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SUBJECT: Toxicological Assessment of ISS Air and Water Quality: October 4, 2018 – December 20, 2018 (Increment 57), Including NG-10 and SpaceX-16 Ingress

SUMMARY: Based on these data, air quality was acceptable on ISS for this period and potable water remains acceptable for crew consumption.

AIR QUALITY

Four archive air samples were collected in mini grab sample containers (mGSCs) on ISS during Increment 57, two each on October 8 and November 19, 2018. mGSC samples were also collected during first ingress operations in NG-10 (November 19) and SpX-16 (December 9, 2018). All air samples were returned on SpX-16. Due to ongoing analytical issues, data for formaldehyde is not available for Increment 57.

On October 11, 2018, an anomaly occurred during the launch of Soyuz MS-10. The crew aboard that vehicle landed safely. As a result, the ISS crew complement was 3 until the arrival of Soyuz MS-11 on December 3, 2018.

Table 1. Analytical summary of ISS air analyses (Increment 57)

Return Flight	Sample Location	Sample Date	Freon 218 (mg/m3)	Alcohols ^a (mg/m3)	T-Value ^b (units)	Formaldehyde (µg/m3)
SpaceX-16	Lab	10/8/2018	69	9.3	0.3	---
SpaceX-16	JPM	10/8/2018	82	9.3	0.3	---
SpaceX-16	Lab	11/19/2018	61	6.9	0.2	---
SpaceX-16	Columbus	11/19/2018	60	6.6	0.3	---
SpaceX-16	NG-10 Ingress	11/19/2018	9.2	3.9	0.9 (0.6)	---
SpaceX-16	SpX-16 Ingress	12/9/2018	37	6.5	0.2 (0.1)	---
<i>Guideline</i>			---	<5	<1 ^c	<120

^aIncludes acetone

^bSum of the ratios of the measured concentration and the corresponding 180-day SMAC for each compound, excluding CO₂; parentheses indicate value based on 7-day SMACs and applicable to first ingress

^cT-value <1 used to evaluate routine monthly sampling; <3 used to evaluate first ingress.

^dFormaldehyde badge data are not available for Increment 57 due to analytical concerns.

Data tables containing measured concentrations and corresponding T-values based on appropriate Spacecraft Maximum Allowable Concentrations (SMACs) for compounds present at levels above the laboratory reporting limit are attached to this report. Complete data tables, which include compounds assessed but not detected, are available upon request. The mean relative recoveries of the three surrogate standards from the mGSC samples returned on SpX-16 were within acceptable limits.

The Air Quality Monitors (AQMs) automatically collect samples every 73 hours, which results in 2-3 sampling sessions per unit per week. Monthly average concentrations as well as the Increment average concentrations for compounds measured on the AQMs are presented in Table 2. During this Increment, one of the two AQMs failed and so for much of November and all of December, no data were available for several compounds. The AQMs were replaced in January 2019, during Increment 58.

Table 2. Average monthly concentrations (mg/m³) of AQM target compounds

Compound	October Average	November Average	December Average	Increment Average
2-Propanol	0.1	TRACE	--	0.1
Acetone	0.1	0.1	--	0.1
Acrolein	ND	ND	--	ND
Benzene	ND	ND	--	ND
1,2-Dichloroethane	ND	ND	--	ND
Decamethylcyclopentasiloxane#	0.2	0.2	0.2	0.2
Hexanal	ND	ND	--	ND
Hexane	ND	ND	--	ND
m,p-Xylenes#	ND	ND	ND	ND
Methanol	0.2	0.2	--	0.2
o-Xylene#	TRACE	TRACE	TRACE	TRACE
Octamethylcyclotetrasiloxane#	TRACE	TRACE	TRACE	TRACE
Toluene#	ND	ND	ND	ND
2-Butanone	ND	ND	ND	ND
Acetaldehyde	0.3	0.2	0.2	0.2
Dichloromethane	ND	ND	ND	ND
Ethanol	4.8	4.3	4.1	4.4
Ethyl Acetate	0.04	0.05	TRACE	0.04
Hexamethylcyclotrisiloxane#	0.1	0.1	0.1	0.1
n-Butanol	0.1	0.1	0.1	0.1
Trimethylsilanol	0.1	0.1	0.1	0.1

Obtained from prime unit

ND: Not detected; <MDL (Minimum Detection Limit)

TRACE= >MDL, <MQL (Minimum Quantification Limit)

--: Not assessed due to AQM failure.

Note: An AQM unit failed in early November, and so data for several compounds is lacking for November and December 2018.

Toxicological Evaluation of ISS Air Quality

Routine air quality monitoring is performed in-flight using the AQMs. Archive air samples (mGSCs and formaldehyde badges) are collected during each Increment and returned for analysis in the Toxicology and Environmental Chemistry (TEC) Air Quality Laboratory. Data from the ground analyses complement the in-flight data and provide a more complete understanding of air quality on the ISS. The routine archive samples for this Increment that returned on SpX-16 confirmed air quality was acceptable during October to December. **All measured values for routine samples (mGSC and AQM) met 180-d T-value guideline criteria ($T < 1$), indicating no concern for crew health.** The average, rounded T-value calculated from the Increment 57 mGSC samples was 0.3 (Figure 1). T-values calculated from GSC results and AQM (Figure 2) were in reasonable agreement given the differences between the analytical techniques and the number of target compounds used in the calculation.

