



Verification Division  
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**NOTE BY THE TECHNICAL SECRETARIAT**

**REPORT OF THE FORTIETH MEETING OF THE VALIDATION GROUP  
FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE  
9 AND 10 SEPTEMBER 2014**

1. The Validation Group (hereinafter “the Group”) met on 9 and 10 September 2014 to discuss the evaluation of new analytical data for possible inclusion in the OPCW Central Analytical Database (OCAD) and to consider matters related to it. Mr James Riches of the United Kingdom of Great Britain and Northern Ireland acted as Chairperson of the meeting.
2. The Group was informed that Mr Mohammad Taghi Naseri (Islamic Republic of Iran) has been nominated to join the gas-chromatography (retention index) (GC(RI)) Subgroup.
3. The Group was informed that Mr Mozaffar Eslami has resigned.
4. The evaluators for the analytical techniques evaluated new data and data postponed from previous meetings 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 is responsible, are listed below:

GC(RI)	Mr Gary Mallard (Acting) (United States of America)
Mass spectrometry (MS)	Mr Sten-Åke Fredriksson (Sweden)
Infrared (IR) spectroscopy	Mr Armando Alcaraz (United States of America)
Nuclear magnetic resonance (NMR) spectroscopy	Mr Damian Magiera (Germany)

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

5. This report of the Group’s Fortieth Meeting presents the sets of validated analytical data of scheduled chemicals (see Annex 1) to be forwarded to the Director-General for appropriate action.
6. The Technical Secretariat (hereinafter “the Secretariat”) informed the Group that the data on scheduled chemicals validated by the Group at previous meetings had been



approved by the Executive Council (hereinafter “the Council”) at its Seventy-Sixth Session (EC-76/DEC.4, dated 10 July 2014).

7. The Group was informed that none of the laboratories that replied to a request for NMR data in electronic format was able to provide it. Mr Marc-Michael Blum from the OPCW Laboratory agreed to discuss and update, before the next meeting, the guidelines for the submission of NMR data to include electronic data submission.
8. The Group agreed that the removal of data entries 02-1-0017, 16-2-0067, 16-2-0190, 16-2-0191, 16-2-0192r, 16-2-0193, 16-2-0194r, 16-2-0195, 16-2-0196r, 16-2-0197r, 16-2-0199r, 16-2-0200, 16-2-0201, 16-2-0202r, 16-2-0203r, and 16-2-0204r should be recommended to the Council at its next meeting because superior data had been submitted and approved at later meetings of this Group.
9. The Group re-examined previously approved MS and GC(RI) data for three chemicals (see the report of the Thirty-Eight Meeting of the Group) and recommends that the data for them should not be added to the OCAD (V17) pending clarification and possible resubmission. The submissions in question are 28-2-0156 to 28-2-0158 and 28-4-0159 to 28-4-0161.
10. Proposed additions to the working list of chemicals relevant to investigations of alleged use, which is managed by the OPCW Laboratory, were distributed to the Group for comment. The Group agreed that the working list should be updated with all proposed additions.
11. As agreed at the Thirty-Ninth Meeting of the Group, four MS/MS data sets from three laboratories (Czech Republic, Sweden, and the United Kingdom of Great Britain and Northern Ireland) were distributed by the MS subgroup coordinator for discussion by the MS subgroup at this meeting. The MS subgroup considered the data and agreed on a suitable electronic format for the submission and collation of the data. It was agreed that these data sets would be reviewed at the next meeting.
12. The Group discussed the possibility of including Raman spectroscopy data in the OCAD and requested data to further the discussions.
13. Some changes to the “Procedures for Evaluation of Data to Be Included in the OPCW Central Analytical Database” (S/969/2011, dated 2 November 2011) were recommended. Specifically, it was recommended that for GC(RI) data the term accuracy be replaced by standard deviation and data submitted to unit RI values and that MS data be submitted with a minimum ion intensity of 0.1%.
14. The Group was presented with a list of differences in chemical names between previous Group reports and those in the OCAD. The Group agreed to two minor name changes.
15. The use of a system to coordinate data evaluation across the subgroups was discussed by the Group. It was agreed that the use of a chemical ID number is useful for administrative and auditing purposes.
16. In a Note by the Secretariat concerning the declaration of riot control agents (RCAs) (S/1177/2014, dated 1 May 2014), the Scientific Advisory Board advised the

