

# Chemical Characterization and Identification of Organosilicon Contaminants in ISS Potable Water

John E. Straub II<sup>1</sup>, Debrah K. Plumlee<sup>2</sup> and William T. Wallace<sup>3</sup>

*Wyle Science, Technology and Engineering Group, Houston, Texas, 77058*

*and*

Daniel B. Gazda<sup>4</sup>

*NASA Johnson Space Center, Houston, Texas, 77058*

2015 marked the 15th anniversary of continuous human presence on board the International Space Station. During the past year crewmembers from Expeditions 42-46, including two participating in a 1-year mission, continued to rely on reclaimed water as their primary source of potable water. This paper presents and discusses results from chemical analyses performed on ISS water samples returned in 2015. Since the U.S. water processor assembly (WPA) became operational in 2008, there have been 5 instances of organic contaminants breaking through the treatment process. On each occasion, the breakthrough was signaled by an increase in the total organic carbon (TOC) concentration in the product water measured by the onboard TOC analyzer (TOCA). Although the fifth and most recent TOC rise in 2015 was not unexpected, it was the first time where dimethylsilanediol (DMSD) was not the primary compound responsible for the increase. Results from ground analysis of a product water sample collected in June of 2015 and returned on Soyuz 41 showed that DMSD only accounted for <10% of the measured TOC. After considerable laboratory investigation, the compound responsible for the majority of the TOC was identified as monomethylsilanetriol (MMST). MMST is a low-toxicity compound that is structurally similar to DMSD.

## Nomenclature

CE	Capillary Electrophoresis
DAI	Direct Aqueous Injection
DMSD	Dimethylsilanediol
EDV	Russian Portable Water Tank (22 liters)
EPA	Environmental Protection Agency
GC/MS	Gas Chromatography/Mass Spectrometry
HX	Heat Exchanger
IC	Ion Chromatography
ICP/MS	Inductively Coupled Plasma/Mass Spectrometry
ISS	International Space Station
JSC	Johnson Space Center
LC	Liquid Chromatography
LC/MS	Liquid Chromatography/Mass Spectrometry
LCV	Leuco Crystal Violet
MCL	Maximum Contaminant Level
MMST	Monomethylsilanediol
MORD	Medical Operations Requirements Document
N/A	Not Applicable
NA	Not Analyzed
NASA	National Aeronautics and Space Administration
NTU	Nephelometric Turbidity Unit
PFU	Protoflight unit

<sup>1</sup> Senior Engineer, Wyle Science, Technology and Engineering Group, Mail Stop: Wyle/HEF/37A.

<sup>2</sup> Senior Scientist, Wyle Science, Technology and Engineering Group, Mail Stop: Wyle/HEF/37A.

<sup>3</sup> Senior Scientist, Wyle Science, Technology and Engineering Group, Mail Stop: Wyle/HEF/37A.

<sup>4</sup> Environmental Chemistry Laboratory Technical Monitor, NASA Johnson Space Center, Mail Stop: SK4.

PWD	Potable-Water Dispenser
RL	Reporting Limit
RI	Refractive Index
SRV-K	System for Regeneration of Condensate Water
SVO-ZV	System for Water Storage and Dispensing
SWEG	Spacecraft Water Exposure Guideline
TEC	Toxicology and Environmental Chemistry
THM	Trihalomethanes
TOCA	Total Organic Carbon Analyzer
U.S.	United States
UV-VIS	Ultraviolet-Visible
WPA	Water Processor Assembly

## I. Introduction

Analytical results from characterization of chemical contaminants in archival-water samples returned in 2015 from the International Space Station (ISS) Expeditions 42-45 are presented and discussed herein. These results have been evaluated for compliance with the potable-water quality requirements for Russian Segment water supplies in the *ISS Medical Operations Requirement Document (MORD)*<sup>1</sup> and for U.S. Segment water supplies in the *System Specification for the ISS* document<sup>2</sup>. Spacecraft specific limits have also been defined as Spacecraft Water Exposure Guidelines (SWEGs)<sup>3</sup> for some contaminants of interest to NASA and have been used when available. Analytical data for archival-water samples returned from Expeditions 1-41 have previously been published and presented at the International Conference on Environmental Systems<sup>4-16</sup>.

Table 1 summarizes the details for the archival samples that were collected and returned in 2015. All water samples returned on Russian Soyuz vehicles were transported to the United States in the same NASA aircraft as the returning U.S. crewmembers. A representative of the NASA Johnson Space Center (JSC) Toxicology and Environmental Chemistry (TEC) laboratory took possession of these samples upon their arrival in Houston, Texas, then delivered them directly to the laboratory for processing and analysis.

Sample allocation was determined based upon the volume of each return water sample. Samples with sufficient volume received full chemical characterization while those with insufficient volume required reductions in allocated volumes and/or elimination of some analyses. A list of the analytical methods used for sample analysis is provided in Table 2.

Expedition	Flight No.	Samples Received	Sample Type	Sample Collection Date	Sample Receipt Date
42	Soyuz 40	1	PWD Ambient	2/2/2015	3/13/2015
		1	PWD Hot	3/4/2015	
		1	SRV-K Hot	3/4/2015	
		1	SVO-ZV	3/4/2015	
	<b>Total:</b>	<b>4</b>			
43	SpaceX-6	1	PWD Ambient	3/31/2015	5/26/2015
		1	PWD Hot	5/4/2015	
		1	SRV-K Warm	5/4/2015	
		1	SVO-ZV	5/4/2015	
	Soyuz 41	1	PWD Aux	6/10/2015	6/12/2015
<b>Total:</b>	<b>5</b>				
44	Soyuz 42	1	PWD Aux	9/10/2015	9/19/2015
	<b>Total:</b>	<b>1</b>			
45	Soyuz 43	1	PWD Hot	11/10/2015	12/14/2015
		1	PWD Ambient	12/1/2015	
		1	SRV-K Warm	12/1/2015	
		1	SVO-ZV	12/1/2015	
	<b>Total:</b>	<b>4</b>			

**Table 2. TEC Laboratory Methods for Water Analysis**

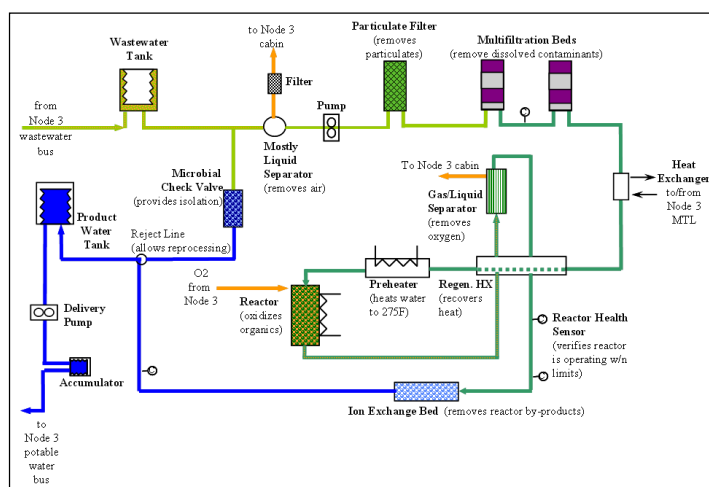
Parameter	Analytical Method
pH and conductivity	Potentiometric
Total Solids	Gravimetric
Turbidity	Nephelometric
Iodine and iodide	Leuco crystal violet (LCV)
Metals/Minerals	Inductively coupled plasma/mass spectrometry (ICP/MS)
Inorganic anions & cations	Ion chromatography (IC)
Total organic carbon (TOC)	Ultraviolet or heated persulfate oxidation
Alcohols and glycols	Direct aqueous injection gas chromatography/mass spectrometry (DAI/GC/MS)
Volatile organics	GC/MS with a purge and trap concentrator
Semivolatile organics	GC/MS after liquid/liquid extraction
Organic acids and amines	Capillary electrophoresis (CE) and IC
Urea/Caprolactam	Liquid chromatography with ultraviolet-visible detector (LC/UV-VIS)
Formaldehyde	GC/MS after derivatization and extraction
Dimethylsilanediol, Monomethylsilanetriol	Liquid chromatography with refractive index detector (LC/RI)

## II. Background

The onboard potable water supplies available for use by the ISS Expeditions 42-45 crews included reclaimed water from the U.S. Segment and both regenerated and stored potable water from the Russian Segment.