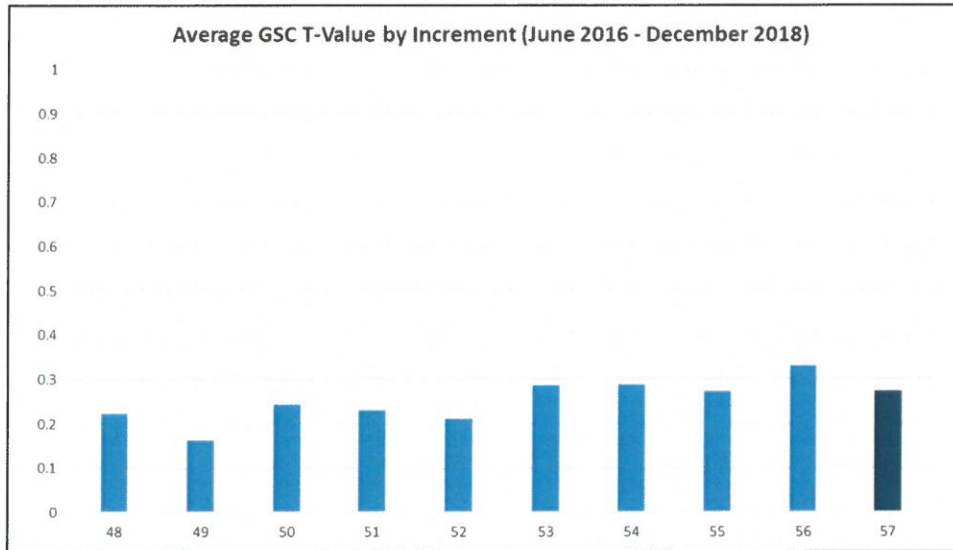


Figure 1. GSC-Derived T-values for Increments 47- 57. Average T-values do not include CO₂, first ingress, or contingency samples.

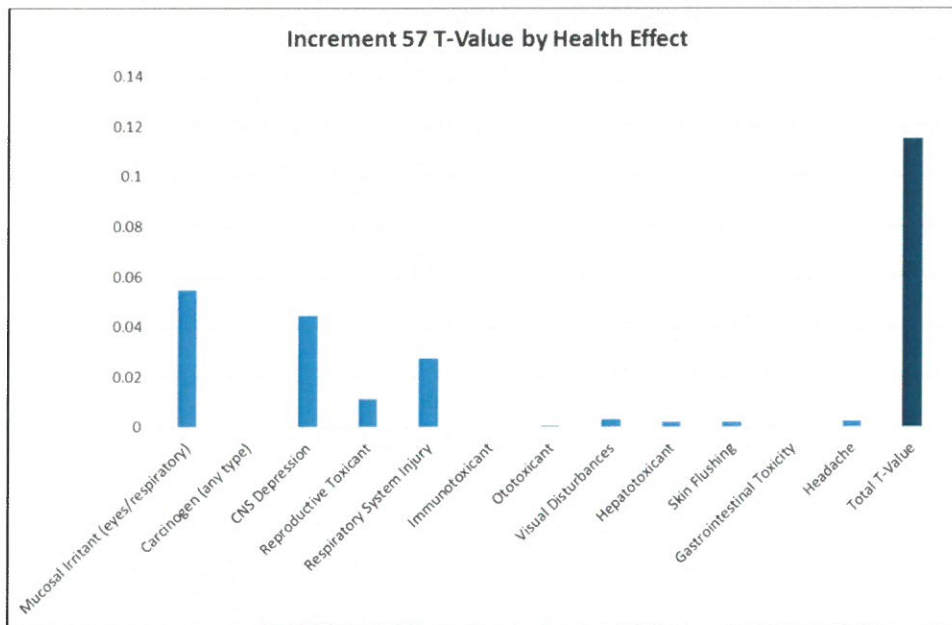


Figure 2. AQM-Derived T-Values by Health Effect for Increment 57

Generally, the reported concentrations for the compounds detected during Increment 57 are similar to levels detected during recent increments. Atmospheric concentrations of siloxanes (i.e., TMS, OMCTS, and HMCTS) were similar to those observed during Increment 55.

All mGSC samples contained a CO₂ concentration below the Increment limit documented in Chit 14468, which requests that the 24 hour average concentration not exceed 3.0 mmHg (7100 mg/m³) on the US segment. While mGSC CO₂ sampling provides a snap-shot of the CO₂ concentration, the major constituent analyzer (MCA) routinely monitors CO₂ levels in the US segment. For this reason, data from the MCA are

better suited for evaluation of short and long-term trends in CO₂ (Figure 3). Concentrations measured by the MCA fluctuate as a result of multiple factors including the number of crew on ISS, current scrubbing capability, and processes and activities that generate CO₂.

