An Assessment of the *International Space Station*'s Trace Contaminant Control Subassembly Process Economics

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*August 2005*
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August 2005
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<td>BMP</td>
<td>microcontaminant filtering system (Russian acronym)</td>
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<tr>
<td>CBA</td>
<td>charcoal bed assembly</td>
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<tr>
<td>CH$_3$SO$_3$H</td>
<td>methanesulfonic acid</td>
</tr>
<tr>
<td>CH$_4$</td>
<td>methane</td>
</tr>
<tr>
<td>Cl</td>
<td>chlorine</td>
</tr>
<tr>
<td>CO</td>
<td>carbon monoxide</td>
</tr>
<tr>
<td>CO$_2$</td>
<td>carbon dioxide</td>
</tr>
<tr>
<td>COA</td>
<td>catalytic oxidizer assembly</td>
</tr>
<tr>
<td>CSA-CP</td>
<td>compound-specific analyzer for combustion products</td>
</tr>
<tr>
<td>ECLSS</td>
<td>Environmental Control and Life Support System</td>
</tr>
<tr>
<td>EPA</td>
<td>Environmental Protection Agency</td>
</tr>
<tr>
<td>F</td>
<td>fluorine</td>
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<td>GANK</td>
<td>gas analyzer (Russian acronym)</td>
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<td>GC</td>
<td>gas chromatography</td>
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<tr>
<td>H</td>
<td>hydrogen</td>
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<tr>
<td>H$_2$O</td>
<td>water</td>
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<td>H$_3$PO$_4$</td>
<td>phosphoric acid</td>
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<tr>
<td>HCl</td>
<td>hydrogen chloride</td>
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<tr>
<td>HF</td>
<td>hydrogen fluoride</td>
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<td>ISS</td>
<td><em>International Space Station</em></td>
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<td>KSC</td>
<td>Kennedy Space Center</td>
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<tr>
<td>Li</td>
<td>lithium</td>
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<td>Li$_2$CO$_3$</td>
<td>lithium carbonate</td>
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<tr>
<td>Acronym</td>
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<tr>
<td>LiOH</td>
<td>lithium hydroxide</td>
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<td>MS</td>
<td>mass spectrometry</td>
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<tr>
<td>N₂</td>
<td>nitrogen</td>
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<tr>
<td>Na₂CO₃</td>
<td>sodium carbonate</td>
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<td>sodium hydroxide</td>
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<td>NOₓ</td>
<td>oxides of nitrogen</td>
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<td>OFP</td>
<td>octafluoropropane/Freon 218</td>
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<td>ORU</td>
<td>on-orbit replaceable unit</td>
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<td>Pd</td>
<td>palladium</td>
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<td>relative percent difference</td>
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<td>Russian on-orbit segment</td>
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<td>resistance temperature detector</td>
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<td>SBA</td>
<td>sorbent bed assembly</td>
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<td>SKV</td>
<td>air conditioning and humidity removal assembly (Russian acronym)</td>
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<td>service module</td>
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<td>spacecraft maximum allowable concentration</td>
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<td>Space Transportation System</td>
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<td>TCCS</td>
<td>trace contaminant control subassembly</td>
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<td>temperature and humidity control</td>
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<td>utilization flight</td>
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<td>VOC</td>
<td>volatile organic compound</td>
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1. INTRODUCTION

Key characteristics of a crewed spacecraft cabin—low leakage rates, a small specific volume, and the use of a host of advanced materials of construction—qualify it as the “ultimate in tight building design” and may contribute to conditions leading to unhealthy air quality if appropriate care is not exercised.\[1\] Within the boundary defined by the air quality standards set for crew health purposes, the design approach must balance a number of competing design elements to achieve acceptable cabin air quality.\[2\] Specific attention to these design elements during the spacecraft cabin design, manufacturing, and subsequent operations can passively minimize trace chemical contaminant generation; however, it is not possible to completely eliminate all sources. Therefore, active controls are needed on board the spacecraft to fully address the air quality control challenge.

The International Space Station (ISS) Environmental Control and Life Support System (ECLSS) includes equipment specifically designed to actively remove trace chemical contamination from the cabin atmosphere. This equipment includes two primary control units—one in the United States on-orbit segment (USOS) and the other in the Russian on-orbit segment (ROS). Trace contaminant control is provided by the trace contaminant control subassembly (TCCS) located in the atmosphere revitalization subsystem (ARS) rack that is housed in the laboratory module, Destiny. The microcontaminant filtering system, known by its Russian acronym BMP, located in the service module, Zvezda, provides the trace contaminant control function in the ROS. Both the TCCS and BMP operate simultaneously. The BMP employs regenerable activated charcoal beds and therefore has a lower logistics penalty leading to a low life cycle cost associated with its operation. In contrast, the TCCS beds cannot be regenerated in situ leading to a greater relative life cycle cost. Because maintaining the TCCS’s proper function is logistically intensive, its performance in flight has been studied in detail to determine where savings may be achieved. The following discussion provides details of these studies and recommendations for improving the TCCS’s process economics without compromising its performance or crew health and safety.

1.1 Active Trace Contaminant Control On Board the International Space Station’s United States On-Orbit Segment

The TCCS provides active trace chemical contamination control on board the ISS’s USOS. Employing physical adsorption, thermal catalytic oxidation, and chemical adsorption processes to remove trace chemical contaminants from the cabin atmosphere, the TCCS is a mature equipment design with more than 25 yr of development and refinement behind it that began in the early 1970s. It is mounted in the ARS rack located in the laboratory module, Destiny.\[3\] Figures 1 and 2, a simplified
process flow diagram and isometric view, show the primary on-orbit replaceable units (ORUs) within the TCCS. They include a charcoal bed assembly (CBA), a thermal catalytic oxidizer assembly (COA), and a post-sorbent bed assembly (SBA) as well as a blower assembly, flowmeter assembly, and electrical assembly. The CBA and SBA are expendable while the COA is subject to potentially life-limiting catalyst poisoning and component wearout. Other TCCS components are replaced as they wear out. Figures 2 and 3 show the spatial arrangement of the TCCS and its location in the ARS rack. The TCCS is mounted on slides in the ARS rack to facilitate on-orbit maintenance.
The CBA, COA, and SBA are the primary components that remove contaminants as the TCCS processes the cabin atmosphere. The process begins as the cabin atmosphere enters the TCCS directly from the cabin at 15.29 m$^3$/hr (9 ft$^3$/min) and first flows through the CBA. The CBA is an expendable, fixed bed containing 22.7 kg (50 lb) of 4 x 6 mesh Barnebeye-Sutcliffe Corporation Type 3032 granular activated charcoal. The charcoal is treated with 10 percent phosphoric acid (H$_3$PO$_4$) by weight. Its key design compounds are ammonia (NH$_3$) and dichloromethane. While the CBA removes a broad spectrum of other volatile organic compounds (VOCs) from the process air stream, NH$_3$ and dichloromethane are the key design components that determine the bed’s size.

While the CBA is quite effective for removing a variety of chemical contaminants from the process air stream, some compounds such as methane (CH$_4$), carbon monoxide (CO), and low molecular weight alcohols are not removed or poorly removed by adsorption. The COA oxidizes these poorly adsorbed compounds, thereby supplementing the CBA to achieve a broad spectrum control capability. The COA consists of a recuperative heat exchanger, electrical heater, and a fixed bed of catalyst pellets (fig. 4). The catalyst bed consists of 0.5 kg (1.1 lb) of 3.2-mm cylindrical alumina pellets that support a 0.5-percent palladium (Pd) catalyst manufactured by Engelhard Corporation. The process condition within the COA is normally maintained at 400 °C (750 °F), although the unit is capable of achieving a temperature as high as 538 °C (1,000 °F). While it is specifically designed to convert CH$_4$ and CO to carbon dioxide (CO$_2$), the COA will also oxidize a variety of other VOCs. Because CH$_4$ and CO control do not require a high flow rate, only one-third of the total process air stream entering the TCCS, approximately 4.59 m$^3$/hr (2.7 ft$^3$/min) flows through the COA. This reduces the TCCS’s overall power consumption.
Upon exiting the COA, the air flows through a fixed bed containing 1.4 kg (3 lb) of 6×14 mesh granular anhydrous lithium hydroxide (LiOH); the LiOH is manufactured by the Cyprus Foote Mineral Company. Because many light halocarbons can break through the CBA and oxidize in the COA to produce acid gases, the SBA provides posttreatment to prevent these oxidation products from entering the cabin. Downstream of the SBA, the flow streams combine and exit the TCCS.

1.2 Preflight Assessment of Trace Contaminant Control Subassembly Process Economics

1.2.1 Design Basis and Sources of Conservatism

Because the TCCS employs consumable charcoal and LiOH resources, it has a potentially high life cycle cost associated with its operation. Service intervals established for the CBA, SBA, and COA dictate the TCCS’s process economics. Since other components are replaced as they wear out, they are not considered to be candidates for reducing the TCCS’s process economics.

As the TCCS design and operational approach has matured, there have been refinements in the recommended service interval for the CBA, SBA, and COA. Early in the ISS developmental phase, the service interval for the CBA and SBA was set at 90 days and the COA service interval was set at 1 yr. This early service interval estimate was based upon a highly conservative trace contaminant loading assumption combined with the assumption that the TCCS would not receive any assistance from humidity condensate absorption. The CBA, SBA, and COA weigh 36.6, 4.1, and 11 kg, respectively. For the initially specified service intervals, a total of 174 kg would need to be delivered to the ISS.
annually. As well, a total of 4.2 hr of crew time would be required to carry out the maintenance. Beyond this, there are the annual costs for refurbishing the CBA, SBA, and COA on the ground.

Developmental testing established two areas of conservatism associated with the TCCS design. First, trace contaminant removal via absorption in humidity condensate provides a significant assist to the overall trace contaminant control function. For instance, contaminant removal via absorption in humidity condensate was found to provide more than 55 percent of the total NH$_3$ removal. As stated earlier, NH$_3$ is a key design-driven compound for the CBA design and service interval. Its design did not consider a reduced load resulting from the assist from absorption in humidity condensate. Second, catalyst poisoning by halocarbons relative to CH$_4$’s conversion to CO$_2$ is a function of the poison concentration entering the COA; this poisoning is for the most part reversible. The original COA service interval was based upon the assumption that catalyst poisoning is cumulative over time. The testing showed that only poison concentration affects the degree of poisoning. Therefore, the COA service interval may be reevaluated with respect to the degree of CBA saturation and actual halocarbon concentration in the cabin atmosphere.

The trace contaminant load model used as the design specification was also a source of conservatism. The early model was derived from raw equipment offgassing test data collected at 50 °C. These data were then adjusted by a mass index that scaled the offgassing rates by the ratio of the station mass to Spacelab mass. Extensive evaluation by NASA found that the raw offgassing test data are conservative by a factor of >10. As a result of this evaluation, NASA established a new trace contaminant load specification based upon equipment offgassing data from six Spacelab missions that included an adjustment for temperature. The new load model specification established specific offgassing rates for a kilogram of typical internally mounted spacecraft equipment. Also, an estimate for the total internal, nonstructural equipment mass was developed along with a recommended crew size for design. These specifications were set at 75,000 kg and 5.25 people, respectively.

### 1.2.2 Preflight On-Orbit Replaceable Unit Service Interval Estimates

Considering these areas of conservatism, further preflight analysis was conducted. Engineering analysis conducted by Lockheed and confirmed by NASA before Destiny was launched in February 2001 extended the CBA’s service life to 1 yr. Lockheed also extended the COA and SBA service intervals to 1.28 and 2.56 yr, respectively. The analysis conducted by Lockheed actually showed that a single CBA could be in service for 100 yr before the concentration of any single compound in the design load model would exceed 90 percent of its individual spacecraft maximum allowable concentration (SMAC). While this might appear to be acceptable strictly from a performance viewpoint, it is in reality a situation that must be avoided because it could lead to the TCCS itself becoming a source of contamination. For instance, if NH$_3$ is allowed to break through the CBA and enter the COA, it will be converted to oxides of nitrogen (NO$_x$). As well, any halocarbons that break through the CBA will be converted to acid gases in the COA. While the SBA controls these acid gases, a heavier loading may lead to a shorter service interval for the SBA, negatively affecting process economics.

To confirm Lockheed’s analysis, NASA conducted a similar evaluation. In this analysis, the TCCS was challenged with the design trace contaminant load specification—offgassing from 75,000 kg of internal equipment and the metabolic contribution from 5.25 people. The station assembly
was assumed to be completed; therefore, the cabin volume for the analysis was $\approx 600 \text{ m}^3$. The assist to the TCCS by five condensing heat exchangers was included in the assessment with an average latent load of 14 kg of condensate/day divided evenly among the condensing heat exchanger units for simplicity.

Results from NASA’s analysis showed that dichloromethane, one of the CBA’s principal compounds for design, is expected to begin to break through after 20 days and completely saturate the bed after 164 days. Data from developmental TCCS catalyst poisoning testing and the predicted dichloromethane concentration of 1.2 mg/m$^3$ indicate that the effect on the TCCS’s CH$_4$ oxidation efficiency is negligible. Furthermore, testing showed that the reduction in CH$_4$ oxidation efficiency by halogen poisoning is reversible. Combined with the fact that a minimum of 1-percent efficiency is necessary to maintain the CH$_4$ concentration below its SMAC of 3,800 mg/m$^3$, it becomes evident that the TCCS possesses a substantial design margin to accommodate catalyst poisoning by the trace halocarbon load.\textsuperscript{5} It was concluded from this analysis that allowing low concentration halocarbon breakthrough of the CBA is acceptable because it does not adversely affect the TCCS’s function. Evidence supporting this conclusion is presented later.

While halocarbon breakthrough presents no significant adverse effect on the TCCS’s intended function or process economics, as will be presented later, NH$_3$—another key design driver for the CBA—must be considered. The analysis conducted by NASA includes the key assumption that the TCCS receives an assist in NH$_3$ removal from absorption in humidity condensate. When this assist is considered, the time to NH$_3$ breakthrough is 694 days. In contrast, breakthrough is predicted to begin after 62 days without the assist. It can be seen why early service interval estimates established 90 days. Developmental testing showed that the TCCS may handle no more than 23 percent of the total NH$_3$ load.\textsuperscript{4} Because uncertainty is inherent in any preflight engineering analysis, it was assumed, conservatively, that it was reasonable for NH$_3$ breakthrough to begin at any time between 62 and 694 days. The median between these periods is 316 days. Therefore, it was considered reasonable and conservative to expect the charcoal bed to provide effective NH$_3$ control for a least 62 days plus the magnitude of the median, or 378 days. This was considered reasonable since the estimate is an extrapolation of ground testing that has not exceeded 45 days duration.

Compared to their originally specified service intervals, the most recent preflight estimates for the CBA, COA, and SBA service intervals reduce the logistics mass requirements by nearly 75 percent to 44.1 kg/yr. Even so, logistics mass, stowage volume, and crew time associated with routine maintenance is at a premium and impacts the time the crew may spend on scientific research. Efforts to further reduce the annual logistics requirements for operating the TCCS are considered appropriate given that there are three remaining areas of conservatism:

(1) The 1-yr CBA service interval estimate is for a crew of more than five compared to the present crew size of three.

(2) It was assumed that all the urea in human sweat decomposes to NH$_3$. In reality, this may not be the case, and the total NH$_3$ load in practice may be much lower than was used for design.
(3) The total offgassing rate is based upon the completely assembled station while the station is presently only about one-half complete with respect to its habitable volume.

Considering these areas of conservatism combined with the fact that the 1-yr CBA service interval estimate is actually an extrapolation that far exceeds ground testing experience, it was deemed appropriate to return the first CBA after 1 yr of operation and determine the extent that it was loaded. Because the CBA service interval has a direct bearing on the service interval for both the COA and SBA, the postflight assessment of the extent of the CBA’s loading is central to establishing the overall plan to managing the TCCS’s logistics needs. Essentially, the TCCS’s end-to-end performance must be understood thoroughly to achieve an effective management approach to its proper and safe operation. The following discussion presents the data and engineering evaluation required to achieve this.
2. CHARCOAL BED ASSEMBLY SERVICE INTERVAL

2.1 Trace Contaminant Control Subassembly Flight History and Charcoal Bed Assembly Sampling

To evaluate the CBA’s actual loading under flight conditions, charcoal samples were collected from the unit launched on board Destiny after \( \approx 14 \) mo in flight. The CBA had been installed in the TCCS after Destiny completed its preflight functional validation testing so all of its operational time was accumulated during flight. The TCCS was activated on February 13, 2001. Over the next 14 mo, the TCCS operated for 7,389 hr out of the total 9,984 in-service hours. It was shut down periodically for a total of 2,595 hr, or 26 percent of the total in-service hours. On April 6, 2002, the CBA was replaced with a spare unit containing fresh charcoal.

The CBA was returned by STS–111/UF–2 in June 2002 and delivered to the maintenance depot at NASA Kennedy Space Center (KSC). During refurbishment, twenty-five 100-g charcoal samples were collected for analysis. Figure 5 depicts the approximate sample locations and figure 6 shows the CBA just before sample collection. Samples were collected at five depths or segments through the CBA’s entire packed length—0, 15.2, 25.4, 40.6, and 55.9 cm from the charcoal packing inlet. Five samples were collected at each depth from four radial quadrants—designated A, B, C, and D—and the center. In addition, a sample of the fresh charcoal used to repack the CBA during the refurbishment was also collected. All of the samples were delivered to Boeing’s Analytical Services Laboratory, Huntsville, AL, for analysis of their VOC and \( \text{NH}_3 \) loading. In addition, the samples were analyzed for their \( \text{H}_3\text{PO}_4 \) content to characterize the theoretical \( \text{NH}_3 \) capacity.

![CBA sampling geometry](image-url)
2.2 Analytical Methods

2.2.1 Phosphate and Ammonia

Two methods were used for characterizing the phosphate and \( \text{NH}_3 \) loading—pH titration and ion chromatography. For both methods, it is necessary to desorb the \( \text{H}_3\text{PO}_4 \) by water (\( \text{H}_2\text{O} \)) extraction. To accomplish this, a portion of each sample was selected and ground into a powder using a mortar and pestle. First, 4-g aliquots of the powder were transferred to a bottle containing 50 mL of deionized \( \text{H}_2\text{O} \). Then, the \( \text{H}_2\text{O} \) and charcoal mixtures were shaken vigorously and allowed to stand for 24 hr. For the titration method, the \( \text{H}_2\text{O} \) desorbate was not filtered, while for the ion chromatography method, the desorbate was passed through a 0.45-\( \mu \) hydrophobic polyethersulfone filter before analysis.

For the titration method, the titrant was a 0.3-molar sodium hydroxide (NaOH) solution standardized against a primary standard of potassium hydrogen phthalate (\( \text{HOOC}_6\text{H}_4\text{COOK} \)). The titration was conducted in the bottle containing both the \( \text{H}_2\text{O} \) and charcoal. The pH was measured using a pH meter and recorded after adding successive 0.5-mL aliquots of titrant to ensure good resolution of the pH transitions.

