



Verification Division  
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### REPORT OF THE TWENTY-NINTH MEETING OF THE VALIDATION GROUP FOR THE UPDATING OF THE OPCW CENTRAL ANALYTICAL DATABASE 3 AND 4 MARCH 2009

1. The Validation Group (hereinafter “the Group”) met for the twenty-ninth time on 3 and 4 March 2009 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 Hugh Gregg 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 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)
Infrared spectrometry (IR)	Mr Armando Alcaraz (United States of America)
Mass spectrometry (MS)	Mr Sten-Åke Fredriksson (Sweden)
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 the data approved is technically valid.
4. The Group forwarded lists of the validated analytical data to the Director-General for appropriate action (see Annex 1).
5. The Group reviewed some of the data in the OCAD, and recommended the removal of the data listed in Annex 2, due to the fact that this Annex lists data that is not scheduled, that is not an analytical derivative of scheduled compounds, and that is not a degradation product of scheduled chemicals. However, the Group recommended that this data be retained in the Validation Group Working Database.
6. The Group updated the Rules for Naming Compounds in the OCAD (see paragraph 2.14 and paragraph 3 of Annex 3) to clarify the names of scheduled chemicals. The



Technical Secretariat (hereinafter “the Secretariat”) is requested to review the OCAD and update names as necessary.

7. The Group recommended that the Secretariat create a standard protocol for the naming of chemicals relevant to the Chemical Weapons Convention (hereinafter “the Convention”). The Group would approve the protocol (and any changes to it) as the method to be used for generating chemical names. The Group would then no longer publish the Rules for Naming Compounds in the Group’s reports; however, the Group’s report shall note the approval of an updated protocol.
8. The Secretariat reported that all the data on scheduled chemicals submitted by the Group up to and including its Twenty-Seventh Meeting have been approved by the Executive Council, and have been incorporated into the OCAD (v.11\_2008). This version was released in December 2008.
9. The Secretariat reported that a Validation Group Working Database (VGWD), containing all the data validated by the Group, up to and including the data approved during its Twenty-Eighth Meeting, was prepared in January 2009 and is available from the Secretariat on request.
10. The Group continued to discuss the possibility of establishing a liquid chromatography-mass spectrometry (LC-MS) database for potential inclusion in the OCAD. The Group discussed a presentation that had been given by the Secretariat, and agreed to continue to explore the creation of an LC-MS database, which is likely to be an ion-trap based LC-MS-MS database.
11. The Secretariat noted that several mass spectra are present in the OCAD without corresponding GC(RI) data. These omissions have led to false positive identifications during inspections. As a result, the Secretariat strongly encourages that experimental GC(RI) data be submitted for the following compounds:

Schedule	Priority	Chemical Name
1.A.03	High	Ethyl S-2-diethylaminoethyl isopropylphosphonothiolate
1.A.03	High	Ethyl S-2-diethylaminoethyl propylphosphonothiolate
1.A.03	High	Isopropyl S-2-diethylaminoethyl methylphosphonothiolate
1.A.03	High	sec-Butyl S-2-diethylaminoethyl methylphosphonothiolate
2.B.04	High	Bis(S-2-diisopropylaminoethyl) methylphosphonodithiolate
2.B.04	High	Bis(S-2-diethylaminoethyl) methylphosphonodithiolate
1.A.03	Medium	2-Isopropyl-5-methylcyclohexyl S-2-dimethylaminoethyl ethylphosphonothiolate
1.A.03	Medium	2-Isopropyl-5-methylcyclohexyl S-2-dimethylaminoethyl methylphosphonothiolate
1.A.03	Medium	2-Methylbutyl S-2-diethylaminoethyl propylphosphonothiolate
1.A.03	Medium	Cyclohexylmethyl S-2-dimethylaminoethyl propylphosphonothiolate
1.A.03	Medium	Cyclooctyl S-2-dimethylaminoethyl propylphosphonothiolate
1.A.03	Medium	Cyclopentyl S-2-diisopropylaminoethyl methylphosphonothiolate
1.A.03	Medium	Ethyl S-2-diisopropylaminoethyl propylphosphonothiolate

Schedule	Priority	Chemical Name
1.A.03	Medium	Ethyl S-2-dimethylaminoethyl isopropylphosphonothiolate
1.A.03	Medium	Ethyl S-2-dipropylaminoethyl isopropylphosphonothiolate
1.A.03	Medium	Ethyl S-2-dipropylaminoethyl propylphosphonothiolate
1.A.03	Medium	Methyl S-2-diisopropylaminoethyl propylphosphonothiolate
1.A.03	Medium	Pentyl S-2-diethylaminoethyl propylphosphonothiolate
1.A.03	Medium	Propyl S-2-dimethylaminoethyl isopropylphosphonothiolate
1.A.03	Medium	tert-Butyl S-2-diisopropylaminoethyl methylphosphonothiolate
2.B.04	Medium	O-Trimethylsilyl S-2-diethylaminoethyl methylphosphonothiolate
2.B.12	Medium	2-(N-Methyl-N-propylamino)ethanethiol
2.B.12	Medium	2-(N-Isopropyl-N-methylamino)ethanethiol
DS	Medium	N,N-Diethyl-N-(2-trimethylsilylthioethyl)amine