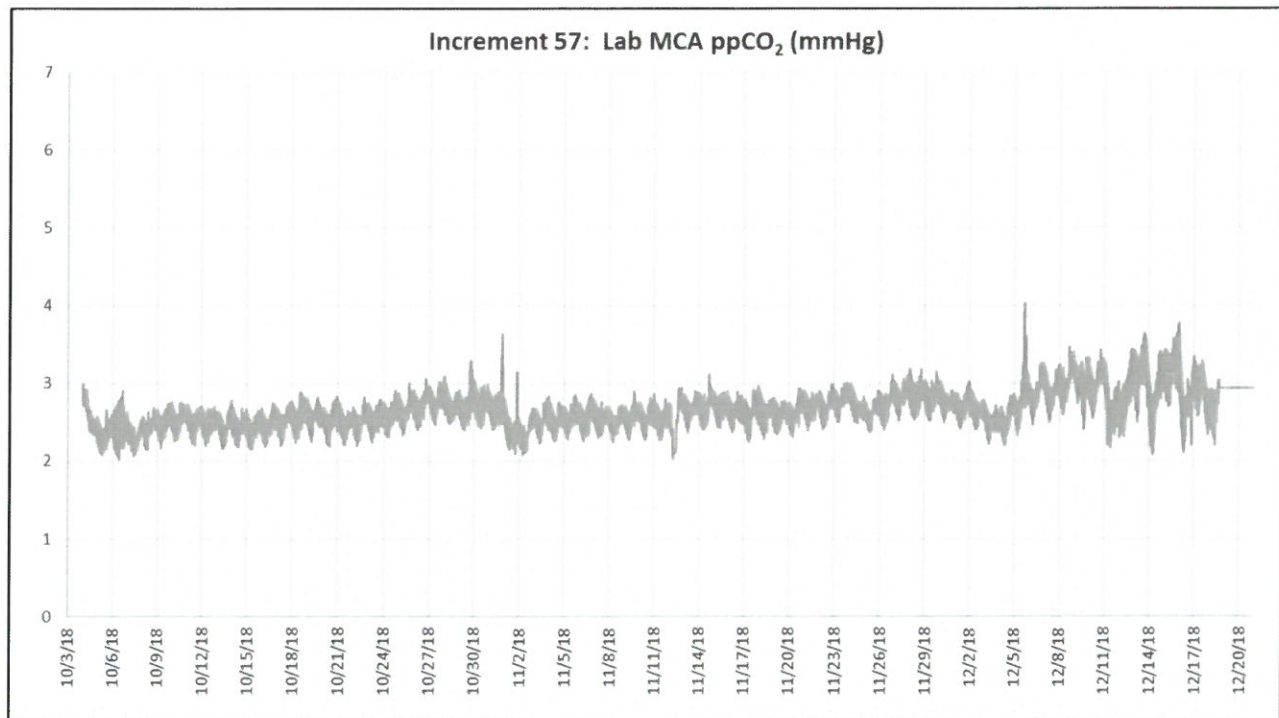


Figure 3. Environmental CO₂ Concentrations on ISS Increment 57 in mmHg

All CO₂ data for Increment 57 were obtained from the MCA in the US LAB. Overall, CO₂ concentrations were well-controlled throughout the Increment. CO₂ levels are often maintained between 1.5 and 2 mmHg with 3-person crew. A gradual increase in CO₂ levels were observed in October due to degraded function of Vozdukh and use of the Node 3 CDRA which operates at slower fan speeds. Three additional crew arrived on Soyuz MS-11 on December 3, 2018. Several excursions above 3 mmHg were observed at the end of October and the beginning of November; these were associated with calibration procedures and are not thought to reflect CO₂ concentrations in ISS air. There was also a brief loss of communication with the MCA on November 12th. On December 5, 2018, the MCA was sampling the airlock and registered higher CO₂ levels during servicing of the Extravehicular Mobility Unit (EMU). The Lab MCA failed on December 18, 2018. The Node 3 MCA was activated on December 23, 2018 (Increment 58) and was functioning within specified parameters.

Alcohol values in all routine archive samples continued to exceed the guideline of <5 mg/m³, which is intended to protect the water recovery system from risk of overloading. These levels are primarily due to ethanol in the ISS atmosphere. AQM results for ethanol continued to fall in Increment 57 from a peak of 6.6 mg/m³ in August. Ethanol levels observed in mGSC samples in October (8.2 mg/m³) were similar to the low end of results from Increment 56 (8.3-15 mg/m³) but were markedly lower in November (5.6-5.9 mg/m³). Total alcohols (including acetone) were 9.3 mg/m³ in October GSC samples but declined to 6.6-6.9 mg/m³ in November. Results from GSC and AQM sampling indicate that alcohol levels declined in Increment 57, reversing the trend from Increments 55 and 56.

Octafluoropropane (Freon 218) levels continued to decrease (~60 mg/m³ in October) following the release during Increment 53 (865 mg/m³). This concentration is more than three orders of magnitude below the 180d SMAC value (85,000 mg/m³) and does not constitute a toxicological risk.

Analytical and quality concerns with the formaldehyde monitoring kits is ongoing, and thus no data on formaldehyde in ISS air is available for Increment 57.

NG-10 Ingress

A GSC sample was collected upon ingress into NG-10 on November 19, 2018 at 17:30 GMT, approximately 13 minutes after hatch opening. The concentration of Freon 218 (octafluoropropane), a marker for ISS air dilution of first hatch samples, was 60 mg/m³ approximately 9 hours prior to first ingress sampling for comparison. The concentration of Freon 218 in the ingress sample was 9.2 mg/m³, indicating a low level of dilution. This is somewhat surprising, given the 13 minute delay between ingress and sample collection. The total T-value (excluding CO₂) was 0.60, which was well below the 7-d T-value limit of 3.0 units for first ingress. The primary contributors were trimethylsilanol (0.8 mg/m³), acetaldehyde (0.5 mg/m³) and carbon disulfide (0.1 mg/m³). Based on the available information, mixing of air between NG-10 and the ISS stack had occurred to a low extent at the time of sampling (<15%). However, even considering a 20% mixing rate, the T-value would not rise to a level of concern for health after docking.