For the ion chromatography method, the phosphate loading was measured by anion chromatography using a Dionex LC 20 ion chromatograph equipped with a conductivity detector. A Dionex AS12A 4-mm ID column with an eluent consisting of 2.7 millimolar (mM) sodium carbonate (\( \text{Na}_2\text{CO}_3 \)) and 0.3 mM sodium bicarbonate (\( \text{NaHCO}_3 \)) was used for the chromatographic analysis. \( \text{NH}_3 \) content was also determined similarly but with a Dionex CS16 Ionpac 5-mm column using a 26-mM methanesulfonic acid (\( \text{CH}_3\text{SO}_3\text{H} \)) eluent.
2.2.2 Volatile Organic Compounds

VOC loading was determined by gas chromatography/mass spectrometry (GC/MS) using a modified version of the U.S. Environmental Protection Agency (EPA) method TO-14 for air sample analyses. First, charcoal sample aliquots were thermally desorbed at 240 °C with a flow of 50 cm³/min over a period of 4 min into evacuated 500-cm³ Summa® passivated canisters. An Entech 5100 thermal desorption unit was used for the desorption step. Desorption into a canister allows the components to be diluted to a concentration within the optimum range of linearity for the GC/MS instrument. The canisters were pressurized to 103.4 kPa (15 psia) with high purity nitrogen (N₂) for the initial dilution analyses. Because a broad range of component concentrations were observed within the first segment of charcoal samples, the canister samples containing the desorbed components were analyzed multiple times at different dilutions to ensure minimum detection limits and optimum method accuracy across a broad dynamic range for both major and minor component loading. These additional dilutions were accomplished by additional pressurizations of the canister.

The canisters were connected to a Tekmar Model 2100 purge-and-trap unit where the volume of sample introduced into the purge-and-trap instrument was controlled by timed flow of the pressurized canister contents onto the purge-and-trap column utilizing a mass flow controller. The trap column was a Supelco model VOCARB column composed of Carbopack B, Carboxen 1000, and Carboxen 1001 sorbents. To minimize the amount of H₂O ultimately reaching the instrument, the purge-and-trap column was first thermally desorbed into an Entech model 7000 cryofocusing unit where the components were trapped at –175 °C. Before desorbing and transferring the purged and trapped components, known quantities of volatile internal standards are added. The cryofocusing unit temperature is then rapidly raised to 80 °C, and the components are transferred to the gas chromatographic column via a heated transfer line maintained at 110 °C. The GC receiving the desorbed components is equipped with a J&W Model DB 624 60-m × 0.32-mm capillary column coated with 1.8-μ film thickness. Collection of the components on the GC column is performed at an equilibrated column temperature of 35 °C. Analysis is then conducted by ramping the GC oven to 220 °C at a rate of 8 °C/min.

2.3 Analytical Results

2.3.1 Phosphoric Acid Loading

Two analytical approaches were used to measure the H₃PO₄ and NH₃ loading on the samples—pH titration and ion chromatography. Figure 7 is a typical H₃PO₄ titration curve that shows two equivalence points. H₃PO₄ contains three hydrogen (H) atoms capable of neutralization with pKa values of 2.16, 7.21, and 12.32. Because the pH transition of the third H takes place at a very high pH, the change in pH at that equivalence point is not shown in figure 7.
Figure 7 shows that the second equivalence point is exactly twice the volume of the first, as is expected for a polyprotic acid. The number of NH$_3$ equivalents chemisorbed by the H$_3$PO$_4$ is calculated based upon the difference between the titrant volumes required to neutralize the first two H atoms. Replicate samples of unused acid-treated charcoal were subjected to the analytical method to serve as a check for this approach. Figure 8, which shows the results from the unused charcoal samples, indicates that the titrant volumes necessary to neutralize the first two H atoms of the H$_3$PO$_4$ are not equivalent. The titrant volume required to neutralize the first H was consistently lower, suggesting that the charcoal neutralizes a percentage of the first H when the H$_3$PO$_4$ is loaded onto it. Calculations based upon the two equivalence points indicate an average first H depletion of 50.5 percent for the unused charcoal sample. The depletion varied from 46 to 56 percent for the different replicates.
Charcoal sample replicates collected from the CBA were prepared and analyzed by the same method. Figure 9 shows the data obtained from the first and second segments of a representative sample. The segment 1B sample is typical of all segment 1 samples, while the segment 2B sample is typical of all samples from segments 2 through 5. Examination of figure 9 indicates that there is no good end point for the second H for the segment 1 samples. Because the samples contain adsorbed NH$_3$ and the ammonium ion is a weak acid, the end points for ammonium ion conjugate acid and the dihydrogen phosphate of the H$_3$PO$_4$ may merge, resulting in a poor end point.
Because all data from segments 2 through 5 have good end points, they can be used to calculate an average depletion of the $\text{H}_3\text{PO}_4$’s first H. Analysis of five replicate samples from segment 2 samples established a range of depletion from 26 to 43 percent with an average of 37 percent.

Although the titration method provided useful insight into the depletion of the first H, the variability and poor end points observed for segment 1 using the titration method indicated further analysis via a second method was necessary. Ion chromatography was used for further analysis of the phosphate and NH$_3$ loading of segment 1. Three replicate samples were collected from each of the five quadrant samples from segment 1, ground to a powder, and desorbed by soaking with deionized H$_2$O for $\approx$20 hr. Table 1 summarizes the phosphate data acquired for these samples and two fresh charcoal samples that were submitted for comparative purposes. More detailed data are found in appendix A. The first fresh charcoal sample was from the batch used to repack the CBA, and the second was collected from a separate batch for evaluation of potential batch-to-batch $\text{H}_3\text{PO}_4$ loading differences.

Table 1. CBA charcoal phosphate loading.

<table>
<thead>
<tr>
<th>Sample Description</th>
<th>Average (mg/g)</th>
<th>Range (mg/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Segment 1 center</td>
<td>101</td>
<td>98–107</td>
</tr>
<tr>
<td>Segment 1A</td>
<td>93</td>
<td>83–105</td>
</tr>
<tr>
<td>Segment 1B</td>
<td>98</td>
<td>90–103</td>
</tr>
<tr>
<td>Segment 1C</td>
<td>74</td>
<td>62–82</td>
</tr>
<tr>
<td>Segment 1D</td>
<td>84</td>
<td>62–99</td>
</tr>
<tr>
<td>Segment 1 average</td>
<td>90</td>
<td>62–107</td>
</tr>
<tr>
<td>Unused sample 1</td>
<td>56</td>
<td>54–58</td>
</tr>
<tr>
<td>Unused sample 2</td>
<td>100</td>
<td>98–102</td>
</tr>
</tbody>
</table>
The ion chromatography method indicates an average $\text{H}_3\text{PO}_4$ loading data of 90 mg/g for the used charcoal and 100 mg/g for the unused charcoal sample 2. These loadings are in good agreement with the 10 wt. % (100 mg/g) $\text{H}_3\text{PO}_4$ specification. It should be noted that the average of 90 percent for all the used charcoal replicates is the average of all the replicate data. The loading for the unused charcoal sample 1, however, was considerably different. Its loading averaged 56 percent, indicating potential batch-wise variation in $\text{H}_3\text{PO}_4$ loading as delivered from the vendor. Also, this sample of unused charcoal was collected from the batch used to repack the CBA. Therefore, the newly repacked CBA would appear to be out of specification for $\text{H}_3\text{PO}_4$ loading.

2.3.2 Further Evaluation of Batch-Wise Phosphoric Acid Content

Further evaluation of the potential batch-wise variation in $\text{H}_3\text{PO}_4$ loading was conducted on random samples collected from eight drums of activated charcoal in storage at KSC. Table 2 shows the results of replicate analyses of the eight samples. As can be seen, the average $\text{H}_3\text{PO}_4$ loading is 88 mg/g with a range from 48 to 145 mg/g. These data indicate that $\text{H}_3\text{PO}_4$ variation within a batch of charcoal is characteristic of the material. Because a discrete, random sampling technique was used in favor of more sophisticated methods that involve collecting core samples, the observed variation may actually be enhanced by the technique used to collect samples from the drums. Therefore, the sampling technique makes it possible to collect a sample from a pocket of charcoal with low, moderate, or high loading merely by chance. For the purpose of the CBA service interval, however, this variation must be accounted for to ensure the TCCS’s proper performance and safe operation.

Table 2. Phosphate loading for charcoal in depot storage.

<table>
<thead>
<tr>
<th>Sample No.</th>
<th>Sample Mass in 500 mL (g)</th>
<th>Loading Summary</th>
<th>Precision Summary</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Average Phosphate (mg/L)</td>
<td>Analysis Average (mg/g charcoal)</td>
</tr>
<tr>
<td>1A</td>
<td>4.9996</td>
<td>1,040</td>
<td>100</td>
</tr>
<tr>
<td>1B</td>
<td>4.9879</td>
<td>1,098</td>
<td>110</td>
</tr>
<tr>
<td>2A</td>
<td>4.9826</td>
<td>1,212</td>
<td>122</td>
</tr>
<tr>
<td>2B</td>
<td>4.9933</td>
<td>1,236</td>
<td>124</td>
</tr>
<tr>
<td>3A</td>
<td>5.0403</td>
<td>1,071</td>
<td>106</td>
</tr>
<tr>
<td>3B</td>
<td>5.003</td>
<td>758</td>
<td>76</td>
</tr>
<tr>
<td>4A</td>
<td>5.0194</td>
<td>1,456</td>
<td>145</td>
</tr>
<tr>
<td>4B</td>
<td>4.9752</td>
<td>1,169</td>
<td>117</td>
</tr>
<tr>
<td>5A</td>
<td>4.982</td>
<td>851</td>
<td>85</td>
</tr>
<tr>
<td>5B</td>
<td>4.9778</td>
<td>609</td>
<td>61</td>
</tr>
<tr>
<td>6A</td>
<td>4.9964</td>
<td>927</td>
<td>93</td>
</tr>
<tr>
<td>6B</td>
<td>4.9946</td>
<td>824</td>
<td>82</td>
</tr>
<tr>
<td>7A</td>
<td>5.0077</td>
<td>847</td>
<td>85</td>
</tr>
<tr>
<td>7B</td>
<td>4.966</td>
<td>865</td>
<td>87</td>
</tr>
<tr>
<td>8A</td>
<td>4.9918</td>
<td>714</td>
<td>71</td>
</tr>
<tr>
<td>8B</td>
<td>4.9756</td>
<td>632</td>
<td>63</td>
</tr>
<tr>
<td>3A*</td>
<td>5.009</td>
<td>718</td>
<td>72</td>
</tr>
<tr>
<td>3B*</td>
<td>5.0034</td>
<td>540</td>
<td>54</td>
</tr>
<tr>
<td>5A*</td>
<td>5.0058</td>
<td>562</td>
<td>56</td>
</tr>
<tr>
<td>5B*</td>
<td>5.0058</td>
<td>477</td>
<td>48</td>
</tr>
<tr>
<td>Average</td>
<td></td>
<td>88</td>
<td>88</td>
</tr>
</tbody>
</table>
2.3.3 Ammonia Loading

Table 3 shows the average results for analyses of duplicate 1-g quantities of charcoal samples. The samples were ground to a powder and desorbed with H₂O over a 24-hr period. The desorbates were filtered and analyzed for NH₃ by ion chromatography. Appendix B contains a more detailed summary of these data. These data show NH₃ loading in the first segment with very small trace loading through the remainder of the bed. The actual depth of NH₃ loading cannot be accurately determined from the sampling approach used, so it is assumed that the loading may decrease linearly through the length of the first segment.

Table 3. CBA ammonia loading summary.

<table>
<thead>
<tr>
<th>Description</th>
<th>Ammonia (mg/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Segment 1 center</td>
<td>3.55</td>
</tr>
<tr>
<td>Segment 1A</td>
<td>4.38</td>
</tr>
<tr>
<td>Segment 1B</td>
<td>5.74</td>
</tr>
<tr>
<td>Segment 1C</td>
<td>4.83</td>
</tr>
<tr>
<td>Segment 1D</td>
<td>3.58</td>
</tr>
<tr>
<td>Segment 2 center</td>
<td>0.007</td>
</tr>
<tr>
<td>Segment 2A</td>
<td>0.008</td>
</tr>
<tr>
<td>Segment 2B</td>
<td>0.006</td>
</tr>
<tr>
<td>Segment 2C</td>
<td>0.008</td>
</tr>
<tr>
<td>Segment 2D</td>
<td>0.008</td>
</tr>
<tr>
<td>Segment 3 center</td>
<td>0.007</td>
</tr>
<tr>
<td>Segment 3A</td>
<td>0.006</td>
</tr>
<tr>
<td>Segment 3B</td>
<td>0.007</td>
</tr>
<tr>
<td>Segment 3C</td>
<td>0.006</td>
</tr>
<tr>
<td>Segment 3D</td>
<td>0.006</td>
</tr>
<tr>
<td>Segment 4 center</td>
<td>0.009</td>
</tr>
<tr>
<td>Segment 4A</td>
<td>0.007</td>
</tr>
<tr>
<td>Segment 4B</td>
<td>0.007</td>
</tr>
<tr>
<td>Segment 4C</td>
<td>0.005</td>
</tr>
<tr>
<td>Segment 4D</td>
<td>0.004</td>
</tr>
<tr>
<td>Segment 5 center</td>
<td>0.006</td>
</tr>
<tr>
<td>Segment 5A</td>
<td>0.006</td>
</tr>
<tr>
<td>Segment 5B</td>
<td>0.006</td>
</tr>
<tr>
<td>Segment 5C</td>
<td>0.006</td>
</tr>
<tr>
<td>Segment 5D</td>
<td>0.006</td>
</tr>
</tbody>
</table>

2.3.4 Volatile Organic Compound Loading

VOC analysis identified 58 target compounds and 40 tentatively identified compounds. Twenty-five compounds in seven functional classes comprise the major portion of the loading. Table 4 summarizes the VOC loading by functional class and compound. Appendix C contains detailed data for each sample analyzed.
Table 4. Functional classes and VOCs loaded on CBA charcoal.

<table>
<thead>
<tr>
<th>Functional Class</th>
<th>Compounds</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alcohols</td>
<td>Ethanol</td>
</tr>
<tr>
<td></td>
<td>2-propanol</td>
</tr>
<tr>
<td></td>
<td>n-propanol</td>
</tr>
<tr>
<td></td>
<td>n-butanol</td>
</tr>
<tr>
<td></td>
<td>2-butanol</td>
</tr>
<tr>
<td>Aldehydes</td>
<td>Ethanal</td>
</tr>
<tr>
<td></td>
<td>Propanal</td>
</tr>
<tr>
<td></td>
<td>Butanal</td>
</tr>
<tr>
<td>Esters</td>
<td>Ethyl acetate</td>
</tr>
<tr>
<td></td>
<td>Butyl acetate</td>
</tr>
<tr>
<td></td>
<td>Propyl acetate</td>
</tr>
<tr>
<td>Ketones</td>
<td>2-propanone</td>
</tr>
<tr>
<td></td>
<td>2-butanone</td>
</tr>
<tr>
<td></td>
<td>4-methyl-2-pentanone</td>
</tr>
<tr>
<td>Aromatics</td>
<td>Benzene</td>
</tr>
<tr>
<td></td>
<td>Methylbenzene</td>
</tr>
<tr>
<td></td>
<td>Dimethylbenzenes</td>
</tr>
<tr>
<td>Halocarbons</td>
<td>Dichloromethane</td>
</tr>
<tr>
<td></td>
<td>Chlorobenzene</td>
</tr>
<tr>
<td></td>
<td>Octafluoropropane</td>
</tr>
<tr>
<td>Aliphatic hydrocarbons</td>
<td>Octane</td>
</tr>
<tr>
<td></td>
<td>Cyclohexane</td>
</tr>
<tr>
<td></td>
<td>Heptane</td>
</tr>
<tr>
<td></td>
<td>Hexane</td>
</tr>
</tbody>
</table>

2.3.4.1 Axial Loading. Analysis of the data shows three patterns of VOC loading. The first pattern is heavily loaded in the first segment with trace loading in segments 2 through 5. Figures 10–12 illustrate this pattern for the esters, aromatics, and hydrocarbons, respectively. Compounds in these functional classes tend to have a higher average molecular weight and lower volatility than those in the other four classes. The second pattern, exhibited by the alcohols and shown in figure 13, has a peak loading in the second segment with lower loading through the remainder of the bed. This pattern indicates a rollup effect. Rollup occurs when high molecular weight, lower volatility compounds push the lighter, more volatile compounds off the first segment of the bed. Similar loading is exhibited by octafluoropropane (OFP or Freon 218) as shown in figure 14. The rollup effect for OFP is more pronounced in that no detectable loading was observed in the first segment with the peak loading in the second segment. From these data, it is concluded that the OFP has been displaced from the first segment of the bed by more easily adsorbed compounds. Loading through the remaining three segments was found to be fairly uniform. The aldehydes, ketones, and halocarbons exhibit the third loading pattern. Figures 15–17 show that loading for these functional classes is highest in the first segment samples followed by what appears to be a plateau for the second and third segments and decreasing loading through the last two bed segments.
Figure 10. Average total ester loading.

Figure 11. Average total aromatic loading.
Figure 12. Average total hydrocarbon loading.

Figure 13. Average total alcohol loading.
Figure 14. Average OFP loading.

Figure 15. Average total aldehyde loading.
Figure 16. Average total ketone loading.

Figure 17. Average total halocarbon loading less OFP.
These data are interesting because coadsorption phenomena are being exhibited by the observed loading. After its time in service, the heavier, less volatile compounds were found to load the leading segment of the bed while comparatively lighter, more volatile compounds were observed in the remaining segments. It is anticipated that had the CBA remained in service for a longer period, the loading peaks exhibited by the alcohols and OFP would move deeper into the bed as the heavier, less volatile compounds continued to load the segments closer to the bed inlet. Ultimately, the CBA would provide no net removal of alcohols, OFP, and other highly volatile compounds leaving the COA and humidity condensate as the primary removal processes.

2.3.4.2 Radial Loading. Analysis of samples collected from the different quadrants and the center of each segment show radial variation. Figure 18 shows the total radial loading for all functional classes. While the general trend in loading through the length of the bed is fairly consistent and follows a pattern consistent with the first and third axial distributions, there is noticeable variation across the cross section. Segment 1 shows a wide radial variation, indicating possible nonuniform inlet flow. Loading at the center of the first segment is typically higher followed in descending order by quadrants A, C, D, and B. With the exception of quadrant D, radial loading is more uniform for sections 2 and 3. Loading in quadrant D varies significantly in sections 3 and 5, contrary to loading in the other sections. Sections 4 and 5 also show variation between the center and quadrant C. The bed center and quadrant C also show comparatively low loading in sections 4 and 5. Sections 2 through 5 are the most uniformly loaded in quadrants A and B. Overall, these variations may indicate flow channeling and exit flow effects. Evaluating each functional class independently shows much more pronounced variations for the lighter, more volatile compounds. The alcohols, ketones, and halocarbons exhibited much greater variation at the bed inlet and outlet sections as well as in the middle sections but all follow the general trends shown in figure 18. Appendix D contains plots showing the radial loading for the individual functional classes.

