OPCW

Technical Secretariat

Verification Division
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REPORT OF THE TWENTY-FOURTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 14 AND 15 NOVEMBER 2006

1. The Validation Group (hereinafter "the Group") held its Twenty-Fourth Meeting on 14 and 15 November 2006 to discuss the evaluation of new analytical data for possible inclusion in the OPCW Central Analytical Database (OCAD), and to consider related matters. Mr Gary Mallard of the United States of America chaired 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 table below lists the names of the coordinators who were present at the Meeting, along with the technique for which each is responsible.

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

3. 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 those approved are technically valid.

4. At its Twenty-Third Meeting the Group forwarded lists of validated analytical data on scheduled chemicals for appropriate action to the Director-General, who had submitted them to the Executive Council (hereinafter "the Council") (EC-46/DG.1, dated 7 June 2006). The Group noted that the Council had approved the inclusion of these data in the OCAD (EC-46/DEC.5, dated 7 June 2006).

5. The Technical Secretariat (hereinafter "the Secretariat") announced that version 9 (electronic version 7) of the OCAD was ready for release.

6. The Group discussed naming rules for a number of derivatives and decomposition products of the lewisites (Schedule 1.A.05), and established names for specific unscheduled compounds. It decided to name the derivatives of chemicals containing arsenic, in those cases where butanethiol is used in the derivatisation, in accordance with the rules of the International Union of Pure and Applied Chemistry, as follows:

butyl bis(2-chlorovinyl)arsinothiolite, dibutyl 2-chlorovinylarsonodithiolite, and tributyl arsenotrithiolite.

7. A presentation on the OCAD Management System, a new database-management tool developed by the Secretariat, was given by Secretariat staff members Mr Valeri Timakov and Mr Daniele Parravicini. The System includes tools for tracking new submissions, edits to data to be incorporated into the OCAD, results of evaluations by the Group, decisions of the Council on data to be incorporated into the OCAD, and the data themselves. There was general agreement that the System would be a valuable tool for reducing the number of errors of various kinds that have occurred in the past. The Group requested that a read-only version of the database that contains all analytical data be made available to all evaluators for use in the evaluation process.

8. The Secretariat informed the Group that the Council was still considering the Secretariat's note on the implications of incorporating into the OCAD analytical data on riot-control agents and on unscheduled degradation products of scheduled chemicals. The Group requested that, while this issue remained under consideration, the Secretariat create a database, the Validation Group Working Database (VGWD), containing the analytical data on these chemicals, and that it distribute it to the members of the Group members and to the laboratories participating in OPCW Proficiency Tests. The Group decided that the VGWD should contain only data that have been approved as technically valid by the Group, and that it should be given the same status as the OCAD for the purpose of identifying chemicals in the Proficiency Tests.

9. The Group considered the comparison of the electronic and hard-copy versions of the infrared (IR) data in the OCAD, and made a number of recommendations, which it summarised and provided to the Secretariat. The Group recommended that in the future, to facilitate the evaluation of data, submitting laboratories indicate what other data, if any, they have submitted, based on different analytical techniques, for the same batch of samples.

10. At its Twenty-Second Meeting the Group forwarded a list of mass-spectrometry data to the Director-General for appropriate action (EC-44/DG.3, dated 13 February 2006). Among these data, whose inclusion in the OCAD the Council subsequently approved (EC-45/DEC.6, dated 18 May 2006), was one that the Group had inadvertently put on the list: (04-2-0374). The Group requested that the Secretariat take appropriate action to correct this error.

11. The following new mass-spectrometry data are available for re-evaluation:

    04-2-0374r, 04-2-0415, 04-2-0449, 17-2-0103, 24-2-0033, 24-2-0036, 24-2-0043 to 0045, 24-2-0047, 24-2-0052, 24-2-0054, 24-2-0069 to 0070, 24-2-0073 to 0074, and 24-2-0078

12. Additional nuclear-magnetic-resonance (NMR), MS, GC(RI), and IR data are expected.

13. The Group appointed evaluators for the analytical techniques. Annex 3 to this report lists the evaluators by technique. The evaluators agreed to send their written evaluation reports to the appointed coordinators no later than 13 March 2007. The coordinators agreed to send evaluation summary reports to the Chairperson of the Group and to the evaluators no later than 20 March 2007, so that the reports can be discussed at the Group's Twenty-Fifth Meeting, which is scheduled for 27 and 28 March 2007. The evaluators agreed to come to that Meeting prepared to finalise the evaluation of the analytical data referred to in paragraphs 11 and 12 above.

