



Verification Division
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NOTE BY THE TECHNICAL SECRETARIAT**REPORT OF THE THIRTY-NINTH MEETING OF THE VALIDATION GROUP
FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE
1 AND 2 APRIL 2014**

1. The Validation Group (hereinafter “the Group”) met on 1 and 2 April 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 James Jones (United Kingdom) and Mr Roberto Alvarez (Spain) have been accepted as new members.
3. The Group was informed that Mr Mike Salt has resigned.
4. The Group was informed that Mr Damian Magiera has been unanimously elected to coordinate the nuclear magnetic resonance (NMR) subgroup.
5. 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:

Gas chromatography (retention index) (GC(RI))	Mr Martin Söderström (Finland)
Mass spectrometry (MS)	Mr Sten-Åke Fredriksson (Sweden)
Infrared (IR) spectroscopy	Mr Armando Alcaraz (United States of America)
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.

6. This report of the Group’s Thirty-Ninth Meeting presents the sets of validated analytical data of scheduled chemicals and derivatives of scheduled chemicals (see Annex 1) to be forwarded to the Director-General for appropriate action.



7. The Group was informed that the latest versions of the OCAD (version 16) and the Validation Group Working Database have been released and are available to members of the Group.
8. The Group discussed electronic formats for the submission of NMR data and was made aware that software is available, at modest cost, which can convert data acquired on instruments from different manufacturers into a single format. The NMR subgroup, with support from Mr Marc-Michael Blum from the OPCW Laboratory, agreed to discuss and update the guidelines for submission of NMR data to include electronic data submission before the next meeting.
9. A list of chemicals proposed to be relevant to investigations of alleged use was collated by Mr Armando Alcaraz and distributed to the Group for comments. The list will be managed by the OPCW Laboratory for use by the Group members. The Group welcomes additions to this list.
10. The Group was informed of progress on the submission of MS/MS data. Three laboratories have now submitted MS/MS data. The MS subgroup coordinator agreed to distribute all three sets of data for discussion before the next meeting.
11. A proposal by the OPCW Laboratory for a system to coordinate data evaluation across the subgroups was discussed. The Group agreed to evaluate this approach and provide feedback. The proposal involves the presentation of a chemical ID number with each data submission, which will ensure that any change to chemical names proposed by any of the subgroups is captured in the tables produced by all evaluators.
12. Mr Mehran Babri pointed out a corrupted data file in the IR data for 04-1-0196v in the current version of the OCAD. This will be corrected in the next version of the OCAD.
13. 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 the next scheduled Group meeting.
14. The next meeting is scheduled to take place on 9 and 10 September 2014. The evaluators agreed to send their written evaluation reports to the appointed coordinators no later than 26 August 2014. The evaluators have agreed to come to the meeting prepared to finalise the evaluation of the analytical data referred to in the previous paragraph.
15. Annex 3 to this report lists the evaluators.

Annexes:

- Annex 1: Lists of Approved Data Recommended for Inclusion in the OPCW Central Analytical Database
- Annex 2: Lists of Approved Data for Chemicals Relevant to the Convention
- Annex 3: 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

OPCW Code	Chemical Name	Schedule	Decision
04-2-0464	3,5-Dimethylcyclohexyl S-2-diethylaminoethyl ethylphosphonothiolate	1.A.03	A
04-2-0515	1-Methylpentyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
04-2-0516	2-Methylpentyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
04-2-0518	1-Methylhexyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
04-2-0552	2-Ethylhexyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
04-2-0553	Nonyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
04-2-0554	1-Methyloctyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
04-2-0555	Decyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
04-2-0556	1-Methylnonyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	A
05-2-0178	3,5,5-Trimethylhexyl S-2-dimethylaminoethyl propylphosphonothiolate	1.A.03	A
07-2-2051	2-Diisopropylaminoethyl ethylphosphonofluoridate	2.B.04	A
08-2-0118	O-Methyl S-pentyl methylphosphonothiolate	2.B.04	A
14-2-0035	4-tert-Butylcyclohexyl S-2-dimethylaminoethyl methylphosphonothiolate	1.A.03	A
17-2-0371	2,4-Dimethylhexahydro-1,3,5,2,4-benzotrioxadiphosphopine-2,4-disulfide	2.B.04	A
17-2-0372	2,4-Dimethylhexahydro-1,5,3,2,4-benzodioxathiadiphosphopine-2,4-disulfide	2.B.04	A
17-2-0373	2,4-Diethylhexahydro-1,3,5,2,4-benzotrioxadiphosphopine-2,4-disulfide	2.B.04	A
17-2-0374	6-(2-Chloroethyl)-2-propyl-1,3,6,2-dioxazaphosphocane-2-sulfide	2.B.04	A
17-2-0375	6-(2-Chloroethyl)-2-ethyl-1,3,6,2-dioxazaphosphocane-2-sulfide	2.B.04	A
17-2-0376	6-(2-Chloroethyl)-2-methyl-1,3,6,2-dioxazaphosphocane-2-sulfide	2.B.04	A