SpaceX-16 Ingress

A GSC sample was collected upon ingress into SpaceX-16 on December 9, 2018 at 8:35 GMT, approximately 5 minutes after hatch opening. No contemporaneous samples are available to assess atmospheric mixing, but based on Freon 218 results from November 19th and December 31st (Increment 58), it appears that the atmosphere in SpaceX-16 had been diluted 50% or more prior to mGSC sampling. The total T-value (excluding CO₂) was 0.1, which was well below the 7-d T-value limit of 3.0 units. The primary contributors to the T-value were acetaldehyde (0.2 mg/m³) and trimethylsilanol (0.1 mg/m³). Even considering a 75% mixing rate, the T-value would not rise to a level of concern after docking.

WATER QUALITY

Two archive water samples were collected from the US segment during Increment 57 and returned on Soyuz 55. A condensate sample was collected from the Russian Service Module (SM) and returned on SpaceX-16. Complete data tables with results for all measured parameters are available upon request. A summary of select analytical results from the Increment 57 samples is provided in Table 3. Expanded summary tables containing organic carbon recoveries and results for all analytes present at concentrations above reporting limits are included as attachments to this report.

Table 3. Analytical Summary of ISS Water Analyses (Increment 57)

Return Mission	Sample Location	Sample Date	TOC (mg/L)	DMSD (mg/L)	Methyl Sulfone (mg/L)	Conductivity (μS/cm)	Total Iodine (mg/L)
Soyuz 55	PWD Hot	11/12/2018	1.08	2.0	0.1	1	<0.05
Soyuz 55	PWD Ambient	12/11/2018	1.19	3.3	0.1	1	<0.05
SpaceX-16	Russian Condensate	11/24/2018	96.9	7.3	0.1	150	NA

NA: not analyzed

Toxicological Evaluation of ISS Water Quality

Routine water quality monitoring is performed in-flight using the total organic carbon analyzer (TOCA). Results from these analyses provide a general indication of overall water quality. Archive water samples are collected during each increment and returned for comprehensive analysis in ground laboratories. Data from the ground analyses complement the in-flight data and provide a more complete understanding of water quality on the ISS.

Potable Water

Concentrations of all chemicals detected in the potable water samples met the requirements listed in SSP 41000, System Specification for the International Space Station and JSC 63414, Spacecraft Water Exposure Guidelines (SWEGs). Total organic carbon (TOC) concentrations from in-flight (PWD TOC and WPA TOC) and ground analyses (Archive TOC) performed between October 2016 and December 2018 are shown in Figure 4. The TOC concentration in the potable samples was similar to the previous Increment (PWD Hot 1.1 mg/L, PWD Ambient 1.2 mg/L) and measured concentrations were well below both the U.S. Segment Specification (3000 µg/L) and the 100-day SWEG (5000 µg/L). DMSD is the primary compound responsible for the TOC in both potable samples.

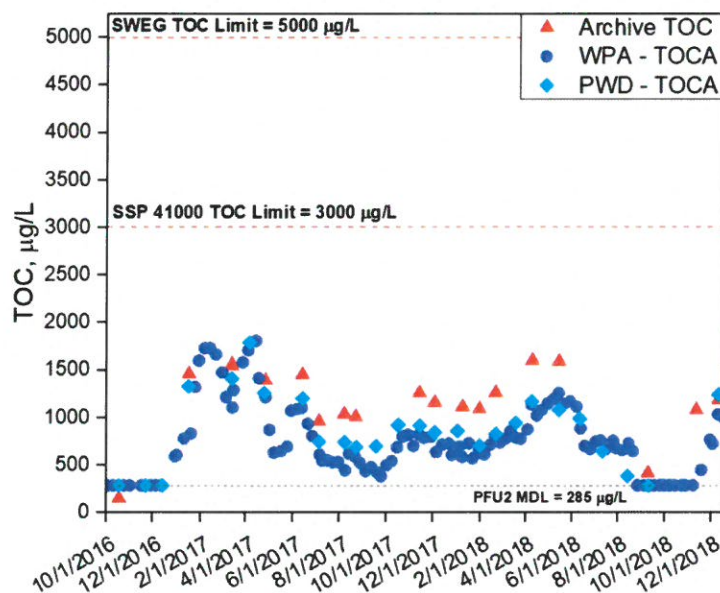


Figure 4. Total Organic Carbon (TOC) trending in US Potable Water

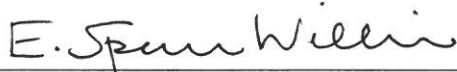
Methyl sulfone, often a minor contributor to the TOC, was detected in the PWD Hot and Ambient samples at slightly lower concentrations than the previous Increment (0.12 vs. 0.15 mg/L) and still well below the SWEG of 1,500 mg/L. Silicon was present at 0.9 and 1.1 mg/L, markedly higher than the levels observed in Increment 56. Much of this silicon can be attributed to DMSD levels (69-86%), which were markedly higher in these samples compared to Increment 56. Nickel was detected at very low levels in both PWD samples (0.002 mg/L).

Iodine is a biocide used on the US segment. It is added to the water produced by the WPA, but removed prior to crew consumption to avoid potential thyroid dysfunction. The total iodine level in the potable

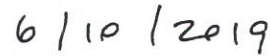
samples collected from the PWD was below the reporting limit (0.05 mg/L), indicating effective removal of iodine in water intended for consumption. For additional information regarding microbial analyses, please see the Increment 57 post-flight report issued by the JSC Environmental Microbiology Laboratory.