Director-General of a number of RCAs that are not currently on the OCAD. The Group was provided with a list of these chemicals and requested to consider the submission of data for these compounds.

17. MS, GC(RI), and IR data are available for the next meeting. Available data from all analytical techniques will be sent to the Group at least six weeks before its next scheduled meeting.
18. The next meeting is scheduled to take place on 24 and 25 March 2015. The evaluators agreed to send their written evaluation reports to the appointed coordinators no later than 10 March 2015. The evaluators have agreed to come to the meeting prepared to finalise the evaluation of the analytical data referred to in the previous paragraph.
19. Annex 2 to this report lists the evaluators.

Annexes:

- Annex 1: Lists of Approved Data Recommended for Inclusion in the OPCW Central Analytical Database
- Annex 2: List of Members of the Validation Group

## Annex 1

**LISTS OF APPROVED DATA RECOMMENDED FOR INCLUSION  
IN THE OPCW CENTRAL ANALYTICAL DATABASE**

Note: In the last column of the tables that follow, “A” means “accepted”; “B”, “accepted subject to minor corrections”.

**TABLE 1: LIST OF APPROVED MS DATA OF SCHEDULED CHEMICALS**

<b>OPCW Code</b>	<b>Chemical Name</b>	<b>Schedule</b>	<b>Decision</b>
16-2-0205a	1,2-Dimethylpropyl propyl methylphosphonate	2.B.04	A
16-2-0205b	1,2-Dimethylpropyl propyl methylphosphonate	2.B.04	A
16-2-0206a	1,2-Dimethylpropyl propyl ethylphosphonate	2.B.04	A
16-2-0206b	1,2-Dimethylpropyl propyl ethylphosphonate	2.B.04	A
16-2-0207a	1,2-Dimethylpropyl propyl propylphosphonate	2.B.04	A
16-2-0207b	1,2-Dimethylpropyl propyl propylphosphonate	2.B.04	A
16-2-0208	2-Ethoxy-1-methylethyl methyl methylphosphonate	2.B.04	A
16-2-0209a	2-Ethoxy-1-methylethyl methyl ethylphosphonate	2.B.04	A
16-2-0209b	2-Ethoxy-1-methylethyl methyl ethylphosphonate	2.B.04	A
16-2-0210a	2-Ethoxy-1-methylethyl methyl propylphosphonate	2.B.04	A
16-2-0210b	2-Ethoxy-1-methylethyl methyl propylphosphonate	2.B.04	A
16-2-0211a	2-Ethoxy-1-methylethyl ethyl methylphosphonate	2.B.04	A
16-2-0211b	2-Ethoxy-1-methylethyl ethyl methylphosphonate	2.B.04	A
16-2-0212	2-Ethoxy-1-methylethyl ethyl ethylphosphonate	2.B.04	A
16-2-0213a	2-Ethoxy-1-methylethyl ethyl propylphosphonate	2.B.04	A
16-2-0213b	2-Ethoxy-1-methylethyl ethyl propylphosphonate	2.B.04	A
16-2-0214a	2-Ethoxy-1-methylethyl isopropyl methylphosphonate	2.B.04	A
16-2-0214b	2-Ethoxy-1-methylethyl isopropyl methylphosphonate	2.B.04	A
16-2-0215	2-Ethoxy-1-methylethyl isopropyl ethylphosphonate	2.B.04	A
16-2-0216	2-Ethoxy-1-methylethyl isopropyl propylphosphonate	2.B.04	A
16-2-0217a	2-Ethoxy-1-methylethyl propyl methylphosphonate	2.B.04	A
16-2-0217b	2-Ethoxy-1-methylethyl propyl methylphosphonate	2.B.04	A
16-2-0218a	2-Ethoxy-1-methylethyl propyl ethylphosphonate	2.B.04	A
16-2-0218b	2-Ethoxy-1-methylethyl propyl ethylphosphonate	2.B.04	A
16-2-0219a	2-Ethoxy-1-methylethyl propyl propylphosphonate	2.B.04	A
16-2-0219b	2-Ethoxy-1-methylethyl propyl propylphosphonate	2.B.04	A
16-2-0220a	Bis(2-ethoxy-1-methylethyl) methylphosphonate	2.B.04	B
16-2-0220b	Bis(2-ethoxy-1-methylethyl) methylphosphonate	2.B.04	B
16-2-0220c	Bis(2-ethoxy-1-methylethyl) methylphosphonate	2.B.04	B
16-2-0221a	Bis(2-ethoxy-1-methylethyl) ethylphosphonate	2.B.04	B
16-2-0221b	Bis(2-ethoxy-1-methylethyl) ethylphosphonate	2.B.04	B
16-2-0221c	Bis(2-ethoxy-1-methylethyl) ethylphosphonate	2.B.04	B
16-2-0222a	Bis(2-ethoxy-1-methylethyl) propylphosphonate	2.B.04	B
16-2-0222b	Bis(2-ethoxy-1-methylethyl) propylphosphonate	2.B.04	B
16-2-0222c	Bis(2-ethoxy-1-methylethyl) propylphosphonate	2.B.04	B
16-2-0223	2-Isopropoxyethyl methyl methylphosphonate	2.B.04	A
16-2-0224	2-Isopropoxyethyl methyl ethylphosphonate	2.B.04	A