![Figure 18. Radial loading of total VOCs.](image-url)
2.4 Correlation to Predicted Loading

2.4.1 Ammonia Loading

Previous TCCS developmental testing conducted by Lockheed found complete $\text{H}_3\text{PO}_4$ neutralization in the inlet section of the CBA. In this testing, reaction with $\text{NH}_3$ consumed 2.74 wt. % $\text{H}_3\text{PO}_4$. The charcoal was loaded with 8.22 wt. % $\text{H}_3\text{PO}_4$. Thus, the 5.48 wt. % $\text{H}_3\text{PO}_4$ did not react. Titration was the only method used by Lockheed to determine $\text{H}_3\text{PO}_4$ neutralization. As well, no analyses for $\text{NH}_3$ or $\text{H}_3\text{PO}_4$ depletion on the fresh charcoal were reported. It must be assumed that the remaining $\text{H}_3\text{PO}_4$ was depleted by interaction with the charcoal or remained unavailable for reaction due to mass transfer hindrances. The amount of $\text{H}_3\text{PO}_4$ consumed by reaction with $\text{NH}_3$ during this test was equivalent to 28.2 mg $\text{H}_3\text{PO}_4$/gram of charcoal. Reaction of this quantity of $\text{H}_3\text{PO}_4$ indicates $\text{NH}_3$ loading of 4.9 mg/g of charcoal.

Like Lockheed’s results, nearly all of the $\text{NH}_3$ is adsorbed on the first segment of the charcoal bed as table 3 shows. Unlike Lockheed’s results, only traces are found throughout the remaining segments, indicating a greater overall capacity. The average $\text{NH}_3$ loading for segment 1 samples is 4.4 mg/g of charcoal. This is similar in magnitude to the 4.9 mg/g observed by Lockheed. It is interesting to note that Lockheed’s evaluation indicated that the $\text{H}_3\text{PO}_4$ was completely consumed in the bed inlet segment. If it is assumed that the remaining $\text{H}_3\text{PO}_4$ was depleted by its interaction with the charcoal, then $\approx$58 mg $\text{H}_3\text{PO}_4$/gram charcoal could neutralize via this reaction. Comparatively, as much as 43 percent of the $\text{H}_3\text{PO}_4$, or 43 mg/g, for a 10 wt. % loading, on the charcoal collected from the CBA is neutralized similarly. Based on both of these evaluations, $\approx$50 mg $\text{H}_3\text{PO}_4$/gram charcoal could be neutralized on the fresh charcoal.

2.4.2 Volatile Organic Compound Loading

Calculation of charcoal loading is based upon the adsorption potential theory. The adsorption potential, as defined in equation (1), is used to calculate the equilibrium charcoal loading:

$$A = \left(\frac{T}{V_m}\right) \log_{10}\left(\frac{C_s}{C}\right) , \quad (1)$$

where

- $A$ = adsorption potential
- $T$ = temperature (K)
- $V_m$ = liquid molar volume at the normal boiling point (cm³/gmole)
- $C_s$ = vapor pressure expressed in concentration units (mg/m³)
- $C$ = cabin concentration (mg/m³).

The potential factor is used in a Freundlich-type isotherm equation shown in its general form in equation (2):

$$q = \alpha e^{-BA} , \quad (2)$$
where

\[ q = \text{charcoal loading (cm}^3\text{ liquid contaminant/gram of charcoal)} \]
\[ \alpha = \text{preexponential factor (2.1 for soluble compounds and 1.41 for insoluble compounds at 50 percent relative humidity)} \]
\[ \beta = \text{exponential factor (0.31).} \]

Based upon the average prevailing cabin concentration reported from analysis of air quality samples collected in the USOS, the predicted equilibrium charcoal loading is obtained from equations (1) and (2). Table 5 compares the calculated charcoal loading with the maximum measured loading. The maximum loading was in the second segment for the alcohols and the first segment for all other compounds.

Table 5. Calculated versus measured charcoal loading.

<table>
<thead>
<tr>
<th>Compound</th>
<th>C (mg/m³)</th>
<th>A</th>
<th>( q_p^* ) (mg/g)</th>
<th>( q_m^{**} ) (mg/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethanol</td>
<td>2.42</td>
<td>22.1</td>
<td>1.7</td>
<td>0.939</td>
</tr>
<tr>
<td>2-propanol</td>
<td>0.17</td>
<td>21.1</td>
<td>2.2</td>
<td>0.83</td>
</tr>
<tr>
<td>n-propanol</td>
<td>0.07</td>
<td>21.1</td>
<td>2.4</td>
<td>0.382</td>
</tr>
<tr>
<td>n-butanol</td>
<td>0.16</td>
<td>14.5</td>
<td>17.2</td>
<td>0.866</td>
</tr>
<tr>
<td>2-butanol</td>
<td>0.0125</td>
<td>18.8</td>
<td>5</td>
<td>0.005</td>
</tr>
<tr>
<td>Ethanal</td>
<td>0.17</td>
<td>36.2</td>
<td>0.02</td>
<td>0.105</td>
</tr>
<tr>
<td>Propanal</td>
<td>0.026</td>
<td>29.4</td>
<td>0.2</td>
<td>0.037</td>
</tr>
<tr>
<td>Butanal</td>
<td>0.025</td>
<td>17.8</td>
<td>5.9</td>
<td>0.022</td>
</tr>
<tr>
<td>Ethyl acetate</td>
<td>0.025</td>
<td>19.9</td>
<td>4</td>
<td>0.017</td>
</tr>
<tr>
<td>Butyl acetate</td>
<td>0.018</td>
<td>12.6</td>
<td>32.3</td>
<td>0.457</td>
</tr>
<tr>
<td>Propyl acetate</td>
<td>0.0125</td>
<td>16.1</td>
<td>12.8</td>
<td>0.025</td>
</tr>
<tr>
<td>2-propanone</td>
<td>0.2</td>
<td>24.5</td>
<td>0.8</td>
<td>0.083</td>
</tr>
<tr>
<td>2-butane</td>
<td>0.027</td>
<td>21.4</td>
<td>2.1</td>
<td>0.017</td>
</tr>
<tr>
<td>4-methyl-2-pentanone</td>
<td>0.0125</td>
<td>14.3</td>
<td>17.6</td>
<td>0.053</td>
</tr>
<tr>
<td>Benzene</td>
<td>0.00125</td>
<td>25.6</td>
<td>0.4</td>
<td>0.049</td>
</tr>
<tr>
<td>Methylbenzene</td>
<td>0.024</td>
<td>16.6</td>
<td>6.5</td>
<td>1.032</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>0.0162</td>
<td>13.5</td>
<td>18.6</td>
<td>0.284</td>
</tr>
<tr>
<td>Dimethylbenzenes</td>
<td>0.064</td>
<td>12</td>
<td>25.7</td>
<td>2.584</td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>0.16</td>
<td>31.6</td>
<td>0.1</td>
<td>0.047</td>
</tr>
<tr>
<td>Octafluoropropane</td>
<td>113</td>
<td>14.7</td>
<td>19</td>
<td>1.7</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>0.025</td>
<td>16.3</td>
<td>8.9</td>
<td>0.114</td>
</tr>
<tr>
<td>Octane</td>
<td>0.0001</td>
<td>13.9</td>
<td>13.3</td>
<td>0.092</td>
</tr>
<tr>
<td>Cyclohexane</td>
<td>0.0001</td>
<td>24</td>
<td>0.7</td>
<td>0.095</td>
</tr>
<tr>
<td>Heptane</td>
<td>0.0001</td>
<td>16.8</td>
<td>5.3</td>
<td>0.427</td>
</tr>
<tr>
<td>Hexane</td>
<td>0.0001</td>
<td>20.5</td>
<td>1.6</td>
<td>0.014</td>
</tr>
</tbody>
</table>

* Predicted loading.
** Highest measured loading.

Evaluation of the data in table 5 shows that the loading for all compounds is well below that predicted for the average air quality conditions on board the ISS with the exception of ethanal. The maximum loading measured for ethanal is more than 5 times greater than predicted. The alcohols, particularly ethanol, 2-propanol, and n-propanol, are within a factor of 3 of their predicted loading. Measured loading for the heavier aromatics and hydrocarbons also approach predictions for most compounds. The loading for 2-butanol, ethyl acetate, propyl acetate, 2-butane, 4-methyl-2-pentanone, and octane
is more than 100 times lower than predicted. Effectively, it can be concluded that the most highly loaded sections of the CBA have significant capacity remaining.

2.5 Predicted Charcoal Bed Assembly Service Interval

2.5.1 Ammonia Basis

Predicting the service life requires an assessment of the measured NH\textsubscript{3} loading against the prevailing cabin concentration. To accomplish this, the percentage of NH\textsubscript{3} loading relative to the amount of H\textsubscript{3}PO\textsubscript{4} measured in segment 1 is assessed. This requires converting both the phosphate and NH\textsubscript{3} loading to millimoles to account for stoichiometry. Using this convention, the average 4.4 mg NH\textsubscript{3}/gram loading is converted to 0.26 mmole NH\textsubscript{3}/gram and the average 90 mg phosphate/gram is converted to 0.92 mmole H\textsubscript{3}PO\textsubscript{4}/gram. Data established that \approx 37 percent of the H\textsubscript{3}PO\textsubscript{4}’s first H is partially neutralized or depleted by its interaction with the charcoal. Correcting for depletion leaves 0.56 mmole H\textsubscript{3}PO\textsubscript{4}/gram available for reaction. Given that 1 mmole of the first H of H\textsubscript{3}PO\textsubscript{4} reacts with 1 mmole of NH\textsubscript{3}, then the NH\textsubscript{3} has consumed 46 percent (0.26/0.56 mmole) of the theoretical capacity of H\textsubscript{3}PO\textsubscript{4} on the first segment of the bed.

Analysis of the NH\textsubscript{3} loading in humidity condensate indicates that the prevailing NH\textsubscript{3} concentration in the ISS cabin has been \approx 0.12 mg/m\textsuperscript{3}. The theoretical capacity for a typical CBA containing 22.7 kg (50 lb) of charcoal based upon 0.56 mmole H\textsubscript{3}PO\textsubscript{4}/gram charcoal is 12.7 total moles of H\textsubscript{3}PO\textsubscript{4} available for reaction. With 1 mole of H\textsubscript{3}PO\textsubscript{4} reacting with 1 mole of NH\textsubscript{3}, that means the typical CBA theoretical capacity for NH\textsubscript{3} is 12.7 mole or 215.9 g. At the prevailing cabin concentration of 0.12 mg/m\textsuperscript{3}, the bed will not reach saturation for 13 yr. Conservatively, if it is assumed that further hindrances to H\textsubscript{3}PO\textsubscript{4} reaction exist such that only 0.26 mmole H\textsubscript{3}PO\textsubscript{4}/gram charcoal react, then the theoretical capacity is 5.9 mole (100 g) and bed saturation will occur after more than 6 yr of operational service.

These predicted service intervals do not consider the fact that more than 22.7 kg (50 lb) is usually loaded into the CBA during refurbishment. Up to 27.2 kg (60 lb) has been installed. This means that there is additional capacity available that can serve as margin. For the lower loading, this margin amounts to 1.2 mole (20 g) of NH\textsubscript{3}. At the prevailing NH\textsubscript{3} concentration, this is \approx 1.25 yr or up to 20 percent additional capacity margin compared to a 6-yr service interval.

2.5.2 Batch-Wise Phosphoric Acid Consideration

Analysis of the H\textsubscript{3}PO\textsubscript{4} loading has indicated batch-wise variation. When recommending a service interval, this variation must be accounted for. Further analysis, summarized in table 2 and appendix A, shows that when all the charcoal purchased for the TCCS is considered, the average loading is 88 mg H\textsubscript{3}PO\textsubscript{4}/gram of charcoal loading. The analytical method relative percent difference (RPD) is 16.8 percent. Assuming that –16.8 percent applies to account for the worst-case analytical method error, then the worst average loading is 73.2 mg H\textsubscript{3}PO\textsubscript{4}/gram. At 37 percent depletion, the average from previous samples and higher than that measured subsequently, 46.1 mg H\textsubscript{3}PO\textsubscript{4}/gram is available. This is 0.47 mmole H\textsubscript{3}PO\textsubscript{4}/gram of charcoal. The 6-yr service interval indicated above is based on an active H\textsubscript{3}PO\textsubscript{4} loading of 0.26 mmole/gram of charcoal. Effectively, the worst-case H\textsubscript{3}PO\textsubscript{4} loading variation provides on average 81 percent excess active H\textsubscript{3}PO\textsubscript{4} on the charcoal to achieve the recommended service interval.
Even for the three samples analyzed with the lowest loading, the active $\text{H}_3\text{PO}_4$ loading is 0.369 mmole/g. That is nearly 42 percent excess $\text{H}_3\text{PO}_4$ loading to achieve the recommended service interval. This accounts for −19 percent analytical method RPD for these samples plus an average 26.45 percent first H depletion for these same samples.

Considering that the CBA has sufficient capacity to accommodate the observed batch-wise $\text{H}_3\text{PO}_4$ variation and depletion as well as the fact that it typically contains more than 22.7 kg (50 lb) of charcoal that is not considered in the service interval calculation, the 6-yr service interval is deemed conservative and provides substantial margin to ensure proper, safe, and economical TCCS function. From this assessment, it is concluded that activated charcoal housed in the TCCS maintenance depot may be used as is.

2.5.3 Volatile Organic Compound Basis

Dichloromethane is the most interesting VOC with respect to the CBA’s service interval because it, along with $\text{NH}_3$, is a key design component. During testing of a TCCS flight unit in 1998, dichloromethane breakthrough was observed after $\approx$500 hr. The average concentration entering the CBA was 0.45 mg/m$^3$. Over the 500 hr, $\approx$3,442 mg dichloromethane was loaded onto the charcoal before breakthrough was observed. This loading is equivalent to 0.15 mg dichloromethane/gram charcoal. This agrees very closely to the predicted 0.1 mg/g. According to table 5, the highest observed loading of dichloromethane had not yet reached half the predicted loading. From these data, it can be assumed that either dichloromethane has not reached saturation in the bed or that the analytical technique achieves partial desorption. With this in mind, it is appropriate to assume that the actual loading may fall somewhere between the predicted and observed levels. Therefore, dichloromethane saturation may occur anywhere from 69.7 hr (2.9 days) to 926 hr (38 days) at the prevailing average 0.16 mg/m$^3$ concentration. The time to saturation is much less than the time in service; therefore, the effect of halocarbon breakthrough on the proper operation and function of the COA and the effect on the SBA service interval must be considered before recommending a final CBA service interval.
3. CATALYTIC OXIDIZER ASSEMBLY SERVICE INTERVAL

The 2.56-yr service interval recommended by Lockheed is primarily based upon catalyst poisoning. Developmental testing conducted by Lockheed demonstrated a decrease in the CH$_4$ oxidation efficiency over time. While this testing demonstrated that the poisoning effect is partially reversible, it did not address repeated poisoning episodes nor did it consider poisoning as a function of concentration. As a result, the service interval is based upon a calculated cumulative poisoning over time. More detailed testing was sponsored by NASA and documented in reference 5. Analysis of the data from reference 5 shows that the effect of halocarbons on CH$_4$ oxidation in the COA strongly correlates to the free halogen concentration in the process air stream rather than a cumulative effect over time. This correlation, shown in figure 19, means that rather than a cumulative effect over time, the halocarbon concentration entering the COA and the extent of oxidation of the halocarbons determine the degree of poisoning. Evaluation of air quality data reported from analyses of cabin atmospheric samples collected in flight shows that the prevailing 0.44-mg/m$^3$ total non-OFP halocarbon concentration results in a 0.41-mg/m$^3$ free halogen concentration in the COA. According to figure 19, no measurable decrease in CH$_4$ oxidation efficiency is expected at the prevailing total non-OFP halocarbon concentration observed on board the ISS.

![Figure 19. Effect of free halogen concentration on methane oxidation.](image)
Because OFP has been present in the ISS cabin atmosphere at very high concentrations over a 1-yr period, its potential to poison the COA’s catalyst must be evaluated. Figure 20 shows the OFP cabin concentration beginning with the first crew visit to the ISS during STS–88/2A. Testing was conducted to evaluate OFP oxidation in the COA because of the high cabin concentration and concern that the TCCS’s performance may be affected.\textsuperscript{13} As table 6 shows, no measurable hydrogen fluoride (HF) production was observed during the test, and it was concluded that OFP does not oxidize in the COA.

![Figure 20. OFP concentration in the ISS cabin.](image)

Table 6. Test conditions and results.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Test Condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection rate</td>
<td>1.605 mL/s</td>
</tr>
<tr>
<td>Concentration</td>
<td>154 mg/m$^3$</td>
</tr>
<tr>
<td>Start flow rate</td>
<td>4.69 m$^3$/hr</td>
</tr>
<tr>
<td>Temperature 1</td>
<td>384.4 °C</td>
</tr>
<tr>
<td>End flow rate</td>
<td>4.69 m$^3$/hr</td>
</tr>
<tr>
<td>Temperature 2</td>
<td>384.3 °C</td>
</tr>
<tr>
<td>Color change*</td>
<td>None</td>
</tr>
</tbody>
</table>

* Observed HF detector tube color change.

In addition to testing on the ground, flight-related observations pertaining to the potential effect that OFP’s presence may have had on the COA and its ability to control cabin CH$_4$ concentration support the test results. The fact that the average non-OFP halocarbon cabin concentration of 0.44 mg/m$^3$ will not affect CH$_4$ oxidation efficiency and, therefore, CH$_4$ concentration control makes it important...
to evaluate the in-flight CH₄ concentration profile during periods that the OFP concentration was high and the TCCS was known to be operating. Because the OFP concentration reached very high levels, a significant increase in cabin CH₄ concentration would be predicted if only 1 percent of the OFP oxidized in the TCCS’s COA.

The ISS cabin CH₄ concentration profile over the period beginning in December 1998 and ending in May 2002 provides further evidence concerning OFP’s effect upon CH₄ oxidation in the COA. Figure 21 shows that residual amounts of CH₄ were introduced into the ISS’s cabin by visiting crews before the first permanent crew arrived. Although the ROS BMP unit was activated after the first crew arrived, it does not provide active CH₄ removal. Therefore, the cabin CH₄ concentration rose and peaked at more than 200 mg/m³ before the USOS Laboratory module containing the TCCS was activated. Once the TCCS began operating, the CH₄ concentration quickly fell to <100 mg/m³ and continued to fall to <2 mg/m³. This low concentration was maintained throughout the ensuing station operations regardless of the concentration of OFP. The only instances when the CH₄ concentration increased correspond to periods when the TCCS was shut off. The observation that there was no change in cabin CH₄ concentration while the TCCS was operating in the presence of high OFP concentrations further supports the test observation that OFP does not oxidize in the COA.

Figure 21. CH₄ concentration in the ISS cabin.

Additional evidence that OFP does not react in the TCCS’s COA is found by examining figure 20. After ground-based testing cleared the TCCS to be restarted in February 2002, its operation did not have a noticeable effect on the rate that the OFP concentration decayed. An engineering analysis of OFP removal from the cabin found that the concentration decay rate correlates most closely to the
ROS BMP, accounting for the removal at <1 percent efficiency. This analysis is depicted in figure 20 as the solid curve. This observation led to the conclusion that not only was the TCCS CBA saturated with OFP but also supported the conclusion that OFP does not oxidize in the COA.

