OPCW

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# REPORT OF THE TWENTIETH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 7- 8 DECEMBER 2004

1. The Validation Group (hereinafter the "Group") met for the twentieth time on 7 and 8 December 2004 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 Eric Wils of the Netherlands chaired the Meeting.

2. The evaluators for the analytical techniques evaluated new data and sent their written reports to the appointed coordinators. The names of the coordinators who were present at the meeting are listed hereunder, along with the techniques for which they are responsible:

   Gas chromatography (retention index) GC(RI): Mr Martin Söderström (Finland)
   Mass spectrometry (MS): Mr Edward White (United States of America)

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

3. The Group submitted the list of validated analytical data to the Director-General for appropriate action. These data include the MS data from laboratory 22, which have been resubmitted in the fall of 2004.

4. Some data on riot control agents were evaluated by the Group, which submitted a list to the Technical Secretariat (hereinafter the "Secretariat") for future action. The Group noted that the Secretariat had started a process of procuring data on riot control agents and unscheduled degradation products of scheduled chemicals. These data will be available for evaluation starting in 2005.

5. The results of the evaluation of the data from the Nineteenth Meeting of the Group were approved by the Executive Council (hereinafter "the Council") at its Thirty-Eighth Session in October 2004 (EC-38/2, dated 15 October 2004). The Secretariat will begin the process of authenticating these data. The Secretariat will also release the new version of the OCAD (hard-copy version 8 and electronic version 6) on a DVD in the beginning of 2005. It will contain all data approved by the Council up to its Thirty-Seventh Session. All work on the authentication

documents has been finalised by the Group. The new OCAD version will also include the latest version of the on-site database.

6. Chemical Abstracts Service (CAS) numbers for the chemicals in the OCAD have been checked by CAS. The CAS numbers suggested for the Schedule 1.A.4 chemicals 2-chlorovinyldichloroarsine (lewisite 1) and bis(2-chlorovinyl)chloroarsine (lewisite 2) differed from those given in the Convention. These new numbers have been assigned to the trans (or E) isomers. The Group recommended that the Secretariat not alter the CAS numbers for the two lewisite chemicals in the OCAD.

7. The Group was informed that the procedure for the removal of data from the OCAD, which the Group established at their Nineteenth Meeting, was not forwarded to the Council, and that the Council decision "Proposed Mechanism for Updating the OPCW Central Analytical Database" (EC-IV/DEC.2, dated 5 September 1997) also provides for the removal of data from the OCAD. The Group recommended that the process of re-evaluation, described in the proposed procedure for the removal of data from the OCAD, be inserted in a future version of the Secretariat's standard operating procedure on "the organisation of the OCAD and the extraction of data to on-site databases". The Group produced a list of data recommended for removal from the OCAD and forwarded this list to the Director-General for appropriate action.

8. The Group considered the issue of naming chiral compounds. The database does not contain spectral data on optical isomers, and the Group does not need to produce the naming of chiral compounds. The position of the Group is that optical isomers should be declared in the same way as the racemic mixture. The spelling of "sulphide" has been corrected to "sulfide". A new example has been added. The latest version of the naming rules appears in Annex 1 to this report.

9. The Secretariat indicated that it wants to improve access to the infrared (IR) data in the OCAD by installing an IR browser. Mr Steven Choquette (United States of America) is currently looking at various browsers and will report to the Group at a later stage.

10. The Group discussed the possibility of adding a chemical identifier to the chemical information on each compound in the OCAD, a possibility that may also have a bearing on the Secretariat's Handbook on Chemicals. Mr Gary Mallard (United States of America) gave a presentation on the subject. He told the Group that a IUPAC identifier could automatically be created from a chemical structure, and that all software for this process is available. The Group recommended that the Secretariat explore the possibility of incorporating the IUPAC chemical identifier into the OCAD.