14. The Group welcomed Mrs Sally Swindlehurst of the United Kingdom of Great Britain and Northern Ireland, and Mr Devendra K. Dubey of India, as new evaluators for MS data.

15. The Group expressed its appreciation for the work of Mr David Cooper as an evaluator of MS data and an expert of long standing on the use of the Queen's English.

16. The Group also expressed its appreciation to its outgoing Chairperson, Mr Gary Mallard of the United States of America. The Group nominated Mr Hugh Gregg, also of the United States of America, as its new Chairperson, and forwarded this nomination to the Director-General for approval. Mr Colin Pottage of the United Kingdom of Great Britain and Northern Ireland will continue to serve as Vice-Chairperson of the Group.

Annexes:

Annex1: Lists of Approved Data Recommended for Inclusion in the OPCW Central Analytical Database
Annex 2: List of Technically Valid Data Not Recommended for Inclusion in the OPCW Central Analytical Database
Annex 3: Lists of Evaluators by Analytical Technique

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 in this and the next Annex, "A" means "accepted"; "B", "accepted subject to minor corrections". A "1" under the "Column" heading means an HP5 or an SE54 column.

TABLE 1: LIST OF APPROVED MS DATA

OPCW Code	Chemical Name	Schedule	Decision
08-2-0067	Diisopropyl N,N-dimethylphosphoramidate	2.B.06	A
08-2-0068	S-2-Ethylthioethyl N-ethyl-N-propyl propylphosphonamidothiolate	2.B.04	A
08-2-0069	S-2-Ethylthioethyl N,N-dipropyl ethylphosphonamidothiolate	2.B.04	A
08-2-0074	2-Ethylbutyl propyl ethylphosphonate	2.B.04	A
08-2-0075	Dimethyl ethylphosphonate	2.B.04	A
08-2-0076	O-Ethyl S-ethyl methylphosphonothiolate	2.B.04	A
08-2-0077	Cyclohexyl methyl methylphosphonate	2.B.04	A
08-2-0078	Methyl pinacolyl methylphosphonate	2.B.04	A
08-2-0079	Ethyl 1-methyl-2-methoxyethyl methylphosphonate	2.B.04	A
08-2-0080	Diethyl N,N-dimethylphosphoramidate	2.B.06	A
08-2-0081	Cyclohexyl ethylphosphonofluoridate	1.A.01	A
08-2-0083	Bis(2-methoxyethyl) ethylphosphonate	2.B.04	A
08-2-0084	Cyclohexyl 2-methoxyethyl ethylphosphonate	2.B.04	A
08-2-0085	Propyl S-2-diisopropylaminoethyl methylphosphonothiolate	1.A.03	A
09-2-0007	Butyl N,N-dimethylphosphoramidocyanidate	1.A.02	B
09-2-0008	Isobutyl N,N-dimethylphosphoramidocyanidate	1.A.02	B
09-2-0009	sec-Butyl N,N-dimethylphosphoramidocyanidate	1.A.02	B
09-2-0010	2-Ethylhexyl N,N-dimethylphosphoramidocyanidate	1.A.02	B
09-2-0012	Isopropyl N,N-diethylphosphoramidocyanidate	1.A.02	B
09-2-0016	2-Ethylhexyl N,N-diethylphosphoramidocyanidate	1.A.02	B
09-2-0017	Methyl N,N-dipropylphosphoramidocyanidate	1.A.02	B
09-2-0018	Propyl N,N-dipropylphosphoramidocyanidate	1.A.02	B
09-2-0019	Isopropyl N,N-dipropylphosphoramidocyanidate	1.A.02	B
09-2-0020	Butyl N,N-dipropylphosphoramidocyanidate	1.A.02	B
09-2-0021	Isobutyl N,N-dipropylphosphoramidocyanidate	1.A.02	B
09-2-0025	Butyl N,N-diisopropylphosphoramidocyanidate	1.A.02	B
09-2-0026	2-Ethylhexyl N,N-diisopropylphosphoramidocyanidate	1.A.02	B
09-2-0030	Ethyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0031	Butyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0032	Hexyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0033	Octyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0034	Isobutyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0035	Pentyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B