### U.S. Potable Water System

The U.S. Segment water processor assembly (WPA) and total organic carbon analyzer (TOCA) both arrived at the ISS in late 2008. The WPA processes a combined wastewater feed (humidity condensate and urine distillate) using a combination of treatment processes including multifiltration beds, high-temperature catalytic oxidation reactor, and ion exchange bed (Figure 1).<sup>4</sup> Iodine biocide is added as part of the final ion exchange process to maintain



**Figure 1 - U.S. Segment Water Processor Assembly (WPA)<sup>1</sup>.**

microbial control in the product water. The U.S potable water dispenser (PWD) provides the ISS crews access to WPA product water. Deiodinated potable water is provided via the ambient and hot ports and iodinated product water is available via the auxiliary (Aux) port. The TOCA provides the capability to measure total organic carbon (TOC) concentrations in WPA product either directly via hose (weekly) or indirectly via bag filled from the PWD (monthly).

## Russian Segment Water Systems

The Russian Segment regenerated potable water system (SRV-K) removes contaminants from humidity condensate using multiple processes, including catalytic oxidation, phase separation, and multifiltration. Silver biocide and minerals are added to the product water before storage. In the SRV-K galley dispenser the product water is pasteurized for microbial control then made available to the ISS crews from either hot or warm ports (Figure 2). The Russian Segment stored water system (SVO-ZV) provides the crews with access to ground-supplied potable water that has been delivered on Russian Progress vehicles and transferred to an EDV bladder tank. The SVO-ZV provides water at ambient temperature from a dispenser port (Figure 3). Both the SRV-K and SVO-ZV water systems have been previously described in detail.<sup>4</sup>



**Figure 2 - SRV-K galley.**  
*Collection of archival sample from SRV-K by Donald Pettit  
(NASA/JSC Photo #ISS006E08616)*



**Figure 3 - SVO-ZV water dispenser.**  
*Collection of water sample from SVO-ZV by Donald Pettit  
(NASA/JSC Photo #ISS006E08628)*

## III. Discussion of Analytical Results

The ISS water samples returned from Expeditions 42-45 were analyzed in the TEC laboratory at JSC. The results from chemical analyses are presented in tabular format in Appendix 1 for SRV-K (regenerated) water, Appendix 2 for SVO-ZV (stored) water, and Appendix 3 for WPA reclaimed water. ISS potability limits have been included in each table for easy comparison to analytical results and a discussion of these results by expedition follows.

### EXPEDITION 42

Four archival potable-water samples were collected during Expedition 42 of 2015 from the PWD ambient, PWD hot, SRV-K hot, and SVO-ZV ports (see Table 1). After their return on the Soyuz 40 vehicle, these samples were received in the TEC laboratory for chemical analysis on March 13, 2015. All samples were analyzed for pH, conductivity, anions, cations, metals, total silicon, minerals, TOC, carboxylates, amines, alcohols, glycols, dimethylsilanediol (DMSD), and formaldehyde, as well as volatile, semivolatile, and nonvolatile organics. Iodine was also analyzed on the PWD samples, dissolved silver on the SVO-ZV and SRV-K samples, and turbidity on the SVO-ZV sample. Total solids were not measured on any of the samples due to limited sample volume.

## ISS U.S. Segment

### PWD Potable-Water Samples

For the PWD ambient and hot water samples collected on February 2 and March 4, 2015, all chemical parameters measured met the ISS potability limits for the U.S. Segment in the *System Specification for the International Space Station, SSP 41000*<sup>2</sup>. Total iodine was not detected (<0.05 mg/L) in either sample, thereby meeting the ISS potability limit at the point of consumption of <0.2 mg/L. An updated historical plot of iodine levels in WPA archival-water samples is shown in Figure 4. Total organic carbon (TOC) levels for both samples were below the method reporting limit of <0.1 mg/L and well below the ISS potability limit of 3.0 mg/L. An updated historical plot of TOC levels in WPA archival-water samples is shown in Figure 5. These results are also consistent with TOC concentrations measured in flight using the TOCA as shown in Table 3. No individual target organic constituents were detected in either sample.

**Table 3. Comparison of Expedition 42 Archive Samples to In-flight TOCA Results**

In-flight TOCA Results			Archive Results		
Date	Location	TOC (mg/L)	Date	Location	TOC (mg/L)
2/02/15	PWD ambient	<0.285	2/02/15	PWD ambient	<0.10
3/02/15	WPA*	<0.285	3/04/15	PWD hot	<0.10

\*TOCA PWD analysis scheduled for 3/04/15 was cancelled due to crew time limitations.

## ISS Russian Segment

### SRV-K Potable-Water Sample

All chemical parameters measured in the SRV-K hot water sample collected on March 4, 2015 met the ISS potability limits for the Russian Segment listed in the *ISS Medical Operations Requirements Document (MORD)*<sup>1</sup>. The total silver concentration of 33 µg/L was below the desired minimum biocidal level of 100 µg/L, which may increase the risk of microbial growth in the system. An updated historical plot of organic carbon levels in SRV-K archival-water samples is shown in Figure 6. The TOC level in the SRV-K sample from Expedition 42 was 0.69 mg/L and well below the ISS limit (Figure 6). The only specific target organic constituent detected in the sample was acetone at 14 µg/L.

### SVO-ZV Potable-Water Sample

All chemical parameters measured in the SVO-ZV water sample collected on March 4, 2015 met the ISS potability limits for the Russian Segment listed in the ISS MORD<sup>1</sup> with the exception of manganese. An updated historical plot of manganese in SVO-ZV archival-water samples is shown in Figure 7. The manganese level of 75 µg/L in the SVO-ZV sample from Expedition 42 was slightly above the ISS limit of 50 µg/L (Figure 7) but well below the SWEG of 300 µg/L<sup>3</sup>. The total silver concentration of 52 µg/L was below the desired minimum biocidal level of 100 µg/L, which may increase the risk of microbial growth in the system. The TOC concentration in the sample was 0.9 mg/L well below the ISS limit. No individual target organic constituents were detected.