12. The Secretariat enquired about the status of predicting GC(RI) data for those compounds for which only MS data is available in the OCAD. The GC(RI) subgroup reviewed the paper provided on the subject by the Secretariat, and accepted the utilisation of the prediction method that had been suggested. The GC(RI) subgroup will evaluate predicted GC(RI) data during the next Meeting of the Group.
13. The Group noted that the GC(RI) subgroup is down to a minimum number of members. It is critical that the GC(RI) subgroup remain strong, and the Group urgently requests Member States to nominate technical experts to join this subgroup.
14. The Group strongly encourages laboratories that submit mass spectral data for inclusion in the OCAD to submit GC(RI) data of those compounds as well.
15. The Secretariat has procured Attenuated Total Reflection (ATR) Fourier Transform Infrared (FTIR) portable systems for use during inspections. In order to make optimal use of these systems, the IR database will be augmented with ATR spectra. To distinguish the ATR FTIR spectra from condensed-phase IR spectra, ATR IR spectra will have an "x" after the OPCW IR code. However, before the submission of ATR FTIR spectra from contributors, the Group has proposed conducting experiments with various ATR FTIR instruments to evaluate the software algorithms that convert the ATR raw data to FTIR transmission spectra. The results of these experiments will help define the requirements for the submission of ATR FTIR spectra in the near future.
16. The Secretariat is looking for assistance in collecting ATR IR spectra. The Secretariat is willing to make arrangements with laboratories to obtain these sets of data. Accordingly, laboratories with stocks of chemicals are encouraged to contact the Secretariat.
17. The Group requests that the Secretariat update document S/373/2003, dated 18 August 2003), "Procedures for the Evaluation of Data to be Included in the OPCW

Central Analytical Database”, to include a new paragraph 7 in the Annex, which would read as follows:

- “7. Submission of data on compounds that have multiple chromatographic peaks**
- 7.1 If the mass or infrared spectra of individual chromatographic peaks of the compound are different, then multiple spectra shall be requested from the submitting laboratory.
- 7.2 The compound shall be given one single OPCW code number that is followed by a letter. The letters shall start at “a” for the first peak eluting, “b” for the second, and so on.
- 7.3 There shall be a consistent set of data from each laboratory. For example, if a laboratory submits three mass spectra, there shall be three retention indices, ordered in such a way that the first peak to elute has an OPCW code ending in “a” for both spectra corresponding to the GC(RI) “RI(a)” column, “RI(b)” the second, and “RI(c)” the third.”
18. MS and GC(RI) data for over 100 compounds are expected before the next Meeting. Some IR data may also be available at that time.
19. The evaluators agreed to send their written evaluation reports to the appointed coordinators **no later than 22 September 2009**. The next Meeting is scheduled to take place on 29 and 30 September 2009. The evaluator has agreed to come to that Meeting prepared to finalise the evaluation of the analytical data referred to in the previous paragraph.
20. The Group appreciates the past evaluations by Mr Chongxi Wei, and accepts his resignation from the Group as he takes up his new post as an inspector for the OPCW.
21. Annex 4 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 Recommended Changes to the OPCW Central Analytical Database
- Annex 3: Rules for Naming Compounds in the OPCW Central Analytical Database
- Annex 4: 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 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**

<b>OPCW Code</b>	<b>Chemical Name</b>	<b>Schedule</b>	<b>Decision</b>
04-2-0472	Isobutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0473	1-Methylbutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0474	Hexyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0475	1-Methylpentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0476	2-Methylpentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0477	Heptyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0478	1-Methylhexyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0479	1-Isopropyl-2-methylpropyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0480	Octyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-2-0481	1-Methylheptyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
07-2-2595	2-Methyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	A
07-2-2596	2-Methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	A
07-2-2597a	2,5-Dimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2597b	2,5-Dimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2599a	2,4-Dimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2599b	2,4-Dimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2601a	2,4,6-Trimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2601b	2,4,6-Trimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2601c	2,4,6-Trimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2604	2-Methyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	A
07-2-2605	2-Methyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	A
07-2-2606	2-Methyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	A
07-2-2607	2-Ethyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	A
07-2-2608	2-Ethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	A
07-2-2609a	2-Ethyl-5-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2609b	2-Ethyl-5-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2611a	2-Ethyl-4-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2611b	2-Ethyl-4-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2613a	4,6-Dimethyl-2-ethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2613b	4,6-Dimethyl-2-ethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2613c	4,6-Dimethyl-2-ethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B