11. The Group finalised its discussion of the significant differences between the GC(RI) values of some compounds measured on a DB5-MS column and those measured on SE-54 types of column. The correction to be made to the GC(RI) data (multiplication by a factor of 1.0087) corresponds with the data measured by the Secretariat on their column. The Group agreed that the original data on a DB5-MS column will be stored in the OCAD together with the corrected values. Furthermore, the type of column for all GC(RI) data in the OCAD needs to be tabulated alongside the data. The Group recommended that for the creation of the on-site database this factor should be applied

retrospectively to the data measured on a DB5-MS column. Starting from this Meeting the approved GC(RI) data will be accompanied by the following note: "Due to differences in the brands of GC columns available on the market, a small correction factor must be applied to the GC(RI) values in some columns to reflect these differences. This applies in particular to the values used in the on-site database."

12. The Group concurred with Secretariat's practice of including multiple mass spectra in the on-site database when the span between the lowest and the highest values of the GC(RI) indices of isomers exceeds 20 units. An average GC(RI) value will be incorporated when the span is 20 units or less.

13. The Group again discussed the gaps in the OCAD, in particular those between the MS and the GC(RI) data. The Group recommended that, because these two types of data are used in the on-site database, these internal gaps should be filled as a matter of priority. Mr Gary Mallard agreed to produce a consolidated list of gaps between the MS and the GC(RI) data to be considered at the Twenty-First Meeting of the Group.

14. There were no new analytical data available for evaluation. The Secretariat will distribute any new data once available. The Group decided that for the Twenty-First Meeting of the Group the previously postponed mass spectra: 04-2-0110, 04-2-0115, 04-2-0116, 04-2-0118, 04-2-0120, 04-2-0161, 04-2-0162, 04-2-0259, 05-2-0154, 05-2-0178, 05-2-0188, 05-2-0194, 06-2-0382, 07-2-0380, 07-2-0383, 07-2-0384, 07-2-0389, 07-2-0542, 07-2-0543, 07-2-0580, 07-2-0591, 07-2-0800, 07-2-0889, 07-2-0890, 07-2-1800, 07-2-1834, 07-2-1930, 07-2-1931, 07-2-2051, 07-2-2164, 07-2-2164r, 07-2-2165, 07-2-2167, 07-2-2170r, 07-2-2338, 08-2-0051, 08-2-0061, 08-2-0065, 16-2-0016, 16-2-0022, 16-2-0023, 18-2-0034, 18-2-0036, 18-2-0040, 18-2-0042, 18-2-0044, 18-2-0054, 18-2-0056, 18-2-0058, 18-2-0059, 18-2-0062, 18-2-0063, 18-2-0064, 18-2-0069, 18-2-0070, 18-2-0073, 18-2-0076, 18-2-0077, 18-2-0080, 18-2-0081, 18-2-0082, 21-2-0004, 21-2-0004r, 21-2-0005, 21-2-0005r, and 22-2-0001 will be re-evaluated. Additionnally, the resubmitted GC(RI) data 19-4-0007r, 19-4-0009r, 19-4-0010r, 19-4-0013r, 19-4-0014r, 19-4-0017r and 19-4-0018r and all postponed GC(RI) data will be reconsidered.

15. The Group appointed evaluators for the analytical techniques. Annex 2 to this report lists the evaluators by analytical technique. The evaluators agreed to send their written evaluation reports to the appointed coordinators no later than 1 June 2005. The coordinators agreed to send evaluation summary reports to the Group's Chairman and to the evaluators no later than 14 June 2005, so that the reports can be discussed at the Group's next meeting, which is scheduled for 21 and 22 June 2005. The evaluators agreed to come to that meeting prepared to finalise the evaluation of the analytical data referred to in paragraph 14.

Annexes:

Annex 1: Rules for Naming Compounds in the OPCW Central Analytical Database
Annex 2: List of Evaluators by Analytical Technique

## Annex 1

## RULES FOR NAMING COMPOUNDS IN THE OPCW CENTRAL ANALYTICAL DATABASE

1. In general, the name (spelling, punctuation, spaces, and so on) is to be based on the name given in the Convention's Annex on Chemicals.

2. The following additional rules should be followed in cases where the information in the Schedules of Chemicals is insufficient to designate only one name.