Because the prevailing ISS cabin halocarbon concentration and high OFP concentrations have been demonstrated to have negligible effects upon the COA’s performance, other COA components besides the catalyst dictate the COA’s service interval. These components include the connector seals on the COA exhaust, the resistance temperature detectors (RTDs), and the heater assembly. The connector seals may be replaced on orbit without returning the COA to the ground, while maintenance on the RTDs and heater assembly require disassembly. Therefore, the COA’s service interval must be revised based upon wearout of the RTDs and heater assembly. Lockheed documented recommended service intervals of 3 yr for these components. However, experience with ground testing of a similar thermal catalytic oxidizer—also built by Lockheed—has indicated that many of these components have a shelf life of 30 yr and operational lives exceeding 5 yr of accumulated operation. The available evidence establishes that the COA is not a consumable item and its service interval is dictated by wearout mechanisms.
4. PREDICTED SORBENT BED ASSEMBLY SERVICE LIFE

4.1 Background

Evaluation by Lockheed in 1993 through 1995 established a service interval of 467 days (1.28 yr) for the TCCS expendable beds.9,10 This interval was based primarily upon catalyst poisoning considerations that may result from the design specification loading of halocarbons in the cabin. In Lockheed’s evaluation, halocarbons loaded the CBA and then entered the COA where their oxidation poisoned the CH$_4$ oxidation reaction. After 1.28 yr of operation, Lockheed’s assessment predicted that CH$_4$ would reach its SMAC based upon assumption of cumulative catalyst poisoning over time. Reaching the CH$_4$ SMAC, therefore, was used to specify the bed replacement interval. Specific SBA loading was not considered in this evaluation, but SBA replacement was tied to CBA loading and replacement.

Acid gas removal is described by the following net reaction equation where LiOH reacts with an acid gas in the presence of H$_2$O vapor and CO$_2$. The X in the net equation denotes halogens such as chlorine (Cl) and fluorine (F):

$$\text{LiOH} + \text{HX} \rightarrow \text{LiX} + \text{H}_2\text{O}.$$  (3)

Essentially, the reaction involves the production of an intermediate lithium carbonate (Li$_2$CO$_3$) product that reacts with the acid gas, producing H$_2$O and a nonvolatile salt.

TCCS developmental testing conducted by Lockheed and documented in 1992 showed that the measured acid gas removal performance of the SBA was 0.0194 g acid gas as hydrogen chloride (HCl)/gram LiOH (0.0128 mole HCl/mole LiOH). This was much lower than the expected performance of 0.276 g acid gas as HCl/gram LiOH (0.181 mole HCl/mole LiOH) reported by the material’s vendor, Cyprus Foote Mineral Company.11 On a molar basis, the observed performance represents 7 percent of the bed’s rated capacity. This equates to 3.98 mole or 95.25 g of LiOH available for reaction.

Lockheed proposed no explanation for the reduced capacity. However, review of the literature shows that granule size and flow distribution, temperature, contact time, and acid gas concentration entering the bed may be factors. Evaluation of Li$_2$CO$_3$ as an acid gas control medium by Gully et al. showed an experimental loading of 0.675 g HCl/gram Li$_2$CO$_3$.14 This converts to 0.684 mole HCl/mole LiOH which is higher than the loading reported by Cyprus Foote Mineral Company. It is noted that the experiments conducted by Gully were carried out at 69 °C (156 °F) at a molar air flow rate of 2.9 mole/hr (0.065 standard m$^3$/hr) using a Li$_2$CO$_3$ material having a 12 × 14 mesh granule size. The LiOH used in the TCCS’s SBA is sieved to 6 × 14 mesh, so slightly larger granules are packed into the SBA. This means that there is less surface area available for contact with the process air and that there may be a greater potential for flow channeling in the bed. The TCCS’s process gas temperature upon exiting the COA is approximately 63 °C (145 °F). That is very close to the experimental temperature used by Gully, so any temperature effect is negligible. The contact time in the experimental bed
used by Gully was ≈0.05 s versus 2.5 s provided by the SBA. Therefore, contact time in the SBA is considered more than sufficient. In Gully’s experiments, the inlet HCl concentration was maintained at 45 ppm. This is substantially higher than the <10 ppm that entered the SBA during Lockheed’s test. Most vendors acquire loading data at higher concentrations of the contaminant of interest rather than the trace levels that are experienced on board spacecraft because most industrial applications deal with much higher loadings. From this assessment, the most likely factors are the granule size, which may allow flow channeling and lost performance, combined with poor flow distribution at the bed inlet, causing dead zones where the LiOH does not contact the flowing air stream sufficiently. Nonetheless, the performance reported by Lockheed is considered real and the SBA service life should be based upon it.

4.2 Design Versus Actual Halocarbon Load

Assessment of the design specification load indicates that not all of the halocarbons will break through the charcoal bed during its 1-yr service life. Using predicted concentrations from Lockheed’s TCCS performance analysis, table 7 shows that 19 out of the 25 halocarbons break through the charcoal bed within a 6-yr service interval. This would produce approximately $3.58 \times 10^{-4}$ mole of acid gases as HF and HCl/hour. Table 8 lists the compounds contributing to this acid gas load. Using the LiOH utilization observed during the developmental testing, the SBA’s capacity would be exhausted in approximately 464 days (1.27 yr). Saturation occurs rapidly for the halocarbons that break through the charcoal so this would imply a 460-day specification service life. As such, Lockheed’s original service life recommendation of 467 days (1.28 yr) actually allowed some breakthrough of acid gases.

Table 7. Charcoal loading at design specification conditions.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$C$ (mg/m$^3$)</th>
<th>$M_{sat}$ (mg)</th>
<th>$T_{sat}$ (days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chloromethane</td>
<td>0.006</td>
<td>0.05</td>
<td>0.023</td>
</tr>
<tr>
<td>Chloroethene</td>
<td>0.00006</td>
<td>0.5</td>
<td>2.2</td>
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<tr>
<td>Chloroethane</td>
<td>0.00002</td>
<td>0.85</td>
<td>116</td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>1.6</td>
<td>1,640</td>
<td>2.8</td>
</tr>
<tr>
<td>1,1-dichloroethene</td>
<td>0.0001</td>
<td>19.4</td>
<td>527</td>
</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>0.02</td>
<td>5,445</td>
<td>741</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>0.31</td>
<td>227,704</td>
<td>2,000</td>
</tr>
<tr>
<td>1,2-dichloropropane</td>
<td>0.0015</td>
<td>8,569</td>
<td>15,557</td>
</tr>
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<td>Trichloromethane</td>
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<td>612</td>
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<tr>
<td>Trichloroethene</td>
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<tr>
<td>1,2-dichlorobenzene</td>
<td>0.0013</td>
<td>153,440</td>
<td>321,434</td>
</tr>
<tr>
<td>Tetrachloromethane</td>
<td>0.002</td>
<td>5,966</td>
<td>8,124</td>
</tr>
<tr>
<td>Tetrachloroethene</td>
<td>0.15</td>
<td>183,891</td>
<td>3,339</td>
</tr>
<tr>
<td>Chlorodifluoromethane</td>
<td>0.05</td>
<td>7.4</td>
<td>0.4</td>
</tr>
<tr>
<td>Dichlorofluoromethane</td>
<td>0.00013</td>
<td>2.2</td>
<td>45.2</td>
</tr>
<tr>
<td>1-chloro-1,2,2-trifluoroethane</td>
<td>0.001</td>
<td>104</td>
<td>284</td>
</tr>
<tr>
<td>Dichlorodifluoromethane</td>
<td>0.0028</td>
<td>22.5</td>
<td>22</td>
</tr>
<tr>
<td>Dichlorodifluoroethene</td>
<td>0.00039</td>
<td>187.5</td>
<td>1,309</td>
</tr>
<tr>
<td>Trichlorofluoromethane</td>
<td>0.29</td>
<td>6,015</td>
<td>56.5</td>
</tr>
<tr>
<td>Bromotrifluoromethane</td>
<td>0.24</td>
<td>28</td>
<td>0.32</td>
</tr>
<tr>
<td>Dichlorotetrafluoroethane</td>
<td>0.0054</td>
<td>3,307</td>
<td>1,668</td>
</tr>
<tr>
<td>Trichlorotrifluoroethane</td>
<td>3.86</td>
<td>249,898</td>
<td>176</td>
</tr>
<tr>
<td>Tetrachlorodifluoroethane</td>
<td>0.0068</td>
<td>85,640</td>
<td>34,298</td>
</tr>
</tbody>
</table>
Table 8. Acid gas production at design specification conditions.

<table>
<thead>
<tr>
<th>Compound</th>
<th>C  (mg/m³)</th>
<th>COA Efficiency (%)</th>
<th>Rate (moles/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chloromethane</td>
<td>0.006</td>
<td>80</td>
<td>4.36 × 10⁻⁷</td>
</tr>
<tr>
<td>Chloroethene</td>
<td>0.0006</td>
<td>80</td>
<td>3.53 × 10⁻⁶</td>
</tr>
<tr>
<td>Chloroethane</td>
<td>0.00002</td>
<td>80</td>
<td>1.14 × 10⁻⁹</td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>1.6</td>
<td>80</td>
<td>1.38 × 10⁻⁴</td>
</tr>
<tr>
<td>1,1-dichloroethene</td>
<td>0.0001</td>
<td>60</td>
<td>5.68 × 10⁻⁹</td>
</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>0.02</td>
<td>60</td>
<td>1.11 × 10⁻⁶</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>0.31</td>
<td>80</td>
<td>1.01 × 10⁻⁵</td>
</tr>
<tr>
<td>Trichloromethane</td>
<td>0.0036</td>
<td>70</td>
<td>2.91 × 10⁻⁷</td>
</tr>
<tr>
<td>Trichloroethene</td>
<td>0.016</td>
<td>60</td>
<td>1.13 × 10⁻⁶</td>
</tr>
<tr>
<td>1,1,1-trichloroethane</td>
<td>0.14</td>
<td>60</td>
<td>8.67 × 10⁻⁶</td>
</tr>
<tr>
<td>Chlorodifluoromethane</td>
<td>0.05</td>
<td>80</td>
<td>6.37 × 10⁻⁶</td>
</tr>
<tr>
<td>Dichlorodifluoromethane</td>
<td>0.00013</td>
<td>80</td>
<td>1.39 × 10⁻⁶</td>
</tr>
<tr>
<td>1-chloro-1,2,2-trifluoroethane</td>
<td>0.001</td>
<td>30</td>
<td>4.65 × 10⁻⁶</td>
</tr>
<tr>
<td>Dichlorodifluoromethane</td>
<td>0.0028</td>
<td>70</td>
<td>2.98 × 10⁻⁷</td>
</tr>
<tr>
<td>Dichlorodifluoroethene</td>
<td>0.00039</td>
<td>60</td>
<td>3.23 × 10⁻⁶</td>
</tr>
<tr>
<td>Trichlorodifluoromethane</td>
<td>0.29</td>
<td>70</td>
<td>2.71 × 10⁻⁵</td>
</tr>
<tr>
<td>Bromotrifluoromethane</td>
<td>0.24</td>
<td>10</td>
<td>2.96 × 10⁻⁶</td>
</tr>
<tr>
<td>Dichlorotetrafluoroethane</td>
<td>0.0054</td>
<td>30</td>
<td>2.81 × 10⁻⁷</td>
</tr>
<tr>
<td>Trichlorotrifluoroethane</td>
<td>3.86</td>
<td>30</td>
<td>1.70 × 10⁻⁴</td>
</tr>
</tbody>
</table>

Total acid gas production (moles/hr) = 3.58 × 10⁻⁴

The prevailing halocarbon loading in the ISS cabin, however, has been much lower than the design specification. Figure 22 shows the trend in total halocarbon concentration reported from air quality monitoring samples collected between February 2001 and March 2004. Tabular data used to construct figure 22 are provided in appendix E. Based upon the observed loading, there are 11 halocarbons that may contribute to acid gas production. Table 9 shows the predicted saturation time for the observed halocarbons. Considering the degree of charcoal breakthrough that can occur for these halocarbon compounds, the compounds listed in table 10 are the contributors to acid gas production in the COA. Using this observed loading, the maximum predicted acid gas production in the COA is 3.58 × 10⁻⁵ mole/hr when it is assumed the CBA is completely saturated. This is 10 times lower than the loading predicted by the design specification. Using the same LiOH utilization observed during the TCCS development testing, the SBA’s projected service life is 4,632 days (12.7 yr).
Figure 22. ISS cabin air quality trend for halocarbons.

Table 9. Charcoal loading based on observed ISS cabin air quality conditions.

<table>
<thead>
<tr>
<th>Compound</th>
<th>$C$ (mg/m$^3$)</th>
<th>$M_{sat}$ (mg)</th>
<th>$T_{sat}$ (days)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dichlorodifluoromethane</td>
<td>0.09</td>
<td>1,690</td>
<td>51.1</td>
</tr>
<tr>
<td>Chloromethane</td>
<td>0.027</td>
<td>5.3</td>
<td>0.54</td>
</tr>
<tr>
<td>Trichlorofluoromethane</td>
<td>0.013</td>
<td>6,421</td>
<td>1,305</td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>0.22</td>
<td>2,504</td>
<td>31.6</td>
</tr>
<tr>
<td>Trichlorotrifluoroethane</td>
<td>0.0038</td>
<td>54,871</td>
<td>39,324</td>
</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>0.026</td>
<td>25,344</td>
<td>2,707</td>
</tr>
<tr>
<td>1,2-dichloropropane</td>
<td>0.0059</td>
<td>54,305</td>
<td>25,066</td>
</tr>
<tr>
<td>Tetrachloroethene</td>
<td>0.0059</td>
<td>141,760</td>
<td>65,433</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>0.0038</td>
<td>100,296</td>
<td>71,878</td>
</tr>
<tr>
<td>Bromotrifluoromethane</td>
<td>0.14</td>
<td>222</td>
<td>4.3</td>
</tr>
<tr>
<td>Chloropentafluoroethane</td>
<td>0.011</td>
<td>9,982</td>
<td>2,517</td>
</tr>
</tbody>
</table>
Table 10. Acid gas production at observed ISS air quality conditions.

<table>
<thead>
<tr>
<th>Compound</th>
<th>C (mg/m³)</th>
<th>COA Efficiency (%)</th>
<th>Rate (moles/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dichlorodifluoromethane</td>
<td>0.09</td>
<td>70</td>
<td>8.88 × 10⁻⁶</td>
</tr>
<tr>
<td>Chloromethane</td>
<td>0.027</td>
<td>80</td>
<td>1.92 × 10⁻⁶</td>
</tr>
<tr>
<td>Trichlorofluoromethane</td>
<td>0.013</td>
<td>70</td>
<td>1.32 × 10⁻⁶</td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>0.22</td>
<td>80</td>
<td>1.93 × 10⁻⁵</td>
</tr>
<tr>
<td>Trichlorotrifluoroethane</td>
<td>0.0038</td>
<td>30</td>
<td>1.76 × 10⁻⁷</td>
</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>0.026</td>
<td>60</td>
<td>1.47 × 10⁻⁶</td>
</tr>
<tr>
<td>1,2-dichloropropane</td>
<td>0.0059</td>
<td>80</td>
<td>4.05 × 10⁻⁵</td>
</tr>
<tr>
<td>Tetrachloroethene</td>
<td>0.0059</td>
<td>60</td>
<td>4.14 × 10⁻⁷</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>0.0038</td>
<td>80</td>
<td>1.32 × 10⁻⁷</td>
</tr>
<tr>
<td>Bromotrifluoromethane</td>
<td>0.14</td>
<td>10</td>
<td>1.40 × 10⁻⁶</td>
</tr>
<tr>
<td>Chloropentafluoroethane</td>
<td>0.011</td>
<td>20</td>
<td>4.07 × 10⁻⁷</td>
</tr>
<tr>
<td><strong>Total acid gas production (moles/hr)</strong></td>
<td></td>
<td></td>
<td><strong>3.58 × 10⁻⁵</strong></td>
</tr>
</tbody>
</table>

4.3 Sorbent Bed Assembly Functional Failure Impact on Cabin Air Quality

In the event that the SBA fails, the present halocarbon loading the cabin air can result in acid gas production as high as $5.78 \times 10^{-5}$ mole/hr when including compounds in table 7 that may be below the in-flight air quality sample analytical method’s detection limit. HCl accounts for 60 percent while HF makes up 40 percent of the acid gas production. Using these percentages, HCl and HF generation into the cabin can be as high as 1.26 mg/hr and 0.46 mg/hr, respectively. The primary route for removal from the cabin in the case of a failed SBA is absorption by humidity condensate. Single-pass removal efficiency of the Russian segment’s condensing heat exchanger when removing a two-person latent load is 0.12 percent for HCl and 0.025 percent for HF. The SMACs for HCl and HF are 1.5 mg/m³ and 0.1 mg/m³, respectively. Threshold generation rates to maintain cabin concentrations <90 percent of SMAC are 0.23 mg/hr for HCl and 0.0032 mg/hr for HF for the stage 4R station configuration with two crew-members. Therefore, to avoid impacts to the cabin environment, SBA failure must be avoided. This is best accomplished by imposing a substantial margin upon the service interval estimate.

In the event of complete SBA failure and using projected maximum generation rates, HCl concentration in the cabin rises to 7.3 mg/m³ and the HF concentration rises to 12.8 mg/m³. These concentrations approach HCl’s 1-hr SMAC of 8 mg/m³ and far exceed HF’s 1-hr SMAC of 2 mg/m³. As noted earlier, the 180-day SMACs are 1.5 mg/m³ and 0.1 mg/m³ for HCl and HF, respectively. With no active removal and assuming a 100-percent SBA failure, the elapsed time to exceed the 180-day SMAC for HF occurs in 3.4 days. HCl will exceed its SMAC in 18.4 days.

Given the potential for a significant impact to cabin air quality, routine monitoring of the cabin for either HCl or HF is necessary as the SBA nears the end of its service life. The predicted HCl concentration can be measured by the compound-specific analyzer for combustion products (CSA-CPs) as well as detector tubes included in the Russian complement of air quality monitoring equipment. The recently launched GANK–4M instrument may also prove useful in monitoring HCl concentration. Monitoring HF is more difficult; while both the detector tubes and the GANK–4M provide capability, their sensitivity may not be sufficient to detect it. At predicted maximum concentrations, odor thresholds will be exceeded; therefore, it is possible that SBA failure may be detected by odor. The odor threshold for HCl is 1.5 mg/m³ while HF’s odor threshold is 0.03 mg/m³. Crewmembers may also experience eye and mucous membrane irritation.
4.4 Summary

It should also be noted that the service life estimate is based upon actual operational time rather than calendar time. During the period between February 2001 and March 2004, the TCCS did not operate for a total of 107 days. To provide some factor of safety, it is recommended that any one SBA not exceed 50 percent of the calculated service life. Therefore, the recommended SBA service life, based upon the prevailing halocarbon load in the ISS cabin, is 2,190 days (6 yr). This margin also allows for the potential that some of the compounds in table 7 that have not been isolated in air quality sample analyses could be present at concentrations below the in-flight air quality sample analytical method’s detection limit. If such a situation exists, the acid gas production rate may be as high as $5.78 \times 10^{-5}$. At that rate, the recommended 6 yr still provides a 24-percent margin.
5. DISCUSSION

Managing the TCCS’s ORU service intervals requires its end-to-end performance to be considered. The data presented from postflight evaluation of the CBA’s performance after 7,389 cumulative operating hours (307.9 days) have established that NH$_3$ is the key compound driving its service interval. Conservatively, the postflight evaluation indicates the CBA’s service interval may be as long as 6 yr.

By extending the CBA’s service interval, the data also indicate that alcohols, halocarbons, and other VOCs can be expected to break through the CBA and enter the COA. Test data have demonstrated that the total prevailing halocarbon loading of 0.44 mg/m$^3$ is expected to have a negligible impact on the capability to oxidize CH$_4$ and CO. Further, no operational constraints exist for the TCCS in the event of OFP leaks because testing and evaluation of in-flight air quality data have demonstrated that it is not oxidized in the COA. Therefore, the COA becomes a wearout item with its maintenance driven by its heater assembly and RTD components. Seals in the COA’s outlet coupling also must be maintained; however, this can be accomplished on orbit. Experience with a functionally similar thermal catalytic oxidizer during years of developmental testing indicate that the heater assembly and RTDs may have shelf lives exceeding 10 yr, maybe even approaching 30 yr, and the capacity for at least 5 yr of accumulated operation. Functional redundancy is provided for the COA; therefore, the unit may be classified as a wearout item with no specified service interval.

