



Toxicological Assessment of ISS Air Quality: Contingency Sampling – February 2013

Two grab sample containers (GSCs) were collected by crew members onboard ISS in response to a vinegar-like odor in the US Lab. On February 5, the first sample was collected approximately 1 hour after the odor was noted by the crew in the forward portion of the Lab. The second sample was collected on February 22 when a similar odor was noted and localized to the end ports of the microgravity science glovebox (MSG). The crewmember removed a glove from the MSG and collected the GSC inside the glovebox volume. Both samples were returned on SpaceX-2 for ground analysis.

Complete data tables of all measured concentrations and corresponding T-values based on 180-day SMACs are enclosed. A summary of those results is shown in Table 1. Shaded rows indicate data that are limited due to low sample pressures. Recoveries of the 3 surrogate standards from the GSCs were as follows:

- Lab sample (Feb 5) – ¹³C-acetone, 101%; fluorobenzene, 98%; and chlorobenzene, 78%
- MSG sample (Feb 22) – ¹³C-acetone, 125%; fluorobenzene, 110%; and chlorobenzene, 97%

The sample pressure of the GSC collected in the Lab was low (4.9 psia) relative to the typical pressure range of 13-14 psia, indicating a problem with sample acquisition. Due to the low pressure, the detection limit was 0.083 mg/m³ (compared to the normal detection limit of 0.05 mg/m³). Despite the low sample pressure, the sample was deemed valid due to the presence of alcohols, Freon 218 (octafluoropropane), and carbon dioxide at levels that were typical of historic samples and due to adequate surrogate recoveries.

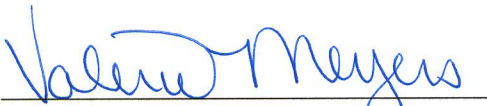
Table 1. Analytical Summary of ISS results

Sample Location	Sample Date	NMVOCs ^a (mg/m ³)	Freon 218 (mg/m ³)	CO ₂ (mg/m ³)	Alcohols (mg/m ³)	T-Value ^b (units)
Lab	2/5/2013	6.8	26	5266	4.6	0.23
MSG	2/22/2013	6.9	15	7518	4.9	0.22
<i>Guideline</i>		<25	---	<9300	<5	<1

^aNon-methane volatile organic hydrocarbons, excluding Freon 218

^bBased on 180-d SMACs and calculated excluding CO₂

Toxicological Evaluation of ISS Air Quality: No compounds of concern for crew health were detected in these contingency samples. Concentrations of target compounds and the corresponding combined T-value were low compared to typical routine monthly samples collected on ISS. The vinegar-like smell noted by the crew is likely to be acetic acid. Acetic acid was not detected in these samples; however, the reported odor threshold range for this compound (0.2 – 1 ppm) is well below the detection limit for standard GC/MS analysis of GSCs. In addition, whole air sample collection in evacuated canisters is not the ideal sampling method for acetic acid. A different sampling/analysis method would be required to evaluate on-orbit acetic acid concentrations.


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5/15/2013
Date

- Enclosures Table 1: Analytical concentrations of compounds found in the contingency GSCs
- Table 2: T-values corresponding to analytical concentrations in Table 1.

