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Trace Chemical Contaminant Generation Rates for Spacecraft Contamination Control System Design

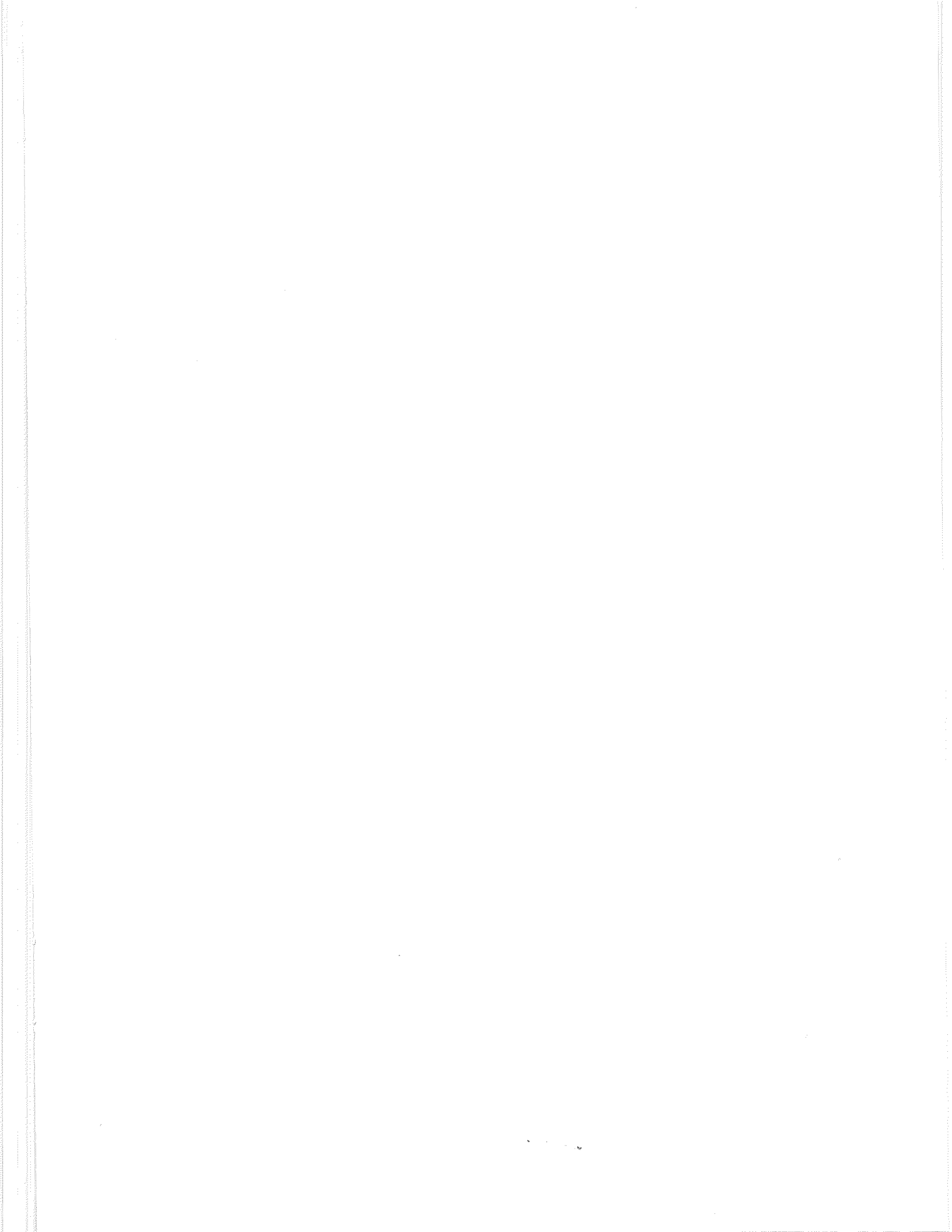
J.L. Perry

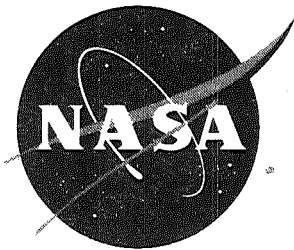
(NASA-TM-108497) TRACE CHEMICAL
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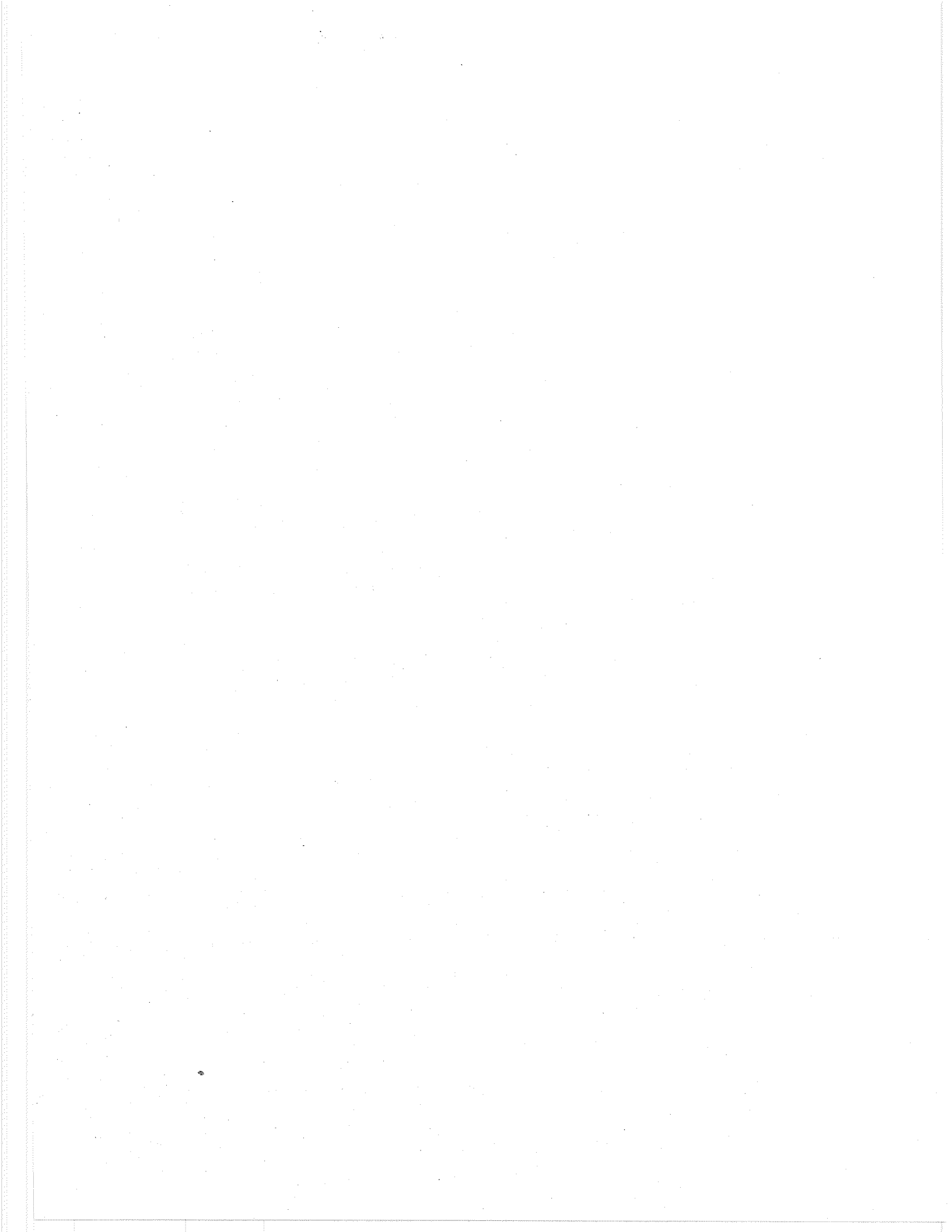


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TECHNICAL MEMORANDUM

TRACE CHEMICAL CONTAMINANT GENERATION RATES FOR SPACECRAFT CONTAMINATION CONTROL SYSTEM DESIGN

INTRODUCTION

A spacecraft presents a unique design challenge with respect to providing a comfortable environment in which people can live and work. All aspects of the spacecraft environmental design must be considered to ensure the comfort and health of the occupants. These include the size of the habitable volume, the temperature, the relative humidity, and the composition of the cabin atmosphere. The crewmembers and the materials selected for outfitting the spacecraft play an integral part in designing a habitable spacecraft. Trace chemicals from these sources that can contaminate the spacecraft atmosphere must be controlled to achieve an acceptable living environment. Otherwise, crewmembers may become ill or unproductive.

Material offgassing and human metabolism are the primary sources for continuous trace chemical contaminant generation onboard a spacecraft. Therefore, these sources are subjected to control via both passive and active means. Passive control involves screening and selecting materials according to established offgassing criteria. These tests are designed to minimize the amount of trace chemical offgassing by limiting the amount of materials that contribute to the total contamination load. Since the material offgassing source cannot be completely eliminated and the crewmembers continuously generate contaminants, active control means are deployed onboard the spacecraft to ensure an acceptably clean cabin atmosphere.

Other sources of trace contaminant generation exist. These include contaminants from house-keeping, personal hygiene, food preparation, extravehicular, and other activities onboard the spacecraft. Contaminants may also be generated from experimental payloads; however, their contribution is normally limited to material offgassing. Even so, occasionally, a contingency contamination event may occur. These events may involve the release of a chemical used as a reagent in a payload or the malfunction of hardware resulting in the release of combustion or pyrolysis products into the cabin atmosphere. Overall, these sources can be controlled by carefully planning activities onboard the spacecraft and using approved material handling procedures for experimental payloads. Since contamination from these sources is difficult at best to quantify, they are generally not used for designing active contamination control systems for spacecraft. Their impacts over time on the performance of the onboard contamination control systems are assessed on a case-by-case basis.

BACKGROUND

Designing active contamination control systems for use onboard spacecraft is a difficult task even though the technologies used are simple and well defined. This difficulty results from the fact that the contamination control system design generally precedes the overall spacecraft design. For this reason, the trace chemical contamination load that the system must process is unknown. Fortunately, a trace chemical contamination load for designing active contamination control systems can now be defined based upon past space mission experience. This experience begins with early contamination control system design and continues to be updated as more space missions are flown. In

addition, the experiences from Russian space missions provide additional information, especially for contamination produced by human metabolic processes.

Initial trace chemical contaminant load models for designing spacecraft contamination control systems use the best estimate of the load from past spacecraft design experience. As the spacecraft design proceeds, more details on the materials of construction and crew size are available, which allows the design load model to be refined. Upon completing the spacecraft design, the original load model can be replaced by contaminant generation rates obtained from the actual materials offgassing data for that spacecraft design. This process has been used successfully for the *Spacelab* and space station programs.

Historically, definition of trace chemical contaminant load models began as early as 1965 when the first design concepts for spacecraft contamination control systems were being developed. This initial work on contamination control systems for *Apollo* defined a load model for offgassing and generation rates for hydrogen and methane.¹ Unfortunately, no references for these data are provided. A study conducted about 1966, however, established a load model that was based upon offgassing test data obtained from materials qualified for spacecraft cabin use, contaminants observed in *Mercury* and *Gemini* charcoal beds, and contaminants observed during several life support tests using human test subjects. Generation rates for these contaminants were based upon offgassing rate tests for materials used onboard *Apollo* spacecraft. It was assumed that the mass of internal materials and equipment was proportional to the total gross mass of the spacecraft. This allowed the contaminant generation load for any spacecraft to be estimated by comparing its estimated mass to the 4,989.52-kg *Apollo* command module. Metabolic contaminants were based upon those documented by P. Webb. A crew of nine was assumed.^{2 3}

Later contamination control system development documented in 1972 used the same load model basis as in 1966 but with metabolic contaminants based upon the work of R.A. Dora.^{4 5} Additional work was done in 1972 to determine the effects of time on equipment offgassing rate. Based upon an assessment of the average offgassing rate, the study suggested that the offgassing rate may decrease by a factor of 4.9 over a period of 180 days.⁶ This load model continued to be used through 1975 during preliminary development of contamination control systems.⁷

A new trace contaminant load model was not developed until 1977. This model was based upon data obtained from the space shuttle program by assessing the offgassing rate per unit equipment mass for various pieces of commercial equipment and spacecraft components. Also, data from materials offgassing tests were assessed to determine rates for contaminants not observed during the component tests. Preliminary data from the *Spacelab* program were also considered. Historical information from *Skylab* and *Apollo* were added to the model in addition to data from spacecraft ground simulation tests. Metabolic contamination production was based upon data documented by P. Webb and R.A. Dora.⁸

This model continued to be the basis well into the design of the *International Space Station*. By 1989, Leban and Wagner documented a model that modified the one developed in 1977 by adding data from *Spacelab* missions 1 and 3 for equipment offgassing rate. The highest generation rate observed from the total *Spacelab* mission hardware for these two missions was used. Historical data from *Skylab* and *Apollo* were still considered, and metabolic data were again based upon the data documented by P. Webb and R.A. Dora.⁹ The time dependence associated with contaminant generation from equipment was not considered in this model or the model developed in 1977.

Although the trace contaminant generation rate models used in the past were effective in providing a design basis for active contamination control systems used onboard *Spacelab*, several problems existed with them. First, the generation rates do not take into account the effects of time on rate resulting in very conservative generation rates. These rates were based upon new hardware and materials. Second, many of the data obtained from *Skylab* and *Apollo* atmospheric samples were taken at different cabin temperature and pressure conditions than those experienced onboard *Spacelab* or to be experienced onboard the *International Space Station*. Future spacecraft most likely will have cabin conditions that are similar to the *International Space Station* and it is difficult to apply data from past programs to them. A third problem exists with the ability to scale the contaminant load to new spacecraft designs. With the exception of the model developed in 1977, scaling the model from one spacecraft to another was accomplished by determining the ratio of the gross spacecraft mass to the gross mass of the *Apollo* command module and then multiplying the generation rate from *Apollo* by the ratio. Although Leban and Wagner updated the ratio to use *Spacelab* as a basis, it becomes increasingly difficult to use this approach because of the differences in the *Skylab*, *Apollo*, *Spacelab*, and future vehicles with respect to material selection and cabin atmospheric conditions. Fourth, the metabolic contaminant generation basis has not been updated to include more data collected during sealed chamber tests on humans. For these reasons, a new model that is based upon on more recent materials selection processes, spacecraft cabin atmospheric conditions, and more metabolic production data is needed.

Since 1989, efforts have been made at the NASA Marshall Space Flight Center to develop an improved trace chemical contaminant load model which addresses these issues. Recently, the *Spacelab* program has provided the most useful set of data to date for defining a trace chemical contaminant generation from spacecraft hardware. These data are based upon the most recent materials selection criteria and reflect cabin atmospheric conditions that will be experienced onboard the *International Space Station*. In addition, American and Russian literature on contaminant generation from metabolic sources has been researched to arrive at a new metabolic load model. The data used to develop the trace chemical contamination control load model are summarized in the following discussion.

EQUIPMENT SOURCES

Spacelab Missions as the Generation Rate Basis

The original basis used for the improved trace chemical contaminant load model is that of Leban and Wagner. This model identified 215 chemical compounds which have been observed during the *Spacelab* missions 1 and 3, *Skylab*, and *Apollo* programs. The list of 215 compounds was modified by deleting the entry for mercury since this chemical would only be observed during an unlikely contingency situation. This left 214 chemical compounds in the model listing.

Data obtained from *Spacelab* missions 1 and 3 were supplemented by four additional missions. These were *Spacelab* missions USML-1, IML-1, D-1, and J. The environmental control system trace contaminant control capability assessments for the six *Spacelab* missions documented by references 10 through 15 were assessed to determine the percentage of overall equipment offgassing that the list of 214 chemical compounds captured. This percentage was based upon the total observed offgassing rate for each mission. Table 1 shows the total generation rate observed during each mission, the total generation rate not accounted for, and the total rate accountability. On average, the list of 214 compounds provided for a 99.61-percent generation rate accountability. This

shows that the primary chemical compounds evolved from equipment offgassing are accounted for by the chemical listing documented by Leban and Wagner. The raw offgassing data from the six *Spacelab* missions for these chemical compounds are listed in appendix A.

Table 1. *Spacelab* trace contaminant generation rate accountability.

<i>Spacelab</i> Mission	Total Rate (mg/day)	Rate Unaccounted for (mg/day)	Total Rate Accountability (Percent)
<i>Spacelab</i> 1	1,580.48	4.4691	99.72
<i>Spacelab</i> 3	9,578.45	5.8424	99.94
<i>Spacelab</i> D-1	732.95	9.5741	98.71
<i>Spacelab</i> IML-1	2,543.90	11.22	99.56
<i>Spacelab</i> USML-1	3,130.48	3.1394	99.90
<i>Spacelab</i> J	1,941.65	3.3300	99.83
Average			99.61

Statistical Analysis of *Spacelab* Equipment Offgassing Data

When dealing with the raw *Spacelab* mission offgassing data, statistical considerations must also be made. Statistics for these data are listed in appendix B. As can be seen by this listing, the standard deviation for many of the chemical compound generation rates is roughly the same order of magnitude as the mean. No data trend is readily observed; therefore, it is assumed that the generation rates are random and should fall within a normal statistical distribution. Data associated with several compounds, however, have a standard deviation that is larger than the mean. This presents a problem to the normal distribution assumption because data outliers may exist. In order to correct this problem, a test was conducted using a data analysis technique used to reconstruct process measurement data. Since no data trend is evident, outliers may be identified by applying the test shown by equation (1).¹⁶

$$(|x_k - \bar{x}_k| > \gamma \cdot s, \gamma > 0) \Rightarrow x_k \text{ is an outlier} \quad (1)$$

In this equation, x_k is compared to the mean, \bar{x}_k . The absolute value of the difference is compared to a set multiple, γ , of the standard deviation, s . In this case, γ is set to one. One standard deviation about the mean was selected since it represents the 95.993 confidence interval of the mean for a single-tail normal distribution.

Results of the outlier analysis are documented in appendix C. If a piece of data is determined to be an outlier by the test of equation (1), then a "1" is entered in the column. Those data points that were designated as outliers then were reconstructed within one standard deviation of the mean according to equation (2).¹⁷

$$\hat{x}_k = \bar{x}_k + \text{sgn}(x_k - \bar{x}_k) \cdot \gamma \cdot s \quad (2)$$

This equation determines the sign of the difference between the outlier data point and the mean, $\text{sgn}(x_k - \bar{x}_k)$, to determine whether the multiple of the standard deviation should be added or subtracted from the mean. This reconstructs all the data within the bounds of a normal distribution. *Spacelab* data reconstructed according to this process are listed in appendix D.

Considerations of Time, Temperature, and Equipment Mass

As previously noted, the offgassing rate is a function of time. The raw data obtained from the *Spacelab* missions, however, is not adjusted for the effects of time. Not only is time a factor but also temperature. Offgassing tests are conducted at 48.89 °C. This elevated temperature can have a profound effect on generation rate. Since the equipment inside a spacecraft typically does not see this type of temperature, an adjustment was investigated to account not only for time but also temperature. Recent studies that compare results from flight grab sample analyses to predictions of *Spacelab* cabin concentration show that using raw offgassing test data as a basis for trace contaminant generation causes cabin concentration to be overestimated by a factor of 11.48.¹⁸ It is assumed that this factor accounts for the effects of both time and temperature since the flight hardware were at normal operating conditions of 21 °C.

In addition, the raw offgassing data expressed as milligrams per day (mg/day) are not readily scaled to future spacecraft designs. In order to facilitate scaleup, the rates must be expressed as mg/day per unit mass of internal, nonstructural hardware. Data on the internal, nonstructural hardware masses were obtained from mass properties reports for the six *Spacelab* missions documented in references 19 through 24. These masses are 5,547.23, 5,831.79, 5,300.13, 6,253.18, 5,791.92, and 5,788.20 kg for *Spacelab* missions 1, 3, D-1, USML-1, IML-1, and J, respectively. These masses include a 1,832.33-kg mass for the *Spacelab* long-module subsystem equipment. The additional mass includes all the experiments, mission dependent equipment, and mission peculiar equipment that contribute to the internal equipment launch load.

The adjusted *Spacelab* trace chemical contaminant generation rates listed in appendix D have been adjusted by dividing by the time and temperature adjustment factor of 11.48 and then dividing by the respective mission equipment mass. The results are documented in appendix E. These rates are easily scaled to any spacecraft design and are consistent with normal spacecraft cabin temperature conditions.

METABOLIC SOURCES

Trace chemical contaminants produced by human metabolism enter the cabin atmosphere via several routes. Chief among these are expired air, flatus, and sweat. Other routes include offgassing from feces and urine; however, these routes are considered insignificant since human waste products are normally isolated from a spacecraft cabin atmosphere. Endogenous production of carbon monoxide is also very important and its route into the cabin atmosphere is via expired air.

During the development of past trace chemical contaminant load models, very limited information on metabolic contaminant sources was used. The primary references were those documented by P. Webb and R.A. Dora. Although useful for spacecraft contamination control system design,

these references are limited. More recently, M.A. Golub and T. Wydeven reported on waste sources onboard spacecraft. Their initial study documented the load model developed by Leban and Wagner as a basis.²⁵ However, in an update on their initial study, M.A. Golub and T. Wydeven reported a more recent study by M.T. Dmitriyev, A.G. Malysheva, and Y.G. Rastyannikov on trace chemical contaminants from human metabolic sources. These metabolic source data were recommended to replace those contained in the model developed by Leban and Wagner.²⁶

Although it would be convenient to use only one study as a basis for the metabolic contribution to a spacecraft contamination load model, this approach does not allow comparison of these data to those obtained during other recent studies. In order to obtain the most data possible, the American and Russian aerospace literature on human metabolic contamination production were surveyed. These literature sources were surveyed since their primary intent was to provide data to support the design, development, and operation of long-duration space missions. It is acknowledged that additional data may be obtained from medical literature; however, those data most likely are not in a format that is readily used for spacecraft design purposes.

Contamination From Expired Air

The data reported by M.T. Dmitriyev, A.G. Malysheva, and Y.G. Rastyannikov are the most extensive available in the aerospace literature. In their study, 136 gaseous waste products entering the air via expired air, sweat, urine, and feces were identified by gas chromatography-mass spectrometry analysis.²⁷ Similar analytical techniques were used by J.P. Conkle, B.J. Camp, and B.E. Welch to study the composition of expired air from eight test subjects. In their study, 43 chemical compounds from metabolic sources were found in expired air.²⁸ As can be seen by the listing in appendix F, the results from these two studies are comparable. In general, the generation rates are within the same order of magnitude. It should be noted that the data from the test subjects designated as nonsmokers were used from the report of Conkle, Camp, and Welch. It is assumed that the test subjects used in the work by Dmitriyev, Malysheva, and Rastyannikov are nonsmokers.

Two additional studies showed very few chemical contaminants in expired air. M.A. Golub and T. Wydeven reported a study by Y.G. Nefedov and B.A. Adamovich which documented the chemical composition of expired air for 22 compounds.²⁹ These same compounds and their respective expired air concentrations are also reported by Y. Nefedov, S.N. Zaloguev, and V.P. Savina.³⁰ These compounds are ethanal (up to 0.1 mg/m³); methanal (up to 0.1 mg/m³); 2-propanone (0.35±0.30 mg/m³); 2-butanone (0.12±0.02 mg/m³); propanal (up to 0.1 mg/m³); ethanol (0.86±0.50 mg/m³); methanol (0.19±0.10 mg/m³); propanol (up to 0.1 mg/m³); 2-propanol (up to 0.1 mg/m³); methanoic acid, ethanoic acid, propionic acid, isovaleric acid, and valeric acid (0.41±0.8 mg/m³); ammonia (0.51±0.07 mg/m³); dimethylamine (up to 0.1 mg/m³); methane (1.24±0.07 mg/m³); ethane (up to 0.1 mg/m³); ethylene (up to 0.1 mg/m³); propane (up to 0.1 mg/m³); hexane (up to 0.1 mg/m³); and carbon monoxide (4.9±1.1 mg/m³ for nonsmokers). Early work by V.V. Kustov and L.A. Tiunov report expired air data for carbon monoxide (0.011 mg/L average), 2-propanone (0.954 mg/h average), and methane (1 to 99 parts per trillion).³¹ Data from these sources were included in the overall assessment of contamination from expired air to account for the possibility that expired air from some people will be a greater source of contaminants than others. Generation rates were obtained from these sources by using a normal ventilation rate of 4.27 L/min.³²

The respective lists of chemical compounds from expired air were compared to the list of 214 compounds identified in spacecraft equipment offgassing studies. Only those compounds found in this

list have been used. Average generation rates for the four references cited were used. These data are presented in appendix F.

Contamination From Flatus

Composition of human flatus has been reported by E. Kirk to be 9-percent carbon dioxide, 3.9-percent oxygen, 7.2-percent methane, 20.9-percent hydrogen, 59-percent nitrogen, and 0.00028-percent hydrogen sulfide on average. Kirk also reported an average production rate of 1.48 mL/min.³³ Additional data reported by E.L. Murphy show a 20 to 50 mL/h production rate with a composition of 10-percent carbon dioxide, 3-percent oxygen, 18-percent methane, 9-percent hydrogen, and 60-percent nitrogen.³⁴ Literature sources cited by V.V. Kustov and L.A. Tiunov report composition ranges of 5.9- to 24.7-percent carbon dioxide, 0- to 10.3-percent oxygen, 0- to 55-percent methane, 0- to 54-percent hydrogen, 10- to 87.7-percent nitrogen, and 0- to 0.00064-percent hydrogen sulfide. Production rates from Kirk and Murphy were also presented.³⁵ These data are summarized in the listing found in appendix G. Generation rates documented in appendix G are based upon the largest reported production rate of 1.48 mL/min reported by Kirk.

Contamination From Sweat

Past contaminant generation from sweat primarily concentrated on ammonia production. Typical ammonia nitrogen concentrations are reported by P.L. Altman and D.S. Dittmer to be 2.0 to 35 mg per 100 mL of sweat.³⁶ P. Webb referenced these data and also reported sweat production rates of 33 to 50 mL of sweat produced per hour for a normal size adult. Production rates during exercise and other environmental conditions are reported to range from 125 to 3,900 mL/h.³⁷ However, this approach to determining gaseous contaminant production from sweat has to rely upon determining an acceptable sweat production rate. Also, as shown by Dmitriyev, Malysheva, and Rastyannikov, many more contaminants can be produced. In order to avoid determining an average sweat production rate and to account for the largest number of contaminants possible, the data of Dmitriyev, Malysheva, and Rastyannikov are used as the basis for contaminant production from sweat. These data are listed in appendix H.

Endogenous Carbon Monoxide Production

Previous carbon monoxide production rates were based upon the 23-mg/day or 0.958-mg/h rate developed by R.B. Jagow in 1977 during early trace chemical contaminant load model development.³⁸ Since that time, no additional data sources have been investigated. Also, the seven data sources used to determine this rate were not reported; therefore it cannot be verified. Other data are reported by Y.G. Nefyodov, V.P. Savina, and N.L. Sokolov. In their study, a rate of 0.384 mg/h was observed based upon a 1 to 2 mg/m³ carbon monoxide composition for expired air.³⁹ This rate is comparable to that reported by R.F. Coburn, W.S. Blakemore, and R.E. Forster who observed an average production rate of 0.42 mL/h or 0.776 mg/h.⁴⁰ In comparison, analysis of expired air reported by Dmitriyev, Malysheva, and Rastyannikov shows a 0.574 mg/h production rate.⁴¹ As can be seen, the rates agree fairly well. Since the references used by R.B. Jagow are not cited, the rate reported was not used to determine a carbon monoxide generation rate. Based upon the other three references, an average rate of 0.575 mg/h was calculated. These data are summarized in appendix I.

LOAD MODEL FOR CONTAMINATION CONTROL SYSTEMS DESIGN

The complete trace chemical contaminant load model combines the contaminants generated from spacecraft materials and equipment with those generated by the crew. Table 2 summarizes the load model for 214 compounds. The mean equipment rate per unit mass of hardware is based on the analysis of *Spacelab* program data summarized in appendices A through E and described previously. The mass of equipment used to determine a spacecraft generation rate should use the mass for all internally mounted, nonstructural hardware. Metabolic data presented in table 2 represent the summation of data for expired air, flatus, sweat, and endogenous carbon monoxide production tabulated in appendices F through I. These rates are for a single person.

The load model presented in table 2 is designed to be easily scaled to any spacecraft. The primary information necessary for estimating trace chemical contaminant generation rates for a spacecraft include the mass of internally mounted, nonstructural equipment and the size of the crew. It should be noted that a central assumption for using this load model as a basis for spacecraft contamination control system design is that materials used in the cabin are similar to those used for *Spacelab* module missions. This assumption is considered to be appropriate since all future spacecraft must select materials from the same approved list of spacecraft materials and any new materials must meet the same offgassing acceptability criteria.

OTHER DESIGN CONSIDERATIONS

Other considerations that must be addressed when designing a contamination control system for a spacecraft include the specific volume and the environmental conditions of the cabin. Specific volume refers to the cabin volume per person and is expressed in cubic meters per person. Studies conducted by V.P. Savina, Y.G. Nefyodov, T.I. Kuznetsova, and V.Y. Ryzhkova demonstrate that the smaller the specific volume, the more critical the need for active contamination control. Some of the data indicate that the contaminant accumulation rate increases exponentially as specific volume decreases.⁴² These data show that in order to ensure an economical spacecraft trace contaminant control system, a large specific volume is recommended. The study results indicate that an optimum specific volume lies between 12 and 24 m³ per person.

This study also investigated the effects of temperature in the range of 32 to 36 °C and a relative humidity of 90 percent on metabolic contaminant generation. Increases in 2-propanone and ethanal production were observed to be 70 percent and 130 percent, respectively.⁴³ More extensive studies were conducted by Y.G. Nefyodov, V.P. Savina, and S.N. Zaloguev on the effects of temperature and relative humidity on metabolic contaminant generation. These studies show that changes in cabin temperature and relative humidity conditions may increase metabolic contamination production by factors of 2 to 5.⁴⁴

As can be seen from these studies, spacecraft volume, crew size, and cabin environmental conditions play an important role in trace chemical contaminant production. With consideration given to these parameters, the load model presented by table 2 assumes normal cabin environmental conditions of 21 °C and 50-percent relative humidity are maintained. Additional considerations beyond cabin conditions that are important to designing active spacecraft contamination control systems are the contaminant physical properties. Molecular weight, liquid density, molar volume, vapor pressure, and Henry's Law constant are parameters that allow for the proper design and

Table 2. Spacecraft trace chemical contaminant generation load model.