2.1 The name is to be capitalised the only exceptions being the structural and stereo-descriptors, sec-, tert-, cis-, and trans-. In cases where a structural or stereo-descriptor prefixes a name, the name is to be capitalised.

2.2 The trivial names for the following radicals are to be used:
Saturated branched: Isopropyl, Isobutyl, sec-Butyl, tert-Butyl.
Pinacolyl is to be used instead of 1,2,2-trimethylpropyl.
However, pinacolyl alcohol should be referred to as 3,3-dimethyl-2-butanol.
Unsaturated: Vinyl, Allyl, Isopropenyl.

2.3 When a compound has several substituents, they are to be listed in alphabetical order, irrespective of the presence of N-, O-, or S- prefixes, and of the descriptors, sec-, tert-, cis- or trans-; but see rule 2.5 below.

2.4 The radicals isobutyl, isopropenyl, and isopropyl are considered to be one entity and are to be listed in alphabetical order starting from 'iso'.

2.5 The substituents in Schedule 1.A.03 and 1.B.10 compounds are to be listed in the order 'alkyl 2-dialkylaminoethyl' in line with the names given in the Convention, but constituting an exception to rule 2.3. The same exception applies to Schedule 2.B.4 compounds containing the 'alkyl 2-dialkylaminoethyl' moieties.

2.6 Parentheses are to be used in the following cases: around prefixes defining substituted substituents; after the numerical multiplicative prefixes 'bis', 'tris', and so on; around simple substituent prefixes to separate locants of the same type referring to different structural elements; and to avoid ambiguity.

2.7 For radicals with a branching structure, the name should be derived from the longest continuous chain starting (position 1) at the conjunction with the parent structure. Examples:

(a) The methylphosphonofluoridate made using 5-methyl-3-hexanol is 1-Ethyl-3-methylbutyl methylphosphonofluoridate.

(b) The name 1-ethyl-2-methylpropyl is to be used instead of 1-isopropylpropyl.

2.8 Thiolate and thionate are to be differentiated according to whether the S-atom is single- or double-bonded to the phosphorus atom.

2.9 For phosphorous compounds containing two S-sec-butyl or S-tert-butyl groups linked to phosphorus, the name has to be started with bis(S-sec-butyl) or bis(S-tert-butyl).

2.10 The name is to be as short as possible, and unnecessary characters such as the following are to be left out:

(a) the n- in n-alkyl;

(b) the 1- before 1-alkyl in case of a normal alkyl chain;

(c) the O in O-Alkyl alkylphosphonohalidates;

(d) the O in O-Alkyl S-2-dialkylaminoethyl alkylphosphonothiolates belonging to Schedule 1.A.03; and

(e) unnecessary brackets and parentheses.

2.11 Hydrochloride salts of schedule 2.B.10, 2.B.11 and 2.B.12 chemicals are to be named as free amines with the addition of hydrochloride.

2.12 Substituents to an aromatic ring are to be numbered numerically.

3. These rules are illustrated below by examples of scheduled compounds and by derivatives associated with the scheduled compounds.

**Examples of Names of Scheduled Compounds**

| Schedule | Name |
|---|---|
| 1.A.01 | Alkyl alkylphosphonofluoridate |
| 1.A.02 | Alkyl N,N-dialkylphosphoramidocyanidate |
| 1.A.03 | Alkyl S-2-dialkylaminoethyl alkylphosphonothiolate |
| | Alkyl S-trialkylammoniumethyl alkylphosphonothiolate halide (i.e. chloride, iodide) |
| 1.A.04 | 2-Chloroethylchloromethylsulfide |
| | Bis(2-chloroethyl)sulfide |
| | Bis(2-chloroethylthio)methane |
| | 1,2-Bis(2-chloroethylthio)ethane |
| | 1,3-Bis(2-chloroethylthio)propane |
| | 1,4-Bis(2-chloroethylthio)butane |
| | 1,5-Bis(2-chloroethylthio)pentane |
| | Bis(2-chloroethylthiomethyl)ether |
| | Bis(2-chloroethylthioethyl)ether |
| 1.A.05 | 2-Chlorovinyldichloroarsine |
| | Bis(2-chlorovinyl)chloroarsine |
| | Tris(2-chlorovinyl)arsine |
| 1.A.06 | Bis(2-chloroethyl)ethylamine |
| | Bis(2-chloroethyl)methylamine |
| | Tris(2-chloroethyl)amine |
| 1.A.07 | Saxitoxin |
| 1.A.08 | Ricin |