OPCW Code	Chemical Name	Schedule	Decision
07-2-2616	2-Ethyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	A
07-2-2617	2-Ethyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	A
07-2-2618	2-Ethyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	A
07-2-2619	2-Propyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	A
07-2-2621a	5-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2621b	5-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2623a	4-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2623b	4-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2625a	4,6-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2625b	4,6-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2625c	4,6-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2628	2-Propyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	A
07-2-2629	2-Propyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	A
07-2-2630	2-Propyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	A
07-2-2631	2-Isopropyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	A
07-2-2632	2-Isopropyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	A
07-2-2633a	2-Isopropyl-5-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2633b	2-Isopropyl-5-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2635a	2-Isopropyl-4-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2635b	2-Isopropyl-4-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2637a	4,6-Dimethyl-2-isopropyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2637b	4,6-Dimethyl-2-isopropyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2637c	4,6-Dimethyl-2-isopropyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	B
07-2-2640	2-Isopropyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	A
07-2-2641	2-Isopropyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	A
07-2-2642	2-Isopropyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	A
07-2-2643	2-Methyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	A
07-2-2644	2-Methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	A
07-2-2645a	2,5-Dimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2645b	2,5-Dimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2647a	2,4-Dimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2647b	2,4-Dimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2649a	2,4,6-Trimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2649b	2,4,6-Trimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2649c	2,4,6-Trimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2652	2-Methyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	A
07-2-2653	2-Methyl-1,3,2-dioxaphosphocane-2-sulfide	2.B.04	A
07-2-2654	2-Methyl-1,3,6,2-dioxathiaphosphocane-2-sulfide	2.B.04	A
07-2-2655	2-Ethyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	A
07-2-2656	2-Ethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	A
07-2-2657a	2-Ethyl-5-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2657b	2-Ethyl-5-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2659a	2-Ethyl-4-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2659b	2-Ethyl-4-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2661a	4,6-Dimethyl-2-ethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B

OPCW Code	Chemical Name	Schedule	Decision
07-2-2661b	4,6-Dimethyl-2-ethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2661c	4,6-Dimethyl-2-ethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2664	2-Ethyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	A
07-2-2665	2-Ethyl-1,3,2-dioxaphosphocane-2-sulfide	2.B.04	A
07-2-2666	2-Ethyl-1,3,6,2-dioxathiaphosphocane-2-sulfide	2.B.04	A
07-2-2667	2-Propyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	A
07-2-2668	2-Propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	A
07-2-2669a	5-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2669b	5-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2672	4-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2673a	4,6-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2673b	4,6-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2673c	4,6-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2676	2-Propyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	A
07-2-2677	2-Propyl-1,3,2-dioxaphosphocane-2-sulfide	2.B.04	A
07-2-2678	2-Propyl-1,3,6,2-dioxathiaphosphocane-2-sulfide	2.B.04	A
07-2-2679	2-Isopropyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	A
07-2-2680	2-Isopropyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	A
07-2-2681a	2-Isopropyl-5-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2681b	2-Isopropyl-5-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2683a	2-Isopropyl-4-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2683b	2-Isopropyl-4-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2685a	4,6-Dimethyl-2-isopropyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2685b	4,6-Dimethyl-2-isopropyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2685c	4,6-Dimethyl-2-isopropyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	B
07-2-2688	2-Isopropyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	A
07-2-2689	2-Isopropyl-1,3,2-dioxaphosphocane-2-sulfide	2.B.04	A
07-2-2690	2-Isopropyl-1,3,6,2-dioxathiaphosphocane-2-sulfide	2.B.04	A
07-2-2691	2-Methyl-1,3,2-oxathiaphosphinane-2-oxide	2.B.04	A
07-2-2692	2-Ethyl-1,3,2-oxathiaphosphinane-2-oxide	2.B.04	A
07-2-2693	2-Propyl-1,3,2-oxathiaphosphinane-2-oxide	2.B.04	A
07-2-2694	2-Isopropyl-1,3,2-oxathiaphosphinane-2-oxide	2.B.04	A
07-2-2695	2-Methyl-1,3,2-dithiaphosphinane-2-oxide	2.B.04	A
07-2-2696	2-Ethyl-1,3,2-dithiaphosphinane-2-oxide	2.B.04	A
07-2-2697	2-Propyl-1,3,2-dithiaphosphinane-2-oxide	2.B.04	A
07-2-2698	2-Isopropyl-1,3,2-dithiaphosphinane-2-oxide	2.B.04	A
07-2-2699	2-Methyl-1,3,2-oxathiaphosphepane-2-oxide	2.B.04	A
07-2-2700	2-Ethyl-1,3,2-oxathiaphosphepane-2-oxide	2.B.04	A
07-2-2701	2-Propyl-1,3,2-oxathiaphosphepane-2-oxide	2.B.04	A
07-2-2702	2-Isopropyl-1,3,2-oxathiaphosphepane-2-oxide	2.B.04	A
07-2-2704	2-Ethyl-1,3,2-dithiaphosphepane-2-oxide	2.B.04	A
07-2-2705	2-Propyl-1,3,2-dithiaphosphepane-2-oxide	2.B.04	A
07-2-2706	2-Isopropyl-1,3,2-dithiaphosphepane-2-oxide	2.B.04	A
07-2-2707	2-Methyl-1,3,2-oxathiaphosphinane-2-sulfide	2.B.04	A
07-2-2708	2-Ethyl-1,3,2-oxathiaphosphinane-2-sulfide	2.B.04	A