COMMON NAME	IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	MEAN	STANDARD	METABOLIC	STANDARD
		WEIGHT		RATE	DEVIATION	RATE	DEVIATION
		g/mole	mg/m ³	mg/day*kg	mg/day*kg	mg/day	mg/day
methyl alcohol	methanol	32.04	9.000	8.55E-04	4.18E-04	3.96E-01	4.78E-01
ethyl alcohol	ethanol	46.07	2000.000	3.53E-03	4.32E-03	2.18E+00	2.08E+00
allyl alcohol	2-propen-1-ol	58.08	1.000	1.00E-06	1.35E-06	8.14E-03	1.41E-02
isopropyl alcohol	2-propanol	60.09	150.000	2.51E-03	1.48E-03	1.02E+00	6.71E-01
n-propyl alcohol	1-propanol	60.09	98.000	1.11E-04	1.30E-04	4.08E-01	1.68E-01
ethylene glycol	1,2-ethanediol	62.07	13.000	2.03E-06	4.00E-06	0.00E+00	0.00E+00
sec-butyl alcohol	2-butanol	74.12	120.000	5.67E-06	3.95E-06	0.00E+00	0.00E+00
isobutyl alcohol	2-methyl-1-propanol	74.12	120.000	4.14E-04	4.33E-04	4.77E-02	8.27E-02
tert-butyl alcohol	2-methyl-2-propanol	74.12	120.000	4.36E-05	3.02E-05	0.00E+00	0.00E+00
n-butyl alcohol	1-butanol	74.12	80.000	2.27E-03	2.44E-03	3.95E-01	1.22E-01
propylene glycol	1,2-propanediol	76.10	0.100	8.29E-08	1.85E-07	0.00E+00	0.00E+00
isoamyl alcohol	3-methyl-1-butanol	88.15	0.100	1.00E-05	1.33E-05	3.26E-01	1.23E-01
n-amyl alcohol	1-pentanol	88.15	130.000	7.20E-05	9.00E-05	8.66E-04	1.50E-03
carbolic acid	phenol	94.11	7.700	1.59E-04	3.24E-04	2.58E-01	5.99E-02
hexahydrophenol	cyclohexanol	100.16	120.000	2.67E-04	4.89E-04	3.70E-01	1.30E-01
2-ethyl butyl alcohol	2-ethyl-1-butanol	102.17	0.100	4.16E-08	9.31E-08	0.00E+00	0.00E+00
sec-hexyl alcohol	2-hexanol	102.18	170.000	1.59E-06	8.90E-07	0.00E+00	0.00E+00
dichloro isopropyl alcohol	1,3-dichloro-2-propanol	128.99	0.100	7.90E-09	1.21E-08	0.00E+00	0.00E+00
2-ethyl hexyl alcohol	2-ethylhexanol	130.23	0.100	4.68E-06	5.17E-06	0.00E+00	0.00E+00
n-nonyl alcohol	nonanol	144.26	0.100	1.11E-06	2.47E-06	0.00E+00	0.00E+00
n-decyl alcohol	decanol	159.29	0.100	1.13E-08	1.19E-08	0.00E+00	0.00E+00
formaldehyde	methanal	30.03	0.050	1.74E-08	2.67E-08	1.67E-01	2.64E-01
acetaldehyde	ethanal	44.05	4.000	6.86E-05	3.99E-05	3.38E-01	2.58E-01
acrolein	2-propenal	56.06	0.030	1.20E-06	2.26E-06	0.00E+00	0.00E+00
propionaldehyde	propanal	58.08	95.000	1.62E-04	1.57E-04	1.54E-01	2.66E-01
methacrolein	2-methylpropenal	70.09	0.100	6.70E-07	1.34E-06	0.00E+00	0.00E+00
n-butylaldehyde	butanal	72.10	120.000	3.11E-04	5.48E-04	0.00E+00	0.00E+00
valeraldehyde	pentanal	86.13	110.000	3.54E-05	4.30E-05	1.39E-02	5.21E-03
sorbaldehyde	2,4-hexadien-1-al	96.13	0.100	2.42E-07	5.42E-07	2.58E-02	4.47E-03
caproaldehyde	hexanal	100.16	0.100	2.60E-05	2.74E-05	1.59E-02	6.57E-03
benzenecarbonal	benzaldehyde	106.12	173.000	8.84E-06	1.11E-05	6.20E-03	2.80E-03
enanthaldehyde	heptanal	114.19	0.100	8.02E-06	9.69E-06	1.46E-02	5.46E-02
p-tolualdehyde	4-methylbenzaldehyde	120.15	0.100	7.47E-08	1.67E-07	0.00E+00	0.00E+00
caprylaldehyde	octanal	128.22	0.100	2.17E-06	2.17E-06	1.71E-02	6.14E-03
phene	benzene	78.11	0.200	1.51E-05	1.00E-05	1.18E+00	9.72E-01
toluene	methylbenzene	92.15	60.000	1.53E-03	4.55E-04	4.62E-01	1.79E-01
styrene	ethenylbenzene	104.14	43.000	1.54E-05	1.59E-05	4.02E-04	2.13E-04
o-xylene	1,2-dimethylbenzene	106.16	220.000	3.07E-04	2.49E-04	3.23E-02	2.42E-02
m-xylene	1,3-dimethylbenzene	106.16	220.000	7.03E-04	1.32E-03	3.23E-02	2.42E-02
p-xylene	1,4-dimethylbenzene	106.16	220.000	6.68E-04	4.12E-04	3.23E-02	2.42E-02
ethylbenzene	ethylbenzene	106.16	130.000	8.38E-05	6.60E-05	3.73E-01	1.56E-01
indonaphthene	indene	116.16	9.500	0.00E+00	0.00E+00	1.10E-02	1.90E-02
alpha-methylstyrene	alpha-methylstyrene	118.18	140.000	7.13E-08	9.59E-08	0.00E+00	0.00E+00
pseudocumene	1,2,4-trimethylbenzene	120.20	15.000	2.17E-05	2.32E-05	1.31E-03	2.26E-03
mesitylene	1,3,5-trimethylbenzene	120.20	15.000	2.67E-06	9.64E-07	7.89E-04	1.37E-03
ethylmethylbenzene	1-ethyl-2-methylbenzene	120.20	25.000	2.05E-06	2.83E-06	0.00E+00	0.00E+00
cumene	isopropylbenzene	120.20	74.000	1.00E-05	4.00E-06	1.11E-04	1.93E-04
propylbenzene	propylbenzene	120.20	49.000	9.61E-05	1.19E-04	2.76E-02	1.07E-02
methylpropylbenzene	1-methyl-3-propylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
butylbenzene	n-butylbenzene	134.12	0.100	6.04E-07	8.79E-07	1.65E-03	2.86E-03
p-cymene	1-isopropyl-4-methylbenzene	134.22	0.100	7.98E-08	1.78E-07	0.00E+00	0.00E+00
methyl formate	methanoic acid methyl ester	60.05	0.100	2.04E-06	2.35E-06	0.00E+00	0.00E+00
ethyl formate	methanoic acid ethyl ester	74.08	91.000	2.13E-06	2.38E-06	0.00E+00	0.00E+00
methyl acetate	ethanoic acid methyl ester	74.08	120.000	6.18E-05	7.91E-05	0.00E+00	0.00E+00
ethyl acetate	ethanoic acid ethyl ester	88.11	180.000	1.58E-04	1.38E-04	3.91E-01	3.84E-01
allyl acetate	ethanoic acid allyl ester	100.12	0.100	1.68E-06	2.03E-06	0.00E+00	0.00E+00
methyl methacrylate	2-methyl propenoic acid methyl ester	100.12	100.000	6.78E-05	6.19E-05	0.00E+00	0.00E+00
isopropyl acetate	ethanoic acid isopropyl ester	102.13	210.000	2.77E-06	3.05E-06	0.00E+00	0.00E+00
butyl formate	methanoic acid butyl ester	102.13	0.100	4.34E-07	6.24E-07	0.00E+00	0.00E+00

Table 2. Spacecraft trace chemical contaminant generation load model—Continued.

COMMON NAME	IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	MEAN	STANDARD	METABOLIC	STANDARD
		WEIGHT		RATE	DEVIATION	RATE	DEVIATION
		g/mole	mg/m ³	mg/day*kg	mg/day*kg	mg/day	mg/day
propyl acetate	ethanoic acid propyl ester	102.13	170.000	1.18E-04	2.20E-04	1.46E-03	2.52E-03
ethyl methacrylate	2-methyl propenoic acid ethyl ester	114.15	0.100	6.02E-06	1.35E-05	0.00E+00	0.00E+00
butyl acetate	ethanoic acid butyl ester	116.16	190.000	3.98E-04	3.48E-04	1.32E-01	5.12E-02
isobutyl acetate	ethanoic acid isobutyl ester	116.16	190.000	5.85E-05	9.32E-05	7.61E-02	3.01E-02
ethyl lactate	lactic acid ethyl ester	118.13	190.000	1.12E-06	2.51E-06	0.00E+00	0.00E+00
methyl cellosolve acetate	ethanoic acid 2-methoxy ethyl ester	118.36	0.100	8.65E-07	1.94E-06	0.00E+00	0.00E+00
isoamyl acetate	ethanoic acid isoamyl ester	130.18	0.100	9.03E-06	1.74E-05	1.14E-01	4.71E-02
n-amyl acetate	ethanoic acid amyl ester	130.18	160.000	1.85E-05	2.93E-05	0.00E+00	0.00E+00
cellosolve acetate	ethanoic acid 2-ethoxyethyl ester	132.16	160.000	4.61E-04	2.85E-04	0.00E+00	0.00E+00
ethyl acetylglucolate	hydroxyethanoic acid ethyl ester	146.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dibutyl oxalate	oxalic acid dibutyl ester	202.25	0.100	6.21E-09	1.39E-08	0.00E+00	0.00E+00
furan	1,4-epoxy-1,3-butadiene	68.07	0.111	7.58E-07	1.08E-06	2.07E-01	1.10E-01
tetrahydrofuran	1,4-epoxybutane	72.11	120.000	3.38E-05	3.55E-05	0.00E+00	0.00E+00
allyl methyl ether	3-methoxy-1-propene	72.11	0.100	1.06E-08	2.37E-08	0.00E+00	0.00E+00
ether	diethyl ether	74.12	240.000	3.88E-05	5.02E-05	0.00E+00	0.00E+00
sylvan	2-methylfuran	82.10	0.130	1.66E-06	1.80E-06	0.00E+00	0.00E+00
gluconal	2,3-dihydropyran	84.13	0.100	6.75E-08	1.51E-07	0.00E+00	0.00E+00
p-dioxane	1,4-dioxane	88.11	0.100	5.76E-05	5.60E-05	3.17E-01	1.42E-01
metaformaldehyde	1,3,5-trioxane	90.08	0.100	1.48E-06	1.65E-06	0.00E+00	0.00E+00
ethyl cellosolve	2-ethoxyethanol	90.12	0.300	2.18E-04	3.83E-04	0.00E+00	0.00E+00
chloropropylene oxide	epichlorohydrin	92.53	0.100	8.23E-07	1.84E-06	0.00E+00	0.00E+00
tetramethyl oxirane	1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	2.63E-07	5.88E-07	0.00E+00	0.00E+00
N-ethyl-diethylenimine oxide	4-ethylmorpholine	115.18	0.100	3.79E-05	8.47E-05	0.00E+00	0.00E+00
butyl propyl ether	1-propoxybutane	116.21	0.100	1.53E-05	2.36E-05	0.00E+00	0.00E+00
glycol monobutyl ether	2-butoxyethanol	118.18	0.100	1.36E-07	1.86E-07	0.00E+00	0.00E+00
methyl chloride	chloromethane	50.49	41.000	3.52E-06	3.24E-06	5.99E-02	2.80E-02
vinyl chloride	chloroethene	62.50	3.000	6.07E-07	8.49E-07	0.00E+00	0.00E+00
ethyl chloride	chloroethane	64.52	260.000	2.96E-08	6.02E-08	0.00E+00	0.00E+00
allyl chloride	3-chloropropene	76.53	0.100	2.36E-08	5.29E-08	0.00E+00	0.00E+00
methylene chloride	dichloromethane	84.93	10.000	1.12E-03	1.03E-03	6.47E-02	2.45E-02
butyl chloride	1-chlorobutane	92.57	150.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dichloroethene	1,1-dichloroethene	96.95	7.900	1.90E-07	3.75E-07	0.00E+00	0.00E+00
ethylene dichloride	1,2-dichloroethane	98.97	1.000	4.24E-05	3.50E-05	0.00E+00	0.00E+00
dichloropropene	1,2-dichloropropene	110.97	0.100	8.07E-06	1.80E-05	0.00E+00	0.00E+00
chlorophene	chlorobenzene	112.56	46.000	7.84E-04	7.60E-04	4.97E-02	2.08E-02
propylene chloride	1,2-dichloropropane	112.99	42.000	3.01E-06	4.41E-06	0.00E+00	0.00E+00
chloroform	trichloromethane	119.38	4.900	8.90E-06	8.71E-06	7.21E-02	3.24E-02
isobutylene chloride	1,2-dichloro-2-methylpropane	127.01	0.100	6.31E-07	9.04E-07	0.00E+00	0.00E+00
trichloroethylene	trichloroethene	131.39	10.000	5.06E-05	3.56E-05	5.30E-02	2.17E-02
methyl chloroform	1,1,1-trichloroethane	133.41	160.000	4.14E-04	2.58E-04	1.61E-01	2.49E-01
vinyl trichloride	1,1,2-trichloroethane	133.41	0.100	3.39E-08	4.85E-08	1.23E-02	0.00E+00
dichlorobenzene	1,2-dichlorobenzene	147.01	30.000	1.96E-06	4.37E-06	0.00E+00	0.00E+00
chloromethylheptane	3-chloromethylheptane	148.68	0.100	5.17E-08	1.16E-07	0.00E+00	0.00E+00
carbon tetrachloride	tetrachloromethane	153.82	13.000	5.05E-06	4.55E-06	7.54E-03	3.12E-03
tetrachloroethylene	tetrachloroethene	165.83	34.000	3.80E-04	3.48E-04	4.72E-02	1.95E-02
Freon 22	chlorodifluoromethane	86.47	350.000	2.01E-05	3.74E-05	0.00E+00	0.00E+00
Freon 21	dichlorofluoromethane	102.90	21.000	2.63E-07	3.73E-07	0.00E+00	0.00E+00
chlorotrifluoroethane	1-chloro-1,2,2-trifluoroethane	118.50	480.000	4.64E-06	2.41E-07	0.00E+00	0.00E+00
Freon 12	dichlorodifluoromethane	120.91	490.000	6.25E-06	7.21E-06	0.00E+00	0.00E+00
dichlorodifluoroethylene	1,2-dichloro-1,2-difluoroethene	132.93	140.000	1.44E-06	4.47E-07	0.00E+00	0.00E+00
Freon 124	chlorotetrafluoroethane	136.48	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
Freon 11	trichlorofluoromethane	137.40	560.000	7.71E-04	6.37E-04	0.00E+00	0.00E+00
Halon 1301	bromotrifluoromethane	148.90	11000.000	8.06E-05	1.80E-04	0.00E+00	0.00E+00
Freon 114	1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	8.10E-06	1.81E-05	0.00E+00	0.00E+00
Freon 113	1,1,2-trichloro-1,2,2-trifluoroethane	187.40	400.000	8.64E-03	1.03E-02	0.00E+00	0.00E+00
Freon 112	1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	1.55E-05	1.78E-05	0.00E+00	0.00E+00
methane	methane	16.04	3800.000	5.43E-04	9.61E-05	2.34E+02	9.47E+01
acetylene	ethyne	26.04	530.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethylene	ethene	28.05	340.000	7.00E-08	1.57E-07	2.45E-01	2.55E-01

Table 2. Spacecraft trace chemical contaminant generation load model—Continued.

COMMON NAME	IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	MEAN	STANDARD	METABOLIC	STANDARD
		WEIGHT		RATE	DEVIATION	RATE	DEVIATION
		g/mole	mg/m ³	mg/day*kg	mg/day*kg	mg/day	mg/day
ethane	ethane	30.07	1200.000	4.07E-07	7.60E-07	4.29E+00	2.41E+00
allene	propadiene	40.07	82.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methylacetylene	propyne	40.07	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propylene	propene	42.08	860.000	1.03E-06	1.53E-06	0.00E+00	0.00E+00
propane	propane	44.09	900.000	4.27E-07	4.94E-07	3.29E+00	2.10E+00
vinylethylene	1,3-butadiene	54.09	0.130	8.22E-07	1.84E-06	0.00E+00	0.00E+00
ethylethylene	1-butene	56.10	460.000	5.66E-05	2.37E-05	1.63E-01	1.86E-01
isobutane	2-methylpropane	58.12	240.000	3.54E-06	7.47E-06	0.00E+00	0.00E+00
butane	butane	58.12	240.000	2.43E-06	2.70E-06	1.59E-02	2.76E-02
pentamethylene	cyclopentene	68.11	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00
isoprene	2-methyl-1,3-butadiene	68.12	560.000	0.00E+00	0.00E+00	9.13E-01	6.43E-01
propylethylene	1-pentene	70.13	190.000	9.10E-09	1.29E-08	0.00E+00	0.00E+00
isopentane	2-methylbutane	72.15	300.000	6.25E-07	1.18E-06	2.28E-01	3.95E-01
pentane	pentane	72.15	590.000	4.46E-05	5.08E-05	7.65E-01	4.57E-01
cyclohexene	3,4,5,6-tetrahydrobenzene	82.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexene	2-hexene	84.16	0.100	1.42E-07	2.84E-07	1.48E-02	2.56E-02
hexamethylene	cyclohexane	84.16	210.000	1.48E-04	2.31E-04	1.21E-01	5.12E-02
methylpentamethylene	methylcyclopentane	84.16	52.000	1.10E-05	1.87E-05	9.61E-02	4.28E-02
neohexane	2,2-dimethylbutane	86.17	88.000	5.17E-07	1.16E-06	0.00E+00	0.00E+00
diethylmethylethane	3-methylpentane	86.18	1800.000	3.64E-06	2.33E-06	3.26E-02	5.64E-02
hexane	hexane	86.18	180.000	3.55E-05	3.40E-05	2.55E-01	2.50E-01
methylcyclohexene	4-methylcyclohexene	96.17	390.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00
heptylene	1-heptene	98.18	200.000	3.40E-09	7.60E-09	3.74E-02	1.62E-02
hexahydrotoluene	methylcyclohexane	98.18	60.000	3.52E-05	2.57E-05	0.00E+00	0.00E+00
dimethylpentane	2,2-dimethylpentane	100.21	0.100	9.79E-06	1.61E-05	0.00E+00	0.00E+00
dimethylpentane	2,4-dimethylpentane	100.21	0.100	1.11E-07	1.56E-07	0.00E+00	0.00E+00
triethylmethane	3-ethylpentane	100.21	0.100	1.11E-07	1.77E-07	0.00E+00	0.00E+00
heptane	heptane	100.21	200.000	3.16E-05	2.44E-05	8.50E-02	4.10E-02
dimethylcyclohexane	1,1-dimethylcyclohexane	112.22	120.000	8.11E-06	1.80E-05	0.00E+00	0.00E+00
2-octene	2-octene	112.22	230.000	9.78E-09	1.39E-08	0.00E+00	0.00E+00
methylheptylene	6-methyl-1-heptene	112.22	0.100	2.40E-09	5.37E-09	0.00E+00	0.00E+00
trans-1,2-dimethylhexamethylene	trans-1,2-dimethylcyclohexane	112.22	120.000	1.73E-05	3.51E-05	0.00E+00	0.00E+00
trimethylpentane	2,2,3-trimethylpentane	114.23	0.100	1.05E-07	2.35E-07	0.00E+00	0.00E+00
dimethylhexane	3,3-dimethylhexane	114.23	0.100	2.63E-06	1.94E-07	0.00E+00	0.00E+00
ethylhexane	3-ethylhexane	114.23	0.100	2.93E-07	4.19E-07	0.00E+00	0.00E+00
octane	octane	114.23	350.000	9.36E-06	6.75E-06	7.91E-02	4.34E-02
ethylheptane	4-ethylheptane	128.26	0.100	3.16E-08	3.79E-08	0.00E+00	0.00E+00
nonane	nonane	128.26	320.000	4.75E-06	2.59E-06	5.22E-02	2.34E-02
citrene (limonene)	4-isopropenyl-1-methylcyclohexene	136.23	0.100	1.11E-06	2.47E-06	0.00E+00	0.00E+00
methylethylheptane	2-methyl-3-ethylheptane	142.28	0.100	3.42E-06	7.76E-07	0.00E+00	0.00E+00
decane	decane	142.28	230.000	1.18E-05	1.60E-05	3.00E-02	0.00E+00
hendecane	undecane	156.31	320.000	1.00E-05	1.51E-05	4.33E-02	1.99E-02
dodecane	dodecane	170.34	280.000	2.86E-07	4.05E-07	3.89E-02	1.87E-02
acetone	2-propanone	58.08	50.000	2.23E-03	1.39E-03	9.63E+00	9.12E+00
methyl vinyl ketone	3-buten-2-one	70.00	0.100	6.27E-08	9.69E-08	0.00E+00	0.00E+00
methyl ethyl ketone	2-butanone	72.11	30.000	2.81E-03	3.20E-03	8.74E+00	2.86E-01
cyclopentanone (adipic ketone)	cyclopentanone	84.11	0.100	1.48E-04	3.22E-04	0.00E+00	0.00E+00
methyl propenyl ketone	3-penten-2-one	84.12	0.100	8.89E-09	1.99E-08	0.00E+00	0.00E+00
cyclopropyl methyl ketone	acetyl cyclopropane	84.13	0.100	1.47E-08	3.28E-08	0.00E+00	0.00E+00
methyl propyl ketone	2-pentanone	86.13	70.000	2.01E-06	2.02E-06	0.00E+00	0.00E+00
methyl isopropyl ketone	3-methyl-2-butanone	86.13	70.000	1.18E-05	1.94E-05	0.00E+00	0.00E+00
mesityl oxide (methyl isobutenyl ketone)	4-methyl-3-penten-2-one	98.14	40.000	1.16E-04	7.47E-05	0.00E+00	0.00E+00
cyclohexanone (pimelic ketone)	cyclohexanone	98.14	60.000	4.34E-04	2.28E-04	0.00E+00	0.00E+00
pinacolone	3,3-dimethyl-2-butanone	100.16	0.100	3.78E-06	3.90E-06	0.00E+00	0.00E+00
methyl isobutyl ketone	4-methyl-2-pentanone	100.16	140.000	8.64E-04	5.46E-04	7.47E-02	2.51E-02
diisopropyl ketone	2,4-dimethyl-3-pentanone	114.18	0.100	2.65E-08	3.91E-08	0.00E+00	0.00E+00
methyl n-amyl ketone	2-heptanone	114.18	0.100	2.35E-05	5.08E-05	4.18E-02	0.00E+00
methyl isoamyl ketone	5-methyl-2-hexanone	114.18	0.100	1.05E-06	1.10E-06	0.00E+00	0.00E+00

Table 2. Spacecraft trace chemical contaminant generation load model—Continued.

COMMON NAME	IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	MEAN	STANDARD	METABOLIC	STANDARD
		WEIGHT		RATE	DEVIATION	RATE	DEVIATION
		g/mole	mg/m ³	mg/day*kg	mg/day*kg	mg/day	mg/day
phenyl methyl ketone	acetophenone	120.14	250.000	2.21E-07	3.45E-07	0.00E+00	0.00E+00
methyl hexyl ketone	2-octanone	128.21	100.000	5.09E-08	1.14E-07	0.00E+00	0.00E+00
methylheptanone	5-methyl-3-heptanone	128.21	0.100	1.34E-06	1.48E-06	0.00E+00	0.00E+00
diisobutyl ketone	2,6-dimethyl-4-heptanone	142.20	58.000	1.03E-06	2.31E-06	0.00E+00	0.00E+00
hydrogen sulfide	hydrogen sulfide	34.08	2.800	0.00E+00	0.00E+00	9.23E-03	7.89E-03
carbon oxisulfide	carbonyl sulfide	60.07	12.000	3.18E-06	2.87E-06	0.00E+00	0.00E+00
ethylene sulfide	ethylene sulfide	60.11	0.100	9.32E-09	2.08E-08	0.00E+00	0.00E+00
methyl sulfide	dimethyl sulfide	62.14	2.500	5.80E-08	1.30E-07	8.76E-02	1.52E-01
carbon disulfide	carbon disulfide	76.14	16.000	1.58E-05	1.65E-05	0.00E+00	0.00E+00
tetrahydrothiopyran	pentamethylene sulfide	102.20	0.100	5.22E-08	7.38E-08	0.00E+00	0.00E+00
nitric oxide	nitric oxide	30.01	6.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nitrogen dioxide	nitrogen dioxide	46.01	0.940	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nitrogen tetroxide	nitrogen tetroxide	92.01	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
acetic acid	ethanoic acid	60.05	7.400	5.92E-07	8.31E-07	7.14E-01	2.93E-01
ethylhexanoic acid	2-ethylhexanoic acid	144.21	0.100	1.19E-07	2.65E-07	0.00E+00	0.00E+00
diamine	hydrazine	32.05	0.005	0.00E+00	0.00E+00	0.00E+00	0.00E+00
acetonitrile	methyl cyanide	41.05	6.700	6.77E-09	1.03E-08	1.12E-01	4.38E-02
monomethyl hydrazine	methyl hydrazine	46.07	0.004	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nitromethane	nitromethane	61.04	13.000	1.40E-05	3.12E-05	0.00E+00	0.00E+00
dimethylformamide	N,N-dimethylformamide	73.10	0.100	9.27E-07	1.17E-06	0.00E+00	0.00E+00
nitroethane	nitroethane	75.07	0.100	1.40E-08	1.98E-08	0.00E+00	0.00E+00
indole	2,3-benzopyrrole	117.15	0.250	0.00E+00	0.00E+00	4.50E-05	1.11E-05
hydrogen	hydrogen	2.02	340.000	2.41E-06	3.50E-06	3.13E+01	1.09E+01
ammonia	ammonia	17.00	7.000	4.11E-05	4.35E-05	7.84E-01	1.36E+00
carbon monoxide	carbon monoxide	28.01	10.000	1.37E-03	6.58E-04	1.38E+01	3.74E+00
dioxosilane	disiloxane	78.10	0.100	5.73E-06	1.24E-05	0.00E+00	0.00E+00
trimethylsilanol	trimethylsilanol	90.21	40.000	7.89E-05	8.98E-05	0.00E+00	0.00E+00
trioxosilane	trisiloxane	124.30	0.100	1.02E-05	1.20E-05	0.00E+00	0.00E+00
hexamethyldioxosilane	hexamethyldisiloxane	162.48	0.100	3.73E-06	4.79E-06	0.00E+00	0.00E+00
tetraoxosilane	tetrasiloxane	170.40	0.100	4.40E-05	9.40E-05	0.00E+00	0.00E+00
diphenylsilane	diphenylsilane	184.32	0.100	4.23E-09	9.47E-09	0.00E+00	0.00E+00
hexamethylcyclotrioxosilane	hexamethylcyclotrisiloxane	222.40	230.000	1.15E-04	4.65E-05	0.00E+00	0.00E+00
octamethyltrioxosilane	octamethyltrisiloxane	236.54	40.000	6.91E-05	1.42E-04	0.00E+00	0.00E+00
octamethylcyclotetraoxosilane	octamethylcyclotetrasiloxane	296.62	0.100	1.84E-04	8.64E-05	0.00E+00	0.00E+00
decamethylcyclopentaoxosilane	decamethylcyclopentasiloxane	370.64	0.100	2.30E-05	2.66E-05	0.00E+00	0.00E+00
decamethylcyclohexaoxosilane	decamethylcyclohexasiloxane	444.71	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
tetradecamethylcycloheptaoxosilane	tetradecamethylcycloheptasiloxane	519.09	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hexadecamethylcyclooctaoxosilane	hexadecamethylcyclooctasiloxane	593.24	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00

analysis of adsorption beds at the normal spacecraft cabin conditions. Appendix J provides a listing of these properties.

SUMMARY

Development of a spacecraft trace chemical contaminant control system requires the definition of the expected contaminant load onboard. In order to define the load, past load model development has been reviewed, recent space mission data have been tabulated and analyzed, and the major human metabolic sources have been defined. It is assumed that all materials used onboard the spacecraft are selected according to material selection and control procedures used by the *Spacelab* program. Also, cabin conditions are assumed to be 21 °C and 50-percent relative humidity. The resulting trace chemical contaminant load model provides a basis for designing future spacecraft contamination control systems and also assessing the capabilities of current systems in use by the shuttle, *Spacelab*, and *International Space Station* programs.

CONCLUSION

A trace chemical contamination load model has been developed for both equipment and human sources based upon past space flight experience. This model, which includes considerations for the effects of time and temperature on equipment contaminant generation, can serve as the design basis for active trace contaminant control systems for spacecraft and possibly other aerospace applications.