| Schedule | Name |
|---|---|
| 1.B.09 | Alkylphosphonic difluoride |
| 1.B.10 | Alkyl 2-dialkylaminoethyl alkylphosphonite |
| 1.B.11 | Isopropyl methylphosphonochloridate |
| 1.B.12 | Pinacolyl methylphosphonochloridate |
| 2.A.01 | O,O-Diethyl S-2-diethylaminoethyl phosphorothiolate |
| 2.A.02 | 1,1,3,3,3-Pentafluoro-2-(trifluoromethyl)-1-propene |
| 2.A.03 | 3-Quinuclidinyl benzilate |
| 2.B.04 | To avoid any confusion the O and S groups, should be indicated in esters when sulfur is present. |
| | Examples: |
| | Methylphosphonothioic acid [$(CH_3P(=S)(OH)_2$] |
| | O-Ethyl methylphosphonothionate [$(C_2H_5O)P(=S)(CH_3)(OH)$] |
| | O,O-Diethyl methylphosphonothionate [$(C_2H_5O)_2P(=S)(CH_3)$] |
| | O-Propyl O-trimethylsilyl propylphosphonothionate |
| | O-Ethyl S-ethyl methylphosphonothiolate [$(C_2H_5O)P(=O)(CH_3)(SC_2H_5)$] |
| | S-Ethyl O-methyl methylphosphonothiolate |
| | O-Ethyl S-2-methylthioethyl methylphosphonothiolate |
| | O-Ethyl S-ethyl methylphosphonothiolothionate [$(C_2H_5O)P(=S)(CH_3)(SC_2H_5)$] |
| | Bis(S-sec-butyl) methylphosphonodithiolate |
| | O-Ethyl methylphosphonothionochloridate [$(C_2H_5O)P(=S)(CH_3)(Cl)$] |
| | Methylphosphonous dichloride ($CH_3P\text{-}Cl_2$) |
| | Methylphosphonic dichloride [$(CH_3P(=O)\text{-}Cl_2)$] |
| | Methylphosphonothioic dichloride [$(CH_3P(=S)\text{-}Cl_2)$] |
| | Dimethyl methylphosphonate |
| | Bis(1,2-dimethylpropyl) methylphosphonate |
| | Benzyl 1,2-dimethylpropyl ethylphosphonate |
| | Methyl methylphosphonate instead of methyl methylphosphonic acid |
| | Methylphosphonic acid |
| | Isobutyl methylphosphonochloridate |
| | Isopropyl methylphosphonoazidate |
| | 2-Diisopropylaminoethyl methylphosphinate [$(i\text{-}C_3H_7)_2N\text{-}CH_2CH_2\text{-}O\text{-}P(=O)(H)(CH_3)$] |
| | Methyl 2-diethylaminoethyl methylphosphonate |
| | O-Ethyl S-2-dibutylaminoethyl methylphosphonothiolate |
| | Bis(S-2-diethylaminoethyl) methylphosphonodithiolate |
| | O-Ethyl S-3-dimethylaminopropyl methylphosphonothiolate |
| | Diethyl methylphosphonite [$(C_2H_5O)_2P(CH_3)$] |
| | Dicyclohexyl dimethylpyrophosphonate [$(C_6H_{11}O)(CH_3)P(=O)\text{-}O\text{-}P(=O)(CH_3)(C_6H_{11}O)$] |
| | Dicyclohexyl dimethylpyrophosphonodithionate [$(C_6H_{11}O)(CH_3)P(=S)\text{-}O\text{-}P(=S)(CH_3)(C_6H_{11}O)$] |
| 2.B.05 | N,N-Dialkylphosphoramidic dihalide |
| 2.B.06 | Dialkyl N,N-dialkylphosphoramidate |
| | Dimethyl N-ethyl-N-methylphosphoramidate |