## EXPEDITION 43

Five archival water samples were collected during Expedition 43 of 2015 from the PWD ambient, PWD hot, SRV-K warm, SVO-ZV, and PWD Aux ports (see Table 1). After their return on the SpaceX-6 and Soyuz 41 vehicles, these samples were received in the TEC laboratory for chemical analysis on May 26 and June 12, 2015, respectively. The four potable water samples that returned on SpaceX-6 were analyzed for pH, conductivity, anions, cations, metals, total silicon, minerals, TOC, carboxylates, amines, alcohols, glycols, DMSD, and formaldehyde, as well as volatile, semivolatile, and nonvolatile organics. Iodine was also analyzed on the PWD potable water samples as well as turbidity and dissolved silver on the SRV-K and SVO-ZV samples. Total solids were not measured on any of the potable samples due to limited sample volume. The product water sample returned on Soyuz 41 was analyzed for cations, metals, total silicon, reactive silica, minerals, TOC, carboxylates, amines, alcohols, glycols, DMSD, formaldehyde, volatile organics, and nonvolatile organics, based on limited sample volume.

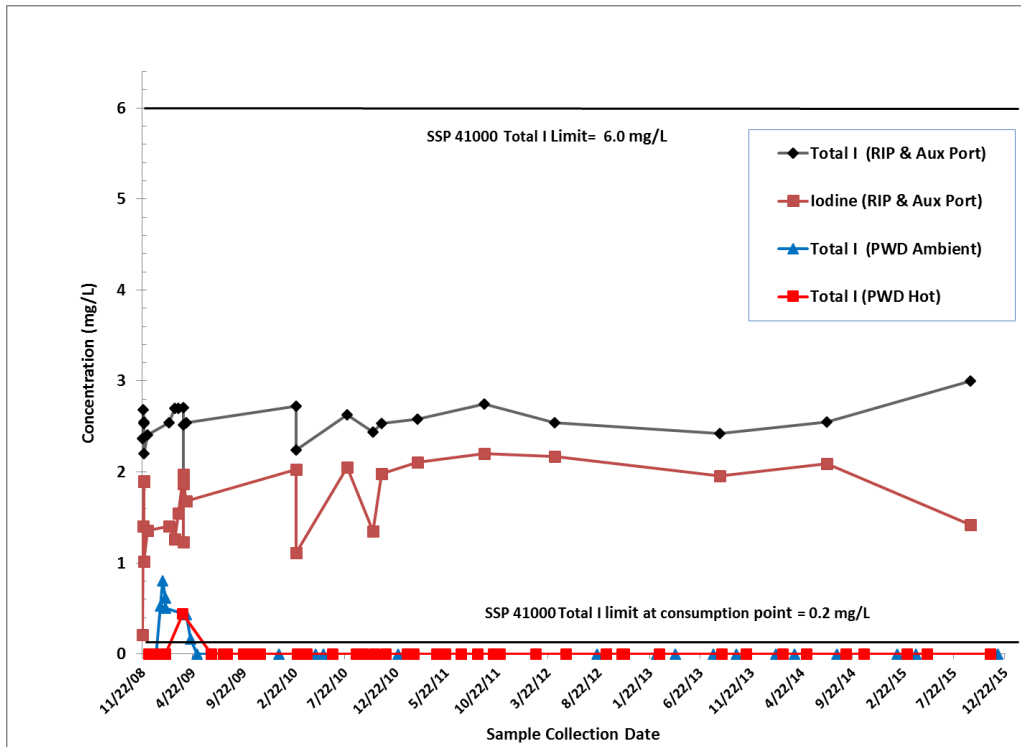


Figure 4 - Total I & iodine levels in WPA archival-water samples from ISS ULF2 to Soyuz 43<sup>4-10</sup>. 2015 data is from Expeditions 42-45

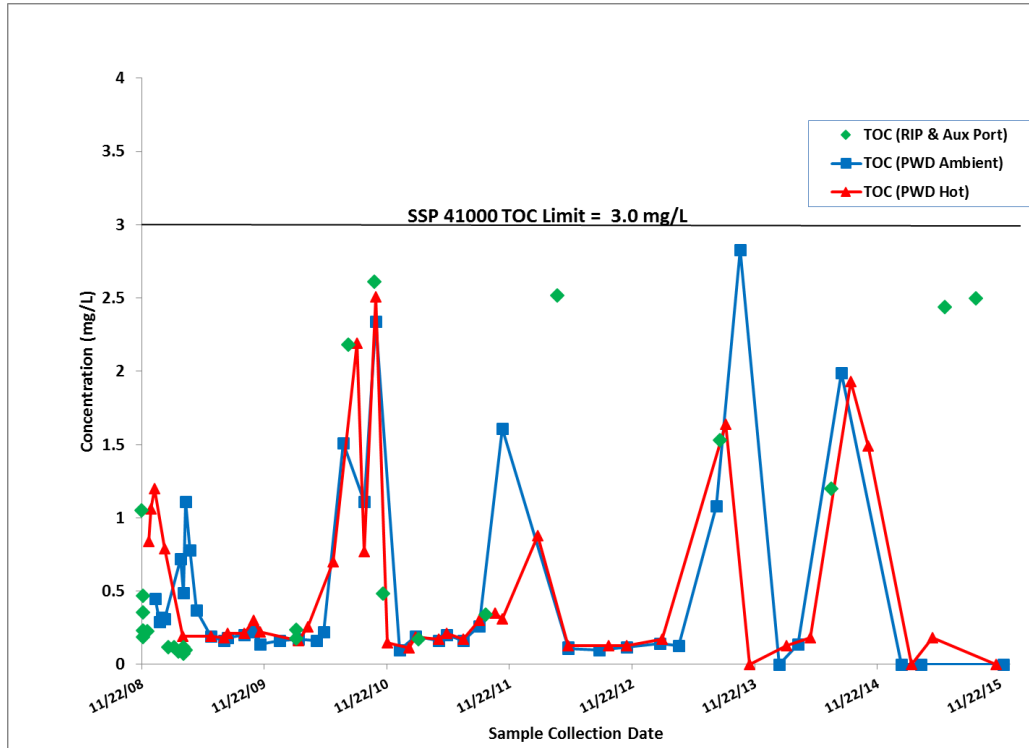
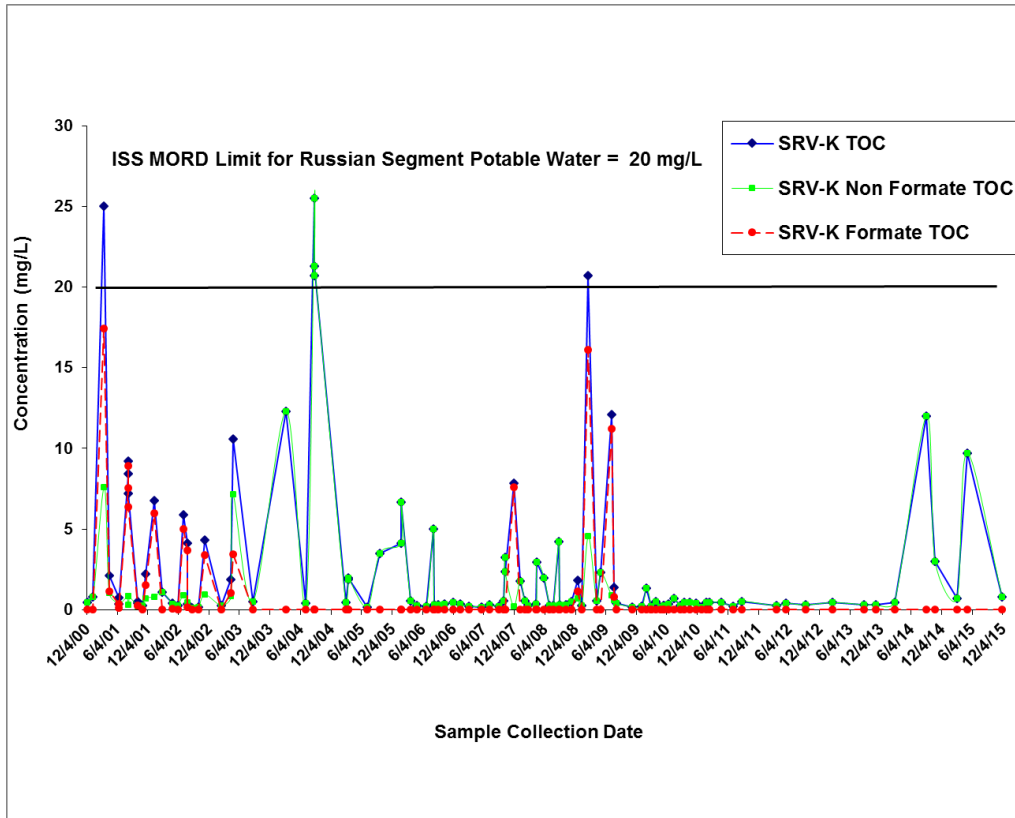
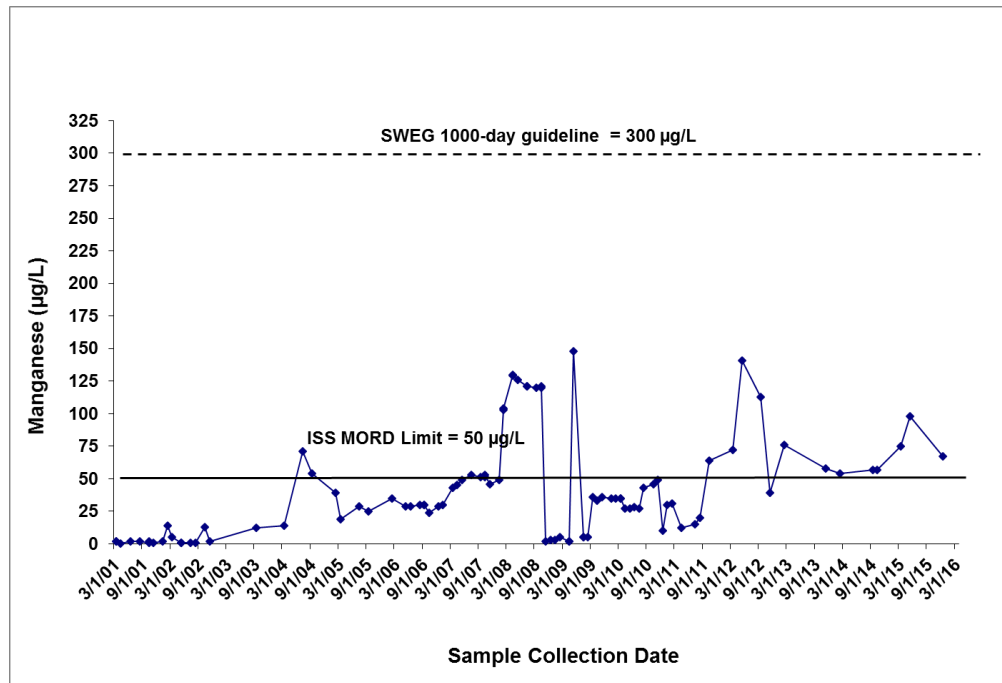