TABLE 1
ANALYTICAL RESULTS OF
SPACE-X-2 RETURN GSC AIR SAMPLES

CHEMICAL CONTAMINANT	CONCENTRATION (mg/M ³)	
	AA05496 + Contingency Sample 1 Lab1 D1 02/05/13 @ 18:00 GMT S/N 2010	AA05497 Contingency Sample 2 Inside MSG 02/22/13 @ 17:40 GMT S/N 2019
	TARGET COMPOUNDS (TO-14/POLAR)	
FREON12	<0.083	<0.050
CHLOROMETHANE	<0.083	<0.050
FREON114	<0.083	<0.050
METHANOL	0.43	0.54
ACETALDEHYDE	0.18	0.25
VINYLCHLORIDE	<0.083	<0.050
BROMOMETHANE	<0.083	<0.050
ETHANOL *	3.3	3.7
CHLOROETHANE	<0.083	<0.050
ACETONITRILE	<0.083	<0.050
PROPENAL	<0.083	<0.050
ACETONE	0.36	0.29
PROPANAL	TRACE	TRACE
ISOPROPANOL	0.49	0.26
FREON11	<0.083	<0.050
FURAN	<0.083	<0.050
ACRYLONITRILE	<0.083	<0.050
PENTANE	<0.083	<0.050
2-METHYL-2-PROPANOL	<0.083	<0.050
METHYLACETATE	<0.083	<0.050
1,1-DICHLOROETHENE	<0.083	<0.050
DICHLOROMETHANE	<0.083	<0.050
3-CHLOROPROPENE	<0.083	<0.050
FREON113	<0.083	<0.050
N-PROPANOL	TRACE	TRACE
1,1-DICHLOROETHANE	<0.083	<0.050
BUTANAL	<0.083	<0.050
2-BUTANONE	<0.083	<0.050
CIS-1,2-DICHLOROETHENE	<0.083	<0.050
2-METHYLFURAN	<0.083	<0.050
ETHYLACETATE	TRACE	0.057
HEXANE	<0.083	<0.050
CHLOROFORM	<0.083	<0.050
2-BUTENAL	<0.083	<0.050
1,2-DICHLOROETHANE	<0.083	TRACE
1,1,1-TRICHLOROETHANE	<0.083	<0.050
N-BUTANOL	TRACE	0.089
BENZENE	<0.083	<0.050
CARBONTETRACHLORIDE	<0.083	<0.050
2-PENTANONE	<0.083	<0.050
2-METHYLHEXANE	<0.083	<0.050
2,3-DIMETHYLPENTANE	<0.083	<0.050
PENTANAL	<0.083	<0.050
3-METHYLHEXANE	<0.083	<0.050
1,2-DICHLOROPROPANE	<0.083	<0.050
1,4-DIOXANE	<0.083	<0.050
TRICHLOROETHENE	<0.083	<0.050
2,5-DIMETHYLFURAN	<0.083	<0.050
N-HEPTANE	<0.083	<0.050
4-METHYL2-PENTANONE	<0.083	<0.050
CIS-1,3-DICHLOROPROPENE	<0.083	<0.050
2-PENTENAL	<0.083	<0.050
TRANS-1,3-DICHLOROPROPENE	<0.083	<0.050
1,1,2-TRICHLOROETHANE	<0.083	<0.050
TOLUENE	TRACE	TRACE
HEXANAL	<0.083	<0.050
MESITYLOXIDE	<0.083	<0.050
1,2-DIBROMOETHANE	<0.083	<0.050
BUTYLACETATE	<0.083	<0.050
OCTANE	<0.083	<0.050
TETRACHLOROETHENE	<0.083	<0.050
CHLOROBENZENE	<0.083	<0.050
ETHYLBENZENE	<0.083	<0.050
M/P-XYLENES	<0.083	<0.050
2-HEPTANONE	<0.083	<0.050
CYCLOHEXANONE	<0.083	<0.050
HEPTANAL	<0.083	<0.050
STYRENE	<0.083	<0.050
1,1,2,2-TETRACHLOROETHANE	<0.083	<0.050
O-XYLENE	TRACE	0.085
NONANE	<0.083	<0.050
1,3,5-TRIMETHYLBENZENE	<0.083	<0.050
1,2,4-TRIMETHYLBENZENE	<0.083	<0.050
1,3-DICHLOROBENZENE	<0.083	<0.050
1,4-DICHLOROBENZENE	<0.083	<0.050
1,2-DICHLOROBENZENE	<0.083	<0.050
1,2,4-TRICHLOROBENZENE	<0.083	<0.050
HEXACHLORO-1,3-BUTADIENE	<0.083	<0.050