Russian SM Condensate

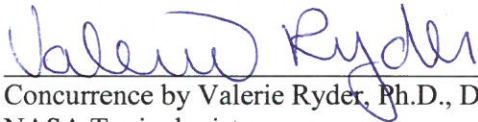
A condensate sample was collected from the SM as part of an effort to characterize the role of hydrophilic coatings in the condensing heat exchangers in the generation of DMSD on ISS. The TOC in this sample was 96.9 mg/L. Organic compounds present in concentrations >1 mg/L included ethanol (75.6 mg/L), acetate (48.2 mg/L), benzyl alcohol (10.2 mg/L), DMSD (7.3 mg/L), methanol (5.2 mg/L), 1-butanol (4.4 mg/L), propylene glycol (3.8 mg/L), benzoic acid (2.4 mg/L), and acetone (2.0 mg/L). Silver (3.2 mg/L) and calcium (1.1 mg/L) were the only metals detected at levels above 1 mg/L.



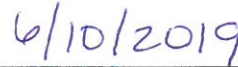
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Concurrence by Valerie Ryder, Ph.D., DABT
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Date

- Enclosures
- Table 1: Analytical concentrations of compounds quantified in the mGSC returned on SpaceX-16
 - Table 2A: T-values corresponding to concentrations for samples returned on SpX-16 in Table 1, based on 7-day and 180-day SMACs
 - Table 2B: T-values corresponding to concentrations from NG-10 and SpaceX-16 ingress, based on 7-day and 180-day SMACs
 - Table 3: Analytical concentrations of compounds quantified in PWD Hot and Ambient samples returned on Soyuz 55 and SM Condensate Sample returned on SpaceX-16.

TABLE 1
ANALYTICAL RESULTS OF SPACEX-16 RETURN

CHEMICAL CONTAMINANT	CONCENTRATION (mg/M ³)					
	AQ190017 SN2110	AQ190018 SN2114	AQ190019 SN2008	AQ190020 SN2116	AQ190021 SN2011	AQ190022 SN2012
	LAB 10/8/18 @ 11:50 GMT	JPM 10/8/18 @ 11:50 GMT	LAB 11/19/18 @ 8:15 GMT	COL 11/19/18 @ 8:20 GMT	NG-10 Ingress 11/19/18 @ 17:30 GMT	SpaceX-16 Ingress 12/9/18 @ 8:35 GMT
TARGET COMPOUNDS (TO-15) **						
1,1,1,2-Tetrafluoroethane (Norflurane)	<0.050	<0.050	<0.050	<0.050	0.21	0.063
Propene	<0.025	<0.025	<0.025	<0.025	<0.025	TRACE
Propane	<0.025	<0.025	<0.025	<0.025	TRACE	0.042
Carbonyl sulfide (Carbon oxide sulfide)	<0.025	<0.025	<0.025	<0.025	0.054	<0.025
Isobutane	<0.025	<0.025	<0.025	0.039	0.81	<0.025
Methanol *	0.36	0.38	0.38	0.32	0.23	0.47
Acetaldehyde	0.36	0.33	0.24	0.24	0.50	0.20
2-Methyl-1-propene	<0.025	<0.025	<0.025	<0.025	0.29	<0.025
Butane	<0.025	<0.025	<0.025	<0.025	0.035	<0.025
Ethanol *	8.3	8.2	5.9	5.6	1.3	5.1
Acetone	0.31	0.28	0.29	0.26	0.52	0.23
Propanal (Propionaldehyde)	<0.025	<0.025	<0.025	<0.025	0.051	<0.025
2-Propanol (Isopropanol) *	0.26	0.27	0.27	0.28	1.6	0.67
Isoprene (2-Methyl-1,3-butadiene)	0.038	0.036	0.028	0.029	<0.025	TRACE
2-Methyl-2-propanol	<0.025	<0.025	<0.025	<0.025	0.069	<0.025
Carbon disulfide	TRACE	TRACE	<0.025	<0.025	0.11	<0.025
1-Propanol	0.041	0.035	TRACE	0.036	0.031	TRACE
Trimethylsilanol	0.11	0.16	0.094	0.20	0.82	0.067
Butanal (Butyraldehyde)	<0.025	<0.025	<0.025	<0.025	0.044	<0.025
2-Butanone (Methyl ethyl ketone)	<0.025	<0.025	<0.025	<0.025	0.24	<0.025
Ethyl acetate	0.029	0.028	0.028	0.034	0.12	<0.025
1-Butanol	0.061	0.059	0.056	0.066	0.22	0.032
4-Methyl-2-pentanone (MIBK)	<0.025	<0.025	<0.025	<0.025	0.089	<0.025
Toluene	<0.025	<0.025	<0.025	<0.025	0.11	<0.025
Hexanal	<0.025	<0.025	<0.025	<0.025	0.056	<0.025
Butyl acetate	<0.050	<0.050	<0.050	<0.050	0.089	<0.050
Ethylbenzene	<0.050	<0.050	<0.050	<0.050	0.093	<0.050
m & p-Xylene	<0.050	<0.050	<0.050	<0.050	0.38	<0.050
Heptanal	<0.050	<0.050	<0.050	<0.050	0.056	<0.050
o-Xylene	<0.050	<0.050	TRACE	<0.050	0.12	<0.050
Octamethylcyclotetrasiloxane	<0.125	<0.125	<0.125	<0.125	0.23	<0.125
Decamethylcyclopentasiloxane	0.41	0.49	0.26	0.37	TRACE	0.30
Octafluoropropane (Perfluoropropane) *	69	82	61	60	9.2	37
SPECIAL INTEREST COMPOUNDS						
Hexamethylcyclotrisiloxane #	0.30	0.47	0.21	0.29	1.07	<0.20
NON-TARGET COMPOUNDS ***						
Fluorotrimethylsilane	<0.050	<0.050	<0.050	<0.050	0.22	<0.050
1-Methoxy-2-propyl acetate	<0.050	<0.050	<0.050	<0.050	0.12	<0.050
Octamethyltrisiloxane	<0.050	<0.050	<0.050	<0.050	0.25	<0.050
2-Pinene	<0.050	<0.050	<0.050	<0.050	0.075	<0.050
C12-Alkane	<0.050	<0.050	<0.050	<0.050	0.11	<0.050
C10-Siloxane	<0.050	<0.050	<0.050	<0.050	0.18	<0.050
C12-Alkane	<0.050	<0.050	<0.050	<0.050	0.14	<0.050
C11-Alkane	<0.050	<0.050	<0.050	<0.050	0.15	<0.050
C12-Alkane	<0.050	<0.050	<0.050	<0.050	0.15	<0.050
C12-Alkane	<0.050	<0.050	<0.050	<0.050	0.13	<0.050
TOTAL ALCOHOLS PLUS ACETONE	9.3	9.3	6.9	6.6	3.9	6.5
TARGET COMPOUNDS (GC) **						
Methane	58	59	44	42	5.9	29
Carbon dioxide	5200	5200	5400	5400	1800	4600
Hydrogen	4.3	4.3	2.7	2.6	1.0	3.1
Carbon monoxide	0.82	0.75	0.68	0.77	1.9	1.9
TOTAL CONCENTRATION (NON-METHANE HYDROCARBONS)	79	93	68	68	20	44
TOTAL CONCENTRATION - OFP (NON-METHANE HYDROCARBONS)	11	11	7.8	7.8	11	7.2

