Houston, Texas

Jeffrey A. Rutz*, John R. Schultz, and C. Mike Kuo Wyle Integrated Science & Engineering Group

Harold E. Cole and Sam Manuel Boeing Huntsville Laboratory Huntsville, Alabama

Matthew Curtis, Patrick R. Jones, and O. David Sparkman University of the Pacific Department of Chemistry Stockton, California

J. Torin McCoy NASA Johnson Space Center Houston, Texas

ABSTRACT

<u>Discovery and Identification of Dimethylsilanediol as a Contaminant in ISS Potable</u> Water

In September of 2010, analysis of ISS potable water samples was undertaken to determine the contaminant responsible for a rise in total organic carbon (TOC). As analysis of the routine target list of organic compounds did not reveal the contaminant, efforts to look for unknown compounds was initiated, resulting in an unknown peak being discovered in the gas chromatography/mass spectrometry (GC/MS) analysis for glycols. A mass spectrum of the contaminant was then generated by concentrating one of the samples by evaporation and analyzing by GC/MS in full-scan mode. Although a computer match of the compound's identity could not be obtained with the instrument's database, a search with a more up to date mass spectral library yielded a good match with dimethylsilanediol (DMSD). Inductively Coupled Plasma/Mass Spectrometry (ICP/MS) analyses showed abnormally high silicon levels in the samples, confirming that the unknown contained silicon. DMSD was then synthesized to confirm the identification and provide a standard to develop a calibration curve. Further confirmation was provided by external Direct Analysis in Real Time (DART) GC/MS analysis. A preliminary GC/MS method was then developed and archived samples from various locations on ISS were analyzed to determine the extent of the contamination and provide data for troubleshooting. This paper describes these events in more detail as well as problems encountered in routine GC/MS analyses and the subsequent development of high performance liquid chromatography and LC/MS/MS methods for quantitation of DMSD.

*Wyle Integrated Science & Engineering Group 1290 Hercules Drive, Suite 120 Houston, TX 77058 Phone: 281-483-6425

Fax: 281-483-3058 Jeffrey.a.rutz@nasa.gov