| Schedule | Name |
|---|---|
| 2.B.07 | Arsenic trichloride |
| 2.B.08 | 2,2-Diphenyl-2-hydroxyacetic acid |
| 2.B.09 | 3-Quinuclidinol |
| 2.B.10 | 2-(N,N-Dialkylamino)ethylchloride |
| | 2-(N-Ethyl-N-methylamino)ethylchloride |
| 2.B.11 | 2-(N,N-Dialkylamino)ethanol |
| | 2-(N-Ethyl-N-methylamino)ethanol |
| 2.B.12 | 2-(N,N-Dialkylamino)ethanethiol |
| | 2-(N-Ethyl-N-methylamino)ethanethiol |
| 2.B.13 | Bis(2-hydroxyethyl)sulfide |
| 2.B.14 | 3,3-Dimethyl-2-butanol |
| 3.A.01 | Carbonyl dichloride |
| 3.A.02 | Cyanogen chloride |
| 3.A.03 | Hydrogen cyanide |
| 3.A.04 | Trichloronitromethane |
| 3.B.05 | Phosphorous oxychloride |
| 3.B.06 | Phosphorous trichloride |
| 3.B.07 | Phosphorous pentachloride |
| 3.B.08 | Trimethyl phosphate |
| 3.B.09 | Triethyl phosphate |
| 3.B.10 | Dimethyl phosphate |
| 3.B.11 | Diethyl phosphate |
| 3.B.12 | Sulfur monochloride |
| 3.B.13 | Sulfur dichloride |
| 3.B.14 | Thionyl chloride |
| 3.B.15 | Ethyldiethanolamine |
| 3.B.16 | Methyldiethanolamine |
| 3.B.17 | Triethanolamine |

**Examples of Names for Derivatives (D.S.)**

| D.S. | Type of Name |
|---|---|
| 1.A.05 | 2-(2-Chlorovinyl)-5-methyl-1,3,2-benzodithiarsole |
| 2.B.08 | Bis(trimethylsilyl)benzilate |
| 2.B.09 | 3-Quinuclidinyl trimethylsilyl ether |
| 2.B.07 | 2-Chloro-5-methyl-1,3,2-benzodithiarsole |
| 2.B.11 | N,N-Dialkyl-N-(2-trimethylsilyloxyethyl)amine |
| | N,N-Dialkyl-N-(2-tert-butyldimethylsilyloxyethyl)amine |
| 2.B.12 | N,N-Dialkyl-N-(2-trimethylsilylthioethyl)amine |
| 2.B.13 | Bis(2-trimethylsilyloxyethyl)sulphide |
| 3.B.15 | Bis(2-trimethylsilyloxyethyl)ethylamine |
| 3.B.16 | Bis(2-trimethylsilyloxyethyl)methylamine |
| 3.B.17 | Tris(2-trimethylsilyloxyethyl)amine |
| | Tris(2-tert-butyldimethylsilyloxyethyl)amine |