OPCW Code	Chemical Name	Schedule	Decision
07-2-2709	2-Propyl-1,3,2-oxathiaphosphinane-2-sulfide	2.B.04	A
07-2-2710	2-Isopropyl-1,3,2-oxathiaphosphinane-2-sulfide	2.B.04	A
07-2-2711	2-Methyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	A
07-2-2712	2-Ethyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	A
07-2-2713	2-Propyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	A
07-2-2714	2-Isopropyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	A
07-2-2716	2-Ethyl-1,3,2-oxathiaphosphhepane-2-sulfide	2.B.04	A
07-2-2717	2-Propyl-1,3,2-oxathiaphosphhepane-2-sulfide	2.B.04	A
07-2-2719	2-Methyl-1,3,2-dithiaphosphhepane-2-sulfide	2.B.04	A
07-2-2722	2-Isopropyl-1,3,2-dithiaphosphhepane-2-sulfide	2.B.04	A
17-2-0179	Bis[(1S,2S)-2-chlorocyclohexyl] ethylphosphonate	2.B.04	A
17-2-0180	Bis[(1S,2S)-2-chlorocyclohexyl] propylphosphonate	2.B.04	A
17-2-0181	2-Propyl-1,3,6,2-trioxaphosphocane-2-oxide	2.B.04	A
17-2-0182	2-Propyl-1,3,6,2-trithiaphosphocane-2-oxide	2.B.04	A
17-2-0183	2-Ethyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	A
17-2-0184	2-Isopropyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	A
17-2-0185	2-Propyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	A
17-2-0186	2-Propyl-1,3,2-dioxaphosphhepane-2-sulfide	2.B.04	A
17-2-0187	2-Propyl-1,3,2-dithiaphosphhepane-2-oxide	2.B.04	A
17-2-0188	2-Methyl-1,3,2-dithiaphosphhepane-2-sulfide	2.B.04	A
17-2-0189	2-Methyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	A
17-2-0190	5-Propyl-1,4,6,5-oxadithiaphosphocane-5-oxide	2.B.04	A
17-2-0191	6-Propyldodecahydrodibenzo[d,g][1,3,6,2]trioxaphosphocine-6-oxide	2.B.04	A
17-2-0192	6-Ethyldodecahydrodibenzo[d,g][1,3,6,2]trioxaphosphocine-6-oxide	2.B.04	A
17-2-0193	6-Methyldodecahydrodibenzo[d,g][1,3,6,2]trioxaphosphocine-6-oxide	2.B.04	A
17-2-0194	(3aR,7aR)-2-Propylhexahydro-1,3,2-benzodioxaphosphole-2-oxide	2.B.04	A
17-2-0195a	(3aR,7aS)-2-Propylhexahydro-1,3,2-benzodioxaphosphole-2-oxide	2.B.04	B
17-2-0195b	(3aR,7aS)-2-Propylhexahydro-1,3,2-benzodioxaphosphole-2-oxide	2.B.04	B
17-2-0197	S-(4-Mercaptobutyl) methylphosphonothiolothionochloridate	2.B.04	B
17-2-0198	S-(4-Mercaptobutyl) ethylphosphonothiolothionochloridate	2.B.04	B
17-2-0199	S-(5-Mercaptopentyl) methylphosphonothiolothionochloridate	2.B.04	B
17-2-0200	S-(5-Mercaptopentyl) isopropylphosphonothiolothionochloridate	2.B.04	B
17-2-0201	S-(5-Mercaptopentyl) ethylphosphonothiolothionochloridate	2.B.04	B
17-2-0202	S-(5-Mercaptopentyl) propylphosphonothiolothionochloridate	2.B.04	B
17-2-0203	5-Methyl-2-propyl-1,3,2-benzodithiaphosphole-2-oxide	2.B.04	A
17-2-0204	2-Ethyl-5-methyl-1,3,2-benzodithiaphosphole-2-oxide	2.B.04	A
17-2-0205	2-Ethyl-5-methyl-1,3,2-benzoxathiaphosphole-2-oxide	2.B.04	A
17-2-0206	S-(3-Mercaptopropyl) methylphosphonothiolothionochloridate	2.B.04	B
17-2-0207	2-Ethyl-1,3,2-dithiaphosphhepane-2-sulfide	2.B.04	A
17-2-0208	2-Isopropyl-1,3,2-dithiaphosphhepane-2-sulfide	2.B.04	A
17-2-0209	S-(4-Mercaptobutyl) isopropylphosphonothiolothionochloridate	2.B.04	B
17-2-0210	2-Ethyl-1,3,2-oxathiaphosphhepane-2-sulfide	2.B.04	A
17-2-0211	2-Isopropyl-1,3,2-oxathiaphosphhepane-2-sulfide	2.B.04	A
17-2-0212	2-Methyl-1,3,2-oxathiaphosphhepane-2-sulfide	2.B.04	A
17-2-0213	2-Propyl-1,3,2-oxathiaphosphhepane-2-sulfide	2.B.04	A