Figure 5 - TOC levels in WPA archival-water samples from ISS ULF2 to Soyuz 43<sup>4-10</sup>. Note the 4 previous TOC rises in 2010, 2012, 2013, and 2014 from dimethylsilanediol breakthrough, 2015 data is from Expeditions 42-45



**Figure 6 - Total, formate, and nonformate organic carbon levels in SRV-K water samples from ISS Flights 4A to Soyuz 43<sup>4-16</sup>. 2015 data is from Expeditions 42-45**



**Figure 7 - Manganese levels in SVO-ZV water samples from ISS Flights 5A to Soyuz 43<sup>4-16</sup>. 2015 data is from Expeditions 42-45**

## ISS U.S. Segment

### *PWD Potable-Water Samples*

For the PWD ambient and hot water samples collected on March 31 and May 4, 2015, all chemical parameters measured met the ISS potability limits in SSP 41000<sup>2</sup>. Total organic carbon (TOC) levels were <0.1 mg/L and 0.18 mg/L, respectively, and well below the potability limit of 3.0 mg/L as shown in Figure 5. These results are also consistent with TOC concentrations measured in flight using the TOCA as shown in Table 4. The only individual target organic constituents identified in the samples were methyl sulfone at 86 and 71 µg/L and diethylphthalate at 14 µg/L (PWD hot only). Total iodine was not detected (<0.05 mg/L) in either sample as shown in Figure 4.

**Table 4. Comparison of Expedition 43 Archive Samples to In-flight TOCA Results**

In-flight TOCA Results			Archive Results		
Date	Location	TOC (mg/L)	Date	Location	TOC (mg/L)
3/31/15	PWD ambient	<0.285	3/31/15	PWD ambient	<0.10
5/4/15	PWD hot	<0.285	5/4/15	PWD hot	0.180

### *Product Water Sample (PWD Aux)*

A contingency sample was collected from the PWD Aux port during Expedition 43 on June 10, 2015 in response to a rapid increase in the TOC concentration in the WPA product water as measured by the in-flight TOCA. The measured TOC of 2.44 mg/L in the PWD Aux sample was much higher than that found in the May 4 PWD hot sample (0.18 mg/L), but remained below the TOC potability limit of 3.0 mg/L (Figure 5). Since the U.S. water processor assembly (WPA) became operational in 2008, there have been 5 previous instances of organic contaminants breaking through the WPA treatment process. On each occasion, the breakthrough was signaled by an increase in the TOC concentration in the product water as measured by the in-flight TOCA. For all of the previous TOC increases, dimethylsilanediol (DMSD) was determined to be the primary source.<sup>4-9</sup> Although DMSD was measured at a concentration of 0.85 mg/L in the June PWD Aux sample, that level was only sufficient to account for 9% of the measured TOC. Therefore DMSD was not the primary compound responsible for the elevated TOC and no other individual target organic constituents were detected in the sample. The total silicon concentration in the sample of 4.3 mg/L was much higher than typically found in WPA water when DMSD is not present, so analysis for reactive silica (inorganic silicon) was performed in the Advanced Water Recovery Lab at JSC. Results from that analysis showed 2.0 mg/L SiO<sub>2</sub> (or 0.94 mg/L total silicon equivalent), which suggested that organosilicon compounds other than DMSD must be present but unidentified in the sample. After considerable laboratory investigation the unknown compound was determined to be monomethylsilanetriol (MMST), an organosilicon compound structurally similar to DMSD. After reviewing the available toxicologic data on MMST an interim SWEG was set at 110 mg/L, which is much higher than the concentration that could potentially have been present in the June PWD Aux sample. Accordingly, the presence of MMST at levels well below the SWEG was not expected to pose a significant crew health risk, so a waiver was put in place. This allowed the ISS crews to temporarily continue consumption of WPA water until replacement ion exchange and multifiltration beds arrived on the HTV-5 resupply vehicle. The replacement beds were installed in early October to remediate the TOC rise.