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APPENDIX A

Raw *Spacelab* Trace Contaminant Generation Rate Data

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IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J
	WEIGHT		RAW RATE	RAW RATE	RAW RATE	RAW RATE	RAW RATE	RAW RATE
	g/mole	mg/m ³	mg/day	mg/day	mg/day	mg/day	mg/day	mg/day
methanol	32.04	9.000	6.27E+01	8.83E+01	1.84E+01	1.83E+01	6.45E+01	1.40E+02
ethanol	46.07	2000.000	6.12E+01	1.36E+03	4.58E+00	4.10E+02	7.70E+01	5.46E+01
2-propen-1-ol	58.08	1.000	0.00E+00	4.38E-01	0.00E+00	0.00E+00	8.90E-02	6.40E-02
2-propanol	60.09	150.000	8.17E+01	2.56E+02	4.97E+01	7.62E+01	2.27E+02	4.17E+02
1-propanol	60.09	98.000	9.49E-01	3.23E+00	2.71E-01	7.78E+00	6.55E+00	4.41E+01
1,2-ethanediol	62.07	13.000	0.00E+00	0.00E+00	7.80E-02	1.33E+00	0.00E+00	0.00E+00
2-butanol	74.12	120.000	4.42E-02	8.78E-02	2.51E-01	7.80E-01	3.98E-01	8.63E-01
2-methyl-1-propanol	74.12	120.000	1.05E+01	9.08E+01	8.05E+00	1.33E+00	8.12E+01	8.00E+00
2-methyl-2-propanol	74.12	120.000	1.55E+00	1.23E+00	9.67E-01	2.11E+00	9.21E+00	5.45E+00
1-butanol	74.12	80.000	8.36E+01	8.75E+02	1.84E+01	1.17E+02	1.11E+02	7.18E+01
1,2-propanediol	76.10	0.100	5.87E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methyl-1-butanol	88.15	0.100	1.31E-02	0.00E+00	1.00E-03	1.78E+00	1.72E-01	3.11E+00
1-pentanol	88.15	130.000	1.74E+01	1.44E+01	1.10E-02	1.22E+00	0.00E+00	1.05E+00
phenol	94.11	7.700	8.59E-01	6.12E-02	3.18E+00	1.08E+02	0.00E+00	3.04E-01
cyclohexanol	100.16	120.000	1.64E+01	1.63E+02	1.20E-01	0.00E+00	0.00E+00	0.00E+00
2-ethyl-1-butanol	102.17	0.100	2.95E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexanol	102.18	170.000	0.00E+00	1.49E-01	0.00E+00	1.10E-01	2.16E-01	1.53E-01
1,3-dichloro-2-propanol	128.99	0.100	1.00E-03	0.00E+00	3.30E-03	0.00E+00	0.00E+00	0.00E+00
2-ethylhexanol	130.23	0.100	6.10E-01	0.00E+00	1.20E+00	0.00E+00	5.00E-03	3.52E-01
nonanol	144.26	0.100	0.00E+00	8.24E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
decanol	159.29	0.100	0.00E+00	0.00E+00	2.00E-03	0.00E+00	2.00E-03	1.00E-03
methanal	30.03	0.050	0.00E+00	2.30E-03	0.00E+00	0.00E+00	0.00E+00	8.00E-03
ethanal	44.05	4.000	2.85E+00	6.33E+00	9.06E-01	1.22E+00	7.57E+00	9.67E+00
2-propenal	56.06	0.030	6.50E-03	6.50E-03	2.00E-02	0.00E+00	8.19E-01	3.00E-02
propanal	58.08	95.000	5.93E+00	1.12E+01	1.90E-03	5.22E+00	1.03E+01	5.44E+01
2-methylpropenal	70.09	0.100	0.00E+00	2.44E-02	0.00E+00	0.00E+00	0.00E+00	4.46E-01
butanal	72.10	120.000	4.38E+00	1.86E+02	1.62E-01	1.24E+01	2.68E+00	2.82E+00
pentanal	86.13	110.000	1.07E+00	7.88E-01	4.83E-02	0.00E+00	1.43E+01	4.30E+00
2,4-hexadien-1-al	96.13	0.100	1.72E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hexanal	100.16	0.100	5.19E+00	1.32E+00	1.71E-02	4.40E-01	1.35E-01	4.75E+00
benzaldehyde	106.12	173.000	1.41E+00	0.00E+00	2.41E+00	0.00E+00	3.80E-02	2.61E-01
heptanal	114.19	0.100	1.41E-02	4.78E-01	2.89E-01	3.30E-01	1.40E-01	3.36E+00
4-methylbenzaldehyde	120.15	0.100	5.29E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
octanal	128.22	0.100	0.00E+00	3.62E-01	3.12E-01	2.20E-01	1.20E-02	2.00E-03
benzene	78.11	0.200	5.29E-01	3.43E+00	6.80E-01	2.20E-01	8.74E-01	1.45E+00
methylbenzene	92.15	60.000	9.42E+01	1.71E+02	8.11E+01	7.18E+01	1.55E+02	6.73E+01
ethenylbenzene	104.14	43.000	1.17E+00	5.60E-03	1.15E+00	2.20E-01	3.26E-01	5.19E+00
1,2-dimethylbenzene	106.16	220.000	7.47E+00	1.34E+01	1.71E+01	1.56E+00	9.00E+01	2.91E+01
1,3-dimethylbenzene	106.16	220.000	9.04E+00	4.48E+02	7.25E+00	2.33E+00	1.19E+01	6.54E+00
1,4-dimethylbenzene	106.16	220.000	8.03E+01	1.01E+02	8.50E-03	3.04E+01	3.96E+01	2.36E+01
ethylbenzene	106.16	130.000	7.34E+00	2.26E+01	5.11E+00	1.33E+00	2.67E+00	2.26E+00
indene	116.16	9.500	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
alpha-methylstyrene	118.18	140.000	0.00E+00	0.00E+00	9.00E-04	0.00E+00	2.00E-02	1.50E-02
1,2,4-trimethylbenzene	120.20	15.000	1.98E+00	1.49E-02	4.52E-02	0.00E+00	6.92E+00	2.48E+00
1,3,5-trimethylbenzene	120.20	15.000	1.29E-01	2.20E-01	2.95E-01	0.00E+00	1.81E-01	1.84E-01
1-ethyl-2-methylbenzene	120.20	25.000	6.29E-01	1.47E-02	3.46E-01	0.00E+00	0.00E+00	0.00E+00
isopropylbenzene	120.20	74.000	8.20E-01	1.35E+00	6.87E-01	2.20E-01	7.38E-01	3.28E-01
propylbenzene	120.20	49.000	3.39E+00	3.32E+01	4.17E-01	1.10E-01	1.47E+01	1.20E-02
1-methyl-3-propylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
n-butylbenzene	134.12	0.100	0.00E+00	2.81E-01	0.00E+00	0.00E+00	6.80E-02	1.70E-02
1-isopropyl-4-methylbenzene	134.22	0.100	0.00E+00	5.94E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanoic acid methyl ester	60.05	0.100	0.00E+00	7.30E-03	0.00E+00	1.10E-01	6.29E-01	3.18E-01
methanoic acid ethyl ester	74.08	91.000	0.00E+00	1.13E-01	0.00E+00	2.20E-01	8.21E-01	6.40E-02
ethanoic acid methyl ester	74.08	120.000	1.43E+00	1.41E+00	2.53E+01	1.44E+00	3.06E+00	1.68E+00
ethanoic acid ethyl ester	88.11	180.000	1.11E+01	4.68E+01	1.44E+00	1.21E+01	1.42E+00	7.83E+00
ethanoic acid allyl ester	100.12	0.100	2.20E-03	6.05E-01	0.00E+00	1.10E-01	2.08E-01	0.00E+00
2-methyl propenoic acid methyl ester	100.12	100.000	2.11E+00	2.94E+00	2.47E-01	1.39E+01	1.35E+00	1.02E+01
ethanoic acid isopropyl ester	102.13	210.000	3.95E-01	1.14E-01	5.76E-02	0.00E+00	4.00E-03	7.91E-01
methanoic acid butyl ester	102.13	0.100	5.70E-03	0.00E+00	0.00E+00	0.00E+00	2.02E-01	5.80E-02

PRECEDING PAGE BLANK NOT FILLED

PAGE 20 INTENTIONALLY BLANK

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J
	WEIGHT		RAW RATE	RAW RATE	RAW RATE	RAW RATE	RAW RATE	RAW RATE
	g/mole	mg/m ³	mg/day	mg/day	mg/day	mg/day	mg/day	mg/day
ethanoic acid propyl ester	102.13	170.000	4.67E+00	7.42E+01	2.90E-03	5.60E-01	2.87E-01	8.83E-01
2-methyl propenoic acid ethyl ester	114.15	0.100	0.00E+00	4.48E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid butyl ester	116.16	190.000	1.93E+01	1.20E+02	8.33E+00	6.00E+00	3.84E+01	1.45E+01
ethanoic acid isobutyl ester	116.16	190.000	4.20E+00	3.12E+01	7.85E-01	0.00E+00	3.70E-02	7.01E-01
lactic acid ethyl ester	118.13	190.000	0.00E+00	0.00E+00	7.61E-01	0.00E+00	0.00E+00	0.00E+00
ethanoic acid 2-methoxy ethyl ester	118.36	0.100	6.13E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid isoamyl ester	130.18	0.100	0.00E+00	3.46E-01	3.95E-02	0.00E+00	4.30E-02	5.80E+00
ethanoic acid amyl ester	130.18	160.000	1.21E+00	9.82E+00	0.00E+00	0.00E+00	6.91E-01	0.00E+00
ethanoic acid 2-ethoxyethyl ester	132.16	160.000	6.90E+01	1.45E+01	3.61E+01	1.16E+01	5.37E+01	1.16E+01
hydroxyethanoic acid ethyl ester	146.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
oxalic acid dibutyl ester	202.25	0.100	4.40E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-epoxy-1,3-butadiene	68.07	0.111	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.93E-01	1.34E-01
1,4-epoxybutane	72.11	120.000	2.92E+00	1.21E+01	4.73E-01	5.60E-01	7.65E-01	1.49E+00
3-methoxy-1-propene	72.11	0.100	7.50E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
diethyl ether	74.12	240.000	6.58E+00	0.00E+00	1.03E+01	0.00E+00	1.02E+00	4.00E-03
2-methylfuran	82.10	0.130	5.00E-04	1.18E-01	1.90E-02	0.00E+00	2.16E-01	5.06E-01
2,3-dihydroxypropan	84.13	0.100	4.78E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-dioxane	88.11	0.100	8.09E+00	5.92E+00	1.89E-02	2.20E-01	1.13E+01	3.49E-01
1,3,5-trioxane	90.08	0.100	1.10E-03	1.90E-03	0.00E+00	2.20E-01	1.07E-01	3.99E-01
2-ethoxyethanol	90.12	0.300	3.62E+00	1.31E+02	3.52E+00	3.56E+00	4.00E-02	4.30E+00
epichlorohydrin	92.53	0.100	5.83E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	0.00E+00	1.96E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-ethylmorpholine	115.18	0.100	2.68E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-propoxybutane	116.21	0.100	6.83E+00	1.97E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-butoxyethanol	118.18	0.100	6.00E-04	0.00E+00	5.00E-04	0.00E+00	3.20E-02	3.60E-02
chloromethane	50.49	41.000	3.77E-02	2.02E-02	2.70E-03	6.70E-01	4.27E-01	4.22E-01
chloroethene	62.50	3.000	1.67E-01	0.00E+00	0.00E+00	0.00E+00	2.00E-03	1.22E-01
chloroethane	64.52	260.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E-03	2.00E-02
3-chloropropene	76.53	0.100	0.00E+00	0.00E+00	1.60E-02	0.00E+00	0.00E+00	0.00E+00
dichloromethane	84.93	10.000	3.52E+01	2.21E+02	4.50E+00	3.41E+01	3.20E+01	1.87E+02
1-chlorobutane	92.57	150.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1-dichloroethene	96.95	7.900	1.50E-03	0.00E+00	0.00E+00	0.00E+00	1.35E-01	6.00E-03
1,2-dichloroethane	98.97	1.000	1.45E+00	2.48E+00	8.23E-02	1.44E+00	4.51E+00	1.12E+01
1,2-dichloropropene	110.97	0.100	0.00E+00	6.01E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chlorobenzene	112.56	46.000	1.05E+01	1.65E+02	7.33E-01	1.22E+02	4.55E+01	1.61E+01
1,2-dichloropropane	112.99	42.000	0.00E+00	4.69E-01	0.00E+00	1.22E+00	0.00E+00	0.00E+00
trichloromethane	119.38	4.900	7.07E-01	1.18E+00	1.88E+00	0.00E+00	1.27E-01	4.70E-02
1,2-dichloro-2-methylpropane	127.01	0.100	1.05E-01	0.00E+00	2.05E-01	0.00E+00	0.00E+00	0.00E+00
trichloroethene	131.39	10.000	6.73E+00	4.91E+00	8.33E-01	7.80E-01	6.69E+00	1.27E+00
1,1,1-trichloroethane	133.41	160.000	2.92E+01	2.78E+01	3.43E+00	6.78E+00	4.05E+01	7.82E+01
1,1,2-trichloroethane	133.41	0.100	0.00E+00	0.00E+00	1.06E-02	0.00E+00	0.00E+00	6.00E-03
1,2-dichlorobenzene	147.01	30.000	1.38E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E-03
3-chloromethylheptane	148.68	0.100	3.66E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
tetrachloromethane	153.82	13.000	2.08E-01	2.08E-01	7.84E-02	8.90E-01	9.68E-01	0.00E+00
tetrachloroethene	165.83	34.000	6.63E+01	6.98E+01	5.46E+00	8.22E+00	1.53E+01	7.82E+00
chlorodifluoromethane	86.47	350.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.34E+01	1.21E+00
dichlorofluoromethane	102.90	21.000	0.00E+00	0.00E+00	4.56E-02	0.00E+00	0.00E+00	8.60E-02
1-chloro-1,2,2-trifluoroethane	118.50	480.000	3.03E-01	3.03E-01	3.03E-01	3.30E-01	3.03E-01	3.02E-01
dichlorodifluoromethane	120.91	490.000	1.83E+00	0.00E+00	7.38E-02	0.00E+00	3.01E-01	9.01E-01
1,2-dichloro-1,2-difluoroethene	132.93	140.000	9.10E-02	9.10E-02	9.10E-02	1.10E-01	1.91E-01	0.00E+00
chlorotetrafluoroethane	136.48	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichlorofluoromethane	137.40	560.000	2.16E+01	5.95E+00	9.40E+01	1.51E+02	9.10E+00	5.90E+01
bromotrifluoromethane	148.90	11000.000	0.00E+00	6.00E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	1.20E-03	0.00E+00	0.00E+00	0.00E+00	6.46E+00	0.00E+00
1,1,2-trichloro-1,2,2-trifluoroethane	187.40	400.000	8.09E+01	2.91E+03	1.32E+01	2.54E+02	1.29E+03	8.65E+01
1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	0.00E+00	0.00E+00	0.00E+00	3.56E+00	3.02E+00	9.26E-01
methane	16.04	3800.000	4.30E+01	2.76E+01	4.15E+01	3.32E+01	3.90E+01	2.80E+01
ethyne	26.04	530.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethene	28.05	340.000	4.96E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J
	WEIGHT		RAW RATE	RAW RATE	RAW RATE	RAW RATE	RAW RATE	RAW RATE
	g/mole	mg/m ³	mg/day	mg/day	mg/day	mg/day	mg/day	mg/day
ethane	30.07	1200.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.72E-01	2.40E-02
propadiene	40.07	82.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propyne	40.07	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propene	42.08	860.000	3.74E-02	5.50E-02	1.00E-04	0.00E+00	2.70E-02	5.18E-01
propane	44.09	900.000	0.00E+00	6.21E-02	0.00E+00	0.00E+00	2.80E-02	1.27E-01
1,3-butadiene	54.09	0.130	0.00E+00	6.13E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-butene	56.10	460.000	4.81E+00	4.95E+00	4.56E+00	4.56E+00	1.87E-01	1.61E+00
2-methylpropane	58.12	240.000	0.00E+00	0.00E+00	5.40E-03	0.00E+00	2.68E+00	6.20E-02
butane	58.12	240.000	0.00E+00	1.62E-01	3.10E-03	0.00E+00	4.59E-01	5.38E-01
cyclopentene	68.11	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-1,3-butadiene	68.12	560.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-pentene	70.13	190.000	0.00E+00	0.00E+00	2.30E-03	0.00E+00	0.00E+00	2.00E-03
2-methylbutane	72.15	300.000	0.00E+00	3.92E-01	0.00E+00	0.00E+00	3.80E-02	0.00E+00
pentane	72.15	590.000	5.59E+00	1.48E+01	4.00E-02	1.10E-01	2.21E+00	6.75E-01
3,4,5,6-tetrahydrobenzene	82.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexene	84.16	0.100	0.00E+00	9.55E-02	0.00E+00	0.00E+00	2.00E-03	3.00E-03
cyclohexane	84.16	210.000	7.34E+00	7.88E+01	3.17E-01	0.00E+00	4.94E+00	2.85E+00
methylcyclopentane	84.16	52.000	1.44E-02	6.37E+00	1.21E-01	2.20E-01	4.12E-01	1.45E-01
2,2-dimethylbutane	86.17	88.000	0.00E+00	3.85E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methylpentane	86.18	1800.000	3.46E-01	3.13E-01	0.00E+00	0.00E+00	2.49E-01	5.97E-01
hexane	86.18	180.000	6.48E-01	1.03E+01	2.66E-01	3.30E-01	4.06E+00	2.55E+00
4-methylcyclohexane	96.17	390.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-heptene	98.18	200.000	0.00E+00	0.00E+00	2.30E-03	0.00E+00	0.00E+00	0.00E+00
methylcyclohexane	98.18	60.000	2.31E+00	6.37E+00	3.11E-02	4.22E+00	2.19E+00	1.05E-01
2,2-dimethylpentane	100.21	0.100	0.00E+00	5.36E+00	0.00E+00	0.00E+00	7.36E-01	2.45E-01
2,4-dimethylpentane	100.21	0.100	0.00E+00	4.94E-02	3.30E-03	0.00E+00	1.30E-02	0.00E+00
3-ethylpentane	100.21	0.100	0.00E+00	1.27E-02	0.00E+00	0.00E+00	6.00E-02	0.00E+00
heptane	100.21	200.000	1.29E-01	4.23E+00	3.12E-02	1.11E+00	5.18E+00	2.80E+00
1,1-dimethylcyclohexane	112.22	120.000	5.69E+00	2.67E-02	6.00E-04	0.00E+00	0.00E+00	0.00E+00
2-octene	112.22	230.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E-03	3.00E-03
6-methyl-1-heptene	112.22	0.100	1.70E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trans-1,2-dimethylcyclohexane	112.22	120.000	0.00E+00	1.18E+01	4.83E-02	0.00E+00	3.52E-01	1.66E-01
2,2,3-trimethylpentane	114.23	0.100	7.45E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3,3-dimethylhexane	114.23	0.100	1.69E-01	1.69E-01	1.69E-01	2.20E-01	1.69E-01	1.68E-01
3-ethylhexane	114.23	0.100	4.87E-02	0.00E+00	9.50E-02	0.00E+00	0.00E+00	0.00E+00
octane	114.23	350.000	2.95E-01	3.06E-01	2.95E-01	2.90E-01	1.75E+00	1.31E+00
4-ethylheptane	128.26	0.100	6.70E-03	6.70E-03	1.30E-03	0.00E+00	0.00E+00	0.00E+00
nonane	128.26	320.000	2.17E-01	2.17E-01	2.47E-01	0.00E+00	6.67E-01	6.25E-01
4-isopropenyl-1-methylcyclohexene	136.23	0.100	7.84E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-3-ethylheptane	142.28	0.100	2.41E-01	2.41E-01	2.41E-01	0.00E+00	2.58E-01	2.57E-01
decane	142.28	230.000	0.00E+00	1.13E-02	1.02E-01	0.00E+00	2.99E+00	2.90E+00
undecane	156.31	320.000	0.00E+00	4.12E-01	3.93E-02	1.10E-01	5.50E+00	5.80E-01
dodecane	170.34	280.000	0.00E+00	0.00E+00	4.98E-02	0.00E+00	0.00E+00	9.30E-02
2-propanone	58.08	50.000	1.15E+02	5.33E+02	1.68E+02	8.93E+01	1.02E+02	6.59E+01
3-buten-2-one	70.00	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.20E-02	8.00E-03
2-butanone	72.11	30.000	3.69E+01	4.76E+02	1.11E+01	7.25E+02	6.23E+01	3.96E+01
cyclopentanone	84.11	0.100	2.10E-03	1.07E+02	0.00E+00	1.44E+00	6.10E-02	1.80E-02
3-penten-2-one	84.12	0.100	6.30E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
acetyl cyclopropane	84.13	0.100	1.04E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-pentanone	86.13	70.000	3.20E-02	5.64E-01	0.00E+00	0.00E+00	2.19E-01	2.00E-01
3-methyl-2-butanone	86.13	70.000	0.00E+00	5.50E-01	7.90E-02	6.55E+00	2.22E-01	2.20E-01
4-methyl-3-penten-2-one	98.14	40.000	3.71E+00	5.97E+00	3.71E+00	3.78E+00	2.83E+01	1.16E+01
cyclohexanone	98.14	60.000	7.98E+00	3.72E+01	8.91E+00	2.08E+01	6.42E+01	4.57E+01
3,3-dimethyl-2-butanone	100.16	0.100	0.00E+00	8.05E-01	5.75E-01	0.00E+00	2.07E-01	1.04E-01
4-methyl-2-pentanone	100.16	140.000	4.48E+01	1.69E+02	9.81E+00	2.68E+01	9.80E+01	4.79E+01
2,4-dimethyl-3-pentanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.20E-02	4.00E-03
2-heptanone	114.18	0.100	4.80E-02	2.75E-02	2.20E-03	1.10E-01	1.82E+01	5.20E-02
5-methyl-2-hexanone	114.18	0.100	7.67E-02	7.35E-02	0.00E+00	0.00E+00	3.95E-01	4.90E-02

APPENDIX B

Raw *Spacelab* Trace Contaminant Generation Rate Data Statistics

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	MAXIMUM	MINIMUM	MEAN	RAW RATE	STANDARD
	WEIGHT		RAW RATE	RAW RATE	RAW RATE	VARIANCE	DEVIATION
	g/mole	mg/m ³	mg/day	mg/day	mg/day	mg ² /day ²	mg/day
methanol	32.04	9.000	1.40E+02	1.83E+01	6.53E+01	1.75E+03	4.18E+01
ethanol	46.07	2000.000	1.36E+03	4.58E+00	3.28E+02	2.31E+05	4.81E+02
2-propen-1-ol	58.08	1.000	4.38E-01	0.00E+00	9.85E-02	2.43E-02	1.56E-01
2-propanol	60.09	150.000	4.17E+02	4.97E+01	1.85E+02	1.69E+04	1.30E+02
1-propanol	60.09	98.000	4.41E+01	2.71E-01	1.05E+01	2.34E+02	1.53E+01
1,2-ethanediol	62.07	13.000	1.33E+00	0.00E+00	2.35E-01	2.41E-01	4.91E-01
2-butanol	74.12	120.000	8.63E-01	4.42E-02	4.04E-01	1.01E-01	3.18E-01
2-methyl-1-propanol	74.12	120.000	9.08E+01	1.33E+00	3.33E+01	1.40E+03	3.75E+01
2-methyl-2-propanol	74.12	120.000	9.21E+00	9.67E-01	3.42E+00	8.95E+00	2.99E+00
1-butanol	74.12	80.000	8.75E+02	1.84E+01	2.13E+02	8.86E+04	2.98E+02
1,2-propanediol	76.10	0.100	5.87E-02	0.00E+00	9.78E-03	4.79E-04	2.19E-02
3-methyl-1-butanol	88.15	0.100	3.11E+00	0.00E+00	8.46E-01	1.43E+00	1.20E+00
1-pentanol	88.15	130.000	1.74E+01	0.00E+00	5.68E+00	5.32E+01	7.29E+00
phenol	94.11	7.700	1.08E+02	0.00E+00	1.87E+01	1.59E+03	3.99E+01
cyclohexanol	100.16	120.000	1.63E+02	0.00E+00	2.99E+01	3.58E+03	5.98E+01
2-ethyl-1-butanol	102.17	0.100	2.95E-02	0.00E+00	4.92E-03	1.21E-04	1.10E-02
2-hexanol	102.18	170.000	2.16E-01	0.00E+00	1.05E-01	6.44E-03	8.02E-02
1,3-dichloro-2-propanol	128.99	0.100	3.30E-03	0.00E+00	7.17E-04	1.47E-06	1.21E-03
2-ethylhexanol	130.23	0.100	1.20E+00	0.00E+00	3.60E-01	1.91E-01	4.37E-01
nonanol	144.26	0.100	8.24E-01	0.00E+00	1.37E-01	9.43E-02	3.07E-01
decanol	159.29	0.100	2.00E-03	0.00E+00	8.33E-04	8.06E-07	8.98E-04
methanal	30.03	0.050	8.00E-03	0.00E+00	1.72E-03	8.60E-06	2.93E-03
ethanal	44.05	4.000	9.67E+00	9.06E-01	4.76E+00	1.09E+01	3.30E+00
2-propenal	56.06	0.030	8.19E-01	0.00E+00	1.47E-01	9.04E-02	3.01E-01
propanal	58.08	95.000	5.44E+01	1.90E-03	1.45E+01	3.32E+02	1.82E+01
2-methylpropenal	70.09	0.100	4.46E-01	0.00E+00	7.84E-02	2.71E-02	1.65E-01
butanal	72.10	120.000	1.86E+02	1.62E-01	3.47E+01	4.58E+03	6.77E+01
pentanal	86.13	110.000	1.43E+01	0.00E+00	3.42E+00	2.58E+01	5.08E+00
2,4-hexadien-1-al	96.13	0.100	1.72E-01	0.00E+00	2.86E-02	4.09E-03	6.40E-02
hexanal	100.16	0.100	5.19E+00	1.71E-02	1.98E+00	4.67E+00	2.16E+00
benzaldehyde	106.12	173.000	2.41E+00	0.00E+00	6.87E-01	8.41E-01	9.17E-01
heptanal	114.19	0.100	3.36E+00	1.41E-02	7.68E-01	1.36E+00	1.17E+00
4-methylbenzaldehyde	120.15	0.100	5.29E-02	0.00E+00	8.82E-03	3.89E-04	1.97E-02
octanal	128.22	0.100	3.62E-01	0.00E+00	1.51E-01	2.33E-02	1.53E-01
benzene	78.11	0.200	3.43E+00	2.20E-01	1.20E+00	1.14E+00	1.07E+00
methylbenzene	92.15	60.000	1.71E+02	6.73E+01	1.07E+02	1.67E+03	4.09E+01
ethenylbenzene	104.14	43.000	5.19E+00	5.60E-03	1.34E+00	3.16E+00	1.78E+00
1,2-dimethylbenzene	106.16	220.000	9.00E+01	1.56E+00	2.64E+01	8.80E+02	2.97E+01
1,3-dimethylbenzene	106.16	220.000	4.48E+02	2.33E+00	8.08E+01	2.70E+04	1.64E+02
1,4-dimethylbenzene	106.16	220.000	1.01E+02	8.50E-03	4.58E+01	1.18E+03	3.44E+01
ethylbenzene	106.16	130.000	2.26E+01	1.33E+00	6.89E+00	5.34E+01	7.31E+00
indene	116.16	9.500	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
alpha-methylstyrene	118.18	140.000	2.00E-02	0.00E+00	5.98E-03	6.85E-05	8.28E-03
1,2,4-trimethylbenzene	120.20	15.000	6.92E+00	0.00E+00	1.91E+00	6.02E+00	2.45E+00
1,3,5-trimethylbenzene	120.20	15.000	2.95E-01	0.00E+00	1.68E-01	8.18E-03	9.04E-02
1-ethyl-2-methylbenzene	120.20	25.000	6.29E-01	0.00E+00	1.65E-01	5.87E-02	2.42E-01
isopropylbenzene	120.20	74.000	1.35E+00	2.20E-01	6.91E-01	1.35E-01	3.68E-01
propylbenzene	120.20	49.000	3.32E+01	1.20E-02	8.64E+00	1.47E+02	1.21E+01
1-methyl-3-propylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
n-butylbenzene	134.12	0.100	2.81E-01	0.00E+00	6.09E-02	1.02E-02	1.01E-01
1-isopropyl-4-methylbenzene	134.22	0.100	5.94E-02	0.00E+00	9.90E-03	4.90E-04	2.21E-02
methanoic acid methyl ester	60.05	0.100	6.29E-01	0.00E+00	1.77E-01	5.34E-02	2.31E-01
methanoic acid ethyl ester	74.08	91.000	8.21E-01	0.00E+00	2.03E-01	8.20E-02	2.86E-01
ethanoic acid methyl ester	74.08	120.000	2.53E+01	1.41E+00	5.71E+00	7.68E+01	8.76E+00
ethanoic acid ethyl ester	88.11	180.000	4.68E+01	1.42E+00	1.34E+01	2.40E+02	1.55E+01
ethanoic acid allyl ester	100.12	0.100	6.05E-01	0.00E+00	1.54E-01	4.65E-02	2.16E-01
2-methyl propenoic acid methyl ester	100.12	100.000	1.39E+01	2.47E-01	5.13E+00	2.58E+01	5.08E+00
ethanoic acid isopropyl ester	102.13	210.000	7.91E-01	0.00E+00	2.27E-01	8.15E-02	2.85E-01
methanoic acid butyl ester	102.13	0.100	2.02E-01	0.00E+00	4.43E-02	5.41E-03	7.35E-02

PRECEDING PAGE BLANK NOT FILMED

PART 20

INDIVIDUALLY BLANK

IUPAC/ACCEPTED NAME	MOLECULAR WEIGHT g/mole	SMAC mg/m ³	MAXIMUM RAW RATE mg/day	MINIMUM RAW RATE mg/day	MEAN RAW RATE mg/day	RAW RATE VARIANCE mg ² /day ²	STANDARD DEVIATION mg/day
ethanoic acid propyl ester	102.13	170.000	7.42E+01	2.90E-03	1.34E+01	7.41E+02	2.72E+01
2-methyl propenoic acid ethyl ester	114.15	0.100	4.48E+00	0.00E+00	7.47E-01	2.79E+00	1.67E+00
ethanoic acid butyl ester	116.16	190.000	1.20E+02	6.00E+00	3.44E+01	1.57E+03	3.97E+01
ethanoic acid isobutyl ester	116.16	190.000	3.12E+01	0.00E+00	6.16E+00	1.28E+02	1.13E+01
lactic acid ethyl ester	118.13	190.000	7.61E-01	0.00E+00	1.27E-01	8.05E-02	2.84E-01
ethanoic acid 2-methoxy ethyl ester	118.36	0.100	6.13E-01	0.00E+00	1.02E-01	5.22E-02	2.28E-01
ethanoic acid isoamyl ester	130.18	0.100	5.80E+00	0.00E+00	1.04E+00	4.55E+00	2.13E+00
ethanoic acid amyl ester	130.18	160.000	9.82E+00	0.00E+00	1.95E+00	1.26E+01	3.55E+00
ethanoic acid 2-ethoxyethyl ester	132.16	160.000	6.90E+01	1.16E+01	3.27E+01	4.98E+02	2.23E+01
hydroxyethanoic acid ethyl ester	146.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
oxalic acid dibutyl ester	202.25	0.100	4.40E-03	0.00E+00	7.33E-04	2.69E-06	1.64E-03
1,4-epoxy-1,3-butadiene	68.07	0.111	2.93E-01	0.00E+00	7.12E-02	1.22E-02	1.11E-01
1,4-epoxybutane	72.11	120.000	1.21E+01	4.73E-01	3.06E+00	1.72E+01	4.15E+00
3-methoxy-1-propene	72.11	0.100	7.50E-03	0.00E+00	1.25E-03	7.81E-06	2.80E-03
diethyl ether	74.12	240.000	1.03E+01	0.00E+00	2.99E+00	1.63E+01	4.03E+00
2-methylfuran	82.10	0.130	5.06E-01	0.00E+00	1.43E-01	3.23E-02	1.80E-01
2,3-dihydropyran	84.13	0.100	4.78E-02	0.00E+00	7.97E-03	3.17E-04	1.78E-02
1,4-dioxane	88.11	0.100	1.13E+01	1.89E-02	4.32E+00	1.94E+01	4.41E+00
1,3,5-trioxane	90.08	0.100	3.99E-01	0.00E+00	1.22E-01	2.17E-02	1.47E-01
2-ethoxyethanol	90.12	0.300	1.31E+02	4.00E-02	2.43E+01	2.27E+03	4.76E+01
epichlorohydrin	92.53	0.100	5.83E-01	0.00E+00	9.72E-02	4.73E-02	2.17E-01
1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	1.96E-01	0.00E+00	3.26E-02	5.32E-03	7.30E-02
4-ethylmorpholine	115.18	0.100	2.68E+01	0.00E+00	4.47E+00	9.99E+01	1.00E+01
1-propoxybutane	116.21	0.100	6.83E+00	0.00E+00	1.47E+00	6.27E+00	2.50E+00
2-butoxyethanol	118.18	0.100	3.60E-02	0.00E+00	1.15E-02	2.54E-04	1.59E-02
chloromethane	50.49	41.000	6.70E-01	2.70E-03	2.63E-01	6.59E-02	2.57E-01
chloroethene	62.50	3.000	1.67E-01	0.00E+00	4.85E-02	4.77E-03	6.90E-02
chloroethane	64.52	260.000	2.00E-02	0.00E+00	3.50E-03	5.46E-05	7.39E-03
3-chloropropene	76.53	0.100	1.60E-02	0.00E+00	2.67E-03	3.56E-05	5.96E-03
dichloromethane	84.93	10.000	2.21E+02	4.50E+00	8.56E+01	7.20E+03	8.48E+01
1-chlorobutane	92.57	150.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1-dichloroethene	96.95	7.900	1.35E-01	0.00E+00	2.38E-02	2.48E-03	4.98E-02
1,2-dichloroethane	98.97	1.000	1.12E+01	8.23E-02	3.53E+00	1.36E+01	3.69E+00
1,2-dichloropropene	110.97	0.100	6.01E+00	0.00E+00	1.00E+00	5.02E+00	2.24E+00
chlorobenzene	112.56	46.000	1.65E+02	7.33E-01	6.00E+01	3.84E+03	6.19E+01
1,2-dichloropropane	112.99	42.000	1.22E+00	0.00E+00	2.81E-01	2.05E-01	4.53E-01
trichloromethane	119.38	4.900	1.88E+00	0.00E+00	6.58E-01	4.77E-01	6.91E-01
1,2-dichloro-2-methylpropane	127.01	0.100	2.05E-01	0.00E+00	5.16E-02	6.16E-03	7.85E-02
trichloroethene	131.39	10.000	6.73E+00	7.80E-01	3.53E+00	7.01E+00	2.65E+00
1,1,1-trichloroethane	133.41	160.000	7.82E+01	3.43E+00	3.10E+01	6.13E+02	2.48E+01
1,1,2-trichloroethane	133.41	0.100	1.06E-02	0.00E+00	2.77E-03	1.71E-05	4.13E-03
1,2-dichlorobenzene	147.01	30.000	1.38E+00	0.00E+00	2.31E-01	2.66E-01	5.16E-01
3-chloromethylheptane	148.68	0.100	3.66E-02	0.00E+00	6.10E-03	1.86E-04	1.36E-02
tetrachloromethane	153.82	13.000	9.68E-01	0.00E+00	3.92E-01	1.50E-01	3.87E-01
tetrachloroethene	165.83	34.000	6.98E+01	5.46E+00	2.88E+01	7.80E+02	2.79E+01
chlorodifluoromethane	86.47	350.000	1.34E+01	0.00E+00	2.43E+00	2.42E+01	4.92E+00
dichlorofluoromethane	102.90	21.000	8.60E-02	0.00E+00	2.19E-02	1.10E-03	3.31E-02
1-chloro-1,2,2-trifluoroethane	118.50	480.000	3.30E-01	3.02E-01	3.07E-01	1.02E-04	1.01E-02
dichlorodifluoromethane	120.91	490.000	1.83E+00	0.00E+00	5.17E-01	4.39E-01	6.63E-01
1,2-dichloro-1,2-difluoroethene	132.93	140.000	1.91E-01	0.00E+00	9.57E-02	3.09E-03	5.55E-02
chlorotetrafluoroethane	136.48	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichlorofluoromethane	137.40	560.000	1.51E+02	5.95E+00	5.68E+01	2.73E+03	5.23E+01
bromotrifluoromethane	148.90	11000.000	6.00E+01	0.00E+00	1.00E+01	5.00E+02	2.24E+01
1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	6.46E+00	0.00E+00	1.08E+00	5.80E+00	2.41E+00
1,1,2-trichloro-1,2,2-trifluoroethane	187.40	400.000	2.91E+03	1.32E+01	7.73E+02	1.11E+06	1.05E+03
1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	3.56E+00	0.00E+00	1.25E+00	2.21E+00	1.49E+00
methane	16.04	3800.000	4.30E+01	2.76E+01	3.54E+01	3.81E+01	6.17E+00
ethyne	26.04	530.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethene	28.05	340.000	4.96E-02	0.00E+00	8.27E-03	3.42E-04	1.85E-02