OPCW Code	Chemical Name	Schedule	Decision
09-2-0036	Isopropyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0037	Cyclohexyl N-ethyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0052	Methyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0053	Ethyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0054	Propyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0055	Butyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0056	Pentyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0058	Isopropyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0059	Isobutyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0060	1-Ethylpropyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0062	Cyclohexyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0063	sec-Butyl N-isopropyl-N-methylphosphoramidocyanidate	1.A.02	B
09-2-0067	Methyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0068	Ethyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0069	Propyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0070	Butyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0071	Pentyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0073	sec-Butyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0077	Isobutyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0078	Cyclohexyl N-ethyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0082	Methyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	B
09-2-0083	Ethyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	B
09-2-0084	Propyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	B
09-2-0085	Butyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	B
09-2-0088	Isopropyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	B
09-2-0091	Cyclohexyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	B
09-2-0093	3-Methylbutyl N-ethyl-N-isopropylphosphoramidocyanidate	1.A.02	B
09-2-0096	Methyl N-isopropyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0098	Propyl N-isopropyl-N-propylphosphoramidocyanidate	1.A.02	B
09-2-0102	Methyl N,N-diethylphosphoramidocyanidate	1.A.02	B

TABLE 2. LIST OF APPROVED MS DATA FOR DERIVATIVES OF SCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
17-2-0104	Dibutyl 2-chlorovinylarsonodithiolite	DS	B
17-2-0105	Tributyl arsenotrithiolite	DS	B

TABLE 3. LIST OF APPROVED GC(RI) DATA

OPCW Code	Chemical Name	Schedule	Column	A	B	Decision
17-4-0078	Butyl bis(2-chlorovinyl)arsinothiolite	DS	1	1697	1702	B

OPCW Code	Chemical Name	Schedule	Column	A	B	Decision
17-4-0080	Tributyl arsenotrithiolite	DS	1	2170		B

Tables 4 and 5 show data on compounds recommended by the Scientific Advisory Board in (see Annex 4 to SAB-IV/1, dated 6 February 2001).

TABLE 4. LIST OF APPROVED MS DATA FOR UNSCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
17-2-0096	2-Chloroethyl vinyl sulfone	NS	B
17-2-0098	Bis(2-chloroethyl)sulfone	NS	B
17-2-0099	Bis(2-chloroethyl)sulfoxide	NS	B
17-2-0101	Divinylsulfoxide	NS	B
17-2-0102	Divinylsulfone	NS	B

TABLE 5. LIST OF APPROVED GC(RI) DATA

OPCW Code	Chemical Name	Schedule	Column	A	Decision
17-4-0070	2-Chloroethyl vinyl sulfoxide	NS	1	1168	A
17-4-0071	2-Chloroethyl vinyl sulfone	NS	1	1212	A
17-4-0073	Bis(2-chloroethyl)sulfone	NS	1	1429	A
17-4-0074	Bis(2-chloroethyl)sulfoxide	NS	1	1452	A
17-4-0076	Divinylsulfoxide	NS	1	912	A
17-4-0077	Divinylsulfone	NS	1	1000	A