## Annex 2

## LIST OF EVALUATORS BY ANALYTICAL TECHNIQUE

**IR Evaluators**

| Name | Country | Address | Phone/Fax/E-Mail | Speciality |
|---|---|---|---|---|
| Colin Pottage | United Kingdom | DSTL, Porton Down<br>Salisbury, Wilts<br>SP4 0JQ<br>UK | +44 1980 613397<br>+44 1980 613822<br>cpottage@dstl.gov.uk | **IR Co-ordinator,** NMR |
| Martin Söderström | Finland | VERIFIN<br>P.O. Box 55<br>00014 University of Helsinki<br>Finland | +358-9-19150442<br>+358-9-19150437<br>martin.soderstrom@helsinki.fi | GC, IR |
| Stefan Kremer | Germany | WIS 29623 Munster, Germany | 0049-5192-136-433<br>0049-5192-136-355<br>stefankremer@bwb.org | IR |
| Steven Choquette | United States of America | NIST<br>100 Bureau Drive<br>Stop 8394<br>Gaithersburg, MD<br>20899-8394 USA | +1 301-975-3096<br>+1 301-977-0587<br>steven.choquette@nist.gov | IR |
| Vladimir Podborsky | The Czech Republic | MTIP Brno, Veslarskâ 230<br>P.O. Box 547<br>602 00 BRNO Czech Republic | +420-5-41182629<br>+420-5-41183152<br>podborsky@email.cz | IR |
| Armando Alcaraz | United States of America | Lawrence Livermore National Laboratory, University of California, Forensic Science Center, P.O. Box 808, L-178, Livermore, CA 94551<br>USA | +1-925 423-6889<br>+1-925 423-9014<br>Alcaraz1@llnl.gov | GC, IR |
| Bedrich Uchytil | Czech Republic | Institute for Protection of Population<br>Laboratory<br>Korunni 2<br>25168 Kamenice<br>Czech Republic | +420-323-673052<br>+420-323-673054<br>sscokamenice@iol.cz | GC, IR |

**MS Evaluators**

| Name | Country | Address | Phone/Fax/E-Mail | Speciality |
|---|---|---|---|---|
| Edward White* | United States of America | NIST<br>100 Bureau Drive<br>Stop 8392<br>Gaithersburg, MD<br>20899-8392 USA | +1 301-975-3101<br>+1 301-977-0685<br>edward.white@nist.gov | **MS Co-ordinator** |
| Vesa Häkkinen* | Finland | VERIFIN<br>P.O. Box 55<br>00014 University of Helsinki<br>Finland | +358-9-19150439<br>+358-9-19150437<br>vesa.hakkinen@helsinki.fi | MS |
| Jirí Cermak | Czech Republic | Research Institute for Organic Syntheses<br>53218 Pardubice<br>Czech Republic | +420 466 822 351<br>+420 466 822 978<br>jiri.cermak@vuosas.cz | MS |
| David Brian Cooper* | United Kingdom | DSTL, Porton Down<br>Salisbury, Wilts<br>SP4 0JQ | +44 1980 613599<br>+44 1980 613822<br>dbcooper@dstl.gov.uk | MS |
| Danian Xu* | China | Research Institute of Chemical Defence<br>Laboratory of Analytical Chemistry<br>P.O. Box 1044<br>102205 Beijing, China | +86 10 69760259<br>+86 10 69760254<br>xu600@263.net | MS |
| Shigeyuki Hanaoka* | Japan | Chemicals Evaluation and Research Institute, 1600, Shimo-Takano, Sugito-machi, Kitakatsushika-gun, Saitama 345-0043, Japan | +81-480 37 2601<br>+81-480 37 2521<br>hanaoka-shigeyuki@ceri.jp | MS |
| Luis Ramalho* | Portugal | Instituto Nacional De Engenharia E Tecnologia Industrial (INETI), Estrada Paco Lumiar Lisbon, Portugal | +351 21 7165141<br>+351 21 7168100<br>luis.ramalho@ineti.pt | MS |

| Name | Country | Address | Phone/Fax/E-Mail | Speciality |
|---|---|---|---|---|
| Sten-Åke Fredriksson* | Sweden | FOI, Swedish Defence Research Agency Div. NBC Defence Cementvagen 20 SE-90182 Umea Sweden | +46 90 106712<br>fax: +46 90 106809<br>sten-ake.fredriksson@foi.se | MS |
| Mozaffar Eslami | Islamic Republic of Iran | Research Institute of Petroleum Industry (RIPI)<br>P.O. Box 18745-4391, Tehran, Iran | 98-21-5901021 to 51 (ext. 4817)<br>direct tel. -5901092<br>Fax: 98-21-6153397<br>Eslamim@nioc-ripi.org | MS |
| Hugh Gregg* | United States of America | Lawrence Livermore National Laboratory, University of California, P.O. Box 808, L-091, Livermore, CA 94551 | 1-925-423-7501<br>1-925-424-2626<br>Hugh-gregg@llnl.gov | MS |

* Present at the Twentieth Meeting of the Validation Group.