**TABLE 1
ANALYTICAL RESULTS OF
SPACEX-2 RETURN GSC AIR SAMPLES**

CHEMICAL CONTAMINANT	CONCENTRATION (mg/M ³)	
	AA05496 + Contingency Sample 1 Lab1 D1 02/05/13 @ 18:00 GMT S/N 2010	AA05497 Contingency Sample 2 Inside MSG 02/22/13 @ 17:40 GMT S/N 2019
	SPECIAL INTEREST COMPOUNDS **	
1,3-BUTADIENE	<0.083	<0.050
ETHYLENE OXIDE	<0.083	<0.050
2-METHYL-2-PROPENAL	<0.083	<0.050
3-BUTEN-2-ONE	<0.083	<0.050
2-ETHOXYETHANOL	<0.083	<0.050
DIMETHYL DISULFIDE	<0.083	<0.050
OCTAFLUOROPROPANE &	26	15
PERFLUORO-2-METHYLPENTANE &	<0.083	<0.050
CARBONYL SULFIDE &	<0.083	<0.050
ISOBUTANE &	0.71	<0.050
2-METHYL-1-PROPENE &	TRACE	TRACE
DIMETHYL SULFIDE &	<0.083	<0.050
CARBON DISULFIDE &	<0.083	<0.050
TRIMETHYLSILANOL &	0.29	0.13
OCTAMETHYLCYCLOTETRASILOXANE &	0.12	0.10
DECAMETHYLCYCLOPENTASILOXANE &	0.54	0.86
HEXAMETHYLCYCLOTRIASILOXANE %	<0.083	<0.050
NON-TARGET COMPOUNDS **		
SULFUR HEXAFLUORIDE	0.086	0.12
1,1,1,2-TETRAFLUOROETHANE	0.13	0.20
1,1-DIFLUOROETHANE	<0.083	<0.050
PROPENE	<0.083	<0.050
PROPANE	<0.083	<0.050
TOTAL ALCOHOLS PLUS ACETONE	4.6	4.9
TARGET COMPOUNDS (GC)		
CARBON MONOXIDE	<0.38	<0.23
METHANE	7	7.3
HYDROGEN	3.7	3.1
CARBON DIOXIDE	5266	7518
TOTAL CONCENTRATION (NON-METHANE HYDROCARBONS)	33	22
TOTAL CONCENTRATION - OFP (NON-METHANE HYDROCARBONS)	6.8	6.9

+ Detection limits are higher due to low initial sample pressure and high dilution factor

< : Value is less than the laboratory report detection limit.

* GC/FID data results are in bold

** Quantified using "B" response factor except where noted

& Quantified using a multi-point calibration

% Response factor generated from an internal study

TRACE: Amount detected is sufficient for compound identification only.