Annex 2

LIST OF TECHNICALLY VALID DATA NOT RECOMMENDED FOR INCLUSION IN THE OPCW CENTRAL ANALYTICAL DATABASE

TABLE 1: LIST OF TECHNICALLY VALID MS DATA ON UNSCHEDULED CHEMICALS

OPCW Code	Chemical Name	Schedule	Decision
08-2-0070	Diethyl N,N-dipropylphosphoramidodithiolate	NS	B
08-2-0071	Ethyl isobutyl N,N-dipropylphosphoramidodithiolate	NS	B
08-2-0072	Diisobutyl N,N-dipropylphosphoramidodithiolate	NS	B
08-2-0073	Dipropyl N,N-dipropylphosphoramidodithiolate	NS	B
08-2-0082	Ethyl 2-methoxyethyl N,N-dimethylphosphoramidate	NS	A
09-2-0050	2-Ethoxyethyl N-methyl-N-propylphosphoramidocyanidate	NS	B
09-2-0065	2-Ethoxyethyl N-isopropyl-N-methylphosphoramidocyanidate	NS	B
09-2-0072	2-Methoxyethyl N-ethyl-N-propylphosphoramidocyanidate	NS	B
09-2-0076	2-Ethoxyethyl N-ethyl-N-propylphosphoramidocyanidate	NS	B
09-2-0087	2-Methoxyethyl N-ethyl-N-isopropylphosphoramidocyanidate	NS	B
09-2-0095	2-Ethoxyethyl N-ethyl-N-isopropylphosphoramidocyanidate	NS	B
17-2-0094	2-Chloroethylthioethyl 2-chloroethyldithioethyl ether	NS	B
17-2-0097	Bis(2-chloroethyl)disulfide	NS	B
17-2-0100	Bis(2-chloroethyl)trisulfide	NS	B
17-2-0106	Methyl bis(2-chlorovinyl)arsinite	NS	B
17-2-0107	Dimethyl (2-chlorovinyl)arsonite	NS	B
17-2-0108	Trimethyl arsenite	NS	B
17-2-0109	Bis(trimethylsilyl) 2-chlorovinylarsonite	NS	B
17-2-0110	Trimethylsilyl bis(2-chlorovinyl)arsinite	NS	B
17-2-0111	2-(2-Chlorovinyl)-1,3,6,2-dioxathiarsocane	NS	B
17-2-0112	Tetrakis(2-chlorovinyl)diarsoxane	NS	B

TABLE 2. LIST OF TECHNICALLY VALID GC(RI) DATA

OPCW Code	Chemical Name	Schedule	Column	A	Decision
17-4-0069	2-Chloroethylthioethyl 2-chloroethyldithioethyl ether	NS	1	2241	A
17-4-0072	Bis(2-chloroethyl)disulfide	NS	1	1402	A
17-4-0075	Bis(2-chloroethyl)trisulfide	NS	1	1640	B

Annex 3

LISTS OF EVALUATORS BY ANALYTICAL TECHNIQUE[1]

TABLE 1: IR EVALUATORS

Name	Country	Address	Phone, Fax, and E-Mail	Specialty
Colin Pottage*	United Kingdom of Great Britain and Northern Ireland	Dstl, Porton Down Salisbury, Wilts SP4 0JQ United Kingdom of Great Britain and Northern Ireland	+44 1980 613397 +44 1980 613830 cpottage@dstl.gov.uk	**IR co-ordinator,** NMR
Martin Söderström*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki Finland	+358 9 19150438 +358 9 19150437 martin.soderstrom@helsinki.fi	GC, IR
Stefan Kremer*	Germany	WIS 29623 Munster Germany	+49 5192 136 433 +49 5192 136 355 stefankremer@bwb.org	IR
Steven Choquette	United States of America	NIST 100 Bureau Drive Stop 8312 Gaithersburg, MD 20899-8312 United States of America	+1 301 975 3096 +1 301 977 0587 steven.choquette@nist.gov	IR
Vladimir Podborsky	Czech Republic	MTIP Brno Veslarskâ 230 P.O. Box 547 602 00 BRNO Czech Republic	+420 5 4118 2629 +420 5 4118 3152 podborsky@email.cz	IR

[1] An asterisk indicates that the evaluator in question was present at the Twenty-Fourth Meeting of the Group.

Name	Country	Address	Phone, Fax, and E-Mail	Specialty
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 United States of America	+1 925 423 6889 +1 925 423 9014 Alcaraz1@llnl.gov	GC, IR
Bedrich Uchytil*	Czech Republic	Institute for Protection of the Population Laboratory Korunni 2 25168 Kamenice Czech Republic	+420 724 355 197 +420 323 673 054 bedrich.uchytil@ioolb.izscr.cz	GC, IR

TABLE 2: MS EVALUATORS

Name	Country	Address	Phone, Fax, and E-Mail	Specialty
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Vesa Häkkinen*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki Finland	+358 9 1915 0439 +358 9 1915 0437 vesa.hakkinen@helsinki.fi	MS
Jirí Cermak*	Czech Republic	Research Institute for Organic Syntheses 53218 Pardubice Czech Republic	+420 466 822 351 +420 466 822 978 jiri.cermak@vuos.com	MS