* GC/FID data results are in bold

** Quantified using a multi-point calibration

*** Quantified using "B" response factor except where noted; concentrations are estimates only.

Response factor generated from an internal study

< : Value is less than the laboratory reporting limit.

TRACE: Amount detected is sufficient for compound identification only. One-half of the reporting limit was used in the Total Concentration summation.

OFP - Octafluoropropane

**TABLE 2A
T-VALUES FOR SPACEX-16 RETURN**

CHEMICAL CONTAMINANT	T-VALUE (180-d SMAC)			
	AQ190017 SN2110 LAB 10/8/18 @ 11:50 GMT	AQ190018 SN2114 JPM 10/8/18 @ 11:50 GMT	AQ190019 SN2008 LAB 11/19/18 @ 8:15 GMT	AQ190020 SN2116 COL 11/19/18 @ 8:20 GMT
TARGET COMPOUNDS (TO-15)				
Isobutane	ND	ND	ND	0.00020
Methanol	0.00405	0.00419	0.00421	0.00361
Acetaldehyde	0.09096	0.08170	0.05890	0.05971
Ethanol	0.00413	0.00412	0.00293	0.00279
Acetone	0.00589	0.00545	0.00567	0.00509
2-Propanol (Isopropanol)	0.00173	0.00179	0.00178	0.00190
Isoprene (2-Methyl-1,3-butadiene)	0.01262	0.01211	0.00941	0.00976
Carbon disulfide	0.01136	0.01136	ND	ND
1-Propanol	0.00056	0.00048	0.00017	0.00049
Trimethylsilanol	0.02745	0.03969	0.02355	0.05064
Ethyl acetate	0.00016	0.00016	0.00016	0.00019
1-Butanol	0.00153	0.00148	0.00140	0.00164
o-Xylene	ND	ND	0.00068	ND
Decamethylcyclopentasiloxane	0.02701	0.03245	0.01754	0.02471
Octafluoropropane (Perfluoropropane)	0.00081	0.00096	0.00071	0.00070
SPECIAL INTEREST COMPOUNDS				
Hexamethylcyclotrisiloxane	0.03279	0.05255	0.02358	0.03245
NON-TARGET COMPOUNDS				
All Non-Target Compounds were below their reporting limit.				
TARGET COMPOUNDS (GC)				
Methane	0.01647	0.01689	0.01264	0.01187
Hydrogen	0.01257	0.01254	0.00783	0.00757
Carbon monoxide	0.04851	0.04420	0.03976	0.04527
TOTAL T-VALUE	0.29858	0.32210	0.21092	0.25859

ND : Value is less than the laboratory reporting limit.

Note: Number of decimal places in T-Values do not represent significant figures of measurements.