OPCW Code	Chemical Name	Schedule	Decision
23-2-0001	2,4,6-Tripropyl-1,3,5,2,4,6-trioxatriphosphorinane- 2,4,6-trioxide	2.B.04	A
28-2-0050	Phenyl N,N-dimethyl-P-methylphosponamidate	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)	RI(d)	RI(e)	Decision
04-4-0277	Pentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2023					A
04-4-0278	2-Methylbutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	1971					A
04-4-0279	Ethyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	1758					A
04-4-0282	1-Methylbutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	1920					A
04-4-0284	1-Methylpentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2004					A
04-4-0287	1-Methylhexyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2096					A
04-4-0290	1-Methylheptyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2189					A
04-4-0322r	2,2-Dimethylpropyl S-2-diethylaminoethyl isopropylphosphonothiolate	1.A.03	1	1857					A
09-4-0028	Benzyl butyl methylphosphonate	2.B.04	1	1738					A
09-4-0029	Benzyl methylphosphonofluoridate	2.B.04	1	1318					A
09-4-0032	Bis(tert-butyldimethylsilyl) ethylphosphonate	2.B.04	1	1653					A
09-4-0033	Bis(tert-butyldimethylsilyl) isopropylphosphonate	2.B.04	1	1702					A
09-4-0034	Bis(tert-butyldimethylsilyl) methylphosphonate	2.B.04	1	1571					A
09-4-0035	Bis(tert-butyldimethylsilyl) propylphosphonate	2.B.04	1	1712					A
15-4-0047	3,3,5,5-Tetramethylcyclohexyl N,N-diethyl-P-ethylphosphonamidate	2.B.04	1	1869					A
15-4-0048	3-Methylpentyl N,N-diethyl-P,P'-dimethyldiphosphono-P-amidate	2.B.04	1	1971					A
15-4-0049	3-Methylpentyl N,N-diethyl-P-methylphosphonamidate	2.B.04	1	1569					A
15-4-0050	4-Methylcyclohexyl N,N-diethyl-P,P'-dimethyldiphosphono-P-amidate	2.B.04	1	2107	2112	2129	2130		A
15-4-0051	4-Methylcyclohexyl N,N-diethyl-P-ethylphosphonamidate	2.B.04	1	1758	1764	1771	1782		A
15-4-0052	4-Methylcyclohexyl N,N-diethyl-P-methylphosphonamidate	2.B.04	1	1684	1691	1700	1711		A

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	Decision
15-4-0056	N,N,N',N'-Tetraethyl-P,P'-diisopropylpyrophosphonic diamide	2.B.04	1	1993	2043				B
15-4-0057	N,N,N',N'-Tetraethyl-P-methylphosphonic diamide	2.B.04	1	1488					B
15-4-0058	N,N,N',N'-Tetraethyl-P,P'-diethylpyrophosphonic diamide	2.B.04	1	1958					B
15-4-0059	N,N,N',N'-Tetraethyl-P,P'-dimethylpyrophosphonic diamide	2.B.04	1	1818	1834				B
15-4-0060	N,N,N',N'-Tetraethyl-P-ethylphosphonic diamide	2.B.04	1	1561					B
15-4-0062	Cyclohexyl N,N-diethyl-P,P'-dimethyldiphosphono-P-amidate	2.B.04	1	2065	2069				A
15-4-0063	Cyclohexyl N,N-diethyl-P-methylphosphonamidate	2.B.04	1	1645					A
15-4-0074	Isobutyl N,N-diethyl-P-isopropylphosphonamidate	2.B.04	1	1479					A
15-4-0075	Isobutyl N,N-diethyl-P-methylphosphonamidate	2.B.04	1	1371					B
15-4-0077	Isopropyl N,N-diethyl-P-isopropylphosphonamidate	2.B.04	1	1362					A
15-4-0078	Isopropyl N,N-diethyl-P,P'-diisopropyldiphosphono-P-amidate	2.B.04	1	1817	1838				A
15-4-0079	N,N-Diethyl-P-isopropylphosphonamidic chloride	2.B.04	1	1358					A
15-4-0080	N,N-Diethyl-P-methylphosphonamidic chloride	2.B.04	1	1235					A
15-4-0082	Pinacolyl N,N-diethyl-P,P'-diethyldiphosphono-P-amidate	2.B.04	1	1975	1988	1988	2016		A
15-4-0083	Pinacolyl N,N-diethyl-P-methylphosphonamidate	2.B.04	1	1474					A
15-4-0084	Pinacolyl N,N-diethyl-P-ethylphosphonamidate	2.B.04	1	1547	1554				A
15-4-0085	sec-Butyl N,N-diethyl-P,P'-dimethyldiphosphono-P-amidate	2.B.04	1	1734	1744	1746	1754		A
15-4-0086	sec-Butyl N,N-diethyl-P-methylphosphonamidate	2.B.04	1	1351					B
17-4-0203	Dibutyl diisopropylpyrophosphonate	2.B.04	1	1937					A
17-4-0207	(5-Ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl methyl methylphosphonate	2.B.04	1	2068	2099				A
17-4-0208	Butyl (5-ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl methylphosphonate	2.B.04	1	2300	2314				A
17-4-0209	Bis[(5-ethyl-2-methyl-2-oxido-1,3,2-dioxaphosphinan-5-yl)methyl] methylphosphonate	2.B.04	1	3296	3298	3309			A
28-4-0016r	2,4-Dimethyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	1	1176	1191				A
28-4-0017	4-Ethyl-2-methyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	1	1265	1293				A

