tangjijun2012@163.com	GC
Dušan Trefilík	Czech Republic	NBC Defence institute Vita Nejedleho 1, Vyskov, Czech Republic	+420 777 255 274 dusan.trefilik@seznam.cz	MS
Ferdinand Visser	South Africa	PROTECHNIK P.O. Box 8855 Pretoria 0001, South Africa	+27 845173852 ferdiev@protechnik.co.za	GC Coordinator of the GC subgroup

- - - o - - -