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	MAXIMUM	MINIMUM	MEAN	RAW RATE	STANDARD
	WEIGHT		RAW RATE	RAW RATE	RAW RATE	VARIANCE	DEVIATION
	g/mole	mg/m ³	mg/day	mg/day	mg/day	mg ² /day ²	mg/day
ethane	30.07	1200.000	2.72E-01	0.00E+00	4.93E-02	9.99E-03	1.00E-01
propadiene	40.07	82.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propyne	40.07	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propene	42.08	860.000	5.18E-01	0.00E+00	1.06E-01	3.43E-02	1.85E-01
propane	44.09	900.000	1.27E-01	0.00E+00	3.62E-02	2.15E-03	4.64E-02
1,3-butadiene	54.09	0.130	6.13E-01	0.00E+00	1.02E-01	5.21E-02	2.28E-01
1-butene	56.10	460.000	4.95E+00	1.87E-01	3.45E+00	3.43E+00	1.85E+00
2-methylpropane	58.12	240.000	2.68E+00	0.00E+00	4.58E-01	9.89E-01	9.94E-01
butane	58.12	240.000	5.38E-01	0.00E+00	1.94E-01	5.02E-02	2.24E-01
cyclopentene	68.11	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-1,3-butadiene	68.12	560.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-pentene	70.13	190.000	2.30E-03	0.00E+00	7.17E-04	1.03E-06	1.02E-03
2-methylbutane	72.15	300.000	3.92E-01	0.00E+00	7.16E-02	2.07E-02	1.44E-01
pentane	72.15	590.000	1.48E+01	4.00E-02	3.91E+00	2.74E+01	5.24E+00
3,4,5,6-tetrahydrobenzene	82.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexene	84.16	0.100	9.55E-02	0.00E+00	1.68E-02	1.24E-03	3.52E-02
cyclohexane	84.16	210.000	7.88E+01	0.00E+00	1.57E+01	8.03E+02	2.83E+01
methylcyclopentane	84.16	52.000	6.37E+00	1.44E-02	1.21E+00	5.33E+00	2.31E+00
2,2-dimethylbutane	86.17	88.000	3.85E-01	0.00E+00	6.41E-02	2.06E-02	1.43E-01
3-methylpentane	86.18	1800.000	5.97E-01	0.00E+00	2.51E-01	4.31E-02	2.08E-01
hexane	86.18	180.000	1.03E+01	2.66E-01	3.03E+00	1.26E+01	3.55E+00
4-methylcyclohexene	96.17	390.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-heptene	98.18	200.000	2.30E-03	0.00E+00	3.83E-04	7.35E-07	8.57E-04
methylcyclohexane	98.18	60.000	6.37E+00	3.11E-02	2.54E+00	4.98E+00	2.23E+00
2,2-dimethylpentane	100.21	0.100	5.36E+00	0.00E+00	1.06E+00	3.77E+00	1.94E+00
2,4-dimethylpentane	100.21	0.100	4.94E-02	0.00E+00	1.10E-02	3.17E-04	1.78E-02
3-ethylpentane	100.21	0.100	6.00E-02	0.00E+00	1.21E-02	4.80E-04	2.19E-02
heptane	100.21	200.000	5.18E+00	3.12E-02	2.25E+00	3.91E+00	1.98E+00
1,1-dimethylcyclohexane	112.22	120.000	5.69E+00	0.00E+00	9.53E-01	4.49E+00	2.12E+00
2-octene	112.22	230.000	3.00E-03	0.00E+00	8.33E-04	1.47E-06	1.21E-03
6-methyl-1-heptene	112.22	0.100	1.70E-03	0.00E+00	2.83E-04	4.01E-07	6.34E-04
trans-1,2-dimethylcyclohexane	112.22	120.000	1.18E+01	0.00E+00	2.06E+00	1.89E+01	4.34E+00
2,2,3-trimethylpentane	114.23	0.100	7.45E-02	0.00E+00	1.24E-02	7.71E-04	2.78E-02
3,3-dimethylhexane	114.23	0.100	2.20E-01	1.68E-01	1.77E-01	3.64E-04	1.91E-02
3-ethylhexane	114.23	0.100	9.50E-02	0.00E+00	2.40E-02	1.33E-03	3.64E-02
octane	114.23	350.000	1.75E+00	2.90E-01	7.08E-01	3.54E-01	5.95E-01
4-ethylheptane	128.26	0.100	6.70E-03	0.00E+00	2.45E-03	9.24E-06	3.04E-03
nonane	128.26	320.000	6.67E-01	0.00E+00	3.29E-01	5.70E-02	2.39E-01
4-isopropenyl-1-methylcyclohexene	136.23	0.100	7.84E-01	0.00E+00	1.31E-01	8.54E-02	2.92E-01
2-methyl-3-ethylheptane	142.28	0.100	2.58E-01	0.00E+00	2.06E-01	8.58E-03	9.26E-02
decane	142.28	230.000	2.99E+00	0.00E+00	1.00E+00	1.89E+00	1.38E+00
undecane	156.31	320.000	5.50E+00	0.00E+00	1.11E+00	3.90E+00	1.98E+00
dodecane	170.34	280.000	9.30E-02	0.00E+00	2.38E-02	1.29E-03	3.59E-02
2-propanone	58.08	50.000	5.33E+02	6.59E+01	1.79E+02	2.60E+04	1.61E+02
3-buten-2-one	70.00	0.100	3.20E-02	0.00E+00	6.67E-03	1.37E-04	1.17E-02
2-butanone	72.11	30.000	7.25E+02	1.11E+01	2.25E+02	7.59E+04	2.75E+02
cyclopentanone	84.11	0.100	1.07E+02	0.00E+00	1.82E+01	1.60E+03	3.99E+01
3-penten-2-one	84.12	0.100	6.30E-03	0.00E+00	1.05E-03	5.51E-06	2.35E-03
acetyl cyclopropane	84.13	0.100	1.04E-02	0.00E+00	1.73E-03	1.50E-05	3.88E-03
2-pentanone	86.13	70.000	5.64E-01	0.00E+00	1.69E-01	3.93E-02	1.98E-01
3-methyl-2-butanone	86.13	70.000	6.55E+00	0.00E+00	1.27E+00	5.60E+00	2.37E+00
4-methyl-3-penten-2-one	98.14	40.000	2.83E+01	3.71E+00	9.51E+00	7.85E+01	8.86E+00
cyclohexanone	98.14	60.000	6.42E+01	7.98E+00	3.08E+01	4.13E+02	2.03E+01
3,3-dimethyl-2-butanone	100.16	0.100	8.05E-01	0.00E+00	2.82E-01	9.26E-02	3.04E-01
4-methyl-2-pentanone	100.16	140.000	1.69E+02	9.81E+00	6.61E+01	2.86E+03	5.35E+01
2,4-dimethyl-3-pentanone	114.18	0.100	1.20E-02	0.00E+00	2.67E-03	1.96E-05	4.42E-03
2-heptanone	114.18	0.100	1.82E+01	2.20E-03	3.07E+00	4.58E+01	6.77E+00
5-methyl-2-hexanone	114.18	0.100	3.95E-01	0.00E+00	9.90E-02	1.85E-02	1.36E-01

IUPAC/ACCEPTED NAME	MOLECULAR WEIGHT g/mole	SMAC mg/m ³	MAXIMUM RAW RATE mg/day	MINIMUM RAW RATE mg/day	MEAN RAW RATE mg/day	RAW RATE VARIANCE mg ² /day ²	STANDARD DEVIATION mg/day
acetophenone	120.14	250.000	9.64E-02	0.00E+00	2.06E-02	1.25E-03	3.53E-02
2-octanone	128.21	100.000	3.79E-02	0.00E+00	6.32E-03	2.00E-04	1.41E-02
5-methyl-3-heptanone	128.21	0.100	3.85E-01	0.00E+00	1.14E-01	2.00E-02	1.42E-01
2,6-dimethyl-4-heptanone	142.20	58.000	7.64E-01	0.00E+00	1.27E-01	8.11E-02	2.85E-01
hydrogen sulfide	34.08	2.800	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
carbonyl sulfide	60.07	12.000	6.88E-01	0.00E+00	2.44E-01	5.98E-02	2.45E-01
ethylene sulfide	60.11	0.100	6.60E-03	0.00E+00	1.10E-03	6.05E-06	2.46E-03
dimethyl sulfide	62.14	2.500	4.32E-02	0.00E+00	7.20E-03	2.59E-04	1.61E-02
carbon disulfide	76.14	16.000	5.57E+00	8.80E-03	1.43E+00	3.62E+00	1.90E+00
pentamethylene sulfide	102.20	0.100	1.27E-02	0.00E+00	4.23E-03	3.58E-05	5.99E-03
nitric oxide	30.01	6.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nitrogen dioxide	46.01	0.940	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nitrogen tetroxide	92.01	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid	60.05	7.400	1.90E-01	0.00E+00	5.03E-02	5.51E-03	7.42E-02
2-ethylhexanoic acid	144.21	0.100	8.40E-02	0.00E+00	1.40E-02	9.80E-04	3.13E-02
hydrazine	32.05	0.005	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methyl cyanide	41.05	6.700	3.00E-03	0.00E+00	6.67E-04	1.22E-06	1.11E-03
methyl hydrazine	46.07	0.004	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nitromethane	61.04	13.000	1.03E+01	0.00E+00	1.72E+00	1.48E+01	3.85E+00
N,N-dimethylformamide	73.10	0.100	3.49E-01	0.00E+00	8.21E-02	1.50E-02	1.22E-01
nitroethane	75.07	0.100	3.40E-03	0.00E+00	1.13E-03	2.57E-06	1.60E-03
2,3-benzopyrrole	117.15	0.250	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hydrogen	2.02	340.000	9.42E-01	0.00E+00	2.26E-01	1.25E-01	3.53E-01
ammonia	17.00	7.000	1.04E+01	0.00E+00	3.29E+00	1.47E+01	3.83E+00
carbon monoxide	28.01	10.000	2.10E+02	3.94E+01	1.00E+02	3.59E+03	5.99E+01
disiloxane	78.10	0.100	3.93E+00	0.00E+00	6.66E-01	2.13E+00	1.46E+00
trimethylsilanol	90.21	40.000	2.36E+01	1.20E-02	6.66E+00	7.30E+01	8.54E+00
trisiloxane	124.30	0.100	3.01E+00	0.00E+00	8.43E-01	1.22E+00	1.11E+00
hexamethyldisiloxane	162.48	0.100	1.53E+00	0.00E+00	3.53E-01	2.95E-01	5.43E-01
tetrasiloxane	170.40	0.100	2.99E+01	0.00E+00	5.09E+00	1.23E+02	1.11E+01
diphenylsilane	184.32	0.100	3.00E-03	0.00E+00	5.00E-04	1.25E-06	1.12E-03
hexamethylcyclotrisiloxane	222.40	230.000	1.58E+01	2.30E+00	8.00E+00	1.93E+01	4.39E+00
octamethyltrisiloxane	236.54	40.000	4.76E+01	0.00E+00	8.24E+00	3.10E+02	1.76E+01
octamethylcyclotetrasiloxane	296.62	0.100	2.69E+01	3.94E+00	1.31E+01	6.38E+01	7.99E+00
decamethylcyclopentasiloxane	370.64	0.100	5.98E+00	0.00E+00	1.88E+00	5.34E+00	2.31E+00
decamethylcyclohexasiloxane	444.71	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
tetradecamethylcycloheptasiloxane	519.09	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hexadecamethylcyclooctasiloxane	593.24	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

APPENDIX C

Raw *Spacelab* Trace Contaminant Generation Rate Data Outlier Analysis

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J
	WEIGHT		OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST
	g/mole	mg/m ³	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n
methanol	32.04	9.000	0	0	1	1	0	1
ethanol	46.07	2000.000	0	1	0	0	0	0
2-propen-1-ol	58.08	1.000	0	1	0	0	0	0
2-propanol	60.09	150.000	0	0	1	0	0	1
1-propanol	60.09	98.000	0	0	0	0	0	1
1,2-ethanediol	62.07	13.000	0	0	0	1	0	0
2-butanol	74.12	120.000	1	0	0	1	0	1
2-methyl-1-propanol	74.12	120.000	0	1	0	0	1	0
2-methyl-2-propanol	74.12	120.000	0	0	0	0	1	0
1-butanol	74.12	80.000	0	1	0	0	0	0
1,2-propanediol	76.10	0.100	1	0	0	0	0	0
3-methyl-1-butanol	88.15	0.100	0	0	0	0	0	1
1-pentanol	88.15	130.000	1	1	0	0	0	0
phenol	94.11	7.700	0	0	0	1	0	0
cyclohexanol	100.16	120.000	0	1	0	0	0	0
2-ethyl-1-butanol	102.17	0.100	1	0	0	0	0	0
2-hexanol	102.18	170.000	1	0	1	0	1	0
1,3-dichloro-2-propanol	128.99	0.100	0	0	1	0	0	0
2-ethylhexanol	130.23	0.100	0	0	1	0	0	0
nonanol	144.26	0.100	0	1	0	0	0	0
decanol	159.29	0.100	0	0	1	0	1	0
methanal	30.03	0.050	0	0	0	0	0	1
ethanal	44.05	4.000	0	0	1	1	0	1
2-propenal	56.06	0.030	0	0	0	0	1	0
propanal	58.08	95.000	0	0	0	0	0	1
2-methylpropenal	70.09	0.100	0	0	0	0	0	1
butanal	72.10	120.000	0	1	0	0	0	0
pentanal	86.13	110.000	0	0	0	0	1	0
2,4-hexadien-1-al	96.13	0.100	1	0	0	0	0	0
hexanal	100.16	0.100	1	0	0	0	0	1
benzaldehyde	106.12	173.000	0	0	1	0	0	0
heptanal	114.19	0.100	0	0	0	0	0	1
4-methylbenzaldehyde	120.15	0.100	1	0	0	0	0	0
octanal	128.22	0.100	0	1	1	0	0	0
benzene	78.11	0.200	0	1	0	0	0	0
methylbenzene	92.15	60.000	0	1	0	0	1	0
ethenylbenzene	104.14	43.000	0	0	0	0	0	1
1,2-dimethylbenzene	106.16	220.000	0	0	0	0	1	0
1,3-dimethylbenzene	106.16	220.000	0	1	0	0	0	0
1,4-dimethylbenzene	106.16	220.000	1	1	1	0	0	0
ethylbenzene	106.16	130.000	0	1	0	0	0	0
indene	116.16	9.500	0	0	0	0	0	0
alpha-methylstyrene	118.18	140.000	0	0	0	0	1	1
1,2,4-trimethylbenzene	120.20	15.000	0	0	0	0	1	0
1,3,5-trimethylbenzene	120.20	15.000	0	0	1	1	0	0
1-ethyl-2-methylbenzene	120.20	25.000	1	0	0	0	0	0
isopropylbenzene	120.20	74.000	0	1	0	1	0	0
propylbenzene	120.20	49.000	0	1	0	0	0	0
1-methyl-3-propylbenzene	134.12	0.100	0	0	0	0	0	0
n-butylbenzene	134.12	0.100	0	1	0	0	0	0
1-isopropyl-4-methylbenzene	134.22	0.100	0	1	0	0	0	0
methanoic acid methyl ester	60.05	0.100	0	0	0	0	1	0
methanoic acid ethyl ester	74.08	91.000	0	0	0	0	1	0
ethanoic acid methyl ester	74.08	120.000	0	0	1	0	0	0
ethanoic acid ethyl ester	88.11	180.000	0	1	0	0	0	0
ethanoic acid allyl ester	100.12	0.100	0	1	0	0	0	0
2-methyl propenoic acid methyl ester	100.12	100.000	0	0	0	1	0	1
ethanoic acid isopropyl ester	102.13	210.000	0	0	0	0	0	1
methanoic acid butyl ester	102.13	0.100	0	0	0	0	1	0

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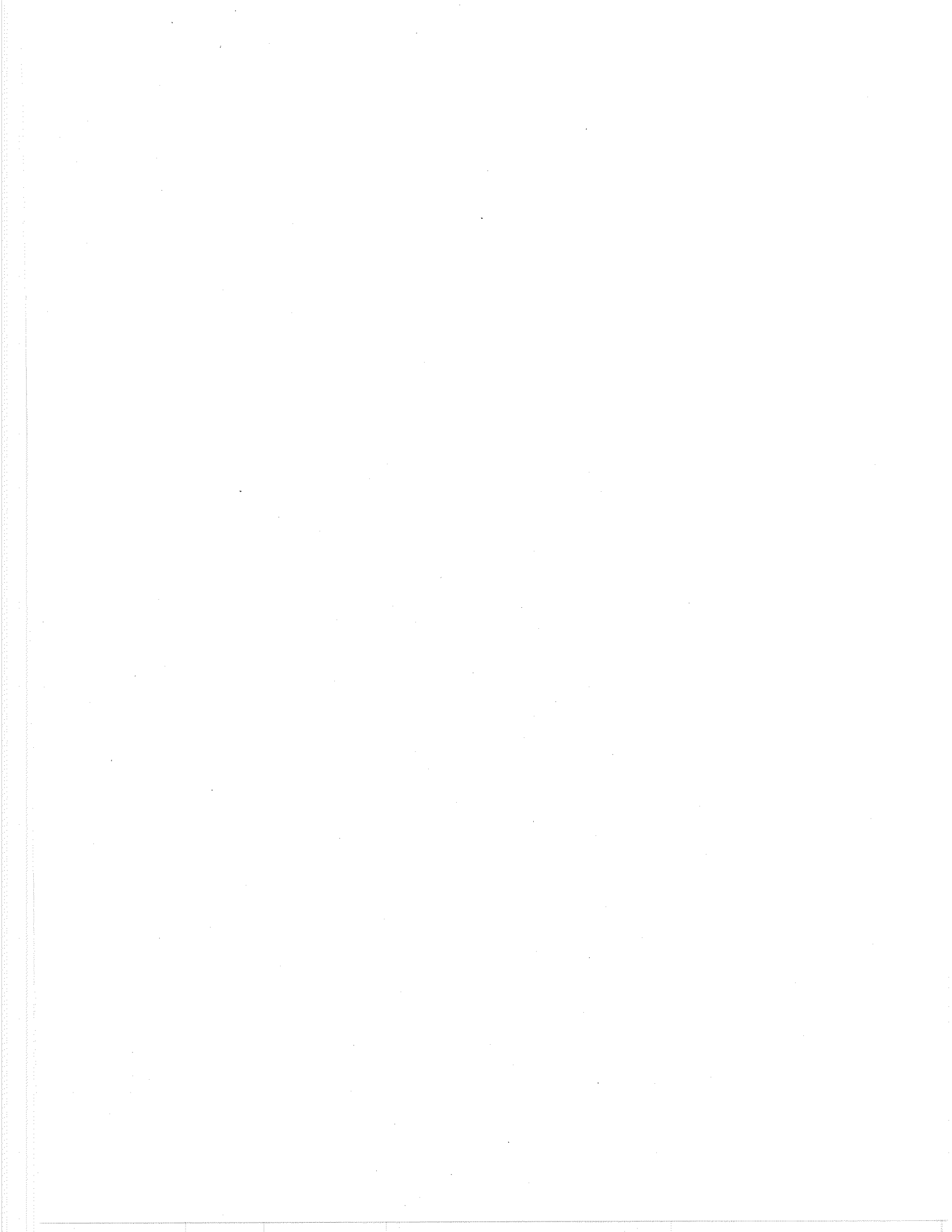
IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J
	WEIGHT		OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST
	g/mole	mg/m ³	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n
ethanoic acid propyl ester	102.13	170.000	0	1	0	0	0	0
2-methyl propenoic acid ethyl ester	114.15	0.100	0	1	0	0	0	0
ethanoic acid butyl ester	116.16	190.000	0	1	0	0	0	0
ethanoic acid isobutyl ester	116.16	190.000	0	1	0	0	0	0
lactic acid ethyl ester	118.13	190.000	0	0	1	0	0	0
ethanoic acid 2-methoxy ethyl ester	118.36	0.100	1	0	0	0	0	0
ethanoic acid isoamyl ester	130.18	0.100	0	0	0	0	0	1
ethanoic acid amyl ester	130.18	160.000	0	1	0	0	0	0
ethanoic acid 2-ethoxyethyl ester	132.16	160.000	1	0	0	0	0	0
hydroxyethanoic acid ethyl ester	146.14	0.100	0	0	0	0	0	0
oxalic acid dibutyl ester	202.25	0.100	1	0	0	0	0	0
1,4-epoxy-1,3-butadiene	68.07	0.111	0	0	0	0	1	0
1,4-epoxybutane	72.11	120.000	0	1	0	0	0	0
3-methoxy-1-propene	72.11	0.100	1	0	0	0	0	0
diethyl ether	74.12	240.000	0	0	1	0	0	0
2-methylfuran	82.10	0.130	0	0	0	0	0	1
2,3-dihdropyran	84.13	0.100	1	0	0	0	0	0
1,4-dioxane	88.11	0.100	0	0	0	0	1	0
1,3,5-trioxane	90.08	0.100	0	0	0	0	0	1
2-ethoxyethanol	90.12	0.300	0	1	0	0	0	0
epichlorohydrin	92.53	0.100	1	0	0	0	0	0
1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	0	1	0	0	0	0
4-ethylmorpholine	115.18	0.100	1	0	0	0	0	0
1-propoxybutane	116.21	0.100	1	0	0	0	0	0
2-butoxyethanol	118.18	0.100	0	0	0	0	1	1
chloromethane	50.49	41.000	0	0	1	1	0	0
chloroethene	62.50	3.000	1	0	0	0	0	1
chloroethane	64.52	260.000	0	0	0	0	0	1
3-chloropropene	76.53	0.100	0	0	1	0	0	0
dichloromethane	84.93	10.000	0	1	0	0	0	1
1-chlorobutane	92.57	150.000	0	0	0	0	0	0
1,1-dichloroethene	96.95	7.900	0	0	0	0	1	0
1,2-dichloroethane	98.97	1.000	0	0	0	0	0	1
1,2-dichloropropene	110.97	0.100	0	1	0	0	0	0
chlorobenzene	112.56	46.000	0	1	0	0	0	0
1,2-dichloropropane	112.99	42.000	0	0	0	1	0	0
trichloromethane	119.38	4.900	0	0	1	0	0	0
1,2-dichloro-2-methylpropane	127.01	0.100	0	0	1	0	0	0
trichloroethene	131.39	10.000	1	0	1	1	1	0
1,1,1-trichloroethane	133.41	160.000	0	0	1	0	0	1
1,1,2-trichloroethane	133.41	0.100	0	0	1	0	0	0
1,2-dichlorobenzene	147.01	30.000	1	0	0	0	0	0
3-chloromethylheptane	148.68	0.100	1	0	0	0	0	0
tetrachloromethane	153.82	13.000	0	0	0	1	1	1
tetrachloroethene	165.83	34.000	1	1	0	0	0	0
chlorodifluoromethane	86.47	350.000	0	0	0	0	1	0
dichlorofluoromethane	102.90	21.000	0	0	0	0	0	1
1-chloro-1,2,2-trifluoroethane	118.50	480.000	0	0	0	1	0	0
dichlorodifluoromethane	120.91	490.000	1	0	0	0	0	0
1,2-dichloro-1,2-difluoroethene	132.93	140.000	0	0	0	0	1	1
chlorotetrafluoroethane	136.48	0.100	0	0	0	0	0	0
trichlorofluoromethane	137.40	560.000	0	0	0	1	0	0
bromotrifluoromethane	148.90	11000.000	0	1	0	0	0	0
1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	0	0	0	0	1	0
1,1,2-trichloro-1,2,2-trifluoroethane	187.40	400.000	0	1	0	0	0	0
1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	0	0	0	1	1	0
methane	16.04	3800.000	1	1	0	0	0	1
ethyne	26.04	530.000	0	0	0	0	0	0
ethene	28.05	340.000	1	0	0	0	0	0

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J
	WEIGHT		OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST
	g/mole	mg/m ³	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n
ethane	30.07	1200.000	0	0	0	0	1	0
propadiene	40.07	82.000	0	0	0	0	0	0
propyne	40.07	0.100	0	0	0	0	0	0
propene	42.08	860.000	0	0	0	0	0	1
propane	44.09	900.000	0	0	0	0	0	1
1,3-butadiene	54.09	0.130	0	1	0	0	0	0
1-butene	56.10	460.000	0	0	0	0	1	0
2-methylpropane	58.12	240.000	0	0	0	0	1	0
butane	58.12	240.000	0	0	0	0	1	1
cyclopentene	68.11	170.000	0	0	0	0	0	0
2-methyl-1,3-butadiene	68.12	560.000	0	0	0	0	0	0
1-pentene	70.13	190.000	0	0	1	0	0	1
2-methylbutane	72.15	300.000	0	1	0	0	0	0
pentane	72.15	590.000	0	1	0	0	0	0
3,4,5,6-tetrahydrobenzene	82.14	0.100	0	0	0	0	0	0
2-hexene	84.16	0.100	0	1	0	0	0	0
cyclohexane	84.16	210.000	0	1	0	0	1	0
methylcyclopentane	84.16	52.000	0	1	0	0	0	0
2,2-dimethylbutane	86.17	88.000	0	1	0	0	0	0
3-methylpentane	86.18	1800.000	0	0	1	1	0	1
hexane	86.18	180.000	0	1	0	0	0	0
4-methylcyclohexane	96.17	390.000	0	0	0	0	0	0
1-heptene	98.18	200.000	0	0	1	0	0	0
methylcyclohexane	98.18	60.000	0	1	1	0	0	1
2,2-dimethylpentane	100.21	0.100	0	1	0	0	0	0
2,4-dimethylpentane	100.21	0.100	0	1	0	0	0	0
3-ethylpentane	100.21	0.100	0	0	0	0	1	0
heptane	100.21	200.000	1	1	1	0	1	0
1,1-dimethylcyclohexane	112.22	120.000	1	0	0	0	0	0
2-octene	112.22	230.000	0	0	0	0	0	1
6-methyl-1-heptene	112.22	0.100	1	0	0	0	0	0
trans-1,2-dimethylcyclohexane	112.22	120.000	0	1	0	0	0	0
2,2,3-trimethylpentane	114.23	0.100	1	0	0	0	0	0
3,3-dimethylhexane	114.23	0.100	0	0	0	1	0	0
3-ethylhexane	114.23	0.100	0	0	1	0	0	0
octane	114.23	350.000	0	0	0	0	1	1
4-ethylheptane	128.26	0.100	1	1	0	0	0	0
nonane	128.26	320.000	0	0	0	1	1	1
4-isopropenyl-1-methylcyclohexane	136.23	0.100	1	0	0	0	0	0
2-methyl-3-ethylheptane	142.28	0.100	0	0	0	1	0	0
decane	142.28	230.000	0	0	0	0	1	1
undecane	156.31	320.000	0	0	0	0	1	0
dodecane	170.34	280.000	0	0	0	0	0	1
2-propanone	58.08	50.000	0	1	0	0	0	0
3-buten-2-one	70.00	0.100	0	0	0	0	1	0
2-butanone	72.11	30.000	0	0	0	1	0	0
cyclopentanone	84.11	0.100	0	1	0	0	0	0
3-penten-2-one	84.12	0.100	1	0	0	0	0	0
acetyl cyclopropane	84.13	0.100	1	0	0	0	0	0
2-pentanone	86.13	70.000	0	1	0	0	0	0
3-methyl-2-butanone	86.13	70.000	0	0	0	1	0	0
4-methyl-3-penten-2-one	98.14	40.000	0	0	0	0	1	0
cyclohexanone	98.14	60.000	1	0	1	0	1	0
3,3-dimethyl-2-butanone	100.16	0.100	0	1	0	0	0	0
4-methyl-2-pentanone	100.16	140.000	0	1	1	0	0	0
2,4-dimethyl-3-pentanone	114.18	0.100	0	0	0	0	1	0
2-heptanone	114.18	0.100	0	0	0	0	1	0
5-methyl-2-hexanone	114.18	0.100	0	0	0	0	1	0