## ISS Russian Segment

### *SRV-K Potable-Water Sample*

All chemical parameters measured in the SRV-K warm water sample collected on May 4, 2015 met the ISS MORD potability limits with the exceptions of manganese and turbidity. The manganese concentration of 95 µg/L was above the MORD limit of 50 µg/L but well below the SWEG of 300 µg/L. The measured turbidity of 1.6 NTU was only slightly above the MORD limit of 1.5 NTU, but turbidity is an aesthetic parameter for which a slight elevation is not considered to pose a risk to crew health. The total silver concentration of 61 µg/L was below the desired minimum biocidal level of 100 µg/L, which may increase the risk of microbial growth in the system. The TOC level in the sample of 9.7 mg/L was below the ISS MORD limit (Figure 6). Organic compounds detected near or above 1 mg/L consisted of ethanol (11.2 mg/L), acetate (4.8 mg/L) and methanol (0.9 mg/L). Trace levels of acetone, acetaldehyde and bis-(2-ethylhexyl)phthalate were also measured.

### *SVO-ZV Potable-Water Sample*

All chemical parameters measured in the SVO-ZV water sample collected on May 4, 2015 met the ISS MORD potability limits with the exception of manganese. The manganese level of 98 µg/L in the sample was slightly above the ISS limit of 50 µg/L (Figure 7) but well below the SWEG of 300 µg/L<sup>15</sup>. The total silver concentration of 108 µg/L was above the desired minimum biocidal level of 100 µg/L. The TOC concentration in the sample was



0.89 mg/L and well below the ISS MORD limit. Trace levels of bis-(2-ethylhexyl) adipate, bis-(2-ethylhexyl) phthalate, and monomethyl phthalate were the only specific target organic constituents detected.

#### EXPEDITION 44

Again, in response to the 2015 TOC rise, a WPA product water sample was collected from the PWD Aux port on September 10, 2015 during Expedition 44 (see Table 1). After returning on the Soyuz 42 vehicle, the sample was received in the TEC laboratory for chemical analyses on September 19, 2015. The sample was analyzed for pH, conductivity, anions, cations, metals, total silicon, reactive silica, minerals, TOC, carboxylates, amines, alcohols, glycols, DMSD, MMST, formaldehyde, volatile organics, and nonvolatile organics. Total solids and semivolatile organics were not analyzed due to limited sample volume.

##### *Product Water Sample (PWD Aux)*

The measured TOC of 2.50 mg/L in the September PWD Aux sample was slightly higher than that found in the June PWD Aux sample (2.44 mg/L), but remained below the TOC potability limit of 3.0 mg/L (Figure 5). The individual target organic constituents detected in the sample were DMSD at 5.5 mg/L, MMST at 3.8 mg/L, and trimethylamine at 0.289 mg/L, accounting for about 83% of the measured TOC. DMSD accounted for the majority of the TOC (57%) in the September sample, whereas MMST was estimated to be the primary source of TOC in the June sample. The total silicon concentration was 16.5 mg/L in the September sample, which was the highest level ever measured for WPA product water samples. Because this value was much higher than the silicon that could be accounted for by DMSD and MMST (~2.8 mg/L), an aliquot of the sample was analyzed for reactive silica in the Advanced Water Recovery Lab at JSC. The result of this analysis was 35 mg/L of SiO<sub>2</sub> (or 16 mg/L total silicon equivalent) confirming that inorganic silicon accounted for a significant portion of the total silicon in the sample. Iodine was present at a concentration of 1.42 mg/L, which fell within the required biocidal range of 1.0 to 4.0 mg/L.

#### EXPEDITION 45

Four archival potable-water samples were collected during Expedition 45 of 2015 from the PWD ambient, PWD hot, SRV-K warm, and SVO-ZV ports (see Table 1). After their return on the Soyuz 43 vehicle, these samples were received in the TEC laboratory for chemical analyses on December 14, 2015. All samples were analyzed for pH, conductivity, iodine, anions, cations, metals, total silicon, minerals, TOC, carboxylates, amines, alcohols, glycols, DMSD, MMST, and formaldehyde, as well as volatile, semivolatile, and nonvolatile organics. Dissolved silver was analyzed on the SRV-K and SVO-ZV samples. Turbidity was also analyzed on the PWD hot and SRV-K warm samples. Total solids were not measured on any of the samples due to limited sample volume.

#### ISS U.S. Segment

##### *PWD Potable-Water Samples*

For the PWD water samples collected on November 10 and December 1, 2015, all chemical parameters measured met the ISS potability limits in SSP 41000<sup>2</sup>. The TOC levels for both samples were below the method reporting limit of <0.1 mg/L and well below the ISS potability limit of 3.0 mg/L (see Figure 5). These results were also consistent with TOC concentrations measured in flight using the TOCA as shown in Table 5. These results together confirmed that the replacement of the ion exchange and multifiltration beds on October 2, 2105 had resulted in a return to nominal TOC levels in the WPA product water. The only individual target organic constituents detected were methyl sulfone at 115 µg/L in PWD ambient and diethylphthalate at 13 µg/L in PWD hot. Total iodine was not detected (<0.05 mg/L) in either sample, thereby meeting the ISS potability limit at the point of consumption of <0.2 mg/L (Figure 4).

**Table 5. Comparison of Expedition 45 Archive Samples to In-flight TOCA Results**

In-flight TOCA Results			Archive Results		
Date	Location	TOC(mg/L)	Date	Location	TOC (mg/L)
11/10/15	PWD hot	<0.285	11/10/15	PWD hot	<0.10
12/1/15	PWD ambient	<0.285	12/1/15	PWD ambient	<0.10

## **ISS Russian Segment**

### ***SRV-K Potable-Water Sample***

All chemical parameters measured in the SRV-K warm water sample collected on December 1, 2015 met the ISS MORD potability limits with the exceptions of manganese and turbidity. Although the manganese level of 59 µg/L was just slightly above the MORD limit of 50 µg/L, it was well below the SWEG of 300 µg/L. The measured turbidity of 2.4 NTU was above the MORD limit of 1.5 NTU; however, slightly elevated turbidity alone is not considered to pose a significant increase in risk to crew health. The total silver concentration of 77 µg/L was below the desired minimum biocidal level of 100 µg/L, which may increase the risk of microbial growth in the system. The TOC level in the sample of 0.78 mg/L was well below the ISS MORD limit (Figure 6). No individual target organic compounds were detected in the sample.

### ***SVO-ZV Potable-Water Sample***

All chemical parameters measured in the SVO-ZV water sample collected on December 1, 2015 met the ISS MORD potability limits with the exception of manganese. The manganese level of 67 µg/L in the sample was slightly above the ISS limit of 50 µg/L but well below the SWEG of 300 µg/L<sup>3</sup> (see Figure 7). The total silver concentration of 102 µg/L was above the desired minimum biocidal level of 100 µg/L. The TOC concentration in the sample was 1.12 mg/L, which is well below the ISS MORD limit. No individual target organic compounds were detected in the sample.