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

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	RI(c)	Decision
04-4-0281	Isobutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	1874			A
04-4-0283	Hexyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2114			A
04-4-0285	2-Methylpentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2052			A
04-4-0286	Heptyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2211			A
04-4-0288	1-Isopropyl-2-methylpropyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2035			A
04-4-0289	Octyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	1	2314			A
07-4-2358	2-Methyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	2	1140			A
07-4-2359	2-Methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1187			A
07-4-2360	2,5-Dimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1230	1272		B
07-4-2362	2,4-Dimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1202	1300		B
07-4-2364	2,4,6-Trimethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1229	1268	1341	B
07-4-2368	2-Methyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	2	1319			A
07-4-2369	2-Methyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	2	1507			A
07-4-2370	2-Ethyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	2	1236			A
07-4-2371	2-Ethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1285			A
07-4-2372	2-Ethyl-5-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1329	1363		B
07-4-2374	2-Ethyl-4-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1298	1374		B
07-4-2376	4,6-Dimethyl-2-ethyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1317	1355	1400	B
07-4-2379	2-Ethyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	2	1352			A
07-4-2380	2-Ethyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	2	1401			A
07-4-2381	2-Ethyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	2	1591			A
07-4-2382	2-Propyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	2	1325			A
07-4-2383	2-Propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1379			A
07-4-2384	5-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1420	1452		B
07-4-2386	4-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1386	1463		B
07-4-2388	4,6-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1400	1440	1484	B

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	RI(c)	Decision
07-4-2391	2-Propyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	2	1443			A
07-4-2392	2-Propyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	2	1492			B
07-4-2393	2-Propyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	2	1682			A
07-4-2394	2-Isopropyl-1,3,2-dioxaphospholane-2-oxide	2.B.04	2	1287			A
07-4-2395	2-Isopropyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1333			A
07-4-2396	2-Isopropyl-5-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1376	1401		B
07-4-2398	2-Isopropyl-4-methyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1343	1398		B
07-4-2400	4,6-Dimethyl-2-isopropyl-1,3,2-dioxaphosphinane-2-oxide	2.B.04	2	1354	1389	1408	B
07-4-2403	2-Isopropyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	2	1389			A
07-4-2404	2-Isopropyl-1,3,2-dioxaphosphocane-2-oxide	2.B.04	2	1434			A
07-4-2405	2-Isopropyl-1,3,6,2-dioxathiaphosphocane-2-oxide	2.B.04	2	1624			A
07-4-2406	2-Methyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	2	1172			A
07-4-2407	2-Methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1207			A
07-4-2408	2,5-Dimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1254	1272		B
07-4-2410	2,4-Dimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1228	1337		B
07-4-2412	2,4,6-Trimethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1246	1302	1385	B
07-4-2415	2-Methyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	2	1311			A
07-4-2416	2-Methyl-1,3,2-dioxaphosphocane-2-sulfide	2.B.04	2	1375			A
07-4-2417	2-Methyl-1,3,6,2-dioxathiaphosphocane-2-sulfide	2.B.04	2	1571			A
07-4-2418	2-Ethyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	2	1268			A
07-4-2419	2-Ethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1306			A
07-4-2420	2-Ethyl-5-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1352	1370		B
07-4-2422	2-Ethyl-4-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1320	1409		B
07-4-2424	4,6-Dimethyl-2-ethyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1330	1386	1442	B
07-4-2427	2-Ethyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	2	1398			A
07-4-2428	2-Ethyl-1,3,2-dioxaphosphocane-2-sulfide	2.B.04	2	1459			A
07-4-2429	2-Ethyl-1,3,6,2-dioxathiaphosphocane-2-sulfide	2.B.04	2	1656			A
07-4-2430	2-Propyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	2	1356			A

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	RI(c)	Decision
07-4-2431	2-Propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1398			A
07-4-2432	5-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1443	1458		B
07-4-2434	4-Methyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1407	1495		B
07-4-2436	4,6-Dimethyl-2-propyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1413	1470	1523	B
07-4-2439	2-Propyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	2	1490			A
07-4-2440	2-Propyl-1,3,2-dioxaphosphocane-2-sulfide	2.B.04	2	1550			A
07-4-2441	2-Propyl-1,3,6,2-dioxathiaphosphocane-2-sulfide	2.B.04	2	1747			A
07-4-2442	2-Isopropyl-1,3,2-dioxaphospholane-2-sulfide	2.B.04	2	1318			A
07-4-2443	2-Isopropyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1359			A
07-4-2444	2-Isopropyl-5-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1402	1420		B
07-4-2446	2-Isopropyl-4-methyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1366	1441		B
07-4-2448	4,6-Dimethyl-2-isopropyl-1,3,2-dioxaphosphinane-2-sulfide	2.B.04	2	1368	1424	1457	B
07-4-2451	2-Isopropyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	2	1441			A
07-4-2452	2-Isopropyl-1,3,2-dioxaphosphocane-2-sulfide	2.B.04	2	1497			A
07-4-2453	2-Isopropyl-1,3,6,2-dioxathiaphosphocane-2-sulfide	2.B.04	2	1694			A
07-4-2454	2-Methyl-1,3,2-oxathiaphosphinane-2-oxide	2.B.04	2	1378			A
07-4-2455	2-Ethyl-1,3,2-oxathiaphosphinane-2-oxide	2.B.04	2	1477			A
07-4-2456	2-Propyl-1,3,2-oxathiaphosphinane-2-oxide	2.B.04	2	1565			A
07-4-2457	2-Isopropyl-1,3,2-oxathiaphosphinane-2-oxide	2.B.04	2	1521			A
07-4-2458	2-Methyl-1,3,2-dithiaphosphinane-2-oxide	2.B.04	2	1600			A
07-4-2459	2-Ethyl-1,3,2-dithiaphosphinane-2-oxide	2.B.04	2	1703			A
07-4-2460	2-Propyl-1,3,2-dithiaphosphinane-2-oxide	2.B.04	2	1788			A
07-4-2461	2-Isopropyl-1,3,2-dithiaphosphinane-2-oxide	2.B.04	2	1751			A
07-4-2462	2-Methyl-1,3,2-oxathiaphosphepane-2-oxide	2.B.04	2	1469			A
07-4-2463	2-Ethyl-1,3,2-oxathiaphosphepane-2-oxide	2.B.04	2	1564			A
07-4-2464	2-Propyl-1,3,2-oxathiaphosphepane-2-oxide	2.B.04	2	1650			A
07-4-2465	2-Isopropyl-1,3,2-oxathiaphosphepane-2-oxide	2.B.04	2	1607			A
07-4-2466	2-Methyl-1,3,2-dithiaphosphepane-2-oxide	2.B.04	2	1673			A