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J
	WEIGHT		OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST	OUTLIER TEST
	g/mole	mg/m ³	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n	1=y/0=n
acetophenone	120.14	250.000	0	0	1	0	0	0
2-octanone	128.21	100.000	0	1	0	0	0	0
5-methyl-3-heptanone	128.21	0.100	0	0	0	0	1	0
2,6-dimethyl-4-heptanone	142.20	58.000	0	0	0	0	0	1
hydrogen sulfide	34.08	2.800	0	0	0	0	0	0
carbonyl sulfide	60.07	12.000	0	1	0	0	0	0
ethylene sulfide	60.11	0.100	1	0	0	0	0	0
dimethyl sulfide	62.14	2.500	0	1	0	0	0	0
carbon disulfide	76.14	16.000	0	1	0	0	0	0
pentamethylene sulfide	102.20	0.100	1	1	0	0	0	0
nitric oxide	30.01	6.100	0	0	0	0	0	0
nitrogen dioxide	46.01	0.940	0	0	0	0	0	0
nitrogen tetroxide	92.01	0.100	0	0	0	0	0	0
ethanoic acid	60.05	7.400	0	0	0	0	0	1
2-ethylhexanoic acid	144.21	0.100	1	0	0	0	0	0
hydrazine	32.05	0.005	0	0	0	0	0	0
methyl cyanide	41.05	6.700	0	0	0	0	0	1
methyl hydrazine	46.07	0.004	0	0	0	0	0	0
nitromethane	61.04	13.000	0	0	0	1	0	0
N,N-dimethylformamide	73.10	0.100	0	0	1	0	0	0
nitroethane	75.07	0.100	1	1	0	0	0	0
2,3-benzopyrrole	117.15	0.250	0	0	0	0	0	0
hydrogen	2.02	340.000	0	0	0	0	0	1
ammonia	17.00	7.000	0	0	0	1	0	0
carbon monoxide	28.01	10.000	0	1	1	0	0	0
disiloxane	78.10	0.100	1	0	0	0	0	0
trimethylsilanol	90.21	40.000	0	0	0	0	0	1
trisiloxane	124.30	0.100	1	0	0	0	0	0
hexamethyldisiloxane	162.48	0.100	0	0	0	0	0	1
tetrasiloxane	170.40	0.100	1	0	0	0	0	0
diphenylsilane	184.32	0.100	1	0	0	0	0	0
hexamethylcyclotrisiloxane	222.40	230.000	0	0	1	0	0	1
octamethyltrisiloxane	236.54	40.000	0	1	0	0	0	0
octamethylcyclotetrasiloxane	296.62	0.100	0	0	1	0	1	0
decamethylcyclopentasiloxane	370.64	0.100	0	0	0	0	0	1
decamethylcyclohexasiloxane	444.71	0.100	0	0	0	0	0	0
tetradecamethylcycloheptasiloxane	519.09	0.100	0	0	0	0	0	0
hexadecamethylcyclooctasiloxane	593.24	0.100	0	0	0	0	0	0

APPENDIX D

Adjusted *Spacelab* Trace Contaminant Generation Rate Data



IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED
	WEIGHT		SL-1 RATE	SL-3 RATE	SL-D1 RATE	SL-IML1 RATE	SL-USML1 RATE	SL-J RATE
	g/mole	mg/m ³	mg/day	mg/day	mg/day	mg/day	mg/day	mg/day
methanol	32.04	9.000	6.27E+01	1.07E+02	2.35E+01	2.35E+01	6.45E+01	6.02E+01
ethanol	46.07	2000.000	6.12E+01	8.09E+02	4.58E+00	4.10E+02	7.70E+01	5.46E+01
2-propen-1-ol	58.08	1.000	0.00E+00	2.54E-01	0.00E+00	0.00E+00	8.90E-02	6.40E-02
2-propanol	60.09	150.000	8.17E+01	2.56E+02	5.47E+01	7.62E+01	2.27E+02	3.15E+02
1-propanol	60.09	98.000	9.49E-01	3.23E+00	2.71E-01	7.78E+00	6.55E+00	2.58E+01
1,2-ethanediol	62.07	13.000	0.00E+00	0.00E+00	7.80E-02	7.25E-01	0.00E+00	0.00E+00
2-butanol	74.12	120.000	8.64E-02	8.78E-02	2.51E-01	7.22E-01	3.98E-01	7.22E-01
2-methyl-1-propanol	74.12	120.000	1.05E+01	7.08E+01	8.05E+00	1.33E+00	7.08E+01	8.00E+00
2-methyl-2-propanol	74.12	120.000	1.55E+00	1.23E+00	9.67E-01	2.11E+00	6.41E+00	5.45E+00
1-butanol	74.12	80.000	8.36E+01	5.10E+02	1.84E+01	1.17E+02	1.11E+02	7.18E+01
1,2-propanediol	76.10	0.100	3.17E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methyl-1-butanol	88.15	0.100	1.31E-02	0.00E+00	1.00E-03	1.78E+00	1.72E-01	2.04E+00
1-pentanol	88.15	130.000	1.30E+01	1.30E+01	1.10E-02	1.22E+00	0.00E+00	1.05E+00
phenol	94.11	7.700	8.59E-01	6.12E-02	3.18E+00	5.87E+01	0.00E+00	3.04E-01
cyclohexanol	100.16	120.000	1.64E+01	8.97E+01	1.20E-01	0.00E+00	0.00E+00	0.00E+00
2-ethyl-1-butanol	102.17	0.100	1.59E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexanol	102.18	170.000	2.44E-02	1.49E-01	2.44E-02	1.10E-01	1.85E-01	1.53E-01
1,3-dichloro-2-propanol	128.99	0.100	1.00E-03	0.00E+00	1.93E-03	0.00E+00	0.00E+00	0.00E+00
2-ethylhexanol	130.23	0.100	6.10E-01	0.00E+00	7.98E-01	0.00E+00	5.00E-03	3.52E-01
nonanol	144.26	0.100	0.00E+00	4.44E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
decanol	159.29	0.100	0.00E+00	0.00E+00	1.73E-03	0.00E+00	1.73E-03	1.00E-03
methanal	30.03	0.050	0.00E+00	2.30E-03	0.00E+00	0.00E+00	0.00E+00	4.65E-03
ethanal	44.05	4.000	2.85E+00	6.33E+00	1.45E+00	1.45E+00	7.57E+00	8.06E+00
2-propenal	56.06	0.030	6.50E-03	6.50E-03	2.00E-02	0.00E+00	4.48E-01	3.00E-02
propanal	58.08	95.000	5.93E+00	1.12E+01	1.90E-03	5.22E+00	1.03E+01	3.27E+01
2-methylpropenal	70.09	0.100	0.00E+00	2.44E-02	0.00E+00	0.00E+00	0.00E+00	2.43E-01
butanal	72.10	120.000	4.38E+00	1.02E+02	1.62E-01	1.24E+01	2.68E+00	2.82E+00
pentanal	86.13	110.000	1.07E+00	7.88E-01	4.83E-02	0.00E+00	8.50E+00	4.30E+00
2,4-hexadien-1-al	96.13	0.100	9.26E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hexanal	100.16	0.100	4.14E+00	1.32E+00	1.71E-02	4.40E-01	1.35E-01	4.14E+00
benzaldehyde	106.12	173.000	1.41E+00	0.00E+00	1.60E+00	0.00E+00	3.80E-02	2.61E-01
heptanal	114.19	0.100	1.41E-02	4.78E-01	2.89E-01	3.30E-01	1.40E-01	1.94E+00
4-methylbenzaldehyde	120.15	0.100	2.85E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
octanal	128.22	0.100	0.00E+00	3.04E-01	3.04E-01	2.20E-01	1.20E-02	2.00E-03
benzene	78.11	0.200	5.29E-01	2.26E+00	6.80E-01	2.20E-01	8.74E-01	1.45E+00
methylbenzene	92.15	60.000	9.42E+01	1.48E+02	8.11E+01	7.18E+01	1.48E+02	6.73E+01
ethenylbenzene	104.14	43.000	1.17E+00	5.60E-03	1.15E+00	2.20E-01	3.26E-01	3.12E+00
1,2-dimethylbenzene	106.16	220.000	7.47E+00	1.34E+01	1.71E+01	1.56E+00	5.61E+01	2.91E+01
1,3-dimethylbenzene	106.16	220.000	9.04E+00	2.45E+02	7.25E+00	2.33E+00	1.19E+01	6.54E+00
1,4-dimethylbenzene	106.16	220.000	8.02E+01	8.02E+01	1.14E+01	3.04E+01	3.96E+01	2.36E+01
ethylbenzene	106.16	130.000	7.34E+00	1.42E+01	5.11E+00	1.33E+00	2.67E+00	2.26E+00
indene	116.16	9.500	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
alpha-methylstyrene	118.18	140.000	0.00E+00	0.00E+00	9.00E-04	0.00E+00	1.43E-02	1.43E-02
1,2,4-trimethylbenzene	120.20	15.000	1.98E+00	1.49E-02	4.52E-02	0.00E+00	4.36E+00	2.48E+00
1,3,5-trimethylbenzene	120.20	15.000	1.29E-01	2.20E-01	2.59E-01	7.77E-02	1.81E-01	1.84E-01
1-ethyl-2-methylbenzene	120.20	25.000	4.07E-01	1.47E-02	3.46E-01	0.00E+00	0.00E+00	0.00E+00
isopropylbenzene	120.20	74.000	8.20E-01	1.06E+00	6.87E-01	3.23E-01	7.38E-01	3.28E-01
propylbenzene	120.20	49.000	3.39E+00	2.08E+01	4.17E-01	1.10E-01	1.47E+01	1.20E-02
1-methyl-3-propylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
n-butylbenzene	134.12	0.100	0.00E+00	1.62E-01	0.00E+00	0.00E+00	6.80E-02	1.70E-02
1-isopropyl-4-methylbenzene	134.22	0.100	0.00E+00	3.20E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanoic acid methyl ester	60.05	0.100	0.00E+00	7.30E-03	0.00E+00	1.10E-01	4.08E-01	3.18E-01
methanoic acid ethyl ester	74.08	91.000	0.00E+00	1.13E-01	0.00E+00	2.20E-01	4.89E-01	6.40E-02
ethanoic acid methyl ester	74.08	120.000	1.43E+00	1.41E+00	1.45E+01	1.44E+00	3.06E+00	1.68E+00
ethanoic acid ethyl ester	88.11	180.000	1.11E+01	2.89E+01	1.44E+00	1.21E+01	1.42E+00	7.83E+00
ethanoic acid allyl ester	100.12	0.100	2.20E-03	3.70E-01	0.00E+00	1.10E-01	2.08E-01	0.00E+00
2-methyl propenoic acid methyl ester	100.12	100.000	2.11E+00	2.94E+00	2.47E-01	1.02E+01	1.35E+00	1.02E+01
ethanoic acid isopropyl ester	102.13	210.000	3.95E-01	1.14E-01	5.76E-02	0.00E+00	4.00E-03	5.12E-01
methanoic acid butyl ester	102.13	0.100	5.70E-03	0.00E+00	0.00E+00	0.00E+00	1.18E-01	5.80E-02

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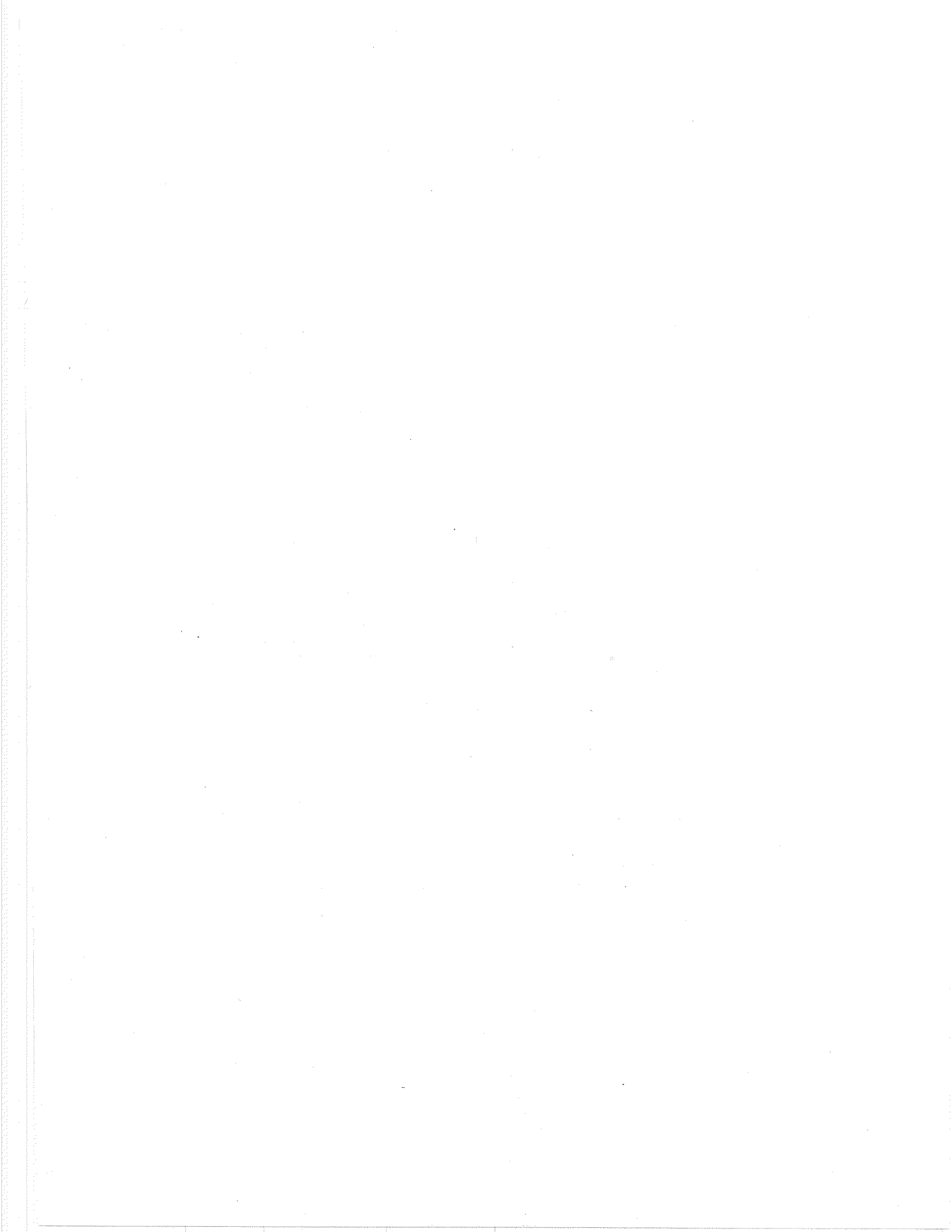
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IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED
	WEIGHT		SL-1 RATE	SL-3 RATE	SL-D1 RATE	SL-IML1 RATE	SL-USML1 RATE	SL-J RATE
	g/mole	mg/m ³	mg/day	mg/day	mg/day	mg/day	mg/day	mg/day
ethanoic acid propyl ester	102.13	170.000	4.67E+00	4.07E+01	2.90E-03	5.60E-01	2.87E-01	8.83E-01
2-methyl propenoic acid ethyl ester	114.15	0.100	0.00E+00	2.42E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid butyl ester	116.16	190.000	1.93E+01	7.41E+01	8.33E+00	6.00E+00	3.84E+01	1.45E+01
ethanoic acid isobutyl ester	116.16	190.000	4.20E+00	1.75E+01	7.85E-01	0.00E+00	3.70E-02	7.01E-01
lactic acid ethyl ester	118.13	190.000	0.00E+00	0.00E+00	4.11E-01	0.00E+00	0.00E+00	0.00E+00
ethanoic acid 2-methoxy ethyl ester	118.36	0.100	3.31E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid isoamyl ester	130.18	0.100	0.00E+00	3.46E-01	3.95E-02	0.00E+00	4.30E-02	3.17E+00
ethanoic acid amyl ester	130.18	160.000	1.21E+00	5.50E+00	0.00E+00	0.00E+00	6.91E-01	0.00E+00
ethanoic acid 2-ethoxyethyl ester	132.16	160.000	5.50E+01	1.45E+01	3.61E+01	1.16E+01	5.37E+01	1.16E+01
hydroxyethanoic acid ethyl ester	146.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
oxalic acid dibutyl ester	202.25	0.100	2.37E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-epoxy-1,3-butadiene	68.07	0.111	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.82E-01	1.34E-01
1,4-epoxybutane	72.11	120.000	2.92E+00	7.20E+00	4.73E-01	5.60E-01	7.65E-01	1.49E+00
3-methoxy-1-propene	72.11	0.100	4.05E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
diethyl ether	74.12	240.000	6.58E+00	0.00E+00	7.02E+00	0.00E+00	1.02E+00	4.00E-03
2-methylfuran	82.10	0.130	5.00E-04	1.18E-01	1.90E-02	0.00E+00	2.16E-01	3.23E-01
2,3-dihydropyran	84.13	0.100	2.58E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-dioxane	88.11	0.100	8.09E+00	5.92E+00	1.89E-02	2.20E-01	8.72E+00	3.49E-01
1,3,5-trioxane	90.08	0.100	1.10E-03	1.90E-03	0.00E+00	2.20E-01	1.07E-01	2.69E-01
2-ethoxyethanol	90.12	0.300	3.62E+00	7.19E+01	3.52E+00	3.56E+00	4.00E-02	4.30E+00
epichlorohydrin	92.53	0.100	3.15E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	0.00E+00	1.06E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-ethylmorpholine	115.18	0.100	1.45E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-propoxybutane	116.21	0.100	3.97E+00	1.97E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-butoxyethanol	118.18	0.100	6.00E-04	0.00E+00	5.00E-04	0.00E+00	2.75E-02	2.75E-02
chloromethane	50.49	41.000	3.77E-02	2.02E-02	6.59E-03	5.20E-01	4.27E-01	4.22E-01
chloroethene	62.50	3.000	1.17E-01	0.00E+00	0.00E+00	0.00E+00	2.00E-03	1.17E-01
chloroethane	64.52	260.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.00E-03	1.09E-02
3-chloropropene	76.53	0.100	0.00E+00	0.00E+00	8.63E-03	0.00E+00	0.00E+00	0.00E+00
dichloromethane	84.93	10.000	3.52E+01	1.70E+02	4.50E+00	3.41E+01	3.20E+01	1.70E+02
1-chlorobutane	92.57	150.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1-dichloroethene	96.95	7.900	1.50E-03	0.00E+00	0.00E+00	0.00E+00	7.35E-02	6.00E-03
1,2-dichloroethane	98.97	1.000	1.45E+00	2.48E+00	8.23E-02	1.44E+00	4.51E+00	7.22E+00
1,2-dichloropropene	110.97	0.100	0.00E+00	3.24E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chlorobenzene	112.56	46.000	1.05E+01	1.22E+02	7.33E-01	1.22E+02	4.55E+01	1.61E+01
1,2-dichloropropane	112.99	42.000	0.00E+00	4.69E-01	0.00E+00	7.35E-01	0.00E+00	0.00E+00
trichloromethane	119.38	4.900	7.07E-01	1.18E+00	1.35E+00	0.00E+00	1.27E-01	4.70E-02
1,2-dichloro-2-methylpropane	127.01	0.100	1.05E-01	0.00E+00	1.30E-01	0.00E+00	0.00E+00	0.00E+00
trichloroethene	131.39	10.000	6.18E+00	4.91E+00	8.88E-01	8.88E-01	6.18E+00	1.27E+00
1,1,1-trichloroethane	133.41	160.000	2.92E+01	2.78E+01	6.23E+00	6.78E+00	4.05E+01	5.58E+01
1,1,2-trichloroethane	133.41	0.100	0.00E+00	0.00E+00	6.90E-03	0.00E+00	0.00E+00	6.00E-03
1,2-dichlorobenzene	147.01	30.000	7.47E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E-03
3-chloromethylheptane	148.68	0.100	1.97E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
tetrachloromethane	153.82	13.000	2.08E-01	2.08E-01	7.84E-02	7.79E-01	7.79E-01	4.83E-03
tetrachloroethene	165.83	34.000	5.67E+01	5.67E+01	5.46E+00	8.22E+00	1.53E+01	7.82E+00
chlorodifluoromethane	86.47	350.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.35E+00	1.21E+00
dichlorofluoromethane	102.90	21.000	0.00E+00	0.00E+00	4.56E-02	0.00E+00	0.00E+00	5.51E-02
1-chloro-1,1,2,2-trifluoroethane	118.50	480.000	3.03E-01	3.03E-01	3.03E-01	3.18E-01	3.03E-01	3.02E-01
dichlorodifluoromethane	120.91	490.000	1.18E+00	0.00E+00	7.38E-02	0.00E+00	3.01E-01	9.01E-01
1,2-dichloro-1,2-difluoroethene	132.93	140.000	9.10E-02	9.10E-02	9.10E-02	1.10E-01	1.51E-01	4.01E-02
chlorotetrafluoroethane	136.48	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichlorofluoromethane	137.40	560.000	2.16E+01	5.95E+00	9.40E+01	1.09E+02	9.10E+00	5.90E+01
bromotrifluoromethane	148.90	11000.000	0.00E+00	3.24E+01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	1.20E-03	0.00E+00	0.00E+00	0.00E+00	3.49E+00	0.00E+00
1,1,2-trichloro-1,2,2-trifluoroethane	187.40	400.000	8.09E+01	1.82E+03	1.32E+01	2.54E+02	1.29E+03	8.65E+01
1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	0.00E+00	0.00E+00	0.00E+00	2.74E+00	2.74E+00	9.26E-01
methane	16.04	3800.000	4.16E+01	2.92E+01	4.15E+01	3.32E+01	3.90E+01	2.92E+01
ethyne	26.04	530.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethene	28.05	340.000	2.68E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED	ADJUSTED
	WEIGHT		SL-1 RATE	SL-3 RATE	SL-D1 RATE	SL-IMLI RATE	SL-USMLI RATE	SL-J RATE
	g/mole	mg/m ³	mg/day	mg/day	mg/day	mg/day	mg/day	mg/day
ethane	30.07	1200.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.49E-01	2.40E-02
propadiene	40.07	82.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propyne	40.07	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propene	42.08	860.000	3.74E-02	5.50E-02	1.00E-04	0.00E+00	2.70E-02	2.91E-01
propane	44.09	900.000	0.00E+00	6.21E-02	0.00E+00	0.00E+00	2.80E-02	8.26E-02
1,3-butadiene	54.09	0.130	0.00E+00	3.30E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-butene	56.10	460.000	4.81E+00	4.95E+00	4.56E+00	4.56E+00	1.59E+00	1.61E+00
2-methylpropane	58.12	240.000	0.00E+00	0.00E+00	5.40E-03	0.00E+00	1.45E+00	6.20E-02
butane	58.12	240.000	0.00E+00	1.62E-01	3.10E-03	0.00E+00	4.18E-01	4.18E-01
cyclopentene	68.11	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-1,3-butadiene	68.12	560.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-pentene	70.13	190.000	0.00E+00	0.00E+00	1.73E-03	0.00E+00	0.00E+00	1.73E-03
2-methylbutane	72.15	300.000	0.00E+00	2.15E-01	0.00E+00	0.00E+00	3.80E-02	0.00E+00
pentane	72.15	590.000	5.59E+00	9.14E+00	4.00E-02	1.10E-01	2.21E+00	6.75E-01
3,4,5,6-tetrahydrobenzene	82.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexene	84.16	0.100	0.00E+00	5.20E-02	0.00E+00	0.00E+00	2.00E-03	3.00E-03
cyclohexane	84.16	210.000	7.34E+00	4.40E+01	3.17E-01	0.00E+00	4.94E+00	2.85E+00
methylcyclopentane	84.16	52.000	1.44E-02	3.52E+00	1.21E-01	2.20E-01	4.12E-01	1.45E-01
2,2-dimethylbutane	86.17	88.000	0.00E+00	2.08E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methylpentane	86.18	1800.000	3.46E-01	3.13E-01	4.33E-02	4.33E-02	2.49E-01	4.59E-01
hexane	86.18	180.000	6.48E-01	6.58E+00	2.66E-01	3.30E-01	4.06E+00	2.55E+00
4-methylcyclohexene	96.17	390.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-heptene	98.18	200.000	0.00E+00	0.00E+00	1.24E-03	0.00E+00	0.00E+00	0.00E+00
methylcyclohexane	98.18	60.000	2.31E+00	4.77E+00	3.06E-01	4.22E+00	2.19E+00	3.06E-01
2,2-dimethylpentane	100.21	0.100	0.00E+00	3.00E+00	0.00E+00	0.00E+00	7.36E-01	2.45E-01
2,4-dimethylpentane	100.21	0.100	0.00E+00	2.87E-02	3.30E-03	0.00E+00	1.30E-02	0.00E+00
3-ethylpentane	100.21	0.100	0.00E+00	1.27E-02	0.00E+00	0.00E+00	3.40E-02	0.00E+00
heptane	100.21	200.000	2.67E-01	4.22E+00	2.67E-01	1.11E+00	4.22E+00	2.80E+00
1,1-dimethylcyclohexane	112.22	120.000	3.07E+00	2.67E-02	6.00E-04	0.00E+00	0.00E+00	0.00E+00
2-octene	112.22	230.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.00E-03	2.05E-03
6-methyl-1-heptene	112.22	0.100	9.17E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trans-1,2-dimethylcyclohexane	112.22	120.000	0.00E+00	6.40E+00	4.83E-02	0.00E+00	3.52E-01	1.66E-01
2,2,3-trimethylpentane	114.23	0.100	4.02E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3,3-dimethylhexane	114.23	0.100	1.69E-01	1.69E-01	1.69E-01	1.96E-01	1.69E-01	1.68E-01
3-ethylhexane	114.23	0.100	4.87E-02	0.00E+00	6.04E-02	0.00E+00	0.00E+00	0.00E+00
octane	114.23	350.000	2.95E-01	3.06E-01	2.95E-01	2.90E-01	1.30E+00	1.30E+00
4-ethylheptane	128.26	0.100	5.49E-03	5.49E-03	1.30E-03	0.00E+00	0.00E+00	0.00E+00
nonane	128.26	320.000	2.17E-01	2.17E-01	2.47E-01	9.03E-02	5.68E-01	5.68E-01
4-isopropenyl-1-methylcyclohexene	136.23	0.100	4.23E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-3-ethylheptane	142.28	0.100	2.41E-01	2.41E-01	2.41E-01	1.14E-01	2.58E-01	2.57E-01
decane	142.28	230.000	0.00E+00	1.13E-02	1.02E-01	0.00E+00	2.38E+00	2.38E+00
undecane	156.31	320.000	0.00E+00	4.12E-01	3.93E-02	1.10E-01	3.08E+00	5.80E-01
dodecane	170.34	280.000	0.00E+00	0.00E+00	4.98E-02	0.00E+00	0.00E+00	5.97E-02
2-propanone	58.08	50.000	1.15E+02	3.40E+02	1.68E+02	8.93E+01	1.02E+02	6.59E+01
3-buten-2-one	70.00	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.84E-02	8.00E-03
2-butanone	72.11	30.000	3.69E+01	4.76E+02	1.11E+01	5.01E+02	6.23E+01	3.96E+01
cyclopentanone	84.11	0.100	2.10E-03	5.81E+01	0.00E+00	1.44E+00	6.10E-02	1.80E-02
3-penten-2-one	84.12	0.100	3.40E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
acetyl cyclopropane	84.13	0.100	5.61E-03	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-pentanone	86.13	70.000	3.20E-02	3.67E-01	0.00E+00	0.00E+00	2.19E-01	2.00E-01
3-methyl-2-butanone	86.13	70.000	0.00E+00	5.50E-01	7.90E-02	3.64E+00	2.22E-01	2.20E-01
4-methyl-3-penten-2-one	98.14	40.000	3.71E+00	5.97E+00	3.71E+00	3.78E+00	1.84E+01	1.16E+01
cyclohexanone	98.14	60.000	1.05E+01	3.72E+01	1.05E+01	2.08E+01	5.11E+01	4.57E+01
3,3-dimethyl-2-butanone	100.16	0.100	0.00E+00	5.86E-01	5.75E-01	0.00E+00	2.07E-01	1.04E-01
4-methyl-2-pentanone	100.16	140.000	4.48E+01	1.20E+02	1.26E+01	2.68E+01	9.80E+01	4.79E+01
2,4-dimethyl-3-pentanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.09E-03	4.00E-03
2-heptanone	114.18	0.100	4.80E-02	2.75E-02	2.20E-03	1.10E-01	9.84E+00	5.20E-02
5-methyl-2-hexanone	114.18	0.100	7.67E-02	7.35E-02	0.00E+00	0.00E+00	2.35E-01	4.90E-02