## **IV. Conclusions and Recommendations**

Despite the fifth and latest TOC rise, the WPA potable water available during ISS Expeditions 42-45 was determined to be chemically acceptable for consumption based upon the analytical data from archival-water samples returned in 2015. There have been 5 instances of organic contamination breaking through the treatment processes of the WPA since it became operational in 2008. Each time that breakthrough occurred, it was signaled by an increase in the TOC concentration of WPA product water as measured by the in-flight TOCA. Although the most recent TOC rise in 2015 was not unexpected, it was the first time that DMSD was not the primary organic constituent contributing to the increase. After considerable laboratory investigation the unknown compound was eventually identified as monomethylsilanetriol (MMST), a low-toxicity organosilicon compound that is structurally similar to DMSD. The 2015 TOC rise in WPA product water was anticipated based upon experience and lessons learned from previous TOC rises, but the need for identification and subsequent confirmation of the presence of MMST was unique. Even though the timing of DMSD breakthrough of the WPA treatment processes is considered predictable based upon historical experience, the root cause for the presence of MMST in WPA product water needs to be further investigated.

Russian Segment potable water supplies (regenerated and stored) were chemically acceptable for crew consumption during Expeditions 42-45 of 2015 based upon the analytical results for archival-water samples collected and returned from the SRV-K and SVO-ZV ports. Although manganese levels in all 3 of the SVO-ZV samples and in 2 of 3 SRV-K samples slightly exceeded the ISS MORD limit of 50 µg/L, all levels were well below the 300 µg/L SWEG limit. Silver biocide levels in all three SRV-K samples and one SVO-ZV sample were below the minimum acceptable biocide level of 100 µg/L, which may increase the risk of microbial growth in the systems. These results suggest that heating of the water by the pasteurization unit serves as the primary means of microbial control in the SRV-K galley. Accordingly, it is recommended to continue collecting archive-samples for ground analysis of manganese and silver biocide levels in both the SRV-K and SVO-ZV water supplies.

## **Appendices**

Chemical analysis results summarizing the analytes detected in archival potable-water samples returned during Expeditions 42-45 of 2015 for Russian Segment SRV-K (regenerated water) and SVO-ZV (stored water) systems are provided in Appendix 1 and Appendix 2, respectively. Results for analytes detected in U.S. Segment archival-water samples collected from the PWD hot, ambient, and auxiliary ports and returned in 2015 during those same expeditions, are provided in Appendix 3.

## **Acknowledgments**

Analytical work described herein was performed at the NASA Johnson Space Center TEC laboratory under NASA contracts NAS9-02078 and NNJ15HK11B. The authors wish to acknowledge the ISS Expeditions 42-45 crews for collecting and storing archival-water samples returned in 2015, as well as TEC laboratory chemists Jim Alverson, Mickie Benoit, Robert Gillispie, David Hunter, Mike Kuo, and Jeff Rutz for performing chemical analyses of the returned samples.

## References

- <sup>1</sup>*ISS Medical Operations Requirements Document*, SSP 50260, Revision C, NASA Johnson Space Center, February 2006, Section 7.2 and Appendix D, Table D-1.
- <sup>2</sup>*System Specification for the International Space Station*, SSP 41000 BY, National Aeronautics and Space Administration, September 21, 2012, Table LXX.
- <sup>3</sup>*Spacecraft Water Exposure Guidelines (SWEGS)*, JSC-63414, NASA Johnson Space Center, November 2008.
- <sup>4</sup>Straub, J.E., Plumlee, D.K., and Mudgett, P.D., “2014 ISS Potable Water Characterization and Continuation of the Dimethylsilanediol Chronicle”, ICES-2015-038, *Proceedings of the 2015 International Conference on Environmental Systems*, 2015.
- <sup>5</sup>Straub, J.E., Plumlee, D. K., Schultz, J. R., and Mudgett, P.D., “International Space Station Potable Water Characterization for 2013”, ICES-2014-190, *Proceedings of the 2014 International Conference on Environmental Systems*, 2014.
- <sup>6</sup>Straub, J.E., Plumlee, D. K., Schultz, J. R., and McCoy, J.T., “Potable-Water Quality for International Space Station Expeditions 30-33”, AIAA-2013-3310, *AIAA Proceedings of the 2013 International Conference on Environmental Systems*, 2013.
- <sup>7</sup>Straub, J.E., Plumlee, D. K., Schultz, J. R., and McCoy, J.T., “International Space Station Potable Water Quality for Expeditions 26 through 29”, AIAA-2012-3413, *AIAA Proceedings of the 2012 International Conference on Environmental Systems*, 2012.
- <sup>8</sup>Straub, J. E., Plumlee, D. K., Schultz, J. R., and McCoy, J.T., “Chemical Analysis Results for Potable Water for ISS Expeditions 21-25”, AIAA-2011-5152, *AIAA Proceedings of the 2011 International Conference on Environmental Systems*, 2011.
- <sup>9</sup>Straub, J. E., Plumlee, D. K., and Schultz, J. R., “ISS Expeditions 16 thru 20: Chemical Analysis Results for Potable Water”, AIAA-2010-6042, *AIAA Proceedings of the 2010 International Conference on Environmental Systems*, 2010.
- <sup>10</sup>Straub, J. E., Plumlee, D. K., and Schultz, J. R., “Chemical Analysis Results for Potable Water Returned from ISS Expeditions 14 and 15”, *SAE International Journal of Aerospace*. 1(1): 556-577, 2008.
- <sup>11</sup>Straub, J. E., Plumlee, D. K., and Schultz, J. R., “Sampling and Chemical Analysis of Potable Water for ISS Expeditions 12 and 13”, *SAE International Journal of Aerospace*, 2007.
- <sup>12</sup>Straub, J. E., Plumlee, D. K., and Schultz, J. R., “ISS Expeditions 10 & 11 Potable Water Sampling and Chemical Analysis Results”, *SAE International Journal of Aerospace*, 2006.
- <sup>13</sup>Straub, J. E., Plumlee, D. K., and Schultz, J. R., “Chemical Analysis of ISS Potable Water from Expeditions 8 and 9”, *SAE International Journal of Aerospace*, 2005.
- <sup>14</sup>Straub, J. E., Plumlee, D. K., and Schultz, J. R., “ISS Potable Water Sampling and Chemical Analysis: Expeditions 6 & 7”, *SAE International Journal of Aerospace*, 2004.
- <sup>15</sup>Plumlee, D. K. and Schultz, J. R., “ISS Potable Water Sampling and Chemical Analysis: Expeditions 4 & 5”, *SAE International Journal of Aerospace*, 2003.
- <sup>16</sup>Plumlee, D. K. and Schultz, J. R., “Chemical Sampling and Analysis of ISS Potable Water: Expeditions 1-3”, *SAE International Journal of Aerospace*, 2002.