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	RI(c)	Decision
07-4-2467	2-Ethyl-1,3,2-dithiaphosphepane-2-oxide	2.B.04	2	1774			A
07-4-2468	2-Propyl-1,3,2-dithiaphosphepane-2-oxide	2.B.04	2	1861			A
07-4-2469	2-Isopropyl-1,3,2-dithiaphosphepane-2-oxide	2.B.04	2	1827			A
07-4-2470	2-Methyl-1,3,2-oxathiaphosphinane-2-sulfide	2.B.04	2	1424			A
07-4-2471	2-Ethyl-1,3,2-oxathiaphosphinane-2-sulfide	2.B.04	2	1524			A
07-4-2472	2-Propyl-1,3,2-oxathiaphosphinane-2-sulfide	2.B.04	2	1612			A
07-4-2473	2-Isopropyl-1,3,2-oxathiaphosphinane-2-sulfide	2.B.04	2	1574			A
07-4-2474	2-Methyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	2	1682			A
07-4-2475	2-Ethyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	2	1785			A
07-4-2476	2-Propyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	2	1868			A
07-4-2477	2-Isopropyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	2	1835			A
07-4-2478	2-Methyl-1,3,2-oxathiaphosphepane-2-sulfide	2.B.04	2	1534			A
07-4-2479	2-Ethyl-1,3,2-oxathiaphosphepane-2-sulfide	2.B.04	2	1628			A
07-4-2480	2-Propyl-1,3,2-oxathiaphosphepane-2-sulfide	2.B.04	2	1714			A
07-4-2481	2-Isopropyl-1,3,2-oxathiaphosphepane-2-sulfide	2.B.04	2	1680			A
07-4-2482	2-Methyl-1,3,2-dithiaphosphepane-2-sulfide	2.B.04	2	1766			A
07-4-2483	2-Ethyl-1,3,2-dithiaphosphepane-2-sulfide	2.B.04	2	1871			A
07-4-2484	2-Propyl-1,3,2-dithiaphosphepane-2-sulfide	2.B.04	2	1958			A
07-4-2485	2-Isopropyl-1,3,2-dithiaphosphepane-2-sulfide	2.B.04	2	1934			A
17-4-0159	Bis[(1S,2S)-2-chlorocyclohexyl] ethylphosphonate	2.B.04	1	2317	2325	2336	A
17-4-0160	Bis[(1S,2S)-2-chlorocyclohexyl] propylphosphonate	2.B.04	1	2382	2388	2397	A
17-4-0161	2-Propyl-1,3,6,2-trioxaphosphocane-2-oxide	2.B.04	1	1480			A
17-4-0162	2-Propyl-1,3,6,2-trithiaphosphocane-2-oxide	2.B.04	1	2157			B
17-4-0163	2-Ethyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	1	1788			A
17-4-0164	2-Isopropyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	1	1838			A
17-4-0165	2-Propyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	1	1876			A
17-4-0166	2-Propyl-1,3,2-dioxaphosphepane-2-sulfide	2.B.04	1	1498			A
17-4-0167	2-Propyl-1,3,2-dithiaphosphepane-2-oxide	2.B.04	1	1866			A