APPENDIX E

Adjusted *Spacelab* Specific Trace Contaminant Generation Rate Data



IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J	MEAN	STANDARD
	WEIGHT		SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	RATE	DEVIATION
	g/mole	mg/m ³	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg
methanol	32.04	9.000	9.85E-04	1.60E-03	3.87E-04	3.54E-04	8.98E-04	9.07E-04	8.55E-04	4.18E-04
ethanol	46.07	2000.000	9.60E-04	1.21E-02	7.53E-05	6.16E-03	1.07E-03	8.21E-04	3.53E-03	4.32E-03
2-propen-1-ol	58.08	1.000	0.00E+00	3.80E-06	0.00E+00	0.00E+00	1.24E-06	9.63E-07	1.00E-06	1.35E-06
2-propanol	60.09	150.000	1.28E-03	3.83E-03	8.99E-04	1.15E-03	3.17E-03	4.73E-03	2.51E-03	1.48E-03
1-propanol	60.09	98.000	1.49E-05	4.83E-05	4.45E-06	1.17E-04	9.12E-05	3.88E-04	1.11E-04	1.30E-04
1,2-ethanediol	62.07	13.000	0.00E+00	0.00E+00	1.28E-06	1.09E-05	0.00E+00	0.00E+00	2.03E-06	4.00E-06
2-butanol	74.12	120.000	1.36E-06	1.31E-06	4.12E-06	1.09E-05	5.54E-06	1.09E-05	5.67E-06	3.95E-06
2-methyl-1-propanol	74.12	120.000	1.65E-04	1.06E-03	1.32E-04	2.00E-05	9.86E-04	1.20E-04	4.14E-04	4.33E-04
2-methyl-2-propanol	74.12	120.000	2.43E-05	1.83E-05	1.59E-05	3.17E-05	8.93E-05	8.21E-05	4.36E-05	3.02E-05
1-butanol	74.12	80.000	1.31E-03	7.62E-03	3.03E-04	1.76E-03	1.55E-03	1.08E-03	2.27E-03	2.44E-03
1,2-propanediol	76.10	0.100	4.97E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.29E-08	1.85E-07
3-methyl-1-butanol	88.15	0.100	2.06E-07	0.00E+00	1.64E-08	2.68E-05	2.40E-06	3.07E-05	1.00E-05	1.33E-05
1-pentanol	88.15	130.000	2.04E-04	1.94E-04	1.81E-07	1.83E-05	0.00E+00	1.57E-05	7.20E-05	9.00E-05
phenol	94.11	7.700	1.35E-05	9.14E-07	5.22E-05	8.82E-04	0.00E+00	4.57E-06	1.59E-04	3.24E-04
cyclohexanol	100.16	120.000	2.57E-04	1.34E-03	1.97E-06	0.00E+00	0.00E+00	0.00E+00	2.67E-04	4.89E-04
2-ethyl-1-butanol	102.17	0.100	2.50E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	4.16E-08	9.31E-08
2-hexanol	102.18	170.000	3.83E-07	2.23E-06	4.01E-07	1.65E-06	2.58E-06	2.30E-06	1.59E-06	8.90E-07
1,3-dichloro-2-propanol	128.99	0.100	1.57E-08	0.00E+00	3.17E-08	0.00E+00	0.00E+00	0.00E+00	7.90E-09	1.21E-08
2-ethylhexanol	130.23	0.100	9.58E-06	0.00E+00	1.31E-05	0.00E+00	6.97E-08	5.30E-06	4.68E-06	5.17E-06
nonanol	144.26	0.100	0.00E+00	6.64E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.11E-06	2.47E-06
decanol	159.29	0.100	0.00E+00	0.00E+00	2.84E-08	0.00E+00	2.41E-08	1.50E-08	1.13E-08	1.19E-08
methanal	30.03	0.050	0.00E+00	3.44E-08	0.00E+00	0.00E+00	0.00E+00	7.00E-08	1.74E-08	2.67E-08
ethanal	44.05	4.000	4.48E-05	9.45E-05	2.39E-05	2.19E-05	1.05E-04	1.21E-04	6.86E-05	3.99E-05
2-propenal	56.06	0.030	1.02E-07	9.71E-08	3.29E-07	0.00E+00	6.24E-06	4.51E-07	1.20E-06	2.26E-06
propanal	58.08	95.000	9.31E-05	1.68E-04	3.12E-08	7.85E-05	1.43E-04	4.92E-04	1.62E-04	1.57E-04
2-methylpropanal	70.09	0.100	0.00E+00	3.64E-07	0.00E+00	0.00E+00	0.00E+00	3.66E-06	6.70E-07	1.34E-06
butanal	72.10	120.000	6.88E-05	1.53E-03	2.66E-06	1.87E-04	3.73E-05	4.24E-05	3.11E-04	5.48E-04
pentanal	86.13	110.000	1.67E-05	1.18E-05	7.94E-07	0.00E+00	1.18E-04	6.47E-05	3.54E-05	4.30E-05
2,4-hexadien-1-al	96.13	0.100	1.45E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.42E-07	5.42E-07
hexanal	100.16	0.100	6.50E-05	1.98E-05	2.81E-07	6.62E-06	1.88E-06	6.22E-05	2.60E-05	2.74E-05
benzaldehyde	106.12	173.000	2.22E-05	0.00E+00	2.64E-05	0.00E+00	5.29E-07	3.93E-06	8.84E-06	1.11E-05
heptanal	114.19	0.100	2.21E-07	7.14E-06	4.75E-06	4.96E-06	1.95E-06	2.91E-05	8.02E-06	9.69E-06
4-methylbenzaldehyde	120.15	0.100	4.48E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.47E-08	1.67E-07
octanal	128.22	0.100	0.00E+00	4.54E-06	4.99E-06	3.31E-06	1.67E-07	3.01E-08	2.17E-06	2.17E-06
benzene	78.11	0.200	8.30E-06	3.38E-05	1.12E-05	3.31E-06	1.22E-05	2.18E-05	1.51E-05	1.00E-05
methylbenzene	92.15	60.000	1.48E-03	2.20E-03	1.33E-03	1.08E-03	2.06E-03	1.01E-03	1.53E-03	4.55E-04
ethenylbenzene	104.14	43.000	1.83E-05	8.36E-08	1.89E-05	3.31E-06	4.54E-06	4.70E-05	1.54E-05	1.59E-05
1,2-dimethylbenzene	106.16	220.000	1.17E-04	2.00E-04	2.81E-04	2.35E-05	7.82E-04	4.39E-04	3.07E-04	2.49E-04
1,3-dimethylbenzene	106.16	220.000	1.42E-04	3.66E-03	1.19E-04	3.50E-05	1.66E-04	9.84E-05	7.03E-04	1.32E-03
1,4-dimethylbenzene	106.16	220.000	1.26E-03	1.20E-03	1.88E-04	4.58E-04	5.51E-04	3.55E-04	6.68E-04	4.12E-04
ethylbenzene	106.16	130.000	1.15E-04	2.12E-04	8.41E-05	2.00E-05	3.72E-05	3.40E-05	8.38E-05	6.60E-05
indene	116.16	9.500	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
alpha-methylstyrene	118.18	140.000	0.00E+00	0.00E+00	1.48E-08	0.00E+00	1.99E-07	2.15E-07	7.13E-08	9.59E-08
1,2,4-trimethylbenzene	120.20	15.000	3.10E-05	2.23E-07	7.43E-07	0.00E+00	6.07E-05	3.74E-05	2.17E-05	2.32E-05
1,3,5-trimethylbenzene	120.20	15.000	2.02E-06	3.28E-06	4.25E-06	1.17E-06	2.52E-06	2.77E-06	2.67E-06	9.64E-07
1-ethyl-2-methylbenzene	120.20	25.000	6.40E-06	2.20E-07	5.68E-06	0.00E+00	0.00E+00	0.00E+00	2.05E-06	2.83E-06
isopropylbenzene	120.20	74.000	1.29E-05	1.58E-05	1.13E-05	4.86E-06	1.03E-05	4.94E-06	1.00E-05	4.00E-06
propylbenzene	120.20	49.000	5.32E-05	3.10E-04	6.85E-06	1.65E-06	2.04E-04	1.81E-07	9.61E-05	1.19E-04
1-methyl-3-propylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
n-butylbenzene	134.12	0.100	0.00E+00	2.42E-06	0.00E+00	0.00E+00	9.47E-07	2.56E-07	6.04E-07	8.79E-07
1-isopropyl-4-methylbenzene	134.22	0.100	0.00E+00	4.79E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.98E-08	1.78E-07
methanoic acid methyl ester	60.05	0.100	0.00E+00	1.09E-07	0.00E+00	1.65E-06	5.69E-06	4.79E-06	2.04E-06	2.35E-06
methanoic acid ethyl ester	74.08	91.000	0.00E+00	1.69E-06	0.00E+00	3.31E-06	6.82E-06	9.63E-07	2.13E-06	2.38E-06
ethanoic acid methyl ester	74.08	120.000	2.24E-05	2.10E-05	2.38E-04	2.17E-05	4.27E-05	2.53E-05	6.18E-05	7.91E-05
ethanoic acid ethyl ester	88.11	180.000	1.74E-04	4.32E-04	2.37E-05	1.82E-04	1.98E-05	1.18E-04	1.58E-04	1.38E-04
ethanoic acid allyl ester	100.12	0.100	3.45E-08	5.52E-06	0.00E+00	1.65E-06	2.90E-06	0.00E+00	1.68E-06	2.03E-06
2-methyl propenoic acid methyl ester	100.12	100.000	3.31E-05	4.38E-05	4.06E-06	1.54E-04	1.88E-05	1.54E-04	6.78E-05	6.19E-05
ethanoic acid isopropyl ester	102.13	210.000	6.20E-06	1.70E-06	9.47E-07	0.00E+00	5.57E-08	7.71E-06	2.77E-06	3.05E-06
methanoic acid butyl ester	102.13	0.100	8.95E-08	0.00E+00	0.00E+00	0.00E+00	1.64E-06	8.73E-07	4.34E-07	6.24E-07

4/6 INTERNAL ONLY

MSFC, ED62/J. L. Perry

ADJUSTED SPACELAB SPECIFIC TRACE CONTAMINANT GENERATION RATE DATA

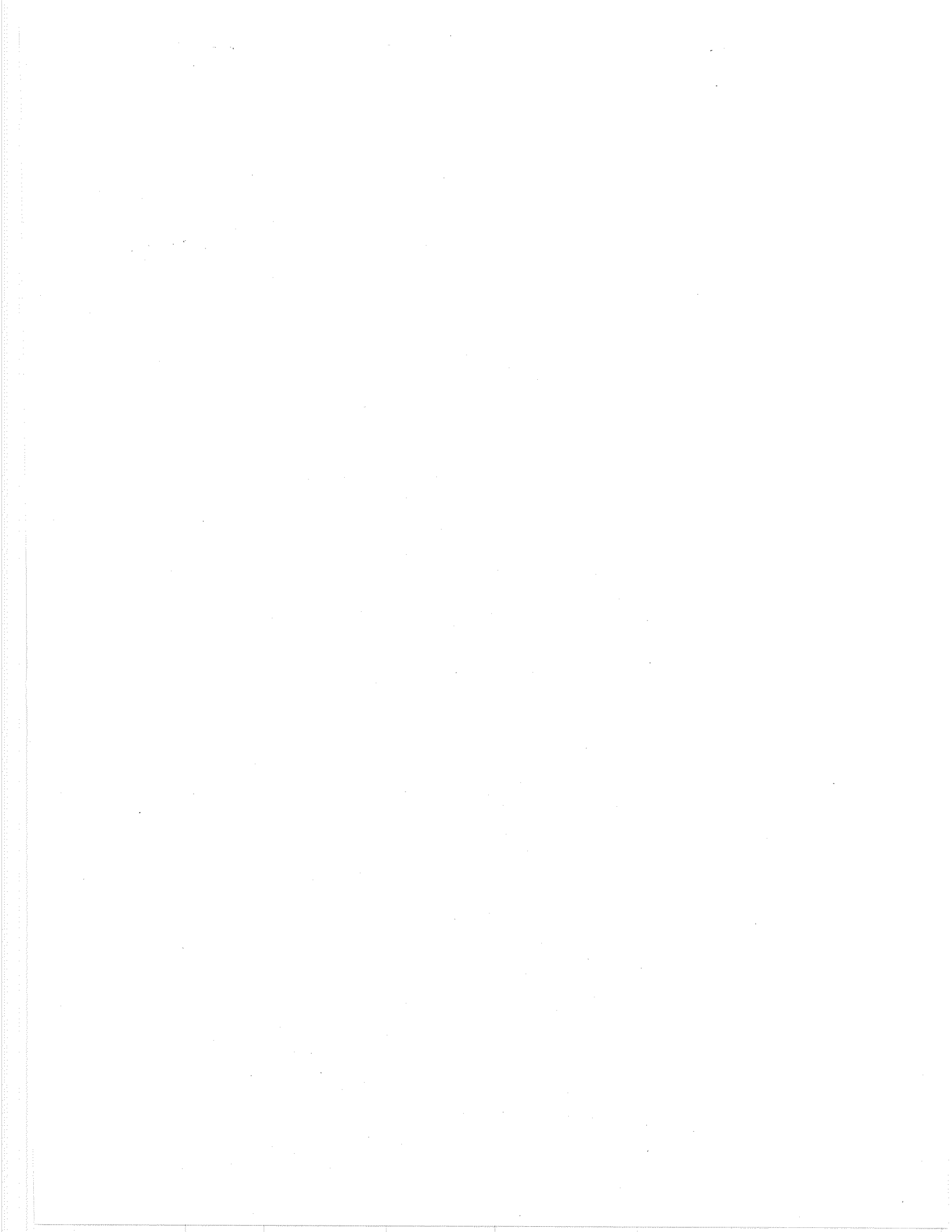
7/13/95

IUPAC/ACCEPTED NAME	MOLECULAR	SHAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J	MEAN	STANDARD
	WEIGHT		SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	RATE	DEVIATION
	g/mole	mg/m ³	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg
ethanoic acid propyl ester	102.13	170.000	7.34E-05	6.07E-04	4.77E-08	8.42E-06	4.00E-06	1.33E-05	1.18E-04	2.20E-04
2-methyl propenoic acid ethyl ester	114.15	0.100	0.00E+00	3.61E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.02E-06	1.35E-05
ethanoic acid butyl ester	116.16	190.000	3.02E-04	1.11E-03	1.37E-04	9.02E-05	5.35E-04	2.18E-04	3.98E-04	3.48E-04
ethanoic acid isobutyl ester	116.16	190.000	6.59E-05	2.61E-04	1.29E-05	0.00E+00	5.15E-07	1.05E-05	5.85E-05	9.32E-05
lactic acid ethyl ester	118.13	190.000	0.00E+00	0.00E+00	6.75E-06	0.00E+00	0.00E+00	0.00E+00	1.12E-06	2.51E-06
ethanoic acid 2-methoxy ethyl ester	118.36	0.100	5.19E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.65E-07	1.94E-06
ethanoic acid isoamyl ester	130.18	0.100	0.00E+00	5.17E-06	6.49E-07	0.00E+00	5.99E-07	4.77E-05	9.03E-06	1.74E-05
ethanoic acid amyl ester	130.18	160.000	1.90E-05	8.22E-05	0.00E+00	0.00E+00	9.63E-06	0.00E+00	1.85E-05	2.93E-05
ethanoic acid 2-ethoxyethyl ester	132.16	160.000	8.64E-04	2.16E-04	5.92E-04	1.74E-04	7.47E-04	1.74E-04	4.61E-04	2.85E-04
hydroxyethanoic acid ethyl ester	146.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
oxalic acid dibutyl ester	202.25	0.100	3.73E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.21E-09	1.39E-08
1,4-epoxy-1,3-butadiene	68.07	0.111	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.53E-06	2.02E-06	7.58E-07	1.08E-06
1,4-epoxybutane	72.11	120.000	4.58E-05	1.08E-04	7.77E-06	8.42E-06	1.07E-05	2.25E-05	3.38E-05	3.55E-05
3-methoxy-1-propene	72.11	0.100	6.35E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.06E-08	2.37E-08
diethyl ether	74.12	240.000	1.03E-04	0.00E+00	1.15E-04	0.00E+00	1.41E-05	6.02E-08	3.88E-05	5.02E-05
2-methylfuran	82.10	0.130	7.85E-09	1.77E-06	3.12E-07	0.00E+00	3.01E-06	4.86E-06	1.66E-06	1.80E-06
2,3-dihydropyran	84.13	0.100	4.05E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	6.75E-08	1.51E-07
1,4-dioxane	88.11	0.100	1.27E-04	8.84E-05	3.11E-07	3.31E-06	1.22E-04	5.25E-06	5.76E-05	5.60E-05
1,3,5-trioxane	90.08	0.100	1.73E-08	2.84E-08	0.00E+00	3.31E-06	1.49E-06	4.05E-06	1.48E-06	1.65E-06
2-ethoxyethanol	90.12	0.300	5.69E-05	1.07E-03	5.78E-05	5.35E-05	5.57E-07	6.47E-05	2.18E-04	3.83E-04
epichlorohydrin	92.53	0.100	4.94E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.23E-07	1.84E-06
1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	0.00E+00	1.58E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.63E-07	5.88E-07
4-ethylmorpholine	115.18	0.100	2.27E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.79E-05	8.47E-05
1-propoxybutane	116.21	0.100	6.23E-05	2.94E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.53E-05	2.36E-05
2-butoxyethanol	118.18	0.100	9.42E-09	0.00E+00	8.22E-09	0.00E+00	3.82E-07	4.13E-07	1.36E-07	1.86E-07
chloromethane	50.49	41.000	5.92E-07	3.02E-07	1.08E-07	7.82E-06	5.95E-06	6.35E-06	3.52E-06	3.24E-06
chloroethene	62.50	3.000	1.84E-06	0.00E+00	0.00E+00	0.00E+00	2.79E-08	1.77E-06	6.07E-07	8.49E-07
chloroethane	64.52	260.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.39E-08	1.64E-07	2.96E-08	6.02E-08
3-chloropropene	76.53	0.100	0.00E+00	0.00E+00	1.42E-07	0.00E+00	0.00E+00	0.00E+00	2.36E-08	5.29E-08
dichloromethane	84.93	10.000	5.53E-04	2.55E-03	7.39E-05	5.13E-04	4.46E-04	2.56E-03	1.12E-03	1.03E-03
1-chlorobutane	92.57	150.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1-dichloroethene	96.95	7.900	2.36E-08	0.00E+00	0.00E+00	0.00E+00	1.02E-06	9.03E-08	1.90E-07	3.75E-07
1,2-dichloroethane	98.97	1.000	2.28E-05	3.71E-05	1.35E-06	2.17E-05	6.28E-05	1.09E-04	4.24E-05	3.50E-05
1,2-dichloropropene	110.97	0.100	0.00E+00	4.84E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.07E-06	1.80E-05
chlorobenzene	112.56	46.000	1.64E-04	1.82E-03	1.20E-05	1.83E-03	6.33E-04	2.43E-04	7.84E-04	7.60E-04
1,2-dichloropropane	112.99	42.000	0.00E+00	7.00E-06	0.00E+00	1.10E-05	0.00E+00	0.00E+00	3.01E-06	4.41E-06
trichloromethane	119.38	4.900	1.11E-05	1.77E-05	2.22E-05	0.00E+00	1.77E-06	7.07E-07	8.90E-06	8.71E-06
1,2-dichloro-2-methylpropane	127.01	0.100	1.65E-06	0.00E+00	2.14E-06	0.00E+00	0.00E+00	0.00E+00	6.31E-07	9.04E-07
trichloroethene	131.39	10.000	9.71E-05	7.33E-05	1.46E-05	1.34E-05	8.61E-05	1.91E-05	5.06E-05	3.56E-05
1,1,1-trichloroethane	133.41	160.000	4.59E-04	4.15E-04	1.02E-04	1.02E-04	5.65E-04	8.39E-04	4.14E-04	2.58E-04
1,1,2-trichloroethane	133.41	0.100	0.00E+00	0.00E+00	1.13E-07	0.00E+00	0.00E+00	9.03E-08	3.39E-08	4.85E-08
1,2-dichlorobenzene	147.01	30.000	1.17E-05	0.00E+00	0.00E+00	0.00E+00	0.00E+00	3.01E-08	1.96E-06	4.37E-06
3-chloromethylheptane	148.68	0.100	3.10E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.17E-08	1.16E-07
tetrachloromethane	153.82	13.000	3.26E-06	3.11E-06	1.29E-06	1.17E-05	1.09E-05	7.26E-08	5.05E-06	4.55E-06
tetrachloroethene	165.83	34.000	8.91E-04	8.47E-04	8.97E-05	1.24E-04	2.13E-04	1.18E-04	3.80E-04	3.48E-04
chlorodifluoromethane	86.47	350.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.02E-04	1.82E-05	2.01E-05	3.74E-05
dichlorofluoromethane	102.90	21.000	0.00E+00	0.00E+00	7.49E-07	0.00E+00	0.00E+00	8.29E-07	2.63E-07	3.73E-07
1-chloro-1,2,2-trifluoroethane	118.50	480.000	4.76E-06	4.53E-06	4.98E-06	4.78E-06	4.22E-06	4.54E-06	4.64E-06	2.41E-07
dichlorodifluoromethane	120.91	490.000	1.85E-05	0.00E+00	1.21E-06	0.00E+00	4.19E-06	1.36E-05	6.25E-06	7.21E-06
1,2-dichloro-1,1,2,2-tetrafluoroethane	132.93	140.000	1.43E-06	1.36E-06	1.50E-06	1.65E-06	2.11E-06	6.04E-07	1.44E-06	4.47E-07
chlorotetrafluoroethane	136.48	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichlorofluoromethane	137.40	560.000	3.39E-04	8.89E-05	1.54E-03	1.64E-03	1.27E-04	8.88E-04	7.71E-04	6.37E-04
bromotrifluoromethane	148.90	11000.000	0.00E+00	4.83E-04	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.06E-05	1.80E-04
1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	1.88E-08	0.00E+00	0.00E+00	0.00E+00	4.86E-05	0.00E+00	8.10E-06	1.81E-05
1,1,2-trichloro-1,2,2-trifluoroethane	187.42	400.000	1.27E-03	2.72E-02	3.81E-04	3.81E-03	1.80E-02	1.30E-02	8.64E-03	1.03E-02
1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	0.00E+00	0.00E+00	0.00E+00	4.12E-05	3.81E-05	1.39E-05	1.55E-05	1.78E-05
methane	16.04	3800.000	6.53E-04	4.37E-04	6.83E-04	5.00E-04	5.43E-04	4.40E-04	5.43E-04	9.61E-05
ethyne	26.04	530.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethene	28.05	340.000	4.20E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	7.00E-08	1.57E-07

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	SL-1	SL-3	SL-D1	SL-IML1	SL-USML1	SL-J	MEAN	STANDARD
	WEIGHT		SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	SPECIFIC RATE	RATE	DEVIATION
	g/mole	mg/m ³	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg	mg/day*kg
ethane	30.07	1200.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.08E-06	3.61E-07	4.07E-07	7.60E-07
propadiene	40.07	82.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propyne	40.07	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propene	42.08	860.000	5.87E-07	8.22E-07	1.64E-09	0.00E+00	3.76E-07	4.39E-06	1.03E-06	1.53E-06
propane	44.09	900.000	0.00E+00	9.28E-07	0.00E+00	0.00E+00	3.90E-07	1.24E-06	4.27E-07	4.94E-07
1,3-butadiene	54.09	0.130	0.00E+00	4.93E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.22E-07	1.84E-06
1-butene	56.10	460.000	7.55E-05	7.39E-05	7.49E-05	6.86E-05	2.22E-05	2.42E-05	5.66E-05	2.37E-05
2-methylpropane	58.12	240.000	0.00E+00	0.00E+00	8.87E-08	0.00E+00	2.02E-05	9.33E-07	3.54E-06	7.47E-06
butane	58.12	240.000	0.00E+00	2.42E-06	5.09E-08	0.00E+00	5.82E-06	6.29E-06	2.43E-06	2.70E-06
cyclopentene	68.11	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-1,3-butadiene	68.12	560.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-pentene	70.13	190.000	0.00E+00	0.00E+00	2.85E-08	0.00E+00	0.00E+00	2.61E-08	9.10E-09	1.29E-08
2-methylbutane	72.15	300.000	0.00E+00	3.22E-06	0.00E+00	0.00E+00	5.29E-07	0.00E+00	6.25E-07	1.18E-06
pentane	72.15	590.000	8.78E-05	1.37E-04	6.57E-07	1.65E-06	3.07E-05	1.02E-05	4.46E-05	5.08E-05
3,4,5,6-tetrahydrobenzene	82.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexene	84.16	0.100	0.00E+00	7.77E-07	0.00E+00	0.00E+00	2.79E-08	4.51E-08	1.42E-07	2.84E-07
cyclohexane	84.16	210.000	1.15E-04	6.58E-04	5.20E-06	0.00E+00	6.88E-05	4.28E-05	1.48E-04	2.31E-04
methylcyclopentane	84.16	52.000	2.26E-07	5.26E-05	1.99E-06	3.31E-06	5.74E-06	2.18E-06	1.10E-05	1.87E-05
2,2-dimethylbutane	86.17	88.000	0.00E+00	3.10E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	5.17E-07	1.16E-06
3-methylpentane	86.18	1800.000	5.44E-06	4.67E-06	7.11E-07	6.51E-07	3.47E-06	6.90E-06	3.64E-06	2.33E-06
hexane	86.18	180.000	1.02E-05	9.83E-05	4.37E-06	4.96E-06	5.66E-05	3.83E-05	3.55E-05	3.40E-05
4-methylcyclohexene	96.17	390.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-heptene	98.18	200.000	0.00E+00	0.00E+00	2.04E-08	0.00E+00	0.00E+00	0.00E+00	3.40E-09	7.60E-09
methylcyclohexane	98.18	60.000	3.62E-05	7.12E-05	5.02E-06	6.35E-05	3.05E-05	4.60E-06	3.52E-05	2.57E-05
2,2-dimethylpentane	100.21	0.100	0.00E+00	4.48E-05	0.00E+00	0.00E+00	1.03E-05	3.69E-06	9.79E-06	1.61E-05
2,4-dimethylpentane	100.21	0.100	0.00E+00	4.29E-07	5.42E-08	0.00E+00	1.81E-07	0.00E+00	1.11E-07	1.56E-07
3-ethylpentane	100.21	0.100	0.00E+00	1.90E-07	0.00E+00	0.00E+00	4.74E-07	0.00E+00	1.11E-07	1.77E-07
heptane	100.21	200.000	4.19E-06	6.31E-05	4.39E-06	1.67E-05	5.88E-05	4.22E-05	3.16E-05	4.42E-05
1,1-dimethylcyclohexane	112.22	120.000	4.83E-05	3.99E-07	9.86E-09	0.00E+00	0.00E+00	0.00E+00	8.11E-06	1.80E-05
2-octene	112.22	230.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.79E-08	3.08E-08	9.78E-09	1.39E-08
6-methyl-1-heptene	112.22	0.100	1.44E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.40E-09	5.37E-09
trans-1,2-dimethylcyclohexane	112.22	120.000	0.00E+00	9.56E-05	7.94E-07	0.00E+00	4.90E-06	2.50E-06	1.73E-05	3.51E-05
2,2,3-trimethylpentane	114.23	0.100	6.31E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.05E-07	2.35E-07
3,3-dimethylhexane	114.23	0.100	2.66E-06	2.52E-06	2.78E-06	2.95E-06	2.35E-06	2.63E-06	2.63E-06	1.94E-07
1-ethylhexane	114.23	0.100	7.65E-07	0.00E+00	7.92E-07	0.00E+00	0.00E+00	0.00E+00	2.93E-07	4.19E-07
octane	114.23	450.000	4.63E-06	4.57E-06	4.04E-06	4.16E-06	1.01E-05	1.96E-05	1.11E-05	6.75E-06
4-ethylheptane	128.26	0.100	8.62E-08	8.20E-08	2.14E-08	0.00E+00	0.00E+00	0.00E+00	1.16E-08	1.79E-08
nonane	128.26	420.000	1.41E-06	1.24E-06	4.06E-06	1.16E-06	7.91E-06	8.54E-06	4.75E-06	2.59E-06
4-isopropenyl-1-methylcyclohexene	136.23	0.100	6.64E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.11E-06	2.47E-06
2-methyl-3-ethylheptane	142.28	0.100	3.79E-06	3.60E-06	3.97E-06	1.71E-06	3.59E-06	3.87E-06	3.42E-06	7.76E-07
decane	142.28	230.000	0.00E+00	1.69E-07	1.68E-06	0.00E+00	3.31E-05	3.58E-05	1.18E-05	1.60E-05
undecane	156.31	320.000	0.00E+00	6.15E-06	6.46E-07	1.65E-06	4.29E-05	8.73E-06	1.00E-05	1.51E-05
dodecane	170.34	280.000	0.00E+00	0.00E+00	8.18E-07	0.00E+00	0.00E+00	8.98E-07	2.86E-07	4.05E-07
2-propanone	58.08	50.000	1.80E-03	5.08E-03	2.76E-03	1.34E-03	1.43E-03	9.92E-04	2.23E-03	1.39E-03
3-buten-2-one	70.00	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.56E-07	1.20E-07	6.27E-08	9.69E-08
2-butanone	72.11	30.000	5.79E-04	7.11E-03	1.83E-04	7.53E-03	8.67E-04	5.95E-04	2.81E-03	3.20E-03
cyclopentanone	84.11	0.100	3.30E-08	8.68E-04	0.00E+00	2.17E-05	8.50E-07	2.71E-07	1.48E-04	3.22E-04
3-penten-2-one	84.12	0.100	5.34E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	8.89E-09	1.99E-08
acetyl cyclopropane	84.13	0.100	8.81E-08	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	1.47E-08	3.28E-08
2-pentanone	86.13	70.000	5.02E-07	5.49E-06	0.00E+00	0.00E+00	3.05E-06	3.01E-06	2.01E-06	2.02E-06
3-methyl-2-butanone	86.13	70.000	0.00E+00	8.21E-06	1.30E-06	5.47E-05	3.09E-06	3.31E-06	1.18E-05	1.94E-05
4-methyl-3-penten-2-one	98.14	40.000	5.83E-05	8.92E-05	6.10E-05	5.68E-05	2.56E-04	1.74E-04	1.16E-04	7.47E-05
cyclohexanone	98.14	60.000	1.64E-04	5.56E-04	1.72E-04	3.13E-04	7.12E-04	6.88E-04	4.34E-04	2.28E-04
3,3-dimethyl-2-butanone	100.16	0.100	0.00E+00	8.76E-06	9.45E-06	0.00E+00	2.88E-06	1.57E-06	3.78E-06	3.90E-06
4-methyl-2-pentanone	100.16	140.000	7.03E-04	1.79E-03	2.07E-04	4.03E-04	1.36E-03	7.20E-04	8.64E-04	5.46E-04
2,4-dimethyl-3-pentanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	9.87E-08	6.02E-08	2.65E-08	3.91E-08
2-heptanone	114.18	0.100	7.54E-07	4.11E-07	3.62E-08	1.65E-06	1.37E-04	7.83E-07	2.35E-05	5.08E-05
5-methyl-2-hexanone	114.18	0.100	1.20E-06	1.10E-06	0.00E+00	0.00E+00	3.27E-06	7.37E-07	1.05E-06	1.10E-06

APPENDIX F

Metabolic Contaminant Generation From Expired Air



IUPAC/ACCEPTED NAME	MOLECULAR WEIGHT (g/mole)	SMAC (mg/m ³)	Conkle Average (mg/h)	Kustov and Tiunov (mg/h)	Nefedov, et al (mg/h)	Dmitriyev, et al (mg/h)	Maximum Rate (mg/h)	Mean Rate (mg/h)	Standard Deviation (mg/h)
methanol	32.04	9.000	3.84E-03	0.00E+00	4.87E-02	4.79E-03	4.87E-02	1.43E-02	1.99E-02
ethanol	46.07	2000.000	7.97E-02	0.00E+00	2.20E-01	1.73E-02	2.20E-01	7.93E-02	8.66E-02
2-propen-1-ol	58.08	1.000	1.36E-03	0.00E+00	0.00E+00	0.00E+00	1.36E-03	3.39E-04	5.88E-04
2-propanol	60.09	150.000	1.18E-02	0.00E+00	2.56E-02	7.36E-02	7.36E-02	2.78E-02	2.80E-02
1-propanol	60.09	98.000	0.00E+00	0.00E+00	0.00E+00	1.61E-02	1.61E-02	4.03E-03	6.98E-03
1,2-ethanediol	62.07	13.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-butanol	74.12	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-1-propanol	74.12	120.000	7.96E-03	0.00E+00	0.00E+00	0.00E+00	7.96E-03	1.99E-03	3.45E-03
2-methyl-2-propanol	74.12	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-butanol	74.12	80.000	6.43E-03	0.00E+00	0.00E+00	1.22E-02	1.22E-02	4.65E-03	5.08E-03
1,2-propanediol	76.10	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methyl-1-butanol	88.15	0.100	1.57E-05	0.00E+00	0.00E+00	1.18E-02	1.18E-02	2.96E-03	5.12E-03
1-pentanol	88.15	130.000	1.44E-04	0.00E+00	0.00E+00	0.00E+00	1.44E-04	3.61E-05	6.25E-05
phenol	94.11	7.700	0.00E+00	0.00E+00	0.00E+00	5.77E-03	5.77E-03	1.44E-03	2.50E-03
cyclohexanol	100.16	120.000	1.01E-04	0.00E+00	0.00E+00	1.26E-02	1.26E-02	3.17E-03	5.43E-03
2-ethyl-1-butanol	102.17	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexanol	102.18	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,3-dichloro-2-propanol	128.99	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-ethylhexanol	130.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nonanol	144.26	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
decanol	159.29	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanal	30.03	0.050	0.00E+00	0.00E+00	2.56E-02	5.39E-04	2.56E-02	6.54E-03	1.10E-02
ethanal	44.05	4.000	1.80E-02	0.00E+00	2.56E-02	2.16E-03	2.56E-02	1.14E-02	1.07E-02
2-propenal	56.06	0.030	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propanal	58.08	95.000	0.00E+00	0.00E+00	2.56E-02	0.00E+00	2.56E-02	6.41E-03	1.11E-02
2-methylpropanal	70.09	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
butanal	72.10	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
pentanal	86.13	110.000	0.00E+00	0.00E+00	0.00E+00	5.02E-04	5.02E-04	1.25E-04	2.17E-04
2,4-hexadien-1-al	96.13	0.100	0.00E+00	0.00E+00	0.00E+00	4.30E-04	4.30E-04	1.08E-04	1.86E-04
hexanal	100.16	0.100	0.00E+00	0.00E+00	0.00E+00	6.32E-04	6.32E-04	1.58E-04	2.74E-04
benzaldehyde	106.12	173.000	0.00E+00	0.00E+00	0.00E+00	2.70E-04	2.70E-04	6.74E-05	1.17E-04
heptanal	114.19	0.100	0.00E+00	0.00E+00	0.00E+00	5.25E-04	5.25E-04	1.31E-04	2.27E-04
4-methylbenzaldehyde	120.15	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
octanal	128.22	0.100	0.00E+00	0.00E+00	0.00E+00	5.91E-04	5.91E-04	1.48E-04	2.56E-04
benzene	78.11	0.200	0.00E+00	0.00E+00	0.00E+00	9.36E-02	9.36E-02	2.34E-02	4.05E-02
methylbenzene	92.15	60.000	0.00E+00	0.00E+00	0.00E+00	1.72E-02	1.72E-02	4.30E-03	7.45E-03
ethenylbenzene	104.14	43.000	0.00E+00	0.00E+00	0.00E+00	2.05E-05	2.05E-05	5.13E-06	8.89E-06
1,2-dimethylbenzene	106.16	220.000	0.00E+00	0.00E+00	0.00E+00	2.33E-03	2.33E-03	5.83E-04	1.01E-03
1,3-dimethylbenzene	106.16	220.000	0.00E+00	0.00E+00	0.00E+00	2.33E-03	2.33E-03	5.83E-04	1.01E-03
1,4-dimethylbenzene	106.16	220.000	0.00E+00	0.00E+00	0.00E+00	2.33E-03	2.33E-03	5.83E-04	1.01E-03
ethylbenzene	106.16	130.000	8.54E-04	0.00E+00	0.00E+00	1.53E-02	1.53E-02	4.03E-03	6.49E-03
indene	116.16	9.500	1.83E-03	0.00E+00	0.00E+00	0.00E+00	1.83E-03	4.58E-04	7.93E-04
alpha-methylstyrene	118.18	140.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2,4-trimethylbenzene	120.20	15.000	0.00E+00	0.00E+00	0.00E+00	2.18E-04	2.18E-04	5.45E-05	9.43E-05
1,3,5-trimethylbenzene	120.20	15.000	1.31E-04	0.00E+00	0.00E+00	0.00E+00	1.31E-04	3.29E-05	5.69E-05
1-ethyl-2-methylbenzene	120.20	25.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
isopropylbenzene	120.20	74.000	1.86E-05	0.00E+00	0.00E+00	0.00E+00	1.86E-05	4.64E-06	8.04E-06
propylbenzene	120.20	49.000	3.27E-04	0.00E+00	0.00E+00	1.09E-03	1.09E-03	3.55E-04	4.47E-04
1-methyl-3-propylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
n-butylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	2.75E-04	2.75E-04	6.88E-05	1.19E-04
1-isopropyl-4-methylbenzene	134.22	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanoic acid methyl ester	60.05	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanoic acid ethyl ester	74.08	91.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid methyl ester	74.08	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid ethyl ester	88.11	180.000	3.86E-02	0.00E+00	0.00E+00	6.30E-03	3.86E-02	1.12E-02	1.60E-02
ethanoic acid allyl ester	100.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl propenoic acid methyl ester	100.12	100.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid isopropyl ester	102.13	210.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanoic acid butyl ester	102.13	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