<b>OPCW Code</b>	<b>Chemical Name</b>	<b>Schedule</b>	<b>Decision</b>
16-2-0225	2-Isopropoxyethyl methyl propylphosphonate	2.B.04	A
16-2-0226	Ethyl 2-isopropoxyethyl methylphosphonate	2.B.04	B
16-2-0227	Ethyl 2-isopropoxyethyl ethylphosphonate	2.B.04	B
16-2-0229	2-Isopropoxyethyl isopropyl methylphosphonate	2.B.04	A
16-2-0230	2-Isopropoxyethyl isopropyl ethylphosphonate	2.B.04	A
16-2-0231	2-Isopropoxyethyl isopropyl propylphosphonate	2.B.04	A
16-2-0232	2-Isopropoxyethyl propyl methylphosphonate	2.B.04	A
16-2-0233	2-Isopropoxyethyl propyl ethylphosphonate	2.B.04	A
16-2-0234	2-Isopropoxyethyl propyl propylphosphonate	2.B.04	A
16-2-0235	Bis(2-isopropoxyethyl) methylphosphonate	2.B.04	A
16-2-0236	Bis(2-isopropoxyethyl) ethylphosphonate	2.B.04	A
16-2-0237	Bis(2-isopropoxyethyl) propylphosphonate	2.B.04	A
16-2-0067r	Isobutyl propyl isopropylphosphonate	2.B.04	A