**Appendix 1. ISS SRV-K Potable Water (Regenerated)**  
**Summary of Analytes Detected in Samples Returned from Expeditions 42 through 45**

Mission				Soyuz 40/Exp. 42	SpaceX-6/Exp. 43	Soyuz 43/Exp. 45
Sample Location		Potable Water		SRV-K Hot	SRV-K Warm	SRV-K Warm
Sample Description		Maximum Contaminant	Maximum Contaminant	Potable Water	Potable Water	Potable Water
Sample Date		Level	Level	3/4/2015	5/4/2015	12/1/2015
Analysis/Sample ID	Units	(MCL)	Source	20150313004	20150526010	20151214004
<b>Physical Characteristics</b>						
pH	pH units	5.5-9.0	MORD	7.56	7.80	7.92
Conductivity	µS/cm			154	296	260
Turbidity	NTU	1.5	MORD	NA	1.6	2.4
<b>Iodine (LCV) - 0 of 1 target analyte above Reporting Limit (RL)</b>						
<b>Anions/Cations (IC) - 7 of 11 target analytes above RL</b>						
Chloride	mg/L	250	MORD	4.4	9.8	8.8
Fluoride	mg/L	1.5/4	MORD/EPA	<0.1	0.1	0.2
Sulfate	mg/L	250	MORD	18.5	27.2	14.8
Calcium	mg/L	100	MORD	20.7	36.4	29.9
Magnesium	mg/L	50	MORD	4.34	8.49	8.59
Potassium	mg/L			0.70	1.83	1.70
Sodium	mg/L			3.28	8.29	7.89
<b>Metals (ICP/MS) - 13 of 23 target analytes above RL</b>						
Calcium	mg/L	100	MORD	22.0	38.6	32.7
Magnesium	mg/L	50	MORD	4.26	9.15	8.52
Potassium	mg/L			0.62	2.00	1.68
Sodium	mg/L			3.24	8.77	7.88
Aluminum	µg/L			32	47	90
Barium	µg/L	1,000/10,000	MORD/SWEG	11	27	53
Copper	µg/L	1,000/1,300	MORD/EPA	4	2	6
Iron	µg/L	300	MORD	15	<5	18
Manganese	µg/L	50/300	MORD/SWEG	37	95	59
Nickel	µg/L	100/300	MORD/SWEG	3	3	2
Silver	µg/L	500/400	MORD/SWEG	33	61	77
Silver, Dissolved	µg/L			2	5	10
Zinc	µg/L	5,000/2,000	MORD/SWEG	49	63	35
<b>Silicon (ICP/MS)</b>						
Silicon (ICP/MS)	µg/L			558	1340	2290
<b>Total Organic Carbon (Heated persulfate oxidation)</b>						
Inorganic Carbon	mg/L			14.2	24.3	25.0
Organic Carbon	mg/L	20	MORD	0.69	9.70	0.78
<b>Volatile Organics (GC/MS) - 2 of 84 target analytes above RL</b>						
Acetone	µg/L	15,000	SWEG	14	52	<5
<b>Volatile Organics -Special Interest Compounds (Semi-quantitative) - 1 of 2 target analytes above RL</b>						
Acetaldehyde	µg/L			not found	99	not found
<b>Semi-volatiles (GC/MS) - 0 of 9 target analytes above RL</b>						
<b>Acid Extractables (GC/MS) -EPA 625 List - 0 of 15 target analytes above RL</b>						
<b>Base/Neutral Extractables (GC/MS)- EPA 625 List - 1 of 45 target analytes above RL</b>						
bis-(2-Ethylhexyl)phthalate	µg/L	20,000/6	SWEG/EPA	<20	60	<8
<b>Alcohols (DAI/GC/MS) - 2 of 14 target analytes above RL</b>						
Ethanol	µg/L			<400	11,200	<400
Methanol	µg/L	40,000	SWEG	<400	886	<400
<b>Glycols (DAI/GC/MS) - 0 of 2 target analytes above RL</b>						
<b>Silanol (DMSD and MMST by LC/RI) - 0 of 2 target analytes above RL</b>						
<b>Carboxylates (CE/IC) - 1 of 11 target analytes above RL</b>						
Acetate	µg/L			MI	4770	<500
<b>Amines (CE/IC) - 0 of 4 target analytes above RL</b>						
<b>Aldehydes (GC/MS) - 0 of 1 target analyte above RL</b>						
<b>Non-volatiles (LC/UV-VIS) - 0 of 2 target analytes above RL</b>						
Organic Carbon Recovery	percent			1.30	84.98	0.00
Unaccounted Organic Carbon	mg/L			0.68	1.46	0.78

NOTES: NA=Not analyzed; MI=Matrix interference; MORD = Medical Operations Requirements Document, SSP 50260;  
EPA = Environmental Protection Agency; SWEG = Spacecraft Water Exposure Guideline, JSC 63414

**Appendix 2. ISS SVO-ZV Potable Water (Stored)**

**Summary of Analytes Detected in Samples Returned from Expeditions 42 through 45**

Mission				Soyuz 40/Exp. 42	SpaceX-6/Exp. 43	Soyuz 43/Exp. 45
Sample Location		Potable Water		SVO-ZV	SVO-ZV	SVO-ZV
Sample Description		Maximum Contaminant	Maximum Contaminant	Potable Water	Potable Water	Potable Water
Sample Date		Level	Level	3/4/2015	5/4/2015	12/1/2015
Analysis/Sample ID	Units	(MCL)	Source	20150313003	20150526009	20151214003
<b>Physical Characteristics</b>						
pH	pH units	5.5-9.0	MORD	7.82	7.88	7.91
Conductivity	µS/cm			357	345	320
Turbidity	NTU	1.5	MORD	0.4	1.3	NA
<b>Iodine (LCV) - 0 of 1 target analyte above Reporting Limit (RL)</b>						
<b>Anions/Cations (IC) - 8 of 11 target analytes above RL</b>						
Chloride	mg/L	250	MORD	10.5	10.9	11.7
Fluoride	mg/L	1.5/4	MORD/EPA	0.1	0.1	0.3
Nitrate as Nitrogen (NO3-N)	mg/L	10	MORD/EPA	0.2	<0.2	<0.2
Sulfate	mg/L	250	MORD	35.2	28.0	21.1
Calcium	mg/L	100	MORD	46.7	42.7	44.1
Magnesium	mg/L	50	MORD	10.4	10.6	10.9
Potassium	mg/L			2.13	2.18	2.27
Sodium	mg/L			8.68	9.63	10.5
<b>Metals (ICP/MS) - 13 of 23 target analytes above RL</b>						
Calcium	mg/L	100	MORD	47.9	45.5	42.4
Magnesium	mg/L	50	MORD	10.2	11.6	10.4
Potassium	mg/L			1.88	2.26	2.17
Sodium	mg/L			8.74	9.67	10.1
Aluminum	µg/L			138	83	232
Barium	µg/L	1,000/10,000	MORD/SWEG	23	30	68
Copper	µg/L	1,000/1,300	MORD/EPA	2	2	2
Iron	µg/L	300	MORD	<5	<5	16
Manganese	µg/L	50/300	MORD/SWEG	75	98	67
Nickel	µg/L	100/300	MORD/SWEG	4	1	3
Silver	µg/L	500/400	MORD/SWEG	52	108	102
Silver, Dissolved	µg/L			2	25	8
Zinc	µg/L	5,000/2,000	MORD/SWEG	175	86	61
<b>Silicon (ICP/MS)</b>						
Silicon (ICP/MS)	µg/L			1960	1990	2950
<b>Total Organic Carbon (Heated persulfate oxidation)</b>						
Inorganic Carbon	mg/L			34.5	30.1	31.3
Organic Carbon	mg/L	20	MORD	0.89	0.89	1.12
<b>Volatile Organics (GC/MS) - 0 of 86 target analytes above RL</b>						
<b>Semi-volatiles (GC/MS) - 1 of 9 target analytes above RL</b>						
bis-(2-Ethylhexyl)adipate	µg/L	400	EPA	<20	90	<20
<b>Acid Extractables (GC/MS) - EPA 625 List - 0 of 15 target analytes above RL</b>						
<b>Base/Neutral Extractables (GC/MS) - EPA 625 List - 1 of 45 target analytes above RL</b>						
bis-(2-Ethylhexyl)phthalate	µg/L	20,000/6	SWEG/EPA	<20	161	<20
<b>Semi-volatiles - Special Interest Compounds (Semi-quantitative - 2 pt curve) - 1 of 47 target analytes above RL</b>						
Monomethylphthalate	µg/L			not found	40	not found
<b>Alcohols (DAI/GC/MS) - 0 of 14 target analytes above RL</b>						
<b>Glycols (DAI/GC/MS) - 0 of 2 target analytes above RL</b>						
<b>Silanols (DMSD and MMST by LC/RI) - 0 of 2 target analytes above RL</b>						
<b>Carboxylates (CE/IC) - 0 of 11 target analytes above RL</b>						
<b>Amines (CE/IC) - 0 of 4 target analytes above RL</b>						
<b>Aldehydes (GC/MS) - 0 of 1 target analyte above RL</b>						
<b>Non-volatiles (LC/UV-VIS) - 0 of 2 target analytes above RL</b>						
Organic Carbon Recovery	percent			0.00	23.14	0.00
Unaccounted Organic Carbon	mg/L			0.89	0.69	1.12