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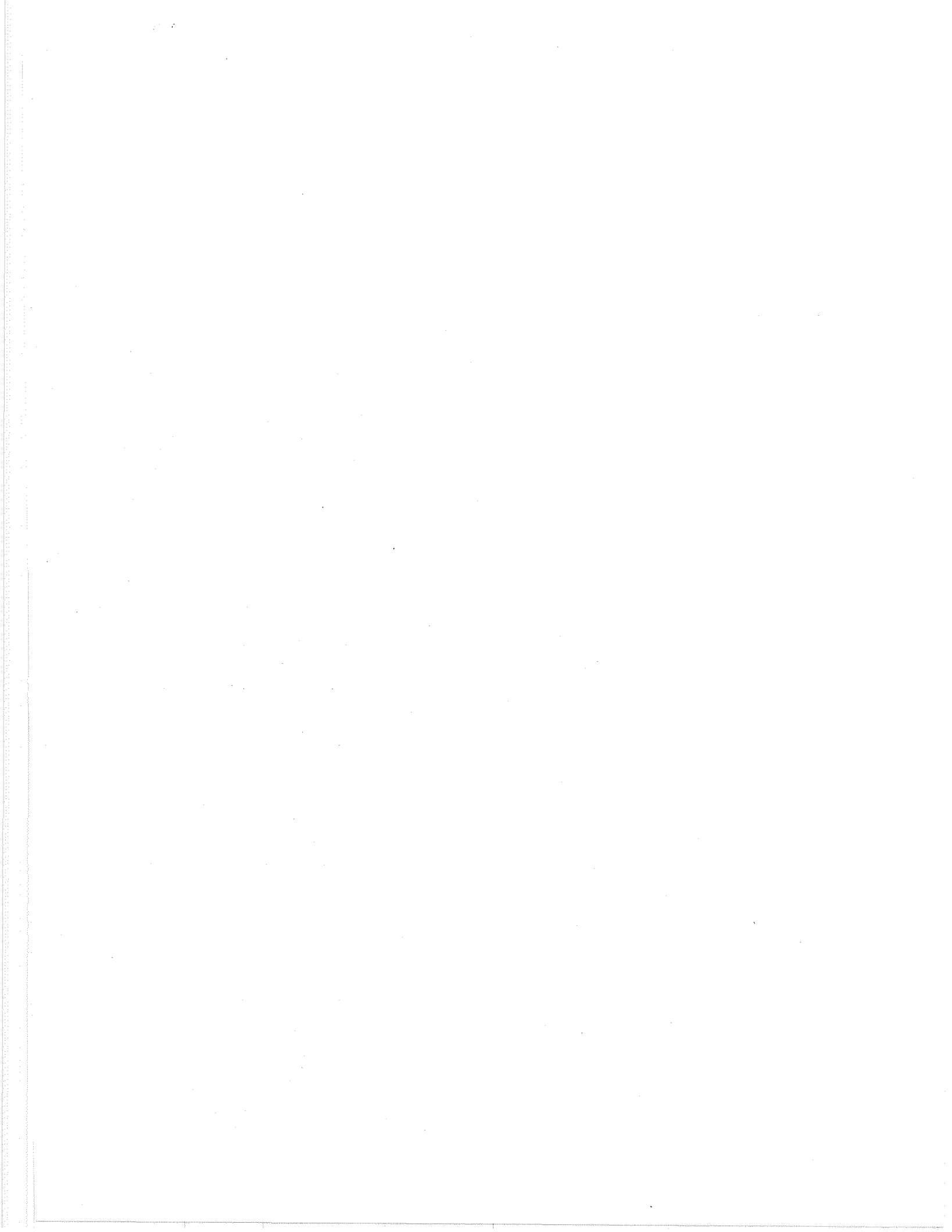
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IUPAC/ACCEPTED NAME	MOLECULAR WEIGHT	SMAC	Conkle Average	Kustov and Tiunov	Nefedov, et al	Dmitriyev, et al	Maximum Rate	Mean Rate	Standard Deviation
	(g/mole)	(mg/m ³)	(mg/h)	(mg/h)	(mg/h)	(mg/h)	(mg/h)	(mg/h)	(mg/h)
ethanoic acid propyl ester	102.13	170.000	2.43E-04	0.00E+00	0.00E+00	0.00E+00	2.43E-04	6.07E-05	1.05E-04
2-methyl propenoic acid ethyl ester	114.15	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid butyl ester	116.16	190.000	3.29E-03	0.00E+00	0.00E+00	4.93E-03	4.93E-03	2.05E-03	2.13E-03
ethanoic acid isobutyl ester	116.16	190.000	0.00E+00	0.00E+00	0.00E+00	2.89E-03	2.89E-03	7.23E-04	1.25E-03
lactic acid ethyl ester	118.13	190.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid 2-methoxy ethyl ester	118.36	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid isoamyl ester	130.18	0.100	0.00E+00	0.00E+00	0.00E+00	4.54E-03	4.54E-03	1.13E-03	1.96E-03
ethanoic acid amyl ester	130.18	160.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid 2-ethoxyethyl ester	132.16	160.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hydroxyethanoic acid ethyl ester	146.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
oxalic acid dibutyl ester	202.25	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-epoxy-1,3-butadiene	68.07	0.111	1.04E-02	0.00E+00	0.00E+00	7.63E-03	1.04E-02	4.49E-03	4.60E-03
1,4-epoxybutane	72.11	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methoxy-1-propene	72.11	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
diethyl ether	74.12	240.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methylfuran	82.10	0.130	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,3-dihydropyran	84.13	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-dioxane	88.11	0.100	5.86E-05	0.00E+00	0.00E+00	1.37E-02	1.37E-02	3.44E-03	5.93E-03
1,3,5-trioxane	90.08	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-ethoxyethanol	90.12	0.300	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
epichlorohydrin	92.53	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-ethylmorpholine	115.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-propoxybutane	116.21	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-butoxyethanol	118.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chloromethane	50.49	41.000	0.00E+00	0.00E+00	0.00E+00	2.70E-03	2.70E-03	6.74E-04	1.17E-03
chloroethene	62.50	3.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chloroethane	64.52	260.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-chloropropene	76.53	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dichloromethane	84.93	10.000	0.00E+00	0.00E+00	0.00E+00	2.36E-03	2.36E-03	5.89E-04	1.02E-03
1-chlorobutane	92.57	150.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1-dichloroethene	96.95	7.900	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloroethane	98.97	1.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloropropene	110.97	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chlorobenzene	112.56	46.000	0.00E+00	0.00E+00	0.00E+00	2.00E-03	2.00E-03	5.00E-04	8.66E-04
1,2-dichloropropane	112.99	42.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichloromethane	119.38	4.900	3.61E-05	0.00E+00	0.00E+00	3.13E-03	3.13E-03	7.90E-04	1.35E-03
1,2-dichloro-2-methylpropane	127.01	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichloroethene	131.39	10.000	0.00E+00	0.00E+00	0.00E+00	2.09E-03	2.09E-03	5.22E-04	9.05E-04
1,1,1-trichloroethane	133.41	160.000	2.42E-02	0.00E+00	0.00E+00	5.98E-04	2.42E-02	6.19E-03	1.04E-02
1,1,2-trichloroethane	133.41	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichlorobenzene	147.01	30.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-chloromethylheptane	148.68	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
tetrachloromethane	153.82	13.000	0.00E+00	0.00E+00	0.00E+00	3.00E-04	3.00E-04	7.50E-05	1.30E-04
tetrachloroethene	165.83	34.000	0.00E+00	0.00E+00	0.00E+00	1.88E-03	1.88E-03	4.69E-04	8.12E-04
chlorodifluoromethane	86.47	350.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dichlorofluoromethane	102.90	21.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-chloro-1,2,2-trifluoroethane	118.50	480.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dichlorodifluoromethane	120.91	490.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloro-1,2-difluoroethene	132.93	140.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chlorotetrafluoroethane	136.48	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichlorofluoromethane	137.40	560.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
bromotrifluoromethane	148.90	11000.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2-trichloro-1,2,2-trifluoroethane	187.40	400.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methane	16.04	3800.000	0.00E+00	1.69E-05	3.18E-01	4.50E-01	4.50E-01	1.92E-01	1.98E-01
ethyne	26.04	530.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethene	28.05	340.000	1.30E-04	0.00E+00	2.56E-02	4.00E-03	2.56E-02	7.44E-03	1.06E-02

IUPAC/ACCEPTED NAME	MOLECULAR WEIGHT (g/mole)	SMAC (mg/m ³)	Conkle Average (mg/h)	Kustov and Tiunov (mg/h)	Nefedov, et al (mg/h)	Dmitriyev, et al (mg/h)	Maximum Rate (mg/h)	Mean Rate (mg/h)	Standard Deviation (mg/h)
ethane	30.07	1200.000	0.00E+00	0.00E+00	2.56E-02	2.39E-01	2.39E-01	6.62E-02	1.00E-01
propadiene	40.07	82.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propyne	40.07	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propene	42.08	860.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propane	44.09	900.000	3.00E-04	0.00E+00	2.56E-02	2.09E-01	2.09E-01	5.87E-02	8.73E-02
1,3-butadiene	54.09	0.130	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-butene	56.10	460.000	1.85E-02	0.00E+00	0.00E+00	2.04E-03	1.85E-02	5.13E-03	7.75E-03
2-methylpropane	58.12	240.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
butane	58.12	240.000	2.65E-03	0.00E+00	0.00E+00	0.00E+00	2.65E-03	6.63E-04	1.15E-03
cyclopentene	68.11	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-1,3-butadiene	68.12	560.000	6.56E-02	0.00E+00	0.00E+00	2.41E-02	6.56E-02	2.24E-02	2.68E-02
1-pentene	70.13	190.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methylbutane	72.15	300.000	0.00E+00	0.00E+00	0.00E+00	3.80E-02	3.80E-02	9.51E-03	1.65E-02
pentane	72.15	590.000	0.00E+00	0.00E+00	0.00E+00	4.39E-02	4.39E-02	1.10E-02	1.90E-02
3,4,5,6-tetrahydrobenzene	82.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexene	84.16	0.100	2.47E-03	0.00E+00	0.00E+00	0.00E+00	2.47E-03	6.17E-04	1.07E-03
cyclohexane	84.16	210.000	0.00E+00	0.00E+00	0.00E+00	4.93E-03	4.93E-03	1.23E-03	2.13E-03
methylcyclopentane	84.16	52.000	1.44E-04	0.00E+00	0.00E+00	4.16E-03	4.16E-03	1.08E-03	1.78E-03
2,2-dimethylbutane	86.17	88.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methylpentane	86.18	1800.000	0.00E+00	0.00E+00	0.00E+00	5.43E-03	5.43E-03	1.36E-03	2.35E-03
hexane	86.18	180.000	1.14E-03	0.00E+00	2.56E-02	4.68E-03	2.56E-02	7.86E-03	1.04E-02
4-methylcyclohexene	96.17	390.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-heptene	98.18	200.000	0.00E+00	0.00E+00	0.00E+00	1.56E-03	1.56E-03	3.90E-04	6.75E-04
methylcyclohexane	98.18	60.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,2-dimethylpentane	100.21	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,4-dimethylpentane	100.21	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-ethylpentane	100.21	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
heptane	100.21	200.000	0.00E+00	0.00E+00	0.00E+00	3.95E-03	3.95E-03	9.87E-04	1.71E-03
1,1-dimethylcyclohexane	112.22	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-octene	112.22	230.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6-methyl-1-heptene	112.22	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trans-1,2-dimethylcyclohexane	112.22	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,2,3-trimethylpentane	114.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3,3-dimethylhexane	114.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-ethylhexane	114.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
octane	114.23	350.000	0.00E+00	0.00E+00	0.00E+00	4.18E-03	4.18E-03	1.04E-03	1.81E-03
4-ethylheptane	128.26	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nonane	128.26	320.000	0.00E+00	0.00E+00	0.00E+00	2.25E-03	2.25E-03	5.63E-04	9.74E-04
4-isopropenyl-1-methylcyclohexene	136.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-3-ethylheptane	142.28	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
decane	142.28	230.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
undecane	156.31	320.000	0.00E+00	0.00E+00	0.00E+00	1.91E-03	1.91E-03	4.78E-04	8.27E-04
dodecane	170.34	280.000	0.00E+00	0.00E+00	0.00E+00	1.80E-03	1.80E-03	4.51E-04	7.81E-04
2-propanone	58.08	50.000	5.39E-01	9.54E-01	8.97E-02	5.91E-03	9.54E-01	3.97E-01	3.80E-01
3-buten-2-one	70.00	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-butanone	72.11	30.000	1.48E-02	0.00E+00	3.07E-02	3.93E-03	3.07E-02	1.24E-02	1.19E-02
cyclopentanone	84.11	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-penten-2-one	84.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
acetyl cyclopropane	84.13	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-pentanone	86.13	70.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methyl-2-butanone	86.13	70.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-methyl-3-penten-2-one	98.14	40.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cyclohexanone	98.14	60.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3,3-dimethyl-2-butanone	100.16	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-methyl-2-pentanone	100.16	140.000	1.97E-03	0.00E+00	0.00E+00	2.20E-03	2.20E-03	1.04E-03	1.04E-03
2,4-dimethyl-3-pentanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-heptanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5-methyl-2-hexanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
acetophenone	120.14	250.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

APPENDIX G

Metabolic Contaminant Generation From Flatus



IUPAC/ACCEPTED NAME	MOLECULAR WEIGHT (g/mole)	SMAC (mg/m ³)	Kustov and Tiunov (percent)	Murphy (percent)	Kirk (percent)	Maximum Rate (mg/h)	Mean Rate (mg/h)	Standard Deviation (mg/h)
methanol	32.04	9.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanol	46.07	2000.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-propen-1-ol	58.08	1.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-propanol	60.09	150.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-propanol	60.09	98.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-ethanediol	62.07	13.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-butanol	74.12	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-1-propanol	74.12	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-2-propanol	74.12	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-butanol	74.12	80.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-propanediol	76.10	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methyl-1-butanol	88.15	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-pentanol	88.15	130.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
phenol	94.11	7.700	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cyclohexanol	100.16	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-ethyl-1-butanol	102.17	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexanol	102.18	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,3-dichloro-2-propanol	128.99	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-ethylhexanol	130.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nonanol	144.26	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
decanol	159.29	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanal	30.03	0.050	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanal	44.05	4.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-propenal	56.06	0.030	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propanal	58.08	95.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methylpropanal	70.09	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
butanal	72.10	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
pentanal	86.13	110.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,4-hexadien-1-al	96.13	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hexanal	100.16	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
benzaldehyde	106.12	173.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
heptanal	114.19	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-methylbenzaldehyde	120.15	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
octanal	128.22	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
benzene	78.11	0.200	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methylbenzene	92.15	60.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethenylbenzene	104.14	43.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dimethylbenzene	106.16	220.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,3-dimethylbenzene	106.16	220.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-dimethylbenzene	106.16	220.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethylbenzene	106.16	130.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
indene	116.16	9.500	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
alpha-methylstyrene	118.18	140.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2,4-trimethylbenzene	120.20	15.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,3,5-trimethylbenzene	120.20	15.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-ethyl-2-methylbenzene	120.20	25.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
isopropylbenzene	120.20	74.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propylbenzene	120.20	49.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-methyl-3-propylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
n-butylbenzene	134.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-isopropyl-4-methylbenzene	134.22	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanoic acid methyl ester	60.05	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanoic acid ethyl ester	74.08	91.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid methyl ester	74.08	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid ethyl ester	88.11	180.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid allyl ester	100.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl propenoic acid methyl ester	100.12	100.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid isopropyl ester	102.13	210.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methanoic acid butyl ester	102.13	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

PRECEDING PAGE BLANK NOT FILLED

PAGE 56 INTERIMONALLY BLANK

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	Kustov	Murphy	Kirk	Maximum	Mean	Standard
	WEIGHT		and Tiunov	(percent)	(percent)	(percent)	Rate	Rate
	(g/mole)	(mg/m ³)	(percent)	(percent)	(percent)	(mg/h)	(mg/h)	(mg/h)
ethanoic acid propyl ester	102.13	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl propenoic acid ethyl ester	114.15	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid butyl ester	116.16	190.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid isobutyl ester	116.16	190.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
lactic acid ethyl ester	118.13	190.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid 2-methoxy ethyl ester	118.36	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid isoamyl ester	130.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid amyl ester	130.18	160.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethanoic acid 2-ethoxyethyl ester	132.16	160.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hydroxyethanoic acid ethyl ester	146.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
oxalic acid dibutyl ester	202.25	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-epoxy-1,3-butadiene	68.07	0.111	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-epoxybutane	72.11	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methoxy-1-propene	72.11	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
diethyl ether	74.12	240.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methylfuran	82.10	0.130	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,3-dihydropyran	84.13	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,4-dioxane	88.11	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,3,5-trioxane	90.08	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-ethoxyethanol	90.12	0.300	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
epichlorohydrin	92.53	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-ethylmorpholine	115.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-propoxybutane	116.21	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-butoxyethanol	118.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chloromethane	50.49	41.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chloroethene	62.50	3.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chloroethane	64.52	260.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-chloropropene	76.53	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dichloromethane	84.93	10.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-chlorobutane	92.57	150.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1-dichloroethene	96.95	7.900	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloroethane	98.97	1.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloropropene	110.97	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chlorobenzene	112.56	46.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloropropane	112.99	42.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichloromethane	119.38	4.900	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloro-2-methylpropane	127.01	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichloroethene	131.39	10.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,1-trichloroethane	133.41	160.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2-trichloroethane	133.41	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichlorobenzene	147.01	30.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-chloromethylheptane	148.68	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
tetrachloromethane	153.82	13.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
tetrachloroethene	165.83	34.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chlorodifluoromethane	86.47	350.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dichlorofluoromethane	102.90	21.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-chloro-1,2,2-trifluoroethane	118.50	480.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dichlorodifluoromethane	120.91	490.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloro-1,2-difluoroethene	132.93	140.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
chlorotetrafluoroethane	136.48	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trichlorofluoromethane	137.40	560.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
bromotrifluoromethane	148.90	11000.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2-trichloro-1,2,2-trifluoroethane	187.40	400.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methane	16.04	3800.000	2.23E-01	1.80E-01	7.20E-02	1.32E+01	9.34E+00	3.75E+00
ethyne	26.04	530.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
ethene	28.05	340.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	Kustov	Murphy	Kirk	Maximum	Mean	Standard
	WEIGHT		and Tiunov	(percent)	(percent)	(percent)	Rate	Rate
	(g/mole)	(mg/m ³)	(percent)	(percent)	(percent)	(mg/h)	(mg/h)	(mg/h)
ethane	30.07	1200.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propadiene	40.07	82.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propyne	40.07	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propene	42.08	860.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
propane	44.09	900.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,3-butadiene	54.09	0.130	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-butene	56.10	460.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methylpropane	58.12	240.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
butane	58.12	240.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cyclopentene	68.11	170.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-1,3-butadiene	68.12	560.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-pentene	70.13	190.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methylbutane	72.15	300.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
pentane	72.15	590.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3,4,5,6-tetrahydrobenzene	82.14	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-hexene	84.16	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cyclohexane	84.16	210.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methylcyclopentane	84.16	52.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,2-dimethylbutane	86.17	88.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methylpentane	86.18	1800.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
hexane	86.18	180.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-methylcyclohexene	96.17	390.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1-heptene	98.18	200.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
methylcyclohexane	98.18	60.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,2-dimethylpentane	100.21	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,4-dimethylpentane	100.21	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-ethylpentane	100.21	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
heptane	100.21	200.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1,1-dimethylcyclohexane	112.22	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-octene	112.22	230.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
6-methyl-1-heptene	112.22	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
trans-1,2-dimethylcyclohexane	112.22	120.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,2,3-trimethylpentane	114.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3,3-dimethylhexane	114.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-ethylhexane	114.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
octane	114.23	350.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-ethylheptane	128.26	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
nonane	128.26	320.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-isopropenyl-1-methylcyclohexene	136.23	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-methyl-3-ethylheptane	142.28	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
decane	142.28	230.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
undecane	156.31	320.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
dodecane	170.34	280.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-propanone	58.08	50.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-buten-2-one	70.00	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-butanone	72.11	30.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cyclopentanone	84.11	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-penten-2-one	84.12	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
acetyl cyclopropane	84.13	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-pentanone	86.13	70.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3-methyl-2-butanone	86.13	70.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-methyl-3-penten-2-one	98.14	40.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
cyclohexanone	98.14	60.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
3,3-dimethyl-2-butanone	100.16	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
4-methyl-2-pentanone	100.16	140.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2,4-dimethyl-3-pentanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
2-heptanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
5-methyl-2-hexanone	114.18	0.100	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
acetophenone	120.14	250.000	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00

APPENDIX H
Metabolic Contaminant Generation From Sweat

METABOLIC CONTAMINANT GENERATION FROM SWEAT

7/13/95

IUPAC/ACCEPTED NAME	MOLECULAR WEIGHT (g/mole)	SMAC (mg/m ³)	Dmitriyev, et al (mg/h)
methanol	32.04	9.000	2.16E-03
ethanol	46.07	2000.000	1.13E-02
2-propen-1-ol	58.08	1.000	0.00E+00
2-propanol	60.09	150.000	1.49E-02
1-propanol	60.09	98.000	1.30E-02
1,2-ethanediol	62.07	13.000	0.00E+00
2-butanol	74.12	120.000	0.00E+00
2-methyl-1-propanol	74.12	120.000	0.00E+00
2-methyl-2-propanol	74.12	120.000	0.00E+00
1-butanol	74.12	80.000	1.18E-02
1,2-propanediol	76.10	0.100	0.00E+00
3-methyl-1-butanol	88.15	0.100	1.06E-02
1-pentanol	88.15	130.000	0.00E+00
phenol	94.11	7.700	9.30E-03
cyclohexanol	100.16	120.000	1.23E-02
2-ethyl-1-butanol	102.17	0.100	0.00E+00
2-hexanol	102.18	170.000	0.00E+00
1,3-dichloro-2-propanol	128.99	0.100	0.00E+00
2-ethylhexanol	130.23	0.100	0.00E+00
nonanol	144.26	0.100	0.00E+00
decanol	159.29	0.100	0.00E+00
methanal	30.03	0.050	4.00E-04
ethanal	44.05	4.000	2.63E-03
2-propenal	56.06	0.030	0.00E+00
propanal	58.08	95.000	0.00E+00
2-methylpropenal	70.09	0.100	0.00E+00
butanal	72.10	120.000	0.00E+00
pentanal	86.13	110.000	4.54E-04
2,4-hexadien-1-al	96.13	0.100	0.00E+00
hexanal	100.16	0.100	5.05E-04
benzaldehyde	106.12	173.000	1.91E-04
heptanal	114.19	0.100	4.75E-04
4-methylbenzaldehyde	120.15	0.100	0.00E+00
octanal	128.22	0.100	5.64E-04
benzene	78.11	0.200	2.57E-02
methylbenzene	92.15	60.000	1.50E-02
ethenylbenzene	104.14	43.000	1.16E-05
1,2-dimethylbenzene	106.16	220.000	7.62E-04
1,3-dimethylbenzene	106.16	220.000	7.62E-04
1,4-dimethylbenzene	106.16	220.000	7.62E-04
ethylbenzene	106.16	130.000	1.15E-02
indene	116.16	9.500	0.00E+00
alpha-methylstyrene	118.18	140.000	0.00E+00
1,2,4-trimethylbenzene	120.20	15.000	0.00E+00
1,3,5-trimethylbenzene	120.20	15.000	0.00E+00
1-ethyl-2-methylbenzene	120.20	25.000	0.00E+00
isopropylbenzene	120.20	74.000	0.00E+00
propylbenzene	120.20	49.000	7.95E-04
1-methyl-3-propylbenzene	134.12	0.100	0.00E+00
n-butylbenzene	134.12	0.100	0.00E+00
1-isopropyl-4-methylbenzene	134.22	0.100	0.00E+00
methanoic acid methyl ester	60.05	0.100	0.00E+00
methanoic acid ethyl ester	74.08	91.000	0.00E+00
ethanoic acid methyl ester	74.08	120.000	0.00E+00
ethanoic acid ethyl ester	88.11	180.000	5.05E-03
ethanoic acid allyl ester	100.12	0.100	0.00E+00
2-methyl propenoic acid methyl ester	100.12	100.000	0.00E+00
ethanoic acid isopropyl ester	102.13	210.000	0.00E+00
methanoic acid butyl ester	102.13	0.100	0.00E+00

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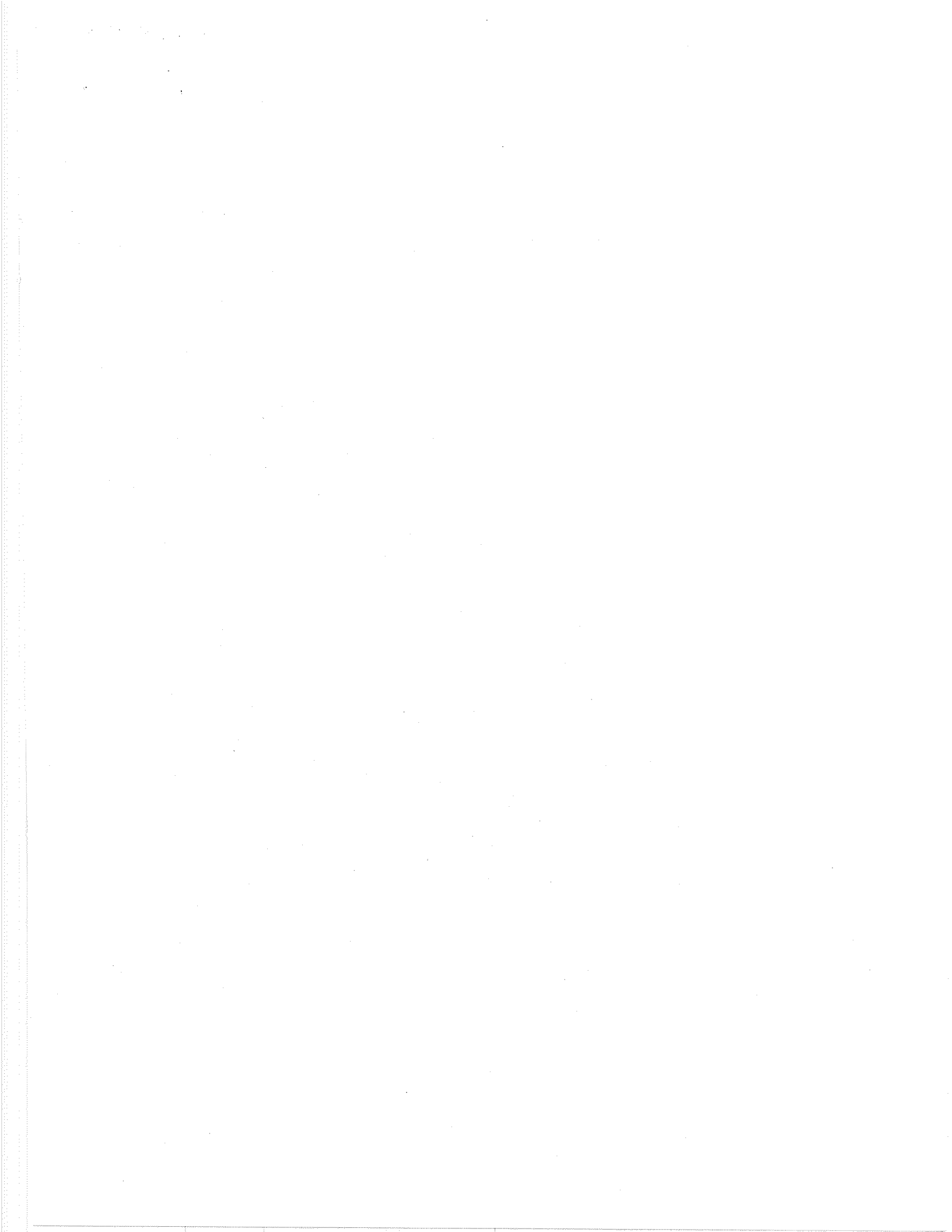
IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	Dmitriyev,
	WEIGHT		et al
	(g/mole)	(mg/m ³)	(mg/h)
ethanoic acid propyl ester	102.13	170.000	0.00E+00
2-methyl propenoic acid ethyl ester	114.15	0.100	0.00E+00
ethanoic acid butyl ester	116.16	190.000	3.43E-03
ethanoic acid isobutyl ester	116.16	190.000	2.45E-03
lactic acid ethyl ester	118.13	190.000	0.00E+00
ethanoic acid 2-methoxy ethyl ester	118.36	0.100	0.00E+00
ethanoic acid isoamyl ester	130.18	0.100	3.63E-03
ethanoic acid amyl ester	130.18	160.000	0.00E+00
ethanoic acid 2-ethoxyethyl ester	132.16	160.000	0.00E+00
hydroxyethanoic acid ethyl ester	146.14	0.100	0.00E+00
oxalic acid dibutyl ester	202.25	0.100	0.00E+00
1,4-epoxy-1,3-butadiene	68.07	0.111	4.13E-03
1,4-epoxybutane	72.11	120.000	0.00E+00
3-methoxy-1-propene	72.11	0.100	0.00E+00
diethyl ether	74.12	240.000	0.00E+00
2-methylfuran	82.10	0.130	0.00E+00
2,3-dihydropyran	84.13	0.100	0.00E+00
1,4-dioxane	88.11	0.100	9.79E-03
1,3,5-trioxane	90.08	0.100	0.00E+00
2-ethoxyethanol	90.12	0.300	0.00E+00
epichlorohydrin	92.53	0.100	0.00E+00
1,1,2,2-tetramethyl-1,2-epoxyethane	100.12	0.100	0.00E+00
4-ethylmorpholine	115.18	0.100	0.00E+00
1-propoxybutane	116.21	0.100	0.00E+00
2-butoxyethanol	118.18	0.100	0.00E+00
chloromethane	50.49	41.000	1.82E-03
chloroethene	62.50	3.000	0.00E+00
chloroethane	64.52	260.000	0.00E+00
3-chloropropene	76.53	0.100	0.00E+00
dichloromethane	84.93	10.000	2.11E-03
1-chlorobutane	92.57	150.000	0.00E+00
1,1-dichloroethene	96.95	7.900	0.00E+00
1,2-dichloroethane	98.97	1.000	0.00E+00
1,2-dichloropropene	110.97	0.100	0.00E+00
chlorobenzene	112.56	46.000	1.57E-03
1,2-dichloropropane	112.99	42.000	0.00E+00
trichloromethane	119.38	4.900	2.21E-03
1,2-dichloro-2-methylpropane	127.01	0.100	0.00E+00
trichloroethene	131.39	10.000	1.69E-03
1,1,1-trichloroethane	133.41	160.000	5.13E-04
1,1,2-trichloroethane	133.41	0.100	5.13E-04
1,2-dichlorobenzene	147.01	30.000	0.00E+00
3-chloromethylheptane	148.68	0.100	0.00E+00
tetrachloromethane	153.82	13.000	2.39E-04
tetrachloroethene	165.83	34.000	1.50E-03
chlorodifluoromethane	86.47	350.000	0.00E+00
dichlorofluoromethane	102.90	21.000	0.00E+00
1-chloro-1,2,2-trifluoroethane	118.50	480.000	0.00E+00
dichlorodifluoromethane	120.91	490.000	0.00E+00
1,2-dichloro-1,2-difluoroethene	132.93	140.000	0.00E+00
chlorotetrafluoroethane	136.48	0.100	0.00E+00
trichlorofluoromethane	137.40	560.000	0.00E+00
bromotrifluoromethane	148.90	11000.000	0.00E+00
1,2-dichloro-1,1,2,2-tetrafluoroethane	170.92	700.000	0.00E+00
1,1,2-trichloro-1,2,2-trifluoroethane	187.40	400.000	0.00E+00
1,1,2,2-tetrachloro-1,2-difluoroethane	204.00	830.000	0.00E+00
methane	16.04	3800.000	2.21E-01
ethyne	26.04	530.000	0.00E+00
ethene	28.05	340.000	2.21E-01