**TABLE 2B
T-VALUES FOR SPACEX-16 RETURN**

CHEMICAL CONTAMINANT	T-VALUE (7- & 180-d)			
	7-d SMAC	180-d SMAC	7-d SMAC	180-d SMAC
	AQ190021 SN2011 NG-10 Ingress 11/19/18 @ 17:30 GMT	AQ190021 SN2011 NG-10 Ingress 11/19/18 @ 17:30 GMT	AQ190022 SN2012 SpaceX-16 Ingress 12/9/18 @ 8:35 GMT	AQ190022 SN2012 SpaceX-16 Ingress 12/9/18 @ 8:35 GMT
TARGET COMPOUNDS (TO-15)				
1,1,1,2-Tetrafluoroethane (Norflurane)	0.00002	0.00002	0.00001	0.00001
Propene	ND	ND	0.00007	0.00007
Propane	0.00000	0.00000	0.00001	0.00001
Carbonyl sulfide (Carbon oxide sulfide)	0.00062	0.00272	ND	ND
Isobutane	0.00425	0.00425	ND	ND
Methanol	0.00254	0.00254	0.00520	0.00520
Acetaldehyde	0.12433	0.12433	0.04932	0.04932
2-Methyl-1-propene	0.00255	0.01275	ND	ND
Butane	0.00001	0.00001	ND	ND
Ethanol	0.00063	0.00063	0.00253	0.00253
Acetone	0.00990	0.00990	0.00439	0.00439
Propanal (Propionaldehyde)	0.00429	0.00429	ND	ND
2-Propanol (Isopropanol)	0.01037	0.01037	0.00448	0.00448
Isoprene (2-Methyl-1,3-butadiene)	ND	ND	0.00208	0.00417
2-Methyl-2-propanol	0.00046	0.00057	ND	ND
Carbon disulfide	0.10240	0.10240	ND	ND
1-Propanol	0.00041	0.00041	0.00017	0.00017
Trimethylsilanol	0.20597	0.20597	0.01666	0.01666
Butanal (Butyraldehyde)	0.00292	0.00292	ND	ND
2-Butanone (Methyl ethyl ketone)	0.00786	0.00786	ND	ND
Ethyl acetate	0.00066	0.00066	ND	ND
1-Butanol	0.00271	0.00542	0.00040	0.00080
4-Methyl-2-pentanone (MIBK)	0.00063	0.00063	ND	ND
Toluene	0.00760	0.00760	ND	ND
Hexanal	0.00278	0.00278	ND	ND
Butyl acetate	0.00047	0.00047	ND	ND
Ethylbenzene	0.00072	0.00186	ND	ND
m & p-Xylene	0.00515	0.01016	ND	ND
Heptanal	0.00242	0.00242	ND	ND
o-Xylene	0.00158	0.00317	ND	ND
Octamethylcyclotetrasiloxane	0.00082	0.01907	ND	ND
Decamethylcyclopentasiloxane	0.00088	0.00583	0.00304	0.02029
Octafluoropropane (Perfluoropropane)	0.00011	0.00011	0.00044	0.00044
SPECIAL INTEREST COMPOUNDS				
Hexamethylcyclotrisiloxane	0.01186	0.11863	ND	ND
NON-TARGET COMPOUNDS				
Fluorotrimethylsilane	0.05732	0.05732	ND	ND
1-Methoxy-2-propyl acetate	0.00218	0.00218	ND	ND
Octamethyltrisiloxane	0.00025	0.00615	ND	ND
2-Pinene	0.00054	0.00054	ND	ND
C12-Alkane	0.00249	0.00249	ND	ND
C10-Siloxane	0.00182	0.00182	ND	ND
C12-Alkane	0.00319	0.00319	ND	ND
C11-Alkane	0.00335	0.00335	ND	ND
C12-Alkane	0.00343	0.00343	ND	ND
C12-Alkane	0.00305	0.00305	ND	ND
TARGET COMPOUNDS (GC)				
Methane	0.00168	0.00168	0.00827	0.00827
Hydrogen	0.00299	0.00299	0.00905	0.00905
Carbon monoxide	0.02948	0.10926	0.03007	0.11143
TOTAL T-VALUE	0.60022	0.86823	0.10612	0.23729

ND : Value is less than the laboratory reporting limit.

Note: Number of decimal places in T-Values do not represent significant figures of measurements.

Table 3: Analytical concentrations of compounds quantified in PWD Hot and Ambient samples returned on Soyuz 55 and SM Condensate sample returned on SpaceX-16