OFP - Octafluoropropane

TABLE 2
T-VALUES for SPACE-X-2 RETURN GSC AIR SAMPLES

CHEMICAL CONTAMINANT	T-VALUE (180-d SMAC)	
	AA05496	AA05497
	Contingency Sample 1 Lab1D1 02/05/13 @ 18:00 GMT S/N 2010	Contingency Sample 2 Inside MSG 02/22/13 @ 17:40 GMT S/N 2019
TARGET COMPOUNDS (TO-14/POLAR)		
FREON12	ND	ND
CHLOROMETHANE	ND	ND
FREON114	ND	ND
METHANOL	0.00473	0.00596
ACETALDEHYDE	0.04566	0.06232
VINYLCHLORIDE	ND	ND
BROMOMETHANE	ND	ND
ETHANOL	0.00165	0.00187
CHLOROETHANE	ND	ND
ACETONITRILE	ND	ND
PROPENAL	ND	ND
ACETONE	0.00690	0.00557
PROPANAL	0.00376	0.00227
ISOPROPANOL	0.00328	0.00172
FREON11	ND	ND
FURAN	ND	ND
ACRYLONITRILE	ND	ND
PENTANE	ND	ND
2-METHYL-2-PROPANOL	ND	ND
METHYLACETATE	ND	ND
1,1-DICHLOROETHENE	ND	ND
DICHLOROMETHANE	ND	ND
3-CHLOROPROPENE	ND	ND
FREON113	ND	ND
N-PROPANOL	0.00042	0.00026
1,1-DICHLOROETHANE	ND	ND
BUTANAL	ND	ND
2-BUTANONE	ND	ND
CIS-1,2-DICHLOROETHENE	ND	ND
2-METHYLFURAN	ND	ND
ETHYLACETATE	0.00023	0.00032
HEXANE	ND	ND
CHLOROFORM	ND	ND
2-BUTENAL	ND	ND
1,2-DICHLOROETHANE	ND	0.01563
1,1,1-TRICHLOROETHANE	ND	ND
N-BUTANOL	0.00103	0.00222
BENZENE	ND	ND
CARBONTETRACHLORIDE	ND	ND
2-PENTANONE	ND	ND
2-METHYLHEXANE	ND	ND
2,3-DIMETHYLPENTANE	ND	ND
PENTANAL	ND	ND
3-METHYLHEXANE	ND	ND
1,2-DICHLOROPROPANE	ND	ND
1,4-DIOXANE	ND	ND
TRICHLOROETHENE	ND	ND
2,5-DIMETHYLFURAN	ND	ND
N-HEPTANE	ND	ND
4-METHYL2-PENTANONE	ND	ND
CIS-1,3-DICHLOROPROPENE	ND	ND
2-PENTENAL	ND	ND
TRANS-1,3-DICHLOROPROPENE	ND	ND
1,1,2-TRICHLOROETHANE	ND	ND
TOLUENE	0.00276	0.00167
HEXANAL	ND	ND
MESITYLOXIDE	ND	ND
1,2-DIBROMOETHANE	ND	ND
BUTYLACETATE	ND	ND
OCTANE	ND	ND
TETRACHLOROETHENE	ND	ND
CHLOROBENZENE	ND	ND
ETHYLBENZENE	ND	ND
M/P-XYLENES	ND	ND
2-HEPTANONE	ND	ND
CYCLOHEXANONE	ND	ND
HEPTANAL	ND	ND
STYRENE	ND	ND
1,1,2,2-TETRACHLOROETHANE	ND	ND
O-XYLENE	0.00112	0.00231
NONANE	ND	ND
1,3,5-TRIMETHYLBENZENE	ND	ND
1,2,4-TRIMETHYLBENZENE	ND	ND
1,3-DICHLOROBENZENE	ND	ND
1,4-DICHLOROBENZENE	ND	ND
1,2-DICHLOROBENZENE	ND	ND
1,2,4-TRICHLOROBENZENE	ND	ND
HEXACHLORO-1,3-BUTADIENE	ND	ND

TABLE 2
T-VALUES for SPACEX-2 RETURN GSC AIR SAMPLES

CHEMICAL CONTAMINANT	T-VALUE (180-d SMAC)	
	AA05496	AA05497
	Contingency Sample 1 Lab1D1 02/05/13 @ 18:00 GMT S/N 2010	Contingency Sample 2 Inside MSG 02/22/13 @ 17:40 GMT S/N 2019
SPECIAL INTEREST COMPOUNDS		
1,3-BUTADIENE	ND	ND
ETHYLENE OXIDE	ND	ND
2-METHYL-2-PROPENAL	ND	ND
3-BUTEN-2-ONE	ND	ND
2-ETHOXYETHANOL	ND	ND
DIMETHYL DISULFIDE	ND	ND
OCTAFLUOROPROPANE	0.00031	0.00018
PERFLUORO-2-METHYLPENTANE	ND	ND
CARBONYL SULFIDE	ND	ND
ISOBUTANE	0.00296	ND
2-METHYL-1-PROPENE	0.00004	0.00002
DIMETHYL SULFIDE	ND	ND
CARBON DISULFIDE	ND	ND
TRIMETHYLSILANOL	0.07261	0.03330
OCTAMETHYLCYCLOTETRA-SILOXANE	0.01040	0.00865
DECAMETHYLCYCLOPENTASILOXANE	0.03574	0.05712
HEXAMETHYLCYCLOTRI-SILOXANE %	ND	ND
NON-TARGET COMPOUNDS		
SULFUR HEXAFLUORIDE	0.00007	0.00010
1,1,1,2-TETRAFLUOROETHANE	0.00128	0.00190
1,1-DIFLUOROETHANE	ND	ND
PROPENE	ND	ND
PROPANE	ND	ND
TARGET COMPOUNDS (GC)		
CARBON MONOXIDE	0.02235	0.00674
METHANE	0.00190	0.00209
HYDROGEN	0.01098	0.00924
CARBON DIOXIDE	0.40504	0.57833
TOTAL T-VALUE	0.63522	0.79978
TOTAL T-VALUE - CO2	0.23018	0.22145

ND : Value is less than the laboratory report detection limit.

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