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

Note: A “1” under the “Column” heading of GC(RI) data 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
16-4-0239	1,2-Dimethylpropyl propyl methylphosphonate	2.B.04	1	1296	1304		A
16-4-0240	1,2-Dimethylpropyl propyl ethylphosphonate	2.B.04	1	1378	1387		A
16-4-0241	1,2-Dimethylpropyl propyl propylphosphonate	2.B.04	1	1449	1455		A
16-4-0242	2-Ethoxy-1-methylethyl methyl methylphosphonate	2.B.04	1	1242			A
16-4-0243	2-Ethoxy-1-methylethyl methyl ethylphosphonate	2.B.04	1	1319	1322		A
16-4-0244	2-Ethoxy-1-methylethyl methyl propylphosphonate	2.B.04	1	1393	1399		A
16-4-0245	2-Ethoxy-1-methylethyl ethyl methylphosphonate	2.B.04	1	1295	1298		A
16-4-0246	2-Ethoxy-1-methylethyl ethyl ethylphosphonate	2.B.04	1	1376			A
16-4-0247	2-Ethoxy-1-methylethyl ethyl propylphosphonate	2.B.04	1	1447	1450		A
16-4-0248	2-Ethoxy-1-methylethyl isopropyl methylphosphonate	2.B.04	1	1322	1328		A
16-4-0249	2-Ethoxy-1-methylethyl isopropyl ethylphosphonate	2.B.04	1	1396			A
16-4-0250	2-Ethoxy-1-methylethyl isopropyl propylphosphonate	2.B.04	1	1467			A
16-4-0251	2-Ethoxy-1-methylethyl propyl methylphosphonate	2.B.04	1	1383	1390		A
16-4-0252	2-Ethoxy-1-methylethyl propyl ethylphosphonate	2.B.04	1	1461	1465		A
16-4-0253	2-Ethoxy-1-methylethyl propyl propylphosphonate	2.B.04	1	1535	1537		A
16-4-0254	Bis(2-ethoxy-1-methylethyl) methylphosphonate	2.B.04	1	1543	1556	1565	B
16-4-0255	Bis(2-ethoxy-1-methylethyl) ethylphosphonate	2.B.04	1	1613	1623	1631	B
16-4-0256	Bis(2-ethoxy-1-methylethyl) propylphosphonate	2.B.04	1	1682	1689	1692	B
16-4-0257	2-Isopropoxyethyl methyl methylphosphonate	2.B.04	1	1281			A
16-4-0258	2-Isopropoxyethyl methyl ethylphosphonate	2.B.04	1	1364			A
16-4-0259	2-Isopropoxyethyl methyl propylphosphonate	2.B.04	1	1446			A
16-4-0260	Ethyl 2-isopropoxyethyl methylphosphonate	2.B.04	1	1344			B
16-4-0261	Ethyl 2-isopropoxyethyl ethylphosphonate	2.B.04	1	1428			B
16-4-0262	Ethyl 2-isopropoxyethyl propylphosphonate	2.B.04	1	1499			B
16-4-0263	2-Isopropoxyethyl isopropyl methylphosphonate	2.B.04	1	1373			A
16-4-0264	2-Isopropoxyethyl isopropyl ethylphosphonate	2.B.04	1	1445			A
16-4-0265	2-Isopropoxyethyl isopropyl propylphosphonate	2.B.04	1	1518			A
16-4-0266	2-Isopropoxyethyl propyl methylphosphonate	2.B.04	1	1436			A
16-4-0267	2-Isopropoxyethyl propyl ethylphosphonate	2.B.04	1	1516			A

<b>OPCW Code</b>	<b>Chemical Name</b>	<b>Schedule</b>	<b>Column</b>	<b>RI(a)</b>	<b>RI(b)</b>	<b>RI(c)</b>	<b>Decision</b>
16-4-0268	2-Isopropoxyethyl propyl propylphosphonate	2.B.04	1	1578			A
16-4-0269	Bis(2-isopropoxyethyl) methylphosphonate	2.B.04	1	1640			A
16-4-0270	Bis(2-isopropoxyethyl) ethylphosphonate	2.B.04	1	1710			A
16-4-0271	Bis(2-isopropoxyethyl) propylphosphonate	2.B.04	1	1780			A

## Annex 2

LIST OF MEMBERS OF THE VALIDATION GROUP<sup>1</sup>

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<sup>1</sup> An asterisk (\*) indicates that the evaluator was present at this meeting of the Group; a double asterisk (\*\*) indicates that the evaluator provided an evaluation but was unable to attend.



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