Name	Country	Address	Phone, Fax, and E-Mail	Specialty
David Brian Cooper*	United Kingdom of Great Britain and Northern Ireland	Dstl, Porton Down Salisbury, Wilts SP4 0JQ United Kingdom of Great Britain and Northern Ireland	+44 1980 613 599 +44 1980 613 822 dbcooper@dstl.gov.uk	MS
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Luis Ramalho	Portugal	Instituto Nacional de Engenharia e Tecnologia Industrial (INETI), Estrada Paco Lumiar Lisbon, Portugal	+351 21 716 5141 +351 21 716 8100 luis.ramalho@ineti.pt	MS
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Name	Country	Address	Phone, Fax, and E-Mail	Specialty
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Hugh Gregg*	United States of America	Lawrence Livermore National Laboratory University of California P.O. Box 808 L-091, Livermore CA 94551 United States of America	+1 925 423 7501 +1 925 424-2626 Hugh-gregg@llnl.gov	MS
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Sally Swindlehurst*	United Kingdom of Great Britain and Northern Ireland	Dstl, Porton Down Salisbury, Wilts SP4 0JQ United Kingdom of Great Britain and Northern Ireland	+44 1980 613 273 +44 1980 613 830 (fax) swilcox@dstl.gov.uk	MS
Marieke van Deursen	Netherlands	TNO Defence, Security and Safety P.O. Box 45 2280 AA Rijswijk Netherlands	+31 15 284 3831 +31 15 284 3963 (fax) M.van.Deursen@pml.tno.nl	MS

TABLE 3: NMR EVALUATORS

Name	Country	Address	Phone, Fax, and E-Mail	Speciality
Luigi Abis	Italy	Polimeri Europa Istituto Donegani Via G.Fauser, 4 28100 Novara Italy	+39 0321 447 548 +39 0321 447 425 luigi.abis@polimerieuropa.com	**NMR coordinator**
Urs Meier	Switzerland	Spiez Laboratory CH-3700 Spiez Switzerland	+41 33 228 1713 +41 33 228 1402 urs.meier@babs.admin.ch	NMR
Harri Koskela	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki Finland	+358 9 1915 0453 +358 9 1915 0437 harri.t.koskela@helsinki.fi	NMR
Lars-Gunnar Hammarström	Sweden	Swedish Defence Research Agency (FOI) Div. of NBC Defence Cementvagen 20 SE-90182 Umea Sweden	+46 90 106 600 +46 90 106 809 lgham@foi.se	NMR
Christine Albaret	France	Centre d'Etudes du Bouchet, BP3 91710 Vert le Petit France	+33 1 6990 8421 +33 1 6493 5266	NMR
Ian Holden	United Kingdom of Great Britain and Northern Ireland	Dstl, Porton Down Salisbury Wilts SP4 0JQ United Kingdom of Great Britain and Northern Ireland	+44 1980 613 770 +44 1980 613 822 ihold@dstl.gov.uk	NMR

Robert Maxwell	United States of America	Lawrence Livermore National Laboratory, University of California, P.O. Box 808, L-091, Livermore CA 94551 United States of America	+1 925 423 4991 +1 925 423 8772 Maxwell7@llnl.gov	NMR

TABLE 4: GC (RI) EVALUATORS

Name	Country	Address	Phone, Fax, and E-Mail	Speciality
Martin Söderström*	Finland	VERIFIN P.O. Box 55 00014 University of Helsinki Finland	+358 9 19150438 +358 9 19150437 martin.soderstrom@helsinki.fi	**GC coordinator** IR
Gary Mallard*	United States of America	NIST 100 Bureau Drive Stop 8380 Gaithersburg, MD 20899-8380 United States of America	+1 301 975 2564 +1 301 869 4020 gary.mallard@nist.gov	GC
Bedrich Uchytil*	Czech Republic	Institute for Protection of Population Laboratory Korunni 2 25168 Kamenice Czech Republic	+420 724 355197 +420 323 673054 bedrich.uchytil@ioolb.izscr.cz	GC, IR
Takeharu Wada	Japan	Chemicals Evaluation and Research Institute 1600, Shimo-Takano Sugito-machi Kitakatsushika-gun, Saitama 345-0043 Japan	+81 480 37 2601 +81 480 37 2521 wada-takeharu@ceri.jp	GC

Name	Country	Address	Phone, Fax, and E-Mail	Speciality
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