NOTES: NA=Not analyzed; MORD = Medical Operations Requirements Document, SSP 50260;  
EPA = Environmental Protection Agency; SWEG = Spacecraft Water Exposure Guideline, JSC 63414

Appendix 3. ISS WPA - PWD Ambient, Hot, and Aux Ports

Summary of Analytes Detected in Samples Returned from Expeditions 42 through 45

Mission				Soyuz 40/Exp. 42		SpaceX-6/Exp. 43		Soyuz 43/Exp. 45		Soyuz 41/Exp. 43	Soyuz 42/Exp. 44
Sample Location	Potable Water			WPA PWD Ambient	WPA PWD Hot	WPA PWD Ambient	WPA PWD Hot	WPA PWD Hot	WPA PWD Ambient	PWD Aux Port	PWD Aux Port
Sample Description	Maximum Contaminant			Potable Water	Potable Water	Potable Water	Potable Water	Potable Water	Potable Water	Product Water	Product Water
Sample Date	Level			2/2/2015	3/4/2015	3/31/2015	5/4/2015	11/10/2015	12/1/2015	6/10/2015	9/10/2015
Analysis/Sample ID	Units	(MCL)	Source	20150313001	20150313002	20150526007	20150526008	20151214001	20151214002	20150612003	20150919001
<b>Physical Characteristics</b>											
pH	pH units	4.5-8.5	41000	6.25	5.65	6.17	6.58	5.59	5.46	NA	6.72
Conductivity	µS/cm			2	3	1	1	2	2	NA	4
Turbidity	NTU	1	41000	NA	NA	NA	NA	<0.4	NA	NA	NA
<b>Iodine (LCV)</b>											
Total I	mg/L	6/0.2	41000 (Total/at pt of consumption)	<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	NA	3.00
Iodine	mg/L			<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	NA	1.42
Iodide	mg/L			<0.05	<0.05	<0.05	<0.05	<0.05	<0.05	NA	1.58
<b>Anions/Cations (IC) - 0 of 11 target analytes above RL</b>											
<b>Metals (ICP/MS) - 9 of 22 target analytes above RL</b>											
Calcium	mg/L	30	41000	<0.01	<0.01	<0.01	0.01	<0.01	<0.01	0.04	0.10
Potassium	mg/L	340	41000	<0.01	<0.01	<0.01	<0.01	0.01	<0.01	0.02	0.11
Sodium	mg/L			<0.01	<0.01	<0.01	<0.01	0.05	0.05	<0.02	0.05
Aluminum	µg/L			2	1	<1	<1	5	<1	<2	<2
Barium	µg/L	10,000	SWEG&41000	<1	6	<1	<1	<1	1	<2	<2
Chromium	µg/L	230	41000	<1	<1	<1	<1	<1	<1	<2	24
Iron	µg/L	300	41000	49	<5	<5	<5	<5	<5	<10	<10
Nickel	µg/L	300	SWEG&41000	4	7	7	6	8	2	96	101
Zinc	µg/L	2000	SWEG&41000	<1	<1	2	2	2	2	<2	4
<b>Silicon (ICP/MS)</b>											
Silicon (ICP/MS)	µg/L			25	18	44	248	62	30	4,260	16,500
<b>Total Organic Carbon (Ultraviolet persulfate oxidation)</b>											
Inorganic Carbon	mg/L			0.96	0.96	0.79	0.80	0.84	0.72	0.81	0.37
Organic Carbon	mg/L	3	41000	<0.10	<0.10	<0.10	0.18	<0.10	<0.10	2.44	2.50
<b>Volatile Organics (GC/MS) - 0 of 86 target analytes above Reporting Limit (RL)</b>											
<b>Semi-volatiles (GC/MS) - 1 of 9 target analytes above RL</b>											
Methylsulfone	µg/L			NA	NA	86	71	<8	115	NA	NA
<b>Acid Extractables (GC/MS) - EPA 625 List - 0 of 15 target analytes above RL</b>											
<b>Base/Neutral Extractables (GC/MS) - EPA 625 List - 1 of 46 target analytes above RL</b>											
Diethylphthalate	µg/L			<8	<8	<8	14	13	<16	NA	NA
<b>Semi-volatiles - Special Interest Compounds (Semi-quantitative - 2 pt curve) - 0 of 47 target analytes above RL</b>											
<b>Alcohols (DAI/GC/MS) - 0 of 14 target analytes above RL</b>											
<b>Glycols (DAI/GC/MS) - 0 of 2 target analytes above RL</b>											
<b>Silanol (DMSD and MMST by LC/RI) - 2 of 2 target analytes above RL</b>											
Dimethylsilanediol (DMSD)	µg/L	35,000	SWEG	<500	<500	<500	<500	<1000	<1000	850	5500
Monomethylsilanetriol (MMST)	µg/L	110,000	SWEG	NA	NA	NA	NA	<1000	<1000	NA	3800
<b>Carboxylates (CE/IC) - 0 of 11 target analytes above RL</b>											
<b>Amines (CE/IC) - 1 of 4 target analytes above RL</b>											
Trimethylamine	µg/L	Trialkylamines 400	SWEG	<500	<500	<250	<250	<250	<250	<250	289
<b>Aldehydes (GC/MS) - 0 of 1 target analyte above RL</b>											
<b>Non-volatiles (LC/UV-VIS) - 0 of 2 target analytes above RL</b>											
Organic Carbon Recovery	percent			NA	NA	NA	15.11	NA	NA	9.07	83.71
Unaccounted Organic Carbon	mg/L			NA	NA	NA	0.15	NA	NA	2.22	0.41

NOTES: NA=Not analyzed; 41000 = System Specification for ISS, SSP 41000; SWEG = Spacecraft Water Exposure Guideline, JSC 63414