Extending the CBA’s service interval also influences the SBA’s service interval. However, the evaluation of in-flight air quality data—considering the COA’s capability for oxidizing the total non-OFP halocarbon load—has found that the SBA may last as long as 12.7 yr. However, because of the potential impacts upon cabin atmospheric quality presented by SBA functional failure, employing a >50-percent margin is prudent. In summary, the prevailing air quality conditions on board the ISS allow for the CBA, COA, and SBA service intervals to be safely extended without compromising the TCCS’s performance.

5.1 Air Quality Monitoring Uncertainty

Most analytical methods employed to measure cabin air quality typically possess an uncertainty within ±20 percent. For single analytes, the uncertainty may be higher or lower. Therefore, it is considered appropriate to apply a 25-percent margin to the CBA and SBA service intervals that are indicated by the supporting data. As well, the NH$_3$ and halocarbon loads can fluctuate depending on the individuals on board the ISS and the new equipment brought on board. Applying a margin to account for these areas of uncertainty is considered prudent and appropriate. The COA is less sensitive to the potential changes in halocarbon loading. A 100-percent halocarbon concentration increase would still allow for a >90 percent CH$_4$ oxidation efficiency and have no bearing on heater assembly and RTD wearout.
5.2 Minimum Trace Contaminant Control Flow Requirement

To extend the service intervals, it must be understood whether the TCCS would still provide sufficient flow capacity to control the primary trace contaminants of interest. Evaluation of air quality dynamics has established the halocarbons, alcohols, acetone, and formaldehyde to be of particular interest. By extending the CBA service interval, these compounds would be controlled by the COA that has a 70 percent lower flow rate. According to its performance specification, the TCCS must control individual trace contaminants below 90 percent of their SMAC. Evaluation of the specification load model and the required flow rate to achieve 90 percent SMAC for all compounds, the TCCS COA can provide this control capability with >500-percent margin. Table 11 summarizes the key trace contaminants and the minimum atmospheric scrubbing flow required to maintain a concentration < 90 percent SMAC. This evaluation indicates that the TCCS ORU service interval changes can be accommodated with respect to trace contaminant control flow rate capacity.

Table 11. Minimum specification trace contaminant control flow requirement.

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Molecular Weight (g/mole)</th>
<th>SMAC (mg/m³)</th>
<th>Equipment Rate (mg/day*kg)</th>
<th>Metabolic Rate (mg/man*day)</th>
<th>Required Flow (m³/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>32.04</td>
<td>9</td>
<td>1.27 x 10⁻³</td>
<td>1.5</td>
<td>0.53</td>
</tr>
<tr>
<td>Ethanol</td>
<td>46.07</td>
<td>2,000</td>
<td>7.85 x 10⁻³</td>
<td>4</td>
<td>0.01</td>
</tr>
<tr>
<td>2-propanol</td>
<td>60.09</td>
<td>150</td>
<td>3.99 x 10⁻³</td>
<td>0</td>
<td>0.09</td>
</tr>
<tr>
<td>n-butanol</td>
<td>74.12</td>
<td>40</td>
<td>4.71 x 10⁻³</td>
<td>1.33</td>
<td>0.42</td>
</tr>
<tr>
<td>Ethanol</td>
<td>44.05</td>
<td>4</td>
<td>1.09 x 10⁻⁶</td>
<td>0.09</td>
<td>0.1</td>
</tr>
<tr>
<td>2-propanal</td>
<td>56.06</td>
<td>0.03</td>
<td>3.46 x 10⁻⁶</td>
<td>0</td>
<td>0.4</td>
</tr>
<tr>
<td>Benzene</td>
<td>78.11</td>
<td>0.32</td>
<td>2.51 x 10⁻⁶</td>
<td>0</td>
<td>0.27</td>
</tr>
<tr>
<td>Methylbenzene</td>
<td>92.15</td>
<td>60</td>
<td>1.98 x 10⁻³</td>
<td>0</td>
<td>0.11</td>
</tr>
<tr>
<td>Dichloromethane</td>
<td>84.93</td>
<td>10</td>
<td>2.15 x 10⁻³</td>
<td>0</td>
<td>0.75</td>
</tr>
<tr>
<td>1,2-dichloroethane</td>
<td>98.97</td>
<td>1</td>
<td>7.74 x 10⁻⁵</td>
<td>0</td>
<td>0.27</td>
</tr>
<tr>
<td>Chlorobenzene</td>
<td>112.56</td>
<td>46</td>
<td>1.54 x 10⁻⁵</td>
<td>0</td>
<td>0.12</td>
</tr>
<tr>
<td>Methane</td>
<td>16.04</td>
<td>3,800</td>
<td>6.39 x 10⁻⁴</td>
<td>160</td>
<td>0.01</td>
</tr>
<tr>
<td>2-propanone</td>
<td>58.08</td>
<td>52</td>
<td>3.62 x 10⁻³</td>
<td>0.2</td>
<td>0.24</td>
</tr>
<tr>
<td>2-butanol</td>
<td>72.11</td>
<td>30</td>
<td>6.01 x 10⁻³</td>
<td>0</td>
<td>0.7</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>2.02</td>
<td>340</td>
<td>5.91 x 10⁻⁶</td>
<td>26</td>
<td>0.02</td>
</tr>
<tr>
<td>Ammonia</td>
<td>17</td>
<td>7</td>
<td>8.46 x 10⁻⁵</td>
<td>321</td>
<td>11.17</td>
</tr>
<tr>
<td>Carbon monoxide</td>
<td>28.01</td>
<td>10</td>
<td>2.03 x 10⁻⁵</td>
<td>23</td>
<td>1.26</td>
</tr>
</tbody>
</table>

Air quality monitoring on board the ISS has determined that formaldehyde is being generated at an unexpected rate. The concentration in the cabin has risen to >0.06 mg/m³ on occasion. After correcting ventilation problems between the USOS and ROS, the concentration appears to have stabilized at ~0.04 mg/m³. Formaldehyde’s SMAC is 0.05 mg/m³. At the prevailing concentration of 0.04 mg/m³, engineering analysis indicates a persistent source generating formaldehyde at ~3.1 mg/hr. Human metabolism from a crew of three accounts for 0.06 mg/hr. At 3.1 mg/hr, the ISS’s total effective trace contaminant control flow rate necessary for maintaining the formaldehyde concentration < 90 percent SMAC is 68.9 m³/hr. With a condensing heat exchanger removing formaldehyde at 39.8-percent efficiency at 144 m³/hr in the ROS, combined with the BMP’s 90-percent efficiency at 27 m³/hr and the TCCS’s 100-percent efficiency at 4.6 m³/hr, the total removal flow capacity is 86.2 m³/hr. This flow may accommodate a cumulative generation rate of 4.3 mg/hr. Effectively, the ISS is approaching
86 percent of its trace contaminant removal flow capacity necessary to maintain the formaldehyde concentration <90 percent SMAC. Several materials, including packaging and acoustic foams, have been evaluated as potential sources.\textsuperscript{18} Efforts to limit accumulation of formaldehyde offgassing sources on board the ISS may be necessary to avoid overwhelming the onboard trace contaminant control capability.

### 5.3 Supporting Air Quality Monitoring

While postflight data, developmental testing data, and engineering analysis are very useful tools for evaluating the TCCS’s performance and managing its logistics needs, a robust environmental monitoring program is a core element for controlling cabin atmospheric quality on board any crewed spacecraft. Data from environmental monitoring are central to the present evaluation and will continue to be important to the continued safe operation of the TCCS and the ISS. To support the service interval changes indicated by this assessment, it is necessary to continue to monitor NH\textsubscript{3}, alcohols, acetone, formaldehyde, total halocarbons, CH\textsubscript{4}, and CO at a minimum. The archival environmental monitoring program presently in use is the minimum acceptable environmental monitoring necessary to provide continuing support to maintain the TCCS.

Trace contaminants not only affect the TCCS’s performance but also other environmental control and life support processes, particularly the H\textsubscript{2}O processing systems. Monitoring allows personnel monitoring both the TCCS and H\textsubscript{2}O processing systems’ performance to understand how the cabin environment may be changing and how those changes may affect logistics decisions. Presently, NH\textsubscript{3} concentration is measured via detector tubes and indirectly monitored via analysis of humidity condensate loading. Formaldehyde is monitored using detector tubes and dosimeter badges, and other trace components are monitored via grab samples that are analyzed on the ground. Most methods have significant time delays between the sample collection and analysis activities. Six months may elapse before data are available in some instances. To best support TCCS operations, the archival environmental monitoring program must be maintained at a minimum. Steps to reduce the time between sample collection and analysis on the ground would provide much better support for maintaining proper TCCS function. Beyond that, supplementing the present monitoring techniques with near real-time monitors for NH\textsubscript{3}, alcohols, total halocarbons, and formaldehyde will approach an ideal situation.
6. CONCLUSIONS

Based upon postflight evaluation of the CBA charcoal loading, ground testing of the COA, and long-term monitoring of the in-flight cabin air quality, the service intervals for the CBA, COA, and SBA may be extended significantly beyond estimates based upon design specification. The CBA service intervals may be extended to no longer than 6 yr, while the SBA service interval may be up to 12.7 yr. The COA service interval may be extended indefinitely as evaluation demonstrates that it is not a consumable item. The CBA service interval applies to a crew of three. For a crew of six, the recommended service interval is 3 yr. Application of a 25-percent margin to the CBA service interval and a 50-percent margin to the SBA service interval is considered appropriate given analytical method uncertainty and the potential variability of the NH$_3$ and halocarbon cabin concentrations. Thus, the recommended CBA and SBA service intervals are 4.5 yr and 6 yr, respectively. The CBA service interval for a crew of six is 2.25 yr.

Further, a well-defined environmental monitoring program is necessary to provide the in-flight air quality data necessary to monitor the trace contaminant control performance. At a minimum, this program must provide airborne concentration data for NH$_3$, total alcohols, acetone, formaldehyde, total halocarbons, CH$_4$, and CO. Such a program provides the ECLSS engineering community with sufficient data to ensure that proper trace contaminant control capability is maintained. Supplemental monitoring for halocarbons provides an excellent enhancement to the minimum environmental monitoring program.
7. RECOMMENDATIONS

Based upon a rigorous evaluation of TCCS performance and in-flight conditions, the recommended service intervals for the CBA and SBA are 4.5 and 6 yr, respectively. For a crew of six, the recommended CBA service interval is 2.25 yr. The COA is not a consumable item and can be operated until it wears out. It is further recommended to conduct a follow-on study of the CBA presently in service after it accumulates 4.5 yr of operation.

To assist in safely operating the TCCS and managing its resources, it is also recommended that a reliable capability to monitor NH$_3$, total alcohols, acetone, formaldehyde, CH$_4$, CO, and total halocarbons in the cabin atmosphere be maintained. Monitoring allows trends to be recognized that may indicate a need to further evaluate the recommended TCCS ORU service intervals. Further, the present archival environmental monitoring program should be maintained with attention given to reduce the time between sample collection and analysis on the ground to provide a continuing means for indirectly monitoring the TCCS performance. Steps to supplement the environmental monitoring capabilities to include selected near real-time monitors is recommended.
APPENDIX A—PHOSPHORIC ACID LOADING ON CHARCOAL

Tables 12 and 13 show $\text{H}_3\text{PO}_4$ loading of CBA charcoal and depot charcoal, respectively.

Table 12. $\text{H}_3\text{PO}_4$ loading of CBA charcoal.

<table>
<thead>
<tr>
<th>Unused Charcoal</th>
<th>grams of charcoal taken</th>
<th>mg/l $\text{PO}_4$</th>
<th>mg $\text{PO}_4$ per g of charcoal</th>
<th>desorb time (hours)</th>
<th>$\text{PO}_4^3$</th>
<th>$\text{H}_3\text{PO}_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHL # 2002-10-04-01982</td>
<td>1.0302</td>
<td>2776.19</td>
<td>20</td>
<td>53.896</td>
<td>19</td>
<td>55.28</td>
</tr>
<tr>
<td></td>
<td>1.0088</td>
<td>2788.27</td>
<td>20</td>
<td>55.279</td>
<td>24</td>
<td>Ave = 55.85</td>
</tr>
<tr>
<td></td>
<td>7.3028</td>
<td>4262.73</td>
<td>100</td>
<td>58.371</td>
<td>21.5</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1-Center Charcoal</th>
<th>grams of charcoal taken</th>
<th>mg/l $\text{PO}_4$</th>
<th>mg $\text{PO}_4$ per g of charcoal</th>
<th>desorb time (hours)</th>
<th>$\text{PO}_4^3$</th>
<th>$\text{H}_3\text{PO}_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHL # 2002-10-04-01977</td>
<td>1.002</td>
<td>5373.0</td>
<td>20</td>
<td>107.246</td>
<td>19</td>
<td>PO$_4^3$</td>
</tr>
<tr>
<td></td>
<td>1.0024</td>
<td>4946.85</td>
<td>20</td>
<td>98.700</td>
<td>24</td>
<td>$\text{H}_3\text{PO}_4$</td>
</tr>
<tr>
<td></td>
<td>10.0749</td>
<td>9916.38</td>
<td>100</td>
<td>98.427</td>
<td>21.5</td>
<td>Ave = 102.81</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1-A Charcoal</th>
<th>grams of charcoal taken</th>
<th>mg/l $\text{PO}_4$</th>
<th>mg $\text{PO}_4$ per g of charcoal</th>
<th>desorb time (hours)</th>
<th>$\text{PO}_4^3$</th>
<th>$\text{H}_3\text{PO}_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHL # 2002-10-04-01978</td>
<td>1.0303</td>
<td>5429.15</td>
<td>20</td>
<td>105.390</td>
<td>19</td>
<td>PO$_4^3$</td>
</tr>
<tr>
<td></td>
<td>1.0026</td>
<td>4578.87</td>
<td>20</td>
<td>91.340</td>
<td>24</td>
<td>$\text{H}_3\text{PO}_4$</td>
</tr>
<tr>
<td></td>
<td>10.0269</td>
<td>8375.41</td>
<td>100</td>
<td>83.529</td>
<td>21.5</td>
<td>Ave = 89.81</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1-B Charcoal</th>
<th>grams of charcoal taken</th>
<th>mg/l $\text{PO}_4$</th>
<th>mg $\text{PO}_4$ per g of charcoal</th>
<th>desorb time (hours)</th>
<th>$\text{PO}_4^3$</th>
<th>$\text{H}_3\text{PO}_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHL # 2002-10-04-01979</td>
<td>1.0762</td>
<td>5491.89</td>
<td>20</td>
<td>102.061</td>
<td>19</td>
<td>PO$_4^3$</td>
</tr>
<tr>
<td></td>
<td>1.0285</td>
<td>5287.04</td>
<td>20</td>
<td>102.811</td>
<td>24</td>
<td>$\text{H}_3\text{PO}_4$</td>
</tr>
<tr>
<td></td>
<td>10.043</td>
<td>9019.32</td>
<td>100</td>
<td>89.807</td>
<td>21.5</td>
<td>Ave = 90.19</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1-C Charcoal</th>
<th>grams of charcoal taken</th>
<th>mg/l $\text{PO}_4$</th>
<th>mg $\text{PO}_4$ per g of charcoal</th>
<th>desorb time (hours)</th>
<th>$\text{PO}_4^3$</th>
<th>$\text{H}_3\text{PO}_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHL # 2002-10-04-01980</td>
<td>1.0113</td>
<td>3120.5</td>
<td>20</td>
<td>61.713</td>
<td>19</td>
<td>PO$_4^3$</td>
</tr>
<tr>
<td></td>
<td>1.0212</td>
<td>4166.45</td>
<td>20</td>
<td>81.599</td>
<td>24</td>
<td>$\text{H}_3\text{PO}_4$</td>
</tr>
<tr>
<td></td>
<td>10.3351</td>
<td>8040.72</td>
<td>100</td>
<td>77.800</td>
<td>21.5</td>
<td>RSD = 14.9%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>1-D Charcoal</th>
<th>grams of charcoal taken</th>
<th>mg/l $\text{PO}_4$</th>
<th>mg $\text{PO}_4$ per g of charcoal</th>
<th>desorb time (hours)</th>
<th>$\text{PO}_4^3$</th>
<th>$\text{H}_3\text{PO}_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>BHL # 2002-10-04-01981</td>
<td>1.0176</td>
<td>5044.3</td>
<td>20</td>
<td>99.141</td>
<td>19</td>
<td>PO$_4^3$</td>
</tr>
<tr>
<td></td>
<td>1.0587</td>
<td>4807.73</td>
<td>20</td>
<td>90.823</td>
<td>24</td>
<td>$\text{H}_3\text{PO}_4$</td>
</tr>
<tr>
<td></td>
<td>10.2067</td>
<td>6374</td>
<td>100</td>
<td>62.449</td>
<td>21.5</td>
<td>Ave = 90.19</td>
</tr>
</tbody>
</table>

STD DEVI = 13.45

RSD = 14.9%
Table 13. \( \text{H}_3\text{PO}_4 \) loading of depot charcoal.