Increment Mission Sample Location Sample Description Sample Date Analysis/Sample ID	Units	Test Conducted by	Potable Water Maximum Contaminant Level (MCL)	Maximum Contaminant Level Source	57		
					Soyuz 55		SpaceX-16
					WPA PWD Hot	WPA PWD Ambient	Service Module
					Potable water 11/12/2018 WQ180821	Potable water 12/11/2018 WQ180822	Raw Condensate 11/24/2018 WQ190028
Physical Characteristics							
Conductivity	µS/cm	U.S.			1	1	147
pH	pH units	U.S.	4.5-8.5	41000	4.90	4.85	7.42
Anions IC							
Sulfate	mg/L	U.S.	250	41000	< 0.5	< 0.5	2.0
Cations IC							
Ammonium (as N)	mg/L	U.S.	1	SWEG&41000	< 0.25	< 0.25	17.7
Minerals ICPMS							
Calcium	mg/L	U.S.	30	41000	0.02	0.02	1.08
Magnesium	mg/L	U.S.	50	41000	< 0.01	< 0.01	0.61
Potassium	mg/L	U.S.	340	41000	< 0.01	< 0.01	0.20
Sodium	mg/L	U.S.			< 0.01	< 0.01	0.10
Trace Metals ICPMS							
Aluminum	µg/L	U.S.			1	2	< 10
Copper	µg/L	U.S.	1,000	41000	< 1	< 1	26
Iron	µg/L	U.S.	300	41000	< 5	< 5	66
Manganese	µg/L	U.S.	300	SWEG&41000	< 1	< 1	26
Nickel	µg/L	U.S.	300	SWEG&41000	2	2	321
Silver	µg/L	U.S.	400	SWEG&41000	< 1	< 1	3,150
Strontium	µg/L	U.S.			< 1	< 1	17
Zinc	µg/L	U.S.	2,000	SWEG&41000	2	1	881
Silicon ICPMS							
Silicon	µg/L	U.S.			882	1,140	3,330
Total Organic Carbon-Sievers							
Total Inorganic Carbon (TIC)	mg/L	U.S.			0.75	0.77	5.79
Total Organic Carbon (TOC)	mg/L	U.S.		SWEG / 41000	1.08	1.19	96.9
Volatile Organics-Special Interest Compounds (Semi-quantitative)							
Trimethylsilanol	µg/L	U.S.			not found	not found	230
Semi-volatile Organics-Targets							
2-Methylthiobenzothiazole	µg/L	U.S.			< 20	< 20	53
Benzothiazole	µg/L	U.S.			< 20	< 20	127
Methyl sulfone	µg/L	U.S.	1,500,000	interim SWEG (06-2017)	124	119	96
Acid Extractables-EPA 625 List GCMS							
Benzoic acid	µg/L	U.S.			< 100	< 100	2,370
Phenol	µg/L	U.S.	4,000	SWEG	< 20	< 20	362
Base and Neutral Extractables-EPA 625 List GCMS							
Benzyl alcohol	µg/L	U.S.			45	< 20	10,200
bis-(2-Ethylhexyl)phthalate	µg/L	U.S.	20,000/6	SWEG/EPA	< 20	< 20	114
Di-n-butylphthalate	µg/L	U.S.	40,000	SWEG	< 20	< 20	56
Diethylphthalate	µg/L	U.S.			< 20	< 20	57
Semi-volatile Organics-Special Interest Compounds (Semi-quantitative)							
2-(2-Butoxyethoxy)ethanol	µg/L	U.S.			not found	not found	410
2-Butoxyethanol	µg/L	U.S.			not found	not found	140
2-Ethoxyethanol	µg/L	U.S.			not found	not found	390
2-Ethyl-1-hexanol	µg/L	U.S.			not found	not found	360
2-Ethylhexanoic acid	µg/L	U.S.			not found	not found	150
2-Phenoxyethanol	µg/L	U.S.			not found	not found	740
2-Phenyl-2-propanol	µg/L	U.S.			not found	not found	130
Benzaldehyde	µg/L	U.S.			not found	not found	120
Butylated hydroxyanisole (BHA)	µg/L	U.S.			not found	not found	130
Dipropylene glycol methyl ether	µg/L	U.S.			not found	not found	280
Monomethyl phthalate	µg/L	U.S.			not found	not found	310
N,N-Diethylformamide	µg/L	U.S.			not found	not found	57
N,N-Dimethyl acetamide	µg/L	U.S.			not found	not found	220

NA=Not analyzed

MI=Matrix Interference

N/A=Not applicable

#previously identified as bis(2-Chloroisopropyl) ether

Table 3: Analytical concentrations of compounds quantified in PWD Hot and Ambient samples returned on Soyuz 55 and SM Condensate sample returned on SpaceX-16

Increment	Mission	Sample Location	Sample Description	Sample Date	Analysis/Sample ID	Units	Test Conducted by	Potable Water Maximum Contaminant Level (MCL)	Maximum Contaminant Level Source	57		
										Soyuz 55		SpaceX-16
										WPA PWD Hot	WPA PWD Ambient	Service Module
										Potable water	Potable water	Raw Condensate
										11/12/2018	12/11/2018	11/24/2018
										WQ180821	WQ180822	WQ190028
N-Phenyl-2-naphthylamine					µg/L	U.S.	260,000	SWEG	not found	not found	86	
Neomenthol					µg/L	U.S.			not found	not found	71	
p-Menth-1-en-8-ol (alpha-Terpineol)					µg/L	U.S.			not found	not found	49	
Tetramethyl thiourea					µg/L	U.S.			not found	not found	320	
Alcohols & Acetone GCMS												
1-Butanol					µg/L	U.S.			< 400	< 400	4,390	
1-Propanol					µg/L	U.S.			< 400	< 400	537	
Acetone					µg/L	U.S.	15,000	SWEG	< 400	< 400	1,980	
Ethanol					µg/L	U.S.			< 400	< 400	75,600	
Methanol					µg/L	U.S.	40,000	SWEG	< 400	< 400	5,170	
Glycols GCMS												
1,2-Propanediol (Propylene glycol)					µg/L	U.S.	1,700,000	SWEG	< 1000	< 1000	3,790	
Silanols LCRI (Semi-Quantitative-NIST traceable standard not available)												
Dimethylsilanediol (DMSD)					µg/L	U.S.	35,000	SWEG	2,000	3,300	7,300	
Carboxylates IC												
Acetate					µg/L	U.S.			< 500	< 500	48,200	
Aldehydes GCMS												
Formaldehyde					µg/L	U.S.	12,000	SWEG	< 10	< 10	34	
Non-volatile Organics LC												
Caprolactam					µg/L	U.S.	100,000	SWEG	< 500	< 500	838	
Organic Carbon Recovery					percent	U.S.			54.35	74.79	85.27	
Unaccounted Organic Carbon					mg/L	U.S.			0.49	0.30	14.28	

Comments: None.

Data Qualifiers: WQ190028: Possible low bias - 2-Ethoxyethanol

NA=Not analyzed
MI=Matrix Interference
N/A=Not applicable
#previously identified as bis(2-Chloroisopropyl) ether