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	Dmitriyev, et al
	WEIGHT		
	(g/mole)	(mg/m ³)	(mg/h)
ethane	30.07	1200.000	1.13E-01
propadiene	40.07	82.000	0.00E+00
propyne	40.07	0.100	0.00E+00
propene	42.08	860.000	0.00E+00
propane	44.09	900.000	7.82E-02
1,3-butadiene	54.09	0.130	0.00E+00
1-butene	56.10	460.000	1.68E-03
2-methylpropane	58.12	240.000	0.00E+00
butane	58.12	240.000	0.00E+00
cyclopentene	68.11	170.000	0.00E+00
2-methyl-1,3-butadiene	68.12	560.000	1.56E-02
1-pentene	70.13	190.000	0.00E+00
2-methylbutane	72.15	300.000	0.00E+00
pentane	72.15	590.000	2.09E-02
3,4,5,6-tetrahydrobenzene	82.14	0.100	0.00E+00
2-hexene	84.16	0.100	0.00E+00
cyclohexane	84.16	210.000	3.82E-03
methylcyclopentane	84.16	52.000	2.93E-03
2,2-dimethylbutane	86.17	88.000	0.00E+00
3-methylpentane	86.18	1800.000	0.00E+00
hexane	86.18	180.000	2.75E-03
4-methylcyclohexene	96.17	390.000	0.00E+00
1-heptene	98.18	200.000	1.17E-03
methylcyclohexane	98.18	60.000	0.00E+00
2,2-dimethylpentane	100.21	0.100	0.00E+00
2,4-dimethylpentane	100.21	0.100	0.00E+00
3-ethylpentane	100.21	0.100	0.00E+00
heptane	100.21	200.000	2.55E-03
1,1-dimethylcyclohexane	112.22	120.000	0.00E+00
2-octene	112.22	230.000	0.00E+00
6-methyl-1-heptene	112.22	0.100	0.00E+00
trans-1,2-dimethylcyclohexane	112.22	120.000	0.00E+00
2,2,3-trimethylpentane	114.23	0.100	0.00E+00
3,3-dimethylhexane	114.23	0.100	0.00E+00
3-ethylhexane	114.23	0.100	0.00E+00
octane	114.23	350.000	2.25E-03
4-ethylheptane	128.26	0.100	0.00E+00
nonane	128.26	320.000	1.61E-03
4-isopropenyl-1-methylcyclohexene	136.23	0.100	0.00E+00
2-methyl-3-ethylheptane	142.28	0.100	0.00E+00
decane	142.28	230.000	1.25E-03
undecane	156.31	320.000	1.33E-03
dodecane	170.34	280.000	1.17E-03
2-propanone	58.08	50.000	4.00E-03
3-buten-2-one	70.00	0.100	0.00E+00
2-butanone	72.11	30.000	3.52E-01
cyclopentanone	84.11	0.100	0.00E+00
3-penten-2-one	84.12	0.100	0.00E+00
acetyl cyclopropane	84.13	0.100	0.00E+00
2-pentanone	86.13	70.000	0.00E+00
3-methyl-2-butanone	86.13	70.000	0.00E+00
4-methyl-3-penten-2-one	98.14	40.000	0.00E+00
cyclohexanone	98.14	60.000	0.00E+00
3,3-dimethyl-2-butanone	100.16	0.100	0.00E+00
4-methyl-2-pentanone	100.16	140.000	2.07E-03
2,4-dimethyl-3-pentanone	114.18	0.100	0.00E+00
2-heptanone	114.18	0.100	1.74E-03
5-methyl-2-hexanone	114.18	0.100	0.00E+00
acetophenone	120.14	250.000	0.00E+00

IUPAC/ACCEPTED NAME	MOLECULAR	SMAC	Dmitriyev,
	WEIGHT		et al
	(g/mole)	(mg/m ³)	(mg/h)
2-octanone	128.21	100.000	0.00E+00
5-methyl-3-heptanone	128.21	0.100	0.00E+00
2,6-dimethyl-4-heptanone	142.20	58.000	0.00E+00
hydrogen sulfide	34.08	2.800	0.00E+00
carbonyl sulfide	60.07	12.000	0.00E+00
ethylene sulfide	60.11	0.100	0.00E+00
dimethyl sulfide	62.14	2.500	0.00E+00
carbon disulfide	76.14	16.000	0.00E+00
pentamethylene sulfide	102.20	0.100	0.00E+00
nitric oxide	30.01	6.100	0.00E+00
nitrogen dioxide	46.01	0.940	0.00E+00
nitrogen tetroxide	92.01	0.100	0.00E+00
ethanoic acid	60.05	7.400	2.27E-02
2-ethylhexanoic acid	144.21	0.100	0.00E+00
hydrazine	32.05	0.005	0.00E+00
methyl cyanide	41.05	6.700	3.63E-03
methyl hydrazine	46.07	0.004	0.00E+00
nitromethane	61.04	13.000	0.00E+00
N,N-dimethylformamide	73.10	0.100	0.00E+00
nitroethane	75.07	0.100	0.00E+00
2,3-benzopyrrole	117.15	0.250	1.61E-06
hydrogen	2.02	340.000	0.00E+00
ammonia	17.00	7.000	0.00E+00
carbon monoxide	28.01	10.000	0.00E+00
disiloxane	78.10	0.100	0.00E+00
trimethylsilanol	90.21	40.000	0.00E+00
trisiloxane	124.30	0.100	0.00E+00
hexamethyldisiloxane	162.48	0.100	0.00E+00
tetrasiloxane	170.40	0.100	0.00E+00
diphenylsilane	184.32	0.100	0.00E+00
hexamethylcyclotrisiloxane	222.40	230.000	0.00E+00
octamethyltrisiloxane	236.54	40.000	0.00E+00
octamethylcyclotetrasiloxane	296.62	0.100	0.00E+00
decamethylcyclopentasiloxane	370.64	0.100	0.00E+00
decamethylcyclohexasiloxane	444.71	0.100	0.00E+00
tetradecamethylcycloheptasiloxane	519.09	0.100	0.00E+00
hexadecamethylcyclooctasiloxane	593.24	0.100	0.00E+00

APPENDIX I

Metabolic Contaminant Generation From Endogenic Carbon Monoxide



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<i>IUPAC/ACCEPTED NAME</i>	<i>MOLECULAR WEIGHT (g/mole)</i>	<i>SMAC (mg/m³)</i>	<i>Coburn, et al (mg/h)</i>	<i>Dmitriyev, et al (mg/h)</i>	<i>Nefedov, et al (mg/h)</i>	<i>Maximum Rate (mg/h)</i>	<i>Mean Rate (mg/h)</i>	<i>Standard Deviation (mg/h)</i>
carbon monoxide	28.01	10.000	7.66E-01	5.74E-01	3.84E-01	7.66E-01	5.75E-01	1.56E-01

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APPENDIX J

Trace Chemical Contaminant Physical Property Data

IUPAC/ACCEPTED NAME	MOLECULAR	LIQUID	MOLAR	VAPOR	HENRY'S
	WEIGHT	DENSITY	VOLUME	PRESSURE	LAW CONST
	g/gmole	g/cm ³	cm ³ /gmole	mg/m ³	atm
methanol	32.04	0.75	42.50	194708.47	0.39
ethanol	46.07	0.74	62.10	127574.70	0.45
2-propen-1-ol	58.08	0.85	74.10	62345.68	0.31
2-propanol	60.09	0.73	80.90	125696.88	0.62
1-propanol	60.09	0.80	81.40	55628.20	0.51
1,2-ethanediol	62.07	1.11	64.90	335.41	0.00
2-butanol	74.12	0.81	103.60	60818.49	0.27
2-methyl-1-propanol	74.12	0.72	101.90	33900.87	0.22
2-methyl-2-propanol	74.12	0.79	102.80	141677.93	2.81
1-butanol	74.12	0.73	102.10	19908.26	1.36
1,2-propanediol	76.10	1.04	90.00	21770.00	0.00
3-methyl-1-butanol	88.15	0.81	123.60	11526.65	0.19
1-pentanol	88.15	0.81	123.70	8854.10	0.68
phenol	94.11	1.07	101.90	1349.94	0.00
cyclohexanol	100.16	0.83	118.20	5440.00	31.32
2-ethyl-1-butanol	102.17	0.83	148.00	35790.00	3.27
2-hexanol	102.18	0.82	146.40	24470.00	1.04
1,3-dichloro-2-propanol	128.99	1.36	115.00	2014.00	0.09
2-ethylhexanol	130.23	0.83	190.00	560.45	0.27
nonanol	144.26	0.83	213.00	644.00	3.41
decanol	159.29	0.83	235.00	25.99	1.48
methanal	30.03	0.82	29.60	6004183.38	0.01
ethanal	44.05	0.78	56.90	2021809.70	5.58
2-propenal	56.06	0.85	65.00	761419.06	64.69
propanal	58.08	0.81	74.80	923684.23	5.31
2-methylpropenal	70.09	0.84	86.00	605400.00	147.08
butanal	72.10	0.69	118.20	395891.04	7.63
pentanal	86.13	0.81	118.20	141349.29	12.49
2,4-hexadien-1-al	96.13	0.90	122.00	6274.00	0.00
hexanal	100.16	0.81	140.00	105900.00	28.46
benzaldehyde	106.12	1.04	118.40	5760.80	2.45
heptanal	114.19	0.85	162.00	14158.00	23.75
4-methylbenzaldehyde	120.15	1.02	140.00	28.00	0.00
octanal	128.22	0.82	184.00	458.00	0.27
benzene	78.11	0.82	96.50	364866.29	257.40
methylbenzene	92.15	0.78	118.20	125752.13	353.10
ethenylbenzene	104.14	0.91	133.00	29789.22	146.30
1,2-dimethylbenzene	106.16	0.76	140.00	41161.04	232.50
1,3-dimethylbenzene	106.16	0.76	137.90	32662.25	370.10
1,4-dimethylbenzene	106.16	0.75	140.50	43504.52	336.90
ethylbenzene	106.16	0.87	139.50	47242.81	446.80
indene	116.16	0.99	136.00	19330.00	0.00
alpha-methylstyrene	118.18	0.92	155.00	9245.87	157.30
1,2,4-trimethylbenzene	120.20	0.88	163.00	11052.71	313.00
1,3,5-trimethylbenzene	120.20	0.86	162.80	13184.68	440.40
1-ethyl-2-methylbenzene	120.20	0.88	161.00	13516.59	157.97
isopropylbenzene	120.20	0.86	163.00	28808.06	805.30
propylbenzene	120.20	0.86	162.20	18514.20	567.10
1-methyl-3-propylbenzene	134.12	0.86	185.00	11410.00	287.35
n-butylbenzene	134.12	0.80	185.00	6141.69	730.70
1-isopropyl-4-methylbenzene	134.22	0.86	184.90	9213.61	13.62
methanoic acid methyl ester	60.05	0.97	62.60	1766656.97	630.50
methanoic acid ethyl ester	74.08	0.91	84.80	1124000.00	6.54
ethanoic acid methyl ester	74.08	0.93	84.80	791433.26	3.81
ethanoic acid ethyl ester	88.11	0.90	106.00	414935.41	6.26
ethanoic acid allyl ester	100.12	0.93	120.00	152800.00	0.00
methyl 2-methyl propenoate	100.12	0.94	120.00	237600.00	0.00
ethanoic acid isopropyl ester	102.13	0.87	128.80	393700.00	182.50
methanoic acid butyl ester	102.13	0.91	128.80	193200.00	0.00

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IUPAC/ACCEPTED NAME	MOLECULAR	LIQUID	MOLAR	VAPOR	HENRY'S
	WEIGHT	DENSITY	VOLUME	PRESSURE	LAW CONST
	g/gmole	g/cm ³	cm ³ /gmole	mg/m ³	atm
ethanoic acid propyl ester	102.13	0.89	128.80	159170.84	0.00
ethyl 2-methyl propenoate	114.15	0.91	143.00	108600.00	0.00
ethanoic acid butyl ester	116.16	0.76	151.00	60813.12	20.84
ethanoic acid isobutyl ester	116.16	0.87	151.00	93222.98	0.00
lactic acid ethyl ester	118.13	1.04	132.00	10260.00	10.07
2-methoxy ethyl ethanoate	118.36	1.01	131.00	22540.00	0.31
ethanoic acid isoamyl ester	130.18	0.87	172.00	43850.00	0.00
ethanoic acid amyl ester	130.18	0.88	172.00	21000.00	0.00
2-ethoxyethyl ethanoate	132.16	0.98	156.00	11640.00	0.72
ethyl acetylglycolate	146.14	1.11	155.00	5151.00	0.00
oxalic acid dibutyl ester	202.25	0.99	249.00	237.00	0.00
1,4-epoxy-1,3-butadiene	68.07	0.93	67.00	2063403.00	299.30
1,4-epoxybutane	72.11	0.89	88.00	578216.81	28.06
3-methoxy-1-propene	72.11	0.77	98.00	1354000.00	0.00
diethyl ether	74.12	0.71	106.40	2001438.92	0.00
2-methylfuran	82.10	0.91	88.00	769200.00	124.60
2,3-dihydropyran	84.13	0.92	97.00	494000.00	1.16
1,4-dioxane	88.11	1.03	94.70	206800.00	0.38
1,3,5-trioxane	90.08	1.20	79.00	132200.00	0.01
2-ethoxyethanol	90.12	0.93	113.00	14000.00	0.26
epichlorohydrin	92.53	1.18	86.00	143000.00	0.00
tetramethyl-1,2-epoxyethane	100.12	0.82	136.00	335340.00	534.40
4-ethylmorpholine	115.18	0.90	140.00	10140.00	0.20
1-propoxybutane	116.21	0.78	174.70	117700.00	0.00
2-butoxyethanol	118.18	0.90	154.00	6939.00	1.40
chloromethane	50.49	1.00	50.40	11417763.50	458.80
chloroethene	62.50	0.97	62.30	8757767.65	1245.00
chloroethane	64.52	0.89	71.70	3891762.21	384.40
3-chloropropene	76.53	0.94	84.40	1387650.04	23219.00
dichloromethane	84.93	1.29	65.10	1860277.31	137.60
1-chlorobutane	92.57	0.87	113.50	465783.19	532.50
1,1-dichloroethene	96.95	1.22	79.90	3404000.00	1241.00
1,2-dichloroethane	98.97	1.24	88.90	381191.36	69.45
1,2-dichloropropene	110.97	1.18	104.00	7245000.00	0.00
chlorobenzene	112.56	0.98	114.60	63522.67	252.10
1,2-dichloropropane	112.99	1.16	107.00	271152.73	73.54
trichloromethane	119.38	1.49	84.50	1155449.48	225.20
1,2-dichloro-2-methylpropane	127.01	1.09	132.00	283300.00	0.00
trichloroethene	131.39	1.39	98.10	477499.71	479.40
1,1,1-trichloroethane	133.41	1.34	108.00	958300.00	832.10
1,1,2-trichloroethane	133.41	1.44	108.00	2240193.37	42.22
1,2-dichlorobenzene	147.01	1.31	130.90	9348.78	163.90
3-chloromethylheptane	148.68	0.88	203.00	26200.00	0.00
tetrachloromethane	153.82	1.59	103.70	867420.54	1634.00
tetrachloroethene	165.83	1.52	114.80	145491.35	1492.00
chlorodifluoromethane	86.47	1.42	62.10	34420537.79	1677.00
dichlorofluoromethane	102.90	1.38	70.40	7151800.00	290.10
1-chloro-1,2,2-trifluoroethane	118.50	1.38	85.00	10420000.00	0.00
dichlorodifluoromethane	120.91	1.48	76.00	31128600.00	21690.00
dichlorodifluoroethene	132.93	1.50	90.00	6168000.00	0.00
chlorotetrafluoroethane	136.48	1.41	90.00	6090000.00	0.00
trichlorofluoromethane	137.40	1.47	88.30	5600894.36	6765.00
bromotrifluoromethane	148.90	0.95	68.00	92661150.00	0.00
dichlorotetrafluoroethane	170.92	1.48	107.60	14265500.00	67140.00
trichlorotrifluoroethane	187.40	1.50	120.00	3146782.38	26940.00
tetrachlorodifluoroethane	204.00	1.61	133.00	502605.00	0.00
methane	16.04	0.43	37.70	168940118.30	35390.00
ethyne	26.04	0.62	42.00	49466774.18	14020.00
ethene	28.05	0.58	49.40	70102917.32	11530.00

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	g/gmole	g/cm ³	cm ³ /gmole	mg/m ³	atm
ethane	30.07	0.55	56.70	47970692.79	26790.00
propadiene	40.07	0.66	63.00	9472430.85	0.00
propyne	40.07	0.71	60.00	8797678.65	591.20
propene	42.08	0.61	66.60	19269552.31	11320.00
propane	44.09	0.58	74.50	16810972.61	38030.00
1,3-butadiene	54.09	0.68	82.00	5925974.40	2424.00
1-butene	56.10	0.60	90.40	6521033.40	13600.00
2-methylpropane	58.12	0.55	96.00	7955325.05	63970.00
butane	58.12	0.60	96.40	5505797.82	50950.00
cyclopentene	68.11	0.77	94.00	1307502.60	3540.00
2-methyl-1,3-butadiene	68.12	0.68	103.60	1904024.04	4265.00
1-pentene	70.13	0.64	110.00	2280929.90	22090.00
2-methylbutane	72.15	0.62	117.40	2539336.87	75840.00
pentane	72.15	0.63	117.80	1878740.32	70250.00
3,4,5,6-tetrahydrobenzene	82.14	0.81	114.00	358424.55	4276.00
2-hexene	84.16	0.68	132.50	625519.56	16420.00
cyclohexane	84.16	0.78	117.00	404326.08	7953.00
methylcyclopentane	84.16	0.75	122.00	573403.28	19840.00
2,2-dimethylbutane	86.17	0.65	138.60	1388740.74	84400.00
3-methylpentane	86.18	0.66	140.60	815695.36	62320.00
hexane	86.18	0.66	139.90	645936.10	50293.00
4-methylcyclohexene	96.17	0.80	138.00	51330.00	0.00
1-heptene	98.18	0.70	154.80	268511.75	22260.00
methylcyclohexane	98.18	0.77	144.00	221051.70	23730.00
2,2-dimethylpentane	100.21	0.67	163.00	520207.81	175200.00
2,4-dimethylpentane	100.21	0.67	163.00	485069.69	163400.00
3-ethylpentane	100.21	0.70	163.00	282978.78	141000.00
heptane	100.21	0.68	162.60	221956.02	149900.00
1,1-dimethylcyclohexane	112.22	0.78	162.60	122128.30	0.00
2-octene	112.22	0.72	177.60	88000.00	34810.00
6-methyl-1-heptene	112.22	0.71	178.00	177700.00	0.00
trans-1,2-dimethylcyclohexane	112.22	0.77	164.30	104038.10	26480.00
2,2,3-trimethylpentane	114.23	0.72	185.00	176566.97	211500.00
3,3-dimethylhexane	114.23	0.71	185.00	157016.64	0.00
3-ethylhexane	114.23	0.71	185.00	108804.39	207000.00
octane	114.23	0.70	186.30	75075.31	273900.00
4-ethylheptane	128.26	0.73	207.00	52700.00	287100.00
nonane	128.26	0.72	207.00	25129.92	329500.00
isopropenylmethylcyclohexene	136.23	0.84	207.00	27900.00	0.00
2-methyl-3-ethylheptane	142.28	0.75	229.00	16690.00	0.00
decane	142.28	0.73	229.00	8188.93	262100.00
undecane	156.31	0.74	252.00	2627.60	101700.00
dodecane	170.34	0.75	274.00	836.22	1191.00
2-propanone	58.08	0.75	77.50	663190.31	2.38
3-buten-2-one	70.00	0.86	86.00	350000.00	5.76
2-butanone	72.11	0.75	96.70	334362.54	0.16
cyclopentanone	84.11	0.80	99.00	39939.49	0.00
3-penten-2-one	84.12	0.86	108.00	39944.24	6.38
acetyl cyclopropane	84.13	0.90	101.00	138100.00	7.65
2-pentanone	86.13	0.81	118.30	144912.91	1.91
3-methyl-2-butanone	86.13	0.81	118.40	214602.23	0.00
4-methyl-3-penten-2-one	98.14	0.86	129.00	56040.00	8.47
cyclohexanone	98.14	0.95	119.00	3583.00	1.36
3,3-dimethyl-2-butanone	100.16	0.80	139.80	189100.00	0.00
4-methyl-2-pentanone	100.16	0.71	140.00	94056.08	3.41
2,4-dimethyl-3-pentanone	114.18	0.81	162.00	44620.00	0.00
2-heptanone	114.18	0.81	162.80	24550.00	53.25
5-methyl-2-hexanone	114.18	0.89	162.00	46920.00	0.00


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	g/gmole	g/cm ³	cm ³ /gmole	mg/m ³	atm
acetophenone	120.14	1.03	140.00	1572.71	1.63
2-octanone	128.21	0.82	186.00	27570.00	8.17
5-methyl-3-heptanone	128.21	0.82	186.00	15500.00	0.00
2,6-dimethyl-4-heptanone	142.20	0.81	208.00	5568.00	36.77
hydrogen sulfide	34.08	0.99	35.00	27004992.20	4.90
carbonyl sulfide	60.07	1.27	49.00	29170300.00	2812.00
ethylene sulfide	60.11	1.01	64.00	1059000.00	337.70
dimethyl sulfide	62.14	0.85	74.00	1518920.52	0.00
carbon disulfide	76.14	1.20	66.00	1391158.36	1067.00
pentamethylene sulfide	102.20	0.99	122.00	42000.00	0.00
nitric oxide	30.01	1.27	23.80	4258094356.42	20686.00
nitrogen dioxide	46.01	1.45	32.00	2052330.89	20428.00
nitrogen tetroxide	92.01	1.45	64.00	5008000.00	20428.00
ethanoic acid	60.05	1.05	56.70	42794.33	0.07
2-ethylhexanoic acid	144.21	0.90	192.00	423.00	3.93
hydrazine	32.05	0.94	42.00	21294.15	39.63
methyl cyanide	41.05	0.83	57.30	172771.77	1.12
methyl hydrazine	46.07	0.88	63.00	108523.59	0.03
nitromethane	61.04	1.08	53.00	97463.92	15.06
N,N-dimethylformamide	73.10	0.94	89.00	17150.00	0.00
nitroethane	75.07	1.05	75.00	108900.00	0.00
2,3-benzopyrrole	117.15	1.22	139.80	74.00	0.02
hydrogen	2.02	0.07	3.00	56774595.77	65178.00
ammonia	17.00	0.67	25.00	6539209.36	0.94
carbon monoxide	28.01	0.80	22.10	433659725.72	63430.00
disiloxane	78.10	0.98	94.00	801400.00	0.00
trimethylsilanol	90.21	0.81	121.00	291300.00	0.00
trisiloxane	124.30	0.92	140.00	116500.00	0.00
hexamethyldisiloxane	162.48	0.76	227.00	361000.00	0.00
tetrasiloxane	170.40	0.96	187.00	100400.00	0.00
diphenylsilane	184.32	1.00	254.00	22.00	0.00
hexamethylcyclotrisiloxane	222.40	1.00	191.70	65880.00	0.00
octamethyltrisiloxane	236.54	0.82	318.00	75460.00	0.00
octamethylcyclotetrasiloxane	296.62	0.96	339.00	26600.00	0.00
decamethylcyclopentasiloxane	370.64	0.96	436.00	33000.00	0.00
decamethylcyclohexasiloxane	444.71	0.97	522.00	1200.00	0.00
tetradecamethylcycloheptasilox	519.09	0.97	607.00	460.00	0.00
hexadecamethylcyclooctasiloxane	593.24	1.18	695.00	265.00	0.00

APPROVAL

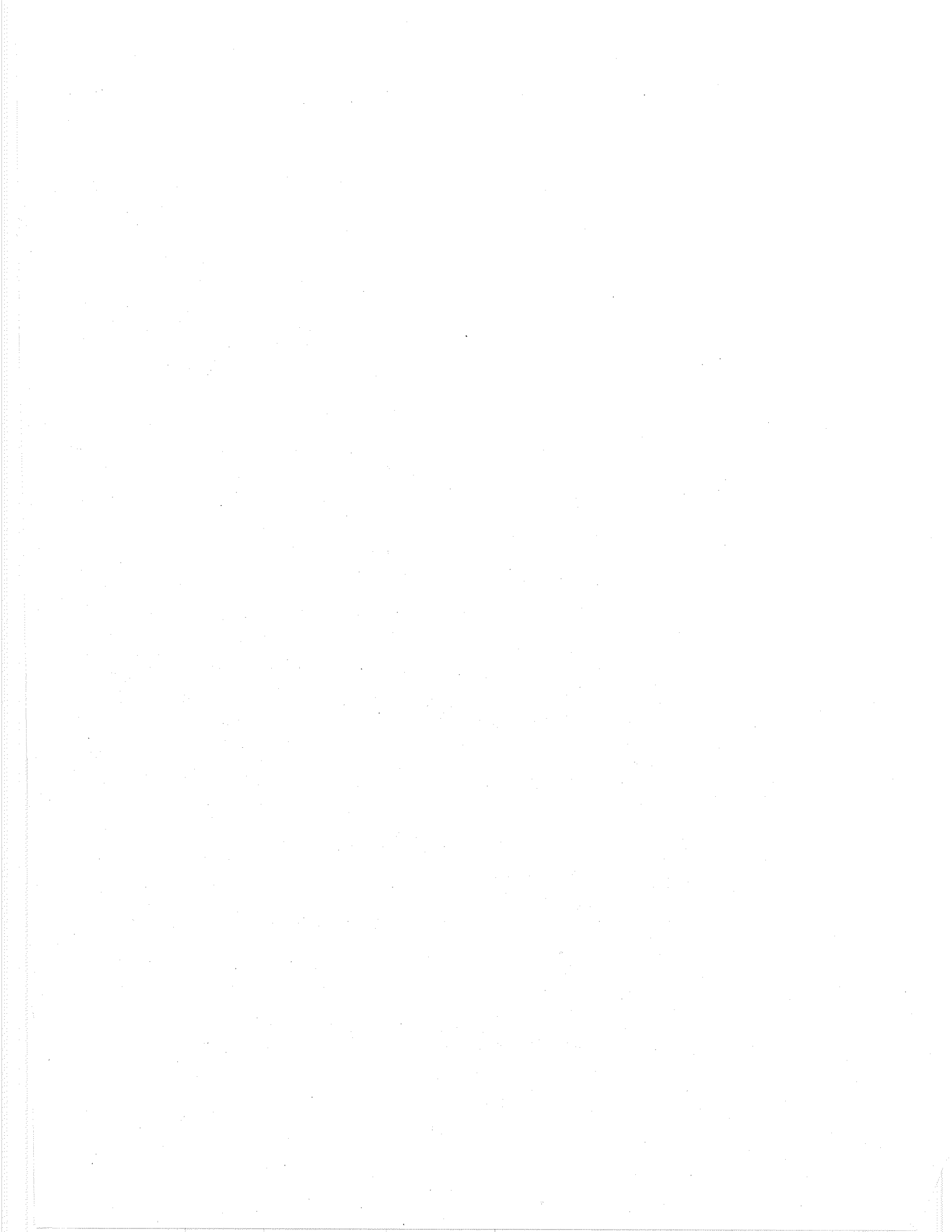
**TRACE CHEMICAL CONTAMINANT GENERATION RATES FOR SPACECRAFT
CONTAMINATION CONTROL SYSTEM DESIGN**

By J.L. Perry

The information in this report has been reviewed for technical content. Review of any information concerning Department of Defense or nuclear energy activities or programs has been made by the MSFC Security Classification Officer. This report, in its entirety, has been determined to be unclassified.



J.C. BLAIR
Director, Structures and Dynamics Laboratory



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13. ABSTRACT (<i>Maximum 200 words</i>) A spacecraft presents a unique design challenge with respect to providing a comfortable environment in which people can live and work. All aspects of the spacecraft environmental design including the size of the habitable volume, its temperature, relative humidity, and composition must be considered to ensure the comfort and health of the occupants. The crewmembers and the materials selected for outfitting the spacecraft play an integral part in designing a habitable spacecraft because material offgassing and human metabolism are the primary sources for continuous trace chemical contaminant generation onboard a spacecraft. Since these contamination sources cannot be completely eliminated, active control processes must be designed and deployed onboard the spacecraft to ensure an acceptably clean cabin atmosphere. Knowledge of the expected rates at which contaminants are generated is very important to the design of these processes. Data from past spacecraft missions and human contaminant production studies have been analyzed to provide this knowledge. The resulting compilation of contaminants and generation rates serve as a firm basis for past, present, and future contamination control system designs for space and aeronautics applications.			
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