<table>
<thead>
<tr>
<th>Charcoal Sample</th>
<th>Weight in 500 mL</th>
<th>mg/L ( \text{PO}_4^{3-} )</th>
<th>mg/L ( \text{PO}_4^{4-} )</th>
<th>Average ( \text{PO}_4 )</th>
<th>Average for Analysis mg/gm Charcoal</th>
<th>Average for Sampling mg/gm Charcoal</th>
<th>Precision Summary</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>RPD (%)</td>
</tr>
<tr>
<td>1A</td>
<td>4.9996</td>
<td>1025</td>
<td>1054</td>
<td>1040</td>
<td>104</td>
<td>107</td>
<td>5.5%</td>
</tr>
<tr>
<td>1B</td>
<td>4.9879</td>
<td>1100</td>
<td>1096</td>
<td>1098</td>
<td>110</td>
<td></td>
<td>0.4%</td>
</tr>
<tr>
<td>2A</td>
<td>4.9826</td>
<td>1200</td>
<td>1223</td>
<td>1212</td>
<td>122</td>
<td>123</td>
<td>2.0%</td>
</tr>
<tr>
<td>2B</td>
<td>4.9933</td>
<td>1225</td>
<td>1246</td>
<td>1236</td>
<td>124</td>
<td></td>
<td>1.7%</td>
</tr>
<tr>
<td>3A</td>
<td>5.0403</td>
<td>1075</td>
<td>1066</td>
<td>1071</td>
<td>106</td>
<td>91</td>
<td>34.2%</td>
</tr>
<tr>
<td>3B</td>
<td>5.0030</td>
<td>750</td>
<td>765</td>
<td>758</td>
<td>76</td>
<td></td>
<td>2.0%</td>
</tr>
<tr>
<td>4A</td>
<td>5.0194</td>
<td>1450</td>
<td>1462</td>
<td>1456</td>
<td>145</td>
<td>131</td>
<td>21.9%</td>
</tr>
<tr>
<td>4B</td>
<td>4.9752</td>
<td>1150</td>
<td>1187</td>
<td>1169</td>
<td>117</td>
<td></td>
<td>3.2%</td>
</tr>
<tr>
<td>5A</td>
<td>4.9820</td>
<td>850</td>
<td>851</td>
<td>851</td>
<td>85</td>
<td>73</td>
<td>33.1%</td>
</tr>
<tr>
<td>5B</td>
<td>4.9778</td>
<td>600</td>
<td>618</td>
<td>609</td>
<td>61</td>
<td></td>
<td>3.0%</td>
</tr>
<tr>
<td>6A</td>
<td>4.9984</td>
<td>913</td>
<td>940</td>
<td>927</td>
<td>93</td>
<td>88</td>
<td>11.8%</td>
</tr>
<tr>
<td>6B</td>
<td>4.9946</td>
<td>825</td>
<td>822</td>
<td>824</td>
<td>82</td>
<td></td>
<td>0.4%</td>
</tr>
<tr>
<td>7A</td>
<td>5.0077</td>
<td>850</td>
<td>843</td>
<td>847</td>
<td>85</td>
<td>86</td>
<td>2.2%</td>
</tr>
<tr>
<td>7B</td>
<td>4.9660</td>
<td>875</td>
<td>855</td>
<td>865</td>
<td>87</td>
<td></td>
<td>2.3%</td>
</tr>
<tr>
<td>8A</td>
<td>4.9918</td>
<td>700</td>
<td>727</td>
<td>714</td>
<td>71</td>
<td>67</td>
<td>12.2%</td>
</tr>
<tr>
<td>8B</td>
<td>4.9756</td>
<td>625</td>
<td>638</td>
<td>632</td>
<td>63</td>
<td></td>
<td>2.1%</td>
</tr>
<tr>
<td>3A*</td>
<td>5.0090</td>
<td>725</td>
<td>711</td>
<td>718</td>
<td>72</td>
<td>63</td>
<td>28.4%</td>
</tr>
<tr>
<td>3B*</td>
<td>5.0034</td>
<td>528</td>
<td>551</td>
<td>540</td>
<td>54</td>
<td></td>
<td>4.3%</td>
</tr>
<tr>
<td>5A*</td>
<td>5.0058</td>
<td>561</td>
<td>564</td>
<td>562</td>
<td>56</td>
<td>52</td>
<td>16.5%</td>
</tr>
<tr>
<td>5B*</td>
<td>5.0058</td>
<td>476</td>
<td>477</td>
<td>477</td>
<td>48</td>
<td></td>
<td>0.2%</td>
</tr>
<tr>
<td></td>
<td>Average =</td>
<td>88</td>
<td>88</td>
<td>88</td>
<td>16.8%</td>
<td>1.8%</td>
<td></td>
</tr>
</tbody>
</table>

RPD = Relative Percent Difference = Absolute Value of the difference in replicate results/average of replicate results (%)

* Repeat Analysis of Samples
APPENDIX B—AMMONIA LOADING ON CHARCOAL

Table 14 shows the breakdown of NH₃ loading on CBA charcoal for segments 1 through 5.

Table 14. NH₃ loading on CBA charcoal.

<table>
<thead>
<tr>
<th>BHL# 2002-10-04-01982</th>
<th>Charcoal (g)</th>
<th>Dilution Factor</th>
<th>NH₄ mg/l</th>
<th>NH₄ mg/g of Charcoal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blank Charcoal</td>
<td>1.0248</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Segment 1 Replicate 1 BHL# 2002-10-04-01977</th>
<th>Charcoal (g)</th>
<th>Dilution Factor</th>
<th>NH₄ mg/l</th>
<th>NH₄ mg/g of Charcoal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Section 1-Center</td>
<td>1.1088</td>
<td>1</td>
<td>212.13</td>
<td>3.83</td>
</tr>
<tr>
<td>Section 1-A</td>
<td>1.007</td>
<td>1</td>
<td>175.64</td>
<td>3.49</td>
</tr>
<tr>
<td>Section 1-B</td>
<td>1.0119</td>
<td>1</td>
<td>256.11</td>
<td>5.06</td>
</tr>
<tr>
<td>Section 1-C</td>
<td>1.0838</td>
<td>1</td>
<td>287.01</td>
<td>5.30</td>
</tr>
<tr>
<td>Section 1-D</td>
<td>1.022</td>
<td>1</td>
<td>157.54</td>
<td>3.08</td>
</tr>
<tr>
<td>Ave</td>
<td></td>
<td></td>
<td></td>
<td>4.15</td>
</tr>
<tr>
<td>Std. Dev</td>
<td></td>
<td></td>
<td></td>
<td>0.87</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Segment 1 Replicate 2 BHL# 2002-10-04-01977</th>
<th>Charcoal (g)</th>
<th>Dilution Factor</th>
<th>NH₄ mg/l</th>
<th>NH₄ mg/g of Charcoal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Section 1-Center</td>
<td>1.0245</td>
<td>1</td>
<td>167.68</td>
<td>3.27</td>
</tr>
<tr>
<td>Section 1-A</td>
<td>1.016</td>
<td>1</td>
<td>267.31</td>
<td>5.26</td>
</tr>
<tr>
<td>Section 1-B</td>
<td>1.0077</td>
<td>1</td>
<td>322.85</td>
<td>6.41</td>
</tr>
<tr>
<td>Section 1-C</td>
<td>1.07</td>
<td>1</td>
<td>233.18</td>
<td>4.36</td>
</tr>
<tr>
<td>Section 1-D</td>
<td>1.0918</td>
<td>1</td>
<td>222.41</td>
<td>4.07</td>
</tr>
<tr>
<td>Ave</td>
<td></td>
<td></td>
<td></td>
<td>4.68</td>
</tr>
<tr>
<td>Std. Dev</td>
<td></td>
<td></td>
<td></td>
<td>1.07</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Segment 2 BHL# 2002-10-04-01978</th>
<th>Charcoal (g)</th>
<th>Dilution Factor</th>
<th>NH₄ mg/l</th>
<th>NH₄ mg/g of Charcoal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Section 2-Center</td>
<td>1.0329</td>
<td>1</td>
<td>0.37</td>
<td>0.007</td>
</tr>
<tr>
<td>Section 2-A</td>
<td>1.0902</td>
<td>1</td>
<td>0.43</td>
<td>0.008</td>
</tr>
<tr>
<td>Section 2-B</td>
<td>1.009</td>
<td>1</td>
<td>0.32</td>
<td>0.006</td>
</tr>
<tr>
<td>Section 2-C</td>
<td>1.0201</td>
<td>1</td>
<td>0.39</td>
<td>0.008</td>
</tr>
<tr>
<td>Section 2-D</td>
<td>1.0146</td>
<td>1</td>
<td>0.42</td>
<td>0.008</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Segment 3 BHL# 2002-10-04-01979</th>
<th>Charcoal (g)</th>
<th>Dilution Factor</th>
<th>NH₄ mg/l</th>
<th>NH₄ mg/g of Charcoal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Section 3-Center</td>
<td>1.032</td>
<td>1</td>
<td>0.36</td>
<td>0.007</td>
</tr>
<tr>
<td>Section 3-A</td>
<td>1.0123</td>
<td>1</td>
<td>0.31</td>
<td>0.006</td>
</tr>
<tr>
<td>Section 3-B</td>
<td>1.0227</td>
<td>1</td>
<td>0.38</td>
<td>0.007</td>
</tr>
<tr>
<td>Section 3-C</td>
<td>1.104</td>
<td>1</td>
<td>0.35</td>
<td>0.006</td>
</tr>
<tr>
<td>Section 3-D</td>
<td>1.025</td>
<td>1</td>
<td>0.32</td>
<td>0.006</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Segment 4 BHL# 2002-10-04-01980</th>
<th>Charcoal (g)</th>
<th>Dilution Factor</th>
<th>NH₄ mg/l</th>
<th>NH₄ mg/g of Charcoal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Section 4-Center</td>
<td>1.0347</td>
<td>1</td>
<td>0.46</td>
<td>0.009</td>
</tr>
<tr>
<td>Section 4-A</td>
<td>1.0278</td>
<td>1</td>
<td>0.35</td>
<td>0.007</td>
</tr>
<tr>
<td>Section 4-B</td>
<td>1.0784</td>
<td>1</td>
<td>0.37</td>
<td>0.007</td>
</tr>
<tr>
<td>Section 4-C</td>
<td>1.0019</td>
<td>1</td>
<td>0.25</td>
<td>0.005</td>
</tr>
<tr>
<td>Section 4-D</td>
<td>1.0009</td>
<td>1</td>
<td>0.21</td>
<td>0.004</td>
</tr>
</tbody>
</table>
Table 14. NH$_3$ loading on CBA charcoal (Continued).

<table>
<thead>
<tr>
<th>Segment 5 BHL# 2002-10-04-01981</th>
<th>Charcoal (g)</th>
<th>Dilution Factor</th>
<th>NH$_4$ mg/l</th>
<th>NH$_4$ mg/g of Charcoal</th>
</tr>
</thead>
<tbody>
<tr>
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APPENDIX C—VOLATILE ORGANIC COMPOUND LOADING ON CHARCOAL

Table 15 shows VOC loading by functional class, table 16 the OFP and NH₃ loading summary, and table 17 the average loading. Target compounds and tentatively identified compounds for all sections and quadrants are shown in tables 18–42.

<table>
<thead>
<tr>
<th>Quadrant</th>
<th>Sample Level</th>
<th>Bed Depth (cm)</th>
<th>Alcohols</th>
<th>Aldehydes</th>
<th>Esters</th>
<th>Ketones</th>
<th>Aromatics</th>
<th>Halocarbons</th>
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Table 16. OFP and NH$_3$ loading summary.

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<th>Ammonia (mg/g)</th>
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Table 17. Average loading.

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<th>Esters</th>
<th>Ketones</th>
<th>Aromatics</th>
<th>Halocarbons</th>
<th>Hydrocarbons</th>
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Loading in mg/g charcoal.
Table 18. Target compounds—section 1, quadrant A.

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<td>3. chloromethane</td>
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<td>22. 2-butanone</td>
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Table 18. Target compounds — section 1, quadrant A (Continued).

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<td>0</td>
</tr>
<tr>
<td>1,1,2-trichloroethane</td>
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</tr>
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<td>tetrachloroethene</td>
<td>0.48</td>
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<tr>
<td>2-hexanone</td>
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<td>0</td>
</tr>
<tr>
<td>n-butyl acetate</td>
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<tr>
<td>1,2-dibromoethane</td>
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<td>styrene</td>
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<td>0</td>
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<td>1,1,2,2-tetrachloroethane</td>
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<tr>
<td>1,3,5-trimethylbenzene</td>
<td>0.64</td>
<td>3.1</td>
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<tr>
<td>1,2,4-trimethylbenzene</td>
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<td>0</td>
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<td>1,3-dichlorobenzene</td>
<td>2.02</td>
<td>12.1</td>
<td>115</td>
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<tr>
<td>1,4-dichlorobenzene</td>
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<td>0</td>
</tr>
<tr>
<td>1,2-dichlorobenzene</td>
<td>0.54</td>
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</tr>
<tr>
<td>1,2,4-trichlorobenzene</td>
<td>0.03</td>
<td>0.2</td>
<td>2.0</td>
</tr>
<tr>
<td>hexachlorobutadiene</td>
<td>0.00</td>
<td>0.0</td>
<td>0</td>
</tr>
</tbody>
</table>

TENTATIVELY IDENTIFIED COMPOUNDS

<table>
<thead>
<tr>
<th>Compound</th>
<th>Concentration (ppm (v))</th>
<th>Loading (mg/m³)</th>
<th>Loading (µg/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Silane, fluorotrimethyl-</td>
<td>0.02</td>
<td>0.08</td>
<td>0.8</td>
</tr>
<tr>
<td>2 Silanol, trimethyl-</td>
<td>0.01</td>
<td>0.03</td>
<td>0.3</td>
</tr>
<tr>
<td>3 Pentane, 2,3-dimethyl</td>
<td>0.02</td>
<td>0.09</td>
<td>0.9</td>
</tr>
<tr>
<td>4 Pentane, 3-ethyl-</td>
<td>0.05</td>
<td>0.27</td>
<td>2.6</td>
</tr>
<tr>
<td>5 Disiloxane, hexamethyl-</td>
<td>0.06</td>
<td>0.26</td>
<td>2.5</td>
</tr>
<tr>
<td>6 Octane, 4,5-dimethyl</td>
<td>0.01</td>
<td>0.03</td>
<td>0.3</td>
</tr>
<tr>
<td>7 Hexane, 2,4-dimethyl</td>
<td>0.01</td>
<td>0.05</td>
<td>0.5</td>
</tr>
<tr>
<td>8 CYCLOPENTANE, 1,2,3-</td>
<td>0.01</td>
<td>0.03</td>
<td>0.3</td>
</tr>
<tr>
<td>9 Ethanol, 2-ethoxy-</td>
<td>0.03</td>
<td>0.13</td>
<td>1.2</td>
</tr>
<tr>
<td>10 Heptane, 2-methyl-</td>
<td>0.03</td>
<td>0.12</td>
<td>1.2</td>
</tr>
<tr>
<td>11 Hexane, 2,3-dimethyl</td>
<td>0.01</td>
<td>0.05</td>
<td>0.5</td>
</tr>
<tr>
<td>12 Heptane, 3-methyl-</td>
<td>0.04</td>
<td>0.18</td>
<td>1.8</td>
</tr>
<tr>
<td>13 Hexane, 2,4-dimethyl</td>
<td>0.01</td>
<td>0.05</td>
<td>0.5</td>
</tr>
<tr>
<td>14 Cyclohexane, 1,4-dimethyl-, trans</td>
<td>0.01</td>
<td>0.04</td>
<td>0.4</td>
</tr>
<tr>
<td>15 Butanoic acid, ethyl ester</td>
<td>0.01</td>
<td>0.05</td>
<td>0.4</td>
</tr>
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</table>
Table 18. Target compounds—section 1, quadrant A (Continued).

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<th>No.</th>
<th>Compound</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>Butanoic acid, 2-methyl-, ethyl ester</td>
<td>0.01</td>
<td>0.07</td>
<td>0.66</td>
</tr>
<tr>
<td>17</td>
<td>Butanoic acid, propyl ester</td>
<td>0.01</td>
<td>0.04</td>
<td>0.37</td>
</tr>
<tr>
<td>18</td>
<td>2-Heptanone</td>
<td>0.01</td>
<td>0.06</td>
<td>0.56</td>
</tr>
<tr>
<td>19</td>
<td>Ethanol, 2-ethoxy-, acetate</td>
<td>0.01</td>
<td>0.03</td>
<td>0.32</td>
</tr>
<tr>
<td>20</td>
<td>Cyclohexane, propyl-</td>
<td>0.01</td>
<td>0.04</td>
<td>0.34</td>
</tr>
<tr>
<td>21</td>
<td>ALPHA-PINENE, (-)-</td>
<td>0.04</td>
<td>0.22</td>
<td>2.14</td>
</tr>
<tr>
<td>22</td>
<td>Isopropylester of 3,3-dimethyltriazine</td>
<td>0.01</td>
<td>0.05</td>
<td>0.52</td>
</tr>
<tr>
<td>23</td>
<td>Cyclohexanone</td>
<td>0.01</td>
<td>0.03</td>
<td>0.26</td>
</tr>
<tr>
<td>24</td>
<td>Cyclohexanone, octamethyl-</td>
<td>0.09</td>
<td>1.12</td>
<td>11</td>
</tr>
<tr>
<td>25</td>
<td>Benzene, 1-ethyl-2-methyl-</td>
<td>0.01</td>
<td>0.06</td>
<td>0.6</td>
</tr>
<tr>
<td>26</td>
<td>Unknown</td>
<td>0.01</td>
<td>0.02</td>
<td>0.2</td>
</tr>
<tr>
<td>27</td>
<td>2-Propenoic acid, 2-methyl-,hexyl</td>
<td>0.05</td>
<td>0.37</td>
<td>3.5</td>
</tr>
<tr>
<td>28</td>
<td>Benzene, (1-methylethenyl)-</td>
<td>0.03</td>
<td>0.13</td>
<td>1.3</td>
</tr>
<tr>
<td>29</td>
<td>Cyclopropane, octyl-</td>
<td>0.01</td>
<td>0.07</td>
<td>0.62</td>
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<td>30</td>
<td>Benzaldehyde</td>
<td>0.25</td>
<td>1.09</td>
<td>10</td>
</tr>
<tr>
<td>31</td>
<td>l-Limonene</td>
<td>0.18</td>
<td>0.98</td>
<td>9.3</td>
</tr>
<tr>
<td>32</td>
<td>Benzene, 1-methyl-2-(1-methylethyl)</td>
<td>0.04</td>
<td>0.20</td>
<td>2.0</td>
</tr>
<tr>
<td>33</td>
<td>1,8-Cineole</td>
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<td>0.08</td>
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<td>34</td>
<td>1-Hexanol, 2-ethyl-</td>
<td>0.07</td>
<td>0.39</td>
<td>3.7</td>
</tr>
<tr>
<td>35</td>
<td>Unknown</td>
<td>0.01</td>
<td>0.07</td>
<td>0.65</td>
</tr>
<tr>
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<td>Benzenemethanol</td>
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<td>0.60</td>
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<tr>
<td>37</td>
<td>Benzene, 1-methyl-2-(2-propenyl)-</td>
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<td>0.06</td>
<td>0.59</td>
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<tr>
<td>38</td>
<td>Siloxane</td>
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<td>0.16</td>
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<tr>
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<td>Tetramethylsuccinonitrile</td>
<td>0.01</td>
<td>0.05</td>
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<td>Ethaneone, 1-phenyl-</td>
<td>0.00</td>
<td>0.02</td>
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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 19. Target compounds—section 2, quadrant A.

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<th>Compound</th>
<th>Concentration</th>
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<td></td>
<td>ppm (v)</td>
<td>mg/m³</td>
</tr>
<tr>
<td>1 dicylorodifluoromethane</td>
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<td>0.0</td>
</tr>
<tr>
<td>2 1,2-dichloro-1,1,2,2-tetrafluoroethane</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>3 chloromethane</td>
<td>0.04</td>
<td>0.07</td>
</tr>
<tr>
<td>4 vinyl chloride</td>
<td>0.0</td>
<td>0.1</td>
</tr>
<tr>
<td>5 acetaldehyde</td>
<td>0.91</td>
<td>1.63</td>
</tr>
<tr>
<td>6 bromomethane</td>
<td>0.0</td>
<td>0.1</td>
</tr>
<tr>
<td>7 chloroethane</td>
<td>0.1</td>
<td>0.2</td>
</tr>
<tr>
<td>8 trichlorofluoromethane</td>
<td>0.0</td>
<td>0.2</td>
</tr>
<tr>
<td>9 pentane</td>
<td>0.41</td>
<td>1.19</td>
</tr>
<tr>
<td>10 ethanol</td>
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</tr>
<tr>
<td>11 propanal</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>12 1,1-dichloroethene</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>13 1,1,2-trichloro-1,2,2-trifluoroethane</td>
<td>0.1</td>
<td>0.7</td>
</tr>
<tr>
<td>14 acetone</td>
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<tr>
<td>17 hexane</td>
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<td>0.0</td>
</tr>
<tr>
<td>18 1,1-dichloroethane</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>19 n-propanol</td>
<td>6.7</td>
<td>16.3</td>
</tr>
<tr>
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<td>0.0</td>
</tr>
<tr>
<td>21 cis-1,2-dichloroethene</td>
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<td>0.0</td>
</tr>
<tr>
<td>22 2-butanol</td>
<td>0.10</td>
<td>0.29</td>
</tr>
<tr>
<td>23 ethyl acetate</td>
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<tr>
<td>24 sec-butanol</td>
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<tr>
<td>25 chloroform</td>
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<td>26 1,1,1-trichloroethane</td>
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<td>0.18</td>
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<tr>
<td>27 cyclohexane</td>
<td>0.04</td>
<td>0.12</td>
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<td>28 carbon tetrachloride</td>
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<tr>
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<td>0.04</td>
</tr>
<tr>
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<td>31 heptane</td>
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<tr>
<td>32 n-Butanol</td>
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</tr>
<tr>
<td>33 trichloroethene</td>
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<td>0.0</td>
</tr>
<tr>
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<td>35 propyl acetate</td>
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<td>0.00</td>
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</tr>
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<td>38 toluene</td>
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<td>2.49</td>
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</table>
Table 19. Target compounds—section 2, quadrant A (Continued).