OPCW Code	Chemical Name	Schedule	Column	RI(a)	RI(b)	RI(c)	Decision
17-4-0168	2-Methyl-1,3,2-dithiaphosphepane-2-sulfide	2.B.04	1	1768			A
17-4-0169	2-Methyl-1,3,2-dithiaphosphinane-2-sulfide	2.B.04	1	1685			A
17-4-0170	5-Propyl-1,4,6,5-oxadithiaphosphocane-5-oxide	2.B.04	1	1955			A
17-4-0171	6-Propyldodecahydrodibenzo[d,g][1,3,6,2]trioxaphosphocine-6-oxide	2.B.04	1	2081			A
17-4-0172	6-Ethyldodecahydrodibenzo[d,g][1,3,6,2]trioxaphosphocine-6-oxide	2.B.04	1	2020			A
17-4-0173	6-Methyldodecahydrodibenzo[d,g][1,3,6,2]trioxaphosphocine-6-oxide	2.B.04	1	1939			A
17-4-0174	(3aR,7aR)-2-Propylhexahydro-1,3,2-benzodioxaphosphole-2-oxide	2.B.04	1	1754			A
17-4-0175	(3aR,7aS)-2-Propylhexahydro-1,3,2-benzodioxaphosphole-2-oxide	2.B.04	1	1690	1739		B
17-4-0177	S-(4-Mercaptobutyl) methylphosphonothiolothionochloridate	2.B.04	1	1781			B
17-4-0178	S-(4-Mercaptobutyl) ethylphosphonothiolothionochloridate	2.B.04	1	1882			B
17-4-0179	S-(5-Mercaptopentyl) methylphosphonothiolothionochloridate	2.B.04	1	1897			B
17-4-0180	S-(5-Mercaptopentyl) isopropylphosphonothiolothionochloridate	2.B.04	1	2065			B
17-4-0181	S-(5-Mercaptopentyl) ethylphosphonothiolothionochloridate	2.B.04	1	1997			B
17-4-0182	S-(5-Mercaptopentyl) propylphosphonothiolothionochloridate	2.B.04	1	2082			B
17-4-0183	5-Methyl-2-propyl-1,3,2-benzodithiaphosphole-2-oxide	2.B.04	1	2191			A
17-4-0184	2-Ethyl-5-methyl-1,3,2-benzodithiaphosphole-2-oxide	2.B.04	1	2106			A
17-4-0186	S-(3-Mercaptopropyl) methylphosphonothiolothionochloridate	2.B.04	1	1658			B
17-4-0187	2-Propyl-1,3,2-dioxaphosphepane-2-oxide	2.B.04	1	1445			A
17-4-0188	2-Ethyl-1,3,2-dithiaphosphepane-2-sulfide	2.B.04	1	1874			A
17-4-0189	2-Isopropyl-1,3,2-dithiaphosphepane-2-sulfide	2.B.04	1	1936			A
17-4-0190	S-(4-Mercaptobutyl) isopropylphosphonothiolothionochloridate	2.B.04	1	1948			B
17-4-0191	2-Ethyl-1,3,2-oxathiaphosphepane-2-sulfide	2.B.04	1	1632			A
17-4-0192	2-Isopropyl-1,3,2-oxathiaphosphepane-2-sulfide	2.B.04	1	1686			A
17-4-0193	2-Methyl-1,3,2-oxathiaphosphepane-2-sulfide	2.B.04	1	1538			A
17-4-0194	2-Propyl-1,3,2-oxathiaphosphepane-2-sulfide	2.B.04	1	1720			A

**TABLE 3: LIST OF APPROVED IR DATA**

<b>OPCW Code</b>	<b>Chemical Name</b>	<b>Schedule</b>	<b>Decision</b>
04-1-0294v	Isobutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0295v	1-Methylbutyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0296v	Hexyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0297v	1-Methylpentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0298v	2-Methylpentyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0299v	Heptyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0300v	1-Methylhexyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0301v	1-Isopropyl-2-methylpropyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A
04-1-0302v	Octyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	B
04-1-0303v	1-Methylheptyl S-2-diethylaminoethyl propylphosphonothiolate	1.A.03	A

**Annex 2**

**LIST OF RECOMMENDED CHANGES TO THE OPCW CENTRAL  
ANALYTICAL DATABASE**

**TABLE 1: LIST OF DATA TO BE REMOVED FROM THE OCAD:  
NON-SCHEDULED DATA INADVERTENTLY INCLUDED  
PREVIOUSLY\***

<b>OPCW Code</b>	<b>Chemical Name</b>	<b>Schedule</b>
02-2-0076	Dibutyl N,N-dimethylphosphoramidate	NS
02-2-0086	Diheptyl N,N-dimethylphosphoramidate	NS
02-2-0084	Dihexyl N,N-dimethylphosphoramidate	NS
02-2-0082	Dioctyl N,N-dimethylphosphoramidate	NS
02-2-0077	Dipentyl N,N-dimethylphosphoramidate	NS
02-1-0092	Dioctyl N,N-dimethylphosphoramidate	NS
02-1-0094	Dihexyl N,N-dimethylphosphoramidate	NS

\* While similar to Schedule 2.B.06 chemicals, these chemicals are not scheduled.

### Annex 3

#### **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 Annex on Chemicals to the Convention.
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 above. 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 phosphorus compounds containing two S-sec-butyl or S-tert-butyl groups linked to phosphorus, the name has to start 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.
- 2.13 Arsenic-containing derivatives or decomposition products of the Lewisites (Schedule 1.A.05) shall be named as follows:
- (a) Derivatives with alkyl thioglycolates shall be named per the following examples:
    - (i) 2-Methoxy-2-oxoethyl bis(2-chlorovinyl)arsinothiolite; and
    - (ii) Bis(2-methoxy-2-oxoethyl) 2-chlorovinylarsonodithiolite.
  - (b) Derivatives with butanethiol shall be named in accordance with the International Union of Pure and Applied Chemistry (IUPAC) rules as follows:
    - (i) Butyl bis(2-chlorovinyl)arsinothiolite;
    - (ii) Dibutyl 2-chlorovinylarsonodithiolite; and
    - (iii) Tributyl arsenotrithiolite.
- 2.14 Compounds with multiple phosphorus atoms shall be named as follows (examples below under 2.B.04):
- (a) A symmetrical phosphonate dimer with an oxygen linkage shall be called a pyrophosphonate.