**NMR Evaluators**

| Name | Country | Address | Phone/Fax/E-Mail | Speciality |
|---|---|---|---|---|
| Luigi Abis | Italy | Polimeri Europa<br>Istituto Donegani<br>Via G.Fauser, 4<br>28100 Novara<br>Italy | +39 0321 447548<br>+39 0321 447425<br>luigi.abis@polimerieuropa.com | **NMR Co-ordinator** |
| Urs Meier | Switzer-land | Spiez Laboratory<br>CH-3700 Spiez<br>Switzerland | +41 332281713<br>+41 332281402<br>urs.meier@babs.admin.ch | NMR |
| Markku Mesilaakso | Finland | VERIFIN<br>P.O.Box 55<br>00014 University of Helsinki<br>Finland | 358-9-19150444<br>358-9-19150437<br>markku.mesilaakso@helsinki.fi | NMR |
| Lars-Gunnar Hammarström | Sweden | FOI, Swedish Defence Research Agency<br>Div. of NBC Defence<br>Cementvagen 20<br>SE-90182 Umea,<br>Sweden | 46-90-106600<br>46-90-106809<br>lgham@foi.se | NMR |
| Christine Albaret | France | Centre d'Etudes du Bouchet, BP3, 91710 Vert le Petit<br>France | 33-1-69908421<br>33-1-64935266 | NMR |
| Ian Holden | United Kingdom | DSTL, Porton Down<br>Salisbury<br>Wilts SP4 0JQ<br>UK | +44 1980 613770<br>+44 1980 613822<br>ihold@dstl.gov.uk | NMR |
| Robert Maxwell | United States of America | Lawrence Livermore National Laboratory, University of California, P.O. Box 808, L-091,<br>Livermore, CA 94551 | 1-925-423-4991<br>1-925-423-8772<br>Maxwell7@llnl.gov | NMR |
| Colin Pottage | United Kingdom | DSTL, Porton Down<br>Salisbury, Wilts<br>SP4 0JQ<br>UK | +44 1980 613397<br>+44 1980 613822<br>cpottage@dstl.gov.uk | IR Co-ordinator, NMR |

**GC (Retention Indices) Evaluators**

| Name | Country | Address | Phone/Fax/E-Mail | Speciality |
|---|---|---|---|---|
| Martin Söderström* | Finland | VERIFIN<br>P.O. Box 55<br>00014 University of Helsinki – Finland | +358-9-19150442<br>+358-9-19150437<br>martin.soderstrom@helsinki.fi | **GC Co-ordinator** IR |
| Gary Mallard* | United States of America | NIST<br>100 Bureau Drive<br>Stop 8380<br>Gaithersburg, MD<br>20899-8380 USA | +1 301-975-2564<br>+1 301-869-4020<br>gary.mallard@nist.gov | GC |
| Bedrich Uchytil* | Czech Republic | Institute for Protection of Population<br>Laboratory<br>Korunni 2<br>25168 Kamenice<br>Czech Republic | +420-323-673052<br>+420-323-673054<br>sscokamenice@iol.cz | GC, IR |
| Takeharu Wada* | Japan | Chemicals Evaluation and Research Institute, 1600, Shimo-Takano, Sugito-machi, Kitakatsushika-gun, Saitama 345-0043<br>Japan | +81 480 37 2601<br>+81 480 37 2521<br>wada-takeharu@ceri.jp | GC |
| Armando Alcaraz* | United States of America | Lawrence Livermore National Laboratory, University of California, Forensic Science Center, P.O. Box 808, L-178, Livermore, CA 94551 | +1 925 423 6889<br>+1 925 423 9014<br>Alcaraz1@llnl.gov | GC, IR |

* Present at the Twentieth Meeting of the Validation Group.

**Chairman**

| Name | Country | Address | Phone/Fax/E-Mail |
|---|---|---|---|
| Eric Wils | The Netherlands | TNO Prins Maurits Laboratory<br>P.O. Box 45<br>2280AA Rijswijk<br>The Netherlands | 31-15-2843494<br>31-15-2843963<br>wils@pml.tno.nl |

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