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	RI(c)	RI(d)	RI(e)	Decision
28-4-0018	2,4,5-Trimethyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	1	1210	1237	1283			A
28-4-0020r	2-Ethyl-4-methyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	1	1267	1287				A
28-4-0021r	2,4-Diethyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	1	1349	1376				A
28-4-0022	2-Ethyl-4,5-dimethyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	1	1296	1317	1356			A
28-4-0023	2,5-Diethyl-4-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	1	1665	1689	1708			A
28-4-0025r	4-Ethyl-2-propyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	1	1432	1460				A
28-4-0026	4,5-Dimethyl-2-propyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	1	1375	1397	1443			A
28-4-0027r	5-Ethyl-2,4-dipropyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	1	1736	1762	1781			A
28-4-0028r	2,4-Dimethyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	1	1199	1209				A
28-4-0029r	4-Ethyl-2-methyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	1	1284	1303				A
28-4-0032	2-Ethyl-4-methyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	1	1292	1305				A
28-4-0033r	2,4-Diethyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	1	1369	1388				A

TABLE 3: LIST OF APPROVED INFRARED DATA OF DERIVATIVES OF SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Associated Chemical Schedule	Decision
09-1-0013	N,N-Diisopropyl-N-(2-trimethylsilyloxyethyl)amine	DS	2.B.11	A
09-1-0015	N-Ethyl-N-methyl-N-(2-trimethylsilyloxyethyl)amine	DS	2.B.11	A
09-1-0016	N-Isopropyl-N-propyl-N-(2-trimethylsilyloxyethyl)amine	DS	2.B.11	A

Annex 2

LISTS OF APPROVED DATA FOR CHEMICALS RELEVANT TO THE CONVENTION

TABLE 1: LIST OF APPROVED DATA FOR DERIVATIVES OF SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Associated Chemical Schedule	Decision
17-2-0230	Bis(2-trifluoroacetoxyethyl)sulfide	DS	2.B.13	A
17-2-0236	Bis(2-heptafluorobutyryloxyethyl)sulfide	DS	2.B.13	A

TABLE 2: LIST OF APPROVED DATA FOR NON-SCHEDULED CHEMICALS RELEVANT TO THE CONVENTION

OPCW Code	Chemical Name	Schedule	Decision
08-2-0092	Dimethyl trimethylsilyl phosphate	NS	A
08-2-0094	Dimethyl tert-butyldimethylsilyl phosphate	NS	A
08-2-0097	tert-Butyldimethylsilyl N,N-diethylaminoethyl-2-sulfonate	NS	A
08-2-0098	tert-Butyldimethylsilyl N,N-diisopropylaminoethyl-2-sulfonate	NS	A
08-2-0099	tert-Butyldimethylsilyl N,N-dipropylaminoethyl-2-sulfonate	NS	A
08-2-0101	Trimethylsilyl N,N-diethylaminoethyl-2-sulfonate	NS	A
08-2-0102	Trimethylsilyl N,N-diisopropylaminoethyl-2-sulfonate	NS	A
08-2-0106	Methyl N,N-diisopropylaminoethyl-2-sulfonate	NS	A
08-2-0107	Methyl N,N-dipropylaminoethyl-2-sulfonate	NS	A
17-2-0095	2-Chloroethyl vinyl sulfoxide	NS	A
24-2-0047	2-Hydroxyethyl vinyl sulfone	NS	A

Annex 3

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