<table>
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<th>Concentration</th>
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</tr>
</thead>
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<td>ppm (v)</td>
<td>mg/m^3</td>
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<tr>
<td>40 trans-1,3-dichloropropene</td>
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<td>0.0</td>
</tr>
<tr>
<td>41 1,1,2-trichloroethane</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>42 tetrachloroethene</td>
<td>0.01</td>
<td>0.07</td>
</tr>
<tr>
<td>43 2-hexanone</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>44 n-butyl acetate</td>
<td>0.12</td>
<td>0.58</td>
</tr>
<tr>
<td>45 1,2-dibromoethane</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>46 chlorobenzene</td>
<td>0.04</td>
<td>0.17</td>
</tr>
<tr>
<td>47 ethylbenzene</td>
<td>0.06</td>
<td>0.28</td>
</tr>
<tr>
<td>48 m,p-xylene</td>
<td>0.23</td>
<td>1.01</td>
</tr>
<tr>
<td>49 o-xylene</td>
<td>0.42</td>
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<tr>
<td>50 styrene</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>51 1,1,2,2-tetrachloroethane</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>52 1,3,5-trimethylbenzene</td>
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<td>0.0</td>
</tr>
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<td>53 1,2,4-trimethylbenzene</td>
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<td>0.0</td>
</tr>
<tr>
<td>54 1,3-dichlorobenzene</td>
<td>0.01</td>
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</tr>
<tr>
<td>55 1,4-dichlorobenzene</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>56 1,2-dichlorobenzene</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>57 1,2,4-trichlorobenzene</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>58 hexachlorobutadiene</td>
<td>0.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01978, Section 2-A
Multiplier: 8
Date Analyzed: 11/12/02
Sample Amt.: 0.0748 g

<table>
<thead>
<tr>
<th>Compound</th>
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<th>Loading</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ppm (v)</td>
<td>mg/m^3</td>
</tr>
<tr>
<td>1 Silane, fluorotrimethyl-</td>
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<td>0.0</td>
</tr>
<tr>
<td>Octafluoropropane</td>
<td>3.6</td>
<td>27.7</td>
</tr>
<tr>
<td>1-Propene</td>
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<td>9.7</td>
</tr>
<tr>
<td>Propane, 2-methyl</td>
<td>0.4</td>
<td>0.9</td>
</tr>
<tr>
<td>1-Propene, 2-methyl</td>
<td>0.4</td>
<td>0.9</td>
</tr>
<tr>
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</tr>
<tr>
<td>2-Propenenitrile, 2-methyl</td>
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</tr>
<tr>
<td>Pentane, 2,3-dimethyl</td>
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<td>0.1</td>
</tr>
<tr>
<td>Pentane, 3-ethyl</td>
<td>0.0</td>
<td>0.2</td>
</tr>
<tr>
<td>Ethanol, 2-ethoxy</td>
<td>0.0</td>
<td>0.1</td>
</tr>
<tr>
<td>Unknown</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Cyclohexene, 1-methyl-5-(1-methylethenyl</td>
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<td>0.1</td>
</tr>
<tr>
<td>1-Hexanol, 2-ethyl</td>
<td>0.1</td>
<td>0.3</td>
</tr>
<tr>
<td>Phenol</td>
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<td>0.1</td>
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<tr>
<td>2-Pyrrolidinone, 1-methyl</td>
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</tr>
<tr>
<td>Benzenemethanol</td>
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</tr>
</tbody>
</table>

1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 20. Target compounds—section 3, quadrant A.

<table>
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<th>Concentration</th>
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</tr>
</thead>
<tbody>
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<td></td>
<td>ppm (v)</td>
<td>mg/m³</td>
</tr>
<tr>
<td>1 dichlorodifluoromethane</td>
<td>0.146</td>
<td>0.713</td>
</tr>
<tr>
<td>2 1,2-dichloro-1,1,2,2-tetrafluoroethane</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>3 chloromethane</td>
<td>0.023</td>
<td>0.047</td>
</tr>
<tr>
<td>4 vinyl chloride</td>
<td>0.038</td>
<td>0.096</td>
</tr>
<tr>
<td>5 acetaldehyde</td>
<td>1.2</td>
<td>2.1</td>
</tr>
<tr>
<td>6 bromomethane</td>
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Table 20. Target compounds—section 3, quadrant A (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01979, Section 3-A
Date Analyzed: 11/12/02
Multiplier: 4

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Table 20. Target compounds—section 3, quadrant A (Continued).

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 21. Target compounds—section 4, quadrant A.

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Table 21. Target compounds — section 4, quadrant A (Continued).

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<td>n-butyl acetate</td>
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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01980, Section 4-A
Date Analyzed: 11/12/02
Multiplier: 4

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
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### Table 22. Target compounds — section 5, quadrant A (Continued).

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### Tentatively Identified Compounds

**Sample Identification:** 2002-10-04-01981, Section 5-A  
**Multiplier:** 4  
**Date Analyzed:** 11/12/02

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 23. Target compounds—section 1, quadrant B.

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</tr>
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<tr>
<td>27 cyclohexane</td>
<td>1.85</td>
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<td>28 carbon tetrachloride</td>
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<tr>
<td>29 benzene</td>
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<tr>
<td>30 1,2-dichloroethane</td>
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<td>31 heptane</td>
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<tr>
<td>32 n-Butanol</td>
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<tr>
<td>33 trichloroethene</td>
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</tr>
<tr>
<td>34 1,2-dichloropropane</td>
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<td>35 propyl acetate</td>
<td>0.448</td>
<td>1.866</td>
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<tr>
<td>36 cis-1,3-dichloropropene</td>
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<tr>
<td>37 4-methyl-2-pentane</td>
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<td>2.916</td>
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Table 23. Target compounds—section 1, quadrant B (Continued).

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<th>Loading</th>
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<td>ppm (v)</td>
<td>mg/m³</td>
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<td>0.018</td>
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</tr>
<tr>
<td>Octafluoropropane</td>
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<td>Pentane, dodecafluoro-</td>
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<td>0.000</td>
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<tr>
<td>Ethane, 1,1,1,2-tetrafluoro-</td>
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<td>0.000</td>
</tr>
<tr>
<td>1-Propene</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Propane, 2-methyl</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1-Propene, 2-methyl</td>
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<td>0.000</td>
</tr>
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<td>Acetic acid, methyl ester</td>
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<td>Silanol, trimethyl-</td>
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<td>0.017</td>
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<tr>
<td>Pentane, 2,2-dimethyl</td>
<td>0.003</td>
<td>0.011</td>
</tr>
<tr>
<td>Pentane, 2,3-dimethyl</td>
<td>0.033</td>
<td>0.133</td>
</tr>
<tr>
<td>Pentane, 3,3-dimethyl</td>
<td>0.011</td>
<td>0.046</td>
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<tr>
<td>Hexane, 2,3-dimethyl</td>
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<tr>
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<td>Disiloxane, hexamethyl-</td>
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<td>Octane, 4,5-dimethyl</td>
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<tr>
<td>1-Butanol, 2-ethyl-</td>
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<td>Hexane, 2,4-dimethyl</td>
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<td>Cyclohexane, methyl-</td>
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<td>CYCLOPENTANE, 1,3-dimethyl-, cis-</td>
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<td>0.013</td>
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<td>CYCLOPENTANE, 1,2-dimethyl-, cis-</td>
<td>0.007</td>
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<tr>
<td>Unknown</td>
<td>0.003</td>
<td>0.009</td>
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<tr>
<td>Cyclopentane, ethyl-</td>
<td>0.003</td>
<td>0.012</td>
</tr>
<tr>
<td>8 CYCLOPENTANE, 1,2,3-</td>
<td>0.000</td>
<td>0.000</td>
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<td>Ethanol, 2-ethoxy-</td>
<td>0.031</td>
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<td>0.003</td>
<td>0.015</td>
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<td>Hexane, 2,3-dimethyl</td>
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<td>1,3-Dioxolane</td>
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<tr>
<td>Heptane, 3-methyl-</td>
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<td>Hexane, 2,4-dimethyl</td>
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<td>0.000</td>
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<tr>
<td>Cyclohexane, 1,4-dimethyl-, trans</td>
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<tr>
<td>Hexane, 3-ethyl-</td>
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<td>0.012</td>
</tr>
<tr>
<td>Cyclotrisiloxane, hexamethyl-</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Heptane, 2,3-methyl-</td>
<td>0.003</td>
<td>0.013</td>
</tr>
<tr>
<td>Unknown</td>
<td>0.005</td>
<td>0.026</td>
</tr>
<tr>
<td>Unknown</td>
<td>0.004</td>
<td>0.017</td>
</tr>
<tr>
<td>15 Butanoic acid, ethyl ester</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Formamide, N,N-dimethyl-</td>
<td>0.002</td>
<td>0.005</td>
</tr>
<tr>
<td>Unknown</td>
<td>0.009</td>
<td>0.026</td>
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<tr>
<td>Trisiloxane, octamethyl-</td>
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<td>16 Butanoic acid, 2-methyl-, ethyl ester</td>
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<tr>
<td>17 Butanoic acid, propyl ester</td>
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<td>0.000</td>
</tr>
<tr>
<td>18 2-Heptanone</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>19 Ethanol, 2-ethoxy-, acetate</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>20 Cyclohexane, propyl-</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>21 (\text{ALPHA.}-\text{PINENE, (\text{\textsc{\textae}})})</td>
<td>0.003</td>
<td>0.019</td>
</tr>
<tr>
<td>Unknown</td>
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<td>0.000</td>
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<tr>
<td>22 Isopropylester of 3,3-dimethytriazine</td>
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<tr>
<td>23 Cyclohexanone</td>
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<tr>
<td>24 Cyclotetrasiloxane, octamethyl-</td>
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<td>0.045</td>
</tr>
<tr>
<td>25 Benzene, 1-ethyl-2-methyl-</td>
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<tr>
<td>26 Unknown</td>
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<td>0.000</td>
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<tr>
<td>27 2-Propenoic acid, 2-methyl-,hexyl</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>28 Benzene, (1-methylthienyl)-</td>
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<td>0.000</td>
</tr>
<tr>
<td>1-Heptanol, 6-methyl-</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>29 Cyclopropane, octyl-</td>
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<tr>
<td>30 Benzaldehyde</td>
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<td>31 (l)-Limonene</td>
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<td>0.025</td>
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<td>32 Benzene, 1-methyl-2-(1-methylethyl)</td>
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Table 23. Target compounds—section 1, quadrant B (Continued).

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<th>Value 1</th>
<th>Value 2</th>
<th>Value 3</th>
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<tr>
<td>33</td>
<td>1,8-Cineole</td>
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<td>Unknown</td>
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<tr>
<td>36</td>
<td>Benzenemethanol</td>
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<td>0.000</td>
<td>0.0000</td>
</tr>
<tr>
<td>37</td>
<td>Benzene, 1-methyl-2-(2-propenyl)-</td>
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<td>0.000</td>
<td>0.0000</td>
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<tr>
<td>38</td>
<td>Siloxane</td>
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<td>0.000</td>
<td>0.0000</td>
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<tr>
<td>39</td>
<td>Tetramethylsuccinonitrile</td>
<td>0.000</td>
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<tr>
<td>40</td>
<td>Ethanone, 1-phenyl-</td>
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<td>0.000</td>
<td>0.0000</td>
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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 24. Target compounds—section 2, quadrant B.

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<th>Compound</th>
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<th>Loading</th>
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<tr>
<td></td>
<td>ppm (v)</td>
<td>mg/m³</td>
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<tr>
<td>1 dichlorodifluoromethane</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2 1,2-dichloro-1,1,2,2-tetrafluoroethane</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>3 chloromethane</td>
<td>0.030</td>
<td>0.062</td>
</tr>
<tr>
<td>4 vinyl chloride</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>5 acetaldehyde</td>
<td>0.838</td>
<td>1.51</td>
</tr>
<tr>
<td>6 bromomethane</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>7 chloroethane</td>
<td>0.151</td>
<td>0.39</td>
</tr>
<tr>
<td>8 trichlorofluoromethane</td>
<td>0.070</td>
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</tr>
<tr>
<td>9 pentane</td>
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<tr>
<td>10 ethanol</td>
<td>29</td>
<td>55</td>
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<tr>
<td>11 propanal</td>
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<td>0.000</td>
</tr>
<tr>
<td>12 1,1-dichloroethene</td>
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<td>0.000</td>
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<td>0.064</td>
<td>0.486</td>
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<td>14 acetone</td>
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<td>0.000</td>
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<tr>
<td>18 1,1-dichloroethane</td>
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<td>0.000</td>
</tr>
<tr>
<td>19 n-propanol</td>
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<td>21 cis-1,2-dichloroethene</td>
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<td>0.000</td>
</tr>
<tr>
<td>22 2-butanone</td>
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<td>0.091</td>
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<td>23 ethyl acetate</td>
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<td>26 1,1,1-trichloroethane</td>
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</tr>
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<td>27 cyclohexane</td>
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<td>0.000</td>
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<td>0.000</td>
</tr>
<tr>
<td>30 1,2-dichloroethane</td>
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<td>31 heptane</td>
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</tr>
<tr>
<td>32 n-Butanol</td>
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<td>0.034</td>
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<tr>
<td>33 trichloroethene</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>34 1,2-dichloropropane</td>
<td>0.000</td>
<td>0.000</td>
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<tr>
<td>35 propyl acetate</td>
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<tr>
<td>36 cis-1,3-dichloropropene</td>
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<td>0.000</td>
</tr>
<tr>
<td>37 4-methyl-2-pentanone</td>
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</table>

Sample Identification: 2002-10-04-01978, Section 2-B
Date Analyzed: 11/12/02
Multiplier: 8
Sample Amt.: 0.0654 g
Table 24. Target compounds—section 2, quadrant B (Continued).

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<th>Compound</th>
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<td>mg/m³</td>
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<td>toluene</td>
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<tr>
<td>octane</td>
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</tr>
<tr>
<td>trans-1,3-dichloropropene</td>
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</tr>
<tr>
<td>1,1,2-trichloroethane</td>
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<td>0.000</td>
</tr>
<tr>
<td>tetrachloroethene</td>
<td>0.000</td>
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</tr>
<tr>
<td>2-hexanone</td>
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</tr>
<tr>
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<td>ethylbenzene</td>
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</tr>
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<td>1,1,2,2-tetrachloroethane</td>
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</tr>
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<td>1,3,5-trimethylbenzene</td>
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<td>0.000</td>
</tr>
<tr>
<td>1,2,4-trimethylbenzene</td>
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</tr>
<tr>
<td>1,3-dichlorobenzene</td>
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<td>0.000</td>
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<tr>
<td>1,4-dichlorobenzene</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1,2-dichlorobenzene</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1,2,4-trichlorobenzene</td>
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<td>0.000</td>
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<tr>
<td>hexachlorobutadiene</td>
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<td>0.000</td>
</tr>
</tbody>
</table>

TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01978, Section 2-B
Date Analyzed: 11/12/02
Multiplier: 8

<table>
<thead>
<tr>
<th>Compound</th>
<th>Concentration</th>
<th>Loading</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ppm (v)</td>
<td>mg/m³</td>
</tr>
<tr>
<td>Octafluoropropane</td>
<td>14.8</td>
<td>114</td>
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<td>1-Propene</td>
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</tr>
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<td>Cyclopentene</td>
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</tr>
<tr>
<td>2-Propanol, 2-methyl-</td>
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</tr>
<tr>
<td>2-Propenenitrile, 2-methyl-</td>
<td>0.043</td>
<td>0.117</td>
</tr>
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<td>Iso-butyronitrile</td>
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<tr>
<td>Benzenemethanol</td>
<td>0.026</td>
<td>0.112</td>
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¹ Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
### Table 25. Target compounds—section 3, quadrant B.

<table>
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<th>Concentration (mg/m³)</th>
<th>Concentration (ug/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 dichlorodifluoromethane</td>
<td>0.000</td>
<td>0.000</td>
<td>0</td>
</tr>
<tr>
<td>2 1,2-dichloro-1,1,2,2-tetrafluoroethane</td>
<td>0.000</td>
<td>0.000</td>
<td>0</td>
</tr>
<tr>
<td>3 chloromethane</td>
<td>0.010</td>
<td>0.020</td>
<td>0</td>
</tr>
<tr>
<td>4 vinyl chloride</td>
<td>0.000</td>
<td>0.000</td>
<td>0</td>
</tr>
<tr>
<td>5 acetaldehyde</td>
<td>0.773</td>
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<td>6 bromomethane</td>
<td>0.000</td>
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<td>0</td>
</tr>
<tr>
<td>7 chloroethane</td>
<td>0.000</td>
<td>0.000</td>
<td>0</td>
</tr>
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<td>8 trichlorofluoromethane</td>
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Table 25. Target compounds—section 3, quadrant B (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01979, Section 3-B  Multiplier: 4
Date Analyzed: 11/12/02

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Table 25. Target compounds—section 3, quadrant B (Continued).

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Table 25. Target compounds—section 3, quadrant B (Continued).

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
### Table 26. Target compounds—section 4, quadrant B.

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Table 26. Target compounds—section 4, quadrant B (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01980, Section 4-B
Date Analyzed: 11/12/02
Multiplier: 4

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Table 26. Target compounds—section 4, quadrant B (Continued).

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*Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard*
Table 27. Target compounds—section 5, quadrant B.

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Table 27. Target compounds—section 5, quadrant B (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

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Table 27. Target compounds—section 5, quadrant B (Continued).

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
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Table 28. Target compounds—section 1, quadrant C (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01977, Section 1-C
Date Analyzed: 11/12/02
Multiplier: 8
Sample Amt.: 0.0591g

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
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Table 29. Target compounds—section 2, quadrant C (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01978, Section 2-C
Multiplier: 4
Date Analyzed: 11/12/02
Sample Amt.: 0.0715 g

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 30. Target compounds—section 3, quadrant C.

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Table 30. Target compounds—section 3, quadrant C (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01979, Section 3-C
Date Analyzed: 11/12/02
Multiplier: 4
Sample Amt.: 0.0568 g

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 31. Target compounds — section 4, quadrant C.

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<th>Compound</th>
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</tr>
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<td>ppm (v)</td>
<td>mg/m³</td>
</tr>
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</tr>
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<td>3 chloromethane</td>
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<td>Loading</td>
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Table 31. Target compounds—section 4, quadrant C (Continued).

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 32. Target compounds — section 5, quadrant C.