- (b) Amidate shall be used instead of amidoate (a term used by some commercial chemical-naming programmes).
- (c) Multiple phosphorus atoms shall be identified as P, P', etc.
- (d) Groups attached to the phosphorus shall be indicated by corresponding prime marks (e.g. "-S-methyl" or "-N',N'-diethyl-", etc.), with P listed before P'.
- (e) Otherwise, the International Union of Pure and Applied Chemistry (IUPAC) names shall be used.
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-trialkylammoniummethyl 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-Chlorovinylchloroarsine
	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
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

Schedule	Name
2.B.04	To avoid any confusion, the O and S groups should be indicated in esters when sulfur is present.
	Examples
	Methylphosphonothioic acid $[(\text{CH}_3\text{P}(=\text{S})(\text{OH}))_2]$
	O-Ethyl methylphosphonothionate $[(\text{C}_2\text{H}_5\text{O})\text{P}(=\text{S})(\text{CH}_3)(\text{OH})]$
	O,O-Diethyl methylphosphonothionate $[(\text{C}_2\text{H}_5\text{O})_2\text{P}(=\text{S})(\text{CH}_3)]$
	O-Propyl O-trimethylsilyl propylphosphonothionate
	O-Ethyl S-ethyl methylphosphonothiolate $[(\text{C}_2\text{H}_5\text{O})\text{P}(=\text{O})(\text{CH}_3)(\text{SC}_2\text{H}_5)]$
	S-Ethyl O-methyl methylphosphonothiolate
	O-Ethyl S-2-methylthioethyl methylphosphonothiolate
	O-Ethyl S-ethyl methylphosphonothiolothionate $[(\text{C}_2\text{H}_5\text{O})\text{P}(=\text{S})(\text{CH}_3)(\text{SC}_2\text{H}_5)]$
	Bis(S-sec-butyl) methylphosphonodithiolate
	O-Ethyl methylphosphonothionochloridate $[(\text{C}_2\text{H}_5\text{O})\text{P}(=\text{S})(\text{CH}_3)(\text{Cl})]$
	S-(4-Mercaptobutyl) isopropylphosphonothiolothionochloridate $[(\text{HS}-\text{C}_4\text{H}_8-\text{S})(\text{i}-\text{C}_3\text{H}_7)\text{P}(=\text{S})(\text{Cl})]$
	Methylphosphonous dichloride $(\text{CH}_3\text{P}-\text{Cl}_2)$
	Methylphosphonic dichloride $[(\text{CH}_3\text{P}(=\text{O})-\text{Cl}_2)]$
	Methylphosphonothioic dichloride $[(\text{CH}_3\text{P}(=\text{S})-\text{Cl}_2)]$
	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 $[(\text{i}-\text{C}_3\text{H}_7)_2\text{N}-\text{CH}_2\text{CH}_2-\text{O}-\text{P}(=\text{O})(\text{H})(\text{CH}_3)]$
	Methyl 2-diethylaminoethyl methylphosphonate
	O-Ethyl S-2-dibutylaminoethyl methylphosphonothiolate
	Bis(S-2-diethylaminoethyl) methylphosphonodithiolate
	O-Ethyl S-3-dimethylaminopropyl methylphosphonothiolate
	Diethyl methylphosphonite $[(\text{C}_2\text{H}_5\text{O})_2\text{P}(\text{CH}_3)]$
	Dicyclohexyl dimethylpyrophosphonate $[(\text{C}_6\text{H}_{11}\text{O})(\text{CH}_3)\text{P}(=\text{O})-\text{O}-\text{P}(=\text{O})(\text{CH}_3)(\text{C}_6\text{H}_{11}\text{O})]$
	Dicyclohexyl dimethylpyrophosphonodithionate $[(\text{C}_6\text{H}_{11}\text{O})(\text{CH}_3)\text{P}(=\text{S})-\text{O}-\text{P}(=\text{S})(\text{CH}_3)(\text{C}_6\text{H}_{11}\text{O})]$
	Cyclohexyl N,N-diethyl-P-propylphosphonamidate $[(\text{C}_6\text{H}_{11}\text{O})(\text{C}_3\text{H}_7)\text{P}(=\text{O})\text{N}(\text{C}_2\text{H}_5)_2]$
	Isopropyl N,N-diethyl-P,P'-dimethyldiphosphono-P-amidate $[(\text{i}-\text{C}_3\text{H}_7\text{O})(\text{CH}_3)\text{P}(=\text{O})-\text{O}-\text{P}(=\text{O})(\text{CH}_3)\text{N}(\text{C}_2\text{H}_5)_2]$
	O'-Isopropyl N,N-diethyl-P-methyl-P'-ethylphosphono-P-amidate $[(\text{i}-\text{C}_3\text{H}_7\text{O})(\text{C}_2\text{H}_5)\text{P}(=\text{O})-\text{O}-\text{P}(=\text{O})(\text{CH}_3)\text{N}(\text{C}_2\text{H}_5)_2]$
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	Phosphorus oxychloride
3.B.06	Phosphorus trichloride
3.B.07	Phosphorus 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.	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-butyl dimethylsilyloxyethyl)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-butyl dimethylsilyloxyethyl)amine

## Annex 4

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