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Table 32. Target compounds—section 5, quadrant C (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01981, Section 5-C
Date Analyzed: 11/12/02
Multiplier: 4

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<td>9 Ethanol, 2-ethoxy-</td>
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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 33. Target compounds—section 1, quadrant D.

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### Table 33. Target compounds — section 1, quadrant D (Continued).

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### Tentatively Identified Compounds

**Sample Identification:** 2002-10-04-01977, Section 1-D  
**Multiplier:** 4  
**Date Analyzed:** 11/12/02  
**Sample Amt.:** 0.1168 g

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Table 33. Target compounds—section 1, quadrant D (Continued).

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<th>Method 2</th>
<th>Method 3</th>
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<tr>
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</table>

1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
### Table 34. Target compounds — section 2, quadrant D.

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<th>Compound</th>
<th>Concentration</th>
<th>Loading</th>
</tr>
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<tbody>
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<td></td>
<td>ppm (v)</td>
<td>mg/m³</td>
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<td>chloromethane</td>
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<td>vinyl chloride</td>
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<td>1,1-dichloroethane</td>
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<td>n-propanol</td>
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### Table 34. Target compounds—section 2, quadrant D (Continued).

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### TENTATIVELY IDENTIFIED COMPOUNDS

**Sample Identification:** 2002-10-04-01978, Section 2-D  
**Multiplier:** 4  
**Sample Amt.:** 0.1063 g  
**Date Analyzed:** 11/12/02

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<td>Ethane, 1,1,1,2-tetrafluoro-</td>
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<td></td>
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<tr>
<td>1-Propene</td>
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Table 34. Target compounds—section 2, quadrant D (Continued).

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<td>Butanoic acid, 2-methyl-, ethyl ester</td>
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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 35. Target compounds—section 3, quadrant D.

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<td>0.01</td>
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<td>0.000</td>
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<tr>
<td>3 chloromethane</td>
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<td>5 Disiloxane, hexamethyl-</td>
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Table 35. Target compounds—section 3, quadrant D (Continued).

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of the Internal Standard
Table 36. Target compounds—section 4, quadrant D.

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Table 36. Target compounds—section 4, quadrant D (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

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</tr>
<tr>
<td>Octafluoropropane</td>
<td>2.386</td>
<td>18.306</td>
</tr>
<tr>
<td>Pentane, dodecafluoro-</td>
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<td>1-Propene</td>
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<td>7 Hexane, 2,4-dimethyl</td>
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<td>Loading</td>
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</tr>
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<td>2.386</td>
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<td>Pentane, dodecafluoro-</td>
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</tr>
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<td>Ethane, 1,1,1,2-tetrafluoro-</td>
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<td>Hexane, 2,3-dimethyl</td>
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<tr>
<td>4 Pentane, 3-ethyl-</td>
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<tr>
<td>5 Disiloxane, hexamethyl-</td>
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Table 36. Target compounds—section 4, quadrant D (Continued).

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<tr>
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<tr>
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<td>Trisiloxane, octamethyl-</td>
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<td>16 Butanoic acid, 2-meth-, ethyl ester</td>
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<tr>
<td>17 Butanoic acid, propyl ester</td>
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<td>18 2-Heptanone</td>
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<td>19 Ethanol, 2-ethoxy-, acetate</td>
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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 37. Target compounds—section 5, quadrant D.

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Table 37. Target compounds—section 5, quadrant D (Continued).

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**TENTATIVELY IDENTIFIED COMPOUNDS**

Sample Identification: 2002-10-04-01981, Section 5-D
Date Analyzed: 11/12/02
Multiplier: 4
Sample Amt.: 0.0796 g

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<tr>
<td>Octafluoropropane</td>
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<tr>
<td>Pentane, dodecafluoro-</td>
<td>0.000</td>
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<tr>
<td>Ethane, 1,1,1,2-tetrafluoro-</td>
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Table 37. Target compounds—section 5, quadrant D (Continued).

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<tr>
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<tr>
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</tr>
<tr>
<td>20</td>
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<td>0.000</td>
<td>0.000</td>
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</tr>
<tr>
<td>21</td>
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<td>0.000</td>
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<tr>
<td>22</td>
<td>Isopropylester of 3,3-dimethyltriazine</td>
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</tr>
<tr>
<td>23</td>
<td>Cyclohexanone</td>
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</tr>
<tr>
<td>24</td>
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<tr>
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<tr>
<td>32</td>
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<tr>
<td>34</td>
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<tr>
<td>35</td>
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<tr>
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<td>38</td>
<td>Siloxane</td>
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<tr>
<td>39</td>
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<tr>
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</table>

1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 38. Target compounds—section 1, center.

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<thead>
<tr>
<th>Compound</th>
<th>Concentration</th>
<th>Loading</th>
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<tr>
<td></td>
<td>ppm (v)</td>
<td>mg/m³</td>
</tr>
<tr>
<td>1. dichlorodifluoromethane</td>
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<td>0.000</td>
</tr>
<tr>
<td>2. 1,2-dichloro-1,1,2,2-tetrafluoroethane</td>
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<tr>
<td>3. chloromethane</td>
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<tr>
<td>4. vinyl chloride</td>
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</tr>
<tr>
<td>5. acetaldehyde</td>
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<td>6.3</td>
</tr>
<tr>
<td>6. bromomethane</td>
<td>0.06</td>
<td>0.22</td>
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<tr>
<td>7. chloroethane</td>
<td>0.03</td>
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</tr>
<tr>
<td>8. trichlorofluoromethane</td>
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</tr>
<tr>
<td>9. pentane</td>
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<td>0.000</td>
</tr>
<tr>
<td>10. ethanol</td>
<td>4.4</td>
<td>8.3</td>
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<tr>
<td>11. propanal</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>12. 1,1-dichloroethene</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>13. 1,1,2-trichloro-1,2,2-trifluoroethane</td>
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<td>0.000</td>
</tr>
<tr>
<td>14. acetone</td>
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<td>19. n-propanol</td>
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<td>20. butanal</td>
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<td>21. cis-1,2-dichloroethene</td>
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<td>22. 2-butanol</td>
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<td>34. 1,2-dichloropropane</td>
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<tr>
<td>35. propyl acetate</td>
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<tr>
<td>36. cis-1,3-dichloropropene</td>
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<tr>
<td>37. 4-methyl-2-pentanone</td>
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Table 38. Target compounds—section 1, center (Continued).

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<tr>
<td>40 trans-1,3-dichloropropene</td>
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<tr>
<td>41 1,1,2-trichloroethane</td>
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<tr>
<td>42 tetrachloroethene</td>
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<td>2.8</td>
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<tr>
<td>43 2-hexanone</td>
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<tr>
<td>44 n-butyl acetate</td>
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<tr>
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</tr>
<tr>
<td>47 ethylbenzene</td>
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<td>48 m,p-xylene</td>
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<td>49 o-xylene</td>
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<td>57 1,2,4-trichlorobenzene</td>
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<tr>
<td>58 hexachlorobutadiene</td>
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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01977, Section 1-Center
Date Analyzed: 11/12/02
Multiplier : 8
Sample Amt. : 0.0601g

<table>
<thead>
<tr>
<th>Compound</th>
<th>Concentration</th>
<th>Loading</th>
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</thead>
<tbody>
<tr>
<td></td>
<td>ppm (v)</td>
<td>mg/m³</td>
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<tr>
<td>1 Pentane, 2,3-dimethyl</td>
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<td>2 Pentane, 3,3-dimethyl</td>
<td>0.006</td>
<td>0.024</td>
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<tr>
<td>3 Hexane, 3-methyl-</td>
<td>0.043</td>
<td>0.174</td>
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<tr>
<td>4 Disiloxane, hexamethyl-</td>
<td>0.034</td>
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<tr>
<td>5 Octane, 4,5-dimethyl</td>
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<td>6 Hexane, 2,4-dimethyl</td>
<td>0.005</td>
<td>0.022</td>
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<tr>
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<tr>
<td>8 CYCLOPENTANE, 1,2,3-</td>
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<tr>
<td>10 Heptane, 2-methyl-</td>
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<tr>
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Table 38. Target compounds—section 1, center (Continued).

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<td></td>
</tr>
<tr>
<td>17</td>
<td>Butanoic acid, 2-methyl-, ethyl ester</td>
<td>0.004</td>
<td>0.019</td>
<td>0.32</td>
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<tr>
<td>18</td>
<td>2-Heptanone</td>
<td>0.004</td>
<td>0.017</td>
<td>0.27</td>
</tr>
<tr>
<td>19</td>
<td>ALPHA-PINENE, (-)-</td>
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<td>Benzene, 1-ethyl-2-methyl-</td>
<td>0.003</td>
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</tr>
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<td>l-Limonene</td>
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</tr>
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<td>24</td>
<td>1,8-Cineole</td>
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<td>0.022</td>
<td>0.37</td>
</tr>
<tr>
<td>25</td>
<td>1-Hexanol, 2-ethyl-</td>
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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 39. Target compounds—section 2, center.

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<th>Concentration</th>
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<td>ppm (v)</td>
<td>mg/m³</td>
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<tr>
<td>1 dichlorodifluoromethane</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>2 1,2-dichloro-1,1,2,2-tetrafluoroethane</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>3 chloromethane</td>
<td>0.000</td>
<td>0.000</td>
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<tr>
<td>4 vinyl chloride</td>
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<td>0.000</td>
</tr>
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<td>5 acetaldehyde</td>
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<tr>
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<td>0.000</td>
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<tr>
<td>7 chloroethane</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>8 trichlorofluoromethane</td>
<td>0.03</td>
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</tr>
<tr>
<td>9 pentane</td>
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<tr>
<td>10 ethanol</td>
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<tr>
<td>11 propanal</td>
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</tr>
<tr>
<td>12 1,1-dichloroethene</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>13 1,1,2-trichloro-1,2,2-trifluoroethane</td>
<td>0.05</td>
<td>0.36</td>
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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01978, Section 2-Center
Date Analyzed: 11/12/02
Multiplier: 4
Sample Amt.: 0.0574 g

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Table 39. Target compounds—section 2, center (Continued).

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 40. Target compounds—section 3, center.

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<td>30 1,2-dichloroethane</td>
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</tr>
<tr>
<td>34 1,2-dichloropropane</td>
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<tr>
<td>35 propyl acetate</td>
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<tr>
<td>37 4-methyl-2-pentanone</td>
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Table 40. Target compounds—section 3, center (Continued).

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<td>40 trans-1,3-dichloropropene</td>
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</tr>
<tr>
<td>41 1,1,2-trichloroethane</td>
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</tr>
<tr>
<td>42 tetrachloroethene</td>
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<td>0.00</td>
</tr>
<tr>
<td>43 2-hexanone</td>
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</tr>
<tr>
<td>44 n-butyl acetate</td>
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</tr>
<tr>
<td>45 1,2-dibromoethane</td>
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<td>46 chlorobenzene</td>
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<tr>
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<td>55 1,4-dichlorobenzene</td>
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<td>56 1,2-dichlorobenzene</td>
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<tr>
<td>57 1,2,4-trichlorobenzene</td>
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<td>58 hexachlorobutadiene</td>
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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01979, Section 3-Center
Multiplier: 4
Date Analyzed: 11/12/02

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<td>mg/m³</td>
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<tr>
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Table 40. Target compounds—section 3, center (Continued).

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<th>Concentration 3</th>
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</tr>
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<td>Disiloxane, hexamethyl-</td>
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<td>Octane, 4,5-dimethyl-</td>
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<td>1-Butanol, 2-ethyl-</td>
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<td>Hexane, 2,4-dimethyl-</td>
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<td>Butanoic acid, 2-methyl-, ethyl ester</td>
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Table 40. Target compounds—section 3, center (Continued).

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
Table 41. Target compounds—section 4, center.

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<td>trichloroethene</td>
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Table 41. Target compounds—section 4, center (Continued).

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TENTATIVELY IDENTIFIED COMPOUNDS

Sample Identification: 2002-10-04-01980, Section 4-Center
Date Analyzed: 11/12/02
Multiplier: 4

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Table 41. Target compounds—section 4, center (Continued).

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1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
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Table 42. Target compounds—section 5, center (Continued).

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<td>octane</td>
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<td>0.000</td>
</tr>
<tr>
<td>58</td>
<td>hexachlorobutadiene</td>
<td>0.000</td>
<td>0.000</td>
</tr>
</tbody>
</table>

**TENTATIVELY IDENTIFIED COMPOUNDS**

Sample Identification: 2002-10-04-01981, Section 5-Center  
Date Analyzed: 11/12/02  
Multiplier : 4  
Sample Amt. : 0.0632 g

| Compound                          | Concentration | Loading |
|---|----------------------------------|------------|---------|
| 1 | Silane, fluorotrimethyl-         | 0.000      | 0.000   |
|   | Octafluoropropane                | 0.000      | 0.000   |
|   | Pentane, dodecafluoro-           | 0.000      | 0.000   |
|   | Ethane, 1,1,1,2-tetrafluoro-     | 0.000      | 0.000   |
|   | 1-Propene                        | 0.029      | 0.050   |
|   | Propane, 2-methyl                | 0.000      | 0.000   |
|   | 1-Propene, 2-methyl              | 0.000      | 0.000   |
|   | Acetic acid, methyl ester        | 0.000      | 0.000   |
| 2 | Silanol, trimethyl-              | 0.000      | 0.000   |
| 3 | Pentane, 2,3-dimethyl            | 0.000      | 0.000   |
|   | Hexane, 2,3-dimethyl             | 0.000      | 0.000   |
| 4 | Pentane, 3-ethyl-                | 0.000      | 0.000   |
| 5 | Disiloxane, hexamethyl-          | 0.000      | 0.000   |
| 6 | Octane, 4,5-dimethyl             | 0.000      | 0.000   |
| 7 | Hexane, 2,4-dimethyl             | 0.000      | 0.000   |
Table 42. Target compounds—section 5, center (Continued).

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<th>Compound</th>
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<th>2</th>
<th>3</th>
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<td>0.000</td>
</tr>
<tr>
<td>CYCLOPENTANE, 1,2,3-</td>
<td>0.000</td>
<td>0.000</td>
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</tr>
<tr>
<td>Ethanol, 2-ethoxy-</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Heptane, 2-methyl-</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Hexane, 2,3-dimethyl</td>
<td>0.000</td>
<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1,3-Dioxolane</td>
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<td>0.000</td>
</tr>
<tr>
<td>Heptane, 3-methyl-</td>
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<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>3-HEXENE, 3-ETHYL-</td>
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<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>1-PENTENE, 2-ETHYL-4-METHYL-</td>
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<td>0.000</td>
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<tr>
<td>2-HEPTENE, 3-METHYL-</td>
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<td>0.000</td>
</tr>
<tr>
<td>Hexane, 2,4-dimethyl</td>
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<td>0.000</td>
</tr>
<tr>
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<td>0.000</td>
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<tr>
<td>Cyclotrisiloxane, hexamethyl-</td>
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<td>0.000</td>
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</tr>
<tr>
<td>Butanoic acid, ethyl ester</td>
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</tr>
<tr>
<td>Trisiloxane, octamethyl-</td>
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<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Butanoic acid, 2-methyl-, ethyl ester</td>
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<td>0.000</td>
<td>0.000</td>
</tr>
<tr>
<td>Butanoic acid, propyl ester</td>
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<td>0.000</td>
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<tr>
<td>2-Heptanone</td>
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<td>0.000</td>
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<td>Ethanol, 2-ethoxy-, acetate</td>
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<td>Cyclohexane, propyl-</td>
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<tr>
<td>ALPHA-PINENE, (-)-</td>
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<tr>
<td>Isopropylester of 3,3-dimethyltriazine</td>
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<td>0.000</td>
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<td>1-Heptanol, 6-methyl-</td>
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<td>0.000</td>
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<td>0.000</td>
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<td>Benzaldehyde</td>
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<td>0.000</td>
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<tr>
<td>l-Limonene</td>
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<tr>
<td>1,8-Cineole</td>
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<td>0.000</td>
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<td>1-Hexanol, 2-ethyl-</td>
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<td>Phenol</td>
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<tr>
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<td>0.000</td>
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<td>0.000</td>
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<tr>
<td>Ethanone, 1-phenyl-</td>
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</table>

1 Qualitatively Estimated by Comparison of Total Ion Current to that of The Internal Standard
APPENDIX D—VOLATILE ORGANIC COMPOUND LOADING BY FUNCTIONAL CLASS

Figures 23–30 show VOC loading by functional class.

![Graph showing alcohol loading](image)

Figure 23. Alcohol loading.
Figure 24. Aldehyde loading.

Figure 25. Ester loading.
Figure 26. Ketone loading.

Figure 27. Aromatic loading.
Figure 28. Halocarbon loading less OFP.

Figure 29. Hydrocarbon loading.
Figure 30. Ammonia loading.
APPENDIX E—HALOCARBON CONCENTRATION SUMMARY FROM INTERNATIONAL SPACE STATION IN-FLIGHT AIR QUALITY SAMPLES

The in-flight air quality samples taken from the International Space Station are shown in table 43.

<table>
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<tr>
<th>SAMPLE DETAILS</th>
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<tr>
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**AVERAGE**

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<th>Dichorodifluoromethane</th>
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<th>Dichloromethane</th>
<th>1,1,2-trichloro-1,2,2-trifluoroethane</th>
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<th>1,2-dichloropropane</th>
<th>Tetrachloroethene</th>
<th>Chlorobenzene</th>
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</tbody>
</table>

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REFERENCES


An Assessment of the International Space Station’s Trace Contaminant Control Subassembly Process Economics

J.L. Perry, H.E. Cole,* and H.N. El-Lessy**

George C. Marshall Space Flight Center
Marshall Space Flight Center, AL 35812

National Aeronautics and Space Administration
Washington, DC 20546–0001

Prepared by the Spacecraft and Vehicle Systems Department, Engineering Directorate

*The Boeing Company, Huntsville, AL **The Boeing Company, Houston, TX

The International Space Station (ISS) Environmental Control and Life Support System includes equipment specifically designed to actively remove trace chemical contamination from the cabin atmosphere. In the U.S. on-orbit segment, this function is provided by the trace contaminant control subassembly (TCCS) located in the atmosphere revitalization subsystem rack housed in the laboratory module, Destiny. The TCCS employs expendable adsorbent beds to accomplish its function leading to a potentially significant life cycle cost over the life of the ISS. Because maintaining the TCCSs proper can be logistically intensive, its performance in flight has been studied in detail to determine where savings may be achieved. Details of these studies and recommendations for improving the TCCS’s process economics without compromising its performance or crew health and safety are presented and discussed.

The International Space Station (ISS) Environmental Control and Life Support System includes equipment specifically designed to actively remove trace chemical contamination from the cabin atmosphere. In the U.S. on-orbit segment, this function is provided by the trace contaminant control subassembly (TCCS) located in the atmosphere revitalization subsystem rack housed in the laboratory module, Destiny. The TCCS employs expendable adsorbent beds to accomplish its function leading to a potentially significant life cycle cost over the life of the ISS. Because maintaining the TCCSs proper can be logistically intensive, its performance in flight has been studied in detail to determine where savings may be achieved. Details of these studies and recommendations for improving the TCCS’s process economics without compromising its performance or crew health and safety are presented and discussed.

air quality, trace contaminants, volatile organic compounds, contamination control, life support, environmental control, International Space Station, activated carbon, catalytic oxidation, adsorption, catalyst

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13. ABSTRACT (Maximum 200 words)

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